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Tables of Internal Partition Functions and Thermodynamic Properties of High-Temperature Mars-Atmosphere Species from 50K to 50000K

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Abstract

High-temperature thermodynamic properties for Mars-atmosphere components (Ar, Ar^{+}, Ar^{2+}, Ar^{3+}, Ar^{4+}, C, C^{+}, C^{2+}, C^{3+}, C^{4+}, C^{-}, C_2, C^{2+}, $C_2{}^{-}$, C_3, CN, CN^{+}, CN^{-}, CO, CO^{+}, CO_2, $CO_2{}^{+}$, e^{-}, N, N^{+}, N^{2+}, N^{3+}, N^{4+}, N^{-}, N_2, $N_2{}^{+}$, $N_2{}^{-}$, N_3, NO, NO^{+}, NO_2, N_2O, N_2O^{+}, CNO, O, O^{+}, O^{2+}, O^{3+}, O^{4+}, O^{-}, O_2, $O_2{}^{+}$, $O_2{}^{-}$, O_3, $O_3{}^{-}$,C_2N, C_2O, $CO_2{}^{-}$) are presented and discussed. The present report is divided into two parts: in the first one, theoretical aspects of the calculation are described. Results are discussed and compared with previous works including aspects such as quasi-bound rotational states for molecules and cut-off criteria and autoionasing states for atomic species. The second part provides tables of spectroscopic data used in the calculation and thermodynamic properties in the temperature range from 50 K to 50000 K at P=1 bar. Finally, fitting coefficients for nondimensional specific heat are included.

Contents

Errata

Replace Eq. (7) at page 5 with

$$\Delta E_i = (Z_i + 1)\, e^3 (\pi / kT)^{1/2} \left(\sum_j n_j Z_j^2 \right)^{1/2}$$

Replace Eq. (20) at page 6 with

$$\frac{C_p(T)}{R} = a_1 \left(\frac{T}{10^5} \right)^{-2} + a_2 \left(\frac{T}{10^5} \right)^{-1} + a_3 + a_4 \left(\frac{T}{10^5} \right) + a_5 \left(\frac{T}{10^5} \right)^{2} + a_6 \left(\frac{T}{10^5} \right)^{3} + a_7 \left(\frac{T}{10^5} \right)^{4}$$

Replace Section B at page 26 with

B Reference Elements

The calculation of the global thermodynamic properties requires the definition of reference elements for the formation of each species. In this work, the Ar atom, the electron e and the molecules in their standard state have been chosen as reference elements that determine the formation of all other species. For carbon compounds, this means that the C2 molecule (gas) is the reference element instead of the C atom (graphite). Corresponding formation enthalpies for all Mars-atmosphere species are listed in table 3.

Replace Table 3 at page 38 with

Table 3: Formation enthalpies at 0 K for Mars-atmosphere species.

Species	$\Delta H_f^0(0K)$ / eV	$\Delta H_f^0(0K)$ / kJ·mol^{-1}
Ar	0.0	0.0
Ar^+	15.7596	1520.5915
Ar^{2+}	43.3893	4186.4895
Ar^{3+}	84.1243	8116.8743
Ar^{4+}	143.8103	13875.7783
C	3.08214787	297.3862
C^+	14.34766863	1384.3589
C^{2+}	38.73094463	3737.0202
C^{3+}	86.61864863	8357.5457
C^{4+}	151.1123946	14580.3331
C^-	1.91063463	184.3508
C_2	0.0[a]	0.0
C_2^+	15.67136537	1512.078
C_2^-	0.99836537	96.3290
C_3	3.8855982	374.9085
CN	0.42128238	40.6481
CN^+	14.01928238	1352.6740
CN^-	−3.44071762	−331.9834
CO	−5.45086931	−525.9363
CO^+	8.56313069	826.2280
CO_2	−8.34611784	−805.2892
CO_2^+	5.43088216	524.0078
e^-	0.0	0.0
N	4.87933027	470.7904
N^+	19.428233	1874.5657
N^{2+}	49.043795	4732.0730
N^{3+}	96.492844	9310.2740
N^{4+}	173.96623	16785.4238
N^-	4.9497068	477.5808
N_2	0.0	0.0
N_2^+	15.581	1503.3589
N_2^-	0.352	33.9633
N_3	4.2931	414.2270
NO	0.930593918	89.7899
NO^+	10.194793918	983.6618
NO_2	0.372497752	35.9411
N_2O	0.885928879	85.4803
N_2O^+	13.77492888	1329.0971
NCO	−2.95506537	−285.1244
O	2.55800581	246.8135
O^+	16.1755	1560.7203
O^{2+}	51.3315	4952.8060
O^{3+}	106.2805	10254.6525
O^{4+}	183.6965	17724.2652
O^-	0.95	91.6623
O_2	0.0	0.0
O_2^+	12.0697	1164.5653
O_2^-	−0.4510	−43.5155
O_3	1.50907122	145.6053
O_3^-	−0.594	−57.3131
CO_2^-	−3.475	−335.2912
C_2N	1.49603463	144.3474
C_2O	2.9704	286.6040

[a]The formation enthalpies for species containing carbon have been calculated with gaseous C_2 as reference element. Formation enthalpies $\{\Delta H_f^0\}$ relative to $C_{graphite}$ as reference element can be obtained from the formula $\{\Delta H_f^0\} = \Delta H_f^0 + 1/2\{\Delta H_f^0\}_{C_2}$ in which $\{\Delta H_f^0\}_{C_2} = 8.54273074$ eV= 824.2483 kJ·mol^{-1}.

Replace Table 244 at page 247 and Table 248 at page 248 with

Table 244: Fitting coefficients for C_p/R of C_2

T interval (K)	a_1	a_2	a_3	a_4	a_5	a_6	a_7
50 - 300	1.044676770E-06	-7.307999310E-03	2.342600887E+01	-2.649742110E+04	1.743107030E+07	-5.051089300E+09	5.318089180E+11
300 - 1000	-1.065174370E-04	1.049508400E-01	-3.245506934E+01	6.400034042E+03	-6.102171840E+05	3.079807170E+07	-6.425149220E+08
1000 - 6000	-5.924921770E-05	2.104802160E-02	1.200705480E+00	2.047496895E+02	-4.911450697E+03	5.899871290E+04	-2.781699550E+05
6000 - 15000	-1.834066580E-02	1.428600830E+00	-4.002295179E+01	7.196492584E+02	-5.868519945E+03	2.313961680E+04	-3.585640240E+04
15000 - 35000	-1.004434600E-01	2.355324930E+00	-1.312263533E+01	5.878405408E+01	-1.270505730E+02	1.473529996E+02	-7.102055798E+01
35000 - 50000	6.305093750E-03	4.430640200E-01	1.169874920E+00	1.876866100E+00	-7.936482100E-02	-2.727636620E+00	2.144150070E+00
Residuals: min=3.7279E - 09, max=6.8648E - 03, mean=3.2416E - 05.							

Table 248: Fitting coefficients for C_p/R of CN

T interval (K)	a_1	a_2	a_3	a_4	a_5	a_6	a_7
50 - 1000	1.111875560E-07	-4.315408230E-04	4.045723650E+00	-2.829786430E+02	6.011850510E+04	-4.021912370E+06	8.588424430E+07
1000 - 3000	2.346656540E-04	-9.401611510E-02	1.776195876E+01	-9.935668245E+02	3.919507110E+04	-7.155456460E+05	4.956335680E+06
3000 - 6000	6.489207950E-04	2.036517310E-02	-5.843742720E+00	6.013747500E+02	-1.282809230E+04	1.251352280E+05	-4.670149390E+05
6000 - 15000	-1.007905870E-03	-2.876327700E-01	2.402454480E+01	-4.148744040E+02	4.309014256E+03	-2.085090700E+04	3.754828280E+04
15000 - 35000	1.818672000E-01	-6.349425130E+00	8.794481536E+01	-5.036671274E+02	1.538130462E+03	-2.402537358E+03	1.525462356E+03
35000 - 50000	-1.627187950E-02	1.206159630E+00	-1.821581190E+00	5.855850010E+00	4.420965150E-03	-7.133790940E+00	4.802415980E+00
Residuals: min=1.5603E - 07, max=4.3060E - 03, mean=4.8932E - 05.							

General Aspects

1 Nomenclature

a_{ij}	:	stoichiometric coefficient for the formation reaction of the i^{th} species
c	:	speed of light
C_p	:	total specific heat
$C_{p,int}$	:	internal specific heat
E_i	:	ionization energy
E_{int}	:	internal energy
E_n	:	energy of the n^{th} quantum level
D_e	:	dissociation energy
F_v	:	rotational energy (polyatomic molecules)
g_n	:	statistical weight of the n^{th} quantum level
G	:	Gibbs free energy
$G_0(v_1, \ldots)$	:	vibrational energy of the state $(v_1, v_2, \ldots, v_m)$
h	:	Planck constant
H_i	:	molar enthalpy of the i^{th} species
I_A, I_B, I_C	:	moments of inertia
J	:	rotational quantum number
k_B	:	Boltzmann constant
m_i	:	mass of the i^{th} species
n	:	principal quantum number
p_i	:	statistical weight of the i^{th} electronic states (polyatomic molecules)
p_v	:	statistical weight of the state $(v_1, v_2, \ldots, v_m)$
$Q_{h.o.}$	:	partition function for the harmonic oscillator (polyatomic molecules)
Q_i	:	total partition function of the i^{th} species
$Q_{int,i}$	:	internal partition function of the i^{th} species
$Q_{r.r.}$	:	partition function for the rigid rotator (polyatomic molecules)
$Q_{tr,i}$	:	translational partition function of the i^{th} species
r_e	:	equilibrium distance
R	:	universal gas constant
Ry	:	Rydberg constant
Ry^*	:	modified Rydberg constant
S	:	entropy
T	:	temperature
$T_0^{(i)}$	:	excitation energy of the i^{th} electronic states (polyatomic molecules)
v	:	vibrational quantum number
V	:	volume
ΔE_i	:	lowering of the ionization potential
$\Delta H_{f,i}$	:	variation of the enthalphy for the formation of the i^{th} species
ω_n	:	frequency of the n-th vibrational mode (polyatomic molecules)
μ	:	reduced mass
π	:	pi greek
σ	:	symmetry factor

2 Introduction

Future missions to Mars foresee hypersonic entries into and aerobraking manoeuvres through the planet's atmosphere. Heatshield design will require the high-speed aerodynamics analysis of spacecraft configurations. In this context, accurate thermodynamic properties of the chemical constituents that may exist in the flow field during hypersonic flight are mandatory. The literature offers a few main sources: the JANAF tables [1], the table series from NASA [2, 3], and the impressive tabulation edited by Gurvich et al. [4]. The JANAF tables are limited to 6000 K, Gurvich et al.'s tables and the recent tables from NASA reach 20000 K. Concerning molecular components, all tabulations can be considered in satisfactory agreement up to 6000 K. However, atomic components and their ions are not dealt with according to the same accuracy because the number of energy levels included in the calculation of electronic partition functions is not sufficient. Concerning this aspect, even the old tables produced by Browne [5] qualify for higher accuracy, although this author included just the observed energy levels as published by Moore [6]. Moreover, the problems connected with the divergence of internal partition functions and related to the completion of the energy-level set were not adequately dealt with.

In this work, we present a new calculation of the thermodynamic properties of Mars-atmosphere components from 50 K up to 50000 K, carried out with the purpose of dealing with the mentioned problems in an as accurate as possible manner. In particular, the problem of the energy-level completion will be confronted by avoiding the hydrogenic approximation recently used by Wang and Rhodes [7] for the calculation of air-component thermodynamic properties. In addition, the thermodynamic properties produced in this work are meant to constitute the platform to support the development of a high-temperature gas mixture thermodynamic model of Mars atmosphere suitable for implementation in hypersonic flow-field solvers. Finally, it is worth noticing that the tables of thermodynamic properties relative to the species that belong also to air are more accurate than and should be considered the update of the corresponding tables presented in ref. [18].

3 Method of Calculation

3.1 The Partition Function

The thermodynamic properties of high-temperature gas mixtures can be obtained if the partition functions of single components are known. In general the partition function can be factorised as the product of the translational $Q_{tr,i}$ and the internal $Q_{int,i}$ contributions

$$Q_i = Q_{tr,i} Q_{int,i} \tag{1}$$

The translational partition function is available in analytical form

$$Q_{tr,i} = \left(\frac{2\pi m_i kT}{h^2} \right)^{3/2} \tag{2}$$

The internal partition function can be written in general terms as

$$Q_{int,i} = \sum_n g_n exp \left(-\frac{E_n}{kT} \right) \tag{3}$$

where g_n and E_n represent the statistical weight and the energy of the n^{th} internal quantum level of the component under consideration In practice, eq. (3) assumes different explicit forms for atoms and for molecules.

3.2 The internal partition function

For an isolated atom, an infinite number of bound states exists below the ionisation limit. The internal partition function is the sum over the infinite electronic levels

$$Q_{int} = \sum_{n}^{\infty} g_n exp\left(-\frac{E_n}{kT}\right) \tag{4}$$

However, the sum in eq. (4) diverges because the statistical weight is not bound when the principal quantum number ($n \to \infty$) increases indefinitely. For example, $g_n = 2n^2$ for atomic hydrogen. Thus, the summation in eq. (4) must be adequately truncated. Unfortunately, there is no universal cut-off criterion. Reviews of various cut-off methods can be found in the literature [4, 8]. The existing cut-off criteria yield partition functions and their derivatives that depend on either the electron density or the gas pressure. This means that the thermodynamic properties of the components depend not only on the temperature but also on the pressure. In addition to the divergence problem, there is also the question of whether to include only experimentally observed energy levels or whether to add the theoretically predicted levels as well. Tables [6, 9] provide energies and statistical weights for many experimentally observed levels. Nonetheless, supplementing that information with semiempirical laws is a useful way to obtain the missing energy levels. Exact quantum-mechanical calculations for high-lying levels, i.e. near the continuum limit, although possible, are still a prohibitive task.

3.3 Cut-off criteria

Let's consider the case of a hydrogen-like atom. A very simple cut-off criterion is to include all the electronic states with a radius of less than the average distance between particles in the electronic partition function. Keeping in mind that this radius in the hydrogen atom is of the order of $a_0 n^2$ and that the average distance between two atoms is of the order of $(1/N)^{1/3}$, N being the particle number density ($p = kNT$), we obtain

$$a_0 n^2 \leq N^{-1/3} \tag{5}$$

a restriction which gives us the maximum permissible principal quantum number n_{max}. This criterion does not account for the presence of electrons and ions in the mixture. In order to include these effects in the calculations similar equations have been developed; in this case the cut-off criterion was derived by equalising the classical semimajor axis of the electron in the considered atom to the Debye shielding distance. The corresponding principal quantum number at which the partition function is to be truncated becomes

$$n_{max} = 36.11 \cdot 10^3 \left(\frac{Z_{eff}^2 T}{\sum_j n_j Z_j^2}\right)^{1/4}, \tag{6}$$

where Z_{eff} is the effective charge of the atom, i.e. the net charge seen by an excited electron, and n_j is the particle number density of the j^{th} component with charge Z_j. In this case the partition function depends not only on the temperature but also on the number densities of the ionised components.

Another class of cut-off criteria is based on the fact that the ionisation energy of an atom in the presence of other components is lowered by a factor which, in general, depends on the number densities of the charged particles, including the electrons. Different theories have been proposed to calculate this lowering; the most popular one is that proposed by Griem [10], which yields the expression

see errata

$$\Delta E_i = (Z_j + 1)\, e^3 (\pi/kT)^{1/2} \left(\sum_j n_j Z_i^2\right)^{1/2} \tag{7}$$

All the levels whose energies are lower than the corrected ionisation potential are accounted for in the sum (4), i.e. we sum up to the last energy level which arises from the limitation

$$E_n = E_i - \Delta E_i \tag{8}$$

In our calculations ΔE_i is set as a parameter, and results are reported for various ΔE_i values.

3.4 Thermodynamic properties

From the partition functions and their first and second derivatives we can calculate all the thermodynamic properties of the components according to the formulae of statistical thermodynamics [11]. The Helmholtz potential, the internal contribution E_{int} to the thermodynamic energy, the entropy, the internal constant-pressure specific heat $C_{p,int}$, are obtained respectively from

$$F - H(0) = -RT \ln Q \tag{9}$$

$$E_{int} = RT^2 \left(\frac{\partial \ln Q_{int}}{\partial T} \right)_V \tag{10}$$

$$U - H(0) = E_{int} + \frac{3}{2} RT \tag{11}$$

$$S = R \ln Q + \frac{RT}{Q} \left(\frac{\partial Q}{\partial T} \right) \tag{12}$$

$$C_{p,int} = R \left[2T \left(\frac{\partial \ln Q_{int}}{\partial T} \right)_V + T^2 \left(\frac{\partial^2 \ln Q_{int}}{\partial T^2} \right)_V \right] \tag{13}$$

The total specific heat is obtained by adding the translational contribution

$$C_p = C_{p,int} + \frac{5}{2} R \tag{14}$$

The enthalpy is given by

$$H - H(0) = E_{int} + \frac{5}{2} RT \tag{15}$$

The Gibbs free energy is calculated from the entropy and the enthalpy as

$$G - H(0) = -RT \ln Q + RT \tag{16}$$

The Helmholtz potential, the internal contribution to the thermodynamic energy and the internal constant-pressure specific heat strongly depend on the assumed sets of energy levels and adopted cut-off criterion.

Finally we calculate the formation enthalpy of the component under consideration from:

$$\Delta H_{f,j} = H_i - \sum_j \sigma_{ij} H_j \tag{17}$$

where H_i, H_j are the molar enthalpies given in eq. (15), σ_{ij} are the stoichiometric coefficients of the formation reaction, and the sum runs on all the forming reactants. For example for N formation

$$\frac{1}{2} N_2 \rightarrow N \tag{18}$$

the formation enthalpy is given by

$$\Delta H_{f,N}(T) = \frac{D}{2} + [H(T) - H(0)]_N - \frac{1}{2} [H(T) - H(0)]_{N_2} \tag{19}$$

Thermodynamic data for many individual components can be conveniently stored for use with computer programs in the form of coefficients associated with equations that reproduce the data. Specific heat can be fitted in different temperature ranges by the following dimensionless form [3]:

see errata

$$\frac{C_p(T)}{R} = a_1 T^{-2} + a_2 T^{-1} + a_3 + a_4 T + a_5 T^2 + a_6 T^3 + a_7 T^4 \tag{20}$$

3.5 The internal partition function of molecular components

The starting point for calculating the internal partition function of molecular components is to solve the Schrödinger equation of a representative molecule to obtain the energy levels corresponding to the independent molecular degree of freedom. The Schrödinger equation is solved in the Born-Oppenheimer approximation, which separates the motion of the electrons from that of the nuclei. The solution of the Schrödinger equation for the electrons yields the approximate wave functions of the infinite electronic states as well as their degeneracies. The energy corresponding to the n^{th} electronic state is expressed as a function of the internuclear distance r and constitutes the potential energy $V_n(r)$ seen by the internal motion of the nuclei, governed by the nuclear Schrödinger equation.

3.5.1 Diatomic molecules

The treatment of the diatomic molecules follows the method developed by Drellishak [12, 13] and by Stupochenko [14]. In this method the energy of a particular state in the molecule E_{nJv} is split into three contributions: the electronic excitation energy $E_{el}(n)$, the vibrational energy $E_{vib}(n,v)$ and the rotational energy $E_{rot}(n,v,J)$. Thus

$$E_{nJv} = E_{el}(n) + E_{vib}(n,v) + E_{rot}(n,v,J) \tag{21}$$

The vibrational energy associated with the v^{th} vibrational level of the n^{th} electronic state of a diatomic molecule is expressed in analytical form as [11]

$$\begin{aligned}\frac{E_{vib}(n,v)}{hc} = {} & \omega_e\left(v+\frac{1}{2}\right) - \omega_e x_e\left(v+\frac{1}{2}\right)^2 + \\ & + \omega_e y_e\left(v+\frac{1}{2}\right)^3 + \omega_e z_e\left(v+\frac{1}{2}\right)^4\end{aligned} \tag{22}$$

where ω_e, $\omega_e x_e$, $\omega_e y_e$, $\omega_e z_e$ are spectroscopic constants for each electronic state, and c is the speed of light. Expression (22) can be rewritten with the energy referenced to the first vibrational level, which reads

$$E_{vib}(n,0) = \frac{1}{2}\omega_e + \frac{1}{4}\omega_e x_e + \frac{1}{8}\omega_e y_e + \frac{1}{16}\omega_e z_e \tag{23}$$

Then expression (22) becomes

$$\frac{E_{vib}(n,v)}{hc} = \frac{E_{vib}(n,0)}{hc} + \omega_0 v - \omega_0 x_0 v^2 + \omega_0 y_0 v^3 + \omega_0 z_0 v^4 \tag{24}$$

where

$$\begin{aligned}\omega_0 &= \omega_e - \omega_e x_e + \tfrac{3}{4}\omega_e y_e + \tfrac{1}{8}\omega_e z_e \\ \omega_0 x_0 &= \omega_e x_e - \tfrac{3}{2}\omega_e y_e - \tfrac{3}{2}\omega_e z_e \\ \omega_0 y_0 &= \omega_e y_e + 2\omega_e z_e \\ \omega_0 z_0 &= \omega_e z_e\end{aligned}$$

Assuming that eq. (22) is valid for all vibrational states up to dissociation, we can determine the maximum permissible value v_{max} of the vibrational quantum number for each rotationless ($J = 0$) molecular state from the equation

$$\omega_0 v_{max} - \omega_0 x_0 v_{max}^2 + \omega_0 y_0 v_{max}^3 + \omega_0 z_0 v_{max}^4 = \frac{D_0(n)}{hc} \tag{25}$$

where $D_0(n)$ is the dissociation energy of the n^{th} electronic state referenced to the energy of the first vibrational level.

Our calculations have been performed by taking as refence for the energy levels the minimum of the potential curve [eq. (22)]. Previous results [18] were obtained taking as reference the first vibrational level ($v = 0$) of the anharmonic oscillator. This determines a difference in the internal partition function

and energy at low temperature[1].

The rotational energy for a non-rigid rotator associated with the v^{th} vibrational level of the n^{th} electronic state reads

$$\frac{E_{rot}(n,v,J)}{hc} = B_v J(J+1) - D_v J^2 (J+1)^2 \tag{26}$$

where

$$B_v = B_e - \alpha_e \left(v + \frac{1}{2}\right) \tag{27}$$

$$D_v = D_e - \beta_e \left(v + \frac{1}{2}\right) \tag{28}$$

The maximum permissible value J_{max} of the rotational quantum number for each vibrational quantum number is determined comparing the vibrational-rotational energy with the dissociation energy relative to the electronic level we are considering. This represents a simplification in which the molecule is considered as a non-rotating system.

For a diatomic molecule the potential curve is given by [15]:

$$U_0 = D_e \left(1 - \exp\left(-\beta(r - r_e)\right)\right)^2 \tag{29}$$

where D_e is the dissociation energy, r_e is the equilibrium distance and b is a constant (in cm^{-1}) whose value will be derived from:

$$\beta = \sqrt{\frac{2\pi^2 c\mu}{D_e h}} \cdot \omega_e \tag{30}$$

When we consider a rotating molecule on the basis of classical mechanics, we must introduce an additional term in eq. (29): a centrifugal potential [13]. Thus, when the angular momentum is J, the effective potential energy (in cm^{-1}) becomes:

$$U_J(r) = U_0 + \frac{h}{8\pi^2 c\mu r^2} J(J+1) \tag{31}$$

A series of potential curves for consecutive J's can be constructed (fig. 1). These potential curves show a maximum at a larger distance respect to the equilibrium distance for $0 < J < J_{max}$. For $J = 0$ no centrifugal distorsion occurs and there is some maximum value of J beyond which the potential curve no longer displays a minimum. This means that for $J = 0$ all vibrational states with energy lower than the dissociation limit are present, while there are no stable states with J larger than J_{max}.

The centrifugal distortion of the potential energy determines the existence of "quasi-bound" states above the dissociation limit of the molecule. In order to calculate the number of rotational states above the dissociation limit for each vibrational state, we differentiate eq. (31) with respect to r, setting this derivative equal to zero and solving the resulting equation for the value of r at the hump (called r_m) as a function of J for any electronic state of the molecule.

$$\frac{\partial U}{\partial r} = 2D_e\beta \left(\exp\left(-\beta(r - r_e)\right) - \exp\left(-2\beta(r - r_e)\right)\right) - \\ - \frac{2}{r^3}\frac{h}{8\pi^2 c\mu} J(J+1) = 0 \tag{32}$$

[1] In general, the energy of the vibrational levels can be calculated with two different criteria. The first one considers as zero-point energy the minimum of the potential curve. If we consider a molecule having just one vibrational level, the internal partition function is given by $Q_{int} = 1$. In the second case, we can choose as zero-point energy the level $v = 0$. Therefore, the vibrational energy is given by eq. (23) and, as a consequence, the internal partition function is $Q_{int} = \exp\left(-\frac{E_{vib}(n,0)}{kT}\right)$.
The difference in the internal partition function and internal energy disappears when considering the internal specific heat because the internal specific heat is given by the derivative of enthalpy in respect to the temperature.

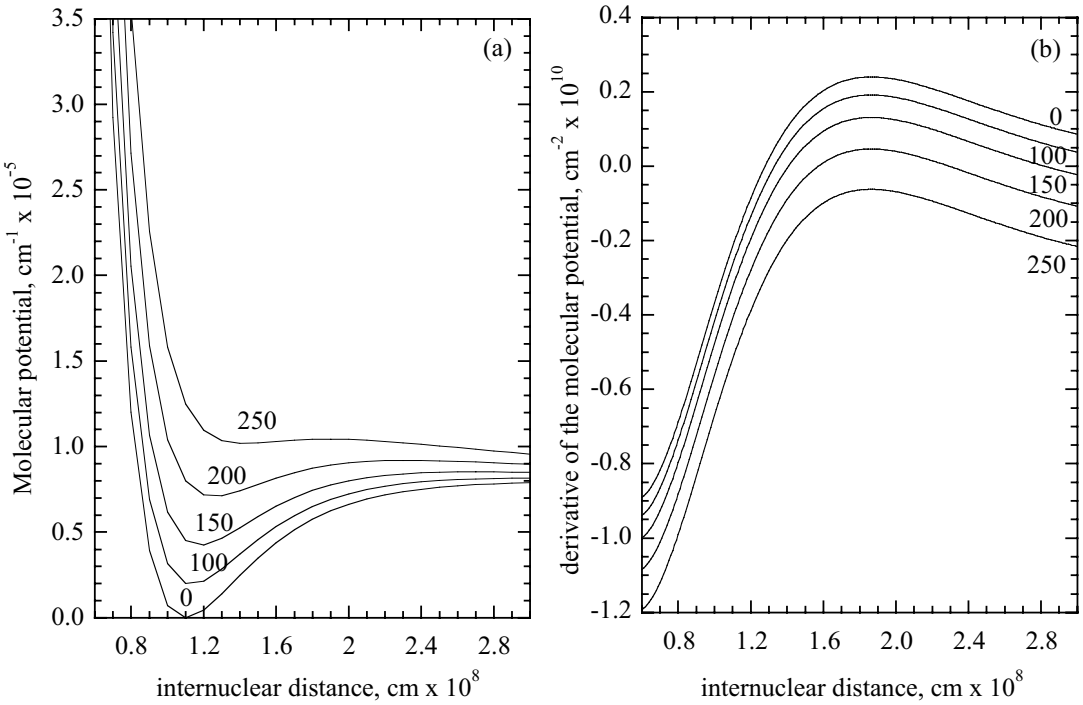

Figure 1: Potential curves and their derivative for N_2 ground state for different centrifugal distorsions (numbers indicate the J's values).

Then the value of the potential at r_m is calculated for each J.

$$U_J(r_m) = D_e \left(1 - \exp\left(-\beta(r_m - r_e)\right)\right)^2 + \frac{h}{8\pi^2 c\mu r_m^2} J(J+1) \tag{33}$$

This potential is compared with the energy as calculated from the coupled vibrational-rotational energy expression for any assumed v

$$E_m = \frac{E_{vib}(n,0)}{hc} + \omega_0 v - \omega_0 x_0 v^2 + \omega_0 y_0 v^3 + \omega_0 z_0 v^4 + B_v J(J+1) - D_v J^2 (J+1)^2 \tag{34}$$

and J is varied until these two energy values are equal. When this point is reached, one has a compatible v, J combination.

Once the maximum number of vibrational levels for each electronic state and the maximum number of rotational states for each vibrational state have been determined, the internal partition function can be calculated by the following expression

$$Q_{int} = \frac{1}{\sigma} \sum_{n}^{n_{max}} g_n \exp\left[-\frac{E_{el}(n)}{kT}\right] \sum_{v}^{v_{max}(n)} \exp\left[-\frac{E_{vib}(n,v)}{kT}\right] \sum_{J}^{J_{max}(v)} (2J+1) \exp\left[-\frac{E_{rot}(n,v,J)}{kT}\right] \tag{35}$$

where σ is a symmetry factor that equals one or two for heteronuclear and homonuclear diatomic molecules, respectively.

In section 4, we present results for selected diatomic molecules and compare them with data from other

compilations. Here, we discuss the influence of quasibound states and of electronically excited states on the thermodynamic properties of molecular components. Figure 2 illustrates the effect of quasi-bound states on nondimensional specific heat of CO and NO. Consideration of the quasi-bound states can introduce differences up to 10% of the maximum specific heat. The nondimensional specific heat at constant pressure starts from the value 3.5 (activation of translational and rotational degrees of freedom) and rapidly reaches the value 4.5 which includes the vibrational contribution from the ground electronic state. The maximum is due to the contribution of the electronically excited states. In any case, depending on the number of electronically excited states considered in the partition function and on the energy values, the nondimensional specific heat slowly converges after the maximum to the translational contribution $(3/2R + R)$. This behaviour is typical for systems containing a finite number of rotational, vibrational and electronic states.

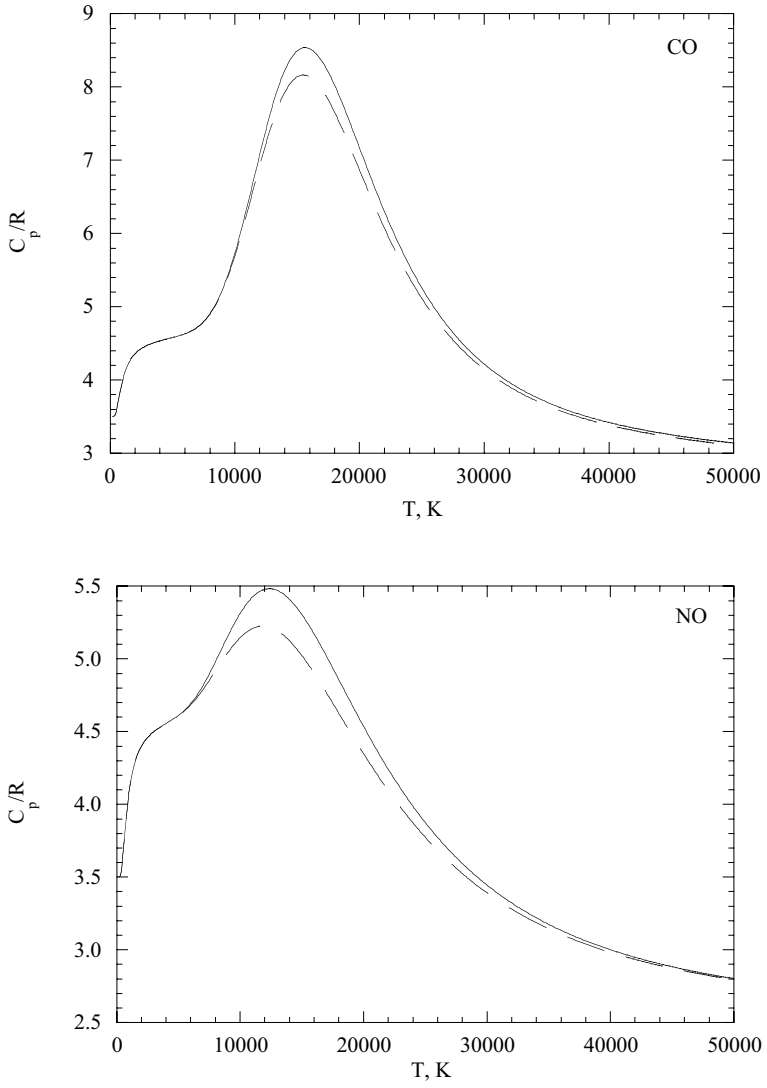

Figure 2: Nondimensional specific heat as a function of temperature for CO and NO without (dashed line) and with (solid line) quasi bound states.

The last observation is better understood by inspection of Fig. 3 which shows the role of electronically

excited states in forming and enhancing the specific heat of O_2 and CN. The curves (a) represent the specific heat of the ground state of the molecules, which rapidly passes from 3.5 to 4.5 for the reasons explained before. Then, there is the presence of a small maximum, after which the specific heat smoothly declines toward the translational contribution. The successive inclusion of electronically excited states (b), (c), (d) (see also Tables 1 and 2) produces a well defined maximum, the absolute value of which depends on the specific molecule.

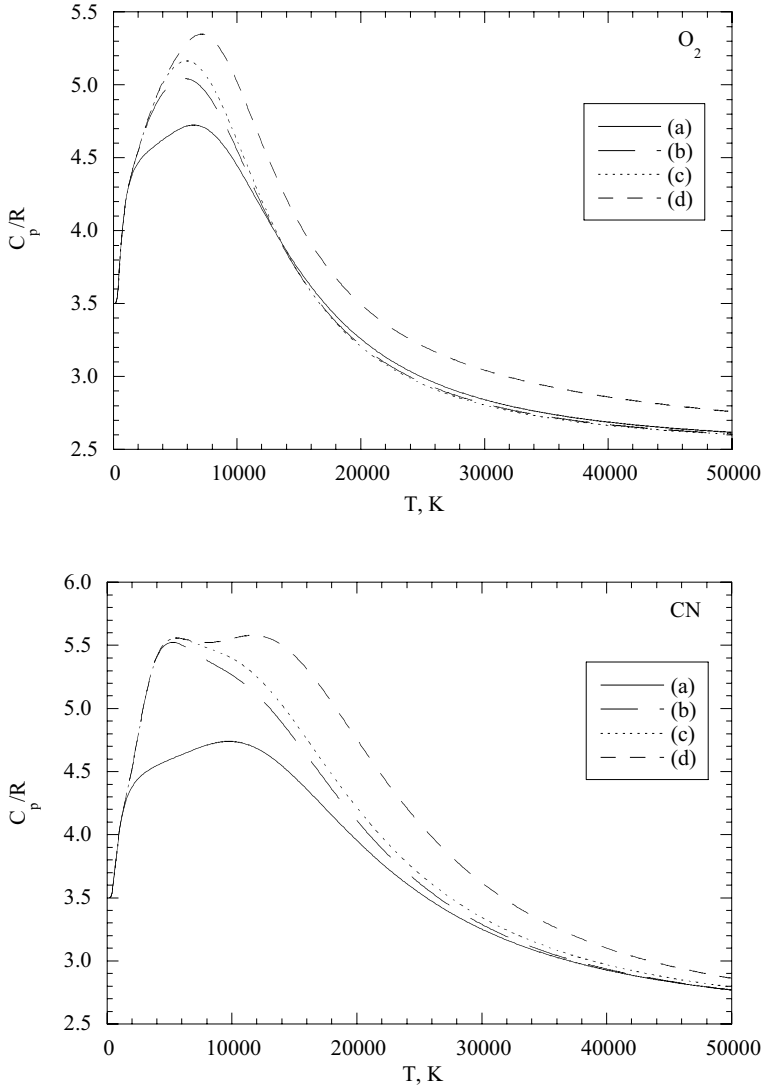

Figure 3: Contribution of electronically excited states to the nondimensional specific heat as a function of temperature for O_2 and CN (see Tables 1 and 2 for details on electronic levels included in each case).

3.5.2 Polyatomic molecules

The internal partition function of polyatomic molecules by analogy with diatomic molecules can be written in the general case in the following way [4, 16]:

$$Q_{int} = \frac{1}{\sigma}\sum_i p_i \exp\left(-\frac{hc}{kT}T_0^{(i)}\right) \cdot \sum_{v_1}\sum_{v_2}\sum_{v_m} p_v \exp\left(-\frac{hc}{kT}G_0^{(i)}(v_1, v_2, \ldots, v_m)\right) \cdot \sum_J \sum_{k=-J}^{k=J} (2J+1)\exp\left(-F_v^{(i)}(J,k)\right) \tag{36}$$

In this expression, the first sum is taken over the electronic states (in general the valence ones) of the molecule, characterised by the energy of excitation $T_0^{(i)}$ and the statistical weight p_i. The electronic states of nonlinear polyatomic molecules are nondegenerate and therefore the statistical weight of these states is determined only by multiplicity $p_i = 2S + 1$. In the case of linear polyatomic molecules, the statistical weights are the same as for the corresponding states of diatomic molecules. The sum over v is carried out for all the m normal vibrations of the molecule. If a molecule, consisting of N atoms, has t degenerate normal vibrations with degeneracy d_n, then $m = 3N - 5 - t$ for linear molecules and $m = 3N - 6 - \sum_{n=1}^{t}(d_n - 1)$ for nonlinear molecules. The statistical weight p_v of the state $(v_1, v_2, \ldots, v_m)$ is equal to:

$$p_v = \prod_{n=1}^{m} \frac{(v_n + d_n - 1)!}{v_n!(d_n - 1)!} \tag{37}$$

The energy of the vibrational levels has been calculated in the approximation of harmonic oscillator:

$$G_0(v_1, v_2, \ldots, v_m) = \sum_{n=1}^{m} \omega_n \left(v_n + \frac{d_n}{2}\right) \tag{38}$$

With an additional simplification through factorising the vibrational partition function, it can be written as:

$$\sum_{v_1}\sum_{v_2}\cdots\sum_{v_m} p_v \exp\left(-\frac{hc}{kT}G_0^{(i)}(v_1, v_2, \ldots, v_m)\right) = \prod_{n=1}^{m}\left(\sum_{v=1}^{v_{max}} p_n(v)\exp\left(-\frac{hc}{kT}G_n^{(i)}(v)\right)\right) \tag{39}$$

where $p_n(v)$ is the statistical weight of v^{th} level in the n^{th} vibrational mode

$$p_n(v) = \frac{(v_n + d_n - 1)!}{v_n!(d_n - 1)!} \tag{40}$$

and $G_n^{(i)}(v)$ is the energy of the of v^{th} level in the n^{th} vibrational mode

$$G_n^{(i)}(v) = \omega_n\left(v_n + \frac{d_n}{2}\right) \tag{41}$$

Summation over J in eq. 36 has been carried out for the value $v = 0$. The energy of the rotational levels of the polyatomic molecules is expressed differently, depending on the symmetry of the molecule. For linear polyatomic molecules and molecules of the type of a spherical top, such as diatomic molecules, the energy of the rotational levels is described by the expression

$$F_v(J) = B_v J(J+1) \tag{42}$$

For molecules of the type of a symmetrical top

$$F_v(J,k) = B_v J(J+1) + (A_v - B_v)k^2 \tag{43}$$

where k assumes values from $-J$ to $+J$. For asymmetrical top molecules:

$$F_v(J) = \frac{1}{2}(B_v + C_v)J(J+1) + (A_v - B_v)k^2 \tag{44}$$

In expressions 42-44, the quantities A_v, B_v, and C_v are the rotational constants related to the principal moments of inertia of the molecule. In particular

$$A_0 = \frac{h}{8\pi^2 c I_A}, B_0 = \frac{h}{8\pi^2 c I_B}, C_0 = \frac{h}{8\pi^2 c I_C} \tag{45}$$

where I_A, I_B, I_C correspond to some average structure of the molecule in the ground vibrational state.

It is important to note that different electronic excited states of the same polyatomic molecule can have different geometries, thus affecting the symmetry number and also determining a different rotational behaviour. Then in order to include these excited states in our calculations it is necessary to take into account this geometry variation.

Increasing temperature, the use of the method of direct summation becomes impossible both because of the absence of data for the high vibrational-rotational energy levels including the ground electronic state of almost all polyatomic molecules, as well as the absence of sufficiently accurate knowledge of the dependence of the energy of these levels on the quantum numbers v_n and J. Then calculations of the thermodynamic functions of polyatomic molecules still use the "rigid rotator-harmonic oscillator" approximation. Deviations from this model, the presence of excited electronic states and other effects are taken into account in the form of corrections. This approximation assumes the vibrations of the molecule in its electronic ground state as harmonic, then the upper limits for v_n and J in the partition function and its derivatives approach infinity. Then, the internal partition function for the molecule in the electronic ground state is given by

$$Q_{int} = p_X Q^{(X)}_{r.r.-h.o.} = p_X Q^{(X)}_{r.r.} Q^{(X)}_{h.o.} \tag{46}$$

where

$$Q_{h.o.} = \prod_{n=1}^{m} \left[1 - \exp\left(-\frac{hc}{kT}\nu_n\right)\right]^{-d_n} \tag{47}$$

and

$$Q_{r.r.} = \frac{1}{\sigma}\frac{kT}{hcB_0} \tag{48}$$

for linear molecules, and

$$Q_{r.r.} = \sqrt{\frac{\pi}{A_0 B_0 C_0}\left(\frac{kT}{hc}\right)^3} \tag{49}$$

for nonlinear molecules.

According to expression (46), the thermodynamic functions can be represented as the sum of the corresponding components.

$$\frac{\left[H^0(T) - H^0(0)\right]_{h.o.}}{RT} = \sum_{n=1}^{m} d_n u_n \exp(-u_n)\left[1 - \exp(-u_n)\right]^{-1} \tag{50}$$

$$\frac{\left[C_p^0(T)\right]_{h.o.}}{R} = \sum_{n=1}^{m} d_n u_n^2 \exp(-u_n)\left[1 - \exp(-u_n)\right]^{-2} \tag{51}$$

where $u_n = (hc/kT)\nu_n$, and

$$\frac{\left[H^0(T) - H^0(0)\right]_{r.r.}}{RT} = \frac{\left[C_p^0(T)\right]_{r.r.}}{R} = 1 \tag{52}$$

for linear molecules, and

$$\frac{\left[H^0(T) - H^0(0)\right]_{r.r.}}{RT} = \frac{\left[C_p^0(T)\right]_{r.r.}}{R} = \frac{3}{2} \tag{53}$$

for nonlinear molecules.

If we assume that the vibrational-rotational partition function of the excited states is equal to that of the ground state, the components of the excited electronic states can be calculated as the corrections to the components of the ground electronic state

$$\frac{\left[H^0(T) - H^0(0)\right]_{e.s.}}{RT} = \frac{\sum_i \frac{p_i}{p_X}\frac{hc}{kT}T_0^{(i)} \exp\left(-\frac{hc}{kT}T_0^{(i)}\right)}{1 + \sum_i \frac{p_i}{p_X}\exp\left(-\frac{hc}{kT}T_0^{(i)}\right)} \tag{54}$$

$$\begin{aligned}\frac{\left[C_p^0(T)\right]_{e.s.}}{R} = & \frac{\left\{\sum_i \frac{p_i}{p_X}\exp\left(-\frac{hc}{kT}T_0^{(i)}\right) + 1\right\}\sum_i \frac{p_i}{p_X}\left[\frac{hc}{kT}T_0^{(i)}\right]^2 \exp\left(-\frac{hc}{kT}T_0^{(i)}\right)}{\left\{1 + \sum_i \frac{p_i}{p_X}\exp\left(-\frac{hc}{kT}T_0^{(i)}\right)\right\}^2} \\ & - \frac{\left\{\sum_i \frac{p_i}{p_X}\frac{hc}{kT}T_0^{(i)} \exp\left(-\frac{hc}{kT}T_0^{(i)}\right)\right\}^2}{\left\{1 + \sum_i \frac{p_i}{p_X}\exp\left(-\frac{hc}{kT}T_0^{(i)}\right)\right\}^2}\end{aligned} \tag{55}$$

where $T_0^{(i)}$ and p_i are the energy and the statistical weight of the i^{th} electronic state respectively and p_X is the statistical weight of the ground state.

4 Results and discussion

4.1 Monoatomic Components

In this section we compare the present results with similar ones from literature. In particular, we compare the present results (called new) with the results obtained by our group some years ago [17, 18] (called old), the recent calculations performed by Wang and Rhodes [7] (called Wang), the old and new calculations of the NASA group [2], the old calculations performed by Browne [5].

The main differences between the calculations are in the set of levels inserted in the partition function and its derivatives.

The present calculations complete the observed levels reported in the tables by Moore [6] and NIST [9] with Rydberg and Ritz extrapolation laws for principal quantum number less than 20, using the hydrogen-like formulation for $n > 20$ (see Appendix A). The calculations are then presented with the lowering of the ionisation potential as a parameter to control the cut-off. The same procedure was used in our previous calculations [17, 18] even though in this case we considered a less complete set of energy levels.

Wang and Rodhes [7] have recently presented new calculations of thermodynamic properties for very high-temperature air components by including a complete set of hydrogen-like levels. Moreover, the results presented by those authors are self-consistent because they calculated the lowering of the ionisation potential provided by the Debye-Huckel theory in their equilibrium code. In principle, their results cannot be directly compared with ours. However, a rough estimate of the lowering of the ionisation potential for atmospheric air plasmas in the temperature range 20000-35000 K should be in the range of 600-500 cm^{-1} for neutral atomic components [19], proportionally scaling with the charge of the considered ion (see eq. 7).

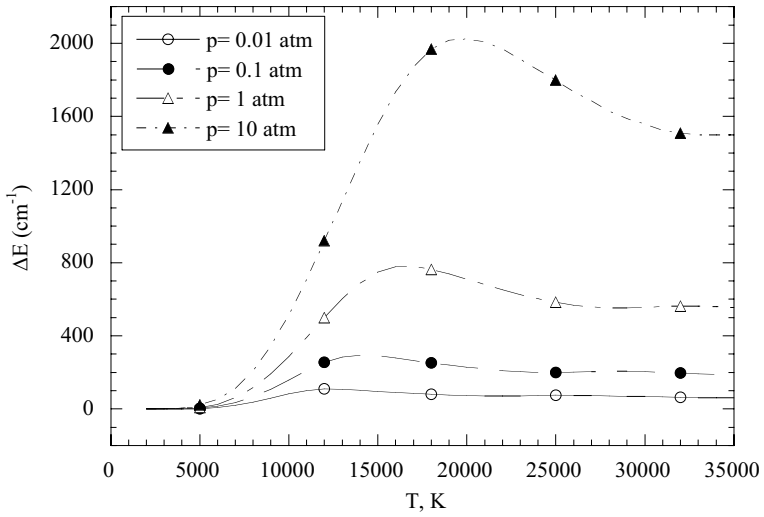

Figure 4: Lowering of the ionisation potential (ΔE) of neutral species in an oxygen plasma as a function of temperature at different pressures.

This point can be understood by looking at Fig. 4, where we have reported the lowering of the ionisation potential for equilibrium oxygen plasmas as a function of temperature for different pressures. Approximately the same lowering should be applied to air plasmas.

Gordon and Mc Bride [2], on the other hand, used the few-level approximation to calculate the partition function of atomic components up to 6000 K. They extended their results above T>6000 K essentially by using Gurvich tables. These also account for a very limited number of excited levels. Finally, the Browne tables [5] are based on the observed levels as reported in the Moore tables [6]. In general we should expect a good agreement about the thermodynamic properties of atomic (neutral and ionised) components for temperatures below 10000 K when only the low-lying excited states contribute to the partition function. Strong differences should appear above 10000 K when the high-lying excited states begin to contribute. The effect becomes evident when complete sets of energy levels are inserted in the partition function. It should also be noted that only our results (new and old) depend on the cut-off. These qualitative observations can be drawn from the results shown in Figs. 5-6, where a comparison of the nondimensional specific heats (C_p/R) for the components N and N^+ is illustrated as a function of temperature for different cut-off values in the temperature range and 0-20000 K.

Wang and Rodhes [7] results at high temperature are in satisfactory agreement with the present results. This means that the hydrogen-like approximation for higher excited states is good. On the other hand, we can observe strong differences in the low-temperature regime. Apparently, Wang and Rhodes have completely disregarded the presence of low-lying levels of the different components. Thus, their specific heat presents a flat behaviour (i.e. only the translational contribution C_p/R=2.5) below 10000 K and a dramatic increase when high-lying excited states are populated.

The Gordon and McBride specific heats closely follow our results below 10000 K but are largely underestimated above 10000 K because of the insufficient number of levels considered by these authors. The same behaviour is observed in relation to Browne's calculations. The insufficient number of levels considered by Gordon and McBride is determined by the cut-off criterion adopted in their calculations. This cut-off criterion is temperature-dependent, the partition function includes only those levels below the ionisation potential lowered by kT, then, as temperature increases, fewer energy levels are used resulting in an underestimation of thermodynamic properties at high temperature. It is also interesting to compare the present results with those obtained by our group some years ago. A satisfactory agreement is observed and the minor differences are due to the improvement of the energy-level sets we have used.

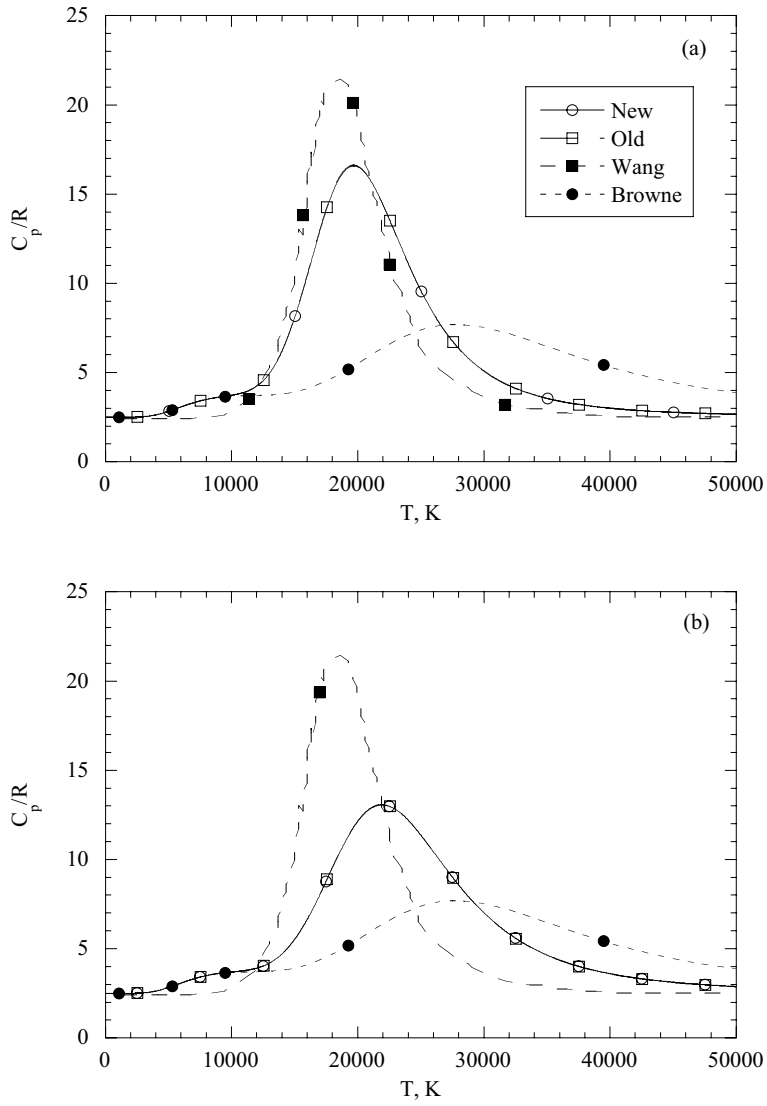

Figure 5: Comparison of nondimensional specific heat as a function of temperature for N for ΔE=500 cm^{-1} and ΔE=1000 cm^{-1}.

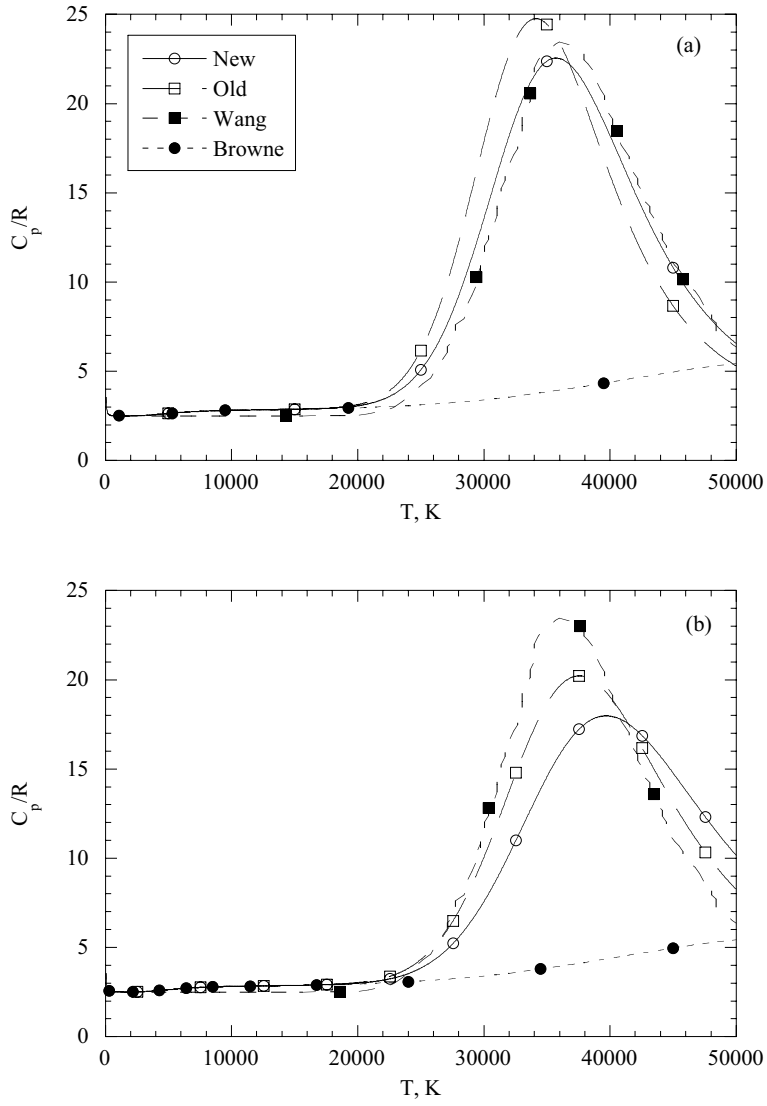

Figure 6: Comparison of nondimensional specific heat as a function of temperature for N^+ for ΔE=500 cm^{-1} and ΔE=1000 cm^{-1}.

Similar considerations can be made from Figs. 7-8 in which we have plotted the nondimensional specific heats of C and C^+. In this case, we limit our comparison to Gordon and Mc Bride's and Browne's data. As in the previous case, the agreement is excellent below 10000 K but becomes poor above that temperature, namely when high-lying excited states begin to contribute substantially to the partition function.

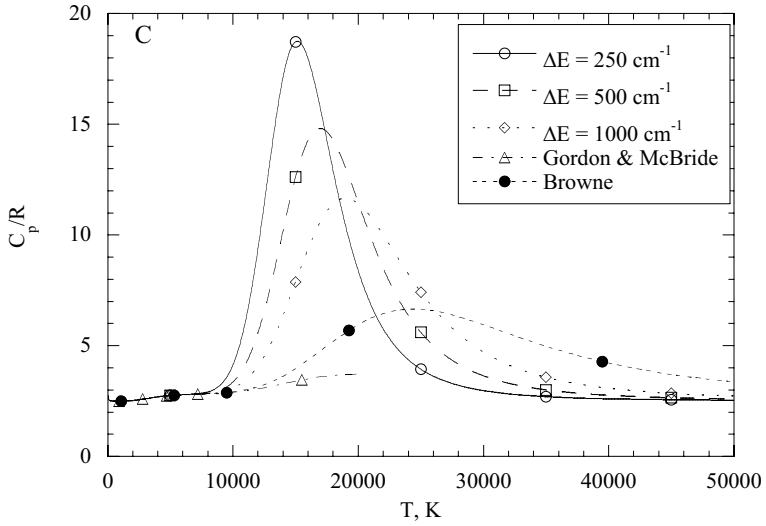

Figure 7: Comparison of nondimensional specific heat as a function of temperature for C for different cut-off.

Before concluding this section, we want to emphasise the problem related to the inclusion of the so-called autoionisation states. These states are derived by considering other series in the completion of energy levels which converge to ionisation potentials greater than the first ionisation potential of the considered component. These levels are usually eliminated in the partition-function calculations by the cut-off procedure even though in many cases those are observed experimentally. To understand their influence, we present in Fig. 9 the nondimensional specific heat for the C^+ and C^{2+} calculated with and without the inclusion of autoionising levels. For both series, we consider levels up to $n = 20$. The figure shows that the autoionisation affects the results above 20000 K and, therefore, originate a further problem for the determination of the electronic partition function.

4.2 Diatomic Species

In this section, we will compare the present results with those given in the JANAF tables [1], by Gordon and Mc Bride [2], in ESA tables [17, 18] and by Jaffe [20]. The present results are calculated using spectroscopic data from Huber and Herzberg [21]. The various calculations differ because of the number of electronically excited states included in the partition function and, in some cases because of the way to account for the rotational and vibrational levels. Results for N_2, O_2, NO and CN are shown in Fig. 10. In the low-temperature range (T<6000 K) our results are in perfect agreement with all other calculations. Small differences emerge at higher temperatures when the contribution of electronically excited states becomes important. Deviations for NO are present only with the recent calculations of Gordon and McBride [2], who have fitted the Gurvich data with polynomial curves.

4.3 Triatomic Species

In this section, we show results for NO_2 and CO_2 calculated using two different methods and two different data sets. The first method consists of the direct summation method, extending the vibrorotational part

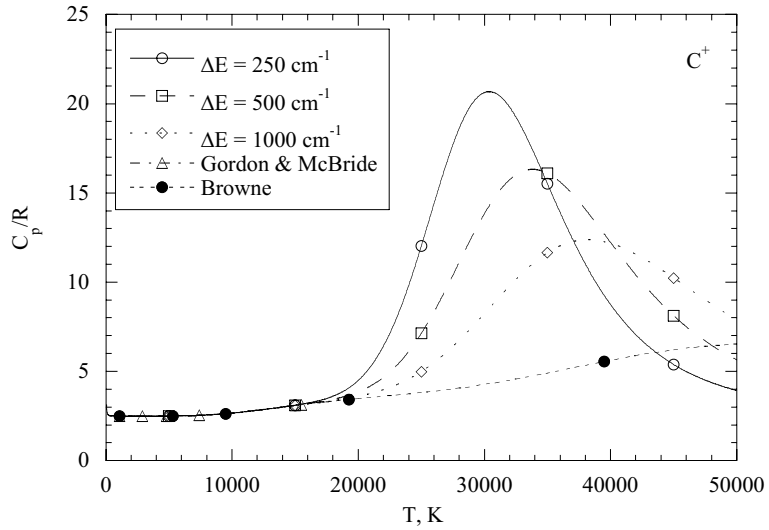

Figure 8: Comparison of nondimensional specific heat as a function of temperature for C^+ for different cut-off.

of electronic excited states with data from the fundamental state if absent, as suggested by Gurvich. The second method uses the "rigid rotator-harmonic oscillator" approximation for the electronic ground state including the correction for the electronic excited states in which the vibrational-rotational partition functions of the ground and excited electronic states are equal. Both data sets include spectroscopic data from Herzberg [11] (vibrational frenquencies and rotational constants), while for the electronic levels energies, in one case we use data from Herzberg, in the second one data are taken from Gurvich [4]. These results are compared with those reported by Gordon and McBride [3] and in JANAF tables [1]. Also for triatomic species the agreement is perfect in the low-temperature range, while differences arise at high temperature when electronically excited states begin contributing to the partition function. These strong differences reflect the differences in the two data sets for the electronic level energies.

The contribution of electronically excited states modulates the corresponding contribution for vibroro-tational partition function of the ground electronic states. In Fig. 12 we have reported the nondimensional specific heat calculated either by the direct summation method or by the rigid rotator-harmonic oscillator method as a function of temperature. Note that in the analytical model the specific heat converge to the value of $7.5R$ and $7R$ respectively for CO_2 and NO_2, as expected by theory.

4.4 Thermodynamic data tabulations

Thermodynamic data are tabulated for each Mars-atmosphere component in the temperature range from 50 K to 50000 K at P=1 bar (Ar, Ar^+, Ar^{2+}, Ar^{3+}, Ar^{4+}, C, C^+, C^{2+}, C^{3+}, C^{4+}, C^-, C_2, C^{2+}, $C_2{}^-$, C_3, CN, CN^+, CN^-, CO, CO^+, CO_2, $CO_2{}^+$, e^-, N, N^+, N^{2+}, N^{3+}, N^{4+}, N^-, N_2, $N_2{}^+$, $N_2{}^-$, N_3, NO, NO^+, NO_2, N_2O, N_2O^+, CNO, O, O^+, O^{2+}, O^{3+}, O^{4+}, O^-, O_2, $O_2{}^+$, $O_2{}^-$, O_3, $O_3{}^-$,C_2N, C_2O, $CO_2{}^-$). We have decided to compile two different kinds of tables. The first one reports partition function, its logarithmic value, the internal contribution to the thermodynamic energy and the internal constant pressure-specific heat as a function of temperature. The second representation reports data in a more traditional format for consistency with the one used in NASA's, JANAF's and Gurvich's tables. A third kind of table shows the curve-fitting coefficients for the constant-pressure specific heat of the various species according to eq. (20) in six temperature subranges. Tables are presented in alphabetic order; for atoms data are tabulated for three different cut-offs (ΔE=250 cm^{-1}, ΔE=500 cm^{-1}, ΔE=1000 cm^{-1}).

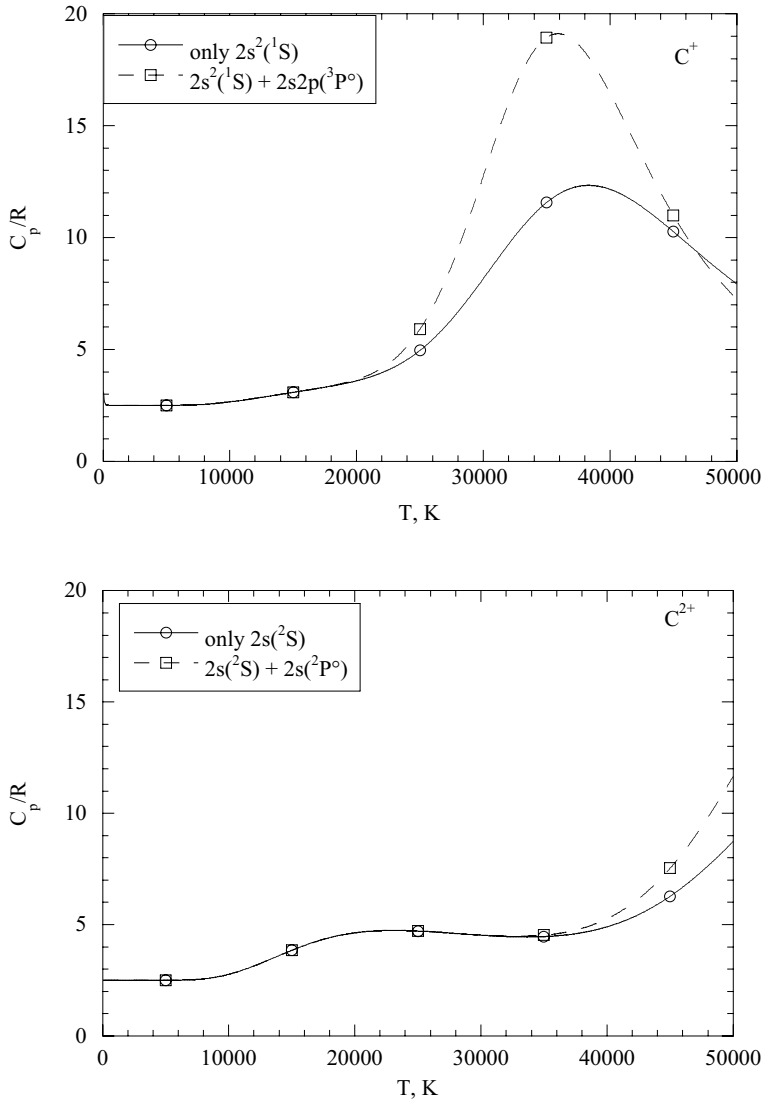

Figure 9: Nondimensional specific heat for C^+ and C^{2+} as a function of temperature calculated with and without autoinising levels (up to $n = 20$).

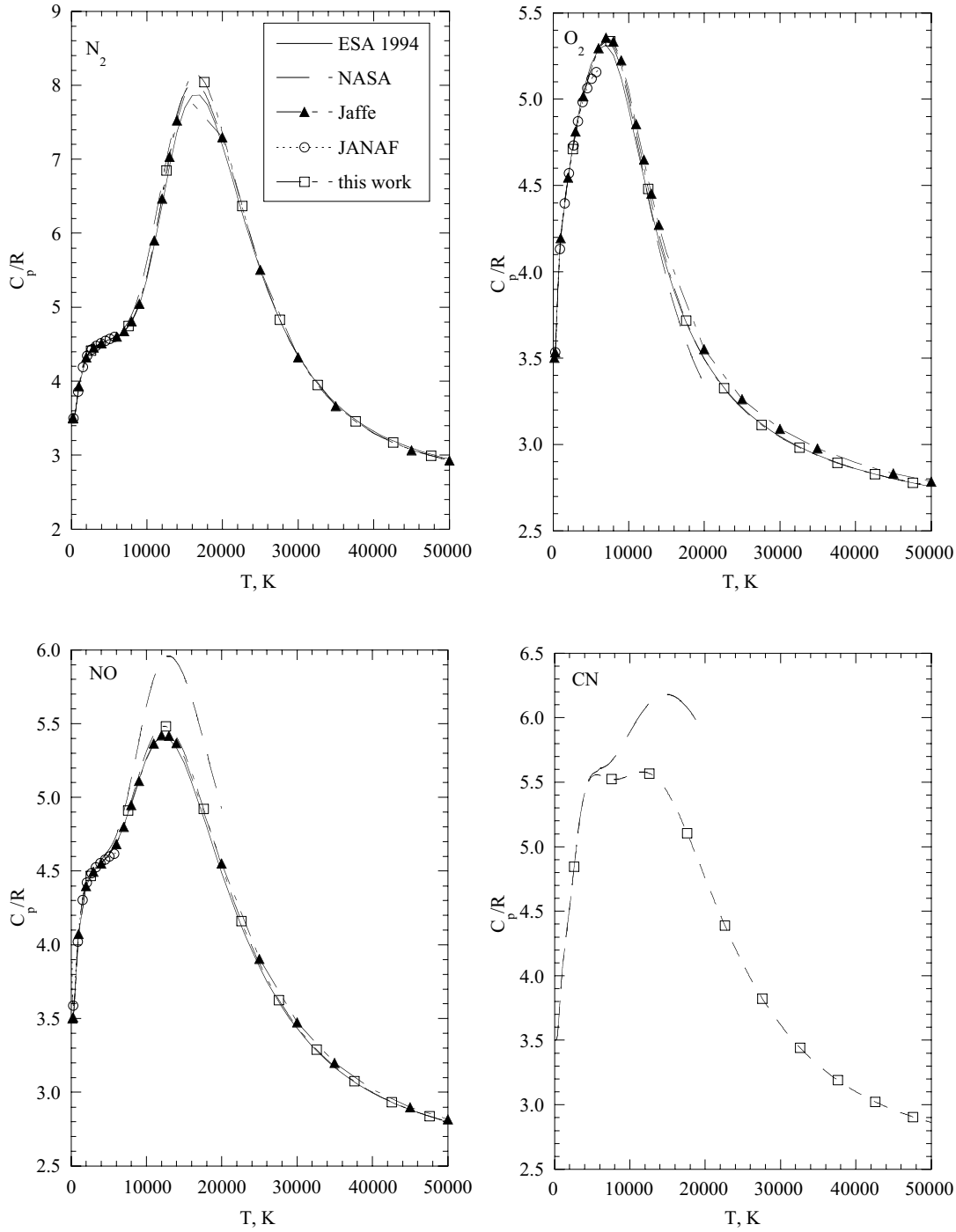

Figure 10: Comparison of nondimensional specific heat as a function of temperature for some selected diatomic species.

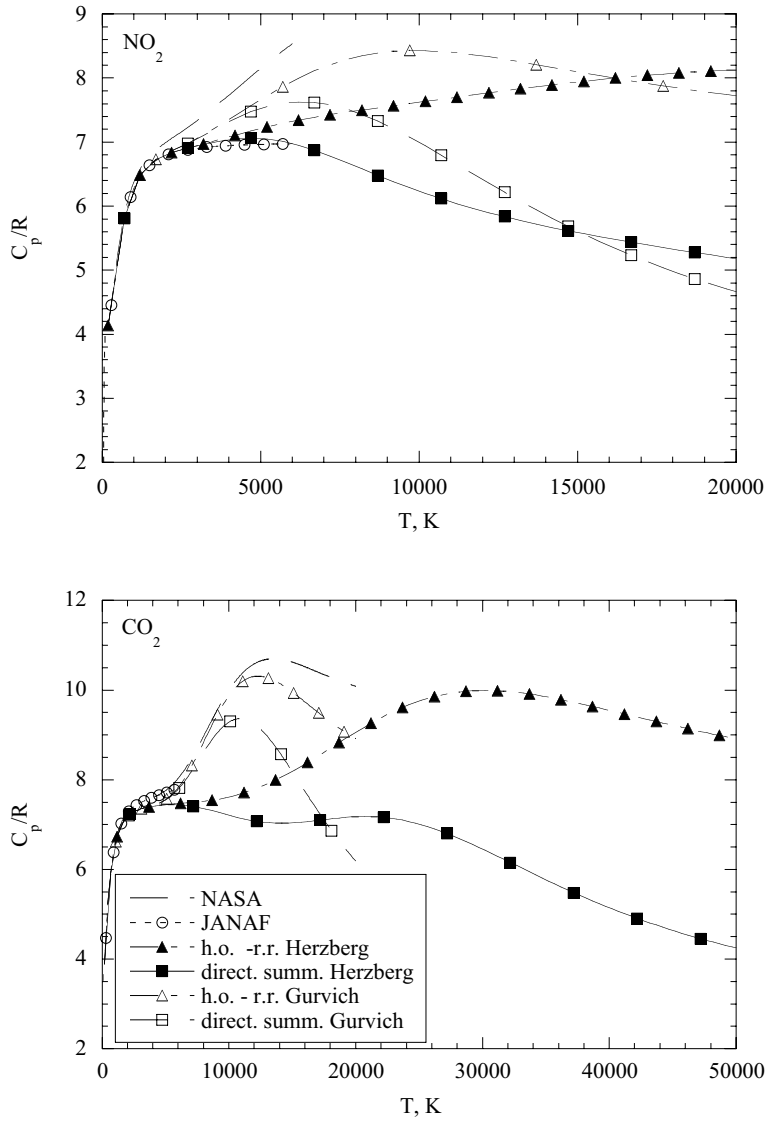

Figure 11: Comparison of nondimensional specific heat as a function of temperature for NO_2 and CO_2.

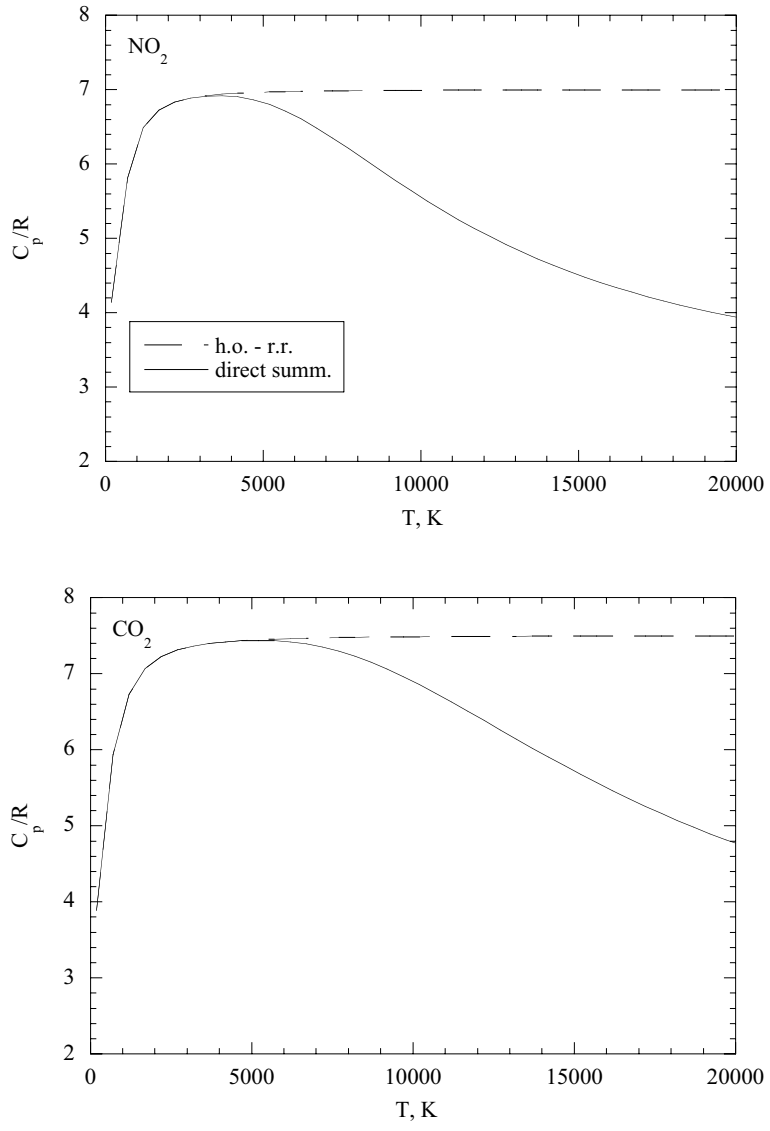

Figure 12: Comparison of nondimensional specific heat as a function of temperature for NO_2 and CO_2 calculated with the direct summation method and the rigid rotator-harmonic oscillator method considering only the ground electronic level.

5 Conclusions

In this report we have described and discussed a recent effort to calculate the high-temperature thermodynamic properties of different Mars atmosphere components. Associated problems, such as the effects of quasi-bound vibrorotational states, cut-off criteria, energy-level completion of the monatomic components, and autoionising states have been considered and have shown to be non-negligible, particularly at high temperature. Indeed, we find agreement with data from other published tables at low temperature and marked differences at high temperature. In particular, for monatomic components the discrepancies are mainly due to the insufficient number of electronic levels usually accounted for in the other tabulations. We have presented examples of tables in two different formats. One is relative to the list of variables of statistical-thermodynamics nature and the other conforms to the format traditionally adopted in other works.

6 Acknowledgements

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A Estimation of energy levels for neutral carbon

The available database for observed atomic electronic energy levels are Moore's tables [6] and the more complete NIST tables [9]. However, many predicted electronic levels are missing, especially for the higher quantum numbers, so the set of electronic levels should be completed using semi-empirical methods. To extend the electronic levels of the ground state configuration we use the iso-electronic sequence method. Let us consider carbon atom C(I) as an example. For carbon the ground state configuration we shall consider:
$2s^2 2p^2$ (^{1}S, ^{3}P, ^{1}D);
$2s^2 p^3$ (^{5}S°, ^{3}S°, ^{3}P°, ^{1}P°, ^{3}D°, ^{1}D°);
$2p^4$ (^{1}S, ^{3}P, ^{1}D).
If one of these terms has not yet been observed, it can be derived through extrapolation from energy levels of iso-electronic species. Practically, for carbon C(I), one missing term is $2p^4$ [^{1}S], so, for example, we consider the energies of N(II), O(III) and F(IV), corresponding to the same term, and reporting them as a function of the atomic number Z, we perform an extrapolation to obtain the missing energy corresponding to the C(I) ($Z = 6$). The method works well, as a matter of fact extrapolating iso-electronic sequences corresponding to $2s^2 p^3$ (^{5}S°) term we obtain a value very close to the observed one. The excited states come from the excitation of one electron towards higher values of the principal quantum numbers ($n > 2$); such series for C(I) are:
$2s^2 2p(^2P°)nx$
$2s2p^2(^4P)nx$
$2s2p^2(^2D)nx'$
$2s2p^2(^2S)nx''$
$2s2p^2(^2P)nx'''$
$2p^3(^4S°)nx^{IV}$
These series arise from the interaction of the atomic core ($2s^2 2p(^2P°)$, $2s2p^2(^4P)$,...) with the excited electron (nx, nx',...) with x=s,p,d,.... Let us focus our attention on the first excited series. In the case of x=s, there are two spectroscopic terms: ^{3}P°(L=1, S=1), and ^{1}P°(L=1, S=0). NIST's tables report observed levels up to $n = 10$ for the former and $n = 14$ (missing values $n = 11$ and $n = 12$) for the latter. To extrapolate to higher principal quantum numbers, the following Ritz-Rydberg series can be used:

$$E_n = E_i - \frac{R^*}{\left(n + A + \frac{B}{n^2}\right)^2} \tag{56}$$

where E_i is the ionisation potential, R^* is the Rydberg constant of the selected series and A, B are adjustable parameters. For each excited series, E_i is calculated as the sum between the ionisation energy of the selected species (in this case C(I)) and the core energy of the successive ionised species (i.e. C(II)). For example, if we consider the $2s2p^2(^4P)nx$ series, E_i is calculated as the sum between the ionisation potential of C(I) (e.g. 90820.42 cm^{-1}) and the energy of the core $2s2p^2(^4P)$ for C(II) (e.g. 43035.78 cm^{-1}). R^* is given by the following equation:

$$R^* = R \cdot (Z' - Z_H)^2 \tag{57}$$

where R is the Rydberg constant (109737 cm^{-1}), Z' is the nuclear charge (atomic number) (for C, Z'=6) and Z_H is the number of core electrons which should be extracted to obtain an hydrogen-like atom (for C(I) Z_H=5). The constants A and B can be determined when at least two observed levels are available. If we have only two levels it is straightforward to solve a system of two equations, while if we have more than two levels it is possible to fit these energy levels as a function of the principal quantum number using equation (41). To extend the spectroscopic term $2s2p^2(^2P°)ns$ (^{3}P°) for $n > 10$, using the latter method, we obtain A=-1.0288 and B=-0.66479. If there is only one observed energy level, instead of equation (56) the following formula should be used:

$$E_n = E_i - \frac{R^*}{(n + C)^2} \tag{58}$$

where C is an adjustable parameter. For the spectroscopic series $2s^2 2p(2P^\circ)nx$, all the spectroscopic terms corresponding to x=g ($n \geq 5$) have not been observed. In this case to obtain the energy level of the terms corresponding to 5g, we report in graph the energy levels (5s, 5p, 5d, 5f) as a function of the azimuthal quantum number l, and extrapolate to $l = 4$. The energy levels of 5s, 5p, 5d, 5f are the average values over all the spectroscopic terms; e.g for 5s we have:

$$\overline{E}_{5s} = \frac{g\left({}^3P^\circ\right) * E_{5s}^{3}P^\circ + g\left({}^1P^\circ\right) * E_{5s}^{1}P^\circ}{g\left({}^3P^\circ\right) + g\left({}^1P^\circ\right)} \tag{59}$$

where g is the statistical weight. The total statistical weight associated to energy level 5g, obtained as previously, is the sum over the statistical weights of all the corresponding predicted spectroscopic terms. From this last energy value, we extrapolate to $n > 5$ using the formula (57). This method has been applied upon $n = 20$ and $l = 19$, with the exception of those series where no observed energies are present. For $n > 20$ energy levels, we assume a hydrogen-like behaviour and use the following formulas:

$$E_n = E_i - \frac{R^*}{n^2} \tag{60}$$

It is possible to demonstrate that, at fixed n and for each series, the sum over the statistical weights of all the corresponding predicted spectroscopic terms for different l is equal to:

$$g_n = 2n^2 \cdot g_{core} \tag{61}$$

so for $n > 20$ we have applied this last equation to determine the total statistical weight.

B Reference States

amended; see errata

The calculation of the global thermodynamic properties requires the definition of reference states for each species. These reference states are chosen according to the standard state and affect the formation enthalpies and the calculation of equilibrium constants. The equilibrium constants refer to the formation reaction of each species from the elements in their standard states. For carbon compounds, the equilibrium constant is calculated taking as reactant the C_2 molecule (gas) instead of carbon (graphite). The formation enthalpy of nitrogen atom is given, for example, by half the dissociation energy of the nitrogen molecule plus the formation enthalphy of the nitrogen molecule, which is zero. For a carbon atom (gas) whose refence state is graphite (solid), the formation enthalpy is equal to the sublimation enthalpy of graphite. Formation enthalpies for all Mars-atmosphere components are reported in table 3.

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[2] In this compilation, the internal partition function of O_2^- has been calculated taking as reference the minimum of the potential curve, while for all other species the reference is the vibrational level $v = 0$.

Tables

List of Tables

Table 1: Electronic levels included in the calculation in Fig. 3 for O_2.

Energy levels cm^{-1} - case (a)	Energy levels cm^{-1} - case (b)	Energy levels cm^{-1} - case (c)	Energy levels cm^{-1} - case (d)
0	0	0	0
–	7918.1	7918.1	7918.1
–	–	13195.1	13195.1
–	–	–	33057.3
–	–	–	34690
–	–	–	35397.8
–	–	–	39279
–	–	–	49793.28
–	–	–	54031
–	–	–	55524
–	–	–	57041
–	–	–	67841
–	–	–	69123
–	–	–	72842
–	–	–	74866
–	–	–	75260
–	–	–	76091
–	–	–	79883
–	–	–	82166

Table 2: Electronic levels included in the calculation in Fig. 3 for CN.

Energy levels cm^{-1} - case (a)	Energy levels cm^{-1} - case (b)	Energy levels cm^{-1} - case (c)	Energy levels cm^{-1} - case (d)
0	0	0	0
–	9245.28	9245.28	9245.28
–	–	25752.0	25752.0
–	–	–	32400
–	–	–	54486.3
–	–	–	59151.18
–	–	–	60095.64
–	–	–	61655
–	–	–	61969.7
–	–	–	65258.19

see errata

Table 3: Formation enthalpy at 0 K for Mars-atmosphere species

Species	$\Delta H_f^0(0K)$ / eV
Ar	0.0
Ar^+	15.7596
Ar^{2+}	43.3893
Ar^{3+}	84.1243
Ar^{4+}	143.8103
C	7.35351324
C^+	18.619034
C^{2+}	43.00231
C^{3+}	90.890014
C^{4+}	155.38376
C^-	6.182
C_2	8.54273074
C_2^+	19.94273074
C_2^-	5.26973074
C_3	8.15696357
CN	4.69264775
CN^+	18.29064775
CN^-	0.83064775
CO	−1.17950394
CO^+	12.83449606
CO_2	−4.07475247
CO_2^+	9.70224753
e^-	0.0
N	4.87933027
N^+	19.428233
N^{2+}	49.043795
N^{3+}	96.492844
N^{4+}	173.96623
N^-	4.9497068
N_2	0.0
N_2^+	15.581
N_2^-	0.352
N_3	4.2931
NO	0.930593918
NO^+	10.194793918
NO_2	0.372497752
N_2O	0.885928879
N_2O^+	13.77492888
NCO	1.3163
O	2.55800581
O^+	16.1755
O^{2+}	51.3315
O^{3+}	106.2805
O^{4+}	183.6965
O^-	0.95
O_2	0.0
O_2^+	12.0697
O_2^-	−0.4510
O_3	1.50907122
O_3^-	−0.594
CO_2^-	−3.475
C_2N	5.7674
C_2O	2.9704

Spectroscopic data tables

Table 4: Spectroscopic data for C_2.

T_e	g_i	ω_e	$\omega_e x_e$	$\omega_e y_e$	$\omega_e z_e$	$\omega_e k_e$	E_{diss}	B_e	$\alpha_e \cdot 10^2$	$\gamma_e \cdot 10^4$	δ_e	ξ_e	$D_e \cdot 10^6$	$\beta_e \cdot 10^6$	g_e	H_{v0}	H_{v1}	r_e
0.	1	1854.71	13.34	-0.172	0	0	50086.62	1.81984	1.765	-2.3	0	0	6.92	0.081	0	0	0	1.2425
716.24	6	1641.35	11.67	0	0	0	0	1.63246	1.661	0	0	0	6.44	0	0	0	0	1.3119
6434.27	3	1470.45	11.19	0.028	0	0	0	1.49852	1.634	-0.87	0	0	6.22	0	0	0	0	1.3693
8391.	2	1608.35	12.078	-0.01	0	0	0	1.61634	1.686	-0.54	0	0	6.44	0.036	0	0	0	1.3184
13312.	3	1961.6	13.7	0	0	0	0	1.87	0.	0	0	0	0.	0	0	0	0	1.23
20022.5	6	1788.22	16.44	-0.5067	0	0	0	1.7527	1.608	-12.74	0	0	6.74	0.103	0	0	0	1.2661
34261.3	2	1809.1	15.81	0	0	0	0	1.7834	1.8	0	0	0	6.8	0	0	0	0	1.2552
40796.65	6	1106.56	39.26	2.805	-0.1271	0	0	1.1922	2.42	0	0	0	6.3	0.29	0	0	0	1.5351
43239.44	1	1829.57	13.94	0	0	0	0	1.8332	1.96	0	0	0	7.32	0.03	0	0	0	1.238
55034.7	1	1671.5	40.02	0.248	0	0	0	1.7897	3.87	-5.5	0	0	8.3	0.6	0	0	0	1.2529
71045.8	3	1360.5	14.8	0	0	0	0	1.448	4.	60.	0	0	10.	0	0	0	0	1.393
73183.6	6	1458.06	0.0	0	0	0	0	1.5238	1.7	0	0	0	6.6	0	0	0	0	1.3579
75456.9	2	1557.5	0.0	0	0	0	0	1.645	1.9	0	0	0	6.	0	0	0	0	1.307

Table 5: Spectroscopic data for C_2^+.

T_e	g_i	ω_e	$\omega_e x_e$	$\omega_e y_e$	$\omega_e z_e$	$\omega_e k_e$	E_{diss}	B_e	α_e	γ_e	δ_e	ξ_e	$D_e \cdot 10^7$	β_e	g_e	H_{v0}	H_{v1}	r_e
0	4	1350	0	0	0	0	42908.35	1.659	0	0	0	0	100	0	0	0	0	1.301
40143	2	1340	0	0	0	0	2765.348	1.648	0	0	0	0	100	0	0	0	0	1.306

Table 6: Spectroscopic data for C_2^-.

T_e	g_i	ω_e	$\omega_e x_e$	$\omega_e y_e$	$\omega_e z_e$	$\omega_e k_e$	E_{diss}	B_e	$\alpha_e \cdot 10^2$	$\gamma_e \cdot 10^4$	δ_e	ξ_e	$D_e \cdot 10^7$	$\beta_e \cdot 10^6$	$g_e \cdot 10^7$	H_{v0}	H_{v1}	r_e
0.	2	1781.04	11.58	-0.027	0	0	68395.26	1.7468	1.67	0	0	0	66.9	0	0	0	0	1.2682
18390.88	2	1968.73	14.43	-0.324	0	0	0	1.8774	1.776	-3.7	0	0	68.4	0.1	0.08	0	0	1.2233
19448.	4	1074.	25.	0	0	0	0	1.135	0.35	0	0	0	0	0	0	0	0	1.573

Table 7: Spectroscopic data for C_3.

T_0	p_i	E_{diss}	A_0	B_0	C_0	r_e	ν_1	ν_2	ν_3	σ	σ_{rot}
0	1	61570.75	0	0.4305	0	1.277	1225.	63.1	2040.	2	0
14000	6	61570.75	0	0.4305	0	1.277	1225.	63.1	2040.	2	0
21500	6	61570.75	0	0.4305	0	1.277	1225.	63.1	2040.	2	0
23800	3	61570.75	0	0.4305	0	1.277	1225.	63.1	2040.	2	0
24675.5	2	61570.75	0	0.4305	0	1.277	1225.	63.1	2040.	2	0
29100	6	61570.75	0	0.4305	0	1.277	1225.	63.1	2040.	2	0
32800	3	61570.75	0	0.4305	0	1.277	1225.	63.1	2040.	2	0
32900	1	61570.75	0	0.4305	0	1.277	1225.	63.1	2040.	2	0
33700	2	61570.75	0	0.4305	0	1.277	1225.	63.1	2040.	2	0
40500	2	61570.75	0	0.4305	0	1.277	1225.	63.1	2040.	2	0

Table 8: Spectroscopic data for CN.

T_e	g_i	ω_e	$\omega_e x_e$	$\omega_e y_e$	$\omega_e z_e$	$\omega_e k_e$	E_{diss}	B_e	$\alpha_e \cdot 10^2$	$\gamma_e \cdot 10^4$	δ_e	ξ_e	$D_e \cdot 10^6$	$\beta_e \cdot 10^6$	g_e	H_{v0}	H_{v1}	r_e
0	2	2068.59	13.087	-0.009093	0	0	62588.63	1.8997	1.737	-0.3107	0	0	6.40	0.012	0	0	0	1.1718
9245.28	4	1812.56	12.609	-0.0118	0	0	0	1.7151	1.708	-0.364	0	0	5.93	0.0425	0	0	0	1.2333
25752.0	2	2163.9	20.2	0	0	0	0	1.973	2.3	0	0	0	6.6	0	0	0	0	1.150
32400	4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
54486.3	4	1004.71	8.78	0	0	0	0	1.162	1.3	0	0	0	7.0	0	0	0	0	1.498
59151.18	2	1681.43	3.60	-1.02	0	0	0	1.4871	0.643	-7.7	0	0	5.0	0	0	0	0	1.3245
60095.64	4	1239.50	12.75	0	0	0	0	1.3834	1.87	0	0	0	7.0	0	0	0	0	1.3373
61655	4	0	0	0	0	0	0	1.085	0.	0	0	0	0	0	0	0	0	1.551
61969.7	4	0	0	0	0	0	0	1.520	0.	0	0	0	0	0	0	0	0	1.310
65258.19	4	1121.76	14.203	0.180	0	0	0	1.3052	2.08	0	0	0	5.8	0	0	0	0	1.4137

Table 9: Spectroscopic data for CN^+.

T_e	g_i	ω_e	$\omega_e x_e$	$\omega_e y_e$	$\omega_e z_e$	$\omega_e k_e$	E_{diss}	B_e	$\alpha_e \cdot 10^2$	$\gamma_e \cdot 10^4$	δ_e	ξ_e	D_e	β_e	g_e	H_{v0}	H_{v1}	r_e
0	6	1580.	12.5	0	0	0	0	39117.89	1.566	170.	0	0	0	0	0	0	0	1.29
1500.	1	1580.	12.5	0	0	0	0	39117.89	1.566	170.	0	0	0	0	0	0	0	1.29
6000.	1	1580.	12.5	0	0	0	0	39117.89	1.566	170.	0	0	0	0	0	0	0	1.29
8000.	1	1580.	12.5	0	0	0	0	39117.89	1.566	170.	0	0	0	0	0	0	0	1.29
15000.	1	1580.	12.5	0	0	0	0	39117.89	1.566	170.	0	0	0	0	0	0	0	1.29

Table 10: Spectroscopic data for CN^-.

T_e	g_i	ω_e	$\omega_e x_e$	$\omega_e y_e$	$\omega_e z_e$	$\omega_e k_e$	E_{diss}	B_e	$\alpha_e \cdot 10^2$	$\gamma_e \cdot 10^4$	δ_e	$D_e \cdot 10^6$	$\beta_e \cdot 10^6$	$g_e \cdot 10^{10}$	H_{v0}	$H_{v1} \cdot 10^{12}$	r_e
0	1	2169.81	13.288	0.0105	5.74E-5	9.83E-7	83155.77	1.9313	1.7504	5.49E-3	2.54E-8	6.122	-1.15E-3	1.805	5.83E-12	-0.1738	1.1283

Table 11: Spectroscopic data for CO.

T_e	g_i	ω_e	$\omega_e x_e$	$\omega_e y_e$	$\omega_e z_e$	$\omega_e k_e$	E_{diss}	B_e	$\alpha_e \cdot 10^2$	$\gamma_e \cdot 10^4$	δ_e	$D_e \cdot 10^6$	$\beta_e \cdot 10^6$	$g_e \cdot 10^{10}$	H_{v0}	$H_{v1} \cdot 10^{12}$	r_e
0	1	2169.81	13.288	0.0105	5.74E-5	9.83E-7	89462.29	1.9313	1.750	5.49E-3	2.54E-8	6.122	-1.15E-3	1.805	5.83E-12	-0.1738	1.1283
48686.7	6	1743.41	14.36	-0.045	0.0025	0	0	1.6912	1.904	-0.41	0	6.36	0.04	0	0	0	1.2057
55825.49	3	1228.6	10.468	0.0091	0.00259	0	0	1.3446	1.892	3.45	0	6.41	0	0	0	0	1.3523
61120.1	6	1171.94	10.635	0.0785	-0.00163	0	0	1.3108	1.782	1.13	0	6.59	0	0	0	0	1.3696
64230.24	3	1117.72	10.686	0.1174	0	0	0	1.2836	1.753	7.1E-2	0	6.77	0	0	0	0	1.384
65075.77	2	1518.24	19.4	0.766	0	0	0	1.6115	2.325	15.9	0	7.33	0.1	0	0	0	1.2353
65084.4	1	1092.22	10.704	0.0554	0	0	0	1.2705	1.848	2.91	0	9.	0	0	0	0	1.3911
65928.	2	1094.	10.2	0	0	0	0	1.257	1.7	0	0	0	0	0	0	0	1.399
83814	3	2199.3	0	0	0	0	0	1.986	4.2	0	0	0	0	0	0	0	1.113
86945.2	1	2112.7	15.22	0	0	0	0.	1.9612	2.61	0	0	7.1	0	0	0	0	1.1197
90975.	3	2166.	15.	0	0	0	0	1.8785	2.	0	0	7.9	0	0	0	0	1.1441
91916.5	1	2175.92	14.76	0	0	0	0	1.9533	1.96	0	0	6.2	0	0	0	0	1.1219
93158.5	6	0	0	0	0	0	0	1.935	0	0	0	-131.	0	0	-1.9E-7	0	1.127
92903.	2	2153.8	42.	0	0	0	0	1.9771	2.54	0	0	6.5	0	0	0	0	1.1152
99803.	1	2112.	198.	0	0	0	0	1.86	0	0	0	80.	0	0	0	0	1.15
101409.	1	2235.3	0	0	0	0	0	1.9203	0	0	0	5.8	0	0	0	0	1.1315
103251.	2	2181.	15.	0	0	0	0	1.9812	0	0	0	14.	0	0	0	0	1.114
105811.	2	1097.	47.	0	0	0	0	0	0	0	0	0	0	0	0	0	0
121137.	2	1570.	13.4	0	0	0	0	0	0	0	0	0	0	0	0	0	0
123656.	1	1521.	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
126729.	2	1560.	13.3	0	0	0	0	0	0	0	0	0	0	0	0	0	0
129043.	1	1558.	10.6	0	0	0	0	0	0	0	0	0	0	0	0	0	0
138038.	1	1771.	29.	0	0	0	0	0	0	0	0	0	0	0	0	0	0
144939.	1	1735.	28.	0	0	0	0	0	0	0	0	0	0	0	0	0	0
147065.	1	1658.	11.	0	0	0	0	0	0	0	0	0	0	0	0	0	0
148929.	1	1750.	30.	0	0	0	0	0	0	0	0	0	0	0	0	0	0
149294.	1	1730.	30.	0	0	0	0	0	0	0	0	0	0	0	0	0	0
153271.	1	1705.	18.5	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Table 12: Spectroscopic data for CO^+.

T_e	g_i	ω_e	$\omega_e x_e$	$\omega_e y_e$	$\omega_e z_e$	$\omega_e k_e$	E_{diss}	B_e	$\alpha_e \cdot 10^2$	γ_e	δ_e	ξ_e	$D_e \cdot 10^6$	$\beta_e \cdot 10^6$	g_e	H_{v0}	H_{v1}	r_e
0	2	2214.24	15.164	-0.0007	0	0	67249.96	1.9772	1.896	0	0	0	6.35	0	0	0	0	1.1151
20733.3	4	1562.06	13.532	0.0131	0	0	0	1.5894	1.942	0	0	0	6.6	0	0	0	0	1.2438
45876.7	2	1734.18	27.927	0.3283	0	0	0	1.7999	3.025	0	0	0	7.75	0.22	0	0	0	1.1688
63012.	4	1144.	33.3	0	0	0	0	1.357	2.4	0	0	0	0	0	0	0	0	1.346
65230.	4	1350.	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
73190.	2	1400.	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
87140.	2	1420.	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
105690.	2	1780.	30.	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Table 13: Spectroscopic data for CO_2.

T_0	p_i	E_{diss}	A_0	B_0	C_0	r_e	ν_1	ν_2	ν_3	σ	σ_{rot}
0	1	43984.062	0	0.3915	0	1.1621	1384.86	667.3	2349.3	2	0
30000.	3	43984.062	0	0.3915	0	1.1621	1384.86	667.3	2349.3	2	0
33000.	6	43984.062	0	0.3915	0	1.1621	1384.86	667.3	2349.3	2	0
36000.	3	43984.062	0	0.3915	0	1.1621	1384.86	667.3	2349.3	2	0
46000.	2	43984.062	5.3	0.426	1.246	1.1621	1384.86	667.3	2349.3	2	2
72480.	2	43984.062	5.3	0.426	1.246	1.1621	1225.	667.3	2349.3	2	2
73100.	1	43984.062	5.3	0.426	1.246	1.1621	1225.	667.3	2349.3	2	2
85160.	1	43984.062	0	0.3915	0	1.1621	1384.86	667.3	2349.3	2	0
85840.	1	43984.062	0	0.3915	0	1.1621	1384.86	667.3	2349.3	2	0
88535	1	43984.062	0	0.3915	0	1.1621	1458.	667.3	2349.3	2	0
89111	1	43984.062	0	0.3915	0	1.1621	1384.86	667.3	2349.3	2	0
91830.	1	43984.062	0	0.3915	0	1.1621	1384.86	667.3	2349.3	2	0
92360	1	43984.062	0	0.39021	0	1.1621	1384.86	667.3	2349.3	2	0
96600.	1	43984.062	0	0.39021	0	1.1621	1384.86	667.3	2349.3	2	0
99331	1	43984.062	0	0.39021	0	1.1621	1384.86	667.3	2349.3	2	0
100570	1	43984.062	0	0.39021	0	1.1621	1384.86	667.3	2349.3	2	0
100650	1	43984.062	0	0.39021	0	1.1621	1384.86	667.3	2349.3	2	0
100940	1	43984.062	0	0.39021	0	1.1621	1384.86	667.3	2349.3	2	0
127065	1	43984.062	0	0.39021	0	1.1621	1384.86	667.3	2349.3	2	0
127443	1	43984.062	0	0.39021	0	1.1621	1384.86	667.3	2349.3	2	0
130774	1	43984.062	0	0.39021	0	1.1621	1384.86	667.3	2349.3	2	0
132977	1	43984.062	0	0.39021	0	1.1621	1384.86	667.3	2349.3	2	0

Table 14: Spectroscopic data for CO_2^+.

T_0	p_i	E_{diss}	A_0	B_0	C_0	r_e	ν_1	ν_2	ν_3	σ	σ_{rot}
0	4	43981.42	0	0.3804	0	1.177	1255.	492.1	1469.	2	0
159.7	4	43981.42	0	0.3804	0	1.177	1255.	492.1	1469.	2	0
28581.	4	43981.42	0	0.3804	0	1.228	1255.	492.1	1469.	2	0
34678.	2	43981.42	0	0.3804	0	1.180	1255.	492.1	1469.	2	0
45320	2	43981.42	0	0.3804	0	0	1255.	492.1	1469.	2	0

Table 15: Spectroscopic data for N_2.

T_e	g_i	ω_e	$\omega_e x_e$	$\omega_e y_e$	$\omega_e z_e \cdot 10^3$	$\omega_e k_e$	E_{diss}	B_e	$\alpha_e \cdot 10^2$	$\gamma_e \cdot 10^4$	$\delta_e \cdot 10^4$	$\xi_e \cdot 10^4$	$D_e \cdot 10^6$	β_e	g_e	H_{v0}	H_{v1}	r_e
0	1	2358.57	14.324	-0.00226	-0.24	0	78714.24	1.9982	1.732	-0.33	0	0	5.76	0	0	0	0	1.0977
50203.6	3	1460.64	13.87	0.0103	-1.97	0	-29694.33	1.4546	1.8	-0.88	0	0	6.15	0	0	0	0	1.2866
59619.35	6	1733.39	14.122	-0.0569	3.61	0	-39490	1.6374	1.791	-0.77	0	0	5.9	0	0	0	0	1.2126
59808	6	1501.4	11.6	0	0	0	-39301	1.47	1.71	0	0	0	0	0	0	0	0	1.28
66272.4	3	1516.88	12.18	0.04186	-0.732	0	-42452	1.4733	1.666	0.	0	0	5.56	0	0	0	0	1.2784
68152.7	1	1530.25	12.07	0.04129	-0.29	0	-50181	1.4799	1.657	0.241	0	0	5.55	0	0	0	0	1.2755
69283.06	2	1694.2	13.949	0.007935	0.291	0	-49051	1.6169	1.793	-0.293	0	0	5.89	0	0	0	0	1.2203
72097	2	1559.26	11.63	0	0	0	-46237	1.498	1.66	0	0	0	0	0	0	0	0	1.268
76436	5	667.	0	0	0	0	-3448	0.921	0.	0	0	0	0	0	0	0	0	1.6170
87900	6	742.49	11.85	0	0	0	-11209	0.928	1.61	0	0	0	5.	0	0	0	0	1.6107
89136	6	2047.18	28.445	2.08833	-535.	0	-9972.	1.8247	1.868	-22.8	7.33	-1.5	0	0	0	0	0	1.1487

Table 16: Spectroscopic data for N_2^+.

T_e	g_i	ω_e	$\omega_e x_e$	$\omega_e y_e$	$\omega_e z_e$	$\omega_e k_e$	E_{diss}	B_e	$\alpha_e \cdot 10^2$	γ_e	δ_e	ξ_e	$D_e \cdot 10^6$	β_e	g_e	H_{v0}	H_{v1}	r_e
0	2	2207	16.1	-0.04	0	0	70272.905	1.93176	1.881	0	0	0	6.1	0	0	0	0	1.1164
9166.9	4	1903.7	15.02	0	0	0	-62217.1	1.7444	1.883	0	0	0	5.6	0	0	0	0	1.1749
25461.4	2	2419.84	23.189	-0.5375	-0.0495	0	-45919.4	2.07456	2.4	0	0	0	6.17	0	0	0	0	1.0742
25467.	4	2398.	14.	0	0	0	-46008.2	2.071	1.4	0	0	0	6.0	0	0	0	0	0
52318.2	4	907.71	11.91	0.016	0	0	-18561.27	1.113	2.	0	0	0	5.0	0	0	0	0	1.471
64608.1	2	2071.5	9.29	-0.43	0	0	-24953.	1.509	0.	0	0	0	4.0	0	0	0	0	1.2628
195000.	2	0	0	0	0	0	0.	0	0.	0	0	0	0	0	0	0	0	0

Table 17: Spectroscopic data for N_2^-.

T_e	g_i	ω_e	$\omega_e x_e$	$\omega_e y_e$	$\omega_e z_e$	$\omega_e k_e$	E_{diss}	B_e	α_e	γ_e	δ_e	ξ_e	$D_e \cdot 10^6$	β_e	g_e	H_{v0}	H_{v1}	r_e
0.	4	1968.	10.	0	0	0	63959.25	0	0	0	0	0	0	0	0	0	0	1.193
77150.	2	2180.	16.	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1.115

Table 18: Spectroscopic data for N_3.

T_0	p_i	E_{diss}	A_0	B_0	C_0	r_e	ν_1	ν_2	ν_3	σ	σ_{rot}
0.	2	36698.23	0	0.43117	0	1.1815	1400.	737.	2150.	2	0
71.9	2	36698.23	0	0.43117	0	1.1815	1400.	737.	2150.	2	0
36739.	2	36698.23	0	0.43238	0	1.1799	1400.	737.	2150.	2	0

Table 19: Spectroscopic data for NO.

T_e	g_i	ω_e	$\omega_e x_e$	$\omega_e y_e$	$\omega_e z_e$	$\omega_e k_e$	E_{diss}	B_e	$\alpha_e \cdot 10^2$	$\gamma_e \cdot 10^4$	δ_e	ξ_e	$D_e \cdot 10^6$	β_e	g_e	H_{v0}	H_{v1}	r_e
0.	4	1904.2	14.075	0.011	0	0	52400.21	1.6719	1.71	-0.37	0	0	0.54	0	0	0	0	1.1508
38807.	8	1019.	12.80	0	0	0	-14537.	1.1275	0.	0	0	0	4.9	0	0	0	0	1.415
43965.7	2	2374.71	16.106	-0.0465	0	0	-28603.	1.9965	1.915	0	0	0	5.4	0	0	0	0	1.0634
45932.	4	1037.2	7.77	0.1	0	0	-26636.7	1.1244	1.2	1.25	0	0	4.9	0	0	0	0	1.4167
48680.	4	1206.	15.0	0	0	0	-21184.	1.3358	0.	0	0	0	6.8	0	0	0	0	0
52126.	4	2395.	15.0	0	0	0	-20383.	2.0	3.	0	0	0	2.8	0	0	0	0	1.062
53084.7	2	2323.9	22.885	0.75	-0.22	0	-19485.	2.0026	2.175	0	0	0	5.8	0	0	0	0	1.0610
53637.	4	1004.4	11.0	0	0	0	-18932.	1.1275	0.	0	0	0	5.0	0	0	0	0	1.4150
60364.2	4	1217.4	15.61	0	0	0	-12205.	1.332	2.1	0	0	0	4.8	0	0	0	0	1.302
60628.8	2	2375.3	16.4	0	0	0	-11940.	1.9863	1.82	0	0	0	5.6	0	0	0	0	1.066
61800.	4	2394.0	20.0	0	0	0	-10769.	1.982	2.3	0	0	0	2.74	0	0	0	0	1.067
62473.4	2	2339.4	0	0	0	0	-10096.	2.003	1.8	0	0	0	2.93	0	0	0	0	1.0617
62913.	2	1085.54	11.083	-0.1439	0	0	-9655.	1.2523	2.04	0	0	0	5.4	0	0	0	0	1.3427
63040.	4	952.0	11.28	0	0	0	-19144.	1.132	2.21	0	0	0	5.6	0	0	0	0	1.4120
64077.5	4	2438.3	48.38	0	0	0	-18106.	2.034	5.6	0	0	0	2.78	0	0	0	0	1.0535

Table 20: Spectroscopic data for NO^+.

T_e	g_i	ω_e	$\omega_e x_e$	$\omega_e y_e$	$\omega_e z_e$	$\omega_e k_e$	E_{diss}	B_e	$\alpha_e \cdot 10^2$	γ_e	δ_e	ξ_e	$D_e \cdot 10^6$	β_e	g_e	H_{v0}	H_{v1}	r_e
0.	1	2376.42	16.262	0	0	0	87515.96	1.99727	1.889	0	0	0	5.64	0	0	0	0	1.0632
52190.	3	1293.	15.1	0	0	0	36505.	1.369	1.92	0	0	0	4.5	0	0	0	0	1.284
59240.	6	1710.	14.	0	0	0	36923.	1.634	1.84	0	0	0	3.6	0	0	0	0	1.175
61880.	6	1313.	10.6	0	0	0	34283.	1.377	1.92	0	0	0	4.41	0	0	0	0	1.28
67720.	3	1284.	10.7	0	0	0	28443.	1.357	1.92	0	0	0	4.5	0	0	0	0	1.29
69540.	1	1283.	13.5	0	0	0	26623.	1.363	1.92	0	0	0	4.5	0	0	0	0	1.287
71450.	2	1278.	16.	0	0	0	24713.	1.361	1.92	0	0	0	4.53	0	0	0	0	1.288
73471.7	2	1601.93	20.207	-0.2683	0	0	22692.	1.586	2.45	0	0	0	5.6	0	0	0	0	1.1931

Table 21: Spectroscopic data for NO_2.

T_0	p_i	E_{diss}	A_0	B_0	C_0	r_e	ν_1	ν_2	ν_3	σ	σ_{rot}
0	2	25123.36	8.0025	0.43364	0.4105	1.1934	1319.95	749.6	1616.05	2	2
11956.	2	25123.36	8.0025	0.43364	0.4105	1.1934	1319.95	749.6	1616.05	2	2
14744.	2	25123.36	8.0025	0.43364	0.4105	1.1934	1319.95	749.6	1616.05	2	2
26000.	4	25123.36	8.0025	0.43364	0.4105	1.1934	1319.95	749.6	1616.05	2	2
27000.	4	25123.36	8.0025	0.43364	0.4105	1.1934	1319.95	749.6	1616.05	2	2
31000.	2	25123.36	8.0025	0.43364	0.4105	1.1934	1319.95	749.6	1616.05	2	2
40125.	2	25123.36	4.132	0.402	0.366	1.314	1319.95	749.6	1616.05	2	2
42500.	2	25123.36	8.0025	0.43364	0.4105	1.1934	940.	749.6	1616.05	2	2
50000.	2	25123.36	8.0025	0.43364	0.4105	1.1934	1319.95	749.6	1616.05	2	2
58309.	2	25123.36	0	0.43364	0	1.13	1420.	596.5	1616.05	2	0
76711.	2	25123.36	8.0025	0.43364	0.4105	1.1934	1319.95	610.	1616.05	2	2
87481.	2	25123.36	8.0025	0.43364	0.4105	1.1934	1319.95	560.	1616.05	2	2
91508.	2	25123.36	8.0025	0.43364	0.4105	1.1934	1319.95	624.	1616.05	2	2
111480.	2	25123.36	8.0025	0.43364	0.4105	1.1934	1319.95	749.6	1616.05	2	2
131680.	2	25123.36	8.0025	0.43364	0.4105	1.1934	1319.95	749.6	1616.05	2	2

Table 22: Spectroscopic data for N_2O.

T_0	p_i	E_{diss}	A_0	B_0	C_0	r_e	ν_1	ν_2	ν_3	σ	σ_{rot}
0.	1	13526.73	0	0.419011	0	-	2223.7	589.2	1276.5	2	0
32630	6	13526.73	0	0.419011	0	-	2223.7	589.2	1276.5	2	0
35460	6	13526.73	0	0.419011	0	-	2223.7	589.2	1276.5	2	0
38500	1	13526.73	0	0.419011	0	-	2223.7	589.2	1276.5	2	0
59590	1	13526.73	0	0.419011	0	-	2223.7	975.	1276.5	2	0
74000	1	13526.73	0	0.419011	0	-	2223.7	589.2	1276.5	2	0
77400	1	13526.73	0	0.419011	0	-	2223.7	589.2	1276.5	2	0
84633	1	13526.73	0	0.419011	0	-	2223.7	589.2	1276.5	2	0
84960	1	13526.73	0	0.419011	0	-	2223.7	589.2	1276.5	2	0
99710	1	13526.73	0	0.419011	0	-	2223.7	589.2	1276.5	2	0
117930	1	13526.73	0	0.419011	0	-	2223.7	589.2	1276.5	2	0

Table 23: Spectroscopic data for N_2O^+.

T_0	p_i	E_{diss}	A_0	B_0	C_0	r_e	ν_1	ν_2	ν_3	σ	σ_{rot}
0	2	13526.72	0	0.41159	0	1.140	1736.6	461.2	1126.4	1	0
132.4	2	13526.72	0	0.41159	0	1.140	1736.6	461.2	1126.4	1	0
28229.	2	13526.72	0	0.433	0	1.155	2451.7	614.	1345.5	1	0

Table 24: Spectroscopic data for CNO.

T_0	p_i	E_{diss}	A_0	B_0	C_0	r_e	ν_1	ν_2	ν_3	σ	σ_{rot}
0	2	33875.29	0	0.38940	0	2.408	1275.	532.7	1922.	1	0
95.2	2	33875.29	0	0.38940	0	2.408	1275.	532.7	1922.	1	0
22802.0	2	33875.29	0	0.4021	0	2.369	2338.0	680.8	1289.3	1	0
31811.0	4	33875.29	0	0.3765	0	2.45	2303.	532.7	1047.	1	0

Table 25: Spectroscopic data for O_2.

T_e	g_i	ω_e	$\omega_e x_e$	$\omega_e y_e$	$\omega_e z_e$	$\omega_e k_e$	E_{diss}	B_e	$\alpha_e \cdot 10^2$	$\gamma_e \cdot 10^4$	$\delta_e \cdot 10^6$	ξ_e	$D_e \cdot 10^6$	β_e	g_e	H_{v0}	H_{v1}	r_e
0.	3	1580.19	11.98	0.04747	-0.001273	0	41260.08	1.43768	1.593	0.641	-2.85	0	4.839	0	0	0	0	1.2075
7918.1	2	1483.5	12.9	0	0	0	33378.	1.4264	1.71	0	0	0	4.86	0	0	0	0	1.2156
13195.1	1	1432.77	14.	0	0	0	-28852.9	1.40037	1.82	-0.42	0	0	5.351	0	0	0	0	1.2269
33057.3	1	794.29	12.736	-0.2444	0.00055	0	-8991.	0.9155	1.391	-7.4	0	0	7.4	0	0	0	0	1.5174
34690.	6	850.	20.	0	0	0	-7358.	0.96	2.6	0	0	0	5.0	0	0	0	0	1.48
35397.8	3	799.07	12.16	-0.55	0	0	-6651.	0.9106	1.41	-9.7	0	0	4.7	0	0	0	0	1.5215
39279.	10	200.	0	0	0	0	-2769.	0.53	0.	0	0	0	0.	0	0	0	0	1.9940
49793.28	3	709.31	10.65	-0.139	0	0	-8044.4	0.819	1.206	-5.56	0	0	4.55	0	0	0	0	1.6043
54031.	3	537.	13.73	0	0	0	-3806.7	0.49	0.	0	0	0	3.33	0	0	0	0	2.074
55524.	6	200.	0	0	0	0	-2637.	0.7117	0.	0	0	0	50.6	0	0	0	0	1.7210
57041.	6	200.	0	0	0	0	-1186.	0.5706	0.	0	0	0	32.5	0	0	0	0	1.9220
67841.	8	1626.4	163.7	0	0	0	-8961.	0.819	3.88	0	0	0	1.01	0	0	0	0	1.62
69123.	8	705.6	9.6	0	0	0	-7299.	0.788	1.01	0	0	0	5.	0	0	0	0	1.6310
72842.	2	499.5	13.5	0	0	0	-3525.	0.547	1.02	0	0	0	4.8	0	0	0	0	1.9610
74866.	2	200.	0	0	0	0	-1581.	0.5259	0.	0	0	0	27.6	0	0	0	0	2.0020
75260.	3	1957.	19.7	0	0	0	-22101.	1.73	2.5	0	0	0	3.12	0	0	0	0	1.104
76091.	1	1927.	19.	0	0	0	-21270.	1.703	2.	0	0	0	3.12	0	0	0	0	1.113
79883.	3	2547.	0	0	0	0	-17478.	1.4638	0	0.	0	0	1.332	0	0	0	0	1.2
82166.	1	792.4	7.7	0	0	0	-13333.	0.811	0.92	0	0	0	4.2	0	0	0	0	1.6110

Table 26: Spectroscopic data for O_2^+.

T_e	g_i	ω_e	$\omega_e x_e$	$\omega_e y_e$	$\omega_e z_e$	$\omega_e k_e$	E_{diss}	B_e	$\alpha_e \cdot 10^2$	$\gamma_e \cdot 10^4$	δ_e	ξ_e	$D_e \cdot 10^6$	$\beta_e \cdot 10^6$	$g_e \cdot 10^6$	H_{v0}	H_{v1}	r_e
0.	4	1904.7	16.25	0	0	0	53740.7	1.6913	1.976	0	0	0	5.32	0	0	0	0	1.1164
32964.	8	1035.69	10.39	0	0	0	-21697.7	1.1046	1.575	0	0	0	4.88	-0.95	0	0	0	1.3814
40669.	4	898.2	13.57	0	0	0	-13992.4	1.0617	1.936	-1.73	0	0	5.94	0.06	0.012	0	0	1.4090
49552.	4	1196.97	17.09	0	0	0	-20969.1	1.2872	2.206	0	0	0	5.81	0.185	0	0	0	1.2796
53620.	4	900.	0	0	0	0	-26861.3	1.2872	2.206	0	0	0	5.811	0	0	0	0	0
62730.	4	920.	12.	0	0	0	-18751.3	1.2872	2.206	0	0	0	5.8	0	0	0	0	1.33
66719.	2	1156.	22.	0	0	0	-14758.9	1.2872	2.206	0	0	0	5.81	0	0	0	0	1.298

Table 27: Spectroscopic data for O_2^-.

T_e	g_i	ω_e	$\omega_e x_e$	$\omega_e y_e$	$\omega_e z_e$	$\omega_e k_e$	E_{diss}	B_e	$\alpha_e \cdot 10^2$	γ_e	δ_e	ξ_e	$D_e \cdot 10^6$	β_e	g_e	H_{v0}	H_{v1}	r_e
0.	4	1090.	8.1	0.	0	0	33529.	1.1566	1.21	0	0	0	4.5	0	0	0	0	0.
25300.	4	574.5	7.1	0.	0	0	-8229.	.615	.95	0	0	0	4.58	0	0	0	0	0.
97800.	8	1044.	10.	0.	0	0	0	0	0	0	0	0	0	0	0	0	0	0.

Table 28: Spectroscopic data for O_3.

T_0	p_i	E_{diss}	A_0	B_0	C_0	r_e	ν_1	ν_2	ν_3	σ	σ_{rot}
0	1	8388.16	3.55381	0.4453	0.39477	1.278	1110.	705.	1043.	2	2
10000.	3	8388.16	3.55381	0.4453	0.39477	-	600.	350.	600.	2	2
12500.	3	8388.16	3.55381	0.4453	0.39477	-	600.	350.	600.	2	2
13000.	1	8388.16	3.55381	0.4453	0.39477	-	850.	500.	0.	2	2
13500.	3	8388.16	3.55381	0.4453	0.39477	-	600.	350.	600.	2	2
14000.	1	8388.16	3.55381	0.4453	0.39477	-	600.	350.	600.	2	2
16600.	1	8388.16	3.55381	0.4453	0.39477	-	600.	350.	600.	2	2
25000.	3	8388.16	3.55381	0.4453	0.39477	-	600.	350.	600.	2	2
28450.	1	8388.16	3.55381	0.4453	0.39477	-	636.	333.	620.	2	2

Table 29: Spectroscopic data for O_3^-.

T_0	p_i	E_{diss}	A_0	B_0	C_0	r_e	ν_1	ν_2	ν_3	σ	σ_{rot}
0	1	12453.195	0	0	0	-	975.	550.	880.	2	2
16508.	1	12453.195	0	0	0	-	815.	275.	880.	2	2
16970.	1	12453.195	0	0	0	-	975.	550.	880.	2	2
21420.	1	12453.195	0	0	0	-	760.	190.	880.	2	2

Table 30: Spectroscopic data for CO_2^-.

T_0	p_i	E_{diss}	A_0	B_0	C_0	r_e	ν_1	ν_2	ν_3	σ	σ_{rot}
0	1	26176.69	6.2054	0.4210	0.3942	0	1400.	800.	1671.	2	2
11300.	1	26176.69	6.2054	0.4210	0.3942	0	1400.	800.	1671.	2	2

Table 31: Spectroscopic data for C_2N.

T_0	p_i	E_{diss}	A_0	B_0	C_0	r_e	ν_1	ν_2	ν_3	σ	σ_{rot}
0	2	49951.21	0	0.4535	0	1.245	1100	321	1453	2	0
26.41	2	49951.21	0	0.4535	0	1.245	1100	321	1453	2	0
30338.53	4	49951.21	0	0.4504	0	1.249	1100	440	1453	2	0
34802.3	2	49951.21	0	0.4430	0	1.259	1100	398	1453	2	0

Table 32: Spectroscopic data for C_2O.

T_0	p_i	E_{diss}	A_0	B_0	C_0	r_e	ν_1	ν_2	ν_3	σ	σ_{rot}
0	3	26895.36	0	0.4085	0	1.160	1074	381	1978	1	0
4050.	2	26895.36	0	0.4085	0	0	1074	381	1978	1	0
6450.	1	26895.36	0	0.4085	0	0	1074	381	1978	1	0
11651.	6	26895.36	0	0.4085	0	0	1074	381	1978	1	0

Thermodynamic data tables

Table 33: Internal thermodynamic properties of Ar ΔE=250 cm^{-1}

T(K)	Q_{int}	$\ln(Q_{int})$	E_{int}/RT	$C_{p,int}/R$
50	$1.000E+00$	$0.000E+00$	$0.000E+00$	$0.000E+00$
100	$1.000E+00$	$0.000E+00$	$0.000E+00$	$0.000E+00$
150	$1.000E+00$	$0.000E+00$	$0.000E+00$	$0.000E+00$
200	$1.000E+00$	$0.000E+00$	$3.345E-288$	$2.241E-285$
298.15	$1.000E+00$	$0.000E+00$	$1.442E-192$	$6.485E-190$
300	$1.000E+00$	$0.000E+00$	$2.293E-191$	$1.025E-188$
400	$1.000E+00$	$0.000E+00$	$5.639E-143$	$1.890E-140$
500	$1.000E+00$	$0.000E+00$	$5.899E-114$	$1.582E-111$
600	$1.000E+00$	$0.000E+00$	$1.281E-94$	$2.864E-92$
700	$1.000E+00$	$0.000E+00$	$8.181E-81$	$1.568E-78$
800	$1.000E+00$	$0.000E+00$	$1.827E-70$	$3.065E-68$
900	$1.000E+00$	$0.000E+00$	$2.028E-62$	$3.025E-60$
1000	$1.000E+00$	$0.000E+00$	$5.498E-56$	$7.383E-54$
2000	$1.000E+00$	$0.000E+00$	$4.217E-27$	$2.838E-25$
3000	$1.000E+00$	$0.000E+00$	$1.584E-17$	$7.125E-16$
4000	$1.000E+00$	$2.731E-14$	$9.516E-13$	$3.252E-11$
5000	$1.000E+00$	$2.876E-11$	$8.223E-10$	$2.381E-08$
6000	$1.000E+00$	$4.100E-09$	$1.065E-07$	$2.823E-06$
7000	$1.000E+00$	$1.924E-07$	$4.592E-06$	$1.113E-04$
8000	$1.000E+00$	$4.036E-06$	$8.747E-05$	$1.914E-03$
9000	$1.000E+00$	$4.593E-05$	$9.012E-04$	$1.779E-02$
10000	$1.000E+00$	$3.300E-04$	$5.883E-03$	$1.053E-01$
11000	$1.002E+00$	$1.676E-03$	$2.729E-02$	$4.453E-01$
12000	$1.007E+00$	$6.517E-03$	$9.737E-02$	$1.453E+00$
13000	$1.021E+00$	$2.053E-02$	$2.818E-01$	$3.834E+00$
14000	$1.056E+00$	$5.438E-02$	$6.826E-01$	$8.349E+00$
15000	$1.132E+00$	$1.241E-01$	$1.406E+00$	$1.498E+01$
16000	$1.281E+00$	$2.473E-01$	$2.477E+00$	$2.190E+01$
17000	$1.546E+00$	$4.355E-01$	$3.759E+00$	$2.593E+01$
18000	$1.986E+00$	$6.862E-01$	$4.995E+00$	$2.534E+01$
19000	$2.675E+00$	$9.839E-01$	$5.970E+00$	$2.132E+01$
20000	$3.698E+00$	$1.308E+00$	$6.611E+00$	$1.624E+01$
21000	$5.154E+00$	$1.640E+00$	$6.957E+00$	$1.169E+01$
22000	$7.150E+00$	$1.967E+00$	$7.089E+00$	$8.203E+00$
23000	$9.801E+00$	$2.282E+00$	$7.080E+00$	$5.725E+00$
24000	$1.322E+01$	$2.582E+00$	$6.986E+00$	$4.018E+00$
25000	$1.754E+01$	$2.864E+00$	$6.842E+00$	$2.854E+00$
26000	$2.286E+01$	$3.130E+00$	$6.673E+00$	$2.057E+00$
27000	$2.931E+01$	$3.378E+00$	$6.491E+00$	$1.507E+00$
28000	$3.699E+01$	$3.611E+00$	$6.306E+00$	$1.121E+00$
29000	$4.600E+01$	$3.829E+00$	$6.122E+00$	$8.477E-01$
30000	$5.644E+01$	$4.033E+00$	$5.943E+00$	$6.505E-01$
32000	$8.192E+01$	$4.406E+00$	$5.603E+00$	$3.992E-01$
34000	$1.140E+02$	$4.736E+00$	$5.293E+00$	$2.574E-01$
36000	$1.530E+02$	$5.030E+00$	$5.010E+00$	$1.732E-01$
38000	$1.992E+02$	$5.294E+00$	$4.754E+00$	$1.210E-01$
40000	$2.527E+02$	$5.532E+00$	$4.522E+00$	$8.726E-02$
42000	$3.134E+02$	$5.748E+00$	$4.310E+00$	$6.474E-02$
44000	$3.813E+02$	$5.944E+00$	$4.117E+00$	$4.924E-02$
46000	$4.560E+02$	$6.123E+00$	$3.939E+00$	$3.827E-02$
48000	$5.374E+02$	$6.287E+00$	$3.777E+00$	$3.032E-02$
50000	$6.250E+02$	$6.438E+00$	$3.627E+00$	$2.443E-02$

Table 34: Total thermodynamic properties of Ar ΔE=250 cm^{-1}

T [K]	C_p [J/mol/K]	S^0 [J/mol/K]	$H^0(T)-H^0(0)$ [KJ/mol]	$H^0(T)-H^0(298)$ [KJ/mol]	$-(G^0-H^0(0))/T$ [J/mol/K]	$-(G^0-H^0(298))/T$ [J/mol/K]	ΔH_f [KJ/mol]	$Log(K_p)$
50	2.079E+01	1.177E+02	1.039E+00	-5.158E+00	9.694E+01	2.209E+02	0.000E+00	0.000E+00
100	2.079E+01	1.321E+02	2.079E+00	-4.119E+00	1.113E+02	1.733E+02	0.000E+00	0.000E+00
150	2.079E+01	1.406E+02	3.118E+00	-3.079E+00	1.198E+02	1.611E+02	0.000E+00	0.000E+00
200	2.079E+01	1.466E+02	4.157E+00	-2.040E+00	1.258E+02	1.568E+02	0.000E+00	0.000E+00
298.15	2.079E+01	1.548E+02	6.197E+00	0.000E+00	1.341E+02	1.548E+02	0.000E+00	0.000E+00
300	2.079E+01	1.550E+02	6.236E+00	3.848E-02	1.342E+02	1.548E+02	0.000E+00	0.000E+00
400	2.079E+01	1.610E+02	8.315E+00	2.117E+00	1.402E+02	1.557E+02	0.000E+00	0.000E+00
500	2.079E+01	1.656E+02	1.039E+01	4.196E+00	1.448E+02	1.572E+02	0.000E+00	0.000E+00
600	2.079E+01	1.694E+02	1.247E+01	6.274E+00	1.486E+02	1.589E+02	0.000E+00	0.000E+00
700	2.079E+01	1.726E+02	1.455E+01	8.353E+00	1.518E+02	1.607E+02	0.000E+00	0.000E+00
800	2.079E+01	1.754E+02	1.663E+01	1.043E+01	1.546E+02	1.623E+02	0.000E+00	0.000E+00
900	2.079E+01	1.778E+02	1.871E+01	1.251E+01	1.570E+02	1.639E+02	0.000E+00	0.000E+00
1000	2.079E+01	1.800E+02	2.079E+01	1.459E+01	1.592E+02	1.654E+02	0.000E+00	0.000E+00
2000	2.079E+01	1.944E+02	4.157E+01	3.538E+01	1.736E+02	1.767E+02	0.000E+00	0.000E+00
3000	2.079E+01	2.028E+02	6.236E+01	5.616E+01	1.821E+02	1.841E+02	0.000E+00	0.000E+00
4000	2.079E+01	2.088E+02	8.314E+01	7.695E+01	1.880E+02	1.896E+02	0.000E+00	0.000E+00
5000	2.079E+01	2.135E+02	1.039E+02	9.773E+01	1.927E+02	1.939E+02	0.000E+00	0.000E+00
6000	2.079E+01	2.172E+02	1.247E+02	1.185E+02	1.965E+02	1.975E+02	0.000E+00	0.000E+00
7000	2.079E+01	2.204E+02	1.455E+02	1.393E+02	1.997E+02	2.006E+02	0.000E+00	0.000E+00
8000	2.080E+01	2.232E+02	1.663E+02	1.601E+02	2.024E+02	2.032E+02	0.000E+00	0.000E+00
9000	2.093E+01	2.257E+02	1.871E+02	1.809E+02	2.049E+02	2.056E+02	0.000E+00	0.000E+00
10000	2.166E+01	2.279E+02	2.083E+02	2.022E+02	2.071E+02	2.077E+02	0.000E+00	0.000E+00
11000	2.449E+01	2.301E+02	2.312E+02	2.249E+02	2.091E+02	2.096E+02	0.000E+00	0.000E+00
12000	3.287E+01	2.325E+02	2.591E+02	2.529E+02	2.109E+02	2.114E+02	0.000E+00	0.000E+00
13000	5.267E+01	2.358E+02	3.007E+02	2.945E+02	2.127E+02	2.132E+02	0.000E+00	0.000E+00
14000	9.020E+01	2.410E+02	3.705E+02	3.643E+02	2.145E+02	2.150E+02	0.000E+00	0.000E+00
15000	1.454E+02	2.490E+02	4.871E+02	4.809E+02	2.165E+02	2.169E+02	0.000E+00	0.000E+00
16000	2.029E+02	2.603E+02	6.621E+02	6.560E+02	2.189E+02	2.193E+02	0.000E+00	0.000E+00
17000	2.364E+02	2.738E+02	8.847E+02	8.785E+02	2.217E+02	2.221E+02	0.000E+00	0.000E+00
18000	2.315E+02	2.873E+02	1.122E+03	1.116E+03	2.250E+02	2.253E+02	0.000E+00	0.000E+00
19000	1.981E+02	2.990E+02	1.338E+03	1.332E+03	2.286E+02	2.289E+02	0.000E+00	0.000E+00
20000	1.558E+02	3.081E+02	1.515E+03	1.509E+03	2.324E+02	2.327E+02	0.000E+00	0.000E+00
21000	1.180E+02	3.148E+02	1.651E+03	1.645E+03	2.361E+02	2.364E+02	0.000E+00	0.000E+00
22000	8.899E+01	3.196E+02	1.754E+03	1.748E+03	2.398E+02	2.401E+02	0.000E+00	0.000E+00
23000	6.839E+01	3.230E+02	1.832E+03	1.826E+03	2.434E+02	2.436E+02	0.000E+00	0.000E+00
24000	5.420E+01	3.256E+02	1.893E+03	1.887E+03	2.467E+02	2.470E+02	0.000E+00	0.000E+00
25000	4.451E+01	3.276E+02	1.942E+03	1.936E+03	2.499E+02	2.502E+02	0.000E+00	0.000E+00
26000	3.789E+01	3.292E+02	1.983E+03	1.977E+03	2.530E+02	2.532E+02	0.000E+00	0.000E+00
27000	3.331E+01	3.306E+02	2.018E+03	2.012E+03	2.558E+02	2.560E+02	0.000E+00	0.000E+00
28000	3.011E+01	3.317E+02	2.050E+03	2.044E+03	2.585E+02	2.587E+02	0.000E+00	0.000E+00
29000	2.783E+01	3.327E+02	2.079E+03	2.073E+03	2.610E+02	2.613E+02	0.000E+00	0.000E+00
30000	2.620E+01	3.336E+02	2.106E+03	2.100E+03	2.634E+02	2.636E+02	0.000E+00	0.000E+00
32000	2.411E+01	3.353E+02	2.156E+03	2.150E+03	2.679E+02	2.681E+02	0.000E+00	0.000E+00
34000	2.293E+01	3.367E+02	2.203E+03	2.197E+03	2.719E+02	2.721E+02	0.000E+00	0.000E+00
36000	2.223E+01	3.380E+02	2.248E+03	2.242E+03	2.755E+02	2.757E+02	0.000E+00	0.000E+00
38000	2.179E+01	3.392E+02	2.292E+03	2.286E+03	2.789E+02	2.790E+02	0.000E+00	0.000E+00
40000	2.151E+01	3.403E+02	2.335E+03	2.329E+03	2.819E+02	2.820E+02	0.000E+00	0.000E+00
42000	2.132E+01	3.413E+02	2.378E+03	2.372E+03	2.847E+02	2.848E+02	0.000E+00	0.000E+00
44000	2.120E+01	3.423E+02	2.421E+03	2.414E+03	2.873E+02	2.874E+02	0.000E+00	0.000E+00
46000	2.110E+01	3.432E+02	2.463E+03	2.457E+03	2.897E+02	2.898E+02	0.000E+00	0.000E+00
48000	2.104E+01	3.441E+02	2.505E+03	2.499E+03	2.919E+02	2.921E+02	0.000E+00	0.000E+00
50000	2.099E+01	3.450E+02	2.547E+03	2.541E+03	2.941E+02	2.942E+02	0.000E+00	0.000E+00

Table 35: Internal thermodynamic properties of Ar ΔE=500 cm^{-1}

T(K)	Q_{int}	$\ln(Q_{int})$	E_{int}/RT	$C_{p,int}/R$
50	$1.000E+00$	$0.000E+00$	$0.000E+00$	$0.000E+00$
100	$1.000E+00$	$0.000E+00$	$0.000E+00$	$0.000E+00$
150	$1.000E+00$	$0.000E+00$	$0.000E+00$	$0.000E+00$
200	$1.000E+00$	$0.000E+00$	$3.345E-288$	$2.241E-285$
298.15	$1.000E+00$	$0.000E+00$	$1.442E-192$	$6.485E-190$
300	$1.000E+00$	$0.000E+00$	$2.293E-191$	$1.025E-188$
400	$1.000E+00$	$0.000E+00$	$5.639E-143$	$1.890E-140$
500	$1.000E+00$	$0.000E+00$	$5.899E-114$	$1.582E-111$
600	$1.000E+00$	$0.000E+00$	$1.281E-94$	$2.864E-92$
700	$1.000E+00$	$0.000E+00$	$8.181E-81$	$1.568E-78$
800	$1.000E+00$	$0.000E+00$	$1.827E-70$	$3.065E-68$
900	$1.000E+00$	$0.000E+00$	$2.028E-62$	$3.025E-60$
1000	$1.000E+00$	$0.000E+00$	$5.498E-56$	$7.383E-54$
2000	$1.000E+00$	$0.000E+00$	$4.217E-27$	$2.838E-25$
3000	$1.000E+00$	$0.000E+00$	$1.584E-17$	$7.123E-16$
4000	$1.000E+00$	$2.731E-14$	$9.408E-13$	$3.203E-11$
5000	$1.000E+00$	$2.661E-11$	$7.437E-10$	$2.095E-08$
6000	$1.000E+00$	$3.160E-09$	$7.795E-08$	$1.955E-06$
7000	$1.000E+00$	$1.201E-07$	$2.709E-06$	$6.219E-05$
8000	$1.000E+00$	$2.159E-06$	$4.469E-05$	$9.382E-04$
9000	$1.000E+00$	$2.230E-05$	$4.224E-04$	$8.084E-03$
10000	$1.000E+00$	$1.508E-04$	$2.615E-03$	$4.570E-02$
11000	$1.001E+00$	$7.360E-04$	$1.173E-02$	$1.878E-01$
12000	$1.003E+00$	$2.788E-03$	$4.096E-02$	$6.036E-01$
13000	$1.009E+00$	$8.643E-03$	$1.174E-01$	$1.594E+00$
14000	$1.023E+00$	$2.278E-02$	$2.862E-01$	$3.567E+00$
15000	$1.054E+00$	$5.242E-02$	$6.072E-01$	$6.871E+00$
16000	$1.113E+00$	$1.073E-01$	$1.136E+00$	$1.143E+01$
17000	$1.219E+00$	$1.976E-01$	$1.888E+00$	$1.635E+01$
18000	$1.392E+00$	$3.309E-01$	$2.804E+00$	$2.010E+01$
19000	$1.663E+00$	$5.083E-01$	$3.761E+00$	$2.141E+01$
20000	$2.062E+00$	$7.238E-01$	$4.621E+00$	$2.017E+01$
21000	$2.629E+00$	$9.664E-01$	$5.297E+00$	$1.729E+01$
22000	$3.402E+00$	$1.224E+00$	$5.766E+00$	$1.390E+01$
23000	$4.426E+00$	$1.488E+00$	$6.049E+00$	$1.074E+01$
24000	$5.745E+00$	$1.748E+00$	$6.188E+00$	$8.122E+00$
25000	$7.404E+00$	$2.002E+00$	$6.223E+00$	$6.096E+00$
26000	$9.446E+00$	$2.246E+00$	$6.187E+00$	$4.577E+00$
27000	$1.191E+01$	$2.478E+00$	$6.106E+00$	$3.457E+00$
28000	$1.485E+01$	$2.698E+00$	$5.996E+00$	$2.633E+00$
29000	$1.828E+01$	$2.906E+00$	$5.869E+00$	$2.027E+00$
30000	$2.226E+01$	$3.103E+00$	$5.733E+00$	$1.577E+00$
32000	$3.193E+01$	$3.464E+00$	$5.453E+00$	$9.870E-01$
34000	$4.408E+01$	$3.786E+00$	$5.179E+00$	$6.445E-01$
36000	$5.883E+01$	$4.075E+00$	$4.921E+00$	$4.375E-01$
38000	$7.626E+01$	$4.334E+00$	$4.681E+00$	$3.074E-01$
40000	$9.641E+01$	$4.569E+00$	$4.460E+00$	$2.226E-01$
42000	$1.193E+02$	$4.781E+00$	$4.257E+00$	$1.657E-01$
44000	$1.447E+02$	$4.975E+00$	$4.070E+00$	$1.262E-01$
46000	$1.728E+02$	$5.152E+00$	$3.898E+00$	$9.824E-02$
48000	$2.033E+02$	$5.315E+00$	$3.739E+00$	$7.790E-02$
50000	$2.361E+02$	$5.464E+00$	$3.593E+00$	$6.281E-02$

Table 36: Total thermodynamic properties of Ar ΔE=500 cm^{-1}

T [K]	C_p [J/mol/K]	S^0 [J/mol/K]	$H^0(T)-H^0(0)$ [KJ/mol]	$H^0(T)-H^0(298)$ [KJ/mol]	$-(G^0-H^0(0))/T$ [J/mol/K]	$-(G^0-H^0(298))/T$ [J/mol/K]	ΔH_f [KJ/mol]	$Log(K_p)$
50	2.079E+01	1.177E+02	1.039E+00	-5.158E+00	9.694E+01	2.209E+02	0.000E+00	0.000E+00
100	2.079E+01	1.321E+02	2.079E+00	-4.119E+00	1.113E+02	1.733E+02	0.000E+00	0.000E+00
150	2.079E+01	1.406E+02	3.118E+00	-3.079E+00	1.198E+02	1.611E+02	0.000E+00	0.000E+00
200	2.079E+01	1.466E+02	4.157E+00	-2.040E+00	1.258E+02	1.568E+02	0.000E+00	0.000E+00
298.15	2.079E+01	1.548E+02	6.197E+00	0.000E+00	1.341E+02	1.548E+02	0.000E+00	0.000E+00
300	2.079E+01	1.550E+02	6.236E+00	3.848E-02	1.342E+02	1.548E+02	0.000E+00	0.000E+00
400	2.079E+01	1.610E+02	8.315E+00	2.117E+00	1.402E+02	1.557E+02	0.000E+00	0.000E+00
500	2.079E+01	1.656E+02	1.039E+01	4.196E+00	1.448E+02	1.572E+02	0.000E+00	0.000E+00
600	2.079E+01	1.694E+02	1.247E+01	6.274E+00	1.486E+02	1.589E+02	0.000E+00	0.000E+00
700	2.079E+01	1.726E+02	1.455E+01	8.353E+00	1.518E+02	1.607E+02	0.000E+00	0.000E+00
800	2.079E+01	1.754E+02	1.663E+01	1.043E+01	1.546E+02	1.623E+02	0.000E+00	0.000E+00
900	2.079E+01	1.778E+02	1.871E+01	1.251E+01	1.570E+02	1.639E+02	0.000E+00	0.000E+00
1000	2.079E+01	1.800E+02	2.079E+01	1.459E+01	1.592E+02	1.654E+02	0.000E+00	0.000E+00
2000	2.079E+01	1.944E+02	4.157E+01	3.538E+01	1.736E+02	1.767E+02	0.000E+00	0.000E+00
3000	2.079E+01	2.028E+02	6.236E+01	5.616E+01	1.821E+02	1.841E+02	0.000E+00	0.000E+00
4000	2.079E+01	2.088E+02	8.314E+01	7.695E+01	1.880E+02	1.896E+02	0.000E+00	0.000E+00
5000	2.079E+01	2.135E+02	1.039E+02	9.773E+01	1.927E+02	1.939E+02	0.000E+00	0.000E+00
6000	2.079E+01	2.172E+02	1.247E+02	1.185E+02	1.965E+02	1.975E+02	0.000E+00	0.000E+00
7000	2.079E+01	2.204E+02	1.455E+02	1.393E+02	1.997E+02	2.006E+02	0.000E+00	0.000E+00
8000	2.079E+01	2.232E+02	1.663E+02	1.601E+02	2.024E+02	2.032E+02	0.000E+00	0.000E+00
9000	2.085E+01	2.257E+02	1.871E+02	1.809E+02	2.049E+02	2.056E+02	0.000E+00	0.000E+00
10000	2.117E+01	2.279E+02	2.081E+02	2.019E+02	2.071E+02	2.077E+02	0.000E+00	0.000E+00
11000	2.235E+01	2.299E+02	2.297E+02	2.235E+02	2.091E+02	2.096E+02	0.000E+00	0.000E+00
12000	2.580E+01	2.320E+02	2.535E+02	2.473E+02	2.109E+02	2.114E+02	0.000E+00	0.000E+00
13000	3.404E+01	2.344E+02	2.829E+02	2.767E+02	2.126E+02	2.131E+02	0.000E+00	0.000E+00
14000	5.045E+01	2.374E+02	3.243E+02	3.181E+02	2.143E+02	2.147E+02	0.000E+00	0.000E+00
15000	7.792E+01	2.418E+02	3.875E+02	3.813E+02	2.159E+02	2.163E+02	0.000E+00	0.000E+00
16000	1.158E+02	2.480E+02	4.837E+02	4.775E+02	2.177E+02	2.181E+02	0.000E+00	0.000E+00
17000	1.567E+02	2.562E+02	6.202E+02	6.140E+02	2.198E+02	2.201E+02	0.000E+00	0.000E+00
18000	1.879E+02	2.661E+02	7.938E+02	7.876E+02	2.221E+02	2.224E+02	0.000E+00	0.000E+00
19000	1.988E+02	2.767E+02	9.890E+02	9.828E+02	2.247E+02	2.250E+02	0.000E+00	0.000E+00
20000	1.885E+02	2.867E+02	1.184E+03	1.178E+03	2.275E+02	2.278E+02	0.000E+00	0.000E+00
21000	1.646E+02	2.954E+02	1.361E+03	1.355E+03	2.305E+02	2.308E+02	0.000E+00	0.000E+00
22000	1.363E+02	3.024E+02	1.512E+03	1.506E+03	2.337E+02	2.339E+02	0.000E+00	0.000E+00
23000	1.100E+02	3.078E+02	1.635E+03	1.629E+03	2.368E+02	2.370E+02	0.000E+00	0.000E+00
24000	8.831E+01	3.121E+02	1.734E+03	1.727E+03	2.398E+02	2.401E+02	0.000E+00	0.000E+00
25000	7.147E+01	3.153E+02	1.813E+03	1.807E+03	2.428E+02	2.430E+02	0.000E+00	0.000E+00
26000	5.884E+01	3.178E+02	1.878E+03	1.872E+03	2.456E+02	2.458E+02	0.000E+00	0.000E+00
27000	4.953E+01	3.199E+02	1.932E+03	1.926E+03	2.483E+02	2.486E+02	0.000E+00	0.000E+00
28000	4.268E+01	3.216E+02	1.978E+03	1.972E+03	2.509E+02	2.511E+02	0.000E+00	0.000E+00
29000	3.764E+01	3.229E+02	2.018E+03	2.012E+03	2.534E+02	2.536E+02	0.000E+00	0.000E+00
30000	3.390E+01	3.242E+02	2.054E+03	2.047E+03	2.557E+02	2.559E+02	0.000E+00	0.000E+00
32000	2.899E+01	3.262E+02	2.116E+03	2.110E+03	2.601E+02	2.602E+02	0.000E+00	0.000E+00
34000	2.614E+01	3.278E+02	2.171E+03	2.165E+03	2.640E+02	2.642E+02	0.000E+00	0.000E+00
36000	2.442E+01	3.293E+02	2.221E+03	2.215E+03	2.676E+02	2.678E+02	0.000E+00	0.000E+00
38000	2.334E+01	3.306E+02	2.269E+03	2.263E+03	2.709E+02	2.710E+02	0.000E+00	0.000E+00
40000	2.264E+01	3.318E+02	2.315E+03	2.309E+03	2.739E+02	2.740E+02	0.000E+00	0.000E+00
42000	2.216E+01	3.328E+02	2.360E+03	2.354E+03	2.767E+02	2.768E+02	0.000E+00	0.000E+00
44000	2.184E+01	3.339E+02	2.404E+03	2.397E+03	2.792E+02	2.794E+02	0.000E+00	0.000E+00
46000	2.160E+01	3.348E+02	2.447E+03	2.441E+03	2.816E+02	2.818E+02	0.000E+00	0.000E+00
48000	2.143E+01	3.358E+02	2.490E+03	2.484E+03	2.839E+02	2.840E+02	0.000E+00	0.000E+00
50000	2.131E+01	3.366E+02	2.533E+03	2.527E+03	2.860E+02	2.861E+02	0.000E+00	0.000E+00

Table 37: Internal thermodynamic properties of Ar ΔE=1000 cm^{-1}

T(K)	Q_{int}	$\ln(Q_{int})$	E_{int}/RT	$C_{p,int}/R$
50	$1.000E+00$	$0.000E+00$	$0.000E+00$	$0.000E+00$
100	$1.000E+00$	$0.000E+00$	$0.000E+00$	$0.000E+00$
150	$1.000E+00$	$0.000E+00$	$0.000E+00$	$0.000E+00$
200	$1.000E+00$	$0.000E+00$	$3.345E-288$	$2.241E-285$
298.15	$1.000E+00$	$0.000E+00$	$1.442E-192$	$6.485E-190$
300	$1.000E+00$	$0.000E+00$	$2.293E-191$	$1.025E-188$
400	$1.000E+00$	$0.000E+00$	$5.639E-143$	$1.890E-140$
500	$1.000E+00$	$0.000E+00$	$5.899E-114$	$1.582E-111$
600	$1.000E+00$	$0.000E+00$	$1.281E-94$	$2.864E-92$
700	$1.000E+00$	$0.000E+00$	$8.181E-81$	$1.568E-78$
800	$1.000E+00$	$0.000E+00$	$1.827E-70$	$3.065E-68$
900	$1.000E+00$	$0.000E+00$	$2.028E-62$	$3.025E-60$
1000	$1.000E+00$	$0.000E+00$	$5.498E-56$	$7.383E-54$
2000	$1.000E+00$	$0.000E+00$	$4.217E-27$	$2.838E-25$
3000	$1.000E+00$	$0.000E+00$	$1.583E-17$	$7.122E-16$
4000	$1.000E+00$	$2.731E-14$	$9.365E-13$	$3.184E-11$
5000	$1.000E+00$	$2.577E-11$	$7.133E-10$	$1.984E-08$
6000	$1.000E+00$	$2.801E-09$	$6.708E-08$	$1.625E-06$
7000	$1.000E+00$	$9.281E-08$	$2.000E-06$	$4.379E-05$
8000	$1.000E+00$	$1.458E-06$	$2.874E-05$	$5.755E-04$
9000	$1.000E+00$	$1.353E-05$	$2.451E-04$	$4.500E-03$
10000	$1.000E+00$	$8.460E-05$	$1.411E-03$	$2.381E-02$
11000	$1.000E+00$	$3.903E-04$	$6.012E-03$	$9.346E-02$
12000	$1.001E+00$	$1.419E-03$	$2.025E-02$	$2.909E-01$
13000	$1.004E+00$	$4.268E-03$	$5.658E-02$	$7.532E-01$
14000	$1.011E+00$	$1.102E-02$	$1.359E-01$	$1.677E+00$
15000	$1.025E+00$	$2.506E-02$	$2.878E-01$	$3.280E+00$
16000	$1.053E+00$	$5.122E-02$	$5.461E-01$	$5.701E+00$
17000	$1.100E+00$	$9.540E-02$	$9.391E-01$	$8.848E+00$
18000	$1.178E+00$	$1.636E-01$	$1.474E+00$	$1.228E+01$
19000	$1.297E+00$	$2.603E-01$	$2.124E+00$	$1.524E+01$
20000	$1.473E+00$	$3.871E-01$	$2.831E+00$	$1.703E+01$
21000	$1.720E+00$	$5.421E-01$	$3.519E+00$	$1.729E+01$
22000	$2.055E+00$	$7.203E-01$	$4.125E+00$	$1.622E+01$
23000	$2.496E+00$	$9.148E-01$	$4.611E+00$	$1.430E+01$
24000	$3.062E+00$	$1.119E+00$	$4.969E+00$	$1.206E+01$
25000	$3.770E+00$	$1.327E+00$	$5.208E+00$	$9.872E+00$
26000	$4.639E+00$	$1.534E+00$	$5.349E+00$	$7.941E+00$
27000	$5.685E+00$	$1.738E+00$	$5.414E+00$	$6.330E+00$
28000	$6.924E+00$	$1.935E+00$	$5.423E+00$	$5.032E+00$
29000	$8.371E+00$	$2.125E+00$	$5.391E+00$	$4.005E+00$
30000	$1.004E+01$	$2.307E+00$	$5.331E+00$	$3.201E+00$
32000	$1.409E+01$	$2.645E+00$	$5.160E+00$	$2.084E+00$
34000	$1.915E+01$	$2.952E+00$	$4.957E+00$	$1.397E+00$
36000	$2.527E+01$	$3.230E+00$	$4.747E+00$	$9.650E-01$
38000	$3.248E+01$	$3.481E+00$	$4.540E+00$	$6.866E-01$
40000	$4.079E+01$	$3.709E+00$	$4.342E+00$	$5.019E-01$
42000	$5.019E+01$	$3.916E+00$	$4.156E+00$	$3.759E-01$
44000	$6.065E+01$	$4.105E+00$	$3.982E+00$	$2.879E-01$
46000	$7.213E+01$	$4.279E+00$	$3.820E+00$	$2.248E-01$
48000	$8.460E+01$	$4.438E+00$	$3.669E+00$	$1.787E-01$
50000	$9.798E+01$	$4.585E+00$	$3.529E+00$	$1.444E-01$

Table 38: Total thermodynamic properties of Ar ΔE=1000 cm^{-1}

T [K]	C_p [J/mol/K]	S^0 [J/mol/K]	$H^0(T)-H^0(0)$ [KJ/mol]	$H^0(T)-H^0(298)$ [KJ/mol]	$-(G^0-H^0(0))/T$ [J/mol/K]	$-(G^0-H^0(298))/T$ [J/mol/K]	ΔH_f [KJ/mol]	$\mathrm{Log}(K_p)$
50	2.079E+01	1.177E+02	1.039E+00	-5.158E+00	9.694E+01	2.209E+02	0.000E+00	0.000E+00
100	2.079E+01	1.321E+02	2.079E+00	-4.119E+00	1.113E+02	1.733E+02	0.000E+00	0.000E+00
150	2.079E+01	1.406E+02	3.118E+00	-3.079E+00	1.198E+02	1.611E+02	0.000E+00	0.000E+00
200	2.079E+01	1.466E+02	4.157E+00	-2.040E+00	1.258E+02	1.568E+02	0.000E+00	0.000E+00
298.15	2.079E+01	1.548E+02	6.197E+00	0.000E+00	1.341E+02	1.548E+02	0.000E+00	0.000E+00
300	2.079E+01	1.550E+02	6.236E+00	3.848E-02	1.342E+02	1.548E+02	0.000E+00	0.000E+00
400	2.079E+01	1.610E+02	8.315E+00	2.117E+00	1.402E+02	1.557E+02	0.000E+00	0.000E+00
500	2.079E+01	1.656E+02	1.039E+01	4.196E+00	1.448E+02	1.572E+02	0.000E+00	0.000E+00
600	2.079E+01	1.694E+02	1.247E+01	6.274E+00	1.486E+02	1.589E+02	0.000E+00	0.000E+00
700	2.079E+01	1.726E+02	1.455E+01	8.353E+00	1.518E+02	1.607E+02	0.000E+00	0.000E+00
800	2.079E+01	1.754E+02	1.663E+01	1.043E+01	1.546E+02	1.623E+02	0.000E+00	0.000E+00
900	2.079E+01	1.778E+02	1.871E+01	1.251E+01	1.570E+02	1.639E+02	0.000E+00	0.000E+00
1000	2.079E+01	1.800E+02	2.079E+01	1.459E+01	1.592E+02	1.654E+02	0.000E+00	0.000E+00
2000	2.079E+01	1.944E+02	4.157E+01	3.538E+01	1.736E+02	1.767E+02	0.000E+00	0.000E+00
3000	2.079E+01	2.028E+02	6.236E+01	5.616E+01	1.821E+02	1.841E+02	0.000E+00	0.000E+00
4000	2.079E+01	2.088E+02	8.314E+01	7.695E+01	1.880E+02	1.896E+02	0.000E+00	0.000E+00
5000	2.079E+01	2.135E+02	1.039E+02	9.773E+01	1.927E+02	1.939E+02	0.000E+00	0.000E+00
6000	2.079E+01	2.172E+02	1.247E+02	1.185E+02	1.965E+02	1.975E+02	0.000E+00	0.000E+00
7000	2.079E+01	2.204E+02	1.455E+02	1.393E+02	1.997E+02	2.006E+02	0.000E+00	0.000E+00
8000	2.079E+01	2.232E+02	1.663E+02	1.601E+02	2.024E+02	2.032E+02	0.000E+00	0.000E+00
9000	2.082E+01	2.257E+02	1.871E+02	1.809E+02	2.049E+02	2.056E+02	0.000E+00	0.000E+00
10000	2.098E+01	2.279E+02	2.080E+02	2.018E+02	2.071E+02	2.077E+02	0.000E+00	0.000E+00
11000	2.156E+01	2.299E+02	2.292E+02	2.230E+02	2.091E+02	2.096E+02	0.000E+00	0.000E+00
12000	2.320E+01	2.318E+02	2.515E+02	2.453E+02	2.109E+02	2.114E+02	0.000E+00	0.000E+00
13000	2.705E+01	2.338E+02	2.763E+02	2.701E+02	2.126E+02	2.130E+02	0.000E+00	0.000E+00
14000	3.473E+01	2.361E+02	3.068E+02	3.006E+02	2.142E+02	2.146E+02	0.000E+00	0.000E+00
15000	4.806E+01	2.389E+02	3.477E+02	3.415E+02	2.157E+02	2.161E+02	0.000E+00	0.000E+00
16000	6.819E+01	2.426E+02	4.052E+02	3.990E+02	2.173E+02	2.177E+02	0.000E+00	0.000E+00
17000	9.436E+01	2.475E+02	4.861E+02	4.799E+02	2.189E+02	2.193E+02	0.000E+00	0.000E+00
18000	1.229E+02	2.537E+02	5.948E+02	5.886E+02	2.207E+02	2.210E+02	0.000E+00	0.000E+00
19000	1.475E+02	2.610E+02	7.305E+02	7.244E+02	2.226E+02	2.229E+02	0.000E+00	0.000E+00
20000	1.624E+02	2.690E+02	8.865E+02	8.803E+02	2.247E+02	2.250E+02	0.000E+00	0.000E+00
21000	1.646E+02	2.771E+02	1.051E+03	1.045E+03	2.270E+02	2.273E+02	0.000E+00	0.000E+00
22000	1.556E+02	2.845E+02	1.212E+03	1.206E+03	2.295E+02	2.297E+02	0.000E+00	0.000E+00
23000	1.397E+02	2.911E+02	1.360E+03	1.354E+03	2.320E+02	2.323E+02	0.000E+00	0.000E+00
24000	1.210E+02	2.967E+02	1.490E+03	1.484E+03	2.346E+02	2.348E+02	0.000E+00	0.000E+00
25000	1.029E+02	3.012E+02	1.602E+03	1.596E+03	2.372E+02	2.374E+02	0.000E+00	0.000E+00
26000	8.681E+01	3.050E+02	1.697E+03	1.691E+03	2.397E+02	2.399E+02	0.000E+00	0.000E+00
27000	7.342E+01	3.080E+02	1.777E+03	1.770E+03	2.422E+02	2.424E+02	0.000E+00	0.000E+00
28000	6.262E+01	3.104E+02	1.844E+03	1.838E+03	2.446E+02	2.448E+02	0.000E+00	0.000E+00
29000	5.409E+01	3.125E+02	1.903E+03	1.896E+03	2.469E+02	2.471E+02	0.000E+00	0.000E+00
30000	4.740E+01	3.142E+02	1.953E+03	1.947E+03	2.491E+02	2.493E+02	0.000E+00	0.000E+00
32000	3.811E+01	3.169E+02	2.038E+03	2.032E+03	2.532E+02	2.534E+02	0.000E+00	0.000E+00
34000	3.240E+01	3.191E+02	2.108E+03	2.102E+03	2.571E+02	2.572E+02	0.000E+00	0.000E+00
36000	2.881E+01	3.208E+02	2.169E+03	2.163E+03	2.606E+02	2.607E+02	0.000E+00	0.000E+00
38000	2.650E+01	3.223E+02	2.224E+03	2.218E+03	2.638E+02	2.639E+02	0.000E+00	0.000E+00
40000	2.496E+01	3.236E+02	2.276E+03	2.269E+03	2.667E+02	2.669E+02	0.000E+00	0.000E+00
42000	2.391E+01	3.248E+02	2.324E+03	2.318E+03	2.695E+02	2.696E+02	0.000E+00	0.000E+00
44000	2.318E+01	3.259E+02	2.371E+03	2.365E+03	2.720E+02	2.721E+02	0.000E+00	0.000E+00
46000	2.266E+01	3.269E+02	2.417E+03	2.411E+03	2.744E+02	2.745E+02	0.000E+00	0.000E+00
48000	2.227E+01	3.279E+02	2.462E+03	2.456E+03	2.766E+02	2.767E+02	0.000E+00	0.000E+00
50000	2.199E+01	3.288E+02	2.506E+03	2.500E+03	2.786E+02	2.788E+02	0.000E+00	0.000E+00

Table 39: Internal thermodynamic properties of Ar^+ ΔE=250 cm^{-1}

T(K)	Q_{int}	$\ln(Q_{int})$	E_{int}/RT	$C_{p,int}/R$
50	$4.000E+00$	$1.386E+00$	$2.651E-17$	$1.092E-15$
100	$4.000E+00$	$1.386E+00$	$1.168E-08$	$2.406E-07$
150	$4.000E+00$	$1.386E+00$	$7.468E-06$	$1.025E-04$
200	$4.000E+00$	$1.386E+00$	$1.734E-04$	$1.786E-03$
298.15	$4.002E+00$	$1.387E+00$	$3.450E-03$	$2.383E-02$
300	$4.002E+00$	$1.387E+00$	$3.578E-03$	$2.456E-02$
400	$4.012E+00$	$1.389E+00$	$1.490E-02$	$7.650E-02$
500	$4.033E+00$	$1.394E+00$	$3.321E-02$	$1.357E-01$
600	$4.065E+00$	$1.402E+00$	$5.455E-02$	$1.843E-01$
700	$4.105E+00$	$1.412E+00$	$7.559E-02$	$2.167E-01$
800	$4.152E+00$	$1.424E+00$	$9.447E-02$	$2.343E-01$
900	$4.203E+00$	$1.436E+00$	$1.104E-01$	$2.406E-01$
1000	$4.255E+00$	$1.448E+00$	$1.234E-01$	$2.390E-01$
2000	$4.714E+00$	$1.551E+00$	$1.560E-01$	$1.363E-01$
3000	$5.007E+00$	$1.611E+00$	$1.380E-01$	$7.572E-02$
4000	$5.195E+00$	$1.648E+00$	$1.185E-01$	$4.696E-02$
5000	$5.325E+00$	$1.672E+00$	$1.025E-01$	$3.172E-02$
6000	$5.419E+00$	$1.690E+00$	$8.989E-02$	$2.278E-02$
7000	$5.490E+00$	$1.703E+00$	$7.987E-02$	$1.712E-02$
8000	$5.546E+00$	$1.713E+00$	$7.177E-02$	$1.333E-02$
9000	$5.591E+00$	$1.721E+00$	$6.512E-02$	$1.067E-02$
10000	$5.628E+00$	$1.728E+00$	$5.958E-02$	$8.753E-03$
11000	$5.658E+00$	$1.733E+00$	$5.489E-02$	$7.406E-03$
12000	$5.685E+00$	$1.738E+00$	$5.090E-02$	$6.689E-03$
13000	$5.707E+00$	$1.742E+00$	$4.750E-02$	$7.165E-03$
14000	$5.727E+00$	$1.745E+00$	$4.472E-02$	$1.074E-02$
15000	$5.744E+00$	$1.748E+00$	$4.278E-02$	$2.270E-02$
16000	$5.760E+00$	$1.751E+00$	$4.240E-02$	$5.589E-02$
17000	$5.775E+00$	$1.753E+00$	$4.526E-02$	$1.377E-01$
18000	$5.791E+00$	$1.756E+00$	$5.483E-02$	$3.202E-01$
19000	$5.811E+00$	$1.760E+00$	$7.750E-02$	$6.922E-01$
20000	$5.841E+00$	$1.765E+00$	$1.240E-01$	$1.390E+00$
21000	$5.887E+00$	$1.773E+00$	$2.107E-01$	$2.602E+00$
22000	$5.964E+00$	$1.786E+00$	$3.604E-01$	$4.548E+00$
23000	$6.090E+00$	$1.807E+00$	$6.015E-01$	$7.429E+00$
24000	$6.293E+00$	$1.839E+00$	$9.636E-01$	$1.132E+01$
25000	$6.610E+00$	$1.889E+00$	$1.470E+00$	$1.602E+01$
26000	$7.088E+00$	$1.958E+00$	$2.125E+00$	$2.098E+01$
27000	$7.791E+00$	$2.053E+00$	$2.907E+00$	$2.531E+01$
28000	$8.794E+00$	$2.174E+00$	$3.763E+00$	$2.814E+01$
29000	$1.019E+01$	$2.321E+00$	$4.624E+00$	$2.893E+01$
30000	$1.208E+01$	$2.492E+00$	$5.419E+00$	$2.774E+01$
32000	$1.787E+01$	$2.883E+00$	$6.641E+00$	$2.168E+01$
34000	$2.735E+01$	$3.309E+00$	$7.318E+00$	$1.478E+01$
36000	$4.193E+01$	$3.736E+00$	$7.576E+00$	$9.486E+00$
38000	$6.322E+01$	$4.147E+00$	$7.578E+00$	$6.002E+00$
40000	$9.296E+01$	$4.532E+00$	$7.441E+00$	$3.836E+00$
42000	$1.330E+02$	$4.890E+00$	$7.235E+00$	$2.503E+00$
44000	$1.852E+02$	$5.222E+00$	$7.000E+00$	$1.675E+00$
46000	$2.515E+02$	$5.527E+00$	$6.756E+00$	$1.151E+00$
48000	$3.336E+02$	$5.810E+00$	$6.515E+00$	$8.105E-01$
50000	$4.331E+02$	$6.071E+00$	$6.282E+00$	$5.848E-01$

Table 40: Total thermodynamic properties of Ar^+ ΔE=250 cm^{-1}

T [K]	C_p [J/mol/K]	S^0 [J/mol/K]	$H^0(T)-H^0(0)$ [KJ/mol]	$H^0(T)-H^0(298)$ [KJ/mol]	$-(G^0-H^0(0))/T$ [J/mol/K]	$-(G^0-H^0(298))/T$ [J/mol/K]	ΔH_f [KJ/mol]	$Log(K_p)$
50	2.079E+01	1.293E+02	1.039E+00	-5.167E+00	1.085E+02	2.326E+02	1.522E+03	-1.590E+03
100	2.079E+01	1.437E+02	2.079E+00	-4.127E+00	1.229E+02	1.849E+02	1.523E+03	-7.948E+02
150	2.079E+01	1.521E+02	3.118E+00	-3.088E+00	1.313E+02	1.727E+02	1.524E+03	-5.296E+02
200	2.080E+01	1.581E+02	4.157E+00	-2.049E+00	1.373E+02	1.683E+02	1.525E+03	-3.969E+02
298.15	2.098E+01	1.664E+02	6.206E+00	0.000E+00	1.456E+02	1.664E+02	1.527E+03	-2.658E+02
300	2.099E+01	1.665E+02	6.245E+00	3.881E-02	1.457E+02	1.664E+02	1.527E+03	-2.641E+02
400	2.142E+01	1.726E+02	8.364E+00	2.158E+00	1.517E+02	1.672E+02	1.529E+03	-1.976E+02
500	2.191E+01	1.775E+02	1.053E+01	4.325E+00	1.564E+02	1.688E+02	1.531E+03	-1.577E+02
600	2.232E+01	1.815E+02	1.274E+01	6.538E+00	1.603E+02	1.706E+02	1.533E+03	-1.310E+02
700	2.259E+01	1.850E+02	1.499E+01	8.784E+00	1.635E+02	1.724E+02	1.536E+03	-1.119E+02
800	2.273E+01	1.880E+02	1.726E+01	1.105E+01	1.664E+02	1.742E+02	1.538E+03	-9.758E+01
900	2.279E+01	1.907E+02	1.953E+01	1.333E+01	1.690E+02	1.759E+02	1.540E+03	-8.642E+01
1000	2.277E+01	1.931E+02	2.181E+01	1.561E+01	1.713E+02	1.775E+02	1.542E+03	-7.747E+01
2000	2.192E+01	2.086E+02	4.417E+01	3.796E+01	1.865E+02	1.896E+02	1.565E+03	-3.696E+01
3000	2.142E+01	2.174E+02	6.580E+01	5.960E+01	1.954E+02	1.975E+02	1.586E+03	-2.326E+01
4000	2.118E+01	2.235E+02	8.708E+01	8.088E+01	2.017E+02	2.033E+02	1.608E+03	-1.631E+01
5000	2.105E+01	2.282E+02	1.082E+02	1.020E+02	2.066E+02	2.078E+02	1.629E+03	-1.209E+01
6000	2.098E+01	2.320E+02	1.292E+02	1.230E+02	2.105E+02	2.115E+02	1.650E+03	-9.234E+00
7000	2.093E+01	2.353E+02	1.502E+02	1.439E+02	2.138E+02	2.147E+02	1.671E+03	-7.170E+00
8000	2.090E+01	2.381E+02	1.711E+02	1.649E+02	2.167E+02	2.175E+02	1.692E+03	-5.602E+00
9000	2.088E+01	2.405E+02	1.919E+02	1.857E+02	2.192E+02	2.199E+02	1.712E+03	-4.368E+00
10000	2.086E+01	2.427E+02	2.128E+02	2.066E+02	2.214E+02	2.221E+02	1.733E+03	-3.368E+00
11000	2.085E+01	2.447E+02	2.337E+02	2.275E+02	2.235E+02	2.240E+02	1.752E+03	-2.541E+00
12000	2.084E+01	2.465E+02	2.545E+02	2.483E+02	2.253E+02	2.258E+02	1.765E+03	-1.845E+00
13000	2.085E+01	2.482E+02	2.754E+02	2.691E+02	2.270E+02	2.275E+02	1.766E+03	-1.253E+00
14000	2.088E+01	2.497E+02	2.962E+02	2.900E+02	2.286E+02	2.290E+02	1.737E+03	-7.496E-01
15000	2.098E+01	2.512E+02	3.171E+02	3.109E+02	2.300E+02	2.304E+02	1.662E+03	-3.255E-01
16000	2.125E+01	2.525E+02	3.382E+02	3.320E+02	2.314E+02	2.318E+02	1.529E+03	2.322E-02
17000	2.193E+01	2.538E+02	3.598E+02	3.536E+02	2.327E+02	2.331E+02	1.349E+03	3.004E-01
18000	2.345E+01	2.551E+02	3.824E+02	3.761E+02	2.339E+02	2.342E+02	1.155E+03	5.144E-01
19000	2.654E+01	2.565E+02	4.072E+02	4.010E+02	2.351E+02	2.354E+02	9.846E+02	6.776E-01
20000	3.235E+01	2.580E+02	4.363E+02	4.301E+02	2.362E+02	2.365E+02	8.576E+02	8.038E-01
21000	4.242E+01	2.598E+02	4.733E+02	4.671E+02	2.372E+02	2.375E+02	7.791E+02	9.052E-01
22000	5.860E+01	2.621E+02	5.232E+02	5.170E+02	2.383E+02	2.386E+02	7.471E+02	9.910E-01
23000	8.256E+01	2.652E+02	5.931E+02	5.869E+02	2.394E+02	2.397E+02	7.597E+02	1.068E+00
24000	1.149E+02	2.694E+02	6.911E+02	6.850E+02	2.406E+02	2.408E+02	8.177E+02	1.143E+00
25000	1.540E+02	2.748E+02	8.252E+02	8.190E+02	2.418E+02	2.421E+02	9.235E+02	1.218E+00
26000	1.952E+02	2.817E+02	9.999E+02	9.937E+02	2.432E+02	2.435E+02	1.078E+03	1.298E+00
27000	2.312E+02	2.898E+02	1.214E+03	1.208E+03	2.448E+02	2.450E+02	1.277E+03	1.385E+00
28000	2.548E+02	2.986E+02	1.458E+03	1.452E+03	2.466E+02	2.468E+02	1.511E+03	1.481E+00
29000	2.614E+02	3.077E+02	1.718E+03	1.712E+03	2.485E+02	2.487E+02	1.762E+03	1.587E+00
30000	2.515E+02	3.165E+02	1.975E+03	1.969E+03	2.506E+02	2.508E+02	2.014E+03	1.700E+00
32000	2.010E+02	3.312E+02	2.432E+03	2.426E+03	2.552E+02	2.554E+02	2.462E+03	1.944E+00
34000	1.437E+02	3.417E+02	2.776E+03	2.769E+03	2.600E+02	2.602E+02	2.800E+03	2.197E+00
36000	9.966E+01	3.486E+02	3.016E+03	3.010E+03	2.648E+02	2.649E+02	3.037E+03	2.446E+00
38000	7.069E+01	3.531E+02	3.184E+03	3.178E+03	2.693E+02	2.695E+02	3.203E+03	2.685E+00
40000	5.268E+01	3.562E+02	3.306E+03	3.300E+03	2.736E+02	2.737E+02	3.323E+03	2.909E+00
42000	4.160E+01	3.585E+02	3.400E+03	3.393E+03	2.776E+02	2.777E+02	3.415E+03	3.119E+00
44000	3.471E+01	3.603E+02	3.475E+03	3.469E+03	2.813E+02	2.814E+02	3.490E+03	3.314E+00
46000	3.035E+01	3.617E+02	3.540E+03	3.534E+03	2.848E+02	2.849E+02	3.554E+03	3.496E+00
48000	2.752E+01	3.629E+02	3.598E+03	3.592E+03	2.880E+02	2.881E+02	3.611E+03	3.665E+00
50000	2.565E+01	3.640E+02	3.651E+03	3.645E+03	2.910E+02	2.911E+02	3.664E+03	3.824E+00

Table 41: Internal thermodynamic properties of Ar^+ ΔE=500 cm^{-1}

T(K)	Q_{int}	$\ln(Q_{int})$	E_{int}/RT	$C_{p,int}/R$
50	$4.000E+00$	$1.386E+00$	$2.651E-17$	$1.092E-15$
100	$4.000E+00$	$1.386E+00$	$1.168E-08$	$2.406E-07$
150	$4.000E+00$	$1.386E+00$	$7.468E-06$	$1.025E-04$
200	$4.000E+00$	$1.386E+00$	$1.734E-04$	$1.786E-03$
298.15	$4.002E+00$	$1.387E+00$	$3.450E-03$	$2.383E-02$
300	$4.002E+00$	$1.387E+00$	$3.578E-03$	$2.456E-02$
400	$4.012E+00$	$1.389E+00$	$1.490E-02$	$7.650E-02$
500	$4.033E+00$	$1.394E+00$	$3.321E-02$	$1.357E-01$
600	$4.065E+00$	$1.402E+00$	$5.455E-02$	$1.843E-01$
700	$4.105E+00$	$1.412E+00$	$7.559E-02$	$2.167E-01$
800	$4.152E+00$	$1.424E+00$	$9.447E-02$	$2.343E-01$
900	$4.203E+00$	$1.436E+00$	$1.104E-01$	$2.406E-01$
1000	$4.255E+00$	$1.448E+00$	$1.234E-01$	$2.390E-01$
2000	$4.714E+00$	$1.551E+00$	$1.560E-01$	$1.363E-01$
3000	$5.007E+00$	$1.611E+00$	$1.380E-01$	$7.572E-02$
4000	$5.195E+00$	$1.648E+00$	$1.185E-01$	$4.696E-02$
5000	$5.325E+00$	$1.672E+00$	$1.025E-01$	$3.172E-02$
6000	$5.419E+00$	$1.690E+00$	$8.989E-02$	$2.278E-02$
7000	$5.490E+00$	$1.703E+00$	$7.987E-02$	$1.712E-02$
8000	$5.546E+00$	$1.713E+00$	$7.177E-02$	$1.333E-02$
9000	$5.591E+00$	$1.721E+00$	$6.512E-02$	$1.067E-02$
10000	$5.628E+00$	$1.728E+00$	$5.958E-02$	$8.752E-03$
11000	$5.658E+00$	$1.733E+00$	$5.489E-02$	$7.401E-03$
12000	$5.685E+00$	$1.738E+00$	$5.090E-02$	$6.639E-03$
13000	$5.707E+00$	$1.742E+00$	$4.749E-02$	$6.834E-03$
14000	$5.726E+00$	$1.745E+00$	$4.465E-02$	$9.084E-03$
15000	$5.744E+00$	$1.748E+00$	$4.247E-02$	$1.611E-02$
16000	$5.759E+00$	$1.751E+00$	$4.130E-02$	$3.399E-02$
17000	$5.774E+00$	$1.753E+00$	$4.192E-02$	$7.496E-02$
18000	$5.788E+00$	$1.756E+00$	$4.588E-02$	$1.615E-01$
19000	$5.804E+00$	$1.759E+00$	$5.596E-02$	$3.314E-01$
20000	$5.823E+00$	$1.762E+00$	$7.677E-02$	$6.426E-01$
21000	$5.850E+00$	$1.766E+00$	$1.154E-01$	$1.177E+00$
22000	$5.890E+00$	$1.773E+00$	$1.817E-01$	$2.038E+00$
23000	$5.950E+00$	$1.783E+00$	$2.890E-01$	$3.345E+00$
24000	$6.044E+00$	$1.799E+00$	$4.530E-01$	$5.206E+00$
25000	$6.184E+00$	$1.822E+00$	$6.906E-01$	$7.682E+00$
26000	$6.393E+00$	$1.855E+00$	$1.017E+00$	$1.073E+01$
27000	$6.694E+00$	$1.901E+00$	$1.439E+00$	$1.417E+01$
28000	$7.118E+00$	$1.963E+00$	$1.957E+00$	$1.765E+01$
29000	$7.702E+00$	$2.041E+00$	$2.553E+00$	$2.070E+01$
30000	$8.489E+00$	$2.139E+00$	$3.197E+00$	$2.287E+01$
32000	$1.088E+01$	$2.387E+00$	$4.477E+00$	$2.367E+01$
34000	$1.475E+01$	$2.691E+00$	$5.525E+00$	$2.044E+01$
36000	$2.066E+01$	$3.028E+00$	$6.221E+00$	$1.563E+01$
38000	$2.925E+01$	$3.376E+00$	$6.596E+00$	$1.118E+01$
40000	$4.120E+01$	$3.719E+00$	$6.735E+00$	$7.758E+00$
42000	$5.724E+01$	$4.047E+00$	$6.722E+00$	$5.355E+00$
44000	$7.810E+01$	$4.358E+00$	$6.621E+00$	$3.725E+00$
46000	$1.045E+02$	$4.649E+00$	$6.470E+00$	$2.629E+00$
48000	$1.371E+02$	$4.921E+00$	$6.293E+00$	$1.889E+00$
50000	$1.766E+02$	$5.174E+00$	$6.106E+00$	$1.382E+00$

Table 42: Total thermodynamic properties of Ar^+ ΔE=500 cm^{-1}

T [K]	C_p [J/mol/K]	S^0 [J/mol/K]	$H^0(T)-H^0(0)$ [KJ/mol]	$H^0(T)-H^0(298)$ [KJ/mol]	$-(G^0-H^0(0))/T$ [J/mol/K]	$-(G^0-H^0(298))/T$ [J/mol/K]	ΔH_f [KJ/mol]	$Log(K_p)$
50	2.079E+01	1.293E+02	1.039E+00	-5.167E+00	1.085E+02	2.326E+02	1.522E+03	-1.590E+03
100	2.079E+01	1.437E+02	2.079E+00	-4.127E+00	1.229E+02	1.849E+02	1.523E+03	-7.948E+02
150	2.079E+01	1.521E+02	3.118E+00	-3.088E+00	1.313E+02	1.727E+02	1.524E+03	-5.296E+02
200	2.080E+01	1.581E+02	4.157E+00	-2.049E+00	1.373E+02	1.683E+02	1.525E+03	-3.969E+02
298.15	2.098E+01	1.664E+02	6.206E+00	0.000E+00	1.456E+02	1.664E+02	1.527E+03	-2.658E+02
300	2.099E+01	1.665E+02	6.245E+00	3.881E-02	1.457E+02	1.664E+02	1.527E+03	-2.641E+02
400	2.142E+01	1.726E+02	8.364E+00	2.158E+00	1.517E+02	1.672E+02	1.529E+03	-1.976E+02
500	2.191E+01	1.775E+02	1.053E+01	4.325E+00	1.564E+02	1.688E+02	1.531E+03	-1.577E+02
600	2.232E+01	1.815E+02	1.274E+01	6.538E+00	1.603E+02	1.706E+02	1.533E+03	-1.310E+02
700	2.259E+01	1.850E+02	1.499E+01	8.784E+00	1.635E+02	1.724E+02	1.536E+03	-1.119E+02
800	2.273E+01	1.880E+02	1.726E+01	1.105E+01	1.664E+02	1.742E+02	1.538E+03	-9.758E+01
900	2.279E+01	1.907E+02	1.953E+01	1.333E+01	1.690E+02	1.759E+02	1.540E+03	-8.642E+01
1000	2.277E+01	1.931E+02	2.181E+01	1.561E+01	1.713E+02	1.775E+02	1.542E+03	-7.747E+01
2000	2.192E+01	2.086E+02	4.417E+01	3.796E+01	1.865E+02	1.896E+02	1.565E+03	-3.696E+01
3000	2.142E+01	2.174E+02	6.580E+01	5.960E+01	1.954E+02	1.975E+02	1.586E+03	-2.326E+01
4000	2.118E+01	2.235E+02	8.708E+01	8.088E+01	2.017E+02	2.033E+02	1.608E+03	-1.631E+01
5000	2.105E+01	2.282E+02	1.082E+02	1.020E+02	2.066E+02	2.078E+02	1.629E+03	-1.209E+01
6000	2.098E+01	2.320E+02	1.292E+02	1.230E+02	2.105E+02	2.115E+02	1.650E+03	-9.234E+00
7000	2.093E+01	2.353E+02	1.502E+02	1.439E+02	2.138E+02	2.147E+02	1.671E+03	-7.170E+00
8000	2.090E+01	2.381E+02	1.711E+02	1.649E+02	2.167E+02	2.175E+02	1.692E+03	-5.602E+00
9000	2.088E+01	2.405E+02	1.919E+02	1.857E+02	2.192E+02	2.199E+02	1.712E+03	-4.368E+00
10000	2.086E+01	2.427E+02	2.128E+02	2.066E+02	2.214E+02	2.221E+02	1.733E+03	-3.368E+00
11000	2.085E+01	2.447E+02	2.337E+02	2.275E+02	2.235E+02	2.240E+02	1.753E+03	-2.541E+00
12000	2.084E+01	2.465E+02	2.545E+02	2.483E+02	2.253E+02	2.258E+02	1.771E+03	-1.843E+00
13000	2.084E+01	2.482E+02	2.754E+02	2.691E+02	2.270E+02	2.275E+02	1.783E+03	-1.248E+00
14000	2.086E+01	2.497E+02	2.962E+02	2.900E+02	2.286E+02	2.290E+02	1.784E+03	-7.359E-01
15000	2.092E+01	2.512E+02	3.171E+02	3.109E+02	2.300E+02	2.304E+02	1.762E+03	-2.943E-01
16000	2.107E+01	2.525E+02	3.381E+02	3.319E+02	2.314E+02	2.318E+02	1.708E+03	8.402E-02
17000	2.141E+01	2.538E+02	3.593E+02	3.531E+02	2.327E+02	2.331E+02	1.613E+03	4.037E-01
18000	2.213E+01	2.551E+02	3.810E+02	3.748E+02	2.339E+02	2.342E+02	1.482E+03	6.685E-01
19000	2.354E+01	2.563E+02	4.038E+02	3.976E+02	2.350E+02	2.354E+02	1.330E+03	8.836E-01
20000	2.613E+01	2.576E+02	4.285E+02	4.223E+02	2.361E+02	2.364E+02	1.181E+03	1.056E+00
21000	3.057E+01	2.589E+02	4.566E+02	4.504E+02	2.372E+02	2.375E+02	1.052E+03	1.195E+00
22000	3.773E+01	2.605E+02	4.905E+02	4.843E+02	2.382E+02	2.385E+02	9.565E+02	1.308E+00
23000	4.860E+01	2.624E+02	5.334E+02	5.271E+02	2.392E+02	2.395E+02	8.972E+02	1.404E+00
24000	6.407E+01	2.648E+02	5.893E+02	5.831E+02	2.402E+02	2.405E+02	8.751E+02	1.487E+00
25000	8.466E+01	2.678E+02	6.632E+02	6.570E+02	2.413E+02	2.415E+02	8.903E+02	1.564E+00
26000	1.100E+02	2.716E+02	7.602E+02	7.540E+02	2.424E+02	2.426E+02	9.433E+02	1.637E+00
27000	1.386E+02	2.763E+02	8.844E+02	8.782E+02	2.435E+02	2.438E+02	1.034E+03	1.710E+00
28000	1.675E+02	2.819E+02	1.038E+03	1.031E+03	2.448E+02	2.450E+02	1.162E+03	1.786E+00
29000	1.929E+02	2.882E+02	1.218E+03	1.212E+03	2.462E+02	2.464E+02	1.324E+03	1.866E+00
30000	2.110E+02	2.951E+02	1.421E+03	1.415E+03	2.477E+02	2.479E+02	1.512E+03	1.951E+00
32000	2.176E+02	3.091E+02	1.856E+03	1.850E+03	2.511E+02	2.513E+02	1.926E+03	2.137E+00
34000	1.907E+02	3.216E+02	2.268E+03	2.262E+03	2.549E+02	2.551E+02	2.325E+03	2.341E+00
36000	1.508E+02	3.314E+02	2.610E+03	2.604E+03	2.589E+02	2.591E+02	2.658E+03	2.554E+00
38000	1.137E+02	3.385E+02	2.874E+03	2.868E+03	2.629E+02	2.631E+02	2.915E+03	2.767E+00
40000	8.529E+01	3.436E+02	3.071E+03	3.065E+03	2.668E+02	2.670E+02	3.108E+03	2.974E+00
42000	6.531E+01	3.472E+02	3.221E+03	3.214E+03	2.706E+02	2.707E+02	3.254E+03	3.172E+00
44000	5.176E+01	3.499E+02	3.337E+03	3.330E+03	2.741E+02	2.742E+02	3.368E+03	3.360E+00
46000	4.265E+01	3.520E+02	3.431E+03	3.424E+03	2.774E+02	2.776E+02	3.460E+03	3.536E+00
48000	3.649E+01	3.537E+02	3.509E+03	3.503E+03	2.806E+02	2.807E+02	3.538E+03	3.701E+00
50000	3.228E+01	3.551E+02	3.578E+03	3.572E+03	2.836E+02	2.837E+02	3.605E+03	3.857E+00

Table 43: Internal thermodynamic properties of Ar^+ ΔE=1000 cm^{-1}

T(K)	Q_{int}	$\ln(Q_{int})$	E_{int}/RT	$C_{p,int}/R$
50	$4.000E+00$	$1.386E+00$	$2.651E-17$	$1.092E-15$
100	$4.000E+00$	$1.386E+00$	$1.168E-08$	$2.406E-07$
150	$4.000E+00$	$1.386E+00$	$7.468E-06$	$1.025E-04$
200	$4.000E+00$	$1.386E+00$	$1.734E-04$	$1.786E-03$
298.15	$4.002E+00$	$1.387E+00$	$3.450E-03$	$2.383E-02$
300	$4.002E+00$	$1.387E+00$	$3.578E-03$	$2.456E-02$
400	$4.012E+00$	$1.389E+00$	$1.490E-02$	$7.650E-02$
500	$4.033E+00$	$1.394E+00$	$3.321E-02$	$1.357E-01$
600	$4.065E+00$	$1.402E+00$	$5.455E-02$	$1.843E-01$
700	$4.105E+00$	$1.412E+00$	$7.559E-02$	$2.167E-01$
800	$4.152E+00$	$1.424E+00$	$9.447E-02$	$2.343E-01$
900	$4.203E+00$	$1.436E+00$	$1.104E-01$	$2.406E-01$
1000	$4.255E+00$	$1.448E+00$	$1.234E-01$	$2.390E-01$
2000	$4.714E+00$	$1.551E+00$	$1.560E-01$	$1.363E-01$
3000	$5.007E+00$	$1.611E+00$	$1.380E-01$	$7.572E-02$
4000	$5.195E+00$	$1.648E+00$	$1.185E-01$	$4.696E-02$
5000	$5.325E+00$	$1.672E+00$	$1.025E-01$	$3.172E-02$
6000	$5.419E+00$	$1.690E+00$	$8.989E-02$	$2.278E-02$
7000	$5.490E+00$	$1.703E+00$	$7.987E-02$	$1.712E-02$
8000	$5.546E+00$	$1.713E+00$	$7.177E-02$	$1.333E-02$
9000	$5.591E+00$	$1.721E+00$	$6.512E-02$	$1.067E-02$
10000	$5.628E+00$	$1.728E+00$	$5.958E-02$	$8.752E-03$
11000	$5.658E+00$	$1.733E+00$	$5.489E-02$	$7.399E-03$
12000	$5.685E+00$	$1.738E+00$	$5.089E-02$	$6.619E-03$
13000	$5.707E+00$	$1.742E+00$	$4.748E-02$	$6.701E-03$
14000	$5.726E+00$	$1.745E+00$	$4.462E-02$	$8.422E-03$
15000	$5.744E+00$	$1.748E+00$	$4.235E-02$	$1.348E-02$
16000	$5.759E+00$	$1.751E+00$	$4.087E-02$	$2.524E-02$
17000	$5.773E+00$	$1.753E+00$	$4.059E-02$	$4.995E-02$
18000	$5.787E+00$	$1.756E+00$	$4.231E-02$	$9.835E-02$
19000	$5.801E+00$	$1.758E+00$	$4.738E-02$	$1.877E-01$
20000	$5.816E+00$	$1.761E+00$	$5.795E-02$	$3.436E-01$
21000	$5.835E+00$	$1.764E+00$	$7.721E-02$	$6.021E-01$
22000	$5.860E+00$	$1.768E+00$	$1.097E-01$	$1.009E+00$
23000	$5.895E+00$	$1.774E+00$	$1.612E-01$	$1.621E+00$
24000	$5.945E+00$	$1.783E+00$	$2.393E-01$	$2.497E+00$
25000	$6.016E+00$	$1.794E+00$	$3.524E-01$	$3.692E+00$
26000	$6.118E+00$	$1.811E+00$	$5.095E-01$	$5.242E+00$
27000	$6.260E+00$	$1.834E+00$	$7.190E-01$	$7.146E+00$
28000	$6.456E+00$	$1.865E+00$	$9.871E-01$	$9.346E+00$
29000	$6.721E+00$	$1.905E+00$	$1.316E+00$	$1.172E+01$
30000	$7.072E+00$	$1.956E+00$	$1.702E+00$	$1.408E+01$
32000	$8.118E+00$	$2.094E+00$	$2.604E+00$	$1.788E+01$
34000	$9.784E+00$	$2.281E+00$	$3.559E+00$	$1.932E+01$
36000	$1.229E+01$	$2.509E+00$	$4.413E+00$	$1.820E+01$
38000	$1.590E+01$	$2.766E+00$	$5.071E+00$	$1.547E+01$
40000	$2.088E+01$	$3.039E+00$	$5.511E+00$	$1.228E+01$
42000	$2.750E+01$	$3.314E+00$	$5.763E+00$	$9.372E+00$
44000	$3.606E+01$	$3.585E+00$	$5.871E+00$	$7.022E+00$
46000	$4.684E+01$	$3.847E+00$	$5.880E+00$	$5.235E+00$
48000	$6.010E+01$	$4.096E+00$	$5.824E+00$	$3.917E+00$
50000	$7.609E+01$	$4.332E+00$	$5.728E+00$	$2.956E+00$

Table 44: Total thermodynamic properties of Ar^+ ΔE=1000 cm^{-1}

T [K]	C_p [J/mol/K]	S^0 [J/mol/K]	$H^0(T)-H^0(0)$ [KJ/mol]	$H^0(T)-H^0(298)$ [KJ/mol]	$-(G^0-H^0(0))/T$ [J/mol/K]	$-(G^0-H^0(298))/T$ [J/mol/K]	ΔH_f [KJ/mol]	$Log(K_p)$
50	2.079E+01	1.293E+02	1.039E+00	-5.167E+00	1.085E+02	2.326E+02	1.522E+03	-1.590E+03
100	2.079E+01	1.437E+02	2.079E+00	-4.127E+00	1.229E+02	1.849E+02	1.523E+03	-7.948E+02
150	2.079E+01	1.521E+02	3.118E+00	-3.088E+00	1.313E+02	1.727E+02	1.524E+03	-5.296E+02
200	2.080E+01	1.581E+02	4.157E+00	-2.049E+00	1.373E+02	1.683E+02	1.525E+03	-3.969E+02
298.15	2.098E+01	1.664E+02	6.206E+00	0.000E+00	1.456E+02	1.664E+02	1.527E+03	-2.658E+02
300	2.099E+01	1.665E+02	6.245E+00	3.881E-02	1.457E+02	1.664E+02	1.527E+03	-2.641E+02
400	2.142E+01	1.726E+02	8.364E+00	2.158E+00	1.517E+02	1.672E+02	1.529E+03	-1.976E+02
500	2.191E+01	1.775E+02	1.053E+01	4.325E+00	1.564E+02	1.688E+02	1.531E+03	-1.577E+02
600	2.232E+01	1.815E+02	1.274E+01	6.538E+00	1.603E+02	1.706E+02	1.533E+03	-1.310E+02
700	2.259E+01	1.850E+02	1.499E+01	8.784E+00	1.635E+02	1.724E+02	1.536E+03	-1.119E+02
800	2.273E+01	1.880E+02	1.726E+01	1.105E+01	1.664E+02	1.742E+02	1.538E+03	-9.758E+01
900	2.279E+01	1.907E+02	1.953E+01	1.333E+01	1.690E+02	1.759E+02	1.540E+03	-8.642E+01
1000	2.277E+01	1.931E+02	2.181E+01	1.561E+01	1.713E+02	1.775E+02	1.542E+03	-7.747E+01
2000	2.192E+01	2.086E+02	4.417E+01	3.796E+01	1.865E+02	1.896E+02	1.565E+03	-3.696E+01
3000	2.142E+01	2.174E+02	6.580E+01	5.960E+01	1.954E+02	1.975E+02	1.586E+03	-2.326E+01
4000	2.118E+01	2.235E+02	8.708E+01	8.088E+01	2.017E+02	2.033E+02	1.608E+03	-1.631E+01
5000	2.105E+01	2.282E+02	1.082E+02	1.020E+02	2.066E+02	2.078E+02	1.629E+03	-1.209E+01
6000	2.098E+01	2.320E+02	1.292E+02	1.230E+02	2.105E+02	2.115E+02	1.650E+03	-9.234E+00
7000	2.093E+01	2.353E+02	1.502E+02	1.439E+02	2.138E+02	2.147E+02	1.671E+03	-7.170E+00
8000	2.090E+01	2.381E+02	1.711E+02	1.649E+02	2.167E+02	2.175E+02	1.692E+03	-5.602E+00
9000	2.088E+01	2.405E+02	1.919E+02	1.857E+02	2.192E+02	2.199E+02	1.712E+03	-4.368E+00
10000	2.086E+01	2.427E+02	2.128E+02	2.066E+02	2.214E+02	2.221E+02	1.733E+03	-3.368E+00
11000	2.085E+01	2.447E+02	2.337E+02	2.275E+02	2.235E+02	2.240E+02	1.754E+03	-2.540E+00
12000	2.084E+01	2.465E+02	2.545E+02	2.483E+02	2.253E+02	2.258E+02	1.773E+03	-1.843E+00
13000	2.084E+01	2.482E+02	2.754E+02	2.691E+02	2.270E+02	2.275E+02	1.790E+03	-1.246E+00
14000	2.086E+01	2.497E+02	2.962E+02	2.900E+02	2.286E+02	2.290E+02	1.801E+03	-7.308E-01
15000	2.090E+01	2.512E+02	3.171E+02	3.109E+02	2.300E+02	2.304E+02	1.802E+03	-2.824E-01
16000	2.100E+01	2.525E+02	3.380E+02	3.318E+02	2.314E+02	2.318E+02	1.786E+03	1.084E-01
17000	2.120E+01	2.538E+02	3.591E+02	3.529E+02	2.327E+02	2.331E+02	1.747E+03	4.481E-01
18000	2.160E+01	2.550E+02	3.805E+02	3.743E+02	2.339E+02	2.342E+02	1.680E+03	7.411E-01
19000	2.235E+01	2.562E+02	4.024E+02	3.962E+02	2.350E+02	2.354E+02	1.587E+03	9.911E-01
20000	2.364E+01	2.574E+02	4.254E+02	4.192E+02	2.361E+02	2.364E+02	1.475E+03	1.202E+00
21000	2.579E+01	2.586E+02	4.500E+02	4.438E+02	2.372E+02	2.375E+02	1.356E+03	1.378E+00
22000	2.918E+01	2.599E+02	4.774E+02	4.711E+02	2.382E+02	2.384E+02	1.243E+03	1.525E+00
23000	3.427E+01	2.613E+02	5.089E+02	5.027E+02	2.391E+02	2.394E+02	1.148E+03	1.648E+00
24000	4.155E+01	2.629E+02	5.466E+02	5.404E+02	2.401E+02	2.403E+02	1.076E+03	1.753E+00
25000	5.149E+01	2.648E+02	5.929E+02	5.867E+02	2.410E+02	2.413E+02	1.031E+03	1.845E+00
26000	6.437E+01	2.670E+02	6.506E+02	6.444E+02	2.420E+02	2.422E+02	1.015E+03	1.927E+00
27000	8.020E+01	2.697E+02	7.226E+02	7.164E+02	2.430E+02	2.432E+02	1.028E+03	2.003E+00
28000	9.849E+01	2.730E+02	8.118E+02	8.056E+02	2.440E+02	2.442E+02	1.070E+03	2.075E+00
29000	1.182E+02	2.768E+02	9.201E+02	9.139E+02	2.451E+02	2.453E+02	1.141E+03	2.146E+00
30000	1.379E+02	2.811E+02	1.048E+03	1.042E+03	2.462E+02	2.464E+02	1.239E+03	2.217E+00
32000	1.695E+02	2.911E+02	1.358E+03	1.352E+03	2.487E+02	2.489E+02	1.506E+03	2.365E+00
34000	1.814E+02	3.019E+02	1.713E+03	1.706E+03	2.515E+02	2.517E+02	1.832E+03	2.525E+00
36000	1.721E+02	3.121E+02	2.069E+03	2.063E+03	2.546E+02	2.547E+02	2.169E+03	2.696E+00
38000	1.494E+02	3.208E+02	2.392E+03	2.386E+03	2.578E+02	2.580E+02	2.478E+03	2.873E+00
40000	1.229E+02	3.278E+02	2.664E+03	2.658E+03	2.612E+02	2.613E+02	2.741E+03	3.053E+00
42000	9.871E+01	3.332E+02	2.885E+03	2.879E+03	2.645E+02	2.646E+02	2.955E+03	3.230E+00
44000	7.917E+01	3.373E+02	3.062E+03	3.056E+03	2.677E+02	2.678E+02	3.126E+03	3.402E+00
46000	6.431E+01	3.405E+02	3.205E+03	3.199E+03	2.708E+02	2.709E+02	3.265E+03	3.567E+00
48000	5.336E+01	3.429E+02	3.322E+03	3.316E+03	2.737E+02	2.739E+02	3.378E+03	3.724E+00
50000	4.537E+01	3.450E+02	3.421E+03	3.414E+03	2.766E+02	2.767E+02	3.474E+03	3.873E+00

Table 45: Internal thermodynamic properties of Ar^{2+} ΔE=250 cm^{-1}

T(K)	Q_{int}	$\ln(Q_{int})$	E_{int}/RT	$C_{p,int}/R$
50	$5.119E+00$	$1.633E+00$	$7.499E-02$	$2.364E-01$
100	$5.597E+00$	$1.722E+00$	$1.722E-01$	$2.483E-01$
150	$6.023E+00$	$1.796E+00$	$1.827E-01$	$1.632E-01$
200	$6.339E+00$	$1.847E+00$	$1.704E-01$	$1.087E-01$
298.15	$6.746E+00$	$1.909E+00$	$1.407E-01$	$6.040E-02$
300	$6.752E+00$	$1.910E+00$	$1.402E-01$	$5.994E-02$
400	$7.007E+00$	$1.947E+00$	$1.182E-01$	$4.862E-02$
500	$7.183E+00$	$1.972E+00$	$1.045E-01$	$5.159E-02$
600	$7.316E+00$	$1.990E+00$	$9.621E-02$	$5.830E-02$
700	$7.422E+00$	$2.004E+00$	$9.125E-02$	$6.440E-02$
800	$7.511E+00$	$2.016E+00$	$8.818E-02$	$6.854E-02$
900	$7.589E+00$	$2.027E+00$	$8.613E-02$	$7.067E-02$
1000	$7.657E+00$	$2.036E+00$	$8.462E-02$	$7.113E-02$
2000	$8.091E+00$	$2.091E+00$	$7.298E-02$	$5.050E-02$
3000	$8.320E+00$	$2.119E+00$	$6.588E-02$	$6.152E-02$
4000	$8.482E+00$	$2.138E+00$	$7.081E-02$	$1.140E-01$
5000	$8.630E+00$	$2.155E+00$	$8.572E-02$	$1.759E-01$
6000	$8.781E+00$	$2.173E+00$	$1.052E-01$	$2.261E-01$
7000	$8.938E+00$	$2.190E+00$	$1.250E-01$	$2.591E-01$
8000	$9.099E+00$	$2.208E+00$	$1.430E-01$	$2.770E-01$
9000	$9.262E+00$	$2.226E+00$	$1.584E-01$	$2.837E-01$
10000	$9.424E+00$	$2.243E+00$	$1.709E-01$	$2.827E-01$
11000	$9.584E+00$	$2.260E+00$	$1.808E-01$	$2.768E-01$
12000	$9.739E+00$	$2.276E+00$	$1.885E-01$	$2.681E-01$
13000	$9.889E+00$	$2.291E+00$	$1.942E-01$	$2.579E-01$
14000	$1.003E+01$	$2.306E+00$	$1.984E-01$	$2.471E-01$
15000	$1.017E+01$	$2.320E+00$	$2.013E-01$	$2.368E-01$
16000	$1.031E+01$	$2.333E+00$	$2.032E-01$	$2.274E-01$
17000	$1.044E+01$	$2.345E+00$	$2.044E-01$	$2.196E-01$
18000	$1.056E+01$	$2.357E+00$	$2.051E-01$	$2.142E-01$
19000	$1.068E+01$	$2.368E+00$	$2.055E-01$	$2.120E-01$
20000	$1.079E+01$	$2.379E+00$	$2.058E-01$	$2.141E-01$
21000	$1.090E+01$	$2.389E+00$	$2.064E-01$	$2.225E-01$
22000	$1.100E+01$	$2.398E+00$	$2.075E-01$	$2.404E-01$
23000	$1.111E+01$	$2.408E+00$	$2.096E-01$	$2.732E-01$
24000	$1.121E+01$	$2.417E+00$	$2.133E-01$	$3.296E-01$
25000	$1.131E+01$	$2.425E+00$	$2.197E-01$	$4.233E-01$
26000	$1.141E+01$	$2.434E+00$	$2.302E-01$	$5.750E-01$
27000	$1.151E+01$	$2.443E+00$	$2.471E-01$	$8.140E-01$
28000	$1.162E+01$	$2.453E+00$	$2.734E-01$	$1.180E+00$
29000	$1.174E+01$	$2.463E+00$	$3.134E-01$	$1.724E+00$
30000	$1.187E+01$	$2.474E+00$	$3.728E-01$	$2.509E+00$
32000	$1.223E+01$	$2.504E+00$	$5.787E-01$	$5.078E+00$
34000	$1.280E+01$	$2.550E+00$	$9.604E-01$	$9.367E+00$
36000	$1.375E+01$	$2.621E+00$	$1.587E+00$	$1.535E+01$
38000	$1.533E+01$	$2.730E+00$	$2.486E+00$	$2.192E+01$
40000	$1.790E+01$	$2.885E+00$	$3.595E+00$	$2.696E+01$
42000	$2.195E+01$	$3.089E+00$	$4.762E+00$	$2.861E+01$
44000	$2.808E+01$	$3.335E+00$	$5.814E+00$	$2.668E+01$
46000	$3.707E+01$	$3.613E+00$	$6.635E+00$	$2.250E+01$
48000	$4.979E+01$	$3.908E+00$	$7.196E+00$	$1.771E+01$
50000	$6.729E+01$	$4.209E+00$	$7.528E+00$	$1.338E+01$

Table 46: Total thermodynamic properties of Ar^{2+} ΔE=250 cm^{-1}

T [K]	C_p [J/mol/K]	S^0 [J/mol/K]	$H^0(T)-H^0(0)$ [KJ/mol]	$H^0(T)-H^0(298)$ [KJ/mol]	$-(G^0-H^0(0))/T$ [J/mol/K]	$-(G^0-H^0(298))/T$ [J/mol/K]	ΔH_f [KJ/mol]	$Log(K_p)$
50	2.275E+01	1.319E+02	1.071E+00	-5.476E+00	1.105E+02	2.414E+02	4.188E+03	-4.377E+03
100	2.285E+01	1.479E+02	2.222E+00	-4.324E+00	1.257E+02	1.911E+02	4.191E+03	-2.188E+03
150	2.214E+01	1.570E+02	3.346E+00	-3.200E+00	1.347E+02	1.783E+02	4.193E+03	-1.458E+03
200	2.169E+01	1.633E+02	4.441E+00	-2.105E+00	1.411E+02	1.738E+02	4.195E+03	-1.093E+03
298.15	2.129E+01	1.719E+02	6.546E+00	0.000E+00	1.499E+02	1.719E+02	4.199E+03	-7.326E+02
300	2.129E+01	1.720E+02	6.585E+00	3.941E-02	1.501E+02	1.719E+02	4.199E+03	-7.280E+02
400	2.119E+01	1.781E+02	8.708E+00	2.162E+00	1.564E+02	1.727E+02	4.204E+03	-5.452E+02
500	2.121E+01	1.829E+02	1.083E+01	4.281E+00	1.612E+02	1.743E+02	4.208E+03	-4.353E+02
600	2.127E+01	1.867E+02	1.295E+01	6.406E+00	1.651E+02	1.761E+02	4.212E+03	-3.621E+02
700	2.132E+01	1.900E+02	1.508E+01	8.535E+00	1.685E+02	1.778E+02	4.216E+03	-3.096E+02
800	2.136E+01	1.929E+02	1.721E+01	1.067E+01	1.713E+02	1.795E+02	4.220E+03	-2.703E+02
900	2.137E+01	1.954E+02	1.935E+01	1.281E+01	1.739E+02	1.812E+02	4.224E+03	-2.397E+02
1000	2.138E+01	1.976E+02	2.149E+01	1.494E+01	1.761E+02	1.827E+02	4.229E+03	-2.151E+02
2000	2.121E+01	2.124E+02	4.279E+01	3.624E+01	1.910E+02	1.943E+02	4.271E+03	-1.043E+02
3000	2.130E+01	2.210E+02	6.400E+01	5.746E+01	1.997E+02	2.018E+02	4.313E+03	-6.694E+01
4000	2.173E+01	2.272E+02	8.550E+01	7.895E+01	2.058E+02	2.074E+02	4.355E+03	-4.808E+01
5000	2.225E+01	2.321E+02	1.075E+02	1.010E+02	2.106E+02	2.119E+02	4.398E+03	-3.666E+01
6000	2.267E+01	2.362E+02	1.300E+02	1.234E+02	2.145E+02	2.156E+02	4.441E+03	-2.896E+01
7000	2.294E+01	2.397E+02	1.528E+02	1.462E+02	2.179E+02	2.188E+02	4.485E+03	-2.341E+01
8000	2.309E+01	2.428E+02	1.758E+02	1.693E+02	2.208E+02	2.216E+02	4.528E+03	-1.921E+01
9000	2.314E+01	2.455E+02	1.989E+02	1.924E+02	2.234E+02	2.241E+02	4.572E+03	-1.591E+01
10000	2.314E+01	2.479E+02	2.221E+02	2.155E+02	2.257E+02	2.264E+02	4.616E+03	-1.324E+01
11000	2.309E+01	2.501E+02	2.452E+02	2.386E+02	2.278E+02	2.284E+02	4.658E+03	-1.104E+01
12000	2.302E+01	2.522E+02	2.682E+02	2.617E+02	2.298E+02	2.303E+02	4.694E+03	-9.193E+00
13000	2.293E+01	2.540E+02	2.912E+02	2.847E+02	2.316E+02	2.321E+02	4.717E+03	-7.617E+00
14000	2.284E+01	2.557E+02	3.141E+02	3.076E+02	2.332E+02	2.337E+02	4.712E+03	-6.263E+00
15000	2.275E+01	2.572E+02	3.369E+02	3.304E+02	2.348E+02	2.352E+02	4.660E+03	-5.096E+00
16000	2.268E+01	2.587E+02	3.596E+02	3.531E+02	2.362E+02	2.367E+02	4.549E+03	-4.093E+00
17000	2.261E+01	2.601E+02	3.823E+02	3.757E+02	2.376E+02	2.380E+02	4.391E+03	-3.233E+00
18000	2.257E+01	2.614E+02	4.048E+02	3.983E+02	2.389E+02	2.393E+02	4.218E+03	-2.498E+00
19000	2.255E+01	2.626E+02	4.274E+02	4.209E+02	2.401E+02	2.404E+02	4.066E+03	-1.866E+00
20000	2.257E+01	2.638E+02	4.499E+02	4.434E+02	2.413E+02	2.416E+02	3.953E+03	-1.315E+00
21000	2.264E+01	2.649E+02	4.726E+02	4.660E+02	2.424E+02	2.427E+02	3.881E+03	-8.286E-01
22000	2.279E+01	2.659E+02	4.952E+02	4.887E+02	2.434E+02	2.437E+02	3.842E+03	-3.923E-01
23000	2.306E+01	2.669E+02	5.182E+02	5.116E+02	2.444E+02	2.447E+02	3.829E+03	3.452E-03
24000	2.353E+01	2.679E+02	5.414E+02	5.349E+02	2.454E+02	2.456E+02	3.833E+03	3.658E-01
25000	2.431E+01	2.689E+02	5.653E+02	5.588E+02	2.463E+02	2.466E+02	3.849E+03	7.001E-01
26000	2.557E+01	2.699E+02	5.902E+02	5.837E+02	2.472E+02	2.474E+02	3.875E+03	1.010E+00
27000	2.755E+01	2.709E+02	6.167E+02	6.101E+02	2.480E+02	2.483E+02	3.907E+03	1.300E+00
28000	3.060E+01	2.719E+02	6.457E+02	6.391E+02	2.489E+02	2.491E+02	3.946E+03	1.571E+00
29000	3.512E+01	2.731E+02	6.784E+02	6.718E+02	2.497E+02	2.499E+02	3.992E+03	1.826E+00
30000	4.165E+01	2.744E+02	7.166E+02	7.100E+02	2.505E+02	2.507E+02	4.044E+03	2.067E+00
32000	6.301E+01	2.777E+02	8.191E+02	8.126E+02	2.521E+02	2.523E+02	4.180E+03	2.514E+00
34000	9.867E+01	2.825E+02	9.782E+02	9.717E+02	2.537E+02	2.539E+02	4.375E+03	2.924E+00
36000	1.484E+02	2.895E+02	1.223E+03	1.217E+03	2.555E+02	2.557E+02	4.658E+03	3.309E+00
38000	2.031E+02	2.990E+02	1.575E+03	1.569E+03	2.575E+02	2.577E+02	5.050E+03	3.679E+00
40000	2.449E+02	3.106E+02	2.027E+03	2.020E+03	2.599E+02	2.600E+02	5.541E+03	4.042E+00
42000	2.587E+02	3.230E+02	2.536E+03	2.529E+03	2.626E+02	2.627E+02	6.090E+03	4.403E+00
44000	2.426E+02	3.347E+02	3.042E+03	3.035E+03	2.656E+02	2.658E+02	6.637E+03	4.763E+00
46000	2.079E+02	3.448E+02	3.494E+03	3.487E+03	2.688E+02	2.690E+02	7.130E+03	5.118E+00
48000	1.681E+02	3.528E+02	3.870E+03	3.863E+03	2.722E+02	2.723E+02	7.547E+03	5.465E+00
50000	1.320E+02	3.589E+02	4.169E+03	4.162E+03	2.755E+02	2.757E+02	7.887E+03	5.801E+00

Table 47: Internal thermodynamic properties of Ar^{2+} ΔE=500 cm^{-1}

T(K)	Q_{int}	$\ln(Q_{int})$	E_{int}/RT	$C_{p,int}/R$
50	$5.119E+00$	$1.633E+00$	$7.499E-02$	$2.364E-01$
100	$5.597E+00$	$1.722E+00$	$1.722E-01$	$2.483E-01$
150	$6.023E+00$	$1.796E+00$	$1.827E-01$	$1.632E-01$
200	$6.339E+00$	$1.847E+00$	$1.704E-01$	$1.087E-01$
298.15	$6.746E+00$	$1.909E+00$	$1.407E-01$	$6.040E-02$
300	$6.752E+00$	$1.910E+00$	$1.402E-01$	$5.994E-02$
400	$7.007E+00$	$1.947E+00$	$1.182E-01$	$4.862E-02$
500	$7.183E+00$	$1.972E+00$	$1.045E-01$	$5.159E-02$
600	$7.316E+00$	$1.990E+00$	$9.621E-02$	$5.830E-02$
700	$7.422E+00$	$2.004E+00$	$9.125E-02$	$6.440E-02$
800	$7.511E+00$	$2.016E+00$	$8.818E-02$	$6.854E-02$
900	$7.589E+00$	$2.027E+00$	$8.613E-02$	$7.067E-02$
1000	$7.657E+00$	$2.036E+00$	$8.462E-02$	$7.113E-02$
2000	$8.091E+00$	$2.091E+00$	$7.298E-02$	$5.050E-02$
3000	$8.320E+00$	$2.119E+00$	$6.588E-02$	$6.152E-02$
4000	$8.482E+00$	$2.138E+00$	$7.081E-02$	$1.140E-01$
5000	$8.630E+00$	$2.155E+00$	$8.572E-02$	$1.759E-01$
6000	$8.781E+00$	$2.173E+00$	$1.052E-01$	$2.261E-01$
7000	$8.938E+00$	$2.190E+00$	$1.250E-01$	$2.591E-01$
8000	$9.099E+00$	$2.208E+00$	$1.430E-01$	$2.770E-01$
9000	$9.262E+00$	$2.226E+00$	$1.584E-01$	$2.837E-01$
10000	$9.424E+00$	$2.243E+00$	$1.709E-01$	$2.827E-01$
11000	$9.584E+00$	$2.260E+00$	$1.808E-01$	$2.768E-01$
12000	$9.739E+00$	$2.276E+00$	$1.885E-01$	$2.681E-01$
13000	$9.889E+00$	$2.291E+00$	$1.942E-01$	$2.579E-01$
14000	$1.003E+01$	$2.306E+00$	$1.984E-01$	$2.471E-01$
15000	$1.017E+01$	$2.320E+00$	$2.013E-01$	$2.368E-01$
16000	$1.031E+01$	$2.333E+00$	$2.032E-01$	$2.274E-01$
17000	$1.044E+01$	$2.345E+00$	$2.044E-01$	$2.196E-01$
18000	$1.056E+01$	$2.357E+00$	$2.051E-01$	$2.141E-01$
19000	$1.068E+01$	$2.368E+00$	$2.055E-01$	$2.116E-01$
20000	$1.079E+01$	$2.379E+00$	$2.058E-01$	$2.129E-01$
21000	$1.090E+01$	$2.389E+00$	$2.062E-01$	$2.193E-01$
22000	$1.100E+01$	$2.398E+00$	$2.071E-01$	$2.323E-01$
23000	$1.111E+01$	$2.407E+00$	$2.086E-01$	$2.544E-01$
24000	$1.121E+01$	$2.416E+00$	$2.112E-01$	$2.895E-01$
25000	$1.130E+01$	$2.425E+00$	$2.154E-01$	$3.431E-01$
26000	$1.140E+01$	$2.434E+00$	$2.217E-01$	$4.233E-01$
27000	$1.150E+01$	$2.442E+00$	$2.312E-01$	$5.415E-01$
28000	$1.160E+01$	$2.451E+00$	$2.452E-01$	$7.133E-01$
29000	$1.170E+01$	$2.460E+00$	$2.653E-01$	$9.586E-01$
30000	$1.181E+01$	$2.469E+00$	$2.938E-01$	$1.302E+00$
32000	$1.207E+01$	$2.491E+00$	$3.880E-01$	$2.407E+00$
34000	$1.242E+01$	$2.519E+00$	$5.577E-01$	$4.292E+00$
36000	$1.291E+01$	$2.558E+00$	$8.404E-01$	$7.177E+00$
38000	$1.366E+01$	$2.615E+00$	$1.272E+00$	$1.106E+01$
40000	$1.480E+01$	$2.694E+00$	$1.872E+00$	$1.550E+01$
42000	$1.650E+01$	$2.803E+00$	$2.622E+00$	$1.961E+01$
44000	$1.900E+01$	$2.944E+00$	$3.463E+00$	$2.234E+01$
46000	$2.258E+01$	$3.117E+00$	$4.307E+00$	$2.306E+01$
48000	$2.758E+01$	$3.317E+00$	$5.069E+00$	$2.184E+01$
50000	$3.436E+01$	$3.537E+00$	$5.692E+00$	$1.930E+01$

Table 48: Total thermodynamic properties of Ar^{2+} ΔE=500 cm^{-1}

T [K]	C_p [J/mol/K]	S^0 [J/mol/K]	$H^0(T)-H^0(0)$ [KJ/mol]	$H^0(T)-H^0(298)$ [KJ/mol]	$-(G^0-H^0(0))/T$ [J/mol/K]	$-(G^0-H^0(298))/T$ [J/mol/K]	ΔH_f [KJ/mol]	$Log(K_p)$
50	2.275E+01	1.319E+02	1.071E+00	-5.476E+00	1.105E+02	2.414E+02	4.188E+03	-4.377E+03
100	2.285E+01	1.479E+02	2.222E+00	-4.324E+00	1.257E+02	1.911E+02	4.191E+03	-2.188E+03
150	2.214E+01	1.570E+02	3.346E+00	-3.200E+00	1.347E+02	1.783E+02	4.193E+03	-1.458E+03
200	2.169E+01	1.633E+02	4.441E+00	-2.105E+00	1.411E+02	1.738E+02	4.195E+03	-1.093E+03
298.15	2.129E+01	1.719E+02	6.546E+00	0.000E+00	1.499E+02	1.719E+02	4.199E+03	-7.326E+02
300	2.129E+01	1.720E+02	6.585E+00	3.941E-02	1.501E+02	1.719E+02	4.199E+03	-7.280E+02
400	2.119E+01	1.781E+02	8.708E+00	2.162E+00	1.564E+02	1.727E+02	4.204E+03	-5.452E+02
500	2.121E+01	1.829E+02	1.083E+01	4.281E+00	1.612E+02	1.743E+02	4.208E+03	-4.353E+02
600	2.127E+01	1.867E+02	1.295E+01	6.406E+00	1.651E+02	1.761E+02	4.212E+03	-3.621E+02
700	2.132E+01	1.900E+02	1.508E+01	8.535E+00	1.685E+02	1.778E+02	4.216E+03	-3.096E+02
800	2.136E+01	1.929E+02	1.721E+01	1.067E+01	1.713E+02	1.795E+02	4.220E+03	-2.703E+02
900	2.137E+01	1.954E+02	1.935E+01	1.281E+01	1.739E+02	1.812E+02	4.224E+03	-2.397E+02
1000	2.138E+01	1.976E+02	2.149E+01	1.494E+01	1.761E+02	1.827E+02	4.229E+03	-2.151E+02
2000	2.121E+01	2.124E+02	4.279E+01	3.624E+01	1.910E+02	1.943E+02	4.271E+03	-1.043E+02
3000	2.130E+01	2.210E+02	6.400E+01	5.746E+01	1.997E+02	2.018E+02	4.313E+03	-6.694E+01
4000	2.173E+01	2.272E+02	8.550E+01	7.895E+01	2.058E+02	2.074E+02	4.355E+03	-4.808E+01
5000	2.225E+01	2.321E+02	1.075E+02	1.010E+02	2.106E+02	2.119E+02	4.398E+03	-3.666E+01
6000	2.267E+01	2.362E+02	1.300E+02	1.234E+02	2.145E+02	2.156E+02	4.441E+03	-2.896E+01
7000	2.294E+01	2.397E+02	1.528E+02	1.462E+02	2.179E+02	2.188E+02	4.485E+03	-2.341E+01
8000	2.309E+01	2.428E+02	1.758E+02	1.693E+02	2.208E+02	2.216E+02	4.528E+03	-1.921E+01
9000	2.314E+01	2.455E+02	1.989E+02	1.924E+02	2.234E+02	2.241E+02	4.572E+03	-1.591E+01
10000	2.314E+01	2.479E+02	2.221E+02	2.155E+02	2.257E+02	2.264E+02	4.616E+03	-1.324E+01
11000	2.309E+01	2.501E+02	2.452E+02	2.386E+02	2.278E+02	2.284E+02	4.659E+03	-1.104E+01
12000	2.302E+01	2.522E+02	2.682E+02	2.617E+02	2.298E+02	2.303E+02	4.700E+03	-9.191E+00
13000	2.293E+01	2.540E+02	2.912E+02	2.847E+02	2.316E+02	2.321E+02	4.735E+03	-7.612E+00
14000	2.284E+01	2.557E+02	3.141E+02	3.076E+02	2.332E+02	2.337E+02	4.758E+03	-6.249E+00
15000	2.275E+01	2.572E+02	3.369E+02	3.304E+02	2.348E+02	2.352E+02	4.759E+03	-5.065E+00
16000	2.268E+01	2.587E+02	3.596E+02	3.531E+02	2.362E+02	2.367E+02	4.728E+03	-4.032E+00
17000	2.261E+01	2.601E+02	3.822E+02	3.757E+02	2.376E+02	2.380E+02	4.655E+03	-3.130E+00
18000	2.257E+01	2.614E+02	4.048E+02	3.983E+02	2.389E+02	2.393E+02	4.546E+03	-2.344E+00
19000	2.255E+01	2.626E+02	4.274E+02	4.209E+02	2.401E+02	2.404E+02	4.415E+03	-1.660E+00
20000	2.256E+01	2.638E+02	4.499E+02	4.434E+02	2.413E+02	2.416E+02	4.284E+03	-1.062E+00
21000	2.261E+01	2.649E+02	4.725E+02	4.660E+02	2.424E+02	2.427E+02	4.170E+03	-5.362E-01
22000	2.272E+01	2.659E+02	4.952E+02	4.886E+02	2.434E+02	2.437E+02	4.084E+03	-6.978E-02
23000	2.290E+01	2.669E+02	5.180E+02	5.114E+02	2.444E+02	2.447E+02	4.026E+03	3.486E-01
24000	2.319E+01	2.679E+02	5.410E+02	5.345E+02	2.454E+02	2.456E+02	3.992E+03	7.278E-01
25000	2.364E+01	2.689E+02	5.644E+02	5.579E+02	2.463E+02	2.466E+02	3.977E+03	1.075E+00
26000	2.431E+01	2.698E+02	5.884E+02	5.818E+02	2.472E+02	2.474E+02	3.978E+03	1.394E+00
27000	2.529E+01	2.707E+02	6.131E+02	6.066E+02	2.480E+02	2.483E+02	3.990E+03	1.690E+00
28000	2.672E+01	2.717E+02	6.391E+02	6.325E+02	2.489E+02	2.491E+02	4.012E+03	1.967E+00
29000	2.876E+01	2.726E+02	6.668E+02	6.602E+02	2.497E+02	2.499E+02	4.041E+03	2.226E+00
30000	3.161E+01	2.737E+02	6.969E+02	6.903E+02	2.504E+02	2.507E+02	4.077E+03	2.469E+00
32000	4.080E+01	2.760E+02	7.684E+02	7.619E+02	2.520E+02	2.522E+02	4.169E+03	2.918E+00
34000	5.647E+01	2.789E+02	8.644E+02	8.579E+02	2.535E+02	2.537E+02	4.294E+03	3.324E+00
36000	8.046E+01	2.828E+02	9.999E+02	9.933E+02	2.550E+02	2.552E+02	4.462E+03	3.697E+00
38000	1.127E+02	2.879E+02	1.192E+03	1.185E+03	2.566E+02	2.567E+02	4.689E+03	4.045E+00
40000	1.496E+02	2.946E+02	1.454E+03	1.447E+03	2.583E+02	2.585E+02	4.988E+03	4.378E+00
42000	1.838E+02	3.028E+02	1.789E+03	1.782E+03	2.602E+02	2.604E+02	5.361E+03	4.699E+00
44000	2.065E+02	3.119E+02	2.181E+03	2.175E+03	2.624E+02	2.625E+02	5.793E+03	5.014E+00
46000	2.125E+02	3.213E+02	2.603E+03	2.597E+03	2.647E+02	2.649E+02	6.255E+03	5.324E+00
48000	2.023E+02	3.302E+02	3.021E+03	3.014E+03	2.673E+02	2.674E+02	6.712E+03	5.631E+00
50000	1.812E+02	3.381E+02	3.405E+03	3.399E+03	2.699E+02	2.701E+02	7.138E+03	5.932E+00

Table 49: Internal thermodynamic properties of Ar^{2+} ΔE=1000 cm^{-1}

T(K)	Q_{int}	$\ln(Q_{int})$	E_{int}/RT	$C_{p,int}/R$
50	$5.119E+00$	$1.633E+00$	$7.499E-02$	$2.364E-01$
100	$5.597E+00$	$1.722E+00$	$1.722E-01$	$2.483E-01$
150	$6.023E+00$	$1.796E+00$	$1.827E-01$	$1.632E-01$
200	$6.339E+00$	$1.847E+00$	$1.704E-01$	$1.087E-01$
298.15	$6.746E+00$	$1.909E+00$	$1.407E-01$	$6.040E-02$
300	$6.752E+00$	$1.910E+00$	$1.402E-01$	$5.994E-02$
400	$7.007E+00$	$1.947E+00$	$1.182E-01$	$4.862E-02$
500	$7.183E+00$	$1.972E+00$	$1.045E-01$	$5.159E-02$
600	$7.316E+00$	$1.990E+00$	$9.621E-02$	$5.830E-02$
700	$7.422E+00$	$2.004E+00$	$9.125E-02$	$6.440E-02$
800	$7.511E+00$	$2.016E+00$	$8.818E-02$	$6.854E-02$
900	$7.589E+00$	$2.027E+00$	$8.613E-02$	$7.067E-02$
1000	$7.657E+00$	$2.036E+00$	$8.462E-02$	$7.113E-02$
2000	$8.091E+00$	$2.091E+00$	$7.298E-02$	$5.050E-02$
3000	$8.320E+00$	$2.119E+00$	$6.588E-02$	$6.152E-02$
4000	$8.482E+00$	$2.138E+00$	$7.081E-02$	$1.140E-01$
5000	$8.630E+00$	$2.155E+00$	$8.572E-02$	$1.759E-01$
6000	$8.781E+00$	$2.173E+00$	$1.052E-01$	$2.261E-01$
7000	$8.938E+00$	$2.190E+00$	$1.250E-01$	$2.591E-01$
8000	$9.099E+00$	$2.208E+00$	$1.430E-01$	$2.770E-01$
9000	$9.262E+00$	$2.226E+00$	$1.584E-01$	$2.837E-01$
10000	$9.424E+00$	$2.243E+00$	$1.709E-01$	$2.827E-01$
11000	$9.584E+00$	$2.260E+00$	$1.808E-01$	$2.768E-01$
12000	$9.739E+00$	$2.276E+00$	$1.885E-01$	$2.681E-01$
13000	$9.889E+00$	$2.291E+00$	$1.942E-01$	$2.579E-01$
14000	$1.003E+01$	$2.306E+00$	$1.984E-01$	$2.471E-01$
15000	$1.017E+01$	$2.320E+00$	$2.013E-01$	$2.368E-01$
16000	$1.031E+01$	$2.333E+00$	$2.032E-01$	$2.274E-01$
17000	$1.044E+01$	$2.345E+00$	$2.044E-01$	$2.196E-01$
18000	$1.056E+01$	$2.357E+00$	$2.051E-01$	$2.141E-01$
19000	$1.068E+01$	$2.368E+00$	$2.054E-01$	$2.114E-01$
20000	$1.079E+01$	$2.379E+00$	$2.058E-01$	$2.125E-01$
21000	$1.090E+01$	$2.389E+00$	$2.062E-01$	$2.181E-01$
22000	$1.100E+01$	$2.398E+00$	$2.070E-01$	$2.293E-01$
23000	$1.111E+01$	$2.407E+00$	$2.083E-01$	$2.475E-01$
24000	$1.120E+01$	$2.416E+00$	$2.105E-01$	$2.746E-01$
25000	$1.130E+01$	$2.425E+00$	$2.138E-01$	$3.133E-01$
26000	$1.140E+01$	$2.433E+00$	$2.186E-01$	$3.670E-01$
27000	$1.149E+01$	$2.442E+00$	$2.253E-01$	$4.404E-01$
28000	$1.159E+01$	$2.450E+00$	$2.347E-01$	$5.398E-01$
29000	$1.169E+01$	$2.459E+00$	$2.474E-01$	$6.731E-01$
30000	$1.179E+01$	$2.467E+00$	$2.644E-01$	$8.500E-01$
32000	$1.201E+01$	$2.486E+00$	$3.163E-01$	$1.383E+00$
34000	$1.227E+01$	$2.507E+00$	$4.026E-01$	$2.252E+00$
36000	$1.260E+01$	$2.534E+00$	$5.398E-01$	$3.576E+00$
38000	$1.304E+01$	$2.568E+00$	$7.462E-01$	$5.441E+00$
40000	$1.365E+01$	$2.614E+00$	$1.039E+00$	$7.843E+00$
42000	$1.449E+01$	$2.673E+00$	$1.428E+00$	$1.062E+01$
44000	$1.565E+01$	$2.751E+00$	$1.911E+00$	$1.344E+01$
46000	$1.725E+01$	$2.848E+00$	$2.467E+00$	$1.586E+01$
48000	$1.940E+01$	$2.965E+00$	$3.062E+00$	$1.747E+01$
50000	$2.225E+01$	$3.102E+00$	$3.653E+00$	$1.802E+01$

Table 50: Total thermodynamic properties of Ar^{2+} ΔE=1000 cm^{-1}

T [K]	C_p [J/mol/K]	S^0 [J/mol/K]	$H^0(T)-H^0(0)$ [KJ/mol]	$H^0(T)-H^0(298)$ [KJ/mol]	$-(G^0-H^0(0))/T$ [J/mol/K]	$-(G^0-H^0(298))/T$ [J/mol/K]	ΔH_f [KJ/mol]	$Log(K_p)$
50	2.275E+01	1.319E+02	1.071E+00	-5.476E+00	1.105E+02	2.414E+02	4.188E+03	-4.377E+03
100	2.285E+01	1.479E+02	2.222E+00	-4.324E+00	1.257E+02	1.911E+02	4.191E+03	-2.188E+03
150	2.214E+01	1.570E+02	3.346E+00	-3.200E+00	1.347E+02	1.783E+02	4.193E+03	-1.458E+03
200	2.169E+01	1.633E+02	4.441E+00	-2.105E+00	1.411E+02	1.738E+02	4.195E+03	-1.093E+03
298.15	2.129E+01	1.719E+02	6.546E+00	0.000E+00	1.499E+02	1.719E+02	4.199E+03	-7.326E+02
300	2.129E+01	1.720E+02	6.585E+00	3.941E-02	1.501E+02	1.719E+02	4.199E+03	-7.280E+02
400	2.119E+01	1.781E+02	8.708E+00	2.162E+00	1.564E+02	1.727E+02	4.204E+03	-5.452E+02
500	2.121E+01	1.829E+02	1.083E+01	4.281E+00	1.612E+02	1.743E+02	4.208E+03	-4.353E+02
600	2.127E+01	1.867E+02	1.295E+01	6.406E+00	1.651E+02	1.761E+02	4.212E+03	-3.621E+02
700	2.132E+01	1.900E+02	1.508E+01	8.535E+00	1.685E+02	1.778E+02	4.216E+03	-3.096E+02
800	2.136E+01	1.929E+02	1.721E+01	1.067E+01	1.713E+02	1.795E+02	4.220E+03	-2.703E+02
900	2.137E+01	1.954E+02	1.935E+01	1.281E+01	1.739E+02	1.812E+02	4.224E+03	-2.397E+02
1000	2.138E+01	1.976E+02	2.149E+01	1.494E+01	1.761E+02	1.827E+02	4.229E+03	-2.151E+02
2000	2.121E+01	2.124E+02	4.279E+01	3.624E+01	1.910E+02	1.943E+02	4.271E+03	-1.043E+02
3000	2.130E+01	2.210E+02	6.400E+01	5.746E+01	1.997E+02	2.018E+02	4.313E+03	-6.694E+01
4000	2.173E+01	2.272E+02	8.550E+01	7.895E+01	2.058E+02	2.074E+02	4.355E+03	-4.808E+01
5000	2.225E+01	2.321E+02	1.075E+02	1.010E+02	2.106E+02	2.119E+02	4.398E+03	-3.666E+01
6000	2.267E+01	2.362E+02	1.300E+02	1.234E+02	2.145E+02	2.156E+02	4.441E+03	-2.896E+01
7000	2.294E+01	2.397E+02	1.528E+02	1.462E+02	2.179E+02	2.188E+02	4.485E+03	-2.341E+01
8000	2.309E+01	2.428E+02	1.758E+02	1.693E+02	2.208E+02	2.216E+02	4.528E+03	-1.921E+01
9000	2.314E+01	2.455E+02	1.989E+02	1.924E+02	2.234E+02	2.241E+02	4.572E+03	-1.591E+01
10000	2.314E+01	2.479E+02	2.221E+02	2.155E+02	2.257E+02	2.264E+02	4.616E+03	-1.324E+01
11000	2.309E+01	2.501E+02	2.452E+02	2.386E+02	2.278E+02	2.284E+02	4.660E+03	-1.104E+01
12000	2.302E+01	2.522E+02	2.682E+02	2.617E+02	2.298E+02	2.303E+02	4.702E+03	-9.191E+00
13000	2.293E+01	2.540E+02	2.912E+02	2.847E+02	2.316E+02	2.321E+02	4.742E+03	-7.610E+00
14000	2.284E+01	2.557E+02	3.141E+02	3.076E+02	2.332E+02	2.337E+02	4.776E+03	-6.244E+00
15000	2.275E+01	2.572E+02	3.369E+02	3.304E+02	2.348E+02	2.352E+02	4.799E+03	-5.053E+00
16000	2.268E+01	2.587E+02	3.596E+02	3.531E+02	2.362E+02	2.367E+02	4.806E+03	-4.008E+00
17000	2.261E+01	2.601E+02	3.822E+02	3.757E+02	2.376E+02	2.380E+02	4.789E+03	-3.086E+00
18000	2.257E+01	2.614E+02	4.048E+02	3.983E+02	2.389E+02	2.393E+02	4.745E+03	-2.272E+00
19000	2.254E+01	2.626E+02	4.274E+02	4.209E+02	2.401E+02	2.404E+02	4.673E+03	-1.552E+00
20000	2.255E+01	2.638E+02	4.499E+02	4.434E+02	2.413E+02	2.416E+02	4.581E+03	-9.156E-01
21000	2.260E+01	2.649E+02	4.725E+02	4.660E+02	2.424E+02	2.427E+02	4.481E+03	-3.520E-01
22000	2.269E+01	2.659E+02	4.951E+02	4.886E+02	2.434E+02	2.437E+02	4.384E+03	1.492E-01
23000	2.284E+01	2.669E+02	5.179E+02	5.114E+02	2.444E+02	2.447E+02	4.301E+03	5.974E-01
24000	2.307E+01	2.679E+02	5.409E+02	5.343E+02	2.454E+02	2.456E+02	4.235E+03	1.001E+00
25000	2.339E+01	2.689E+02	5.641E+02	5.575E+02	2.463E+02	2.466E+02	4.188E+03	1.368E+00
26000	2.384E+01	2.698E+02	5.877E+02	5.811E+02	2.472E+02	2.474E+02	4.158E+03	1.703E+00
27000	2.445E+01	2.707E+02	6.118E+02	6.053E+02	2.480E+02	2.483E+02	4.144E+03	2.012E+00
28000	2.527E+01	2.716E+02	6.367E+02	6.301E+02	2.488E+02	2.491E+02	4.143E+03	2.298E+00
29000	2.638E+01	2.725E+02	6.625E+02	6.559E+02	2.497E+02	2.499E+02	4.152E+03	2.564E+00
30000	2.785E+01	2.734E+02	6.895E+02	6.830E+02	2.504E+02	2.507E+02	4.170E+03	2.814E+00
32000	3.229E+01	2.753E+02	7.493E+02	7.428E+02	2.519E+02	2.521E+02	4.228E+03	3.271E+00
34000	3.951E+01	2.775E+02	8.206E+02	8.140E+02	2.534E+02	2.536E+02	4.312E+03	3.681E+00
36000	5.052E+01	2.801E+02	9.099E+02	9.033E+02	2.548E+02	2.549E+02	4.424E+03	4.053E+00
38000	6.603E+01	2.832E+02	1.026E+03	1.019E+03	2.562E+02	2.564E+02	4.568E+03	4.396E+00
40000	8.600E+01	2.871E+02	1.177E+03	1.170E+03	2.576E+02	2.578E+02	4.751E+03	4.716E+00
42000	1.091E+02	2.918E+02	1.372E+03	1.365E+03	2.591E+02	2.593E+02	4.980E+03	5.018E+00
44000	1.326E+02	2.974E+02	1.614E+03	1.607E+03	2.607E+02	2.609E+02	5.258E+03	5.307E+00
46000	1.527E+02	3.038E+02	1.900E+03	1.893E+03	2.625E+02	2.626E+02	5.581E+03	5.587E+00
48000	1.660E+02	3.106E+02	2.220E+03	2.213E+03	2.643E+02	2.645E+02	5.940E+03	5.859E+00
50000	1.707E+02	3.175E+02	2.558E+03	2.552E+03	2.663E+02	2.665E+02	6.317E+03	6.125E+00

Table 51: Internal thermodynamic properties of Ar^{3+} ΔE=250 cm^{-1}

T(K)	Q_{int}	$\ln(Q_{int})$	E_{int}/RT	$C_{p,int}/R$
50	$4.000E+00$	$1.386E+00$	$1.708E-261$	$1.037E-258$
100	$4.000E+00$	$1.386E+00$	$6.180E-130$	$1.877E-127$
150	$4.000E+00$	$1.386E+00$	$4.058E-86$	$8.225E-84$
200	$4.000E+00$	$1.386E+00$	$3.110E-64$	$4.729E-62$
298.15	$4.000E+00$	$1.386E+00$	$1.162E-42$	$1.185E-40$
300	$4.000E+00$	$1.386E+00$	$2.166E-42$	$2.197E-40$
400	$4.000E+00$	$1.386E+00$	$1.675E-31$	$1.275E-29$
500	$4.000E+00$	$1.386E+00$	$5.450E-25$	$3.318E-23$
600	$4.000E+00$	$1.386E+00$	$1.159E-20$	$5.878E-19$
700	$4.000E+00$	$1.386E+00$	$1.396E-17$	$6.071E-16$
800	$4.000E+00$	$1.386E+00$	$2.805E-15$	$1.067E-13$
900	$4.000E+00$	$1.386E+00$	$1.711E-13$	$5.787E-12$
1000	$4.000E+00$	$1.386E+00$	$4.536E-12$	$1.381E-10$
2000	$4.000E+00$	$1.386E+00$	$9.282E-06$	$1.413E-04$
3000	$4.000E+00$	$1.386E+00$	$9.915E-04$	$1.007E-02$
4000	$4.005E+00$	$1.388E+00$	$9.450E-03$	$7.218E-02$
5000	$4.023E+00$	$1.392E+00$	$3.491E-02$	$2.139E-01$
6000	$4.064E+00$	$1.402E+00$	$8.084E-02$	$4.131E-01$
7000	$4.134E+00$	$1.419E+00$	$1.436E-01$	$6.266E-01$
8000	$4.233E+00$	$1.443E+00$	$2.163E-01$	$8.178E-01$
9000	$4.362E+00$	$1.473E+00$	$2.918E-01$	$9.657E-01$
10000	$4.515E+00$	$1.507E+00$	$3.645E-01$	$1.064E+00$
11000	$4.689E+00$	$1.545E+00$	$4.308E-01$	$1.116E+00$
12000	$4.881E+00$	$1.585E+00$	$4.888E-01$	$1.131E+00$
13000	$5.086E+00$	$1.626E+00$	$5.378E-01$	$1.117E+00$
14000	$5.301E+00$	$1.668E+00$	$5.780E-01$	$1.084E+00$
15000	$5.523E+00$	$1.709E+00$	$6.103E-01$	$1.038E+00$
16000	$5.749E+00$	$1.749E+00$	$6.354E-01$	$9.867E-01$
17000	$5.979E+00$	$1.788E+00$	$6.545E-01$	$9.330E-01$
18000	$6.209E+00$	$1.826E+00$	$6.685E-01$	$8.801E-01$
19000	$6.440E+00$	$1.862E+00$	$6.783E-01$	$8.301E-01$
20000	$6.669E+00$	$1.897E+00$	$6.847E-01$	$7.843E-01$
21000	$6.896E+00$	$1.931E+00$	$6.885E-01$	$7.436E-01$
22000	$7.121E+00$	$1.963E+00$	$6.902E-01$	$7.084E-01$
23000	$7.343E+00$	$1.994E+00$	$6.903E-01$	$6.791E-01$
24000	$7.561E+00$	$2.023E+00$	$6.893E-01$	$6.557E-01$
25000	$7.777E+00$	$2.051E+00$	$6.876E-01$	$6.385E-01$
26000	$7.989E+00$	$2.078E+00$	$6.855E-01$	$6.274E-01$
27000	$8.198E+00$	$2.104E+00$	$6.832E-01$	$6.228E-01$
28000	$8.404E+00$	$2.129E+00$	$6.811E-01$	$6.253E-01$
29000	$8.607E+00$	$2.153E+00$	$6.793E-01$	$6.358E-01$
30000	$8.807E+00$	$2.176E+00$	$6.782E-01$	$6.564E-01$
32000	$9.202E+00$	$2.219E+00$	$6.791E-01$	$7.426E-01$
34000	$9.590E+00$	$2.261E+00$	$6.879E-01$	$9.371E-01$
36000	$9.981E+00$	$2.301E+00$	$7.118E-01$	$1.349E+00$
38000	$1.039E+01$	$2.340E+00$	$7.647E-01$	$2.175E+00$
40000	$1.083E+01$	$2.382E+00$	$8.700E-01$	$3.718E+00$
42000	$1.134E+01$	$2.429E+00$	$1.064E+00$	$6.374E+00$
44000	$1.200E+01$	$2.485E+00$	$1.393E+00$	$1.052E+01$
46000	$1.291E+01$	$2.558E+00$	$1.910E+00$	$1.627E+01$
48000	$1.421E+01$	$2.654E+00$	$2.649E+00$	$2.311E+01$
50000	$1.613E+01$	$2.781E+00$	$3.603E+00$	$2.970E+01$

Table 52: Total thermodynamic properties of Ar^{3+} ΔE=250 cm^{-1}

T [K]	C_p [J/mol/K]	S^0 [J/mol/K]	$H^0(T)-H^0(0)$ [KJ/mol]	$H^0(T)-H^0(298)$ [KJ/mol]	$-(G^0-H^0(0))/T$ [J/mol/K]	$-(G^0-H^0(298))/T$ [J/mol/K]	ΔH_f [KJ/mol]	$Log(K_p)$
50	2.079E+01	1.293E+02	1.039E+00	-5.158E+00	1.085E+02	2.324E+02	8.120E+03	-8.484E+03
100	2.079E+01	1.437E+02	2.079E+00	-4.119E+00	1.229E+02	1.848E+02	8.123E+03	-4.243E+03
150	2.079E+01	1.521E+02	3.118E+00	-3.079E+00	1.313E+02	1.726E+02	8.126E+03	-2.828E+03
200	2.079E+01	1.581E+02	4.157E+00	-2.040E+00	1.373E+02	1.683E+02	8.129E+03	-2.120E+03
298.15	2.079E+01	1.664E+02	6.197E+00	0.000E+00	1.456E+02	1.664E+02	8.135E+03	-1.421E+03
300	2.079E+01	1.665E+02	6.236E+00	3.848E-02	1.457E+02	1.664E+02	8.136E+03	-1.413E+03
400	2.079E+01	1.725E+02	8.315E+00	2.117E+00	1.517E+02	1.672E+02	8.142E+03	-1.058E+03
500	2.079E+01	1.771E+02	1.039E+01	4.196E+00	1.563E+02	1.687E+02	8.148E+03	-8.456E+02
600	2.079E+01	1.809E+02	1.247E+01	6.274E+00	1.601E+02	1.704E+02	8.154E+03	-7.037E+02
700	2.079E+01	1.841E+02	1.455E+01	8.353E+00	1.633E+02	1.722E+02	8.160E+03	-6.022E+02
800	2.079E+01	1.869E+02	1.663E+01	1.043E+01	1.661E+02	1.738E+02	8.167E+03	-5.261E+02
900	2.079E+01	1.893E+02	1.871E+01	1.251E+01	1.686E+02	1.754E+02	8.173E+03	-4.668E+02
1000	2.079E+01	1.915E+02	2.079E+01	1.459E+01	1.707E+02	1.769E+02	8.179E+03	-4.194E+02
2000	2.079E+01	2.059E+02	4.157E+01	3.538E+01	1.852E+02	1.882E+02	8.242E+03	-2.052E+02
3000	2.087E+01	2.144E+02	6.238E+01	5.619E+01	1.936E+02	1.956E+02	8.304E+03	-1.332E+02
4000	2.139E+01	2.204E+02	8.346E+01	7.726E+01	1.996E+02	2.011E+02	8.366E+03	-9.690E+01
5000	2.257E+01	2.253E+02	1.054E+02	9.919E+01	2.042E+02	2.055E+02	8.430E+03	-7.497E+01
6000	2.422E+01	2.296E+02	1.288E+02	1.225E+02	2.081E+02	2.092E+02	8.495E+03	-6.024E+01
7000	2.600E+01	2.334E+02	1.539E+02	1.477E+02	2.115E+02	2.123E+02	8.562E+03	-4.964E+01
8000	2.759E+01	2.370E+02	1.807E+02	1.745E+02	2.144E+02	2.152E+02	8.630E+03	-4.162E+01
9000	2.882E+01	2.403E+02	2.089E+02	2.027E+02	2.171E+02	2.178E+02	8.700E+03	-3.534E+01
10000	2.963E+01	2.434E+02	2.382E+02	2.320E+02	2.196E+02	2.202E+02	8.770E+03	-3.027E+01
11000	3.007E+01	2.463E+02	2.681E+02	2.619E+02	2.219E+02	2.225E+02	8.840E+03	-2.609E+01
12000	3.019E+01	2.489E+02	2.982E+02	2.920E+02	2.241E+02	2.246E+02	8.904E+03	-2.258E+01
13000	3.007E+01	2.513E+02	3.284E+02	3.221E+02	2.261E+02	2.265E+02	8.955E+03	-1.959E+01
14000	2.980E+01	2.535E+02	3.583E+02	3.521E+02	2.279E+02	2.284E+02	8.978E+03	-1.702E+01
15000	2.942E+01	2.556E+02	3.879E+02	3.817E+02	2.297E+02	2.301E+02	8.953E+03	-1.478E+01
16000	2.899E+01	2.575E+02	4.171E+02	4.109E+02	2.314E+02	2.318E+02	8.870E+03	-1.284E+01
17000	2.854E+01	2.592E+02	4.459E+02	4.397E+02	2.330E+02	2.333E+02	8.738E+03	-1.115E+01
18000	2.810E+01	2.608E+02	4.742E+02	4.680E+02	2.345E+02	2.348E+02	8.592E+03	-9.672E+00
19000	2.769E+01	2.623E+02	5.021E+02	4.959E+02	2.359E+02	2.362E+02	8.466E+03	-8.370E+00
20000	2.731E+01	2.637E+02	5.296E+02	5.234E+02	2.373E+02	2.376E+02	8.378E+03	-7.213E+00
21000	2.697E+01	2.651E+02	5.567E+02	5.505E+02	2.386E+02	2.388E+02	8.332E+03	-6.174E+00
22000	2.668E+01	2.663E+02	5.835E+02	5.774E+02	2.398E+02	2.401E+02	8.318E+03	-5.233E+00
23000	2.643E+01	2.675E+02	6.101E+02	6.039E+02	2.410E+02	2.412E+02	8.329E+03	-4.374E+00
24000	2.624E+01	2.686E+02	6.364E+02	6.302E+02	2.421E+02	2.423E+02	8.357E+03	-3.584E+00
25000	2.609E+01	2.697E+02	6.626E+02	6.564E+02	2.432E+02	2.434E+02	8.396E+03	-2.855E+00
26000	2.600E+01	2.707E+02	6.886E+02	6.824E+02	2.442E+02	2.444E+02	8.444E+03	-2.179E+00
27000	2.596E+01	2.717E+02	7.146E+02	7.084E+02	2.452E+02	2.454E+02	8.497E+03	-1.549E+00
28000	2.598E+01	2.726E+02	7.406E+02	7.344E+02	2.462E+02	2.464E+02	8.553E+03	-9.596E-01
29000	2.607E+01	2.735E+02	7.666E+02	7.604E+02	2.471E+02	2.473E+02	8.613E+03	-4.075E-01
30000	2.624E+01	2.744E+02	7.928E+02	7.866E+02	2.480E+02	2.482E+02	8.674E+03	1.114E-01
32000	2.696E+01	2.761E+02	8.459E+02	8.397E+02	2.497E+02	2.499E+02	8.802E+03	1.062E+00
34000	2.858E+01	2.778E+02	9.012E+02	8.950E+02	2.513E+02	2.515E+02	8.935E+03	1.913E+00
36000	3.201E+01	2.795E+02	9.614E+02	9.552E+02	2.528E+02	2.530E+02	9.075E+03	2.682E+00
38000	3.887E+01	2.814E+02	1.032E+03	1.025E+03	2.543E+02	2.544E+02	9.226E+03	3.381E+00
40000	5.170E+01	2.837E+02	1.121E+03	1.115E+03	2.557E+02	2.558E+02	9.397E+03	4.020E+00
42000	7.378E+01	2.867E+02	1.244E+03	1.238E+03	2.571E+02	2.572E+02	9.602E+03	4.611E+00
44000	1.083E+02	2.909E+02	1.424E+03	1.418E+03	2.585E+02	2.587E+02	9.864E+03	5.160E+00
46000	1.561E+02	2.967E+02	1.687E+03	1.680E+03	2.601E+02	2.602E+02	1.021E+04	5.678E+00
48000	2.129E+02	3.046E+02	2.055E+03	2.049E+03	2.618E+02	2.619E+02	1.066E+04	6.171E+00
50000	2.677E+02	3.144E+02	2.537E+03	2.531E+03	2.636E+02	2.638E+02	1.122E+04	6.647E+00

Table 53: Internal thermodynamic properties of Ar^{3+} ΔE=500 cm^{-1}

T(K)	Q_{int}	$\ln(Q_{int})$	E_{int}/RT	$C_{p,int}/R$
50	$4.000E+00$	$1.386E+00$	$1.708E-261$	$1.037E-258$
100	$4.000E+00$	$1.386E+00$	$6.180E-130$	$1.877E-127$
150	$4.000E+00$	$1.386E+00$	$4.058E-86$	$8.225E-84$
200	$4.000E+00$	$1.386E+00$	$3.110E-64$	$4.729E-62$
298.15	$4.000E+00$	$1.386E+00$	$1.162E-42$	$1.185E-40$
300	$4.000E+00$	$1.386E+00$	$2.166E-42$	$2.197E-40$
400	$4.000E+00$	$1.386E+00$	$1.675E-31$	$1.275E-29$
500	$4.000E+00$	$1.386E+00$	$5.450E-25$	$3.318E-23$
600	$4.000E+00$	$1.386E+00$	$1.159E-20$	$5.878E-19$
700	$4.000E+00$	$1.386E+00$	$1.396E-17$	$6.071E-16$
800	$4.000E+00$	$1.386E+00$	$2.805E-15$	$1.067E-13$
900	$4.000E+00$	$1.386E+00$	$1.711E-13$	$5.787E-12$
1000	$4.000E+00$	$1.386E+00$	$4.536E-12$	$1.381E-10$
2000	$4.000E+00$	$1.386E+00$	$9.282E-06$	$1.413E-04$
3000	$4.000E+00$	$1.386E+00$	$9.915E-04$	$1.007E-02$
4000	$4.005E+00$	$1.388E+00$	$9.450E-03$	$7.218E-02$
5000	$4.023E+00$	$1.392E+00$	$3.491E-02$	$2.139E-01$
6000	$4.064E+00$	$1.402E+00$	$8.084E-02$	$4.131E-01$
7000	$4.134E+00$	$1.419E+00$	$1.436E-01$	$6.266E-01$
8000	$4.233E+00$	$1.443E+00$	$2.163E-01$	$8.178E-01$
9000	$4.362E+00$	$1.473E+00$	$2.918E-01$	$9.657E-01$
10000	$4.515E+00$	$1.507E+00$	$3.645E-01$	$1.064E+00$
11000	$4.689E+00$	$1.545E+00$	$4.308E-01$	$1.116E+00$
12000	$4.881E+00$	$1.585E+00$	$4.888E-01$	$1.131E+00$
13000	$5.086E+00$	$1.626E+00$	$5.378E-01$	$1.117E+00$
14000	$5.301E+00$	$1.668E+00$	$5.780E-01$	$1.084E+00$
15000	$5.523E+00$	$1.709E+00$	$6.103E-01$	$1.038E+00$
16000	$5.749E+00$	$1.749E+00$	$6.354E-01$	$9.867E-01$
17000	$5.979E+00$	$1.788E+00$	$6.545E-01$	$9.330E-01$
18000	$6.209E+00$	$1.826E+00$	$6.685E-01$	$8.801E-01$
19000	$6.440E+00$	$1.862E+00$	$6.783E-01$	$8.301E-01$
20000	$6.669E+00$	$1.897E+00$	$6.847E-01$	$7.843E-01$
21000	$6.896E+00$	$1.931E+00$	$6.885E-01$	$7.436E-01$
22000	$7.121E+00$	$1.963E+00$	$6.902E-01$	$7.084E-01$
23000	$7.343E+00$	$1.994E+00$	$6.903E-01$	$6.790E-01$
24000	$7.561E+00$	$2.023E+00$	$6.893E-01$	$6.556E-01$
25000	$7.777E+00$	$2.051E+00$	$6.876E-01$	$6.383E-01$
26000	$7.989E+00$	$2.078E+00$	$6.855E-01$	$6.269E-01$
27000	$8.198E+00$	$2.104E+00$	$6.832E-01$	$6.216E-01$
28000	$8.404E+00$	$2.129E+00$	$6.810E-01$	$6.225E-01$
29000	$8.607E+00$	$2.153E+00$	$6.791E-01$	$6.298E-01$
30000	$8.807E+00$	$2.176E+00$	$6.777E-01$	$6.443E-01$
32000	$9.201E+00$	$2.219E+00$	$6.771E-01$	$6.997E-01$
34000	$9.587E+00$	$2.260E+00$	$6.813E-01$	$8.076E-01$
36000	$9.971E+00$	$2.300E+00$	$6.933E-01$	$1.008E+00$
38000	$1.036E+01$	$2.338E+00$	$7.185E-01$	$1.373E+00$
40000	$1.076E+01$	$2.376E+00$	$7.659E-01$	$2.020E+00$
42000	$1.119E+01$	$2.415E+00$	$8.496E-01$	$3.118E+00$
44000	$1.167E+01$	$2.457E+00$	$9.897E-01$	$4.871E+00$
46000	$1.225E+01$	$2.506E+00$	$1.212E+00$	$7.483E+00$
48000	$1.299E+01$	$2.564E+00$	$1.544E+00$	$1.106E+01$
50000	$1.396E+01$	$2.636E+00$	$2.011E+00$	$1.548E+01$

Table 54: Total thermodynamic properties of Ar^{3+} ΔE=500 cm^{-1}

T [K]	C_p [J/mol/K]	S^0 [J/mol/K]	$H^0(T)-H^0(0)$ [KJ/mol]	$H^0(T)-H^0(298)$ [KJ/mol]	$-(G^0-H^0(0))/T$ [J/mol/K]	$-(G^0-H^0(298))/T$ [J/mol/K]	ΔH_f [KJ/mol]	$Log(K_p)$
50	2.079E+01	1.293E+02	1.039E+00	-5.158E+00	1.085E+02	2.324E+02	8.120E+03	-8.484E+03
100	2.079E+01	1.437E+02	2.079E+00	-4.119E+00	1.229E+02	1.848E+02	8.123E+03	-4.243E+03
150	2.079E+01	1.521E+02	3.118E+00	-3.079E+00	1.313E+02	1.726E+02	8.126E+03	-2.828E+03
200	2.079E+01	1.581E+02	4.157E+00	-2.040E+00	1.373E+02	1.683E+02	8.129E+03	-2.120E+03
298.15	2.079E+01	1.664E+02	6.197E+00	0.000E+00	1.456E+02	1.664E+02	8.135E+03	-1.421E+03
300	2.079E+01	1.665E+02	6.236E+00	3.848E-02	1.457E+02	1.664E+02	8.136E+03	-1.413E+03
400	2.079E+01	1.725E+02	8.315E+00	2.117E+00	1.517E+02	1.672E+02	8.142E+03	-1.058E+03
500	2.079E+01	1.771E+02	1.039E+01	4.196E+00	1.563E+02	1.687E+02	8.148E+03	-8.456E+02
600	2.079E+01	1.809E+02	1.247E+01	6.274E+00	1.601E+02	1.704E+02	8.154E+03	-7.037E+02
700	2.079E+01	1.841E+02	1.455E+01	8.353E+00	1.633E+02	1.722E+02	8.160E+03	-6.022E+02
800	2.079E+01	1.869E+02	1.663E+01	1.043E+01	1.661E+02	1.738E+02	8.167E+03	-5.261E+02
900	2.079E+01	1.893E+02	1.871E+01	1.251E+01	1.686E+02	1.754E+02	8.173E+03	-4.668E+02
1000	2.079E+01	1.915E+02	2.079E+01	1.459E+01	1.707E+02	1.769E+02	8.179E+03	-4.194E+02
2000	2.079E+01	2.059E+02	4.157E+01	3.538E+01	1.852E+02	1.882E+02	8.242E+03	-2.052E+02
3000	2.087E+01	2.144E+02	6.238E+01	5.619E+01	1.936E+02	1.956E+02	8.304E+03	-1.332E+02
4000	2.139E+01	2.204E+02	8.346E+01	7.726E+01	1.996E+02	2.011E+02	8.366E+03	-9.690E+01
5000	2.257E+01	2.253E+02	1.054E+02	9.919E+01	2.042E+02	2.055E+02	8.430E+03	-7.497E+01
6000	2.422E+01	2.296E+02	1.288E+02	1.225E+02	2.081E+02	2.092E+02	8.495E+03	-6.024E+01
7000	2.600E+01	2.334E+02	1.539E+02	1.477E+02	2.115E+02	2.123E+02	8.562E+03	-4.964E+01
8000	2.759E+01	2.370E+02	1.807E+02	1.745E+02	2.144E+02	2.152E+02	8.630E+03	-4.162E+01
9000	2.882E+01	2.403E+02	2.089E+02	2.027E+02	2.171E+02	2.178E+02	8.700E+03	-3.534E+01
10000	2.963E+01	2.434E+02	2.382E+02	2.320E+02	2.196E+02	2.202E+02	8.770E+03	-3.027E+01
11000	3.007E+01	2.463E+02	2.681E+02	2.619E+02	2.219E+02	2.225E+02	8.841E+03	-2.609E+01
12000	3.019E+01	2.489E+02	2.982E+02	2.920E+02	2.241E+02	2.246E+02	8.910E+03	-2.258E+01
13000	3.007E+01	2.513E+02	3.284E+02	3.221E+02	2.261E+02	2.265E+02	8.973E+03	-1.958E+01
14000	2.980E+01	2.535E+02	3.583E+02	3.521E+02	2.279E+02	2.284E+02	9.024E+03	-1.700E+01
15000	2.942E+01	2.556E+02	3.879E+02	3.817E+02	2.297E+02	2.301E+02	9.052E+03	-1.475E+01
16000	2.899E+01	2.575E+02	4.171E+02	4.109E+02	2.314E+02	2.318E+02	9.048E+03	-1.278E+01
17000	2.854E+01	2.592E+02	4.459E+02	4.397E+02	2.330E+02	2.333E+02	9.003E+03	-1.105E+01
18000	2.810E+01	2.608E+02	4.742E+02	4.680E+02	2.345E+02	2.348E+02	8.920E+03	-9.518E+00
19000	2.769E+01	2.623E+02	5.021E+02	4.959E+02	2.359E+02	2.362E+02	8.815E+03	-8.163E+00
20000	2.731E+01	2.637E+02	5.296E+02	5.234E+02	2.373E+02	2.376E+02	8.709E+03	-6.959E+00
21000	2.697E+01	2.651E+02	5.567E+02	5.505E+02	2.386E+02	2.388E+02	8.622E+03	-5.881E+00
22000	2.668E+01	2.663E+02	5.835E+02	5.774E+02	2.398E+02	2.401E+02	8.560E+03	-4.910E+00
23000	2.643E+01	2.675E+02	6.101E+02	6.039E+02	2.410E+02	2.412E+02	8.526E+03	-4.029E+00
24000	2.624E+01	2.686E+02	6.364E+02	6.302E+02	2.421E+02	2.423E+02	8.516E+03	-3.222E+00
25000	2.609E+01	2.697E+02	6.626E+02	6.564E+02	2.432E+02	2.434E+02	8.525E+03	-2.481E+00
26000	2.600E+01	2.707E+02	6.886E+02	6.824E+02	2.442E+02	2.444E+02	8.549E+03	-1.795E+00
27000	2.595E+01	2.717E+02	7.146E+02	7.084E+02	2.452E+02	2.454E+02	8.583E+03	-1.158E+00
28000	2.596E+01	2.726E+02	7.405E+02	7.344E+02	2.462E+02	2.464E+02	8.626E+03	-5.631E-01
29000	2.602E+01	2.735E+02	7.665E+02	7.603E+02	2.471E+02	2.473E+02	8.674E+03	-6.783E-03
30000	2.614E+01	2.744E+02	7.926E+02	7.864E+02	2.480E+02	2.482E+02	8.727E+03	5.155E-01
32000	2.660E+01	2.761E+02	8.453E+02	8.391E+02	2.497E+02	2.499E+02	8.842E+03	1.471E+00
34000	2.750E+01	2.778E+02	8.993E+02	8.931E+02	2.513E+02	2.515E+02	8.965E+03	2.326E+00
36000	2.916E+01	2.794E+02	9.558E+02	9.496E+02	2.528E+02	2.530E+02	9.096E+03	3.096E+00
38000	3.220E+01	2.810E+02	1.017E+03	1.011E+03	2.543E+02	2.544E+02	9.234E+03	3.796E+00
40000	3.759E+01	2.828E+02	1.086E+03	1.080E+03	2.557E+02	2.558E+02	9.382E+03	4.436E+00
42000	4.671E+01	2.848E+02	1.170E+03	1.164E+03	2.570E+02	2.571E+02	9.546E+03	5.024E+00
44000	6.129E+01	2.873E+02	1.277E+03	1.270E+03	2.583E+02	2.584E+02	9.734E+03	5.569E+00
46000	8.300E+01	2.905E+02	1.420E+03	1.413E+03	2.596E+02	2.598E+02	9.958E+03	6.077E+00
48000	1.127E+02	2.946E+02	1.614E+03	1.608E+03	2.610E+02	2.611E+02	1.023E+04	6.554E+00
50000	1.495E+02	3.000E+02	1.875E+03	1.869E+03	2.624E+02	2.626E+02	1.058E+04	7.007E+00

Table 55: Internal thermodynamic properties of Ar^{3+} ΔE=1000 cm^{-1}

T(K)	Q_{int}	$\ln(Q_{int})$	E_{int}/RT	$C_{p,int}/R$
50	$4.000E+00$	$1.386E+00$	$1.708E-261$	$1.037E-258$
100	$4.000E+00$	$1.386E+00$	$6.180E-130$	$1.877E-127$
150	$4.000E+00$	$1.386E+00$	$4.058E-86$	$8.225E-84$
200	$4.000E+00$	$1.386E+00$	$3.110E-64$	$4.729E-62$
298.15	$4.000E+00$	$1.386E+00$	$1.162E-42$	$1.185E-40$
300	$4.000E+00$	$1.386E+00$	$2.166E-42$	$2.197E-40$
400	$4.000E+00$	$1.386E+00$	$1.675E-31$	$1.275E-29$
500	$4.000E+00$	$1.386E+00$	$5.450E-25$	$3.318E-23$
600	$4.000E+00$	$1.386E+00$	$1.159E-20$	$5.878E-19$
700	$4.000E+00$	$1.386E+00$	$1.396E-17$	$6.071E-16$
800	$4.000E+00$	$1.386E+00$	$2.805E-15$	$1.067E-13$
900	$4.000E+00$	$1.386E+00$	$1.711E-13$	$5.787E-12$
1000	$4.000E+00$	$1.386E+00$	$4.536E-12$	$1.381E-10$
2000	$4.000E+00$	$1.386E+00$	$9.282E-06$	$1.413E-04$
3000	$4.000E+00$	$1.386E+00$	$9.915E-04$	$1.007E-02$
4000	$4.005E+00$	$1.388E+00$	$9.450E-03$	$7.218E-02$
5000	$4.023E+00$	$1.392E+00$	$3.491E-02$	$2.139E-01$
6000	$4.064E+00$	$1.402E+00$	$8.084E-02$	$4.131E-01$
7000	$4.134E+00$	$1.419E+00$	$1.436E-01$	$6.266E-01$
8000	$4.233E+00$	$1.443E+00$	$2.163E-01$	$8.178E-01$
9000	$4.362E+00$	$1.473E+00$	$2.918E-01$	$9.657E-01$
10000	$4.515E+00$	$1.507E+00$	$3.645E-01$	$1.064E+00$
11000	$4.689E+00$	$1.545E+00$	$4.308E-01$	$1.116E+00$
12000	$4.881E+00$	$1.585E+00$	$4.888E-01$	$1.131E+00$
13000	$5.086E+00$	$1.626E+00$	$5.378E-01$	$1.117E+00$
14000	$5.301E+00$	$1.668E+00$	$5.780E-01$	$1.084E+00$
15000	$5.523E+00$	$1.709E+00$	$6.103E-01$	$1.038E+00$
16000	$5.749E+00$	$1.749E+00$	$6.354E-01$	$9.867E-01$
17000	$5.979E+00$	$1.788E+00$	$6.545E-01$	$9.330E-01$
18000	$6.209E+00$	$1.826E+00$	$6.685E-01$	$8.801E-01$
19000	$6.440E+00$	$1.862E+00$	$6.783E-01$	$8.301E-01$
20000	$6.669E+00$	$1.897E+00$	$6.847E-01$	$7.843E-01$
21000	$6.896E+00$	$1.931E+00$	$6.885E-01$	$7.436E-01$
22000	$7.121E+00$	$1.963E+00$	$6.902E-01$	$7.084E-01$
23000	$7.343E+00$	$1.994E+00$	$6.903E-01$	$6.790E-01$
24000	$7.561E+00$	$2.023E+00$	$6.893E-01$	$6.556E-01$
25000	$7.777E+00$	$2.051E+00$	$6.876E-01$	$6.382E-01$
26000	$7.989E+00$	$2.078E+00$	$6.855E-01$	$6.267E-01$
27000	$8.198E+00$	$2.104E+00$	$6.832E-01$	$6.211E-01$
28000	$8.404E+00$	$2.129E+00$	$6.809E-01$	$6.214E-01$
29000	$8.607E+00$	$2.153E+00$	$6.790E-01$	$6.275E-01$
30000	$8.807E+00$	$2.176E+00$	$6.774E-01$	$6.397E-01$
32000	$9.200E+00$	$2.219E+00$	$6.763E-01$	$6.834E-01$
34000	$9.586E+00$	$2.260E+00$	$6.788E-01$	$7.584E-01$
36000	$9.967E+00$	$2.299E+00$	$6.862E-01$	$8.779E-01$
38000	$1.035E+01$	$2.337E+00$	$7.009E-01$	$1.067E+00$
40000	$1.073E+01$	$2.373E+00$	$7.261E-01$	$1.366E+00$
42000	$1.113E+01$	$2.410E+00$	$7.670E-01$	$1.837E+00$
44000	$1.155E+01$	$2.447E+00$	$8.310E-01$	$2.561E+00$
46000	$1.201E+01$	$2.486E+00$	$9.281E-01$	$3.633E+00$
48000	$1.253E+01$	$2.528E+00$	$1.071E+00$	$5.149E+00$
50000	$1.314E+01$	$2.575E+00$	$1.273E+00$	$7.177E+00$

Table 56: Total thermodynamic properties of Ar^{3+} ΔE=1000 cm^{-1}

T [K]	C_p [J/mol/K]	S^0 [J/mol/K]	$H^0(T)-H^0(0)$ [KJ/mol]	$H^0(T)-H^0(298)$ [KJ/mol]	$-(G^0-H^0(0))/T$ [J/mol/K]	$-(G^0-H^0(298))/T$ [J/mol/K]	ΔH_f [KJ/mol]	$Log(K_p)$
50	2.079E+01	1.293E+02	1.039E+00	-5.158E+00	1.085E+02	2.324E+02	8.120E+03	-8.484E+03
100	2.079E+01	1.437E+02	2.079E+00	-4.119E+00	1.229E+02	1.848E+02	8.123E+03	-4.243E+03
150	2.079E+01	1.521E+02	3.118E+00	-3.079E+00	1.313E+02	1.726E+02	8.126E+03	-2.828E+03
200	2.079E+01	1.581E+02	4.157E+00	-2.040E+00	1.373E+02	1.683E+02	8.129E+03	-2.120E+03
298.15	2.079E+01	1.664E+02	6.197E+00	0.000E+00	1.456E+02	1.664E+02	8.135E+03	-1.421E+03
300	2.079E+01	1.665E+02	6.236E+00	3.848E-02	1.457E+02	1.664E+02	8.136E+03	-1.413E+03
400	2.079E+01	1.725E+02	8.315E+00	2.117E+00	1.517E+02	1.672E+02	8.142E+03	-1.058E+03
500	2.079E+01	1.771E+02	1.039E+01	4.196E+00	1.563E+02	1.687E+02	8.148E+03	-8.456E+02
600	2.079E+01	1.809E+02	1.247E+01	6.274E+00	1.601E+02	1.704E+02	8.154E+03	-7.037E+02
700	2.079E+01	1.841E+02	1.455E+01	8.353E+00	1.633E+02	1.722E+02	8.160E+03	-6.022E+02
800	2.079E+01	1.869E+02	1.663E+01	1.043E+01	1.661E+02	1.738E+02	8.167E+03	-5.261E+02
900	2.079E+01	1.893E+02	1.871E+01	1.251E+01	1.686E+02	1.754E+02	8.173E+03	-4.668E+02
1000	2.079E+01	1.915E+02	2.079E+01	1.459E+01	1.707E+02	1.769E+02	8.179E+03	-4.194E+02
2000	2.079E+01	2.059E+02	4.157E+01	3.538E+01	1.852E+02	1.882E+02	8.242E+03	-2.052E+02
3000	2.087E+01	2.144E+02	6.238E+01	5.619E+01	1.936E+02	1.956E+02	8.304E+03	-1.332E+02
4000	2.139E+01	2.204E+02	8.346E+01	7.726E+01	1.996E+02	2.011E+02	8.366E+03	-9.690E+01
5000	2.257E+01	2.253E+02	1.054E+02	9.919E+01	2.042E+02	2.055E+02	8.430E+03	-7.497E+01
6000	2.422E+01	2.296E+02	1.288E+02	1.225E+02	2.081E+02	2.092E+02	8.495E+03	-6.024E+01
7000	2.600E+01	2.334E+02	1.539E+02	1.477E+02	2.115E+02	2.123E+02	8.562E+03	-4.964E+01
8000	2.759E+01	2.370E+02	1.807E+02	1.745E+02	2.144E+02	2.152E+02	8.630E+03	-4.162E+01
9000	2.882E+01	2.403E+02	2.089E+02	2.027E+02	2.171E+02	2.178E+02	8.700E+03	-3.534E+01
10000	2.963E+01	2.434E+02	2.382E+02	2.320E+02	2.196E+02	2.202E+02	8.770E+03	-3.027E+01
11000	3.007E+01	2.463E+02	2.681E+02	2.619E+02	2.219E+02	2.225E+02	8.842E+03	-2.609E+01
12000	3.019E+01	2.489E+02	2.982E+02	2.920E+02	2.241E+02	2.246E+02	8.912E+03	-2.258E+01
13000	3.007E+01	2.513E+02	3.284E+02	3.221E+02	2.261E+02	2.265E+02	8.979E+03	-1.958E+01
14000	2.980E+01	2.535E+02	3.583E+02	3.521E+02	2.279E+02	2.284E+02	9.041E+03	-1.700E+01
15000	2.942E+01	2.556E+02	3.879E+02	3.817E+02	2.297E+02	2.301E+02	9.092E+03	-1.474E+01
16000	2.899E+01	2.575E+02	4.171E+02	4.109E+02	2.314E+02	2.318E+02	9.126E+03	-1.276E+01
17000	2.854E+01	2.592E+02	4.459E+02	4.397E+02	2.330E+02	2.333E+02	9.137E+03	-1.100E+01
18000	2.810E+01	2.608E+02	4.742E+02	4.680E+02	2.345E+02	2.348E+02	9.119E+03	-9.445E+00
19000	2.769E+01	2.623E+02	5.021E+02	4.959E+02	2.359E+02	2.362E+02	9.073E+03	-8.056E+00
20000	2.731E+01	2.637E+02	5.296E+02	5.234E+02	2.373E+02	2.376E+02	9.007E+03	-6.813E+00
21000	2.697E+01	2.651E+02	5.567E+02	5.505E+02	2.386E+02	2.388E+02	8.932E+03	-5.697E+00
22000	2.668E+01	2.663E+02	5.835E+02	5.774E+02	2.398E+02	2.401E+02	8.860E+03	-4.691E+00
23000	2.643E+01	2.675E+02	6.101E+02	6.039E+02	2.410E+02	2.412E+02	8.801E+03	-3.780E+00
24000	2.624E+01	2.686E+02	6.364E+02	6.302E+02	2.421E+02	2.423E+02	8.759E+03	-2.949E+00
25000	2.609E+01	2.697E+02	6.626E+02	6.564E+02	2.432E+02	2.434E+02	8.736E+03	-2.188E+00
26000	2.600E+01	2.707E+02	6.886E+02	6.824E+02	2.442E+02	2.444E+02	8.730E+03	-1.486E+00
27000	2.595E+01	2.717E+02	7.146E+02	7.084E+02	2.452E+02	2.454E+02	8.738E+03	-8.363E-01
28000	2.595E+01	2.726E+02	7.405E+02	7.344E+02	2.462E+02	2.464E+02	8.759E+03	-2.319E-01
29000	2.600E+01	2.735E+02	7.665E+02	7.603E+02	2.471E+02	2.473E+02	8.789E+03	3.325E-01
30000	2.611E+01	2.744E+02	7.926E+02	7.864E+02	2.480E+02	2.482E+02	8.827E+03	8.612E-01
32000	2.647E+01	2.761E+02	8.451E+02	8.389E+02	2.497E+02	2.499E+02	8.919E+03	1.827E+00
34000	2.709E+01	2.777E+02	8.986E+02	8.924E+02	2.513E+02	2.515E+02	9.027E+03	2.688E+00
36000	2.809E+01	2.793E+02	9.537E+02	9.475E+02	2.528E+02	2.530E+02	9.146E+03	3.463E+00
38000	2.966E+01	2.809E+02	1.011E+03	1.005E+03	2.543E+02	2.544E+02	9.274E+03	4.167E+00
40000	3.215E+01	2.824E+02	1.073E+03	1.067E+03	2.556E+02	2.558E+02	9.408E+03	4.808E+00
42000	3.606E+01	2.841E+02	1.141E+03	1.135E+03	2.569E+02	2.571E+02	9.552E+03	5.398E+00
44000	4.208E+01	2.859E+02	1.219E+03	1.212E+03	2.582E+02	2.584E+02	9.708E+03	5.942E+00
46000	5.100E+01	2.880E+02	1.311E+03	1.305E+03	2.595E+02	2.596E+02	9.879E+03	6.447E+00
48000	6.360E+01	2.904E+02	1.425E+03	1.419E+03	2.607E+02	2.608E+02	1.007E+04	6.919E+00
50000	8.046E+01	2.933E+02	1.568E+03	1.562E+03	2.619E+02	2.621E+02	1.030E+04	7.362E+00

Table 57: Internal thermodynamic properties of Ar^{4+} ΔE=250 cm^{-1}

T(K)	Q_{int}	$\ln(Q_{int})$	E_{int}/RT	$C_{p,int}/R$
50	$1.000E+00$	$8.205E-10$	$1.807E-08$	$3.978E-07$
100	$1.000E+00$	$4.961E-05$	$5.462E-04$	$6.013E-03$
150	$1.002E+00$	$1.945E-03$	$1.427E-02$	$1.045E-01$
200	$1.012E+00$	$1.213E-02$	$6.638E-02$	$3.613E-01$
298.15	$1.075E+00$	$7.231E-02$	$2.592E-01$	$9.055E-01$
300	$1.077E+00$	$7.393E-02$	$2.632E-01$	$9.130E-01$
400	$1.195E+00$	$1.779E-01$	$4.614E-01$	$1.151E+00$
500	$1.346E+00$	$2.974E-01$	$6.058E-01$	$1.197E+00$
600	$1.517E+00$	$4.170E-01$	$7.027E-01$	$1.170E+00$
700	$1.700E+00$	$5.304E-01$	$7.655E-01$	$1.110E+00$
800	$1.888E+00$	$6.354E-01$	$8.038E-01$	$1.032E+00$
900	$2.078E+00$	$7.314E-01$	$8.243E-01$	$9.443E-01$
1000	$2.268E+00$	$8.187E-01$	$8.319E-01$	$8.556E-01$
2000	$3.892E+00$	$1.359E+00$	$6.805E-01$	$3.089E-01$
3000	$4.970E+00$	$1.603E+00$	$5.266E-01$	$1.638E-01$
4000	$5.703E+00$	$1.741E+00$	$4.330E-01$	$1.536E-01$
5000	$6.242E+00$	$1.831E+00$	$3.803E-01$	$1.886E-01$
6000	$6.671E+00$	$1.898E+00$	$3.518E-01$	$2.291E-01$
7000	$7.034E+00$	$1.951E+00$	$3.366E-01$	$2.606E-01$
8000	$7.353E+00$	$1.995E+00$	$3.285E-01$	$2.802E-01$
9000	$7.641E+00$	$2.034E+00$	$3.237E-01$	$2.897E-01$
10000	$7.905E+00$	$2.067E+00$	$3.205E-01$	$2.917E-01$
11000	$8.149E+00$	$2.098E+00$	$3.177E-01$	$2.888E-01$
12000	$8.377E+00$	$2.125E+00$	$3.151E-01$	$2.830E-01$
13000	$8.590E+00$	$2.151E+00$	$3.124E-01$	$2.760E-01$
14000	$8.790E+00$	$2.174E+00$	$3.095E-01$	$2.689E-01$
15000	$8.979E+00$	$2.195E+00$	$3.066E-01$	$2.625E-01$
16000	$9.157E+00$	$2.215E+00$	$3.037E-01$	$2.575E-01$
17000	$9.327E+00$	$2.233E+00$	$3.008E-01$	$2.543E-01$
18000	$9.488E+00$	$2.250E+00$	$2.982E-01$	$2.533E-01$
19000	$9.641E+00$	$2.266E+00$	$2.959E-01$	$2.546E-01$
20000	$9.788E+00$	$2.281E+00$	$2.939E-01$	$2.584E-01$
21000	$9.929E+00$	$2.295E+00$	$2.924E-01$	$2.648E-01$
22000	$1.006E+01$	$2.309E+00$	$2.913E-01$	$2.738E-01$
23000	$1.020E+01$	$2.322E+00$	$2.908E-01$	$2.854E-01$
24000	$1.032E+01$	$2.334E+00$	$2.908E-01$	$2.995E-01$
25000	$1.045E+01$	$2.346E+00$	$2.915E-01$	$3.160E-01$
26000	$1.057E+01$	$2.358E+00$	$2.928E-01$	$3.348E-01$
27000	$1.068E+01$	$2.369E+00$	$2.947E-01$	$3.559E-01$
28000	$1.080E+01$	$2.380E+00$	$2.973E-01$	$3.791E-01$
29000	$1.091E+01$	$2.390E+00$	$3.006E-01$	$4.043E-01$
30000	$1.103E+01$	$2.400E+00$	$3.045E-01$	$4.313E-01$
32000	$1.125E+01$	$2.420E+00$	$3.142E-01$	$4.907E-01$
34000	$1.147E+01$	$2.440E+00$	$3.265E-01$	$5.570E-01$
36000	$1.169E+01$	$2.459E+00$	$3.414E-01$	$6.316E-01$
38000	$1.191E+01$	$2.478E+00$	$3.589E-01$	$7.196E-01$
40000	$1.214E+01$	$2.497E+00$	$3.796E-01$	$8.340E-01$
42000	$1.237E+01$	$2.516E+00$	$4.050E-01$	$1.002E+00$
44000	$1.262E+01$	$2.535E+00$	$4.377E-01$	$1.273E+00$
46000	$1.288E+01$	$2.556E+00$	$4.832E-01$	$1.732E+00$
48000	$1.316E+01$	$2.578E+00$	$5.500E-01$	$2.506E+00$
50000	$1.349E+01$	$2.602E+00$	$6.516E-01$	$3.774E+00$

Table 58: Total thermodynamic properties of Ar^{4+} ΔE=250 cm^{-1}

T [K]	C_p [J/mol/K]	S^0 [J/mol/K]	$H^0(T)-H^0(0)$ [KJ/mol]	$H^0(T)-H^0(298)$ [KJ/mol]	$-(G^0-H^0(0))/T$ [J/mol/K]	$-(G^0-H^0(298))/T$ [J/mol/K]	ΔH_f [KJ/mol]	$Log(K_p)$
50	2.079E+01	1.177E+02	1.039E+00	-5.801E+00	9.694E+01	2.337E+02	1.388E+04	-1.450E+04
100	2.084E+01	1.321E+02	2.079E+00	-4.761E+00	1.113E+02	1.798E+02	1.388E+04	-7.252E+03
150	2.166E+01	1.407E+02	3.136E+00	-3.704E+00	1.198E+02	1.654E+02	1.389E+04	-4.835E+03
200	2.379E+01	1.472E+02	4.268E+00	-2.572E+00	1.259E+02	1.601E+02	1.389E+04	-3.626E+03
298.15	2.832E+01	1.576E+02	6.840E+00	0.000E+00	1.347E+02	1.576E+02	1.390E+04	-2.431E+03
300	2.838E+01	1.578E+02	6.892E+00	5.240E-02	1.348E+02	1.576E+02	1.390E+04	-2.416E+03
400	3.036E+01	1.663E+02	9.849E+00	3.009E+00	1.417E+02	1.588E+02	1.391E+04	-1.810E+03
500	3.074E+01	1.731E+02	1.291E+01	6.072E+00	1.473E+02	1.610E+02	1.392E+04	-1.447E+03
600	3.052E+01	1.787E+02	1.598E+01	9.137E+00	1.521E+02	1.635E+02	1.393E+04	-1.205E+03
700	3.002E+01	1.834E+02	1.901E+01	1.217E+01	1.562E+02	1.660E+02	1.394E+04	-1.031E+03
800	2.936E+01	1.873E+02	2.198E+01	1.514E+01	1.599E+02	1.684E+02	1.395E+04	-9.014E+02
900	2.864E+01	1.908E+02	2.488E+01	1.804E+01	1.631E+02	1.707E+02	1.396E+04	-8.001E+02
1000	2.790E+01	1.937E+02	2.770E+01	2.086E+01	1.660E+02	1.729E+02	1.397E+04	-7.191E+02
2000	2.336E+01	2.114E+02	5.289E+01	4.605E+01	1.849E+02	1.883E+02	1.405E+04	-3.535E+02
3000	2.215E+01	2.206E+02	7.549E+01	6.865E+01	1.954E+02	1.977E+02	1.414E+04	-2.308E+02
4000	2.206E+01	2.269E+02	9.755E+01	9.071E+01	2.025E+02	2.042E+02	1.422E+04	-1.691E+02
5000	2.235E+01	2.318E+02	1.197E+02	1.129E+02	2.079E+02	2.093E+02	1.431E+04	-1.319E+02
6000	2.269E+01	2.359E+02	1.423E+02	1.354E+02	2.122E+02	2.134E+02	1.439E+04	-1.069E+02
7000	2.295E+01	2.395E+02	1.651E+02	1.583E+02	2.159E+02	2.169E+02	1.448E+04	-8.894E+01
8000	2.312E+01	2.425E+02	1.881E+02	1.813E+02	2.190E+02	2.199E+02	1.456E+04	-7.540E+01
9000	2.320E+01	2.453E+02	2.113E+02	2.045E+02	2.218E+02	2.226E+02	1.465E+04	-6.481E+01
10000	2.321E+01	2.477E+02	2.345E+02	2.277E+02	2.243E+02	2.249E+02	1.473E+04	-5.628E+01
11000	2.319E+01	2.499E+02	2.577E+02	2.509E+02	2.265E+02	2.271E+02	1.482E+04	-4.927E+01
12000	2.314E+01	2.519E+02	2.809E+02	2.740E+02	2.285E+02	2.291E+02	1.490E+04	-4.339E+01
13000	2.308E+01	2.538E+02	3.040E+02	2.971E+02	2.304E+02	2.309E+02	1.496E+04	-3.839E+01
14000	2.302E+01	2.555E+02	3.270E+02	3.202E+02	2.321E+02	2.326E+02	1.500E+04	-3.409E+01
15000	2.297E+01	2.571E+02	3.500E+02	3.432E+02	2.338E+02	2.342E+02	1.499E+04	-3.036E+01
16000	2.293E+01	2.586E+02	3.730E+02	3.661E+02	2.353E+02	2.357E+02	1.492E+04	-2.711E+01
17000	2.290E+01	2.600E+02	3.959E+02	3.891E+02	2.367E+02	2.371E+02	1.480E+04	-2.425E+01
18000	2.289E+01	2.613E+02	4.188E+02	4.119E+02	2.380E+02	2.384E+02	1.467E+04	-2.174E+01
19000	2.290E+01	2.625E+02	4.417E+02	4.348E+02	2.393E+02	2.396E+02	1.456E+04	-1.950E+01
20000	2.293E+01	2.637E+02	4.646E+02	4.578E+02	2.404E+02	2.408E+02	1.449E+04	-1.751E+01
21000	2.299E+01	2.648E+02	4.876E+02	4.807E+02	2.416E+02	2.419E+02	1.446E+04	-1.571E+01
22000	2.306E+01	2.659E+02	5.106E+02	5.037E+02	2.427E+02	2.430E+02	1.446E+04	-1.407E+01
23000	2.316E+01	2.669E+02	5.337E+02	5.269E+02	2.437E+02	2.440E+02	1.449E+04	-1.258E+01
24000	2.328E+01	2.679E+02	5.569E+02	5.501E+02	2.447E+02	2.450E+02	1.454E+04	-1.121E+01
25000	2.341E+01	2.688E+02	5.802E+02	5.734E+02	2.456E+02	2.459E+02	1.459E+04	-9.940E+00
26000	2.357E+01	2.698E+02	6.037E+02	5.969E+02	2.465E+02	2.468E+02	1.466E+04	-8.765E+00
27000	2.375E+01	2.706E+02	6.274E+02	6.206E+02	2.474E+02	2.477E+02	1.473E+04	-7.672E+00
28000	2.394E+01	2.715E+02	6.512E+02	6.444E+02	2.483E+02	2.485E+02	1.480E+04	-6.652E+00
29000	2.415E+01	2.724E+02	6.753E+02	6.684E+02	2.491E+02	2.493E+02	1.488E+04	-5.697E+00
30000	2.437E+01	2.732E+02	6.995E+02	6.927E+02	2.499E+02	2.501E+02	1.496E+04	-4.801E+00
32000	2.487E+01	2.748E+02	7.488E+02	7.419E+02	2.514E+02	2.516E+02	1.513E+04	-3.164E+00
34000	2.542E+01	2.763E+02	7.990E+02	7.922E+02	2.528E+02	2.530E+02	1.530E+04	-1.703E+00
36000	2.604E+01	2.778E+02	8.505E+02	8.436E+02	2.542E+02	2.543E+02	1.547E+04	-3.904E-01
38000	2.677E+01	2.792E+02	9.033E+02	8.964E+02	2.554E+02	2.556E+02	1.565E+04	7.976E-01
40000	2.772E+01	2.806E+02	9.577E+02	9.509E+02	2.566E+02	2.568E+02	1.582E+04	1.879E+00
42000	2.912E+01	2.820E+02	1.014E+03	1.008E+03	2.578E+02	2.580E+02	1.600E+04	2.868E+00
44000	3.137E+01	2.834E+02	1.075E+03	1.068E+03	2.589E+02	2.591E+02	1.619E+04	3.778E+00
46000	3.519E+01	2.849E+02	1.141E+03	1.134E+03	2.601E+02	2.602E+02	1.638E+04	4.619E+00
48000	4.162E+01	2.865E+02	1.217E+03	1.210E+03	2.611E+02	2.613E+02	1.658E+04	5.398E+00
50000	5.217E+01	2.884E+02	1.310E+03	1.303E+03	2.622E+02	2.623E+02	1.680E+04	6.124E+00

Table 59: Internal thermodynamic properties of Ar^{4+} ΔE=500 cm^{-1}

T(K)	Q_{int}	$\ln(Q_{int})$	E_{int}/RT	$C_{p,int}/R$
50	$1.000E+00$	$8.205E-10$	$1.807E-08$	$3.978E-07$
100	$1.000E+00$	$4.961E-05$	$5.462E-04$	$6.013E-03$
150	$1.002E+00$	$1.945E-03$	$1.427E-02$	$1.045E-01$
200	$1.012E+00$	$1.213E-02$	$6.638E-02$	$3.613E-01$
298.15	$1.075E+00$	$7.231E-02$	$2.592E-01$	$9.055E-01$
300	$1.077E+00$	$7.393E-02$	$2.632E-01$	$9.130E-01$
400	$1.195E+00$	$1.779E-01$	$4.614E-01$	$1.151E+00$
500	$1.346E+00$	$2.974E-01$	$6.058E-01$	$1.197E+00$
600	$1.517E+00$	$4.170E-01$	$7.027E-01$	$1.170E+00$
700	$1.700E+00$	$5.304E-01$	$7.655E-01$	$1.110E+00$
800	$1.888E+00$	$6.354E-01$	$8.038E-01$	$1.032E+00$
900	$2.078E+00$	$7.314E-01$	$8.243E-01$	$9.443E-01$
1000	$2.268E+00$	$8.187E-01$	$8.319E-01$	$8.556E-01$
2000	$3.892E+00$	$1.359E+00$	$6.805E-01$	$3.089E-01$
3000	$4.970E+00$	$1.603E+00$	$5.266E-01$	$1.638E-01$
4000	$5.703E+00$	$1.741E+00$	$4.330E-01$	$1.536E-01$
5000	$6.242E+00$	$1.831E+00$	$3.803E-01$	$1.886E-01$
6000	$6.671E+00$	$1.898E+00$	$3.518E-01$	$2.291E-01$
7000	$7.034E+00$	$1.951E+00$	$3.366E-01$	$2.606E-01$
8000	$7.353E+00$	$1.995E+00$	$3.285E-01$	$2.802E-01$
9000	$7.641E+00$	$2.034E+00$	$3.237E-01$	$2.897E-01$
10000	$7.905E+00$	$2.067E+00$	$3.205E-01$	$2.917E-01$
11000	$8.149E+00$	$2.098E+00$	$3.177E-01$	$2.888E-01$
12000	$8.377E+00$	$2.125E+00$	$3.151E-01$	$2.830E-01$
13000	$8.590E+00$	$2.151E+00$	$3.124E-01$	$2.760E-01$
14000	$8.790E+00$	$2.174E+00$	$3.095E-01$	$2.689E-01$
15000	$8.979E+00$	$2.195E+00$	$3.066E-01$	$2.625E-01$
16000	$9.157E+00$	$2.215E+00$	$3.037E-01$	$2.575E-01$
17000	$9.327E+00$	$2.233E+00$	$3.008E-01$	$2.543E-01$
18000	$9.488E+00$	$2.250E+00$	$2.982E-01$	$2.533E-01$
19000	$9.641E+00$	$2.266E+00$	$2.959E-01$	$2.546E-01$
20000	$9.788E+00$	$2.281E+00$	$2.939E-01$	$2.584E-01$
21000	$9.929E+00$	$2.295E+00$	$2.924E-01$	$2.648E-01$
22000	$1.006E+01$	$2.309E+00$	$2.913E-01$	$2.738E-01$
23000	$1.020E+01$	$2.322E+00$	$2.908E-01$	$2.854E-01$
24000	$1.032E+01$	$2.334E+00$	$2.908E-01$	$2.995E-01$
25000	$1.045E+01$	$2.346E+00$	$2.915E-01$	$3.160E-01$
26000	$1.057E+01$	$2.358E+00$	$2.928E-01$	$3.348E-01$
27000	$1.068E+01$	$2.369E+00$	$2.947E-01$	$3.559E-01$
28000	$1.080E+01$	$2.380E+00$	$2.973E-01$	$3.791E-01$
29000	$1.091E+01$	$2.390E+00$	$3.006E-01$	$4.042E-01$
30000	$1.103E+01$	$2.400E+00$	$3.045E-01$	$4.313E-01$
32000	$1.125E+01$	$2.420E+00$	$3.142E-01$	$4.905E-01$
34000	$1.147E+01$	$2.440E+00$	$3.265E-01$	$5.558E-01$
36000	$1.169E+01$	$2.459E+00$	$3.412E-01$	$6.272E-01$
38000	$1.191E+01$	$2.478E+00$	$3.583E-01$	$7.059E-01$
40000	$1.214E+01$	$2.496E+00$	$3.778E-01$	$7.961E-01$
42000	$1.237E+01$	$2.515E+00$	$4.003E-01$	$9.071E-01$
44000	$1.261E+01$	$2.535E+00$	$4.265E-01$	$1.057E+00$
46000	$1.286E+01$	$2.554E+00$	$4.584E-01$	$1.277E+00$
48000	$1.313E+01$	$2.575E+00$	$4.990E-01$	$1.614E+00$
50000	$1.341E+01$	$2.596E+00$	$5.533E-01$	$2.138E+00$

Table 60: Total thermodynamic properties of Ar^{4+} ΔE=500 cm^{-1}

T [K]	C_p [J/mol/K]	S^0 [J/mol/K]	$H^0(T)-H^0(0)$ [KJ/mol]	$H^0(T)-H^0(298)$ [KJ/mol]	$-(G^0-H^0(0))/T$ [J/mol/K]	$-(G^0-H^0(298))/T$ [J/mol/K]	ΔH_f [KJ/mol]	$Log(K_p)$
50	2.079E+01	1.177E+02	1.039E+00	-5.801E+00	9.694E+01	2.337E+02	1.388E+04	-1.450E+04
100	2.084E+01	1.321E+02	2.079E+00	-4.761E+00	1.113E+02	1.798E+02	1.388E+04	-7.252E+03
150	2.166E+01	1.407E+02	3.136E+00	-3.704E+00	1.198E+02	1.654E+02	1.389E+04	-4.835E+03
200	2.379E+01	1.472E+02	4.268E+00	-2.572E+00	1.259E+02	1.601E+02	1.389E+04	-3.626E+03
298.15	2.832E+01	1.576E+02	6.840E+00	0.000E+00	1.347E+02	1.576E+02	1.390E+04	-2.431E+03
300	2.838E+01	1.578E+02	6.892E+00	5.240E-02	1.348E+02	1.576E+02	1.390E+04	-2.416E+03
400	3.036E+01	1.663E+02	9.849E+00	3.009E+00	1.417E+02	1.588E+02	1.391E+04	-1.810E+03
500	3.074E+01	1.731E+02	1.291E+01	6.072E+00	1.473E+02	1.610E+02	1.392E+04	-1.447E+03
600	3.052E+01	1.787E+02	1.598E+01	9.137E+00	1.521E+02	1.635E+02	1.393E+04	-1.205E+03
700	3.002E+01	1.834E+02	1.901E+01	1.217E+01	1.562E+02	1.660E+02	1.394E+04	-1.031E+03
800	2.936E+01	1.873E+02	2.198E+01	1.514E+01	1.599E+02	1.684E+02	1.395E+04	-9.014E+02
900	2.864E+01	1.908E+02	2.488E+01	1.804E+01	1.631E+02	1.707E+02	1.396E+04	-8.001E+02
1000	2.790E+01	1.937E+02	2.770E+01	2.086E+01	1.660E+02	1.729E+02	1.397E+04	-7.191E+02
2000	2.336E+01	2.114E+02	5.289E+01	4.605E+01	1.849E+02	1.883E+02	1.405E+04	-3.535E+02
3000	2.215E+01	2.206E+02	7.549E+01	6.865E+01	1.954E+02	1.977E+02	1.414E+04	-2.308E+02
4000	2.206E+01	2.269E+02	9.755E+01	9.071E+01	2.025E+02	2.042E+02	1.422E+04	-1.691E+02
5000	2.235E+01	2.318E+02	1.197E+02	1.129E+02	2.079E+02	2.093E+02	1.431E+04	-1.319E+02
6000	2.269E+01	2.359E+02	1.423E+02	1.354E+02	2.122E+02	2.134E+02	1.439E+04	-1.069E+02
7000	2.295E+01	2.395E+02	1.651E+02	1.583E+02	2.159E+02	2.169E+02	1.448E+04	-8.894E+01
8000	2.312E+01	2.425E+02	1.881E+02	1.813E+02	2.190E+02	2.199E+02	1.456E+04	-7.540E+01
9000	2.320E+01	2.453E+02	2.113E+02	2.045E+02	2.218E+02	2.226E+02	1.465E+04	-6.481E+01
10000	2.321E+01	2.477E+02	2.345E+02	2.277E+02	2.243E+02	2.249E+02	1.473E+04	-5.628E+01
11000	2.319E+01	2.499E+02	2.577E+02	2.509E+02	2.265E+02	2.271E+02	1.482E+04	-4.927E+01
12000	2.314E+01	2.519E+02	2.809E+02	2.740E+02	2.285E+02	2.291E+02	1.490E+04	-4.339E+01
13000	2.308E+01	2.538E+02	3.040E+02	2.971E+02	2.304E+02	2.309E+02	1.498E+04	-3.839E+01
14000	2.302E+01	2.555E+02	3.270E+02	3.202E+02	2.321E+02	2.326E+02	1.504E+04	-3.408E+01
15000	2.297E+01	2.571E+02	3.500E+02	3.432E+02	2.338E+02	2.342E+02	1.508E+04	-3.033E+01
16000	2.293E+01	2.586E+02	3.730E+02	3.661E+02	2.353E+02	2.357E+02	1.510E+04	-2.705E+01
17000	2.290E+01	2.600E+02	3.959E+02	3.891E+02	2.367E+02	2.371E+02	1.506E+04	-2.415E+01
18000	2.289E+01	2.613E+02	4.188E+02	4.119E+02	2.380E+02	2.384E+02	1.500E+04	-2.158E+01
19000	2.290E+01	2.625E+02	4.417E+02	4.348E+02	2.393E+02	2.396E+02	1.491E+04	-1.930E+01
20000	2.293E+01	2.637E+02	4.646E+02	4.578E+02	2.404E+02	2.408E+02	1.482E+04	-1.726E+01
21000	2.299E+01	2.648E+02	4.876E+02	4.807E+02	2.416E+02	2.419E+02	1.475E+04	-1.542E+01
22000	2.306E+01	2.659E+02	5.106E+02	5.037E+02	2.427E+02	2.430E+02	1.470E+04	-1.375E+01
23000	2.316E+01	2.669E+02	5.337E+02	5.269E+02	2.437E+02	2.440E+02	1.469E+04	-1.224E+01
24000	2.328E+01	2.679E+02	5.569E+02	5.501E+02	2.447E+02	2.450E+02	1.469E+04	-1.085E+01
25000	2.341E+01	2.688E+02	5.802E+02	5.734E+02	2.456E+02	2.459E+02	1.472E+04	-9.566E+00
26000	2.357E+01	2.698E+02	6.037E+02	5.969E+02	2.465E+02	2.468E+02	1.476E+04	-8.381E+00
27000	2.375E+01	2.706E+02	6.274E+02	6.206E+02	2.474E+02	2.477E+02	1.482E+04	-7.281E+00
28000	2.394E+01	2.715E+02	6.512E+02	6.444E+02	2.483E+02	2.485E+02	1.488E+04	-6.255E+00
29000	2.415E+01	2.724E+02	6.753E+02	6.684E+02	2.491E+02	2.493E+02	1.494E+04	-5.296E+00
30000	2.437E+01	2.732E+02	6.995E+02	6.927E+02	2.499E+02	2.501E+02	1.502E+04	-4.397E+00
32000	2.486E+01	2.748E+02	7.488E+02	7.419E+02	2.514E+02	2.516E+02	1.517E+04	-2.755E+00
34000	2.541E+01	2.763E+02	7.990E+02	7.922E+02	2.528E+02	2.530E+02	1.533E+04	-1.291E+00
36000	2.600E+01	2.778E+02	8.504E+02	8.436E+02	2.542E+02	2.543E+02	1.550E+04	2.469E-02
38000	2.666E+01	2.792E+02	9.031E+02	8.962E+02	2.554E+02	2.556E+02	1.567E+04	1.215E+00
40000	2.741E+01	2.806E+02	9.571E+02	9.503E+02	2.566E+02	2.568E+02	1.584E+04	2.297E+00
42000	2.833E+01	2.819E+02	1.013E+03	1.006E+03	2.578E+02	2.580E+02	1.602E+04	3.288E+00
44000	2.958E+01	2.833E+02	1.071E+03	1.064E+03	2.589E+02	2.591E+02	1.620E+04	4.199E+00
46000	3.140E+01	2.846E+02	1.132E+03	1.125E+03	2.600E+02	2.602E+02	1.638E+04	5.040E+00
48000	3.421E+01	2.860E+02	1.197E+03	1.190E+03	2.611E+02	2.612E+02	1.657E+04	5.819E+00
50000	3.856E+01	2.875E+02	1.269E+03	1.262E+03	2.621E+02	2.622E+02	1.677E+04	6.545E+00

Table 61: Internal thermodynamic properties of Ar^{4+} ΔE=1000 cm^{-1}

T(K)	Q_{int}	$\ln(Q_{int})$	E_{int}/RT	$C_{p,int}/R$
50	$1.000E+00$	$8.205E-10$	$1.807E-08$	$3.978E-07$
100	$1.000E+00$	$4.961E-05$	$5.462E-04$	$6.013E-03$
150	$1.002E+00$	$1.945E-03$	$1.427E-02$	$1.045E-01$
200	$1.012E+00$	$1.213E-02$	$6.638E-02$	$3.613E-01$
298.15	$1.075E+00$	$7.231E-02$	$2.592E-01$	$9.055E-01$
300	$1.077E+00$	$7.393E-02$	$2.632E-01$	$9.130E-01$
400	$1.195E+00$	$1.779E-01$	$4.614E-01$	$1.151E+00$
500	$1.346E+00$	$2.974E-01$	$6.058E-01$	$1.197E+00$
600	$1.517E+00$	$4.170E-01$	$7.027E-01$	$1.170E+00$
700	$1.700E+00$	$5.304E-01$	$7.655E-01$	$1.110E+00$
800	$1.888E+00$	$6.354E-01$	$8.038E-01$	$1.032E+00$
900	$2.078E+00$	$7.314E-01$	$8.243E-01$	$9.443E-01$
1000	$2.268E+00$	$8.187E-01$	$8.319E-01$	$8.556E-01$
2000	$3.892E+00$	$1.359E+00$	$6.805E-01$	$3.089E-01$
3000	$4.970E+00$	$1.603E+00$	$5.266E-01$	$1.638E-01$
4000	$5.703E+00$	$1.741E+00$	$4.330E-01$	$1.536E-01$
5000	$6.242E+00$	$1.831E+00$	$3.803E-01$	$1.886E-01$
6000	$6.671E+00$	$1.898E+00$	$3.518E-01$	$2.291E-01$
7000	$7.034E+00$	$1.951E+00$	$3.366E-01$	$2.606E-01$
8000	$7.353E+00$	$1.995E+00$	$3.285E-01$	$2.802E-01$
9000	$7.641E+00$	$2.034E+00$	$3.237E-01$	$2.897E-01$
10000	$7.905E+00$	$2.067E+00$	$3.205E-01$	$2.917E-01$
11000	$8.149E+00$	$2.098E+00$	$3.177E-01$	$2.888E-01$
12000	$8.377E+00$	$2.125E+00$	$3.151E-01$	$2.830E-01$
13000	$8.590E+00$	$2.151E+00$	$3.124E-01$	$2.760E-01$
14000	$8.790E+00$	$2.174E+00$	$3.095E-01$	$2.689E-01$
15000	$8.979E+00$	$2.195E+00$	$3.066E-01$	$2.625E-01$
16000	$9.157E+00$	$2.215E+00$	$3.037E-01$	$2.575E-01$
17000	$9.327E+00$	$2.233E+00$	$3.008E-01$	$2.543E-01$
18000	$9.488E+00$	$2.250E+00$	$2.982E-01$	$2.533E-01$
19000	$9.641E+00$	$2.266E+00$	$2.959E-01$	$2.546E-01$
20000	$9.788E+00$	$2.281E+00$	$2.939E-01$	$2.584E-01$
21000	$9.929E+00$	$2.295E+00$	$2.924E-01$	$2.648E-01$
22000	$1.006E+01$	$2.309E+00$	$2.913E-01$	$2.738E-01$
23000	$1.020E+01$	$2.322E+00$	$2.908E-01$	$2.854E-01$
24000	$1.032E+01$	$2.334E+00$	$2.908E-01$	$2.995E-01$
25000	$1.045E+01$	$2.346E+00$	$2.915E-01$	$3.160E-01$
26000	$1.057E+01$	$2.358E+00$	$2.928E-01$	$3.348E-01$
27000	$1.068E+01$	$2.369E+00$	$2.947E-01$	$3.559E-01$
28000	$1.080E+01$	$2.380E+00$	$2.973E-01$	$3.791E-01$
29000	$1.091E+01$	$2.390E+00$	$3.006E-01$	$4.042E-01$
30000	$1.103E+01$	$2.400E+00$	$3.045E-01$	$4.313E-01$
32000	$1.125E+01$	$2.420E+00$	$3.142E-01$	$4.904E-01$
34000	$1.147E+01$	$2.440E+00$	$3.265E-01$	$5.554E-01$
36000	$1.169E+01$	$2.459E+00$	$3.411E-01$	$6.256E-01$
38000	$1.191E+01$	$2.478E+00$	$3.580E-01$	$7.008E-01$
40000	$1.214E+01$	$2.496E+00$	$3.772E-01$	$7.819E-01$
42000	$1.237E+01$	$2.515E+00$	$3.985E-01$	$8.717E-01$
44000	$1.261E+01$	$2.534E+00$	$4.224E-01$	$9.763E-01$
46000	$1.286E+01$	$2.554E+00$	$4.491E-01$	$1.106E+00$
48000	$1.311E+01$	$2.574E+00$	$4.799E-01$	$1.279E+00$
50000	$1.338E+01$	$2.594E+00$	$5.164E-01$	$1.519E+00$

Table 62: Total thermodynamic properties of Ar^{4+} ΔE=1000 cm^{-1}

T [K]	C_p [J/mol/K]	S^0 [J/mol/K]	$H^0(T)-H^0(0)$ [KJ/mol]	$H^0(T)-H^0(298)$ [KJ/mol]	$-(G^0-H^0(0))/T$ [J/mol/K]	$-(G^0-H^0(298))/T$ [J/mol/K]	ΔH_f [KJ/mol]	$Log(K_p)$
50	2.079E+01	1.177E+02	1.039E+00	-5.801E+00	9.694E+01	2.337E+02	1.388E+04	-1.450E+04
100	2.084E+01	1.321E+02	2.079E+00	-4.761E+00	1.113E+02	1.798E+02	1.388E+04	-7.252E+03
150	2.166E+01	1.407E+02	3.136E+00	-3.704E+00	1.198E+02	1.654E+02	1.389E+04	-4.835E+03
200	2.379E+01	1.472E+02	4.268E+00	-2.572E+00	1.259E+02	1.601E+02	1.389E+04	-3.626E+03
298.15	2.832E+01	1.576E+02	6.840E+00	0.000E+00	1.347E+02	1.576E+02	1.390E+04	-2.431E+03
300	2.838E+01	1.578E+02	6.892E+00	5.240E-02	1.348E+02	1.576E+02	1.390E+04	-2.416E+03
400	3.036E+01	1.663E+02	9.849E+00	3.009E+00	1.417E+02	1.588E+02	1.391E+04	-1.810E+03
500	3.074E+01	1.731E+02	1.291E+01	6.072E+00	1.473E+02	1.610E+02	1.392E+04	-1.447E+03
600	3.052E+01	1.787E+02	1.598E+01	9.137E+00	1.521E+02	1.635E+02	1.393E+04	-1.205E+03
700	3.002E+01	1.834E+02	1.901E+01	1.217E+01	1.562E+02	1.660E+02	1.394E+04	-1.031E+03
800	2.936E+01	1.873E+02	2.198E+01	1.514E+01	1.599E+02	1.684E+02	1.395E+04	-9.014E+02
900	2.864E+01	1.908E+02	2.488E+01	1.804E+01	1.631E+02	1.707E+02	1.396E+04	-8.001E+02
1000	2.790E+01	1.937E+02	2.770E+01	2.086E+01	1.660E+02	1.729E+02	1.397E+04	-7.191E+02
2000	2.336E+01	2.114E+02	5.289E+01	4.605E+01	1.849E+02	1.883E+02	1.405E+04	-3.535E+02
3000	2.215E+01	2.206E+02	7.549E+01	6.865E+01	1.954E+02	1.977E+02	1.414E+04	-2.308E+02
4000	2.206E+01	2.269E+02	9.755E+01	9.071E+01	2.025E+02	2.042E+02	1.422E+04	-1.691E+02
5000	2.235E+01	2.318E+02	1.197E+02	1.129E+02	2.079E+02	2.093E+02	1.431E+04	-1.319E+02
6000	2.269E+01	2.359E+02	1.423E+02	1.354E+02	2.122E+02	2.134E+02	1.439E+04	-1.069E+02
7000	2.295E+01	2.395E+02	1.651E+02	1.583E+02	2.159E+02	2.169E+02	1.448E+04	-8.894E+01
8000	2.312E+01	2.425E+02	1.881E+02	1.813E+02	2.190E+02	2.199E+02	1.456E+04	-7.540E+01
9000	2.320E+01	2.453E+02	2.113E+02	2.045E+02	2.218E+02	2.226E+02	1.465E+04	-6.481E+01
10000	2.321E+01	2.477E+02	2.345E+02	2.277E+02	2.243E+02	2.249E+02	1.473E+04	-5.628E+01
11000	2.319E+01	2.499E+02	2.577E+02	2.509E+02	2.265E+02	2.271E+02	1.482E+04	-4.927E+01
12000	2.314E+01	2.519E+02	2.809E+02	2.740E+02	2.285E+02	2.291E+02	1.490E+04	-4.339E+01
13000	2.308E+01	2.538E+02	3.040E+02	2.971E+02	2.304E+02	2.309E+02	1.498E+04	-3.838E+01
14000	2.302E+01	2.555E+02	3.270E+02	3.202E+02	2.321E+02	2.326E+02	1.506E+04	-3.407E+01
15000	2.297E+01	2.571E+02	3.500E+02	3.432E+02	2.338E+02	2.342E+02	1.512E+04	-3.032E+01
16000	2.293E+01	2.586E+02	3.730E+02	3.661E+02	2.353E+02	2.357E+02	1.517E+04	-2.702E+01
17000	2.290E+01	2.600E+02	3.959E+02	3.891E+02	2.367E+02	2.371E+02	1.520E+04	-2.411E+01
18000	2.289E+01	2.613E+02	4.188E+02	4.119E+02	2.380E+02	2.384E+02	1.520E+04	-2.151E+01
19000	2.290E+01	2.625E+02	4.417E+02	4.348E+02	2.393E+02	2.396E+02	1.517E+04	-1.919E+01
20000	2.293E+01	2.637E+02	4.646E+02	4.578E+02	2.404E+02	2.408E+02	1.512E+04	-1.711E+01
21000	2.299E+01	2.648E+02	4.876E+02	4.807E+02	2.416E+02	2.419E+02	1.506E+04	-1.523E+01
22000	2.306E+01	2.659E+02	5.106E+02	5.037E+02	2.427E+02	2.430E+02	1.500E+04	-1.353E+01
23000	2.316E+01	2.669E+02	5.337E+02	5.269E+02	2.437E+02	2.440E+02	1.496E+04	-1.199E+01
24000	2.328E+01	2.679E+02	5.569E+02	5.501E+02	2.447E+02	2.450E+02	1.494E+04	-1.057E+01
25000	2.341E+01	2.688E+02	5.802E+02	5.734E+02	2.456E+02	2.459E+02	1.493E+04	-9.273E+00
26000	2.357E+01	2.698E+02	6.037E+02	5.969E+02	2.465E+02	2.468E+02	1.494E+04	-8.072E+00
27000	2.375E+01	2.706E+02	6.274E+02	6.206E+02	2.474E+02	2.477E+02	1.497E+04	-6.960E+00
28000	2.394E+01	2.715E+02	6.512E+02	6.444E+02	2.483E+02	2.485E+02	1.501E+04	-5.924E+00
29000	2.415E+01	2.724E+02	6.753E+02	6.684E+02	2.491E+02	2.493E+02	1.506E+04	-4.957E+00
30000	2.437E+01	2.732E+02	6.995E+02	6.927E+02	2.499E+02	2.501E+02	1.512E+04	-4.051E+00
32000	2.486E+01	2.748E+02	7.488E+02	7.419E+02	2.514E+02	2.516E+02	1.525E+04	-2.399E+00
34000	2.540E+01	2.763E+02	7.990E+02	7.922E+02	2.528E+02	2.530E+02	1.539E+04	-9.287E-01
36000	2.599E+01	2.778E+02	8.504E+02	8.436E+02	2.542E+02	2.543E+02	1.555E+04	3.916E-01
38000	2.661E+01	2.792E+02	9.030E+02	8.962E+02	2.554E+02	2.556E+02	1.571E+04	1.585E+00
40000	2.729E+01	2.806E+02	9.569E+02	9.500E+02	2.566E+02	2.568E+02	1.588E+04	2.671E+00
42000	2.803E+01	2.819E+02	1.012E+03	1.005E+03	2.578E+02	2.580E+02	1.606E+04	3.664E+00
44000	2.890E+01	2.832E+02	1.069E+03	1.062E+03	2.589E+02	2.591E+02	1.623E+04	4.576E+00
46000	2.998E+01	2.846E+02	1.128E+03	1.121E+03	2.600E+02	2.602E+02	1.641E+04	5.419E+00
48000	3.142E+01	2.859E+02	1.189E+03	1.182E+03	2.611E+02	2.612E+02	1.659E+04	6.199E+00
50000	3.342E+01	2.872E+02	1.254E+03	1.247E+03	2.621E+02	2.622E+02	1.678E+04	6.926E+00

Table 63: Internal thermodynamic properties of C ΔE=250 cm^{-1}

T(K)	Q_{int}	$\ln(Q_{int})$	E_{int}/RT	$C_{p,int}/R$
50	$4.306E+00$	$1.460E+00$	$6.211E-01$	$2.305E-01$
100	$6.047E+00$	$1.800E+00$	$3.690E-01$	$5.834E-02$
150	$6.861E+00$	$1.926E+00$	$2.588E-01$	$2.553E-02$
200	$7.325E+00$	$1.991E+00$	$1.989E-01$	$1.420E-02$
298.15	$7.827E+00$	$2.058E+00$	$1.365E-01$	$6.302E-03$
300	$7.834E+00$	$2.058E+00$	$1.357E-01$	$6.223E-03$
400	$8.105E+00$	$2.093E+00$	$1.030E-01$	$3.473E-03$
500	$8.275E+00$	$2.113E+00$	$8.292E-02$	$2.212E-03$
600	$8.390E+00$	$2.127E+00$	$6.941E-02$	$1.531E-03$
700	$8.474E+00$	$2.137E+00$	$5.968E-02$	$1.122E-03$
800	$8.537E+00$	$2.144E+00$	$5.234E-02$	$8.592E-04$
900	$8.587E+00$	$2.150E+00$	$4.661E-02$	$6.891E-04$
1000	$8.627E+00$	$2.155E+00$	$4.202E-02$	$6.000E-04$
2000	$8.814E+00$	$2.176E+00$	$2.385E-02$	$1.996E-02$
3000	$8.911E+00$	$2.187E+00$	$3.477E-02$	$1.005E-01$
4000	$9.033E+00$	$2.201E+00$	$6.274E-02$	$1.897E-01$
5000	$9.192E+00$	$2.218E+00$	$9.483E-02$	$2.517E-01$
6000	$9.378E+00$	$2.238E+00$	$1.243E-01$	$2.888E-01$
7000	$9.578E+00$	$2.259E+00$	$1.500E-01$	$3.211E-01$
8000	$9.787E+00$	$2.281E+00$	$1.757E-01$	$4.103E-01$
9000	$1.001E+01$	$2.304E+00$	$2.161E-01$	$7.308E-01$
10000	$1.028E+01$	$2.331E+00$	$3.060E-01$	$1.635E+00$
11000	$1.068E+01$	$2.368E+00$	$5.061E-01$	$3.592E+00$
12000	$1.132E+01$	$2.427E+00$	$8.913E-01$	$6.877E+00$
13000	$1.244E+01$	$2.521E+00$	$1.509E+00$	$1.102E+01$
14000	$1.432E+01$	$2.662E+00$	$2.326E+00$	$1.463E+01$
15000	$1.734E+01$	$2.853E+00$	$3.213E+00$	$1.622E+01$
16000	$2.190E+01$	$3.086E+00$	$4.013E+00$	$1.545E+01$
17000	$2.848E+01$	$3.349E+00$	$4.623E+00$	$1.315E+01$
18000	$3.755E+01$	$3.626E+00$	$5.020E+00$	$1.041E+01$
19000	$4.958E+01$	$3.903E+00$	$5.236E+00$	$7.900E+00$
20000	$6.501E+01$	$4.175E+00$	$5.317E+00$	$5.886E+00$
21000	$8.427E+01$	$4.434E+00$	$5.306E+00$	$4.367E+00$
22000	$1.077E+02$	$4.679E+00$	$5.237E+00$	$3.254E+00$
23000	$1.356E+02$	$4.910E+00$	$5.132E+00$	$2.448E+00$
24000	$1.683E+02$	$5.126E+00$	$5.007E+00$	$1.863E+00$
25000	$2.059E+02$	$5.328E+00$	$4.872E+00$	$1.436E+00$
26000	$2.486E+02$	$5.516E+00$	$4.734E+00$	$1.121E+00$
27000	$2.965E+02$	$5.692E+00$	$4.596E+00$	$8.870E-01$
28000	$3.496E+02$	$5.857E+00$	$4.460E+00$	$7.102E-01$
29000	$4.078E+02$	$6.011E+00$	$4.328E+00$	$5.752E-01$
30000	$4.713E+02$	$6.155E+00$	$4.201E+00$	$4.709E-01$
32000	$6.133E+02$	$6.419E+00$	$3.963E+00$	$3.252E-01$
34000	$7.747E+02$	$6.652E+00$	$3.746E+00$	$2.325E-01$
36000	$9.543E+02$	$6.861E+00$	$3.549E+00$	$1.714E-01$
38000	$1.151E+03$	$7.048E+00$	$3.370E+00$	$1.297E-01$
40000	$1.362E+03$	$7.217E+00$	$3.207E+00$	$1.004E-01$
42000	$1.587E+03$	$7.369E+00$	$3.059E+00$	$7.933E-02$
44000	$1.824E+03$	$7.509E+00$	$2.923E+00$	$6.377E-02$
46000	$2.071E+03$	$7.636E+00$	$2.799E+00$	$5.205E-02$
48000	$2.327E+03$	$7.752E+00$	$2.684E+00$	$4.308E-02$
50000	$2.591E+03$	$7.860E+00$	$2.578E+00$	$3.609E-02$

Table 64: Total thermodynamic properties of C ΔE=250 cm^{-1}

T [K]	C_p [J/mol/K]	S^0 [J/mol/K]	$H^0(T)$-$H^0(0)$ [KJ/mol]	$H^0(T)$-$H^0(298)$ [KJ/mol]	-(G^0-$H^0(0)$)/T [J/mol/K]	-(G^0-$H^0(298)$)/T [J/mol/K]	ΔH_f [KJ/mol]	Log(K_p)
50	2.270E+01	1.200E+02	1.298E+00	-5.238E+00	9.409E+01	2.248E+02	2.980E+02	-3.086E+02
100	2.127E+01	1.352E+02	2.385E+00	-4.151E+00	1.113E+02	1.767E+02	2.983E+02	-1.529E+02
150	2.100E+01	1.437E+02	3.441E+00	-3.095E+00	1.208E+02	1.644E+02	2.986E+02	-1.009E+02
200	2.090E+01	1.498E+02	4.488E+00	-2.048E+00	1.273E+02	1.600E+02	2.987E+02	-7.494E+01
298.15	2.084E+01	1.581E+02	6.536E+00	0.000E+00	1.362E+02	1.581E+02	2.986E+02	-4.927E+01
300	2.084E+01	1.582E+02	6.574E+00	3.855E-02	1.363E+02	1.581E+02	2.986E+02	-4.894E+01
400	2.082E+01	1.642E+02	8.657E+00	2.121E+00	1.426E+02	1.589E+02	2.986E+02	-3.595E+01
500	2.080E+01	1.689E+02	1.074E+01	4.202E+00	1.474E+02	1.605E+02	2.988E+02	-2.814E+01
600	2.080E+01	1.727E+02	1.282E+01	6.282E+00	1.513E+02	1.622E+02	2.991E+02	-2.294E+01
700	2.080E+01	1.759E+02	1.490E+01	8.362E+00	1.546E+02	1.639E+02	2.994E+02	-1.922E+01
800	2.079E+01	1.786E+02	1.698E+01	1.044E+01	1.574E+02	1.656E+02	2.996E+02	-1.643E+01
900	2.079E+01	1.811E+02	1.906E+01	1.252E+01	1.599E+02	1.672E+02	2.999E+02	-1.425E+01
1000	2.079E+01	1.833E+02	2.114E+01	1.460E+01	1.621E+02	1.687E+02	3.002E+02	-1.251E+01
2000	2.095E+01	1.977E+02	4.197E+01	3.543E+01	1.767E+02	1.800E+02	3.024E+02	-4.643E+00
3000	2.162E+01	2.063E+02	6.323E+01	5.669E+01	1.852E+02	1.874E+02	3.037E+02	-2.006E+00
4000	2.236E+01	2.127E+02	8.523E+01	7.870E+01	1.913E+02	1.930E+02	3.048E+02	-6.814E-01
5000	2.288E+01	2.177E+02	1.079E+02	1.013E+02	1.961E+02	1.974E+02	3.061E+02	1.162E-01
6000	2.319E+01	2.219E+02	1.309E+02	1.244E+02	2.001E+02	2.012E+02	3.074E+02	6.502E-01
7000	2.346E+01	2.255E+02	1.542E+02	1.477E+02	2.035E+02	2.044E+02	3.086E+02	1.033E+00
8000	2.420E+01	2.287E+02	1.780E+02	1.714E+02	2.064E+02	2.072E+02	3.101E+02	1.322E+00
9000	2.686E+01	2.316E+02	2.032E+02	1.967E+02	2.091E+02	2.098E+02	3.131E+02	1.548E+00
10000	3.438E+01	2.348E+02	2.333E+02	2.268E+02	2.115E+02	2.121E+02	3.211E+02	1.731E+00
11000	5.065E+01	2.388E+02	2.749E+02	2.684E+02	2.138E+02	2.143E+02	3.411E+02	1.888E+00
12000	7.796E+01	2.443E+02	3.384E+02	3.318E+02	2.161E+02	2.166E+02	3.834E+02	2.030E+00
13000	1.124E+02	2.518E+02	4.334E+02	4.268E+02	2.185E+02	2.190E+02	4.579E+02	2.169E+00
14000	1.424E+02	2.613E+02	5.617E+02	5.552E+02	2.212E+02	2.217E+02	5.664E+02	2.315E+00
15000	1.557E+02	2.717E+02	7.125E+02	7.060E+02	2.242E+02	2.247E+02	6.980E+02	2.472E+00
16000	1.493E+02	2.817E+02	8.664E+02	8.599E+02	2.275E+02	2.279E+02	8.334E+02	2.638E+00
17000	1.302E+02	2.902E+02	1.007E+03	1.000E+03	2.310E+02	2.313E+02	9.558E+02	2.810E+00
18000	1.073E+02	2.970E+02	1.126E+03	1.119E+03	2.344E+02	2.348E+02	1.057E+03	2.982E+00
19000	8.647E+01	3.022E+02	1.222E+03	1.216E+03	2.379E+02	2.382E+02	1.137E+03	3.150E+00
20000	6.972E+01	3.062E+02	1.300E+03	1.293E+03	2.412E+02	2.415E+02	1.198E+03	3.310E+00
21000	5.710E+01	3.093E+02	1.363E+03	1.356E+03	2.444E+02	2.447E+02	1.246E+03	3.462E+00
22000	4.784E+01	3.117E+02	1.415E+03	1.409E+03	2.474E+02	2.477E+02	1.282E+03	3.605E+00
23000	4.114E+01	3.137E+02	1.460E+03	1.453E+03	2.502E+02	2.505E+02	1.311E+03	3.739E+00
24000	3.627E+01	3.153E+02	1.498E+03	1.492E+03	2.529E+02	2.532E+02	1.335E+03	3.864E+00
25000	3.273E+01	3.167E+02	1.532E+03	1.526E+03	2.554E+02	2.557E+02	1.355E+03	3.982E+00
26000	3.011E+01	3.180E+02	1.564E+03	1.557E+03	2.578E+02	2.581E+02	1.372E+03	4.091E+00
27000	2.816E+01	3.191E+02	1.593E+03	1.586E+03	2.601E+02	2.603E+02	1.387E+03	4.194E+00
28000	2.669E+01	3.201E+02	1.620E+03	1.614E+03	2.622E+02	2.624E+02	1.400E+03	4.290E+00
29000	2.557E+01	3.210E+02	1.646E+03	1.640E+03	2.642E+02	2.644E+02	1.413E+03	4.380E+00
30000	2.470E+01	3.218E+02	1.672E+03	1.665E+03	2.661E+02	2.663E+02	1.425E+03	4.466E+00
32000	2.349E+01	3.234E+02	1.720E+03	1.713E+03	2.696E+02	2.698E+02	1.446E+03	4.622E+00
34000	2.272E+01	3.248E+02	1.766E+03	1.759E+03	2.728E+02	2.730E+02	1.467E+03	4.762E+00
36000	2.221E+01	3.261E+02	1.811E+03	1.804E+03	2.758E+02	2.759E+02	1.486E+03	4.888E+00
38000	2.186E+01	3.272E+02	1.855E+03	1.848E+03	2.784E+02	2.786E+02	1.505E+03	5.002E+00
40000	2.162E+01	3.284E+02	1.898E+03	1.892E+03	2.809E+02	2.811E+02	1.524E+03	5.106E+00
42000	2.145E+01	3.294E+02	1.941E+03	1.935E+03	2.832E+02	2.834E+02	1.543E+03	5.201E+00
44000	2.132E+01	3.304E+02	1.984E+03	1.978E+03	2.853E+02	2.855E+02	1.562E+03	5.289E+00
46000	2.122E+01	3.314E+02	2.026E+03	2.020E+03	2.873E+02	2.874E+02	1.580E+03	5.370E+00
48000	2.114E+01	3.323E+02	2.069E+03	2.062E+03	2.891E+02	2.893E+02	1.599E+03	5.445E+00
50000	2.109E+01	3.331E+02	2.111E+03	2.105E+03	2.909E+02	2.910E+02	1.618E+03	5.515E+00

Table 65: Internal thermodynamic properties of C ΔE=500 cm^{-1}

T(K)	Q_{int}	$\ln(Q_{int})$	E_{int}/RT	$C_{p,int}/R$
50	$4.306E+00$	$1.460E+00$	$6.211E-01$	$2.305E-01$
100	$6.047E+00$	$1.800E+00$	$3.690E-01$	$5.834E-02$
150	$6.861E+00$	$1.926E+00$	$2.588E-01$	$2.553E-02$
200	$7.325E+00$	$1.991E+00$	$1.989E-01$	$1.420E-02$
298.15	$7.827E+00$	$2.058E+00$	$1.365E-01$	$6.302E-03$
300	$7.834E+00$	$2.058E+00$	$1.357E-01$	$6.223E-03$
400	$8.105E+00$	$2.093E+00$	$1.030E-01$	$3.473E-03$
500	$8.275E+00$	$2.113E+00$	$8.292E-02$	$2.212E-03$
600	$8.390E+00$	$2.127E+00$	$6.941E-02$	$1.531E-03$
700	$8.474E+00$	$2.137E+00$	$5.968E-02$	$1.122E-03$
800	$8.537E+00$	$2.144E+00$	$5.234E-02$	$8.592E-04$
900	$8.587E+00$	$2.150E+00$	$4.661E-02$	$6.891E-04$
1000	$8.627E+00$	$2.155E+00$	$4.202E-02$	$6.000E-04$
2000	$8.814E+00$	$2.176E+00$	$2.385E-02$	$1.996E-02$
3000	$8.911E+00$	$2.187E+00$	$3.477E-02$	$1.005E-01$
4000	$9.033E+00$	$2.201E+00$	$6.274E-02$	$1.897E-01$
5000	$9.192E+00$	$2.218E+00$	$9.483E-02$	$2.517E-01$
6000	$9.378E+00$	$2.238E+00$	$1.243E-01$	$2.883E-01$
7000	$9.578E+00$	$2.259E+00$	$1.496E-01$	$3.145E-01$
8000	$9.786E+00$	$2.281E+00$	$1.726E-01$	$3.602E-01$
9000	$1.000E+01$	$2.303E+00$	$1.997E-01$	$4.968E-01$
10000	$1.024E+01$	$2.326E+00$	$2.450E-01$	$8.630E-01$
11000	$1.052E+01$	$2.353E+00$	$3.333E-01$	$1.658E+00$
12000	$1.089E+01$	$2.388E+00$	$4.980E-01$	$3.075E+00$
13000	$1.145E+01$	$2.438E+00$	$7.727E-01$	$5.166E+00$
14000	$1.230E+01$	$2.509E+00$	$1.175E+00$	$7.692E+00$
15000	$1.357E+01$	$2.608E+00$	$1.693E+00$	$1.011E+01$
16000	$1.541E+01$	$2.735E+00$	$2.276E+00$	$1.177E+01$
17000	$1.801E+01$	$2.891E+00$	$2.857E+00$	$1.232E+01$
18000	$2.152E+01$	$3.069E+00$	$3.372E+00$	$1.178E+01$
19000	$2.613E+01$	$3.263E+00$	$3.783E+00$	$1.053E+01$
20000	$3.198E+01$	$3.465E+00$	$4.082E+00$	$8.967E+00$
21000	$3.923E+01$	$3.669E+00$	$4.277E+00$	$7.402E+00$
22000	$4.800E+01$	$3.871E+00$	$4.387E+00$	$6.000E+00$
23000	$5.840E+01$	$4.067E+00$	$4.430E+00$	$4.821E+00$
24000	$7.052E+01$	$4.256E+00$	$4.426E+00$	$3.864E+00$
25000	$8.443E+01$	$4.436E+00$	$4.388E+00$	$3.104E+00$
26000	$1.002E+02$	$4.607E+00$	$4.326E+00$	$2.505E+00$
27000	$1.178E+02$	$4.769E+00$	$4.250E+00$	$2.035E+00$
28000	$1.372E+02$	$4.922E+00$	$4.164E+00$	$1.664E+00$
29000	$1.586E+02$	$5.066E+00$	$4.072E+00$	$1.372E+00$
30000	$1.818E+02$	$5.203E+00$	$3.978E+00$	$1.140E+00$
32000	$2.336E+02$	$5.453E+00$	$3.790E+00$	$8.052E-01$
34000	$2.923E+02$	$5.678E+00$	$3.607E+00$	$5.853E-01$
36000	$3.574E+02$	$5.879E+00$	$3.435E+00$	$4.368E-01$
38000	$4.285E+02$	$6.060E+00$	$3.274E+00$	$3.336E-01$
40000	$5.049E+02$	$6.224E+00$	$3.125E+00$	$2.602E-01$
42000	$5.861E+02$	$6.373E+00$	$2.988E+00$	$2.067E-01$
44000	$6.715E+02$	$6.509E+00$	$2.860E+00$	$1.669E-01$
46000	$7.605E+02$	$6.634E+00$	$2.742E+00$	$1.368E-01$
48000	$8.527E+02$	$6.748E+00$	$2.633E+00$	$1.135E-01$
50000	$9.475E+02$	$6.854E+00$	$2.532E+00$	$9.534E-02$

Table 66: Total thermodynamic properties of C ΔE=500 cm^{-1}

T [K]	C_p [J/mol/K]	S^0 [J/mol/K]	$H^0(T)-H^0(0)$ [KJ/mol]	$H^0(T)-H^0(298)$ [KJ/mol]	$-(G^0-H^0(0))/T$ [J/mol/K]	$-(G^0-H^0(298))/T$ [J/mol/K]	ΔH_f [KJ/mol]	$\mathrm{Log}(K_p)$
50	2.270E+01	1.200E+02	1.298E+00	-5.238E+00	9.409E+01	2.248E+02	2.980E+02	-3.086E+02
100	2.127E+01	1.352E+02	2.385E+00	-4.151E+00	1.113E+02	1.767E+02	2.983E+02	-1.529E+02
150	2.100E+01	1.437E+02	3.441E+00	-3.095E+00	1.208E+02	1.644E+02	2.986E+02	-1.009E+02
200	2.090E+01	1.498E+02	4.488E+00	-2.048E+00	1.273E+02	1.600E+02	2.987E+02	-7.494E+01
298.15	2.084E+01	1.581E+02	6.536E+00	0.000E+00	1.362E+02	1.581E+02	2.986E+02	-4.927E+01
300	2.084E+01	1.582E+02	6.574E+00	3.855E-02	1.363E+02	1.581E+02	2.986E+02	-4.894E+01
400	2.082E+01	1.642E+02	8.657E+00	2.121E+00	1.426E+02	1.589E+02	2.986E+02	-3.595E+01
500	2.080E+01	1.689E+02	1.074E+01	4.202E+00	1.474E+02	1.605E+02	2.988E+02	-2.814E+01
600	2.080E+01	1.727E+02	1.282E+01	6.282E+00	1.513E+02	1.622E+02	2.991E+02	-2.294E+01
700	2.080E+01	1.759E+02	1.490E+01	8.362E+00	1.546E+02	1.639E+02	2.994E+02	-1.922E+01
800	2.079E+01	1.786E+02	1.698E+01	1.044E+01	1.574E+02	1.656E+02	2.996E+02	-1.643E+01
900	2.079E+01	1.811E+02	1.906E+01	1.252E+01	1.599E+02	1.672E+02	2.999E+02	-1.425E+01
1000	2.079E+01	1.833E+02	2.114E+01	1.460E+01	1.621E+02	1.687E+02	3.002E+02	-1.251E+01
2000	2.095E+01	1.977E+02	4.197E+01	3.543E+01	1.767E+02	1.800E+02	3.024E+02	-4.643E+00
3000	2.162E+01	2.063E+02	6.323E+01	5.669E+01	1.852E+02	1.874E+02	3.037E+02	-2.006E+00
4000	2.236E+01	2.127E+02	8.523E+01	7.870E+01	1.913E+02	1.930E+02	3.048E+02	-6.814E-01
5000	2.288E+01	2.177E+02	1.079E+02	1.013E+02	1.961E+02	1.974E+02	3.061E+02	1.162E-01
6000	2.318E+01	2.219E+02	1.309E+02	1.244E+02	2.001E+02	2.012E+02	3.074E+02	6.502E-01
7000	2.340E+01	2.255E+02	1.542E+02	1.477E+02	2.035E+02	2.044E+02	3.086E+02	1.033E+00
8000	2.378E+01	2.286E+02	1.778E+02	1.712E+02	2.064E+02	2.072E+02	3.099E+02	1.322E+00
9000	2.492E+01	2.315E+02	2.020E+02	1.955E+02	2.090E+02	2.098E+02	3.119E+02	1.547E+00
10000	2.796E+01	2.342E+02	2.282E+02	2.217E+02	2.114E+02	2.121E+02	3.161E+02	1.729E+00
11000	3.457E+01	2.372E+02	2.591E+02	2.526E+02	2.136E+02	2.142E+02	3.253E+02	1.881E+00
12000	4.636E+01	2.407E+02	2.991E+02	2.926E+02	2.157E+02	2.163E+02	3.442E+02	2.013E+00
13000	6.374E+01	2.450E+02	3.537E+02	3.472E+02	2.178E+02	2.183E+02	3.783E+02	2.133E+00
14000	8.474E+01	2.505E+02	4.278E+02	4.213E+02	2.199E+02	2.204E+02	4.325E+02	2.249E+00
15000	1.048E+02	2.571E+02	5.229E+02	5.164E+02	2.222E+02	2.226E+02	5.084E+02	2.365E+00
16000	1.187E+02	2.643E+02	6.354E+02	6.288E+02	2.246E+02	2.250E+02	6.024E+02	2.486E+00
17000	1.232E+02	2.717E+02	7.571E+02	7.506E+02	2.272E+02	2.275E+02	7.062E+02	2.611E+00
18000	1.188E+02	2.786E+02	8.787E+02	8.722E+02	2.298E+02	2.302E+02	8.104E+02	2.740E+00
19000	1.083E+02	2.848E+02	9.926E+02	9.861E+02	2.326E+02	2.329E+02	9.075E+02	2.872E+00
20000	9.534E+01	2.900E+02	1.095E+03	1.088E+03	2.353E+02	2.356E+02	9.930E+02	3.002E+00
21000	8.233E+01	2.944E+02	1.183E+03	1.177E+03	2.380E+02	2.383E+02	1.066E+03	3.130E+00
22000	7.067E+01	2.979E+02	1.260E+03	1.253E+03	2.407E+02	2.410E+02	1.127E+03	3.254E+00
23000	6.087E+01	3.008E+02	1.325E+03	1.319E+03	2.432E+02	2.435E+02	1.177E+03	3.373E+00
24000	5.292E+01	3.033E+02	1.382E+03	1.376E+03	2.457E+02	2.459E+02	1.219E+03	3.487E+00
25000	4.659E+01	3.053E+02	1.432E+03	1.425E+03	2.480E+02	2.483E+02	1.254E+03	3.594E+00
26000	4.162E+01	3.070E+02	1.476E+03	1.469E+03	2.502E+02	2.505E+02	1.284E+03	3.696E+00
27000	3.770E+01	3.085E+02	1.515E+03	1.509E+03	2.524E+02	2.526E+02	1.309E+03	3.793E+00
28000	3.462E+01	3.098E+02	1.551E+03	1.545E+03	2.544E+02	2.547E+02	1.332E+03	3.884E+00
29000	3.220E+01	3.110E+02	1.585E+03	1.578E+03	2.563E+02	2.566E+02	1.351E+03	3.970E+00
30000	3.027E+01	3.121E+02	1.616E+03	1.609E+03	2.582E+02	2.584E+02	1.369E+03	4.052E+00
32000	2.748E+01	3.139E+02	1.673E+03	1.667E+03	2.616E+02	2.618E+02	1.400E+03	4.203E+00
34000	2.565E+01	3.155E+02	1.726E+03	1.720E+03	2.647E+02	2.649E+02	1.427E+03	4.338E+00
36000	2.442E+01	3.169E+02	1.776E+03	1.770E+03	2.676E+02	2.678E+02	1.452E+03	4.461E+00
38000	2.356E+01	3.182E+02	1.824E+03	1.818E+03	2.702E+02	2.704E+02	1.475E+03	4.573E+00
40000	2.295E+01	3.194E+02	1.871E+03	1.864E+03	2.727E+02	2.728E+02	1.497E+03	4.675E+00
42000	2.250E+01	3.205E+02	1.916E+03	1.910E+03	2.749E+02	2.751E+02	1.518E+03	4.769E+00
44000	2.217E+01	3.216E+02	1.961E+03	1.954E+03	2.770E+02	2.772E+02	1.539E+03	4.855E+00
46000	2.192E+01	3.226E+02	2.005E+03	1.998E+03	2.790E+02	2.791E+02	1.559E+03	4.935E+00
48000	2.173E+01	3.235E+02	2.049E+03	2.042E+03	2.808E+02	2.809E+02	1.579E+03	5.009E+00
50000	2.158E+01	3.244E+02	2.092E+03	2.086E+03	2.825E+02	2.827E+02	1.599E+03	5.079E+00

Table 67: Internal thermodynamic properties of C ΔE=1000 cm^{-1}

T(K)	Q_{int}	$\ln(Q_{int})$	E_{int}/RT	$C_{p,int}/R$
50	$4.306E+00$	$1.460E+00$	$6.211E-01$	$2.305E-01$
100	$6.047E+00$	$1.800E+00$	$3.690E-01$	$5.834E-02$
150	$6.861E+00$	$1.926E+00$	$2.588E-01$	$2.553E-02$
200	$7.325E+00$	$1.991E+00$	$1.989E-01$	$1.420E-02$
298.15	$7.827E+00$	$2.058E+00$	$1.365E-01$	$6.302E-03$
300	$7.834E+00$	$2.058E+00$	$1.357E-01$	$6.223E-03$
400	$8.105E+00$	$2.093E+00$	$1.030E-01$	$3.473E-03$
500	$8.275E+00$	$2.113E+00$	$8.292E-02$	$2.212E-03$
600	$8.390E+00$	$2.127E+00$	$6.941E-02$	$1.531E-03$
700	$8.474E+00$	$2.137E+00$	$5.968E-02$	$1.122E-03$
800	$8.537E+00$	$2.144E+00$	$5.234E-02$	$8.592E-04$
900	$8.587E+00$	$2.150E+00$	$4.661E-02$	$6.891E-04$
1000	$8.627E+00$	$2.155E+00$	$4.202E-02$	$6.000E-04$
2000	$8.814E+00$	$2.176E+00$	$2.385E-02$	$1.996E-02$
3000	$8.911E+00$	$2.187E+00$	$3.477E-02$	$1.005E-01$
4000	$9.033E+00$	$2.201E+00$	$6.274E-02$	$1.897E-01$
5000	$9.192E+00$	$2.218E+00$	$9.483E-02$	$2.517E-01$
6000	$9.378E+00$	$2.238E+00$	$1.243E-01$	$2.882E-01$
7000	$9.578E+00$	$2.259E+00$	$1.495E-01$	$3.121E-01$
8000	$9.785E+00$	$2.281E+00$	$1.715E-01$	$3.422E-01$
9000	$9.997E+00$	$2.302E+00$	$1.938E-01$	$4.130E-01$
10000	$1.022E+01$	$2.324E+00$	$2.231E-01$	$5.855E-01$
11000	$1.046E+01$	$2.347E+00$	$2.707E-01$	$9.457E-01$
12000	$1.074E+01$	$2.374E+00$	$3.513E-01$	$1.585E+00$
13000	$1.110E+01$	$2.407E+00$	$4.817E-01$	$2.564E+00$
14000	$1.158E+01$	$2.449E+00$	$6.754E-01$	$3.870E+00$
15000	$1.224E+01$	$2.505E+00$	$9.381E-01$	$5.383E+00$
16000	$1.313E+01$	$2.575E+00$	$1.264E+00$	$6.885E+00$
17000	$1.434E+01$	$2.663E+00$	$1.633E+00$	$8.127E+00$
18000	$1.591E+01$	$2.767E+00$	$2.018E+00$	$8.910E+00$
19000	$1.792E+01$	$2.886E+00$	$2.389E+00$	$9.157E+00$
20000	$2.044E+01$	$3.017E+00$	$2.723E+00$	$8.916E+00$
21000	$2.351E+01$	$3.157E+00$	$3.005E+00$	$8.314E+00$
22000	$2.718E+01$	$3.302E+00$	$3.229E+00$	$7.503E+00$
23000	$3.150E+01$	$3.450E+00$	$3.395E+00$	$6.613E+00$
24000	$3.649E+01$	$3.597E+00$	$3.511E+00$	$5.734E+00$
25000	$4.218E+01$	$3.742E+00$	$3.583E+00$	$4.920E+00$
26000	$4.858E+01$	$3.883E+00$	$3.620E+00$	$4.198E+00$
27000	$5.571E+01$	$4.020E+00$	$3.630E+00$	$3.572E+00$
28000	$6.356E+01$	$4.152E+00$	$3.618E+00$	$3.039E+00$
29000	$7.213E+01$	$4.278E+00$	$3.590E+00$	$2.590E+00$
30000	$8.141E+01$	$4.400E+00$	$3.550E+00$	$2.213E+00$
32000	$1.021E+02$	$4.626E+00$	$3.448E+00$	$1.635E+00$
34000	$1.253E+02$	$4.831E+00$	$3.328E+00$	$1.229E+00$
36000	$1.511E+02$	$5.018E+00$	$3.203E+00$	$9.404E-01$
38000	$1.790E+02$	$5.188E+00$	$3.078E+00$	$7.325E-01$
40000	$2.090E+02$	$5.342E+00$	$2.957E+00$	$5.802E-01$
42000	$2.408E+02$	$5.484E+00$	$2.841E+00$	$4.667E-01$
44000	$2.741E+02$	$5.613E+00$	$2.731E+00$	$3.807E-01$
46000	$3.087E+02$	$5.732E+00$	$2.627E+00$	$3.146E-01$
48000	$3.445E+02$	$5.842E+00$	$2.530E+00$	$2.630E-01$
50000	$3.813E+02$	$5.944E+00$	$2.438E+00$	$2.222E-01$

Table 68: Total thermodynamic properties of C ΔE=1000 cm^{-1}

T [K]	C_p [J/mol/K]	S^0 [J/mol/K]	$H^0(T)-H^0(0)$ [KJ/mol]	$H^0(T)-H^0(298)$ [KJ/mol]	$-(G^0-H^0(0))/T$ [J/mol/K]	$-(G^0-H^0(298))/T$ [J/mol/K]	ΔH_f [KJ/mol]	$\mathrm{Log}(K_p)$
50	2.270E+01	1.200E+02	1.298E+00	-5.238E+00	9.409E+01	2.248E+02	2.980E+02	-3.086E+02
100	2.127E+01	1.352E+02	2.385E+00	-4.151E+00	1.113E+02	1.767E+02	2.983E+02	-1.529E+02
150	2.100E+01	1.437E+02	3.441E+00	-3.095E+00	1.208E+02	1.644E+02	2.986E+02	-1.009E+02
200	2.090E+01	1.498E+02	4.488E+00	-2.048E+00	1.273E+02	1.600E+02	2.987E+02	-7.494E+01
298.15	2.084E+01	1.581E+02	6.536E+00	0.000E+00	1.362E+02	1.581E+02	2.986E+02	-4.927E+01
300	2.084E+01	1.582E+02	6.574E+00	3.855E-02	1.363E+02	1.581E+02	2.986E+02	-4.894E+01
400	2.082E+01	1.642E+02	8.657E+00	2.121E+00	1.426E+02	1.589E+02	2.986E+02	-3.595E+01
500	2.080E+01	1.689E+02	1.074E+01	4.202E+00	1.474E+02	1.605E+02	2.988E+02	-2.814E+01
600	2.080E+01	1.727E+02	1.282E+01	6.282E+00	1.513E+02	1.622E+02	2.991E+02	-2.294E+01
700	2.080E+01	1.759E+02	1.490E+01	8.362E+00	1.546E+02	1.639E+02	2.994E+02	-1.922E+01
800	2.079E+01	1.786E+02	1.698E+01	1.044E+01	1.574E+02	1.656E+02	2.996E+02	-1.643E+01
900	2.079E+01	1.811E+02	1.906E+01	1.252E+01	1.599E+02	1.672E+02	2.999E+02	-1.425E+01
1000	2.079E+01	1.833E+02	2.114E+01	1.460E+01	1.621E+02	1.687E+02	3.002E+02	-1.251E+01
2000	2.095E+01	1.977E+02	4.197E+01	3.543E+01	1.767E+02	1.800E+02	3.024E+02	-4.643E+00
3000	2.162E+01	2.063E+02	6.323E+01	5.669E+01	1.852E+02	1.874E+02	3.037E+02	-2.006E+00
4000	2.236E+01	2.127E+02	8.523E+01	7.870E+01	1.913E+02	1.930E+02	3.048E+02	-6.814E-01
5000	2.288E+01	2.177E+02	1.079E+02	1.013E+02	1.961E+02	1.974E+02	3.061E+02	1.162E-01
6000	2.318E+01	2.219E+02	1.309E+02	1.244E+02	2.001E+02	2.012E+02	3.074E+02	6.502E-01
7000	2.338E+01	2.255E+02	1.542E+02	1.477E+02	2.035E+02	2.044E+02	3.086E+02	1.033E+00
8000	2.363E+01	2.286E+02	1.777E+02	1.712E+02	2.064E+02	2.072E+02	3.098E+02	1.322E+00
9000	2.422E+01	2.314E+02	2.016E+02	1.950E+02	2.090E+02	2.098E+02	3.114E+02	1.547E+00
10000	2.565E+01	2.341E+02	2.264E+02	2.199E+02	2.114E+02	2.121E+02	3.142E+02	1.728E+00
11000	2.865E+01	2.366E+02	2.534E+02	2.469E+02	2.136E+02	2.142E+02	3.196E+02	1.879E+00
12000	3.397E+01	2.393E+02	2.845E+02	2.779E+02	2.156E+02	2.162E+02	3.295E+02	2.007E+00
13000	4.211E+01	2.423E+02	3.223E+02	3.158E+02	2.176E+02	2.181E+02	3.468E+02	2.120E+00
14000	5.296E+01	2.458E+02	3.696E+02	3.631E+02	2.194E+02	2.199E+02	3.743E+02	2.223E+00
15000	6.554E+01	2.499E+02	4.288E+02	4.223E+02	2.213E+02	2.218E+02	4.143E+02	2.321E+00
16000	7.803E+01	2.546E+02	5.007E+02	4.941E+02	2.233E+02	2.237E+02	4.676E+02	2.416E+00
17000	8.836E+01	2.596E+02	5.841E+02	5.776E+02	2.253E+02	2.256E+02	5.332E+02	2.512E+00
18000	9.487E+01	2.649E+02	6.761E+02	6.696E+02	2.273E+02	2.277E+02	6.078E+02	2.609E+00
19000	9.692E+01	2.701E+02	7.724E+02	7.659E+02	2.294E+02	2.298E+02	6.872E+02	2.708E+00
20000	9.492E+01	2.750E+02	8.686E+02	8.621E+02	2.316E+02	2.319E+02	7.671E+02	2.808E+00
21000	8.992E+01	2.795E+02	9.612E+02	9.547E+02	2.338E+02	2.341E+02	8.438E+02	2.908E+00
22000	8.317E+01	2.836E+02	1.048E+03	1.041E+03	2.359E+02	2.362E+02	9.149E+02	3.007E+00
23000	7.577E+01	2.871E+02	1.127E+03	1.121E+03	2.381E+02	2.384E+02	9.792E+02	3.105E+00
24000	6.846E+01	2.902E+02	1.199E+03	1.193E+03	2.402E+02	2.405E+02	1.036E+03	3.200E+00
25000	6.170E+01	2.928E+02	1.264E+03	1.258E+03	2.422E+02	2.425E+02	1.087E+03	3.293E+00
26000	5.569E+01	2.951E+02	1.323E+03	1.316E+03	2.442E+02	2.445E+02	1.131E+03	3.382E+00
27000	5.048E+01	2.971E+02	1.376E+03	1.370E+03	2.462E+02	2.464E+02	1.170E+03	3.468E+00
28000	4.606E+01	2.989E+02	1.424E+03	1.418E+03	2.480E+02	2.482E+02	1.204E+03	3.550E+00
29000	4.232E+01	3.004E+02	1.468E+03	1.462E+03	2.498E+02	2.500E+02	1.235E+03	3.628E+00
30000	3.919E+01	3.018E+02	1.509E+03	1.503E+03	2.515E+02	2.517E+02	1.262E+03	3.703E+00
32000	3.438E+01	3.042E+02	1.582E+03	1.576E+03	2.547E+02	2.549E+02	1.309E+03	3.843E+00
34000	3.100E+01	3.061E+02	1.648E+03	1.641E+03	2.577E+02	2.579E+02	1.348E+03	3.971E+00
36000	2.861E+01	3.079E+02	1.707E+03	1.701E+03	2.604E+02	2.606E+02	1.382E+03	4.087E+00
38000	2.688E+01	3.094E+02	1.762E+03	1.756E+03	2.630E+02	2.631E+02	1.413E+03	4.194E+00
40000	2.561E+01	3.107E+02	1.815E+03	1.808E+03	2.653E+02	2.655E+02	1.441E+03	4.292E+00
42000	2.467E+01	3.119E+02	1.865E+03	1.859E+03	2.675E+02	2.677E+02	1.467E+03	4.382E+00
44000	2.395E+01	3.131E+02	1.914E+03	1.907E+03	2.696E+02	2.697E+02	1.491E+03	4.466E+00
46000	2.340E+01	3.141E+02	1.961E+03	1.954E+03	2.715E+02	2.716E+02	1.515E+03	4.544E+00
48000	2.297E+01	3.151E+02	2.007E+03	2.001E+03	2.733E+02	2.734E+02	1.538E+03	4.616E+00
50000	2.263E+01	3.160E+02	2.053E+03	2.046E+03	2.750E+02	2.751E+02	1.560E+03	4.683E+00

Table 69: Internal thermodynamic properties of C^+ ΔE=250 cm^{-1}

T(K)	Q_{int}	$\ln(Q_{int})$	E_{int}/RT	$C_{p,int}/R$
50	$2.645E+00$	$9.726E-01$	$4.450E-01$	$6.140E-01$
100	$3.606E+00$	$1.283E+00$	$4.064E-01$	$2.057E-01$
150	$4.177E+00$	$1.430E+00$	$3.170E-01$	$9.234E-02$
200	$4.535E+00$	$1.512E+00$	$2.550E-01$	$5.131E-02$
298.15	$4.945E+00$	$1.598E+00$	$1.823E-01$	$2.256E-02$
300	$4.951E+00$	$1.600E+00$	$1.813E-01$	$2.227E-02$
400	$5.184E+00$	$1.646E+00$	$1.401E-01$	$1.233E-02$
500	$5.333E+00$	$1.674E+00$	$1.141E-01$	$7.806E-03$
600	$5.436E+00$	$1.693E+00$	$9.612E-02$	$5.379E-03$
700	$5.511E+00$	$1.707E+00$	$8.305E-02$	$3.929E-03$
800	$5.569E+00$	$1.717E+00$	$7.310E-02$	$2.994E-03$
900	$5.614E+00$	$1.725E+00$	$6.527E-02$	$2.357E-03$
1000	$5.651E+00$	$1.732E+00$	$5.895E-02$	$1.904E-03$
2000	$5.822E+00$	$1.762E+00$	$2.995E-02$	$4.694E-04$
3000	$5.880E+00$	$1.772E+00$	$2.007E-02$	$2.086E-04$
4000	$5.910E+00$	$1.777E+00$	$1.510E-02$	$2.085E-04$
5000	$5.928E+00$	$1.780E+00$	$1.220E-02$	$1.372E-03$
6000	$5.940E+00$	$1.782E+00$	$1.077E-02$	$7.140E-03$
7000	$5.950E+00$	$1.783E+00$	$1.122E-02$	$2.280E-02$
8000	$5.960E+00$	$1.785E+00$	$1.438E-02$	$5.280E-02$
9000	$5.972E+00$	$1.787E+00$	$2.107E-02$	$9.896E-02$
10000	$5.988E+00$	$1.790E+00$	$3.181E-02$	$1.604E-01$
11000	$6.011E+00$	$1.794E+00$	$4.677E-02$	$2.343E-01$
12000	$6.040E+00$	$1.798E+00$	$6.581E-02$	$3.173E-01$
13000	$6.077E+00$	$1.805E+00$	$8.855E-02$	$4.064E-01$
14000	$6.123E+00$	$1.812E+00$	$1.146E-01$	$5.004E-01$
15000	$6.177E+00$	$1.821E+00$	$1.436E-01$	$6.022E-01$
16000	$6.241E+00$	$1.831E+00$	$1.759E-01$	$7.214E-01$
17000	$6.315E+00$	$1.843E+00$	$2.123E-01$	$8.782E-01$
18000	$6.400E+00$	$1.856E+00$	$2.552E-01$	$1.106E+00$
19000	$6.497E+00$	$1.871E+00$	$3.086E-01$	$1.456E+00$
20000	$6.612E+00$	$1.889E+00$	$3.784E-01$	$1.991E+00$
21000	$6.750E+00$	$1.910E+00$	$4.729E-01$	$2.786E+00$
22000	$6.920E+00$	$1.934E+00$	$6.023E-01$	$3.912E+00$
23000	$7.134E+00$	$1.965E+00$	$7.775E-01$	$5.420E+00$
24000	$7.408E+00$	$2.003E+00$	$1.009E+00$	$7.313E+00$
25000	$7.764E+00$	$2.050E+00$	$1.305E+00$	$9.519E+00$
26000	$8.228E+00$	$2.108E+00$	$1.666E+00$	$1.188E+01$
27000	$8.830E+00$	$2.178E+00$	$2.087E+00$	$1.417E+01$
28000	$9.606E+00$	$2.262E+00$	$2.555E+00$	$1.611E+01$
29000	$1.060E+01$	$2.361E+00$	$3.048E+00$	$1.748E+01$
30000	$1.185E+01$	$2.472E+00$	$3.541E+00$	$1.812E+01$
32000	$1.534E+01$	$2.730E+00$	$4.441E+00$	$1.731E+01$
34000	$2.052E+01$	$3.021E+00$	$5.124E+00$	$1.462E+01$
36000	$2.788E+01$	$3.328E+00$	$5.562E+00$	$1.141E+01$
38000	$3.792E+01$	$3.636E+00$	$5.791E+00$	$8.516E+00$
40000	$5.117E+01$	$3.935E+00$	$5.868E+00$	$6.239E+00$
42000	$6.811E+01$	$4.221E+00$	$5.844E+00$	$4.557E+00$
44000	$8.922E+01$	$4.491E+00$	$5.756E+00$	$3.348E+00$
46000	$1.149E+02$	$4.744E+00$	$5.632E+00$	$2.486E+00$
48000	$1.456E+02$	$4.981E+00$	$5.487E+00$	$1.871E+00$
50000	$1.816E+02$	$5.202E+00$	$5.333E+00$	$1.429E+00$

Table 70: Total thermodynamic properties of C^+ ΔE=250 cm^{-1}

T [K]	C_p [J/mol/K]	S^0 [J/mol/K]	$H^0(T)$-$H^0(0)$ [KJ/mol]	$H^0(T)$-$H^0(298)$ [KJ/mol]	-(G^0-$H^0(0)$)/T [J/mol/K]	-(G^0-$H^0(298)$)/T [J/mol/K]	ΔH_f [KJ/mol]	Log(K_p)
50	2.589E+01	1.145E+02	1.224E+00	-5.425E+00	9.004E+01	2.230E+02	1.386E+03	-1.446E+03
100	2.250E+01	1.312E+02	2.417E+00	-4.233E+00	1.070E+02	1.735E+02	1.387E+03	-7.221E+02
150	2.155E+01	1.401E+02	3.513E+00	-3.136E+00	1.167E+02	1.610E+02	1.389E+03	-4.804E+02
200	2.121E+01	1.462E+02	4.581E+00	-2.068E+00	1.233E+02	1.566E+02	1.390E+03	-3.594E+02
298.15	2.097E+01	1.547E+02	6.649E+00	0.000E+00	1.324E+02	1.547E+02	1.392E+03	-2.399E+02
300	2.097E+01	1.548E+02	6.688E+00	3.878E-02	1.325E+02	1.547E+02	1.392E+03	-2.384E+02
400	2.089E+01	1.608E+02	8.780E+00	2.131E+00	1.389E+02	1.555E+02	1.394E+03	-1.778E+02
500	2.085E+01	1.655E+02	1.087E+01	4.218E+00	1.437E+02	1.570E+02	1.396E+03	-1.413E+02
600	2.083E+01	1.693E+02	1.295E+01	6.302E+00	1.477E+02	1.588E+02	1.399E+03	-1.170E+02
700	2.082E+01	1.725E+02	1.503E+01	8.384E+00	1.510E+02	1.605E+02	1.401E+03	-9.958E+01
800	2.081E+01	1.753E+02	1.711E+01	1.047E+01	1.539E+02	1.622E+02	1.403E+03	-8.650E+01
900	2.081E+01	1.777E+02	1.920E+01	1.255E+01	1.564E+02	1.638E+02	1.406E+03	-7.631E+01
1000	2.080E+01	1.799E+02	2.128E+01	1.463E+01	1.586E+02	1.653E+02	1.408E+03	-6.814E+01
2000	2.079E+01	1.943E+02	4.207E+01	3.542E+01	1.733E+02	1.766E+02	1.431E+03	-3.114E+01
3000	2.079E+01	2.028E+02	6.286E+01	5.621E+01	1.818E+02	1.840E+02	1.453E+03	-1.859E+01
4000	2.079E+01	2.087E+02	8.365E+01	7.700E+01	1.878E+02	1.895E+02	1.473E+03	-1.223E+01
5000	2.080E+01	2.134E+02	1.044E+02	9.779E+01	1.925E+02	1.938E+02	1.494E+03	-8.358E+00
6000	2.085E+01	2.172E+02	1.252E+02	1.186E+02	1.963E+02	1.974E+02	1.513E+03	-5.741E+00
7000	2.098E+01	2.204E+02	1.462E+02	1.395E+02	1.995E+02	2.004E+02	1.533E+03	-3.848E+00
8000	2.123E+01	2.232E+02	1.672E+02	1.606E+02	2.023E+02	2.031E+02	1.553E+03	-2.409E+00
9000	2.161E+01	2.257E+02	1.887E+02	1.820E+02	2.048E+02	2.055E+02	1.573E+03	-1.276E+00
10000	2.212E+01	2.280E+02	2.105E+02	2.039E+02	2.070E+02	2.076E+02	1.593E+03	-3.573E-01
11000	2.273E+01	2.302E+02	2.329E+02	2.263E+02	2.090E+02	2.096E+02	1.615E+03	4.042E-01
12000	2.343E+01	2.322E+02	2.560E+02	2.493E+02	2.108E+02	2.114E+02	1.637E+03	1.047E+00
13000	2.417E+01	2.341E+02	2.798E+02	2.731E+02	2.126E+02	2.131E+02	1.662E+03	1.600E+00
14000	2.495E+01	2.359E+02	3.044E+02	2.977E+02	2.142E+02	2.146E+02	1.687E+03	2.080E+00
15000	2.579E+01	2.376E+02	3.297E+02	3.231E+02	2.157E+02	2.161E+02	1.714E+03	2.503E+00
16000	2.678E+01	2.393E+02	3.560E+02	3.493E+02	2.171E+02	2.175E+02	1.742E+03	2.879E+00
17000	2.809E+01	2.410E+02	3.834E+02	3.767E+02	2.184E+02	2.188E+02	1.773E+03	3.216E+00
18000	2.999E+01	2.427E+02	4.124E+02	4.057E+02	2.197E+02	2.201E+02	1.805E+03	3.522E+00
19000	3.289E+01	2.443E+02	4.437E+02	4.370E+02	2.210E+02	2.213E+02	1.840E+03	3.800E+00
20000	3.734E+01	2.461E+02	4.786E+02	4.720E+02	2.222E+02	2.225E+02	1.880E+03	4.055E+00
21000	4.395E+01	2.481E+02	5.191E+02	5.124E+02	2.234E+02	2.237E+02	1.925E+03	4.292E+00
22000	5.331E+01	2.503E+02	5.675E+02	5.608E+02	2.246E+02	2.249E+02	1.979E+03	4.513E+00
23000	6.586E+01	2.530E+02	6.268E+02	6.201E+02	2.257E+02	2.260E+02	2.044E+03	4.720E+00
24000	8.159E+01	2.561E+02	7.002E+02	6.936E+02	2.269E+02	2.272E+02	2.123E+03	4.917E+00
25000	9.994E+01	2.598E+02	7.908E+02	7.842E+02	2.282E+02	2.284E+02	2.220E+03	5.106E+00
26000	1.196E+02	2.641E+02	9.006E+02	8.939E+02	2.295E+02	2.297E+02	2.336E+03	5.289E+00
27000	1.386E+02	2.690E+02	1.030E+03	1.023E+03	2.308E+02	2.311E+02	2.472E+03	5.467E+00
28000	1.547E+02	2.743E+02	1.177E+03	1.170E+03	2.323E+02	2.325E+02	2.626E+03	5.643E+00
29000	1.661E+02	2.800E+02	1.338E+03	1.331E+03	2.338E+02	2.341E+02	2.794E+03	5.817E+00
30000	1.715E+02	2.857E+02	1.507E+03	1.500E+03	2.355E+02	2.357E+02	2.971E+03	5.990E+00
32000	1.647E+02	2.967E+02	1.847E+03	1.840E+03	2.390E+02	2.392E+02	3.325E+03	6.333E+00
34000	1.423E+02	3.060E+02	2.155E+03	2.149E+03	2.427E+02	2.428E+02	3.650E+03	6.668E+00
36000	1.156E+02	3.134E+02	2.413E+03	2.407E+03	2.464E+02	2.466E+02	3.924E+03	6.991E+00
38000	9.159E+01	3.190E+02	2.620E+03	2.613E+03	2.501E+02	2.502E+02	4.147E+03	7.299E+00
40000	7.266E+01	3.232E+02	2.783E+03	2.776E+03	2.536E+02	2.538E+02	4.327E+03	7.590E+00
42000	5.867E+01	3.264E+02	2.914E+03	2.907E+03	2.570E+02	2.572E+02	4.475E+03	7.864E+00
44000	4.862E+01	3.289E+02	3.020E+03	3.014E+03	2.602E+02	2.604E+02	4.600E+03	8.121E+00
46000	4.146E+01	3.309E+02	3.110E+03	3.103E+03	2.633E+02	2.634E+02	4.707E+03	8.361E+00
48000	3.635E+01	3.325E+02	3.188E+03	3.181E+03	2.661E+02	2.662E+02	4.803E+03	8.586E+00
50000	3.267E+01	3.339E+02	3.256E+03	3.250E+03	2.688E+02	2.689E+02	4.890E+03	8.797E+00

Table 71: Internal thermodynamic properties of C^+ ΔE=500 cm^{-1}

T(K)	Q_{int}	$\ln(Q_{int})$	E_{int}/RT	$C_{p,int}/R$
50	$2.645E+00$	$9.726E-01$	$4.450E-01$	$6.140E-01$
100	$3.606E+00$	$1.283E+00$	$4.064E-01$	$2.057E-01$
150	$4.177E+00$	$1.430E+00$	$3.170E-01$	$9.234E-02$
200	$4.535E+00$	$1.512E+00$	$2.550E-01$	$5.131E-02$
298.15	$4.945E+00$	$1.598E+00$	$1.823E-01$	$2.256E-02$
300	$4.951E+00$	$1.600E+00$	$1.813E-01$	$2.227E-02$
400	$5.184E+00$	$1.646E+00$	$1.401E-01$	$1.233E-02$
500	$5.333E+00$	$1.674E+00$	$1.141E-01$	$7.806E-03$
600	$5.436E+00$	$1.693E+00$	$9.612E-02$	$5.379E-03$
700	$5.511E+00$	$1.707E+00$	$8.305E-02$	$3.929E-03$
800	$5.569E+00$	$1.717E+00$	$7.310E-02$	$2.994E-03$
900	$5.614E+00$	$1.725E+00$	$6.527E-02$	$2.357E-03$
1000	$5.651E+00$	$1.732E+00$	$5.895E-02$	$1.904E-03$
2000	$5.822E+00$	$1.762E+00$	$2.995E-02$	$4.694E-04$
3000	$5.880E+00$	$1.772E+00$	$2.007E-02$	$2.086E-04$
4000	$5.910E+00$	$1.777E+00$	$1.510E-02$	$2.085E-04$
5000	$5.928E+00$	$1.780E+00$	$1.220E-02$	$1.372E-03$
6000	$5.940E+00$	$1.782E+00$	$1.077E-02$	$7.140E-03$
7000	$5.950E+00$	$1.783E+00$	$1.122E-02$	$2.280E-02$
8000	$5.960E+00$	$1.785E+00$	$1.438E-02$	$5.280E-02$
9000	$5.972E+00$	$1.787E+00$	$2.107E-02$	$9.896E-02$
10000	$5.988E+00$	$1.790E+00$	$3.181E-02$	$1.604E-01$
11000	$6.011E+00$	$1.794E+00$	$4.677E-02$	$2.343E-01$
12000	$6.040E+00$	$1.798E+00$	$6.580E-02$	$3.172E-01$
13000	$6.077E+00$	$1.805E+00$	$8.851E-02$	$4.056E-01$
14000	$6.123E+00$	$1.812E+00$	$1.144E-01$	$4.970E-01$
15000	$6.177E+00$	$1.821E+00$	$1.430E-01$	$5.908E-01$
16000	$6.241E+00$	$1.831E+00$	$1.741E-01$	$6.893E-01$
17000	$6.313E+00$	$1.843E+00$	$2.075E-01$	$7.993E-01$
18000	$6.395E+00$	$1.855E+00$	$2.440E-01$	$9.330E-01$
19000	$6.487E+00$	$1.870E+00$	$2.846E-01$	$1.109E+00$
20000	$6.590E+00$	$1.886E+00$	$3.316E-01$	$1.352E+00$
21000	$6.706E+00$	$1.903E+00$	$3.878E-01$	$1.692E+00$
22000	$6.839E+00$	$1.923E+00$	$4.572E-01$	$2.163E+00$
23000	$6.992E+00$	$1.945E+00$	$5.445E-01$	$2.795E+00$
24000	$7.172E+00$	$1.970E+00$	$6.546E-01$	$3.613E+00$
25000	$7.386E+00$	$2.000E+00$	$7.926E-01$	$4.628E+00$
26000	$7.644E+00$	$2.034E+00$	$9.627E-01$	$5.828E+00$
27000	$7.956E+00$	$2.074E+00$	$1.167E+00$	$7.176E+00$
28000	$8.336E+00$	$2.121E+00$	$1.407E+00$	$8.606E+00$
29000	$8.799E+00$	$2.175E+00$	$1.680E+00$	$1.003E+01$
30000	$9.362E+00$	$2.237E+00$	$1.981E+00$	$1.134E+01$
32000	$1.086E+01$	$2.385E+00$	$2.631E+00$	$1.324E+01$
34000	$1.299E+01$	$2.564E+00$	$3.279E+00$	$1.381E+01$
36000	$1.593E+01$	$2.768E+00$	$3.850E+00$	$1.311E+01$
38000	$1.987E+01$	$2.989E+00$	$4.299E+00$	$1.158E+01$
40000	$2.498E+01$	$3.218E+00$	$4.617E+00$	$9.721E+00$
42000	$3.146E+01$	$3.449E+00$	$4.817E+00$	$7.904E+00$
44000	$3.947E+01$	$3.676E+00$	$4.920E+00$	$6.313E+00$
46000	$4.916E+01$	$3.895E+00$	$4.951E+00$	$5.003E+00$
48000	$6.068E+01$	$4.106E+00$	$4.930E+00$	$3.960E+00$
50000	$7.413E+01$	$4.306E+00$	$4.875E+00$	$3.145E+00$

Table 72: Total thermodynamic properties of C^+ ΔE=500 cm^{-1}

T [K]	C_p [J/mol/K]	S^0 [J/mol/K]	$H^0(T)-H^0(0)$ [KJ/mol]	$H^0(T)-H^0(298)$ [KJ/mol]	$-(G^0-H^0(0))/T$ [J/mol/K]	$-(G^0-H^0(298))/T$ [J/mol/K]	ΔH_f [KJ/mol]	$Log(K_p)$
50	2.589E+01	1.145E+02	1.224E+00	-5.425E+00	9.004E+01	2.230E+02	1.386E+03	-1.446E+03
100	2.250E+01	1.312E+02	2.417E+00	-4.233E+00	1.070E+02	1.735E+02	1.387E+03	-7.221E+02
150	2.155E+01	1.401E+02	3.513E+00	-3.136E+00	1.167E+02	1.610E+02	1.389E+03	-4.804E+02
200	2.121E+01	1.462E+02	4.581E+00	-2.068E+00	1.233E+02	1.566E+02	1.390E+03	-3.594E+02
298.15	2.097E+01	1.547E+02	6.649E+00	0.000E+00	1.324E+02	1.547E+02	1.392E+03	-2.399E+02
300	2.097E+01	1.548E+02	6.688E+00	3.878E-02	1.325E+02	1.547E+02	1.392E+03	-2.384E+02
400	2.089E+01	1.608E+02	8.780E+00	2.131E+00	1.389E+02	1.555E+02	1.394E+03	-1.778E+02
500	2.085E+01	1.655E+02	1.087E+01	4.218E+00	1.437E+02	1.570E+02	1.396E+03	-1.413E+02
600	2.083E+01	1.693E+02	1.295E+01	6.302E+00	1.477E+02	1.588E+02	1.399E+03	-1.170E+02
700	2.082E+01	1.725E+02	1.503E+01	8.384E+00	1.510E+02	1.605E+02	1.401E+03	-9.958E+01
800	2.081E+01	1.753E+02	1.711E+01	1.047E+01	1.539E+02	1.622E+02	1.403E+03	-8.650E+01
900	2.081E+01	1.777E+02	1.920E+01	1.255E+01	1.564E+02	1.638E+02	1.406E+03	-7.631E+01
1000	2.080E+01	1.799E+02	2.128E+01	1.463E+01	1.586E+02	1.653E+02	1.408E+03	-6.814E+01
2000	2.079E+01	1.943E+02	4.207E+01	3.542E+01	1.733E+02	1.766E+02	1.431E+03	-3.114E+01
3000	2.079E+01	2.028E+02	6.286E+01	5.621E+01	1.818E+02	1.840E+02	1.453E+03	-1.859E+01
4000	2.079E+01	2.087E+02	8.365E+01	7.700E+01	1.878E+02	1.895E+02	1.473E+03	-1.223E+01
5000	2.080E+01	2.134E+02	1.044E+02	9.779E+01	1.925E+02	1.938E+02	1.494E+03	-8.358E+00
6000	2.085E+01	2.172E+02	1.252E+02	1.186E+02	1.963E+02	1.974E+02	1.513E+03	-5.741E+00
7000	2.098E+01	2.204E+02	1.462E+02	1.395E+02	1.995E+02	2.004E+02	1.533E+03	-3.848E+00
8000	2.123E+01	2.232E+02	1.672E+02	1.606E+02	2.023E+02	2.031E+02	1.553E+03	-2.409E+00
9000	2.161E+01	2.257E+02	1.887E+02	1.820E+02	2.048E+02	2.055E+02	1.573E+03	-1.276E+00
10000	2.212E+01	2.280E+02	2.105E+02	2.039E+02	2.070E+02	2.076E+02	1.593E+03	-3.573E-01
11000	2.273E+01	2.302E+02	2.329E+02	2.263E+02	2.090E+02	2.096E+02	1.615E+03	4.042E-01
12000	2.342E+01	2.322E+02	2.560E+02	2.493E+02	2.108E+02	2.114E+02	1.637E+03	1.047E+00
13000	2.416E+01	2.341E+02	2.798E+02	2.731E+02	2.126E+02	2.131E+02	1.662E+03	1.600E+00
14000	2.492E+01	2.359E+02	3.043E+02	2.977E+02	2.142E+02	2.146E+02	1.687E+03	2.080E+00
15000	2.570E+01	2.376E+02	3.296E+02	3.230E+02	2.157E+02	2.161E+02	1.714E+03	2.503E+00
16000	2.652E+01	2.393E+02	3.557E+02	3.491E+02	2.171E+02	2.175E+02	1.742E+03	2.879E+00
17000	2.743E+01	2.409E+02	3.827E+02	3.761E+02	2.184E+02	2.188E+02	1.772E+03	3.216E+00
18000	2.854E+01	2.426E+02	4.107E+02	4.040E+02	2.197E+02	2.201E+02	1.803E+03	3.521E+00
19000	3.001E+01	2.441E+02	4.399E+02	4.332E+02	2.210E+02	2.213E+02	1.837E+03	3.799E+00
20000	3.203E+01	2.457E+02	4.709E+02	4.642E+02	2.222E+02	2.225E+02	1.872E+03	4.054E+00
21000	3.485E+01	2.473E+02	5.042E+02	4.976E+02	2.233E+02	2.237E+02	1.910E+03	4.289E+00
22000	3.877E+01	2.491E+02	5.409E+02	5.343E+02	2.245E+02	2.248E+02	1.952E+03	4.507E+00
23000	4.402E+01	2.509E+02	5.822E+02	5.756E+02	2.256E+02	2.259E+02	1.999E+03	4.711E+00
24000	5.083E+01	2.529E+02	6.295E+02	6.229E+02	2.267E+02	2.269E+02	2.052E+03	4.903E+00
25000	5.927E+01	2.551E+02	6.844E+02	6.778E+02	2.278E+02	2.280E+02	2.113E+03	5.084E+00
26000	6.925E+01	2.576E+02	7.485E+02	7.419E+02	2.289E+02	2.291E+02	2.184E+03	5.257E+00
27000	8.045E+01	2.605E+02	8.233E+02	8.167E+02	2.300E+02	2.302E+02	2.266E+03	5.422E+00
28000	9.234E+01	2.636E+02	9.097E+02	9.030E+02	2.311E+02	2.314E+02	2.359E+03	5.582E+00
29000	1.042E+02	2.671E+02	1.008E+03	1.001E+03	2.323E+02	2.325E+02	2.464E+03	5.737E+00
30000	1.150E+02	2.708E+02	1.118E+03	1.111E+03	2.335E+02	2.337E+02	2.581E+03	5.888E+00
32000	1.308E+02	2.788E+02	1.365E+03	1.358E+03	2.361E+02	2.363E+02	2.844E+03	6.183E+00
34000	1.357E+02	2.869E+02	1.634E+03	1.627E+03	2.388E+02	2.390E+02	3.128E+03	6.469E+00
36000	1.298E+02	2.945E+02	1.901E+03	1.894E+03	2.417E+02	2.419E+02	3.411E+03	6.748E+00
38000	1.171E+02	3.012E+02	2.148E+03	2.142E+03	2.447E+02	2.449E+02	3.676E+03	7.019E+00
40000	1.016E+02	3.068E+02	2.367E+03	2.360E+03	2.477E+02	2.478E+02	3.912E+03	7.279E+00
42000	8.650E+01	3.114E+02	2.555E+03	2.548E+03	2.506E+02	2.508E+02	4.117E+03	7.529E+00
44000	7.327E+01	3.151E+02	2.714E+03	2.708E+03	2.534E+02	2.536E+02	4.294E+03	7.767E+00
46000	6.238E+01	3.181E+02	2.850E+03	2.843E+03	2.562E+02	2.563E+02	4.447E+03	7.992E+00
48000	5.371E+01	3.206E+02	2.965E+03	2.959E+03	2.588E+02	2.590E+02	4.581E+03	8.206E+00
50000	4.694E+01	3.227E+02	3.066E+03	3.059E+03	2.613E+02	2.615E+02	4.699E+03	8.408E+00

Table 73: Internal thermodynamic properties of C^+ ΔE=1000 cm^{-1}

T(K)	Q_{int}	$\ln(Q_{int})$	E_{int}/RT	$C_{p,int}/R$
50	$2.645E+00$	$9.726E-01$	$4.450E-01$	$6.140E-01$
100	$3.606E+00$	$1.283E+00$	$4.064E-01$	$2.057E-01$
150	$4.177E+00$	$1.430E+00$	$3.170E-01$	$9.234E-02$
200	$4.535E+00$	$1.512E+00$	$2.550E-01$	$5.131E-02$
298.15	$4.945E+00$	$1.598E+00$	$1.823E-01$	$2.256E-02$
300	$4.951E+00$	$1.600E+00$	$1.813E-01$	$2.227E-02$
400	$5.184E+00$	$1.646E+00$	$1.401E-01$	$1.233E-02$
500	$5.333E+00$	$1.674E+00$	$1.141E-01$	$7.806E-03$
600	$5.436E+00$	$1.693E+00$	$9.612E-02$	$5.379E-03$
700	$5.511E+00$	$1.707E+00$	$8.305E-02$	$3.929E-03$
800	$5.569E+00$	$1.717E+00$	$7.310E-02$	$2.994E-03$
900	$5.614E+00$	$1.725E+00$	$6.527E-02$	$2.357E-03$
1000	$5.651E+00$	$1.732E+00$	$5.895E-02$	$1.904E-03$
2000	$5.822E+00$	$1.762E+00$	$2.995E-02$	$4.694E-04$
3000	$5.880E+00$	$1.772E+00$	$2.007E-02$	$2.086E-04$
4000	$5.910E+00$	$1.777E+00$	$1.510E-02$	$2.085E-04$
5000	$5.928E+00$	$1.780E+00$	$1.220E-02$	$1.372E-03$
6000	$5.940E+00$	$1.782E+00$	$1.077E-02$	$7.140E-03$
7000	$5.950E+00$	$1.783E+00$	$1.122E-02$	$2.280E-02$
8000	$5.960E+00$	$1.785E+00$	$1.438E-02$	$5.280E-02$
9000	$5.972E+00$	$1.787E+00$	$2.107E-02$	$9.896E-02$
10000	$5.988E+00$	$1.790E+00$	$3.181E-02$	$1.604E-01$
11000	$6.011E+00$	$1.794E+00$	$4.677E-02$	$2.343E-01$
12000	$6.040E+00$	$1.798E+00$	$6.580E-02$	$3.171E-01$
13000	$6.077E+00$	$1.805E+00$	$8.850E-02$	$4.052E-01$
14000	$6.123E+00$	$1.812E+00$	$1.143E-01$	$4.956E-01$
15000	$6.177E+00$	$1.821E+00$	$1.428E-01$	$5.864E-01$
16000	$6.240E+00$	$1.831E+00$	$1.733E-01$	$6.770E-01$
17000	$6.312E+00$	$1.843E+00$	$2.057E-01$	$7.690E-01$
18000	$6.393E+00$	$1.855E+00$	$2.396E-01$	$8.664E-01$
19000	$6.483E+00$	$1.869E+00$	$2.754E-01$	$9.757E-01$
20000	$6.581E+00$	$1.884E+00$	$3.136E-01$	$1.106E+00$
21000	$6.689E+00$	$1.901E+00$	$3.550E-01$	$1.268E+00$
22000	$6.808E+00$	$1.918E+00$	$4.010E-01$	$1.475E+00$
23000	$6.938E+00$	$1.937E+00$	$4.532E-01$	$1.739E+00$
24000	$7.082E+00$	$1.958E+00$	$5.135E-01$	$2.074E+00$
25000	$7.242E+00$	$1.980E+00$	$5.839E-01$	$2.488E+00$
26000	$7.421E+00$	$2.004E+00$	$6.665E-01$	$2.989E+00$
27000	$7.624E+00$	$2.031E+00$	$7.631E-01$	$3.575E+00$
28000	$7.854E+00$	$2.061E+00$	$8.752E-01$	$4.240E+00$
29000	$8.117E+00$	$2.094E+00$	$1.004E+00$	$4.970E+00$
30000	$8.418E+00$	$2.130E+00$	$1.149E+00$	$5.742E+00$
32000	$9.160E+00$	$2.215E+00$	$1.485E+00$	$7.295E+00$
34000	$1.014E+01$	$2.316E+00$	$1.868E+00$	$8.636E+00$
36000	$1.141E+01$	$2.434E+00$	$2.271E+00$	$9.534E+00$
38000	$1.304E+01$	$2.568E+00$	$2.665E+00$	$9.873E+00$
40000	$1.509E+01$	$2.714E+00$	$3.022E+00$	$9.676E+00$
42000	$1.762E+01$	$2.869E+00$	$3.326E+00$	$9.067E+00$
44000	$2.068E+01$	$3.029E+00$	$3.568E+00$	$8.207E+00$
46000	$2.434E+01$	$3.192E+00$	$3.749E+00$	$7.243E+00$
48000	$2.863E+01$	$3.355E+00$	$3.874E+00$	$6.280E+00$
50000	$3.360E+01$	$3.514E+00$	$3.952E+00$	$5.384E+00$

Table 74: Total thermodynamic properties of C^+ ΔE=1000 cm^{-1}

T [K]	C_p [J/mol/K]	S^0 [J/mol/K]	$H^0(T)$-$H^0(0)$ [KJ/mol]	$H^0(T)$-$H^0(298)$ [KJ/mol]	-(G^0-$H^0(0)$)/T [J/mol/K]	-(G^0-$H^0(298)$)/T [J/mol/K]	ΔH_f [KJ/mol]	Log(K_p)
50	2.589E+01	1.145E+02	1.224E+00	-5.425E+00	9.004E+01	2.230E+02	1.386E+03	-1.446E+03
100	2.250E+01	1.312E+02	2.417E+00	-4.233E+00	1.070E+02	1.735E+02	1.387E+03	-7.221E+02
150	2.155E+01	1.401E+02	3.513E+00	-3.136E+00	1.167E+02	1.610E+02	1.389E+03	-4.804E+02
200	2.121E+01	1.462E+02	4.581E+00	-2.068E+00	1.233E+02	1.566E+02	1.390E+03	-3.594E+02
298.15	2.097E+01	1.547E+02	6.649E+00	0.000E+00	1.324E+02	1.547E+02	1.392E+03	-2.399E+02
300	2.097E+01	1.548E+02	6.688E+00	3.878E-02	1.325E+02	1.547E+02	1.392E+03	-2.384E+02
400	2.089E+01	1.608E+02	8.780E+00	2.131E+00	1.389E+02	1.555E+02	1.394E+03	-1.778E+02
500	2.085E+01	1.655E+02	1.087E+01	4.218E+00	1.437E+02	1.570E+02	1.396E+03	-1.413E+02
600	2.083E+01	1.693E+02	1.295E+01	6.302E+00	1.477E+02	1.588E+02	1.399E+03	-1.170E+02
700	2.082E+01	1.725E+02	1.503E+01	8.384E+00	1.510E+02	1.605E+02	1.401E+03	-9.958E+01
800	2.081E+01	1.753E+02	1.711E+01	1.047E+01	1.539E+02	1.622E+02	1.403E+03	-8.650E+01
900	2.081E+01	1.777E+02	1.920E+01	1.255E+01	1.564E+02	1.638E+02	1.406E+03	-7.631E+01
1000	2.080E+01	1.799E+02	2.128E+01	1.463E+01	1.586E+02	1.653E+02	1.408E+03	-6.814E+01
2000	2.079E+01	1.943E+02	4.207E+01	3.542E+01	1.733E+02	1.766E+02	1.431E+03	-3.114E+01
3000	2.079E+01	2.028E+02	6.286E+01	5.621E+01	1.818E+02	1.840E+02	1.453E+03	-1.859E+01
4000	2.079E+01	2.087E+02	8.365E+01	7.700E+01	1.878E+02	1.895E+02	1.473E+03	-1.223E+01
5000	2.080E+01	2.134E+02	1.044E+02	9.779E+01	1.925E+02	1.938E+02	1.494E+03	-8.358E+00
6000	2.085E+01	2.172E+02	1.252E+02	1.186E+02	1.963E+02	1.974E+02	1.513E+03	-5.741E+00
7000	2.098E+01	2.204E+02	1.462E+02	1.395E+02	1.995E+02	2.004E+02	1.533E+03	-3.848E+00
8000	2.123E+01	2.232E+02	1.672E+02	1.606E+02	2.023E+02	2.031E+02	1.553E+03	-2.409E+00
9000	2.161E+01	2.257E+02	1.887E+02	1.820E+02	2.048E+02	2.055E+02	1.573E+03	-1.276E+00
10000	2.212E+01	2.280E+02	2.105E+02	2.039E+02	2.070E+02	2.076E+02	1.593E+03	-3.573E-01
11000	2.273E+01	2.302E+02	2.329E+02	2.263E+02	2.090E+02	2.096E+02	1.615E+03	4.042E-01
12000	2.342E+01	2.322E+02	2.560E+02	2.493E+02	2.108E+02	2.114E+02	1.637E+03	1.047E+00
13000	2.416E+01	2.341E+02	2.798E+02	2.731E+02	2.126E+02	2.131E+02	1.662E+03	1.600E+00
14000	2.491E+01	2.359E+02	3.043E+02	2.977E+02	2.142E+02	2.146E+02	1.687E+03	2.080E+00
15000	2.566E+01	2.376E+02	3.296E+02	3.229E+02	2.157E+02	2.161E+02	1.714E+03	2.503E+00
16000	2.641E+01	2.393E+02	3.556E+02	3.490E+02	2.171E+02	2.175E+02	1.742E+03	2.879E+00
17000	2.718E+01	2.409E+02	3.824E+02	3.758E+02	2.184E+02	2.188E+02	1.772E+03	3.216E+00
18000	2.799E+01	2.425E+02	4.100E+02	4.034E+02	2.197E+02	2.201E+02	1.803E+03	3.521E+00
19000	2.890E+01	2.441E+02	4.384E+02	4.318E+02	2.210E+02	2.213E+02	1.835E+03	3.799E+00
20000	2.998E+01	2.456E+02	4.679E+02	4.612E+02	2.222E+02	2.225E+02	1.869E+03	4.053E+00
21000	3.133E+01	2.471E+02	4.985E+02	4.919E+02	2.233E+02	2.236E+02	1.904E+03	4.288E+00
22000	3.305E+01	2.486E+02	5.306E+02	5.240E+02	2.244E+02	2.247E+02	1.942E+03	4.505E+00
23000	3.525E+01	2.501E+02	5.648E+02	5.581E+02	2.255E+02	2.258E+02	1.982E+03	4.708E+00
24000	3.803E+01	2.516E+02	6.013E+02	5.947E+02	2.266E+02	2.268E+02	2.024E+03	4.897E+00
25000	4.148E+01	2.532E+02	6.410E+02	6.344E+02	2.276E+02	2.279E+02	2.070E+03	5.075E+00
26000	4.564E+01	2.549E+02	6.845E+02	6.779E+02	2.286E+02	2.289E+02	2.120E+03	5.244E+00
27000	5.051E+01	2.568E+02	7.325E+02	7.259E+02	2.296E+02	2.299E+02	2.175E+03	5.404E+00
28000	5.604E+01	2.587E+02	7.858E+02	7.791E+02	2.306E+02	2.309E+02	2.235E+03	5.556E+00
29000	6.211E+01	2.608E+02	8.448E+02	8.382E+02	2.316E+02	2.319E+02	2.301E+03	5.702E+00
30000	6.853E+01	2.630E+02	9.101E+02	9.035E+02	2.326E+02	2.329E+02	2.374E+03	5.842E+00
32000	8.144E+01	2.678E+02	1.060E+03	1.054E+03	2.347E+02	2.349E+02	2.539E+03	6.109E+00
34000	9.259E+01	2.731E+02	1.235E+03	1.228E+03	2.368E+02	2.370E+02	2.729E+03	6.361E+00
36000	1.001E+02	2.786E+02	1.428E+03	1.421E+03	2.390E+02	2.391E+02	2.939E+03	6.603E+00
38000	1.029E+02	2.841E+02	1.632E+03	1.625E+03	2.412E+02	2.414E+02	3.159E+03	6.835E+00
40000	1.012E+02	2.894E+02	1.837E+03	1.830E+03	2.435E+02	2.436E+02	3.381E+03	7.060E+00
42000	9.617E+01	2.942E+02	2.034E+03	2.028E+03	2.458E+02	2.459E+02	3.596E+03	7.277E+00
44000	8.902E+01	2.985E+02	2.220E+03	2.213E+03	2.481E+02	2.482E+02	3.799E+03	7.486E+00
46000	8.100E+01	3.023E+02	2.390E+03	2.383E+03	2.503E+02	2.505E+02	3.987E+03	7.687E+00
48000	7.300E+01	3.056E+02	2.544E+03	2.537E+03	2.526E+02	2.527E+02	4.159E+03	7.880E+00
50000	6.555E+01	3.084E+02	2.682E+03	2.676E+03	2.548E+02	2.549E+02	4.316E+03	8.064E+00

Table 75: Internal thermodynamic properties of C^{2+} ΔE=250 cm^{-1}

T(K)	Q_{int}	$\ln(Q_{int})$	E_{int}/RT	$C_{p,int}/R$
50	$1.000E+00$	$0.000E+00$	$0.000E+00$	$0.000E+00$
100	$1.000E+00$	$0.000E+00$	$0.000E+00$	$0.000E+00$
150	$1.000E+00$	$0.000E+00$	$2.063E-215$	$1.037E-212$
200	$1.000E+00$	$0.000E+00$	$5.901E-161$	$2.225E-158$
298.15	$1.000E+00$	$0.000E+00$	$3.193E-107$	$8.075E-105$
300	$1.000E+00$	$0.000E+00$	$1.510E-106$	$3.795E-104$
400	$1.000E+00$	$0.000E+00$	$2.223E-79$	$4.191E-77$
500	$1.000E+00$	$0.000E+00$	$4.227E-63$	$6.376E-61$
600	$1.000E+00$	$0.000E+00$	$2.914E-52$	$3.662E-50$
700	$1.000E+00$	$0.000E+00$	$1.570E-44$	$1.691E-42$
800	$1.000E+00$	$0.000E+00$	$9.695E-39$	$9.139E-37$
900	$1.000E+00$	$0.000E+00$	$3.051E-34$	$2.557E-32$
1000	$1.000E+00$	$0.000E+00$	$1.197E-30$	$9.024E-29$
2000	$1.000E+00$	$4.441E-16$	$1.425E-14$	$5.372E-13$
3000	$1.000E+00$	$1.087E-10$	$2.733E-09$	$6.870E-08$
4000	$1.000E+00$	$5.831E-08$	$1.099E-06$	$2.073E-05$
5000	$1.000E+00$	$2.532E-06$	$3.819E-05$	$5.760E-04$
6000	$1.000E+00$	$3.128E-05$	$3.931E-04$	$4.941E-03$
7000	$1.000E+00$	$1.884E-04$	$2.029E-03$	$2.186E-02$
8000	$1.001E+00$	$7.242E-04$	$6.825E-03$	$6.430E-02$
9000	$1.002E+00$	$2.063E-03$	$1.727E-02$	$1.445E-01$
10000	$1.005E+00$	$4.763E-03$	$3.585E-02$	$2.692E-01$
11000	$1.009E+00$	$9.435E-03$	$6.442E-02$	$4.380E-01$
12000	$1.017E+00$	$1.665E-02$	$1.039E-01$	$6.433E-01$
13000	$1.027E+00$	$2.688E-02$	$1.541E-01$	$8.728E-01$
14000	$1.041E+00$	$4.044E-02$	$2.140E-01$	$1.112E+00$
15000	$1.059E+00$	$5.747E-02$	$2.817E-01$	$1.347E+00$
16000	$1.081E+00$	$7.797E-02$	$3.552E-01$	$1.564E+00$
17000	$1.107E+00$	$1.018E-01$	$4.321E-01$	$1.755E+00$
18000	$1.137E+00$	$1.287E-01$	$5.102E-01$	$1.915E+00$
19000	$1.172E+00$	$1.584E-01$	$5.875E-01$	$2.040E+00$
20000	$1.210E+00$	$1.904E-01$	$6.626E-01$	$2.133E+00$
21000	$1.252E+00$	$2.245E-01$	$7.342E-01$	$2.194E+00$
22000	$1.297E+00$	$2.602E-01$	$8.015E-01$	$2.230E+00$
23000	$1.346E+00$	$2.973E-01$	$8.639E-01$	$2.244E+00$
24000	$1.398E+00$	$3.353E-01$	$9.214E-01$	$2.243E+00$
25000	$1.453E+00$	$3.740E-01$	$9.741E-01$	$2.235E+00$
26000	$1.512E+00$	$4.131E-01$	$1.022E+00$	$2.228E+00$
27000	$1.572E+00$	$4.526E-01$	$1.067E+00$	$2.235E+00$
28000	$1.636E+00$	$4.921E-01$	$1.109E+00$	$2.270E+00$
29000	$1.702E+00$	$5.318E-01$	$1.151E+00$	$2.355E+00$
30000	$1.771E+00$	$5.715E-01$	$1.193E+00$	$2.516E+00$
32000	$1.919E+00$	$6.516E-01$	$1.294E+00$	$3.206E+00$
34000	$2.084E+00$	$7.342E-01$	$1.446E+00$	$4.686E+00$
36000	$2.278E+00$	$8.233E-01$	$1.693E+00$	$7.347E+00$
38000	$2.521E+00$	$9.247E-01$	$2.092E+00$	$1.144E+01$
40000	$2.847E+00$	$1.046E+00$	$2.688E+00$	$1.672E+01$
42000	$3.307E+00$	$1.196E+00$	$3.489E+00$	$2.222E+01$
44000	$3.975E+00$	$1.380E+00$	$4.443E+00$	$2.640E+01$
46000	$4.951E+00$	$1.600E+00$	$5.443E+00$	$2.797E+01$
48000	$6.367E+00$	$1.851E+00$	$6.364E+00$	$2.672E+01$
50000	$8.389E+00$	$2.127E+00$	$7.118E+00$	$2.346E+01$

Table 76: Total thermodynamic properties of C^{2+} ΔE=250 cm^{-1}

T [K]	C_p [J/mol/K]	S^0 [J/mol/K]	$H^0(T)-H^0(0)$ [KJ/mol]	$H^0(T)-H^0(298)$ [KJ/mol]	$-(G^0-H^0(0))/T$ [J/mol/K]	$-(G^0-H^0(298))/T$ [J/mol/K]	ΔH_f [KJ/mol]	$Log(K_p)$
50	2.079E+01	1.027E+02	1.039E+00	-5.158E+00	8.196E+01	2.059E+02	3.739E+03	-3.906E+03
100	2.079E+01	1.172E+02	2.079E+00	-4.119E+00	9.636E+01	1.583E+02	3.742E+03	-1.953E+03
150	2.079E+01	1.256E+02	3.118E+00	-3.079E+00	1.048E+02	1.461E+02	3.744E+03	-1.301E+03
200	2.079E+01	1.316E+02	4.157E+00	-2.040E+00	1.108E+02	1.418E+02	3.746E+03	-9.750E+02
298.15	2.079E+01	1.399E+02	6.197E+00	0.000E+00	1.191E+02	1.399E+02	3.750E+03	-6.527E+02
300	2.079E+01	1.400E+02	6.236E+00	3.848E-02	1.192E+02	1.399E+02	3.750E+03	-6.487E+02
400	2.079E+01	1.460E+02	8.315E+00	2.117E+00	1.252E+02	1.407E+02	3.754E+03	-4.854E+02
500	2.079E+01	1.506E+02	1.039E+01	4.196E+00	1.298E+02	1.422E+02	3.759E+03	-3.872E+02
600	2.079E+01	1.544E+02	1.247E+01	6.274E+00	1.336E+02	1.439E+02	3.763E+03	-3.218E+02
700	2.079E+01	1.576E+02	1.455E+01	8.353E+00	1.368E+02	1.457E+02	3.768E+03	-2.749E+02
800	2.079E+01	1.604E+02	1.663E+01	1.043E+01	1.396E+02	1.473E+02	3.772E+03	-2.398E+02
900	2.079E+01	1.628E+02	1.871E+01	1.251E+01	1.420E+02	1.489E+02	3.777E+03	-2.124E+02
1000	2.079E+01	1.650E+02	2.079E+01	1.459E+01	1.442E+02	1.504E+02	3.781E+03	-1.905E+02
2000	2.079E+01	1.794E+02	4.157E+01	3.538E+01	1.586E+02	1.617E+02	3.825E+03	-9.127E+01
3000	2.079E+01	1.878E+02	6.236E+01	5.616E+01	1.671E+02	1.691E+02	3.867E+03	-5.781E+01
4000	2.079E+01	1.938E+02	8.314E+01	7.695E+01	1.730E+02	1.746E+02	3.909E+03	-4.089E+01
5000	2.079E+01	1.985E+02	1.039E+02	9.774E+01	1.777E+02	1.789E+02	3.950E+03	-3.064E+01
6000	2.083E+01	2.023E+02	1.247E+02	1.185E+02	1.815E+02	1.825E+02	3.990E+03	-2.373E+01
7000	2.097E+01	2.055E+02	1.456E+02	1.394E+02	1.847E+02	1.856E+02	4.031E+03	-1.874E+01
8000	2.132E+01	2.083E+02	1.667E+02	1.606E+02	1.875E+02	1.882E+02	4.071E+03	-1.496E+01
9000	2.199E+01	2.108E+02	1.884E+02	1.822E+02	1.899E+02	1.906E+02	4.112E+03	-1.199E+01
10000	2.302E+01	2.132E+02	2.108E+02	2.047E+02	1.921E+02	1.928E+02	4.154E+03	-9.597E+00
11000	2.443E+01	2.155E+02	2.345E+02	2.283E+02	1.942E+02	1.947E+02	4.198E+03	-7.615E+00
12000	2.614E+01	2.177E+02	2.598E+02	2.536E+02	1.960E+02	1.965E+02	4.243E+03	-5.945E+00
13000	2.804E+01	2.198E+02	2.869E+02	2.807E+02	1.978E+02	1.982E+02	4.292E+03	-4.516E+00
14000	3.003E+01	2.220E+02	3.159E+02	3.097E+02	1.994E+02	1.999E+02	4.342E+03	-3.278E+00
15000	3.198E+01	2.241E+02	3.469E+02	3.407E+02	2.010E+02	2.014E+02	4.396E+03	-2.191E+00
16000	3.379E+01	2.262E+02	3.798E+02	3.736E+02	2.025E+02	2.029E+02	4.452E+03	-1.229E+00
17000	3.538E+01	2.283E+02	4.144E+02	4.082E+02	2.040E+02	2.043E+02	4.510E+03	-3.684E-01
18000	3.671E+01	2.304E+02	4.505E+02	4.443E+02	2.054E+02	2.057E+02	4.570E+03	4.065E-01
19000	3.775E+01	2.324E+02	4.878E+02	4.816E+02	2.068E+02	2.071E+02	4.632E+03	1.109E+00
20000	3.852E+01	2.344E+02	5.259E+02	5.197E+02	2.081E+02	2.084E+02	4.695E+03	1.750E+00
21000	3.903E+01	2.363E+02	5.647E+02	5.585E+02	2.094E+02	2.097E+02	4.760E+03	2.338E+00
22000	3.932E+01	2.381E+02	6.039E+02	5.977E+02	2.106E+02	2.109E+02	4.825E+03	2.880E+00
23000	3.944E+01	2.398E+02	6.433E+02	6.371E+02	2.119E+02	2.121E+02	4.891E+03	3.381E+00
24000	3.944E+01	2.415E+02	6.827E+02	6.765E+02	2.131E+02	2.133E+02	4.957E+03	3.847E+00
25000	3.937E+01	2.431E+02	7.221E+02	7.160E+02	2.142E+02	2.145E+02	5.023E+03	4.281E+00
26000	3.931E+01	2.447E+02	7.615E+02	7.553E+02	2.154E+02	2.156E+02	5.090E+03	4.688E+00
27000	3.937E+01	2.462E+02	8.008E+02	7.946E+02	2.165E+02	2.167E+02	5.157E+03	5.069E+00
28000	3.966E+01	2.476E+02	8.403E+02	8.341E+02	2.176E+02	2.178E+02	5.224E+03	5.428E+00
29000	4.037E+01	2.490E+02	8.803E+02	8.741E+02	2.186E+02	2.188E+02	5.292E+03	5.766E+00
30000	4.171E+01	2.504E+02	9.212E+02	9.150E+02	2.197E+02	2.199E+02	5.361E+03	6.085E+00
32000	4.745E+01	2.532E+02	1.010E+03	1.003E+03	2.217E+02	2.219E+02	5.506E+03	6.676E+00
34000	5.975E+01	2.564E+02	1.115E+03	1.109E+03	2.236E+02	2.238E+02	5.669E+03	7.213E+00
36000	8.188E+01	2.604E+02	1.255E+03	1.249E+03	2.256E+02	2.257E+02	5.867E+03	7.704E+00
38000	1.159E+02	2.657E+02	1.451E+03	1.445E+03	2.275E+02	2.277E+02	6.121E+03	8.162E+00
40000	1.598E+02	2.727E+02	1.725E+03	1.719E+03	2.296E+02	2.298E+02	6.454E+03	8.593E+00
42000	2.055E+02	2.817E+02	2.091E+03	2.085E+03	2.319E+02	2.320E+02	6.879E+03	9.007E+00
44000	2.403E+02	2.921E+02	2.540E+03	2.534E+03	2.344E+02	2.345E+02	7.387E+03	9.409E+00
46000	2.534E+02	3.031E+02	3.038E+03	3.032E+03	2.371E+02	2.372E+02	7.944E+03	9.805E+00
48000	2.430E+02	3.138E+02	3.538E+03	3.532E+03	2.401E+02	2.402E+02	8.503E+03	1.019E+01
50000	2.158E+02	3.232E+02	3.998E+03	3.992E+03	2.432E+02	2.433E+02	9.024E+03	1.057E+01

Table 77: Internal thermodynamic properties of C^{2+} ΔE=500 cm^{-1}

T(K)	Q_{int}	$\ln(Q_{int})$	E_{int}/RT	$C_{p,int}/R$
50	$1.000E+00$	$0.000E+00$	$0.000E+00$	$0.000E+00$
100	$1.000E+00$	$0.000E+00$	$0.000E+00$	$0.000E+00$
150	$1.000E+00$	$0.000E+00$	$2.063E-215$	$1.037E-212$
200	$1.000E+00$	$0.000E+00$	$5.901E-161$	$2.225E-158$
298.15	$1.000E+00$	$0.000E+00$	$3.193E-107$	$8.075E-105$
300	$1.000E+00$	$0.000E+00$	$1.510E-106$	$3.795E-104$
400	$1.000E+00$	$0.000E+00$	$2.223E-79$	$4.191E-77$
500	$1.000E+00$	$0.000E+00$	$4.227E-63$	$6.376E-61$
600	$1.000E+00$	$0.000E+00$	$2.914E-52$	$3.662E-50$
700	$1.000E+00$	$0.000E+00$	$1.570E-44$	$1.691E-42$
800	$1.000E+00$	$0.000E+00$	$9.695E-39$	$9.139E-37$
900	$1.000E+00$	$0.000E+00$	$3.051E-34$	$2.557E-32$
1000	$1.000E+00$	$0.000E+00$	$1.197E-30$	$9.024E-29$
2000	$1.000E+00$	$4.441E-16$	$1.425E-14$	$5.372E-13$
3000	$1.000E+00$	$1.087E-10$	$2.733E-09$	$6.870E-08$
4000	$1.000E+00$	$5.831E-08$	$1.099E-06$	$2.073E-05$
5000	$1.000E+00$	$2.532E-06$	$3.819E-05$	$5.760E-04$
6000	$1.000E+00$	$3.128E-05$	$3.931E-04$	$4.941E-03$
7000	$1.000E+00$	$1.884E-04$	$2.029E-03$	$2.186E-02$
8000	$1.001E+00$	$7.242E-04$	$6.825E-03$	$6.430E-02$
9000	$1.002E+00$	$2.063E-03$	$1.727E-02$	$1.445E-01$
10000	$1.005E+00$	$4.763E-03$	$3.585E-02$	$2.692E-01$
11000	$1.009E+00$	$9.435E-03$	$6.442E-02$	$4.380E-01$
12000	$1.017E+00$	$1.665E-02$	$1.039E-01$	$6.433E-01$
13000	$1.027E+00$	$2.688E-02$	$1.541E-01$	$8.728E-01$
14000	$1.041E+00$	$4.044E-02$	$2.140E-01$	$1.112E+00$
15000	$1.059E+00$	$5.747E-02$	$2.817E-01$	$1.347E+00$
16000	$1.081E+00$	$7.797E-02$	$3.552E-01$	$1.564E+00$
17000	$1.107E+00$	$1.018E-01$	$4.321E-01$	$1.755E+00$
18000	$1.137E+00$	$1.287E-01$	$5.102E-01$	$1.915E+00$
19000	$1.172E+00$	$1.584E-01$	$5.875E-01$	$2.040E+00$
20000	$1.210E+00$	$1.904E-01$	$6.626E-01$	$2.132E+00$
21000	$1.252E+00$	$2.245E-01$	$7.342E-01$	$2.194E+00$
22000	$1.297E+00$	$2.602E-01$	$8.014E-01$	$2.228E+00$
23000	$1.346E+00$	$2.972E-01$	$8.638E-01$	$2.241E+00$
24000	$1.398E+00$	$3.352E-01$	$9.211E-01$	$2.236E+00$
25000	$1.453E+00$	$3.739E-01$	$9.735E-01$	$2.220E+00$
26000	$1.511E+00$	$4.130E-01$	$1.021E+00$	$2.198E+00$
27000	$1.572E+00$	$4.524E-01$	$1.064E+00$	$2.176E+00$
28000	$1.635E+00$	$4.918E-01$	$1.104E+00$	$2.162E+00$
29000	$1.701E+00$	$5.312E-01$	$1.140E+00$	$2.165E+00$
30000	$1.769E+00$	$5.704E-01$	$1.175E+00$	$2.195E+00$
32000	$1.913E+00$	$6.484E-01$	$1.244E+00$	$2.396E+00$
34000	$2.067E+00$	$7.261E-01$	$1.324E+00$	$2.905E+00$
36000	$2.236E+00$	$8.048E-01$	$1.437E+00$	$3.904E+00$
38000	$2.427E+00$	$8.868E-01$	$1.608E+00$	$5.580E+00$
40000	$2.652E+00$	$9.753E-01$	$1.865E+00$	$8.062E+00$
42000	$2.929E+00$	$1.075E+00$	$2.235E+00$	$1.131E+01$
44000	$3.286E+00$	$1.190E+00$	$2.730E+00$	$1.499E+01$
46000	$3.759E+00$	$1.324E+00$	$3.341E+00$	$1.850E+01$
48000	$4.396E+00$	$1.481E+00$	$4.032E+00$	$2.113E+01$
50000	$5.258E+00$	$1.660E+00$	$4.745E+00$	$2.233E+01$

Table 78: Total thermodynamic properties of C^{2+} ΔE=500 cm^{-1}

T [K]	C_p [J/mol/K]	S^0 [J/mol/K]	$H^0(T)-H^0(0)$ [KJ/mol]	$H^0(T)-H^0(298)$ [KJ/mol]	$-(G^0-H^0(0))/T$ [J/mol/K]	$-(G^0-H^0(298))/T$ [J/mol/K]	ΔH_f [KJ/mol]	$Log(K_p)$
50	2.079E+01	1.027E+02	1.039E+00	-5.158E+00	8.196E+01	2.059E+02	3.739E+03	-3.906E+03
100	2.079E+01	1.172E+02	2.079E+00	-4.119E+00	9.636E+01	1.583E+02	3.742E+03	-1.953E+03
150	2.079E+01	1.256E+02	3.118E+00	-3.079E+00	1.048E+02	1.461E+02	3.744E+03	-1.301E+03
200	2.079E+01	1.316E+02	4.157E+00	-2.040E+00	1.108E+02	1.418E+02	3.746E+03	-9.750E+02
298.15	2.079E+01	1.399E+02	6.197E+00	0.000E+00	1.191E+02	1.399E+02	3.750E+03	-6.527E+02
300	2.079E+01	1.400E+02	6.236E+00	3.848E-02	1.192E+02	1.399E+02	3.750E+03	-6.487E+02
400	2.079E+01	1.460E+02	8.315E+00	2.117E+00	1.252E+02	1.407E+02	3.754E+03	-4.854E+02
500	2.079E+01	1.506E+02	1.039E+01	4.196E+00	1.298E+02	1.422E+02	3.759E+03	-3.872E+02
600	2.079E+01	1.544E+02	1.247E+01	6.274E+00	1.336E+02	1.439E+02	3.763E+03	-3.218E+02
700	2.079E+01	1.576E+02	1.455E+01	8.353E+00	1.368E+02	1.457E+02	3.768E+03	-2.749E+02
800	2.079E+01	1.604E+02	1.663E+01	1.043E+01	1.396E+02	1.473E+02	3.772E+03	-2.398E+02
900	2.079E+01	1.628E+02	1.871E+01	1.251E+01	1.420E+02	1.489E+02	3.777E+03	-2.124E+02
1000	2.079E+01	1.650E+02	2.079E+01	1.459E+01	1.442E+02	1.504E+02	3.781E+03	-1.905E+02
2000	2.079E+01	1.794E+02	4.157E+01	3.538E+01	1.586E+02	1.617E+02	3.825E+03	-9.127E+01
3000	2.079E+01	1.878E+02	6.236E+01	5.616E+01	1.671E+02	1.691E+02	3.867E+03	-5.781E+01
4000	2.079E+01	1.938E+02	8.314E+01	7.695E+01	1.730E+02	1.746E+02	3.909E+03	-4.089E+01
5000	2.079E+01	1.985E+02	1.039E+02	9.774E+01	1.777E+02	1.789E+02	3.950E+03	-3.064E+01
6000	2.083E+01	2.023E+02	1.247E+02	1.185E+02	1.815E+02	1.825E+02	3.990E+03	-2.373E+01
7000	2.097E+01	2.055E+02	1.456E+02	1.394E+02	1.847E+02	1.856E+02	4.031E+03	-1.874E+01
8000	2.132E+01	2.083E+02	1.667E+02	1.606E+02	1.875E+02	1.882E+02	4.071E+03	-1.496E+01
9000	2.199E+01	2.108E+02	1.884E+02	1.822E+02	1.899E+02	1.906E+02	4.112E+03	-1.199E+01
10000	2.302E+01	2.132E+02	2.108E+02	2.047E+02	1.921E+02	1.928E+02	4.154E+03	-9.597E+00
11000	2.443E+01	2.155E+02	2.345E+02	2.283E+02	1.942E+02	1.947E+02	4.198E+03	-7.615E+00
12000	2.614E+01	2.177E+02	2.598E+02	2.536E+02	1.960E+02	1.965E+02	4.243E+03	-5.945E+00
13000	2.804E+01	2.198E+02	2.869E+02	2.807E+02	1.978E+02	1.982E+02	4.292E+03	-4.516E+00
14000	3.003E+01	2.220E+02	3.159E+02	3.097E+02	1.994E+02	1.999E+02	4.342E+03	-3.278E+00
15000	3.198E+01	2.241E+02	3.469E+02	3.407E+02	2.010E+02	2.014E+02	4.396E+03	-2.191E+00
16000	3.379E+01	2.262E+02	3.798E+02	3.736E+02	2.025E+02	2.029E+02	4.452E+03	-1.229E+00
17000	3.538E+01	2.283E+02	4.144E+02	4.082E+02	2.040E+02	2.043E+02	4.510E+03	-3.684E-01
18000	3.671E+01	2.304E+02	4.505E+02	4.443E+02	2.054E+02	2.057E+02	4.570E+03	4.065E-01
19000	3.775E+01	2.324E+02	4.878E+02	4.816E+02	2.068E+02	2.071E+02	4.632E+03	1.109E+00
20000	3.852E+01	2.344E+02	5.259E+02	5.197E+02	2.081E+02	2.084E+02	4.695E+03	1.750E+00
21000	3.903E+01	2.363E+02	5.647E+02	5.585E+02	2.094E+02	2.097E+02	4.760E+03	2.338E+00
22000	3.931E+01	2.381E+02	6.039E+02	5.977E+02	2.106E+02	2.109E+02	4.825E+03	2.880E+00
23000	3.942E+01	2.398E+02	6.433E+02	6.371E+02	2.119E+02	2.121E+02	4.891E+03	3.381E+00
24000	3.938E+01	2.415E+02	6.827E+02	6.765E+02	2.131E+02	2.133E+02	4.957E+03	3.847E+00
25000	3.924E+01	2.431E+02	7.220E+02	7.158E+02	2.142E+02	2.145E+02	5.023E+03	4.281E+00
26000	3.906E+01	2.447E+02	7.612E+02	7.550E+02	2.154E+02	2.156E+02	5.090E+03	4.688E+00
27000	3.888E+01	2.461E+02	8.001E+02	7.939E+02	2.165E+02	2.167E+02	5.156E+03	5.069E+00
28000	3.876E+01	2.475E+02	8.389E+02	8.327E+02	2.176E+02	2.178E+02	5.223E+03	5.427E+00
29000	3.878E+01	2.489E+02	8.777E+02	8.715E+02	2.186E+02	2.188E+02	5.289E+03	5.765E+00
30000	3.904E+01	2.502E+02	9.166E+02	9.104E+02	2.197E+02	2.199E+02	5.356E+03	6.085E+00
32000	4.071E+01	2.528E+02	9.960E+02	9.898E+02	2.217E+02	2.218E+02	5.493E+03	6.675E+00
34000	4.494E+01	2.554E+02	1.081E+03	1.075E+03	2.236E+02	2.238E+02	5.635E+03	7.209E+00
36000	5.324E+01	2.581E+02	1.178E+03	1.172E+03	2.254E+02	2.256E+02	5.790E+03	7.696E+00
38000	6.718E+01	2.614E+02	1.298E+03	1.292E+03	2.272E+02	2.274E+02	5.968E+03	8.145E+00
40000	8.782E+01	2.653E+02	1.452E+03	1.446E+03	2.290E+02	2.292E+02	6.180E+03	8.562E+00
42000	1.148E+02	2.702E+02	1.653E+03	1.647E+03	2.308E+02	2.310E+02	6.441E+03	8.954E+00
44000	1.454E+02	2.763E+02	1.913E+03	1.907E+03	2.328E+02	2.329E+02	6.760E+03	9.327E+00
46000	1.746E+02	2.834E+02	2.234E+03	2.228E+03	2.348E+02	2.349E+02	7.140E+03	9.685E+00
48000	1.965E+02	2.913E+02	2.607E+03	2.601E+03	2.370E+02	2.371E+02	7.572E+03	1.003E+01
50000	2.064E+02	2.996E+02	3.012E+03	3.006E+03	2.393E+02	2.395E+02	8.037E+03	1.037E+01

Table 79: Internal thermodynamic properties of C^{2+} ΔE=1000 cm^{-1}

T(K)	Q_{int}	$\ln(Q_{int})$	E_{int}/RT	$C_{p,int}/R$
50	$1.000E+00$	$0.000E+00$	$0.000E+00$	$0.000E+00$
100	$1.000E+00$	$0.000E+00$	$0.000E+00$	$0.000E+00$
150	$1.000E+00$	$0.000E+00$	$2.063E-215$	$1.037E-212$
200	$1.000E+00$	$0.000E+00$	$5.901E-161$	$2.225E-158$
298.15	$1.000E+00$	$0.000E+00$	$3.193E-107$	$8.075E-105$
300	$1.000E+00$	$0.000E+00$	$1.510E-106$	$3.795E-104$
400	$1.000E+00$	$0.000E+00$	$2.223E-79$	$4.191E-77$
500	$1.000E+00$	$0.000E+00$	$4.227E-63$	$6.376E-61$
600	$1.000E+00$	$0.000E+00$	$2.914E-52$	$3.662E-50$
700	$1.000E+00$	$0.000E+00$	$1.570E-44$	$1.691E-42$
800	$1.000E+00$	$0.000E+00$	$9.695E-39$	$9.139E-37$
900	$1.000E+00$	$0.000E+00$	$3.051E-34$	$2.557E-32$
1000	$1.000E+00$	$0.000E+00$	$1.197E-30$	$9.024E-29$
2000	$1.000E+00$	$4.441E-16$	$1.425E-14$	$5.372E-13$
3000	$1.000E+00$	$1.087E-10$	$2.733E-09$	$6.870E-08$
4000	$1.000E+00$	$5.831E-08$	$1.099E-06$	$2.073E-05$
5000	$1.000E+00$	$2.532E-06$	$3.819E-05$	$5.760E-04$
6000	$1.000E+00$	$3.128E-05$	$3.931E-04$	$4.941E-03$
7000	$1.000E+00$	$1.884E-04$	$2.029E-03$	$2.186E-02$
8000	$1.001E+00$	$7.242E-04$	$6.825E-03$	$6.430E-02$
9000	$1.002E+00$	$2.063E-03$	$1.727E-02$	$1.445E-01$
10000	$1.005E+00$	$4.763E-03$	$3.585E-02$	$2.692E-01$
11000	$1.009E+00$	$9.435E-03$	$6.442E-02$	$4.380E-01$
12000	$1.017E+00$	$1.665E-02$	$1.039E-01$	$6.433E-01$
13000	$1.027E+00$	$2.688E-02$	$1.541E-01$	$8.728E-01$
14000	$1.041E+00$	$4.044E-02$	$2.140E-01$	$1.112E+00$
15000	$1.059E+00$	$5.747E-02$	$2.817E-01$	$1.347E+00$
16000	$1.081E+00$	$7.797E-02$	$3.552E-01$	$1.564E+00$
17000	$1.107E+00$	$1.018E-01$	$4.321E-01$	$1.755E+00$
18000	$1.137E+00$	$1.287E-01$	$5.102E-01$	$1.915E+00$
19000	$1.172E+00$	$1.584E-01$	$5.875E-01$	$2.040E+00$
20000	$1.210E+00$	$1.904E-01$	$6.626E-01$	$2.132E+00$
21000	$1.252E+00$	$2.245E-01$	$7.342E-01$	$2.194E+00$
22000	$1.297E+00$	$2.602E-01$	$8.014E-01$	$2.228E+00$
23000	$1.346E+00$	$2.972E-01$	$8.638E-01$	$2.240E+00$
24000	$1.398E+00$	$3.352E-01$	$9.210E-01$	$2.234E+00$
25000	$1.453E+00$	$3.739E-01$	$9.732E-01$	$2.215E+00$
26000	$1.511E+00$	$4.130E-01$	$1.020E+00$	$2.187E+00$
27000	$1.572E+00$	$4.523E-01$	$1.063E+00$	$2.154E+00$
28000	$1.635E+00$	$4.917E-01$	$1.101E+00$	$2.122E+00$
29000	$1.701E+00$	$5.310E-01$	$1.136E+00$	$2.094E+00$
30000	$1.768E+00$	$5.700E-01$	$1.168E+00$	$2.076E+00$
32000	$1.910E+00$	$6.472E-01$	$1.225E+00$	$2.094E+00$
34000	$2.061E+00$	$7.231E-01$	$1.279E+00$	$2.234E+00$
36000	$2.221E+00$	$7.979E-01$	$1.340E+00$	$2.567E+00$
38000	$2.393E+00$	$8.724E-01$	$1.420E+00$	$3.181E+00$
40000	$2.580E+00$	$9.478E-01$	$1.530E+00$	$4.159E+00$
42000	$2.790E+00$	$1.026E+00$	$1.687E+00$	$5.562E+00$
44000	$3.032E+00$	$1.109E+00$	$1.904E+00$	$7.395E+00$
46000	$3.320E+00$	$1.200E+00$	$2.189E+00$	$9.571E+00$
48000	$3.671E+00$	$1.300E+00$	$2.545E+00$	$1.190E+01$
50000	$4.107E+00$	$1.413E+00$	$2.964E+00$	$1.411E+01$

Table 80: Total thermodynamic properties of C^{2+} ΔE=1000 cm^{-1}

T [K]	C_p [J/mol/K]	S^0 [J/mol/K]	$H^0(T)$-$H^0(0)$ [KJ/mol]	$H^0(T)$-$H^0(298)$ [KJ/mol]	-(G^0-$H^0(0)$)/T [J/mol/K]	-(G^0-$H^0(298)$)/T [J/mol/K]	ΔH_f [KJ/mol]	Log(K_p)
50	2.079E+01	1.027E+02	1.039E+00	-5.158E+00	8.196E+01	2.059E+02	3.739E+03	-3.906E+03
100	2.079E+01	1.172E+02	2.079E+00	-4.119E+00	9.636E+01	1.583E+02	3.742E+03	-1.953E+03
150	2.079E+01	1.256E+02	3.118E+00	-3.079E+00	1.048E+02	1.461E+02	3.744E+03	-1.301E+03
200	2.079E+01	1.316E+02	4.157E+00	-2.040E+00	1.108E+02	1.418E+02	3.746E+03	-9.750E+02
298.15	2.079E+01	1.399E+02	6.197E+00	0.000E+00	1.191E+02	1.399E+02	3.750E+03	-6.527E+02
300	2.079E+01	1.400E+02	6.236E+00	3.848E-02	1.192E+02	1.399E+02	3.750E+03	-6.487E+02
400	2.079E+01	1.460E+02	8.315E+00	2.117E+00	1.252E+02	1.407E+02	3.754E+03	-4.854E+02
500	2.079E+01	1.506E+02	1.039E+01	4.196E+00	1.298E+02	1.422E+02	3.759E+03	-3.872E+02
600	2.079E+01	1.544E+02	1.247E+01	6.274E+00	1.336E+02	1.439E+02	3.763E+03	-3.218E+02
700	2.079E+01	1.576E+02	1.455E+01	8.353E+00	1.368E+02	1.457E+02	3.768E+03	-2.749E+02
800	2.079E+01	1.604E+02	1.663E+01	1.043E+01	1.396E+02	1.473E+02	3.772E+03	-2.398E+02
900	2.079E+01	1.628E+02	1.871E+01	1.251E+01	1.420E+02	1.489E+02	3.777E+03	-2.124E+02
1000	2.079E+01	1.650E+02	2.079E+01	1.459E+01	1.442E+02	1.504E+02	3.781E+03	-1.905E+02
2000	2.079E+01	1.794E+02	4.157E+01	3.538E+01	1.586E+02	1.617E+02	3.825E+03	-9.127E+01
3000	2.079E+01	1.878E+02	6.236E+01	5.616E+01	1.671E+02	1.691E+02	3.867E+03	-5.781E+01
4000	2.079E+01	1.938E+02	8.314E+01	7.695E+01	1.730E+02	1.746E+02	3.909E+03	-4.089E+01
5000	2.079E+01	1.985E+02	1.039E+02	9.774E+01	1.777E+02	1.789E+02	3.950E+03	-3.064E+01
6000	2.083E+01	2.023E+02	1.247E+02	1.185E+02	1.815E+02	1.825E+02	3.990E+03	-2.373E+01
7000	2.097E+01	2.055E+02	1.456E+02	1.394E+02	1.847E+02	1.856E+02	4.031E+03	-1.874E+01
8000	2.132E+01	2.083E+02	1.667E+02	1.606E+02	1.875E+02	1.882E+02	4.071E+03	-1.496E+01
9000	2.199E+01	2.108E+02	1.884E+02	1.822E+02	1.899E+02	1.906E+02	4.112E+03	-1.199E+01
10000	2.302E+01	2.132E+02	2.108E+02	2.047E+02	1.921E+02	1.928E+02	4.154E+03	-9.597E+00
11000	2.443E+01	2.155E+02	2.345E+02	2.283E+02	1.942E+02	1.947E+02	4.198E+03	-7.615E+00
12000	2.614E+01	2.177E+02	2.598E+02	2.536E+02	1.960E+02	1.965E+02	4.243E+03	-5.945E+00
13000	2.804E+01	2.198E+02	2.869E+02	2.807E+02	1.978E+02	1.982E+02	4.292E+03	-4.516E+00
14000	3.003E+01	2.220E+02	3.159E+02	3.097E+02	1.994E+02	1.999E+02	4.342E+03	-3.278E+00
15000	3.198E+01	2.241E+02	3.469E+02	3.407E+02	2.010E+02	2.014E+02	4.396E+03	-2.191E+00
16000	3.379E+01	2.262E+02	3.798E+02	3.736E+02	2.025E+02	2.029E+02	4.452E+03	-1.229E+00
17000	3.538E+01	2.283E+02	4.144E+02	4.082E+02	2.040E+02	2.043E+02	4.510E+03	-3.684E-01
18000	3.671E+01	2.304E+02	4.505E+02	4.443E+02	2.054E+02	2.057E+02	4.570E+03	4.065E-01
19000	3.775E+01	2.324E+02	4.878E+02	4.816E+02	2.068E+02	2.071E+02	4.632E+03	1.109E+00
20000	3.852E+01	2.344E+02	5.259E+02	5.197E+02	2.081E+02	2.084E+02	4.695E+03	1.750E+00
21000	3.903E+01	2.363E+02	5.647E+02	5.585E+02	2.094E+02	2.097E+02	4.760E+03	2.338E+00
22000	3.931E+01	2.381E+02	6.039E+02	5.977E+02	2.106E+02	2.109E+02	4.825E+03	2.880E+00
23000	3.941E+01	2.398E+02	6.433E+02	6.371E+02	2.119E+02	2.121E+02	4.891E+03	3.381E+00
24000	3.936E+01	2.415E+02	6.827E+02	6.765E+02	2.131E+02	2.133E+02	4.957E+03	3.847E+00
25000	3.920E+01	2.431E+02	7.220E+02	7.158E+02	2.142E+02	2.145E+02	5.023E+03	4.281E+00
26000	3.897E+01	2.447E+02	7.610E+02	7.548E+02	2.154E+02	2.156E+02	5.090E+03	4.688E+00
27000	3.870E+01	2.461E+02	7.999E+02	7.937E+02	2.165E+02	2.167E+02	5.156E+03	5.069E+00
28000	3.843E+01	2.475E+02	8.384E+02	8.322E+02	2.176E+02	2.178E+02	5.222E+03	5.427E+00
29000	3.820E+01	2.489E+02	8.767E+02	8.705E+02	2.186E+02	2.188E+02	5.288E+03	5.765E+00
30000	3.805E+01	2.502E+02	9.149E+02	9.087E+02	2.197E+02	2.199E+02	5.355E+03	6.085E+00
32000	3.820E+01	2.526E+02	9.910E+02	9.848E+02	2.217E+02	2.218E+02	5.488E+03	6.675E+00
34000	3.936E+01	2.550E+02	1.068E+03	1.062E+03	2.235E+02	2.237E+02	5.622E+03	7.208E+00
36000	4.213E+01	2.573E+02	1.150E+03	1.143E+03	2.253E+02	2.255E+02	5.761E+03	7.693E+00
38000	4.723E+01	2.597E+02	1.238E+03	1.232E+03	2.271E+02	2.272E+02	5.908E+03	8.139E+00
40000	5.537E+01	2.623E+02	1.340E+03	1.334E+03	2.288E+02	2.289E+02	6.069E+03	8.550E+00
42000	6.703E+01	2.653E+02	1.462E+03	1.456E+03	2.304E+02	2.306E+02	6.250E+03	8.933E+00
44000	8.227E+01	2.687E+02	1.611E+03	1.605E+03	2.321E+02	2.322E+02	6.458E+03	9.292E+00
46000	1.004E+02	2.728E+02	1.793E+03	1.787E+03	2.338E+02	2.339E+02	6.699E+03	9.631E+00
48000	1.198E+02	2.774E+02	2.013E+03	2.007E+03	2.355E+02	2.356E+02	6.979E+03	9.954E+00
50000	1.381E+02	2.827E+02	2.272E+03	2.265E+03	2.373E+02	2.374E+02	7.297E+03	1.027E+01

Table 81: Internal thermodynamic properties of C^{3+} ΔE=250 cm^{-1}

T(K)	Q_{int}	$\ln(Q_{int})$	E_{int}/RT	$C_{p,int}/R$
50	$2.000E+00$	$6.931E-01$	$0.000E+00$	$0.000E+00$
100	$2.000E+00$	$6.931E-01$	$0.000E+00$	$0.000E+00$
150	$2.000E+00$	$6.931E-01$	$2.256E-266$	$1.397E-263$
200	$2.000E+00$	$6.931E-01$	$2.866E-199$	$1.331E-196$
298.15	$2.000E+00$	$6.931E-01$	$4.770E-133$	$1.486E-130$
300	$2.000E+00$	$6.931E-01$	$3.237E-132$	$1.002E-129$
400	$2.000E+00$	$6.931E-01$	$9.992E-99$	$2.320E-96$
500	$2.000E+00$	$6.931E-01$	$1.179E-78$	$2.190E-76$
600	$2.000E+00$	$6.931E-01$	$2.742E-65$	$4.244E-63$
700	$2.000E+00$	$6.931E-01$	$9.445E-56$	$1.253E-53$
800	$2.000E+00$	$6.931E-01$	$1.319E-48$	$1.532E-46$
900	$2.000E+00$	$6.931E-01$	$4.694E-43$	$4.844E-41$
1000	$2.000E+00$	$6.931E-01$	$1.281E-38$	$1.190E-36$
2000	$2.000E+00$	$6.931E-01$	$9.448E-19$	$4.388E-17$
3000	$2.000E+00$	$6.931E-01$	$3.328E-12$	$1.030E-10$
4000	$2.000E+00$	$6.931E-01$	$5.737E-09$	$1.332E-07$
5000	$2.000E+00$	$6.931E-01$	$4.771E-07$	$8.863E-06$
6000	$2.000E+00$	$6.931E-01$	$8.790E-06$	$1.361E-04$
7000	$2.000E+00$	$6.932E-01$	$6.878E-05$	$9.126E-04$
8000	$2.000E+00$	$6.932E-01$	$3.161E-04$	$3.669E-03$
9000	$2.000E+00$	$6.932E-01$	$1.021E-03$	$1.053E-02$
10000	$2.001E+00$	$6.934E-01$	$2.577E-03$	$2.393E-02$
11000	$2.001E+00$	$6.938E-01$	$5.449E-03$	$4.598E-02$
12000	$2.003E+00$	$6.945E-01$	$1.009E-02$	$7.799E-02$
13000	$2.005E+00$	$6.955E-01$	$1.687E-02$	$1.203E-01$
14000	$2.008E+00$	$6.971E-01$	$2.606E-02$	$1.722E-01$
15000	$2.012E+00$	$6.993E-01$	$3.777E-02$	$2.324E-01$
16000	$2.018E+00$	$7.021E-01$	$5.199E-02$	$2.991E-01$
17000	$2.025E+00$	$7.058E-01$	$6.860E-02$	$3.701E-01$
18000	$2.034E+00$	$7.102E-01$	$8.738E-02$	$4.432E-01$
19000	$2.045E+00$	$7.155E-01$	$1.080E-01$	$5.165E-01$
20000	$2.058E+00$	$7.216E-01$	$1.303E-01$	$5.879E-01$
21000	$2.072E+00$	$7.285E-01$	$1.537E-01$	$6.561E-01$
22000	$2.088E+00$	$7.362E-01$	$1.780E-01$	$7.198E-01$
23000	$2.106E+00$	$7.447E-01$	$2.028E-01$	$7.780E-01$
24000	$2.125E+00$	$7.538E-01$	$2.279E-01$	$8.301E-01$
25000	$2.146E+00$	$7.637E-01$	$2.529E-01$	$8.757E-01$
26000	$2.169E+00$	$7.741E-01$	$2.777E-01$	$9.149E-01$
27000	$2.192E+00$	$7.850E-01$	$3.019E-01$	$9.475E-01$
28000	$2.218E+00$	$7.964E-01$	$3.254E-01$	$9.740E-01$
29000	$2.244E+00$	$8.082E-01$	$3.482E-01$	$9.947E-01$
30000	$2.271E+00$	$8.204E-01$	$3.700E-01$	$1.010E+00$
32000	$2.329E+00$	$8.456E-01$	$4.107E-01$	$1.030E+00$
34000	$2.391E+00$	$8.716E-01$	$4.475E-01$	$1.043E+00$
36000	$2.455E+00$	$8.982E-01$	$4.812E-01$	$1.071E+00$
38000	$2.522E+00$	$9.250E-01$	$5.139E-01$	$1.147E+00$
40000	$2.592E+00$	$9.523E-01$	$5.497E-01$	$1.335E+00$
42000	$2.665E+00$	$9.802E-01$	$5.954E-01$	$1.731E+00$
44000	$2.744E+00$	$1.009E+00$	$6.624E-01$	$2.481E+00$
46000	$2.832E+00$	$1.041E+00$	$7.673E-01$	$3.775E+00$
48000	$2.935E+00$	$1.077E+00$	$9.324E-01$	$5.831E+00$
50000	$3.064E+00$	$1.120E+00$	$1.185E+00$	$8.843E+00$

Table 82: Total thermodynamic properties of C^{3+} ΔE=250 cm^{-1}

T [K]	C_p [J/mol/K]	S^0 [J/mol/K]	$H^0(T)$-$H^0(0)$ [KJ/mol]	$H^0(T)$-$H^0(298)$ [KJ/mol]	-(G^0-$H^0(0)$)/T [J/mol/K]	-(G^0-$H^0(298)$)/T [J/mol/K]	ΔH_f [KJ/mol]	Log(K_p)
50	2.079E+01	1.085E+02	1.039E+00	-5.158E+00	8.772E+01	2.117E+02	8.361E+03	-8.735E+03
100	2.079E+01	1.229E+02	2.079E+00	-4.119E+00	1.021E+02	1.641E+02	8.364E+03	-4.367E+03
150	2.079E+01	1.313E+02	3.118E+00	-3.079E+00	1.106E+02	1.519E+02	8.368E+03	-2.910E+03
200	2.079E+01	1.373E+02	4.157E+00	-2.040E+00	1.165E+02	1.475E+02	8.371E+03	-2.182E+03
298.15	2.079E+01	1.456E+02	6.197E+00	0.000E+00	1.248E+02	1.456E+02	8.377E+03	-1.462E+03
300	2.079E+01	1.458E+02	6.236E+00	3.848E-02	1.250E+02	1.456E+02	8.377E+03	-1.453E+03
400	2.079E+01	1.517E+02	8.315E+00	2.117E+00	1.309E+02	1.464E+02	8.383E+03	-1.088E+03
500	2.079E+01	1.564E+02	1.039E+01	4.196E+00	1.356E+02	1.480E+02	8.390E+03	-8.690E+02
600	2.079E+01	1.602E+02	1.247E+01	6.274E+00	1.394E+02	1.497E+02	8.396E+03	-7.229E+02
700	2.079E+01	1.634E+02	1.455E+01	8.353E+00	1.426E+02	1.514E+02	8.403E+03	-6.185E+02
800	2.079E+01	1.661E+02	1.663E+01	1.043E+01	1.453E+02	1.531E+02	8.409E+03	-5.401E+02
900	2.079E+01	1.686E+02	1.871E+01	1.251E+01	1.478E+02	1.547E+02	8.416E+03	-4.790E+02
1000	2.079E+01	1.708E+02	2.079E+01	1.459E+01	1.500E+02	1.562E+02	8.422E+03	-4.302E+02
2000	2.079E+01	1.852E+02	4.157E+01	3.538E+01	1.644E+02	1.675E+02	8.487E+03	-2.096E+02
3000	2.079E+01	1.936E+02	6.236E+01	5.616E+01	1.728E+02	1.749E+02	8.550E+03	-1.354E+02
4000	2.079E+01	1.996E+02	8.314E+01	7.695E+01	1.788E+02	1.803E+02	8.612E+03	-9.810E+01
5000	2.079E+01	2.042E+02	1.039E+02	9.773E+01	1.834E+02	1.847E+02	8.674E+03	-7.553E+01
6000	2.079E+01	2.080E+02	1.247E+02	1.185E+02	1.872E+02	1.883E+02	8.735E+03	-6.038E+01
7000	2.079E+01	2.112E+02	1.455E+02	1.393E+02	1.904E+02	1.913E+02	8.796E+03	-4.948E+01
8000	2.082E+01	2.140E+02	1.663E+02	1.601E+02	1.932E+02	1.940E+02	8.857E+03	-4.125E+01
9000	2.087E+01	2.165E+02	1.872E+02	1.810E+02	1.957E+02	1.963E+02	8.918E+03	-3.480E+01
10000	2.098E+01	2.187E+02	2.081E+02	2.019E+02	1.978E+02	1.985E+02	8.980E+03	-2.961E+01
11000	2.117E+01	2.207E+02	2.292E+02	2.229E+02	1.998E+02	2.004E+02	9.041E+03	-2.533E+01
12000	2.143E+01	2.225E+02	2.504E+02	2.442E+02	2.017E+02	2.022E+02	9.104E+03	-2.174E+01
13000	2.179E+01	2.242E+02	2.721E+02	2.659E+02	2.033E+02	2.038E+02	9.167E+03	-1.868E+01
14000	2.222E+01	2.259E+02	2.940E+02	2.878E+02	2.049E+02	2.053E+02	9.232E+03	-1.604E+01
15000	2.272E+01	2.274E+02	3.165E+02	3.103E+02	2.063E+02	2.067E+02	9.297E+03	-1.374E+01
16000	2.327E+01	2.289E+02	3.395E+02	3.333E+02	2.077E+02	2.081E+02	9.364E+03	-1.171E+01
17000	2.386E+01	2.303E+02	3.631E+02	3.569E+02	2.090E+02	2.093E+02	9.432E+03	-9.903E+00
18000	2.447E+01	2.317E+02	3.872E+02	3.810E+02	2.102E+02	2.106E+02	9.501E+03	-8.287E+00
19000	2.508E+01	2.331E+02	4.120E+02	4.058E+02	2.114E+02	2.117E+02	9.572E+03	-6.830E+00
20000	2.568E+01	2.344E+02	4.374E+02	4.312E+02	2.125E+02	2.128E+02	9.643E+03	-5.510E+00
21000	2.624E+01	2.356E+02	4.634E+02	4.571E+02	2.136E+02	2.139E+02	9.716E+03	-4.306E+00
22000	2.677E+01	2.369E+02	4.899E+02	4.837E+02	2.146E+02	2.149E+02	9.789E+03	-3.204E+00
23000	2.725E+01	2.381E+02	5.169E+02	5.107E+02	2.156E+02	2.159E+02	9.863E+03	-2.189E+00
24000	2.769E+01	2.392E+02	5.444E+02	5.381E+02	2.166E+02	2.168E+02	9.938E+03	-1.253E+00
25000	2.807E+01	2.404E+02	5.722E+02	5.660E+02	2.175E+02	2.177E+02	1.001E+04	-3.842E-01
26000	2.839E+01	2.415E+02	6.005E+02	5.943E+02	2.184E+02	2.186E+02	1.009E+04	4.235E-01
27000	2.866E+01	2.426E+02	6.290E+02	6.228E+02	2.193E+02	2.195E+02	1.017E+04	1.177E+00
28000	2.889E+01	2.436E+02	6.578E+02	6.516E+02	2.201E+02	2.203E+02	1.024E+04	1.882E+00
29000	2.906E+01	2.446E+02	6.868E+02	6.805E+02	2.209E+02	2.212E+02	1.032E+04	2.543E+00
30000	2.919E+01	2.456E+02	7.159E+02	7.097E+02	2.217E+02	2.219E+02	1.040E+04	3.166E+00
32000	2.935E+01	2.475E+02	7.744E+02	7.682E+02	2.233E+02	2.235E+02	1.056E+04	4.306E+00
34000	2.946E+01	2.493E+02	8.332E+02	8.270E+02	2.248E+02	2.249E+02	1.071E+04	5.327E+00
36000	2.969E+01	2.510E+02	8.924E+02	8.861E+02	2.262E+02	2.263E+02	1.087E+04	6.248E+00
38000	3.032E+01	2.526E+02	9.523E+02	9.461E+02	2.275E+02	2.277E+02	1.103E+04	7.084E+00
40000	3.188E+01	2.542E+02	1.014E+03	1.008E+03	2.288E+02	2.290E+02	1.120E+04	7.848E+00
42000	3.518E+01	2.558E+02	1.081E+03	1.075E+03	2.301E+02	2.302E+02	1.136E+04	8.549E+00
44000	4.142E+01	2.576E+02	1.157E+03	1.151E+03	2.313E+02	2.314E+02	1.154E+04	9.196E+00
46000	5.217E+01	2.596E+02	1.250E+03	1.243E+03	2.325E+02	2.326E+02	1.173E+04	9.796E+00
48000	6.927E+01	2.622E+02	1.370E+03	1.364E+03	2.337E+02	2.338E+02	1.195E+04	1.036E+01
50000	9.431E+01	2.655E+02	1.532E+03	1.526E+03	2.348E+02	2.350E+02	1.222E+04	1.088E+01

Table 83: Internal thermodynamic properties of C^{3+} ΔE=500 cm^{-1}

T(K)	Q_{int}	$\ln(Q_{int})$	E_{int}/RT	$C_{p,int}/R$
50	$2.000E+00$	$6.931E-01$	$0.000E+00$	$0.000E+00$
100	$2.000E+00$	$6.931E-01$	$0.000E+00$	$0.000E+00$
150	$2.000E+00$	$6.931E-01$	$2.256E-266$	$1.397E-263$
200	$2.000E+00$	$6.931E-01$	$2.866E-199$	$1.331E-196$
298.15	$2.000E+00$	$6.931E-01$	$4.770E-133$	$1.486E-130$
300	$2.000E+00$	$6.931E-01$	$3.237E-132$	$1.002E-129$
400	$2.000E+00$	$6.931E-01$	$9.992E-99$	$2.320E-96$
500	$2.000E+00$	$6.931E-01$	$1.179E-78$	$2.190E-76$
600	$2.000E+00$	$6.931E-01$	$2.742E-65$	$4.244E-63$
700	$2.000E+00$	$6.931E-01$	$9.445E-56$	$1.253E-53$
800	$2.000E+00$	$6.931E-01$	$1.319E-48$	$1.532E-46$
900	$2.000E+00$	$6.931E-01$	$4.694E-43$	$4.844E-41$
1000	$2.000E+00$	$6.931E-01$	$1.281E-38$	$1.190E-36$
2000	$2.000E+00$	$6.931E-01$	$9.448E-19$	$4.388E-17$
3000	$2.000E+00$	$6.931E-01$	$3.328E-12$	$1.030E-10$
4000	$2.000E+00$	$6.931E-01$	$5.737E-09$	$1.332E-07$
5000	$2.000E+00$	$6.931E-01$	$4.771E-07$	$8.863E-06$
6000	$2.000E+00$	$6.931E-01$	$8.790E-06$	$1.361E-04$
7000	$2.000E+00$	$6.932E-01$	$6.878E-05$	$9.126E-04$
8000	$2.000E+00$	$6.932E-01$	$3.161E-04$	$3.669E-03$
9000	$2.000E+00$	$6.932E-01$	$1.021E-03$	$1.053E-02$
10000	$2.001E+00$	$6.934E-01$	$2.577E-03$	$2.393E-02$
11000	$2.001E+00$	$6.938E-01$	$5.449E-03$	$4.598E-02$
12000	$2.003E+00$	$6.945E-01$	$1.009E-02$	$7.799E-02$
13000	$2.005E+00$	$6.955E-01$	$1.687E-02$	$1.203E-01$
14000	$2.008E+00$	$6.971E-01$	$2.606E-02$	$1.722E-01$
15000	$2.012E+00$	$6.993E-01$	$3.777E-02$	$2.324E-01$
16000	$2.018E+00$	$7.021E-01$	$5.199E-02$	$2.991E-01$
17000	$2.025E+00$	$7.058E-01$	$6.860E-02$	$3.701E-01$
18000	$2.034E+00$	$7.102E-01$	$8.738E-02$	$4.432E-01$
19000	$2.045E+00$	$7.155E-01$	$1.080E-01$	$5.165E-01$
20000	$2.058E+00$	$7.216E-01$	$1.303E-01$	$5.879E-01$
21000	$2.072E+00$	$7.285E-01$	$1.537E-01$	$6.561E-01$
22000	$2.088E+00$	$7.362E-01$	$1.780E-01$	$7.198E-01$
23000	$2.106E+00$	$7.447E-01$	$2.028E-01$	$7.780E-01$
24000	$2.125E+00$	$7.538E-01$	$2.279E-01$	$8.301E-01$
25000	$2.146E+00$	$7.637E-01$	$2.529E-01$	$8.757E-01$
26000	$2.169E+00$	$7.741E-01$	$2.777E-01$	$9.148E-01$
27000	$2.192E+00$	$7.850E-01$	$3.019E-01$	$9.474E-01$
28000	$2.218E+00$	$7.964E-01$	$3.254E-01$	$9.738E-01$
29000	$2.244E+00$	$8.082E-01$	$3.481E-01$	$9.943E-01$
30000	$2.271E+00$	$8.204E-01$	$3.700E-01$	$1.009E+00$
32000	$2.329E+00$	$8.456E-01$	$4.105E-01$	$1.026E+00$
34000	$2.391E+00$	$8.716E-01$	$4.469E-01$	$1.030E+00$
36000	$2.455E+00$	$8.981E-01$	$4.793E-01$	$1.031E+00$
38000	$2.521E+00$	$9.248E-01$	$5.086E-01$	$1.045E+00$
40000	$2.590E+00$	$9.516E-01$	$5.365E-01$	$1.097E+00$
42000	$2.660E+00$	$9.784E-01$	$5.658E-01$	$1.224E+00$
44000	$2.733E+00$	$1.006E+00$	$6.010E-01$	$1.484E+00$
46000	$2.810E+00$	$1.033E+00$	$6.487E-01$	$1.953E+00$
48000	$2.893E+00$	$1.062E+00$	$7.179E-01$	$2.729E+00$
50000	$2.985E+00$	$1.093E+00$	$8.207E-01$	$3.925E+00$

Table 84: Total thermodynamic properties of C^{3+} ΔE=500 cm^{-1}

T [K]	C_p [J/mol/K]	S^0 [J/mol/K]	$H^0(T)$-$H^0(0)$ [KJ/mol]	$H^0(T)$-$H^0(298)$ [KJ/mol]	-(G^0-$H^0(0)$)/T [J/mol/K]	-(G^0-$H^0(298)$)/T [J/mol/K]	ΔH_f [KJ/mol]	Log(K_p)
50	2.079E+01	1.085E+02	1.039E+00	-5.158E+00	8.772E+01	2.117E+02	8.361E+03	-8.735E+03
100	2.079E+01	1.229E+02	2.079E+00	-4.119E+00	1.021E+02	1.641E+02	8.364E+03	-4.367E+03
150	2.079E+01	1.313E+02	3.118E+00	-3.079E+00	1.106E+02	1.519E+02	8.368E+03	-2.910E+03
200	2.079E+01	1.373E+02	4.157E+00	-2.040E+00	1.165E+02	1.475E+02	8.371E+03	-2.182E+03
298.15	2.079E+01	1.456E+02	6.197E+00	0.000E+00	1.248E+02	1.456E+02	8.377E+03	-1.462E+03
300	2.079E+01	1.458E+02	6.236E+00	3.848E-02	1.250E+02	1.456E+02	8.377E+03	-1.453E+03
400	2.079E+01	1.517E+02	8.315E+00	2.117E+00	1.309E+02	1.464E+02	8.383E+03	-1.088E+03
500	2.079E+01	1.564E+02	1.039E+01	4.196E+00	1.356E+02	1.480E+02	8.390E+03	-8.690E+02
600	2.079E+01	1.602E+02	1.247E+01	6.274E+00	1.394E+02	1.497E+02	8.396E+03	-7.229E+02
700	2.079E+01	1.634E+02	1.455E+01	8.353E+00	1.426E+02	1.514E+02	8.403E+03	-6.185E+02
800	2.079E+01	1.661E+02	1.663E+01	1.043E+01	1.453E+02	1.531E+02	8.409E+03	-5.401E+02
900	2.079E+01	1.686E+02	1.871E+01	1.251E+01	1.478E+02	1.547E+02	8.416E+03	-4.790E+02
1000	2.079E+01	1.708E+02	2.079E+01	1.459E+01	1.500E+02	1.562E+02	8.422E+03	-4.302E+02
2000	2.079E+01	1.852E+02	4.157E+01	3.538E+01	1.644E+02	1.675E+02	8.487E+03	-2.096E+02
3000	2.079E+01	1.936E+02	6.236E+01	5.616E+01	1.728E+02	1.749E+02	8.550E+03	-1.354E+02
4000	2.079E+01	1.996E+02	8.314E+01	7.695E+01	1.788E+02	1.803E+02	8.612E+03	-9.810E+01
5000	2.079E+01	2.042E+02	1.039E+02	9.773E+01	1.834E+02	1.847E+02	8.674E+03	-7.553E+01
6000	2.079E+01	2.080E+02	1.247E+02	1.185E+02	1.872E+02	1.883E+02	8.735E+03	-6.038E+01
7000	2.079E+01	2.112E+02	1.455E+02	1.393E+02	1.904E+02	1.913E+02	8.796E+03	-4.948E+01
8000	2.082E+01	2.140E+02	1.663E+02	1.601E+02	1.932E+02	1.940E+02	8.857E+03	-4.125E+01
9000	2.087E+01	2.165E+02	1.872E+02	1.810E+02	1.957E+02	1.963E+02	8.918E+03	-3.480E+01
10000	2.098E+01	2.187E+02	2.081E+02	2.019E+02	1.978E+02	1.985E+02	8.980E+03	-2.961E+01
11000	2.117E+01	2.207E+02	2.292E+02	2.229E+02	1.998E+02	2.004E+02	9.041E+03	-2.533E+01
12000	2.143E+01	2.225E+02	2.504E+02	2.442E+02	2.017E+02	2.022E+02	9.104E+03	-2.174E+01
13000	2.179E+01	2.242E+02	2.721E+02	2.659E+02	2.033E+02	2.038E+02	9.167E+03	-1.868E+01
14000	2.222E+01	2.259E+02	2.940E+02	2.878E+02	2.049E+02	2.053E+02	9.232E+03	-1.604E+01
15000	2.272E+01	2.274E+02	3.165E+02	3.103E+02	2.063E+02	2.067E+02	9.297E+03	-1.374E+01
16000	2.327E+01	2.289E+02	3.395E+02	3.333E+02	2.077E+02	2.081E+02	9.364E+03	-1.171E+01
17000	2.386E+01	2.303E+02	3.631E+02	3.569E+02	2.090E+02	2.093E+02	9.432E+03	-9.903E+00
18000	2.447E+01	2.317E+02	3.872E+02	3.810E+02	2.102E+02	2.106E+02	9.501E+03	-8.287E+00
19000	2.508E+01	2.331E+02	4.120E+02	4.058E+02	2.114E+02	2.117E+02	9.572E+03	-6.830E+00
20000	2.568E+01	2.344E+02	4.374E+02	4.312E+02	2.125E+02	2.128E+02	9.643E+03	-5.510E+00
21000	2.624E+01	2.356E+02	4.634E+02	4.571E+02	2.136E+02	2.139E+02	9.716E+03	-4.306E+00
22000	2.677E+01	2.369E+02	4.899E+02	4.837E+02	2.146E+02	2.149E+02	9.789E+03	-3.204E+00
23000	2.725E+01	2.381E+02	5.169E+02	5.107E+02	2.156E+02	2.159E+02	9.863E+03	-2.189E+00
24000	2.769E+01	2.392E+02	5.444E+02	5.381E+02	2.166E+02	2.168E+02	9.938E+03	-1.253E+00
25000	2.807E+01	2.404E+02	5.722E+02	5.660E+02	2.175E+02	2.177E+02	1.001E+04	-3.842E-01
26000	2.839E+01	2.415E+02	6.005E+02	5.943E+02	2.184E+02	2.186E+02	1.009E+04	4.235E-01
27000	2.866E+01	2.426E+02	6.290E+02	6.228E+02	2.193E+02	2.195E+02	1.017E+04	1.177E+00
28000	2.888E+01	2.436E+02	6.578E+02	6.516E+02	2.201E+02	2.203E+02	1.024E+04	1.882E+00
29000	2.905E+01	2.446E+02	6.868E+02	6.805E+02	2.209E+02	2.212E+02	1.032E+04	2.543E+00
30000	2.918E+01	2.456E+02	7.159E+02	7.097E+02	2.217E+02	2.219E+02	1.040E+04	3.166E+00
32000	2.932E+01	2.475E+02	7.744E+02	7.682E+02	2.233E+02	2.235E+02	1.056E+04	4.306E+00
34000	2.935E+01	2.493E+02	8.331E+02	8.269E+02	2.248E+02	2.249E+02	1.071E+04	5.327E+00
36000	2.936E+01	2.509E+02	8.918E+02	8.856E+02	2.262E+02	2.263E+02	1.087E+04	6.248E+00
38000	2.948E+01	2.525E+02	9.506E+02	9.444E+02	2.275E+02	2.277E+02	1.103E+04	7.084E+00
40000	2.991E+01	2.541E+02	1.010E+03	1.004E+03	2.288E+02	2.290E+02	1.119E+04	7.847E+00
42000	3.097E+01	2.555E+02	1.071E+03	1.064E+03	2.301E+02	2.302E+02	1.135E+04	8.548E+00
44000	3.312E+01	2.570E+02	1.134E+03	1.128E+03	2.312E+02	2.314E+02	1.152E+04	9.194E+00
46000	3.702E+01	2.586E+02	1.204E+03	1.198E+03	2.324E+02	2.325E+02	1.169E+04	9.793E+00
48000	4.348E+01	2.603E+02	1.284E+03	1.278E+03	2.335E+02	2.337E+02	1.187E+04	1.035E+01
50000	5.342E+01	2.622E+02	1.380E+03	1.374E+03	2.346E+02	2.348E+02	1.207E+04	1.087E+01

Table 85: Internal thermodynamic properties of C^{3+} ΔE=1000 cm^{-1}

T(K)	Q_{int}	$\ln(Q_{int})$	E_{int}/RT	$C_{p,int}/R$
50	$2.000E+00$	$6.931E-01$	$0.000E+00$	$0.000E+00$
100	$2.000E+00$	$6.931E-01$	$0.000E+00$	$0.000E+00$
150	$2.000E+00$	$6.931E-01$	$2.256E-266$	$1.397E-263$
200	$2.000E+00$	$6.931E-01$	$2.866E-199$	$1.331E-196$
298.15	$2.000E+00$	$6.931E-01$	$4.770E-133$	$1.486E-130$
300	$2.000E+00$	$6.931E-01$	$3.237E-132$	$1.002E-129$
400	$2.000E+00$	$6.931E-01$	$9.992E-99$	$2.320E-96$
500	$2.000E+00$	$6.931E-01$	$1.179E-78$	$2.190E-76$
600	$2.000E+00$	$6.931E-01$	$2.742E-65$	$4.244E-63$
700	$2.000E+00$	$6.931E-01$	$9.445E-56$	$1.253E-53$
800	$2.000E+00$	$6.931E-01$	$1.319E-48$	$1.532E-46$
900	$2.000E+00$	$6.931E-01$	$4.694E-43$	$4.844E-41$
1000	$2.000E+00$	$6.931E-01$	$1.281E-38$	$1.190E-36$
2000	$2.000E+00$	$6.931E-01$	$9.448E-19$	$4.388E-17$
3000	$2.000E+00$	$6.931E-01$	$3.328E-12$	$1.030E-10$
4000	$2.000E+00$	$6.931E-01$	$5.737E-09$	$1.332E-07$
5000	$2.000E+00$	$6.931E-01$	$4.771E-07$	$8.863E-06$
6000	$2.000E+00$	$6.931E-01$	$8.790E-06$	$1.361E-04$
7000	$2.000E+00$	$6.932E-01$	$6.878E-05$	$9.126E-04$
8000	$2.000E+00$	$6.932E-01$	$3.161E-04$	$3.669E-03$
9000	$2.000E+00$	$6.932E-01$	$1.021E-03$	$1.053E-02$
10000	$2.001E+00$	$6.934E-01$	$2.577E-03$	$2.393E-02$
11000	$2.001E+00$	$6.938E-01$	$5.449E-03$	$4.598E-02$
12000	$2.003E+00$	$6.945E-01$	$1.009E-02$	$7.799E-02$
13000	$2.005E+00$	$6.955E-01$	$1.687E-02$	$1.203E-01$
14000	$2.008E+00$	$6.971E-01$	$2.606E-02$	$1.722E-01$
15000	$2.012E+00$	$6.993E-01$	$3.777E-02$	$2.324E-01$
16000	$2.018E+00$	$7.021E-01$	$5.199E-02$	$2.991E-01$
17000	$2.025E+00$	$7.058E-01$	$6.860E-02$	$3.701E-01$
18000	$2.034E+00$	$7.102E-01$	$8.738E-02$	$4.432E-01$
19000	$2.045E+00$	$7.155E-01$	$1.080E-01$	$5.165E-01$
20000	$2.058E+00$	$7.216E-01$	$1.303E-01$	$5.879E-01$
21000	$2.072E+00$	$7.285E-01$	$1.537E-01$	$6.561E-01$
22000	$2.088E+00$	$7.362E-01$	$1.780E-01$	$7.198E-01$
23000	$2.106E+00$	$7.447E-01$	$2.028E-01$	$7.780E-01$
24000	$2.125E+00$	$7.538E-01$	$2.279E-01$	$8.301E-01$
25000	$2.146E+00$	$7.637E-01$	$2.529E-01$	$8.757E-01$
26000	$2.169E+00$	$7.741E-01$	$2.777E-01$	$9.148E-01$
27000	$2.192E+00$	$7.850E-01$	$3.019E-01$	$9.474E-01$
28000	$2.218E+00$	$7.964E-01$	$3.254E-01$	$9.737E-01$
29000	$2.244E+00$	$8.082E-01$	$3.481E-01$	$9.941E-01$
30000	$2.271E+00$	$8.204E-01$	$3.699E-01$	$1.009E+00$
32000	$2.329E+00$	$8.456E-01$	$4.105E-01$	$1.024E+00$
34000	$2.391E+00$	$8.716E-01$	$4.466E-01$	$1.025E+00$
36000	$2.455E+00$	$8.980E-01$	$4.785E-01$	$1.016E+00$
38000	$2.521E+00$	$9.247E-01$	$5.066E-01$	$1.007E+00$
40000	$2.589E+00$	$9.513E-01$	$5.315E-01$	$1.007E+00$
42000	$2.659E+00$	$9.778E-01$	$5.546E-01$	$1.032E+00$
44000	$2.729E+00$	$1.004E+00$	$5.777E-01$	$1.103E+00$
46000	$2.802E+00$	$1.030E+00$	$6.034E-01$	$1.249E+00$
48000	$2.877E+00$	$1.057E+00$	$6.352E-01$	$1.509E+00$
50000	$2.955E+00$	$1.083E+00$	$6.779E-01$	$1.926E+00$

Table 86: Total thermodynamic properties of C^{3+} ΔE=1000 cm^{-1}

T [K]	C_p [J/mol/K]	S^0 [J/mol/K]	$H^0(T)$-$H^0(0)$ [KJ/mol]	$H^0(T)$-$H^0(298)$ [KJ/mol]	-(G^0-$H^0(0)$)/T [J/mol/K]	-(G^0-$H^0(298)$)/T [J/mol/K]	ΔH_f [KJ/mol]	Log(K_p)
50	2.079E+01	1.085E+02	1.039E+00	-5.158E+00	8.772E+01	2.117E+02	8.361E+03	-8.735E+03
100	2.079E+01	1.229E+02	2.079E+00	-4.119E+00	1.021E+02	1.641E+02	8.364E+03	-4.367E+03
150	2.079E+01	1.313E+02	3.118E+00	-3.079E+00	1.106E+02	1.519E+02	8.368E+03	-2.910E+03
200	2.079E+01	1.373E+02	4.157E+00	-2.040E+00	1.165E+02	1.475E+02	8.371E+03	-2.182E+03
298.15	2.079E+01	1.456E+02	6.197E+00	0.000E+00	1.248E+02	1.456E+02	8.377E+03	-1.462E+03
300	2.079E+01	1.458E+02	6.236E+00	3.848E-02	1.250E+02	1.456E+02	8.377E+03	-1.453E+03
400	2.079E+01	1.517E+02	8.315E+00	2.117E+00	1.309E+02	1.464E+02	8.383E+03	-1.088E+03
500	2.079E+01	1.564E+02	1.039E+01	4.196E+00	1.356E+02	1.480E+02	8.390E+03	-8.690E+02
600	2.079E+01	1.602E+02	1.247E+01	6.274E+00	1.394E+02	1.497E+02	8.396E+03	-7.229E+02
700	2.079E+01	1.634E+02	1.455E+01	8.353E+00	1.426E+02	1.514E+02	8.403E+03	-6.185E+02
800	2.079E+01	1.661E+02	1.663E+01	1.043E+01	1.453E+02	1.531E+02	8.409E+03	-5.401E+02
900	2.079E+01	1.686E+02	1.871E+01	1.251E+01	1.478E+02	1.547E+02	8.416E+03	-4.790E+02
1000	2.079E+01	1.708E+02	2.079E+01	1.459E+01	1.500E+02	1.562E+02	8.422E+03	-4.302E+02
2000	2.079E+01	1.852E+02	4.157E+01	3.538E+01	1.644E+02	1.675E+02	8.487E+03	-2.096E+02
3000	2.079E+01	1.936E+02	6.236E+01	5.616E+01	1.728E+02	1.749E+02	8.550E+03	-1.354E+02
4000	2.079E+01	1.996E+02	8.314E+01	7.695E+01	1.788E+02	1.803E+02	8.612E+03	-9.810E+01
5000	2.079E+01	2.042E+02	1.039E+02	9.773E+01	1.834E+02	1.847E+02	8.674E+03	-7.553E+01
6000	2.079E+01	2.080E+02	1.247E+02	1.185E+02	1.872E+02	1.883E+02	8.735E+03	-6.038E+01
7000	2.079E+01	2.112E+02	1.455E+02	1.393E+02	1.904E+02	1.913E+02	8.796E+03	-4.948E+01
8000	2.082E+01	2.140E+02	1.663E+02	1.601E+02	1.932E+02	1.940E+02	8.857E+03	-4.125E+01
9000	2.087E+01	2.165E+02	1.872E+02	1.810E+02	1.957E+02	1.963E+02	8.918E+03	-3.480E+01
10000	2.098E+01	2.187E+02	2.081E+02	2.019E+02	1.978E+02	1.985E+02	8.980E+03	-2.961E+01
11000	2.117E+01	2.207E+02	2.292E+02	2.229E+02	1.998E+02	2.004E+02	9.041E+03	-2.533E+01
12000	2.143E+01	2.225E+02	2.504E+02	2.442E+02	2.017E+02	2.022E+02	9.104E+03	-2.174E+01
13000	2.179E+01	2.242E+02	2.721E+02	2.659E+02	2.033E+02	2.038E+02	9.167E+03	-1.868E+01
14000	2.222E+01	2.259E+02	2.940E+02	2.878E+02	2.049E+02	2.053E+02	9.232E+03	-1.604E+01
15000	2.272E+01	2.274E+02	3.165E+02	3.103E+02	2.063E+02	2.067E+02	9.297E+03	-1.374E+01
16000	2.327E+01	2.289E+02	3.395E+02	3.333E+02	2.077E+02	2.081E+02	9.364E+03	-1.171E+01
17000	2.386E+01	2.303E+02	3.631E+02	3.569E+02	2.090E+02	2.093E+02	9.432E+03	-9.903E+00
18000	2.447E+01	2.317E+02	3.872E+02	3.810E+02	2.102E+02	2.106E+02	9.501E+03	-8.287E+00
19000	2.508E+01	2.331E+02	4.120E+02	4.058E+02	2.114E+02	2.117E+02	9.572E+03	-6.830E+00
20000	2.568E+01	2.344E+02	4.374E+02	4.312E+02	2.125E+02	2.128E+02	9.643E+03	-5.510E+00
21000	2.624E+01	2.356E+02	4.634E+02	4.571E+02	2.136E+02	2.139E+02	9.716E+03	-4.306E+00
22000	2.677E+01	2.369E+02	4.899E+02	4.837E+02	2.146E+02	2.149E+02	9.789E+03	-3.204E+00
23000	2.725E+01	2.381E+02	5.169E+02	5.107E+02	2.156E+02	2.159E+02	9.863E+03	-2.189E+00
24000	2.769E+01	2.392E+02	5.444E+02	5.381E+02	2.166E+02	2.168E+02	9.938E+03	-1.253E+00
25000	2.807E+01	2.404E+02	5.722E+02	5.660E+02	2.175E+02	2.177E+02	1.001E+04	-3.842E-01
26000	2.839E+01	2.415E+02	6.005E+02	5.943E+02	2.184E+02	2.186E+02	1.009E+04	4.235E-01
27000	2.866E+01	2.426E+02	6.290E+02	6.228E+02	2.193E+02	2.195E+02	1.017E+04	1.177E+00
28000	2.888E+01	2.436E+02	6.578E+02	6.516E+02	2.201E+02	2.203E+02	1.024E+04	1.882E+00
29000	2.905E+01	2.446E+02	6.868E+02	6.805E+02	2.209E+02	2.212E+02	1.032E+04	2.543E+00
30000	2.918E+01	2.456E+02	7.159E+02	7.097E+02	2.217E+02	2.219E+02	1.040E+04	3.166E+00
32000	2.930E+01	2.475E+02	7.744E+02	7.682E+02	2.233E+02	2.235E+02	1.056E+04	4.306E+00
34000	2.931E+01	2.493E+02	8.330E+02	8.268E+02	2.248E+02	2.249E+02	1.071E+04	5.327E+00
36000	2.924E+01	2.509E+02	8.915E+02	8.854E+02	2.262E+02	2.263E+02	1.087E+04	6.248E+00
38000	2.916E+01	2.525E+02	9.499E+02	9.437E+02	2.275E+02	2.277E+02	1.103E+04	7.084E+00
40000	2.916E+01	2.540E+02	1.008E+03	1.002E+03	2.288E+02	2.290E+02	1.119E+04	7.847E+00
42000	2.936E+01	2.554E+02	1.067E+03	1.060E+03	2.301E+02	2.302E+02	1.135E+04	8.548E+00
44000	2.996E+01	2.568E+02	1.126E+03	1.120E+03	2.312E+02	2.314E+02	1.151E+04	9.194E+00
46000	3.117E+01	2.582E+02	1.187E+03	1.181E+03	2.324E+02	2.325E+02	1.167E+04	9.792E+00
48000	3.333E+01	2.596E+02	1.251E+03	1.245E+03	2.335E+02	2.336E+02	1.184E+04	1.035E+01
50000	3.680E+01	2.610E+02	1.321E+03	1.315E+03	2.346E+02	2.347E+02	1.201E+04	1.087E+01

Table 87: Internal thermodynamic properties of C^{4+} ΔE=250 cm^{-1}

T(K)	Q_{int}	$\ln(Q_{int})$	E_{int}/RT	$C_{p,int}/R$
50	$1.000E+00$	$0.000E+00$	$0.000E+00$	$0.000E+00$
100	$1.000E+00$	$0.000E+00$	$0.000E+00$	$0.000E+00$
150	$1.000E+00$	$0.000E+00$	$0.000E+00$	$0.000E+00$
200	$1.000E+00$	$0.000E+00$	$0.000E+00$	$0.000E+00$
298.15	$1.000E+00$	$0.000E+00$	$0.000E+00$	$0.000E+00$
300	$1.000E+00$	$0.000E+00$	$0.000E+00$	$0.000E+00$
400	$1.000E+00$	$0.000E+00$	$0.000E+00$	$0.000E+00$
500	$1.000E+00$	$0.000E+00$	$0.000E+00$	$0.000E+00$
600	$1.000E+00$	$0.000E+00$	$0.000E+00$	$0.000E+00$
700	$1.000E+00$	$0.000E+00$	$0.000E+00$	$0.000E+00$
800	$1.000E+00$	$0.000E+00$	$0.000E+00$	$0.000E+00$
900	$1.000E+00$	$0.000E+00$	$0.000E+00$	$0.000E+00$
1000	$1.000E+00$	$0.000E+00$	$0.000E+00$	$0.000E+00$
2000	$1.000E+00$	$0.000E+00$	$0.000E+00$	$0.000E+00$
3000	$1.000E+00$	$0.000E+00$	$0.000E+00$	$0.000E+00$
4000	$1.000E+00$	$0.000E+00$	$0.000E+00$	$0.000E+00$
5000	$1.000E+00$	$0.000E+00$	$9.598E-299$	$6.660E-296$
6000	$1.000E+00$	$0.000E+00$	$1.336E-248$	$7.724E-246$
7000	$1.000E+00$	$0.000E+00$	$8.556E-213$	$4.241E-210$
8000	$1.000E+00$	$0.000E+00$	$6.021E-186$	$2.611E-183$
9000	$1.000E+00$	$0.000E+00$	$4.523E-165$	$1.744E-162$
10000	$1.000E+00$	$0.000E+00$	$2.249E-148$	$7.802E-146$
11000	$1.000E+00$	$0.000E+00$	$1.023E-134$	$3.226E-132$
12000	$1.000E+00$	$0.000E+00$	$2.449E-123$	$7.083E-121$
13000	$1.000E+00$	$0.000E+00$	$1.038E-113$	$2.772E-111$
14000	$1.000E+00$	$0.000E+00$	$1.850E-105$	$4.588E-103$
15000	$1.000E+00$	$0.000E+00$	$2.615E-98$	$6.054E-96$
16000	$1.000E+00$	$0.000E+00$	$4.718E-92$	$1.024E-89$
17000	$1.000E+00$	$0.000E+00$	$1.563E-86$	$3.194E-84$
18000	$1.000E+00$	$0.000E+00$	$1.261E-81$	$2.435E-79$
19000	$1.000E+00$	$0.000E+00$	$3.099E-77$	$5.670E-75$
20000	$1.000E+00$	$0.000E+00$	$2.772E-73$	$4.820E-71$
21000	$1.000E+00$	$0.000E+00$	$1.043E-69$	$1.728E-67$
22000	$1.000E+00$	$0.000E+00$	$1.858E-66$	$2.939E-64$
23000	$1.000E+00$	$0.000E+00$	$1.726E-63$	$2.613E-61$
24000	$1.000E+00$	$0.000E+00$	$9.082E-61$	$1.318E-58$
25000	$1.000E+00$	$0.000E+00$	$2.896E-58$	$4.035E-56$
26000	$1.000E+00$	$0.000E+00$	$5.927E-56$	$7.944E-54$
27000	$1.000E+00$	$0.000E+00$	$8.182E-54$	$1.056E-51$
28000	$1.000E+00$	$0.000E+00$	$7.945E-52$	$9.896E-50$
29000	$1.000E+00$	$0.000E+00$	$5.629E-50$	$6.771E-48$
30000	$1.000E+00$	$0.000E+00$	$3.002E-48$	$3.492E-46$
32000	$1.000E+00$	$0.000E+00$	$4.052E-45$	$4.421E-43$
34000	$1.000E+00$	$0.000E+00$	$2.342E-42$	$2.407E-40$
36000	$1.000E+00$	$0.000E+00$	$6.679E-40$	$6.485E-38$
38000	$1.000E+00$	$0.000E+00$	$1.050E-37$	$9.661E-36$
40000	$1.000E+00$	$0.000E+00$	$9.946E-36$	$8.699E-34$
42000	$1.000E+00$	$0.000E+00$	$6.105E-34$	$5.087E-32$
44000	$1.000E+00$	$0.000E+00$	$2.575E-32$	$2.049E-30$
46000	$1.000E+00$	$0.000E+00$	$7.842E-31$	$5.971E-29$
48000	$1.000E+00$	$0.000E+00$	$1.795E-29$	$1.310E-27$
50000	$1.000E+00$	$0.000E+00$	$3.195E-28$	$2.240E-26$

Table 88: Total thermodynamic properties of C^{4+} ΔE=250 cm^{-1}

T [K]	C_p [J/mol/K]	S^0 [J/mol/K]	$H^0(T)-H^0(0)$ [KJ/mol]	$H^0(T)-H^0(298)$ [KJ/mol]	$-(G^0-H^0(0))/T$ [J/mol/K]	$-(G^0-H^0(298))/T$ [J/mol/K]	ΔH_f [KJ/mol]	$Log(K_p)$
50	2.079E+01	1.027E+02	1.039E+00	-5.158E+00	8.195E+01	2.059E+02	1.458E+04	-1.524E+04
100	2.079E+01	1.172E+02	2.079E+00	-4.119E+00	9.636E+01	1.583E+02	1.459E+04	-7.619E+03
150	2.079E+01	1.256E+02	3.118E+00	-3.079E+00	1.048E+02	1.461E+02	1.459E+04	-5.078E+03
200	2.079E+01	1.316E+02	4.157E+00	-2.040E+00	1.108E+02	1.418E+02	1.460E+04	-3.808E+03
298.15	2.079E+01	1.399E+02	6.197E+00	0.000E+00	1.191E+02	1.399E+02	1.461E+04	-2.552E+03
300	2.079E+01	1.400E+02	6.236E+00	3.848E-02	1.192E+02	1.399E+02	1.461E+04	-2.537E+03
400	2.079E+01	1.460E+02	8.315E+00	2.117E+00	1.252E+02	1.407E+02	1.461E+04	-1.901E+03
500	2.079E+01	1.506E+02	1.039E+01	4.196E+00	1.298E+02	1.422E+02	1.462E+04	-1.519E+03
600	2.079E+01	1.544E+02	1.247E+01	6.274E+00	1.336E+02	1.439E+02	1.463E+04	-1.264E+03
700	2.079E+01	1.576E+02	1.455E+01	8.353E+00	1.368E+02	1.457E+02	1.464E+04	-1.082E+03
800	2.079E+01	1.604E+02	1.663E+01	1.043E+01	1.396E+02	1.473E+02	1.465E+04	-9.456E+02
900	2.079E+01	1.628E+02	1.871E+01	1.251E+01	1.420E+02	1.489E+02	1.466E+04	-8.393E+02
1000	2.079E+01	1.650E+02	2.079E+01	1.459E+01	1.442E+02	1.504E+02	1.467E+04	-7.542E+02
2000	2.079E+01	1.794E+02	4.157E+01	3.538E+01	1.586E+02	1.617E+02	1.475E+04	-3.703E+02
3000	2.079E+01	1.878E+02	6.236E+01	5.616E+01	1.671E+02	1.691E+02	1.484E+04	-2.416E+02
4000	2.079E+01	1.938E+02	8.314E+01	7.695E+01	1.730E+02	1.746E+02	1.492E+04	-1.768E+02
5000	2.079E+01	1.985E+02	1.039E+02	9.773E+01	1.777E+02	1.789E+02	1.500E+04	-1.378E+02
6000	2.079E+01	2.023E+02	1.247E+02	1.185E+02	1.815E+02	1.825E+02	1.508E+04	-1.116E+02
7000	2.079E+01	2.055E+02	1.455E+02	1.393E+02	1.847E+02	1.856E+02	1.516E+04	-9.278E+01
8000	2.079E+01	2.082E+02	1.663E+02	1.601E+02	1.874E+02	1.882E+02	1.525E+04	-7.860E+01
9000	2.079E+01	2.107E+02	1.871E+02	1.809E+02	1.899E+02	1.906E+02	1.533E+04	-6.751E+01
10000	2.079E+01	2.129E+02	2.079E+02	2.017E+02	1.921E+02	1.927E+02	1.541E+04	-5.859E+01
11000	2.079E+01	2.148E+02	2.287E+02	2.224E+02	1.941E+02	1.946E+02	1.549E+04	-5.125E+01
12000	2.079E+01	2.167E+02	2.494E+02	2.432E+02	1.959E+02	1.964E+02	1.558E+04	-4.511E+01
13000	2.079E+01	2.183E+02	2.702E+02	2.640E+02	1.975E+02	1.980E+02	1.566E+04	-3.988E+01
14000	2.079E+01	2.199E+02	2.910E+02	2.848E+02	1.991E+02	1.995E+02	1.574E+04	-3.537E+01
15000	2.079E+01	2.213E+02	3.118E+02	3.056E+02	2.005E+02	2.009E+02	1.583E+04	-3.145E+01
16000	2.079E+01	2.226E+02	3.326E+02	3.264E+02	2.019E+02	2.022E+02	1.591E+04	-2.799E+01
17000	2.079E+01	2.239E+02	3.534E+02	3.472E+02	2.031E+02	2.035E+02	1.600E+04	-2.493E+01
18000	2.079E+01	2.251E+02	3.741E+02	3.680E+02	2.043E+02	2.047E+02	1.608E+04	-2.219E+01
19000	2.079E+01	2.262E+02	3.949E+02	3.887E+02	2.054E+02	2.058E+02	1.617E+04	-1.973E+01
20000	2.079E+01	2.273E+02	4.157E+02	4.095E+02	2.065E+02	2.068E+02	1.626E+04	-1.750E+01
21000	2.079E+01	2.283E+02	4.365E+02	4.303E+02	2.075E+02	2.078E+02	1.635E+04	-1.547E+01
22000	2.079E+01	2.293E+02	4.573E+02	4.511E+02	2.085E+02	2.088E+02	1.644E+04	-1.362E+01
23000	2.079E+01	2.302E+02	4.781E+02	4.719E+02	2.094E+02	2.097E+02	1.652E+04	-1.192E+01
24000	2.079E+01	2.311E+02	4.989E+02	4.927E+02	2.103E+02	2.105E+02	1.661E+04	-1.035E+01
25000	2.079E+01	2.319E+02	5.197E+02	5.135E+02	2.111E+02	2.114E+02	1.670E+04	-8.898E+00
26000	2.079E+01	2.327E+02	5.404E+02	5.342E+02	2.119E+02	2.122E+02	1.679E+04	-7.553E+00
27000	2.079E+01	2.335E+02	5.612E+02	5.550E+02	2.127E+02	2.130E+02	1.688E+04	-6.300E+00
28000	2.079E+01	2.343E+02	5.820E+02	5.758E+02	2.135E+02	2.137E+02	1.697E+04	-5.130E+00
29000	2.079E+01	2.350E+02	6.028E+02	5.966E+02	2.142E+02	2.144E+02	1.706E+04	-4.035E+00
30000	2.079E+01	2.357E+02	6.236E+02	6.174E+02	2.149E+02	2.151E+02	1.715E+04	-3.008E+00
32000	2.079E+01	2.371E+02	6.652E+02	6.590E+02	2.163E+02	2.165E+02	1.734E+04	-1.132E+00
34000	2.079E+01	2.383E+02	7.067E+02	7.005E+02	2.175E+02	2.177E+02	1.752E+04	5.410E-01
36000	2.079E+01	2.395E+02	7.483E+02	7.421E+02	2.187E+02	2.189E+02	1.770E+04	2.044E+00
38000	2.079E+01	2.406E+02	7.899E+02	7.837E+02	2.198E+02	2.200E+02	1.788E+04	3.402E+00
40000	2.079E+01	2.417E+02	8.315E+02	8.252E+02	2.209E+02	2.211E+02	1.807E+04	4.637E+00
42000	2.079E+01	2.427E+02	8.730E+02	8.668E+02	2.219E+02	2.221E+02	1.825E+04	5.766E+00
44000	2.079E+01	2.437E+02	9.146E+02	9.084E+02	2.229E+02	2.230E+02	1.843E+04	6.803E+00
46000	2.079E+01	2.446E+02	9.562E+02	9.500E+02	2.238E+02	2.239E+02	1.862E+04	7.759E+00
48000	2.079E+01	2.455E+02	9.977E+02	9.915E+02	2.247E+02	2.248E+02	1.880E+04	8.644E+00
50000	2.079E+01	2.463E+02	1.039E+03	1.033E+03	2.255E+02	2.257E+02	1.899E+04	9.467E+00

Table 89: Internal thermodynamic properties of C^{4+} ΔE=500 cm^{-1}

T(K)	Q_{int}	$\ln(Q_{int})$	E_{int}/RT	$C_{p,int}/R$
50	$1.000E+00$	$0.000E+00$	$0.000E+00$	$0.000E+00$
100	$1.000E+00$	$0.000E+00$	$0.000E+00$	$0.000E+00$
150	$1.000E+00$	$0.000E+00$	$0.000E+00$	$0.000E+00$
200	$1.000E+00$	$0.000E+00$	$0.000E+00$	$0.000E+00$
298.15	$1.000E+00$	$0.000E+00$	$0.000E+00$	$0.000E+00$
300	$1.000E+00$	$0.000E+00$	$0.000E+00$	$0.000E+00$
400	$1.000E+00$	$0.000E+00$	$0.000E+00$	$0.000E+00$
500	$1.000E+00$	$0.000E+00$	$0.000E+00$	$0.000E+00$
600	$1.000E+00$	$0.000E+00$	$0.000E+00$	$0.000E+00$
700	$1.000E+00$	$0.000E+00$	$0.000E+00$	$0.000E+00$
800	$1.000E+00$	$0.000E+00$	$0.000E+00$	$0.000E+00$
900	$1.000E+00$	$0.000E+00$	$0.000E+00$	$0.000E+00$
1000	$1.000E+00$	$0.000E+00$	$0.000E+00$	$0.000E+00$
2000	$1.000E+00$	$0.000E+00$	$0.000E+00$	$0.000E+00$
3000	$1.000E+00$	$0.000E+00$	$0.000E+00$	$0.000E+00$
4000	$1.000E+00$	$0.000E+00$	$0.000E+00$	$0.000E+00$
5000	$1.000E+00$	$0.000E+00$	$9.598E-299$	$6.660E-296$
6000	$1.000E+00$	$0.000E+00$	$1.336E-248$	$7.724E-246$
7000	$1.000E+00$	$0.000E+00$	$8.556E-213$	$4.241E-210$
8000	$1.000E+00$	$0.000E+00$	$6.021E-186$	$2.611E-183$
9000	$1.000E+00$	$0.000E+00$	$4.523E-165$	$1.744E-162$
10000	$1.000E+00$	$0.000E+00$	$2.249E-148$	$7.802E-146$
11000	$1.000E+00$	$0.000E+00$	$1.023E-134$	$3.226E-132$
12000	$1.000E+00$	$0.000E+00$	$2.449E-123$	$7.083E-121$
13000	$1.000E+00$	$0.000E+00$	$1.038E-113$	$2.772E-111$
14000	$1.000E+00$	$0.000E+00$	$1.850E-105$	$4.588E-103$
15000	$1.000E+00$	$0.000E+00$	$2.615E-98$	$6.054E-96$
16000	$1.000E+00$	$0.000E+00$	$4.718E-92$	$1.024E-89$
17000	$1.000E+00$	$0.000E+00$	$1.563E-86$	$3.194E-84$
18000	$1.000E+00$	$0.000E+00$	$1.261E-81$	$2.435E-79$
19000	$1.000E+00$	$0.000E+00$	$3.099E-77$	$5.670E-75$
20000	$1.000E+00$	$0.000E+00$	$2.772E-73$	$4.820E-71$
21000	$1.000E+00$	$0.000E+00$	$1.043E-69$	$1.728E-67$
22000	$1.000E+00$	$0.000E+00$	$1.858E-66$	$2.939E-64$
23000	$1.000E+00$	$0.000E+00$	$1.726E-63$	$2.613E-61$
24000	$1.000E+00$	$0.000E+00$	$9.082E-61$	$1.318E-58$
25000	$1.000E+00$	$0.000E+00$	$2.896E-58$	$4.035E-56$
26000	$1.000E+00$	$0.000E+00$	$5.927E-56$	$7.944E-54$
27000	$1.000E+00$	$0.000E+00$	$8.182E-54$	$1.056E-51$
28000	$1.000E+00$	$0.000E+00$	$7.945E-52$	$9.896E-50$
29000	$1.000E+00$	$0.000E+00$	$5.629E-50$	$6.771E-48$
30000	$1.000E+00$	$0.000E+00$	$3.002E-48$	$3.492E-46$
32000	$1.000E+00$	$0.000E+00$	$4.052E-45$	$4.421E-43$
34000	$1.000E+00$	$0.000E+00$	$2.342E-42$	$2.407E-40$
36000	$1.000E+00$	$0.000E+00$	$6.679E-40$	$6.485E-38$
38000	$1.000E+00$	$0.000E+00$	$1.050E-37$	$9.661E-36$
40000	$1.000E+00$	$0.000E+00$	$9.946E-36$	$8.699E-34$
42000	$1.000E+00$	$0.000E+00$	$6.105E-34$	$5.087E-32$
44000	$1.000E+00$	$0.000E+00$	$2.575E-32$	$2.049E-30$
46000	$1.000E+00$	$0.000E+00$	$7.842E-31$	$5.971E-29$
48000	$1.000E+00$	$0.000E+00$	$1.795E-29$	$1.310E-27$
50000	$1.000E+00$	$0.000E+00$	$3.195E-28$	$2.240E-26$

Table 90: Total thermodynamic properties of C^{4+} ΔE=500 cm^{-1}

T [K]	C_p [J/mol/K]	S^0 [J/mol/K]	$H^0(T)-H^0(0)$ [KJ/mol]	$H^0(T)-H^0(298)$ [KJ/mol]	$-(G^0-H^0(0))/T$ [J/mol/K]	$-(G^0-H^0(298))/T$ [J/mol/K]	ΔH_f [KJ/mol]	$Log(K_p)$
50	2.079E+01	1.027E+02	1.039E+00	-5.158E+00	8.195E+01	2.059E+02	1.458E+04	-1.524E+04
100	2.079E+01	1.172E+02	2.079E+00	-4.119E+00	9.636E+01	1.583E+02	1.459E+04	-7.619E+03
150	2.079E+01	1.256E+02	3.118E+00	-3.079E+00	1.048E+02	1.461E+02	1.459E+04	-5.078E+03
200	2.079E+01	1.316E+02	4.157E+00	-2.040E+00	1.108E+02	1.418E+02	1.460E+04	-3.808E+03
298.15	2.079E+01	1.399E+02	6.197E+00	0.000E+00	1.191E+02	1.399E+02	1.461E+04	-2.552E+03
300	2.079E+01	1.400E+02	6.236E+00	3.848E-02	1.192E+02	1.399E+02	1.461E+04	-2.537E+03
400	2.079E+01	1.460E+02	8.315E+00	2.117E+00	1.252E+02	1.407E+02	1.461E+04	-1.901E+03
500	2.079E+01	1.506E+02	1.039E+01	4.196E+00	1.298E+02	1.422E+02	1.462E+04	-1.519E+03
600	2.079E+01	1.544E+02	1.247E+01	6.274E+00	1.336E+02	1.439E+02	1.463E+04	-1.264E+03
700	2.079E+01	1.576E+02	1.455E+01	8.353E+00	1.368E+02	1.457E+02	1.464E+04	-1.082E+03
800	2.079E+01	1.604E+02	1.663E+01	1.043E+01	1.396E+02	1.473E+02	1.465E+04	-9.456E+02
900	2.079E+01	1.628E+02	1.871E+01	1.251E+01	1.420E+02	1.489E+02	1.466E+04	-8.393E+02
1000	2.079E+01	1.650E+02	2.079E+01	1.459E+01	1.442E+02	1.504E+02	1.467E+04	-7.542E+02
2000	2.079E+01	1.794E+02	4.157E+01	3.538E+01	1.586E+02	1.617E+02	1.475E+04	-3.703E+02
3000	2.079E+01	1.878E+02	6.236E+01	5.616E+01	1.671E+02	1.691E+02	1.484E+04	-2.416E+02
4000	2.079E+01	1.938E+02	8.314E+01	7.695E+01	1.730E+02	1.746E+02	1.492E+04	-1.768E+02
5000	2.079E+01	1.985E+02	1.039E+02	9.773E+01	1.777E+02	1.789E+02	1.500E+04	-1.378E+02
6000	2.079E+01	2.023E+02	1.247E+02	1.185E+02	1.815E+02	1.825E+02	1.508E+04	-1.116E+02
7000	2.079E+01	2.055E+02	1.455E+02	1.393E+02	1.847E+02	1.856E+02	1.516E+04	-9.278E+01
8000	2.079E+01	2.082E+02	1.663E+02	1.601E+02	1.874E+02	1.882E+02	1.525E+04	-7.860E+01
9000	2.079E+01	2.107E+02	1.871E+02	1.809E+02	1.899E+02	1.906E+02	1.533E+04	-6.751E+01
10000	2.079E+01	2.129E+02	2.079E+02	2.017E+02	1.921E+02	1.927E+02	1.541E+04	-5.859E+01
11000	2.079E+01	2.148E+02	2.287E+02	2.224E+02	1.941E+02	1.946E+02	1.549E+04	-5.125E+01
12000	2.079E+01	2.167E+02	2.494E+02	2.432E+02	1.959E+02	1.964E+02	1.558E+04	-4.511E+01
13000	2.079E+01	2.183E+02	2.702E+02	2.640E+02	1.975E+02	1.980E+02	1.566E+04	-3.988E+01
14000	2.079E+01	2.199E+02	2.910E+02	2.848E+02	1.991E+02	1.995E+02	1.574E+04	-3.537E+01
15000	2.079E+01	2.213E+02	3.118E+02	3.056E+02	2.005E+02	2.009E+02	1.583E+04	-3.145E+01
16000	2.079E+01	2.226E+02	3.326E+02	3.264E+02	2.019E+02	2.022E+02	1.591E+04	-2.799E+01
17000	2.079E+01	2.239E+02	3.534E+02	3.472E+02	2.031E+02	2.035E+02	1.600E+04	-2.493E+01
18000	2.079E+01	2.251E+02	3.741E+02	3.680E+02	2.043E+02	2.047E+02	1.608E+04	-2.219E+01
19000	2.079E+01	2.262E+02	3.949E+02	3.887E+02	2.054E+02	2.058E+02	1.617E+04	-1.973E+01
20000	2.079E+01	2.273E+02	4.157E+02	4.095E+02	2.065E+02	2.068E+02	1.626E+04	-1.750E+01
21000	2.079E+01	2.283E+02	4.365E+02	4.303E+02	2.075E+02	2.078E+02	1.635E+04	-1.547E+01
22000	2.079E+01	2.293E+02	4.573E+02	4.511E+02	2.085E+02	2.088E+02	1.644E+04	-1.362E+01
23000	2.079E+01	2.302E+02	4.781E+02	4.719E+02	2.094E+02	2.097E+02	1.652E+04	-1.192E+01
24000	2.079E+01	2.311E+02	4.989E+02	4.927E+02	2.103E+02	2.105E+02	1.661E+04	-1.035E+01
25000	2.079E+01	2.319E+02	5.197E+02	5.135E+02	2.111E+02	2.114E+02	1.670E+04	-8.898E+00
26000	2.079E+01	2.327E+02	5.404E+02	5.342E+02	2.119E+02	2.122E+02	1.679E+04	-7.553E+00
27000	2.079E+01	2.335E+02	5.612E+02	5.550E+02	2.127E+02	2.130E+02	1.688E+04	-6.300E+00
28000	2.079E+01	2.343E+02	5.820E+02	5.758E+02	2.135E+02	2.137E+02	1.697E+04	-5.130E+00
29000	2.079E+01	2.350E+02	6.028E+02	5.966E+02	2.142E+02	2.144E+02	1.706E+04	-4.035E+00
30000	2.079E+01	2.357E+02	6.236E+02	6.174E+02	2.149E+02	2.151E+02	1.715E+04	-3.008E+00
32000	2.079E+01	2.371E+02	6.652E+02	6.590E+02	2.163E+02	2.165E+02	1.734E+04	-1.132E+00
34000	2.079E+01	2.383E+02	7.067E+02	7.005E+02	2.175E+02	2.177E+02	1.752E+04	5.410E-01
36000	2.079E+01	2.395E+02	7.483E+02	7.421E+02	2.187E+02	2.189E+02	1.770E+04	2.044E+00
38000	2.079E+01	2.406E+02	7.899E+02	7.837E+02	2.198E+02	2.200E+02	1.788E+04	3.402E+00
40000	2.079E+01	2.417E+02	8.315E+02	8.252E+02	2.209E+02	2.211E+02	1.807E+04	4.637E+00
42000	2.079E+01	2.427E+02	8.730E+02	8.668E+02	2.219E+02	2.221E+02	1.825E+04	5.766E+00
44000	2.079E+01	2.437E+02	9.146E+02	9.084E+02	2.229E+02	2.230E+02	1.843E+04	6.803E+00
46000	2.079E+01	2.446E+02	9.562E+02	9.500E+02	2.238E+02	2.239E+02	1.862E+04	7.759E+00
48000	2.079E+01	2.455E+02	9.977E+02	9.915E+02	2.247E+02	2.248E+02	1.880E+04	8.644E+00
50000	2.079E+01	2.463E+02	1.039E+03	1.033E+03	2.255E+02	2.257E+02	1.899E+04	9.467E+00

Table 91: Internal thermodynamic properties of C^{4+} ΔE=1000 cm^{-1}

T(K)	Q_{int}	$\ln(Q_{int})$	E_{int}/RT	$C_{p,int}/R$
50	$1.000E+00$	$0.000E+00$	$0.000E+00$	$0.000E+00$
100	$1.000E+00$	$0.000E+00$	$0.000E+00$	$0.000E+00$
150	$1.000E+00$	$0.000E+00$	$0.000E+00$	$0.000E+00$
200	$1.000E+00$	$0.000E+00$	$0.000E+00$	$0.000E+00$
298.15	$1.000E+00$	$0.000E+00$	$0.000E+00$	$0.000E+00$
300	$1.000E+00$	$0.000E+00$	$0.000E+00$	$0.000E+00$
400	$1.000E+00$	$0.000E+00$	$0.000E+00$	$0.000E+00$
500	$1.000E+00$	$0.000E+00$	$0.000E+00$	$0.000E+00$
600	$1.000E+00$	$0.000E+00$	$0.000E+00$	$0.000E+00$
700	$1.000E+00$	$0.000E+00$	$0.000E+00$	$0.000E+00$
800	$1.000E+00$	$0.000E+00$	$0.000E+00$	$0.000E+00$
900	$1.000E+00$	$0.000E+00$	$0.000E+00$	$0.000E+00$
1000	$1.000E+00$	$0.000E+00$	$0.000E+00$	$0.000E+00$
2000	$1.000E+00$	$0.000E+00$	$0.000E+00$	$0.000E+00$
3000	$1.000E+00$	$0.000E+00$	$0.000E+00$	$0.000E+00$
4000	$1.000E+00$	$0.000E+00$	$0.000E+00$	$0.000E+00$
5000	$1.000E+00$	$0.000E+00$	$9.598E-299$	$6.660E-296$
6000	$1.000E+00$	$0.000E+00$	$1.336E-248$	$7.724E-246$
7000	$1.000E+00$	$0.000E+00$	$8.556E-213$	$4.241E-210$
8000	$1.000E+00$	$0.000E+00$	$6.021E-186$	$2.611E-183$
9000	$1.000E+00$	$0.000E+00$	$4.523E-165$	$1.744E-162$
10000	$1.000E+00$	$0.000E+00$	$2.249E-148$	$7.802E-146$
11000	$1.000E+00$	$0.000E+00$	$1.023E-134$	$3.226E-132$
12000	$1.000E+00$	$0.000E+00$	$2.449E-123$	$7.083E-121$
13000	$1.000E+00$	$0.000E+00$	$1.038E-113$	$2.772E-111$
14000	$1.000E+00$	$0.000E+00$	$1.850E-105$	$4.588E-103$
15000	$1.000E+00$	$0.000E+00$	$2.615E-98$	$6.054E-96$
16000	$1.000E+00$	$0.000E+00$	$4.718E-92$	$1.024E-89$
17000	$1.000E+00$	$0.000E+00$	$1.563E-86$	$3.194E-84$
18000	$1.000E+00$	$0.000E+00$	$1.261E-81$	$2.435E-79$
19000	$1.000E+00$	$0.000E+00$	$3.099E-77$	$5.670E-75$
20000	$1.000E+00$	$0.000E+00$	$2.772E-73$	$4.820E-71$
21000	$1.000E+00$	$0.000E+00$	$1.043E-69$	$1.728E-67$
22000	$1.000E+00$	$0.000E+00$	$1.858E-66$	$2.939E-64$
23000	$1.000E+00$	$0.000E+00$	$1.726E-63$	$2.613E-61$
24000	$1.000E+00$	$0.000E+00$	$9.082E-61$	$1.318E-58$
25000	$1.000E+00$	$0.000E+00$	$2.896E-58$	$4.035E-56$
26000	$1.000E+00$	$0.000E+00$	$5.927E-56$	$7.944E-54$
27000	$1.000E+00$	$0.000E+00$	$8.182E-54$	$1.056E-51$
28000	$1.000E+00$	$0.000E+00$	$7.945E-52$	$9.896E-50$
29000	$1.000E+00$	$0.000E+00$	$5.629E-50$	$6.771E-48$
30000	$1.000E+00$	$0.000E+00$	$3.002E-48$	$3.492E-46$
32000	$1.000E+00$	$0.000E+00$	$4.052E-45$	$4.421E-43$
34000	$1.000E+00$	$0.000E+00$	$2.342E-42$	$2.407E-40$
36000	$1.000E+00$	$0.000E+00$	$6.679E-40$	$6.485E-38$
38000	$1.000E+00$	$0.000E+00$	$1.050E-37$	$9.661E-36$
40000	$1.000E+00$	$0.000E+00$	$9.946E-36$	$8.699E-34$
42000	$1.000E+00$	$0.000E+00$	$6.105E-34$	$5.087E-32$
44000	$1.000E+00$	$0.000E+00$	$2.575E-32$	$2.049E-30$
46000	$1.000E+00$	$0.000E+00$	$7.842E-31$	$5.971E-29$
48000	$1.000E+00$	$0.000E+00$	$1.795E-29$	$1.310E-27$
50000	$1.000E+00$	$0.000E+00$	$3.195E-28$	$2.240E-26$

Table 92: Total thermodynamic properties of C^{4+} ΔE=1000 cm^{-1}

T [K]	C_p [J/mol/K]	S^0 [J/mol/K]	$H^0(T)-H^0(0)$ [KJ/mol]	$H^0(T)-H^0(298)$ [KJ/mol]	$-(G^0-H^0(0))/T$ [J/mol/K]	$-(G^0-H^0(298))/T$ [J/mol/K]	ΔH_f [KJ/mol]	$Log(K_p)$
50	2.079E+01	1.027E+02	1.039E+00	-5.158E+00	8.195E+01	2.059E+02	1.458E+04	-1.524E+04
100	2.079E+01	1.172E+02	2.079E+00	-4.119E+00	9.636E+01	1.583E+02	1.459E+04	-7.619E+03
150	2.079E+01	1.256E+02	3.118E+00	-3.079E+00	1.048E+02	1.461E+02	1.459E+04	-5.078E+03
200	2.079E+01	1.316E+02	4.157E+00	-2.040E+00	1.108E+02	1.418E+02	1.460E+04	-3.808E+03
298.15	2.079E+01	1.399E+02	6.197E+00	0.000E+00	1.191E+02	1.399E+02	1.461E+04	-2.552E+03
300	2.079E+01	1.400E+02	6.236E+00	3.848E-02	1.192E+02	1.399E+02	1.461E+04	-2.537E+03
400	2.079E+01	1.460E+02	8.315E+00	2.117E+00	1.252E+02	1.407E+02	1.461E+04	-1.901E+03
500	2.079E+01	1.506E+02	1.039E+01	4.196E+00	1.298E+02	1.422E+02	1.462E+04	-1.519E+03
600	2.079E+01	1.544E+02	1.247E+01	6.274E+00	1.336E+02	1.439E+02	1.463E+04	-1.264E+03
700	2.079E+01	1.576E+02	1.455E+01	8.353E+00	1.368E+02	1.457E+02	1.464E+04	-1.082E+03
800	2.079E+01	1.604E+02	1.663E+01	1.043E+01	1.396E+02	1.473E+02	1.465E+04	-9.456E+02
900	2.079E+01	1.628E+02	1.871E+01	1.251E+01	1.420E+02	1.489E+02	1.466E+04	-8.393E+02
1000	2.079E+01	1.650E+02	2.079E+01	1.459E+01	1.442E+02	1.504E+02	1.467E+04	-7.542E+02
2000	2.079E+01	1.794E+02	4.157E+01	3.538E+01	1.586E+02	1.617E+02	1.475E+04	-3.703E+02
3000	2.079E+01	1.878E+02	6.236E+01	5.616E+01	1.671E+02	1.691E+02	1.484E+04	-2.416E+02
4000	2.079E+01	1.938E+02	8.314E+01	7.695E+01	1.730E+02	1.746E+02	1.492E+04	-1.768E+02
5000	2.079E+01	1.985E+02	1.039E+02	9.773E+01	1.777E+02	1.789E+02	1.500E+04	-1.378E+02
6000	2.079E+01	2.023E+02	1.247E+02	1.185E+02	1.815E+02	1.825E+02	1.508E+04	-1.116E+02
7000	2.079E+01	2.055E+02	1.455E+02	1.393E+02	1.847E+02	1.856E+02	1.516E+04	-9.278E+01
8000	2.079E+01	2.082E+02	1.663E+02	1.601E+02	1.874E+02	1.882E+02	1.525E+04	-7.860E+01
9000	2.079E+01	2.107E+02	1.871E+02	1.809E+02	1.899E+02	1.906E+02	1.533E+04	-6.751E+01
10000	2.079E+01	2.129E+02	2.079E+02	2.017E+02	1.921E+02	1.927E+02	1.541E+04	-5.859E+01
11000	2.079E+01	2.148E+02	2.287E+02	2.224E+02	1.941E+02	1.946E+02	1.549E+04	-5.125E+01
12000	2.079E+01	2.167E+02	2.494E+02	2.432E+02	1.959E+02	1.964E+02	1.558E+04	-4.511E+01
13000	2.079E+01	2.183E+02	2.702E+02	2.640E+02	1.975E+02	1.980E+02	1.566E+04	-3.988E+01
14000	2.079E+01	2.199E+02	2.910E+02	2.848E+02	1.991E+02	1.995E+02	1.574E+04	-3.537E+01
15000	2.079E+01	2.213E+02	3.118E+02	3.056E+02	2.005E+02	2.009E+02	1.583E+04	-3.145E+01
16000	2.079E+01	2.226E+02	3.326E+02	3.264E+02	2.019E+02	2.022E+02	1.591E+04	-2.799E+01
17000	2.079E+01	2.239E+02	3.534E+02	3.472E+02	2.031E+02	2.035E+02	1.600E+04	-2.493E+01
18000	2.079E+01	2.251E+02	3.741E+02	3.680E+02	2.043E+02	2.047E+02	1.608E+04	-2.219E+01
19000	2.079E+01	2.262E+02	3.949E+02	3.887E+02	2.054E+02	2.058E+02	1.617E+04	-1.973E+01
20000	2.079E+01	2.273E+02	4.157E+02	4.095E+02	2.065E+02	2.068E+02	1.626E+04	-1.750E+01
21000	2.079E+01	2.283E+02	4.365E+02	4.303E+02	2.075E+02	2.078E+02	1.635E+04	-1.547E+01
22000	2.079E+01	2.293E+02	4.573E+02	4.511E+02	2.085E+02	2.088E+02	1.644E+04	-1.362E+01
23000	2.079E+01	2.302E+02	4.781E+02	4.719E+02	2.094E+02	2.097E+02	1.652E+04	-1.192E+01
24000	2.079E+01	2.311E+02	4.989E+02	4.927E+02	2.103E+02	2.105E+02	1.661E+04	-1.035E+01
25000	2.079E+01	2.319E+02	5.197E+02	5.135E+02	2.111E+02	2.114E+02	1.670E+04	-8.898E+00
26000	2.079E+01	2.327E+02	5.404E+02	5.342E+02	2.119E+02	2.122E+02	1.679E+04	-7.553E+00
27000	2.079E+01	2.335E+02	5.612E+02	5.550E+02	2.127E+02	2.130E+02	1.688E+04	-6.300E+00
28000	2.079E+01	2.343E+02	5.820E+02	5.758E+02	2.135E+02	2.137E+02	1.697E+04	-5.130E+00
29000	2.079E+01	2.350E+02	6.028E+02	5.966E+02	2.142E+02	2.144E+02	1.706E+04	-4.035E+00
30000	2.079E+01	2.357E+02	6.236E+02	6.174E+02	2.149E+02	2.151E+02	1.715E+04	-3.008E+00
32000	2.079E+01	2.371E+02	6.652E+02	6.590E+02	2.163E+02	2.165E+02	1.734E+04	-1.132E+00
34000	2.079E+01	2.383E+02	7.067E+02	7.005E+02	2.175E+02	2.177E+02	1.752E+04	5.410E-01
36000	2.079E+01	2.395E+02	7.483E+02	7.421E+02	2.187E+02	2.189E+02	1.770E+04	2.044E+00
38000	2.079E+01	2.406E+02	7.899E+02	7.837E+02	2.198E+02	2.200E+02	1.788E+04	3.402E+00
40000	2.079E+01	2.417E+02	8.315E+02	8.252E+02	2.209E+02	2.211E+02	1.807E+04	4.637E+00
42000	2.079E+01	2.427E+02	8.730E+02	8.668E+02	2.219E+02	2.221E+02	1.825E+04	5.766E+00
44000	2.079E+01	2.437E+02	9.146E+02	9.084E+02	2.229E+02	2.230E+02	1.843E+04	6.803E+00
46000	2.079E+01	2.446E+02	9.562E+02	9.500E+02	2.238E+02	2.239E+02	1.862E+04	7.759E+00
48000	2.079E+01	2.455E+02	9.977E+02	9.915E+02	2.247E+02	2.248E+02	1.880E+04	8.644E+00
50000	2.079E+01	2.463E+02	1.039E+03	1.033E+03	2.255E+02	2.257E+02	1.899E+04	9.467E+00

Table 93: Internal thermodynamic properties of C^-

T(K)	Q_{int}	$\ln(Q_{int})$	E_{int}/RT	$C_{p,int}/R$
50	$4.000E+00$	$1.386E+00$	$7.645E-122$	$2.182E-119$
100	$4.000E+00$	$1.386E+00$	$3.693E-60$	$5.271E-58$
150	$4.000E+00$	$1.386E+00$	$1.130E-39$	$1.075E-37$
200	$4.000E+00$	$1.386E+00$	$1.815E-29$	$1.295E-27$
298.15	$4.000E+00$	$1.386E+00$	$1.941E-19$	$9.294E-18$
300	$4.000E+00$	$1.386E+00$	$2.592E-19$	$1.233E-17$
400	$4.000E+00$	$1.386E+00$	$2.845E-14$	$1.015E-12$
500	$4.000E+00$	$1.386E+00$	$2.861E-11$	$8.166E-10$
600	$4.000E+00$	$1.386E+00$	$2.776E-09$	$6.604E-08$
700	$4.000E+00$	$1.386E+00$	$7.118E-08$	$1.451E-06$
800	$4.000E+00$	$1.386E+00$	$7.966E-07$	$1.421E-05$
900	$4.000E+00$	$1.386E+00$	$5.140E-06$	$8.151E-05$
1000	$4.000E+00$	$1.386E+00$	$2.259E-05$	$3.224E-04$
2000	$4.008E+00$	$1.388E+00$	$1.417E-02$	$1.009E-01$
3000	$4.086E+00$	$1.408E+00$	$9.998E-02$	$4.657E-01$
4000	$4.282E+00$	$1.454E+00$	$2.351E-01$	$7.834E-01$
5000	$4.576E+00$	$1.521E+00$	$3.592E-01$	$8.964E-01$
6000	$4.927E+00$	$1.595E+00$	$4.474E-01$	$8.641E-01$
7000	$5.302E+00$	$1.668E+00$	$5.006E-01$	$7.701E-01$
8000	$5.680E+00$	$1.737E+00$	$5.276E-01$	$6.629E-01$
9000	$6.048E+00$	$1.800E+00$	$5.370E-01$	$5.632E-01$
10000	$6.400E+00$	$1.856E+00$	$5.352E-01$	$4.774E-01$
11000	$6.732E+00$	$1.907E+00$	$5.266E-01$	$4.060E-01$
12000	$7.044E+00$	$1.952E+00$	$5.140E-01$	$3.471E-01$
13000	$7.336E+00$	$1.993E+00$	$4.992E-01$	$2.989E-01$
14000	$7.608E+00$	$2.029E+00$	$4.835E-01$	$2.591E-01$
15000	$7.862E+00$	$2.062E+00$	$4.674E-01$	$2.263E-01$
16000	$8.098E+00$	$2.092E+00$	$4.514E-01$	$1.989E-01$
17000	$8.319E+00$	$2.119E+00$	$4.359E-01$	$1.760E-01$
18000	$8.525E+00$	$2.143E+00$	$4.209E-01$	$1.566E-01$
19000	$8.718E+00$	$2.165E+00$	$4.065E-01$	$1.401E-01$
20000	$8.899E+00$	$2.186E+00$	$3.928E-01$	$1.260E-01$
21000	$9.068E+00$	$2.205E+00$	$3.798E-01$	$1.139E-01$
22000	$9.227E+00$	$2.222E+00$	$3.675E-01$	$1.034E-01$
23000	$9.377E+00$	$2.238E+00$	$3.558E-01$	$9.420E-02$
24000	$9.517E+00$	$2.253E+00$	$3.448E-01$	$8.617E-02$
25000	$9.650E+00$	$2.267E+00$	$3.343E-01$	$7.910E-02$
26000	$9.776E+00$	$2.280E+00$	$3.243E-01$	$7.285E-02$
27000	$9.894E+00$	$2.292E+00$	$3.149E-01$	$6.730E-02$
28000	$1.001E+01$	$2.303E+00$	$3.060E-01$	$6.235E-02$
29000	$1.011E+01$	$2.314E+00$	$2.975E-01$	$5.791E-02$
30000	$1.021E+01$	$2.324E+00$	$2.894E-01$	$5.393E-02$
32000	$1.040E+01$	$2.342E+00$	$2.745E-01$	$4.708E-02$
34000	$1.057E+01$	$2.358E+00$	$2.610E-01$	$4.145E-02$
36000	$1.073E+01$	$2.373E+00$	$2.486E-01$	$3.676E-02$
38000	$1.087E+01$	$2.386E+00$	$2.374E-01$	$3.281E-02$
40000	$1.100E+01$	$2.398E+00$	$2.271E-01$	$2.946E-02$
42000	$1.112E+01$	$2.409E+00$	$2.176E-01$	$2.660E-02$
44000	$1.123E+01$	$2.419E+00$	$2.088E-01$	$2.413E-02$
46000	$1.133E+01$	$2.428E+00$	$2.008E-01$	$2.199E-02$
48000	$1.143E+01$	$2.436E+00$	$1.933E-01$	$2.011E-02$
50000	$1.152E+01$	$2.444E+00$	$1.863E-01$	$1.847E-02$

Table 94: Total thermodynamic properties of C^-

T [K]	C_p [J/mol/K]	S^0 [J/mol/K]	$H^0(T)-H^0(0)$ [KJ/mol]	$H^0(T)-H^0(298)$ [KJ/mol]	$-(G^0-H^0(0))/T$ [J/mol/K]	$-(G^0-H^0(298))/T$ [J/mol/K]	ΔH_f [KJ/mol]	$\mathrm{Log}(K_p)$
50	2.079E+01	1.143E+02	1.039E+00	-5.158E+00	9.348E+01	2.174E+02	1.836E+02	-1.886E+02
100	2.079E+01	1.287E+02	2.079E+00	-4.119E+00	1.079E+02	1.699E+02	1.829E+02	-9.287E+01
150	2.079E+01	1.371E+02	3.118E+00	-3.079E+00	1.163E+02	1.576E+02	1.821E+02	-6.108E+01
200	2.079E+01	1.431E+02	4.157E+00	-2.040E+00	1.223E+02	1.533E+02	1.812E+02	-4.526E+01
298.15	2.079E+01	1.514E+02	6.197E+00	0.000E+00	1.306E+02	1.514E+02	1.791E+02	-2.977E+01
300	2.079E+01	1.515E+02	6.236E+00	3.848E-02	1.307E+02	1.514E+02	1.790E+02	-2.957E+01
400	2.079E+01	1.575E+02	8.315E+00	2.117E+00	1.367E+02	1.522E+02	1.769E+02	-2.182E+01
500	2.079E+01	1.621E+02	1.039E+01	4.196E+00	1.413E+02	1.537E+02	1.750E+02	-1.722E+01
600	2.079E+01	1.659E+02	1.247E+01	6.274E+00	1.451E+02	1.555E+02	1.732E+02	-1.419E+01
700	2.079E+01	1.691E+02	1.455E+01	8.353E+00	1.483E+02	1.572E+02	1.714E+02	-1.205E+01
800	2.079E+01	1.719E+02	1.663E+01	1.043E+01	1.511E+02	1.589E+02	1.696E+02	-1.046E+01
900	2.079E+01	1.743E+02	1.871E+01	1.251E+01	1.536E+02	1.604E+02	1.679E+02	-9.232E+00
1000	2.079E+01	1.765E+02	2.079E+01	1.459E+01	1.558E+02	1.619E+02	1.661E+02	-8.262E+00
2000	2.162E+01	1.911E+02	4.181E+01	3.561E+01	1.702E+02	1.733E+02	1.476E+02	-4.110E+00
3000	2.466E+01	2.004E+02	6.485E+01	5.866E+01	1.788E+02	1.808E+02	1.299E+02	-2.893E+00
4000	2.730E+01	2.079E+02	9.096E+01	8.477E+01	1.851E+02	1.867E+02	1.144E+02	-2.359E+00
5000	2.824E+01	2.141E+02	1.189E+02	1.127E+02	1.903E+02	1.916E+02	1.001E+02	-2.077E+00
6000	2.797E+01	2.192E+02	1.470E+02	1.408E+02	1.947E+02	1.958E+02	8.575E+01	-1.915E+00
7000	2.719E+01	2.235E+02	1.746E+02	1.684E+02	1.985E+02	1.994E+02	7.049E+01	-1.817E+00
8000	2.630E+01	2.271E+02	2.014E+02	1.952E+02	2.019E+02	2.027E+02	5.419E+01	-1.758E+00
9000	2.547E+01	2.301E+02	2.273E+02	2.211E+02	2.049E+02	2.056E+02	3.702E+01	-1.725E+00
10000	2.476E+01	2.328E+02	2.524E+02	2.462E+02	2.075E+02	2.081E+02	1.929E+01	-1.708E+00
11000	2.416E+01	2.351E+02	2.768E+02	2.706E+02	2.099E+02	2.105E+02	1.301E+00	-1.703E+00
12000	2.367E+01	2.372E+02	3.007E+02	2.945E+02	2.121E+02	2.126E+02	-1.670E+01	-1.706E+00
13000	2.327E+01	2.391E+02	3.242E+02	3.180E+02	2.141E+02	2.146E+02	-3.453E+01	-1.715E+00
14000	2.294E+01	2.408E+02	3.473E+02	3.411E+02	2.160E+02	2.164E+02	-5.206E+01	-1.727E+00
15000	2.267E+01	2.423E+02	3.701E+02	3.639E+02	2.177E+02	2.181E+02	-6.923E+01	-1.742E+00
16000	2.244E+01	2.438E+02	3.926E+02	3.864E+02	2.192E+02	2.196E+02	-8.601E+01	-1.759E+00
17000	2.225E+01	2.452E+02	4.150E+02	4.088E+02	2.207E+02	2.211E+02	-1.024E+02	-1.777E+00
18000	2.209E+01	2.464E+02	4.371E+02	4.309E+02	2.221E+02	2.225E+02	-1.184E+02	-1.796E+00
19000	2.195E+01	2.476E+02	4.592E+02	4.530E+02	2.234E+02	2.238E+02	-1.340E+02	-1.815E+00
20000	2.183E+01	2.487E+02	4.811E+02	4.749E+02	2.247E+02	2.250E+02	-1.492E+02	-1.835E+00
21000	2.173E+01	2.498E+02	5.028E+02	4.966E+02	2.258E+02	2.261E+02	-1.642E+02	-1.854E+00
22000	2.165E+01	2.508E+02	5.245E+02	5.183E+02	2.270E+02	2.272E+02	-1.788E+02	-1.873E+00
23000	2.157E+01	2.518E+02	5.461E+02	5.399E+02	2.280E+02	2.283E+02	-1.932E+02	-1.893E+00
24000	2.150E+01	2.527E+02	5.677E+02	5.615E+02	2.290E+02	2.293E+02	-2.073E+02	-1.912E+00
25000	2.144E+01	2.536E+02	5.891E+02	5.829E+02	2.300E+02	2.302E+02	-2.212E+02	-1.930E+00
26000	2.139E+01	2.544E+02	6.105E+02	6.044E+02	2.309E+02	2.312E+02	-2.348E+02	-1.949E+00
27000	2.135E+01	2.552E+02	6.319E+02	6.257E+02	2.318E+02	2.320E+02	-2.483E+02	-1.967E+00
28000	2.130E+01	2.560E+02	6.532E+02	6.470E+02	2.326E+02	2.329E+02	-2.616E+02	-1.984E+00
29000	2.127E+01	2.567E+02	6.745E+02	6.683E+02	2.335E+02	2.337E+02	-2.748E+02	-2.001E+00
30000	2.123E+01	2.574E+02	6.958E+02	6.896E+02	2.342E+02	2.344E+02	-2.878E+02	-2.018E+00
32000	2.118E+01	2.588E+02	7.382E+02	7.320E+02	2.357E+02	2.359E+02	-3.134E+02	-2.051E+00
34000	2.113E+01	2.601E+02	7.805E+02	7.743E+02	2.371E+02	2.373E+02	-3.385E+02	-2.082E+00
36000	2.109E+01	2.613E+02	8.227E+02	8.165E+02	2.384E+02	2.386E+02	-3.632E+02	-2.112E+00
38000	2.106E+01	2.624E+02	8.649E+02	8.587E+02	2.397E+02	2.398E+02	-3.875E+02	-2.141E+00
40000	2.103E+01	2.635E+02	9.070E+02	9.008E+02	2.408E+02	2.410E+02	-4.116E+02	-2.168E+00
42000	2.101E+01	2.645E+02	9.490E+02	9.428E+02	2.419E+02	2.421E+02	-4.354E+02	-2.195E+00
44000	2.099E+01	2.655E+02	9.910E+02	9.848E+02	2.430E+02	2.431E+02	-4.589E+02	-2.220E+00
46000	2.097E+01	2.664E+02	1.033E+03	1.027E+03	2.440E+02	2.441E+02	-4.823E+02	-2.244E+00
48000	2.095E+01	2.673E+02	1.075E+03	1.069E+03	2.449E+02	2.451E+02	-5.054E+02	-2.268E+00
50000	2.094E+01	2.682E+02	1.117E+03	1.111E+03	2.459E+02	2.460E+02	-5.284E+02	-2.290E+00

Table 95: Internal thermodynamic properties of C_2

T(K)	Q_{int}	$\ln(Q_{int})$	E_{int}/RT	$C_{p,int}/R$
50	$9.765E+00$	$2.279E+00$	$9.827E-01$	$1.000E+00$
100	$1.938E+01$	$2.964E+00$	$1.001E+00$	$1.080E+00$
150	$2.952E+01$	$3.385E+00$	$1.105E+00$	$1.635E+00$
200	$4.177E+01$	$3.732E+00$	$1.333E+00$	$2.366E+00$
298.15	$7.768E+01$	$4.353E+00$	$1.767E+00$	$2.689E+00$
300	$7.854E+01$	$4.364E+00$	$1.773E+00$	$2.684E+00$
400	$1.347E+02$	$4.903E+00$	$1.950E+00$	$2.269E+00$
500	$2.092E+02$	$5.343E+00$	$1.980E+00$	$1.967E+00$
600	$2.998E+02$	$5.703E+00$	$1.965E+00$	$1.830E+00$
700	$4.052E+02$	$6.004E+00$	$1.942E+00$	$1.785E+00$
800	$5.244E+02$	$6.262E+00$	$1.922E+00$	$1.783E+00$
900	$6.570E+02$	$6.488E+00$	$1.907E+00$	$1.800E+00$
1000	$8.028E+02$	$6.688E+00$	$1.898E+00$	$1.826E+00$
2000	$3.006E+03$	$8.008E+00$	$1.945E+00$	$2.163E+00$
3000	$6.763E+03$	$8.819E+00$	$2.065E+00$	$2.426E+00$
4000	$1.244E+04$	$9.429E+00$	$2.177E+00$	$2.585E+00$
5000	$2.044E+04$	$9.925E+00$	$2.270E+00$	$2.693E+00$
6000	$3.113E+04$	$1.035E+01$	$2.348E+00$	$2.778E+00$
7000	$4.494E+04$	$1.071E+01$	$2.414E+00$	$2.838E+00$
8000	$6.226E+04$	$1.104E+01$	$2.469E+00$	$2.861E+00$
9000	$8.349E+04$	$1.133E+01$	$2.511E+00$	$2.836E+00$
10000	$1.090E+05$	$1.160E+01$	$2.541E+00$	$2.763E+00$
11000	$1.389E+05$	$1.184E+01$	$2.556E+00$	$2.650E+00$
12000	$1.736E+05$	$1.206E+01$	$2.558E+00$	$2.510E+00$
13000	$2.129E+05$	$1.227E+01$	$2.548E+00$	$2.354E+00$
14000	$2.570E+05$	$1.246E+01$	$2.529E+00$	$2.194E+00$
15000	$3.057E+05$	$1.263E+01$	$2.501E+00$	$2.036E+00$
16000	$3.589E+05$	$1.279E+01$	$2.467E+00$	$1.885E+00$
17000	$4.164E+05$	$1.294E+01$	$2.429E+00$	$1.743E+00$
18000	$4.778E+05$	$1.308E+01$	$2.387E+00$	$1.612E+00$
19000	$5.430E+05$	$1.320E+01$	$2.343E+00$	$1.492E+00$
20000	$6.116E+05$	$1.332E+01$	$2.298E+00$	$1.383E+00$
21000	$6.834E+05$	$1.343E+01$	$2.252E+00$	$1.284E+00$
22000	$7.581E+05$	$1.354E+01$	$2.206E+00$	$1.194E+00$
23000	$8.354E+05$	$1.364E+01$	$2.160E+00$	$1.113E+00$
24000	$9.149E+05$	$1.373E+01$	$2.115E+00$	$1.039E+00$
25000	$9.965E+05$	$1.381E+01$	$2.070E+00$	$9.719E-01$
26000	$1.080E+06$	$1.389E+01$	$2.027E+00$	$9.110E-01$
27000	$1.165E+06$	$1.397E+01$	$1.985E+00$	$8.556E-01$
28000	$1.251E+06$	$1.404E+01$	$1.943E+00$	$8.050E-01$
29000	$1.338E+06$	$1.411E+01$	$1.903E+00$	$7.587E-01$
30000	$1.427E+06$	$1.417E+01$	$1.864E+00$	$7.163E-01$
32000	$1.605E+06$	$1.429E+01$	$1.790E+00$	$6.415E-01$
34000	$1.785E+06$	$1.440E+01$	$1.721E+00$	$5.779E-01$
36000	$1.966E+06$	$1.449E+01$	$1.656E+00$	$5.234E-01$
38000	$2.147E+06$	$1.458E+01$	$1.595E+00$	$4.763E-01$
40000	$2.327E+06$	$1.466E+01$	$1.538E+00$	$4.353E-01$
42000	$2.505E+06$	$1.473E+01$	$1.484E+00$	$3.994E-01$
44000	$2.680E+06$	$1.480E+01$	$1.434E+00$	$3.679E-01$
46000	$2.854E+06$	$1.486E+01$	$1.387E+00$	$3.399E-01$
48000	$3.025E+06$	$1.492E+01$	$1.343E+00$	$3.151E-01$
50000	$3.192E+06$	$1.498E+01$	$1.302E+00$	$2.929E-01$

Table 96: Total thermodynamic properties of C_2

T [K]	C_p [J/mol/K]	S^0 [J/mol/K]	$H^0(T)-H^0(0)$ [KJ/mol]	$H^0(T)-H^0(298)$ [KJ/mol]	$-(G^0-H^0(0))/T$ [J/mol/K]	$-(G^0-H^0(298))/T$ [J/mol/K]	ΔH_f [KJ/mol]	$\mathrm{Log}(K_p)$
50	2.910E+01	1.385E+02	1.448E+00	-9.130E+00	1.095E+02	3.211E+02	0.000E+00	0.000E+00
100	2.977E+01	1.588E+02	2.911E+00	-7.667E+00	1.297E+02	2.354E+02	0.000E+00	0.000E+00
150	3.438E+01	1.716E+02	4.496E+00	-6.082E+00	1.416E+02	2.121E+02	0.000E+00	0.000E+00
200	4.046E+01	1.823E+02	6.374E+00	-4.204E+00	1.504E+02	2.033E+02	0.000E+00	0.000E+00
298.15	4.315E+01	1.994E+02	1.058E+01	0.000E+00	1.639E+02	1.994E+02	0.000E+00	0.000E+00
300	4.310E+01	1.997E+02	1.066E+01	7.950E-02	1.641E+02	1.994E+02	0.000E+00	0.000E+00
400	3.965E+01	2.116E+02	1.480E+01	4.222E+00	1.746E+02	2.010E+02	0.000E+00	0.000E+00
500	3.714E+01	2.201E+02	1.863E+01	8.048E+00	1.829E+02	2.041E+02	0.000E+00	0.000E+00
600	3.600E+01	2.268E+02	2.227E+01	1.170E+01	1.897E+02	2.073E+02	0.000E+00	0.000E+00
700	3.562E+01	2.323E+02	2.585E+01	1.527E+01	1.954E+02	2.105E+02	0.000E+00	0.000E+00
800	3.561E+01	2.371E+02	2.941E+01	1.883E+01	2.003E+02	2.135E+02	0.000E+00	0.000E+00
900	3.575E+01	2.413E+02	3.298E+01	2.240E+01	2.046E+02	2.164E+02	0.000E+00	0.000E+00
1000	3.597E+01	2.450E+02	3.656E+01	2.599E+01	2.085E+02	2.191E+02	0.000E+00	0.000E+00
2000	3.877E+01	2.708E+02	7.392E+01	6.334E+01	2.339E+02	2.392E+02	0.000E+00	0.000E+00
3000	4.096E+01	2.870E+02	1.139E+02	1.033E+02	2.490E+02	2.526E+02	0.000E+00	0.000E+00
4000	4.228E+01	2.990E+02	1.555E+02	1.450E+02	2.601E+02	2.627E+02	0.000E+00	0.000E+00
5000	4.318E+01	3.085E+02	1.983E+02	1.877E+02	2.689E+02	2.710E+02	0.000E+00	0.000E+00
6000	4.388E+01	3.164E+02	2.418E+02	2.313E+02	2.761E+02	2.779E+02	0.000E+00	0.000E+00
7000	4.439E+01	3.232E+02	2.860E+02	2.754E+02	2.824E+02	2.839E+02	0.000E+00	0.000E+00
8000	4.457E+01	3.292E+02	3.305E+02	3.199E+02	2.879E+02	2.892E+02	0.000E+00	0.000E+00
9000	4.437E+01	3.344E+02	3.750E+02	3.644E+02	2.928E+02	2.939E+02	0.000E+00	0.000E+00
10000	4.376E+01	3.391E+02	4.191E+02	4.085E+02	2.972E+02	2.982E+02	0.000E+00	0.000E+00
11000	4.282E+01	3.432E+02	4.624E+02	4.518E+02	3.012E+02	3.021E+02	0.000E+00	0.000E+00
12000	4.165E+01	3.469E+02	5.047E+02	4.941E+02	3.048E+02	3.057E+02	0.000E+00	0.000E+00
13000	4.036E+01	3.502E+02	5.457E+02	5.351E+02	3.082E+02	3.090E+02	0.000E+00	0.000E+00
14000	3.903E+01	3.531E+02	5.854E+02	5.748E+02	3.113E+02	3.121E+02	0.000E+00	0.000E+00
15000	3.771E+01	3.558E+02	6.237E+02	6.132E+02	3.142E+02	3.149E+02	0.000E+00	0.000E+00
16000	3.645E+01	3.581E+02	6.608E+02	6.502E+02	3.169E+02	3.175E+02	0.000E+00	0.000E+00
17000	3.528E+01	3.603E+02	6.967E+02	6.861E+02	3.194E+02	3.200E+02	0.000E+00	0.000E+00
18000	3.419E+01	3.623E+02	7.314E+02	7.208E+02	3.217E+02	3.223E+02	0.000E+00	0.000E+00
19000	3.319E+01	3.641E+02	7.651E+02	7.545E+02	3.239E+02	3.244E+02	0.000E+00	0.000E+00
20000	3.228E+01	3.658E+02	7.978E+02	7.872E+02	3.259E+02	3.264E+02	0.000E+00	0.000E+00
21000	3.146E+01	3.674E+02	8.297E+02	8.191E+02	3.279E+02	3.284E+02	0.000E+00	0.000E+00
22000	3.071E+01	3.688E+02	8.608E+02	8.502E+02	3.297E+02	3.302E+02	0.000E+00	0.000E+00
23000	3.004E+01	3.702E+02	8.911E+02	8.805E+02	3.314E+02	3.319E+02	0.000E+00	0.000E+00
24000	2.942E+01	3.714E+02	9.209E+02	9.103E+02	3.331E+02	3.335E+02	0.000E+00	0.000E+00
25000	2.887E+01	3.726E+02	9.500E+02	9.394E+02	3.346E+02	3.350E+02	0.000E+00	0.000E+00
26000	2.836E+01	3.737E+02	9.786E+02	9.680E+02	3.361E+02	3.365E+02	0.000E+00	0.000E+00
27000	2.790E+01	3.748E+02	1.007E+03	9.962E+02	3.375E+02	3.379E+02	0.000E+00	0.000E+00
28000	2.748E+01	3.758E+02	1.034E+03	1.024E+03	3.389E+02	3.392E+02	0.000E+00	0.000E+00
29000	2.709E+01	3.768E+02	1.062E+03	1.051E+03	3.402E+02	3.405E+02	0.000E+00	0.000E+00
30000	2.674E+01	3.777E+02	1.089E+03	1.078E+03	3.414E+02	3.418E+02	0.000E+00	0.000E+00
32000	2.612E+01	3.794E+02	1.142E+03	1.131E+03	3.437E+02	3.441E+02	0.000E+00	0.000E+00
34000	2.559E+01	3.809E+02	1.193E+03	1.183E+03	3.459E+02	3.462E+02	0.000E+00	0.000E+00
36000	2.514E+01	3.824E+02	1.244E+03	1.233E+03	3.479E+02	3.481E+02	0.000E+00	0.000E+00
38000	2.475E+01	3.838E+02	1.294E+03	1.283E+03	3.497E+02	3.500E+02	0.000E+00	0.000E+00
40000	2.441E+01	3.850E+02	1.343E+03	1.332E+03	3.514E+02	3.517E+02	0.000E+00	0.000E+00
42000	2.411E+01	3.862E+02	1.391E+03	1.381E+03	3.531E+02	3.533E+02	0.000E+00	0.000E+00
44000	2.384E+01	3.873E+02	1.439E+03	1.429E+03	3.546E+02	3.548E+02	0.000E+00	0.000E+00
46000	2.361E+01	3.884E+02	1.487E+03	1.476E+03	3.560E+02	3.563E+02	0.000E+00	0.000E+00
48000	2.341E+01	3.894E+02	1.534E+03	1.523E+03	3.574E+02	3.576E+02	0.000E+00	0.000E+00
50000	2.322E+01	3.903E+02	1.580E+03	1.570E+03	3.587E+02	3.589E+02	0.000E+00	0.000E+00

Table 97: Internal thermodynamic properties of C_2^+

T(K)	Q_{int}	$\ln(Q_{int})$	E_{int}/RT	$C_{p,int}/R$
50	$4.242E+01$	$3.748E+00$	$9.842E-01$	$1.001E+00$
100	$8.419E+01$	$4.433E+00$	$9.925E-01$	$1.001E+00$
150	$1.260E+02$	$4.836E+00$	$9.955E-01$	$1.002E+00$
200	$1.678E+02$	$5.123E+00$	$9.976E-01$	$1.008E+00$
298.15	$2.503E+02$	$5.523E+00$	$1.008E+00$	$1.066E+00$
300	$2.519E+02$	$5.529E+00$	$1.009E+00$	$1.067E+00$
400	$3.379E+02$	$5.823E+00$	$1.038E+00$	$1.189E+00$
500	$4.279E+02$	$6.059E+00$	$1.082E+00$	$1.326E+00$
600	$5.235E+02$	$6.261E+00$	$1.133E+00$	$1.449E+00$
700	$6.259E+02$	$6.439E+00$	$1.186E+00$	$1.549E+00$
800	$7.357E+02$	$6.601E+00$	$1.236E+00$	$1.628E+00$
900	$8.534E+02$	$6.749E+00$	$1.283E+00$	$1.691E+00$
1000	$9.791E+02$	$6.887E+00$	$1.327E+00$	$1.740E+00$
2000	$2.704E+03$	$7.903E+00$	$1.595E+00$	$1.932E+00$
3000	$5.297E+03$	$8.575E+00$	$1.716E+00$	$1.978E+00$
4000	$8.767E+03$	$9.079E+00$	$1.784E+00$	$1.998E+00$
5000	$1.312E+04$	$9.482E+00$	$1.828E+00$	$2.008E+00$
6000	$1.836E+04$	$9.818E+00$	$1.858E+00$	$2.002E+00$
7000	$2.449E+04$	$1.011E+01$	$1.877E+00$	$1.971E+00$
8000	$3.149E+04$	$1.036E+01$	$1.885E+00$	$1.910E+00$
9000	$3.931E+04$	$1.058E+01$	$1.883E+00$	$1.820E+00$
10000	$4.792E+04$	$1.078E+01$	$1.871E+00$	$1.710E+00$
11000	$5.722E+04$	$1.095E+01$	$1.851E+00$	$1.588E+00$
12000	$6.715E+04$	$1.111E+01$	$1.824E+00$	$1.463E+00$
13000	$7.761E+04$	$1.126E+01$	$1.792E+00$	$1.340E+00$
14000	$8.851E+04$	$1.139E+01$	$1.755E+00$	$1.223E+00$
15000	$9.977E+04$	$1.151E+01$	$1.716E+00$	$1.115E+00$
16000	$1.113E+05$	$1.162E+01$	$1.675E+00$	$1.015E+00$
17000	$1.231E+05$	$1.172E+01$	$1.634E+00$	$9.254E-01$
18000	$1.349E+05$	$1.181E+01$	$1.592E+00$	$8.443E-01$
19000	$1.469E+05$	$1.190E+01$	$1.551E+00$	$7.716E-01$
20000	$1.589E+05$	$1.198E+01$	$1.510E+00$	$7.064E-01$
21000	$1.709E+05$	$1.205E+01$	$1.470E+00$	$6.481E-01$
22000	$1.828E+05$	$1.212E+01$	$1.432E+00$	$5.959E-01$
23000	$1.947E+05$	$1.218E+01$	$1.394E+00$	$5.491E-01$
24000	$2.064E+05$	$1.224E+01$	$1.358E+00$	$5.071E-01$
25000	$2.180E+05$	$1.229E+01$	$1.324E+00$	$4.694E-01$
26000	$2.295E+05$	$1.234E+01$	$1.290E+00$	$4.354E-01$
27000	$2.408E+05$	$1.239E+01$	$1.258E+00$	$4.047E-01$
28000	$2.519E+05$	$1.244E+01$	$1.227E+00$	$3.769E-01$
29000	$2.629E+05$	$1.248E+01$	$1.197E+00$	$3.518E-01$
30000	$2.736E+05$	$1.252E+01$	$1.169E+00$	$3.289E-01$
32000	$2.946E+05$	$1.259E+01$	$1.115E+00$	$2.892E-01$
34000	$3.147E+05$	$1.266E+01$	$1.065E+00$	$2.559E-01$
36000	$3.340E+05$	$1.272E+01$	$1.019E+00$	$2.279E-01$
38000	$3.525E+05$	$1.277E+01$	$9.771E-01$	$2.041E-01$
40000	$3.702E+05$	$1.282E+01$	$9.379E-01$	$1.838E-01$
42000	$3.872E+05$	$1.287E+01$	$9.016E-01$	$1.662E-01$
44000	$4.035E+05$	$1.291E+01$	$8.678E-01$	$1.510E-01$
46000	$4.191E+05$	$1.295E+01$	$8.364E-01$	$1.378E-01$
48000	$4.340E+05$	$1.298E+01$	$8.070E-01$	$1.262E-01$
50000	$4.483E+05$	$1.301E+01$	$7.796E-01$	$1.160E-01$

Table 98: Total thermodynamic properties of C_2^+

T [K]	C_p [J/mol/K]	S^0 [J/mol/K]	$H^0(T)-H^0(0)$ [KJ/mol]	$H^0(T)-H^0(298)$ [KJ/mol]	$-(G^0-H^0(0))/T$ [J/mol/K]	$-(G^0-H^0(298))/T$ [J/mol/K]	ΔH_f [KJ/mol]	$\mathrm{Log}(K_p)$
50	2.911E+01	1.507E+02	1.448E+00	-7.249E+00	1.218E+02	2.957E+02	1.101E+03	-1.150E+03
100	2.911E+01	1.709E+02	2.904E+00	-5.793E+00	1.419E+02	2.288E+02	1.102E+03	-5.751E+02
150	2.912E+01	1.827E+02	4.359E+00	-4.338E+00	1.537E+02	2.116E+02	1.103E+03	-3.831E+02
200	2.916E+01	1.911E+02	5.816E+00	-2.881E+00	1.620E+02	2.055E+02	1.104E+03	-2.871E+02
298.15	2.965E+01	2.028E+02	8.697E+00	0.000E+00	1.736E+02	2.028E+02	1.104E+03	-1.922E+02
300	2.966E+01	2.030E+02	8.752E+00	5.488E-02	1.738E+02	2.028E+02	1.104E+03	-1.910E+02
400	3.067E+01	2.117E+02	1.177E+01	3.069E+00	1.822E+02	2.040E+02	1.105E+03	-1.429E+02
500	3.181E+01	2.186E+02	1.489E+01	6.194E+00	1.888E+02	2.062E+02	1.107E+03	-1.140E+02
600	3.283E+01	2.245E+02	1.812E+01	9.427E+00	1.943E+02	2.088E+02	1.108E+03	-9.474E+01
700	3.366E+01	2.296E+02	2.145E+01	1.275E+01	1.990E+02	2.114E+02	1.110E+03	-8.095E+01
800	3.433E+01	2.342E+02	2.485E+01	1.615E+01	2.031E+02	2.140E+02	1.112E+03	-7.059E+01
900	3.485E+01	2.382E+02	2.831E+01	1.961E+01	2.068E+02	2.165E+02	1.114E+03	-6.251E+01
1000	3.526E+01	2.419E+02	3.182E+01	2.312E+01	2.101E+02	2.188E+02	1.116E+03	-5.604E+01
2000	3.685E+01	2.670E+02	6.810E+01	5.940E+01	2.330E+02	2.373E+02	1.136E+03	-2.670E+01
3000	3.723E+01	2.821E+02	1.052E+02	9.647E+01	2.470E+02	2.499E+02	1.154E+03	-1.674E+01
4000	3.740E+01	2.928E+02	1.425E+02	1.338E+02	2.572E+02	2.594E+02	1.170E+03	-1.169E+01
5000	3.748E+01	3.011E+02	1.799E+02	1.712E+02	2.652E+02	2.669E+02	1.186E+03	-8.612E+00
6000	3.743E+01	3.080E+02	2.174E+02	2.087E+02	2.718E+02	2.732E+02	1.200E+03	-6.535E+00
7000	3.718E+01	3.137E+02	2.547E+02	2.460E+02	2.774E+02	2.786E+02	1.214E+03	-5.035E+00
8000	3.667E+01	3.187E+02	2.917E+02	2.830E+02	2.822E+02	2.833E+02	1.227E+03	-3.896E+00
9000	3.592E+01	3.229E+02	3.280E+02	3.193E+02	2.865E+02	2.875E+02	1.240E+03	-3.001E+00
10000	3.500E+01	3.267E+02	3.635E+02	3.548E+02	2.903E+02	2.912E+02	1.252E+03	-2.278E+00
11000	3.399E+01	3.300E+02	3.980E+02	3.893E+02	2.938E+02	2.946E+02	1.264E+03	-1.681E+00
12000	3.295E+01	3.329E+02	4.314E+02	4.227E+02	2.969E+02	2.977E+02	1.276E+03	-1.178E+00
13000	3.193E+01	3.355E+02	4.639E+02	4.552E+02	2.998E+02	3.005E+02	1.288E+03	-7.490E-01
14000	3.096E+01	3.378E+02	4.953E+02	4.866E+02	3.024E+02	3.031E+02	1.301E+03	-3.775E-01
15000	3.005E+01	3.399E+02	5.258E+02	5.171E+02	3.049E+02	3.054E+02	1.314E+03	-5.237E-02
16000	2.923E+01	3.418E+02	5.554E+02	5.467E+02	3.071E+02	3.077E+02	1.327E+03	2.350E-01
17000	2.848E+01	3.436E+02	5.843E+02	5.756E+02	3.092E+02	3.097E+02	1.341E+03	4.911E-01
18000	2.781E+01	3.452E+02	6.124E+02	6.037E+02	3.112E+02	3.116E+02	1.355E+03	7.212E-01
19000	2.720E+01	3.467E+02	6.399E+02	6.312E+02	3.130E+02	3.134E+02	1.370E+03	9.292E-01
20000	2.666E+01	3.481E+02	6.668E+02	6.581E+02	3.147E+02	3.151E+02	1.385E+03	1.119E+00
21000	2.618E+01	3.494E+02	6.933E+02	6.846E+02	3.163E+02	3.168E+02	1.400E+03	1.292E+00
22000	2.574E+01	3.506E+02	7.192E+02	7.105E+02	3.179E+02	3.183E+02	1.416E+03	1.451E+00
23000	2.535E+01	3.517E+02	7.448E+02	7.360E+02	3.193E+02	3.197E+02	1.432E+03	1.598E+00
24000	2.500E+01	3.528E+02	7.699E+02	7.612E+02	3.207E+02	3.210E+02	1.448E+03	1.734E+00
25000	2.469E+01	3.538E+02	7.948E+02	7.861E+02	3.220E+02	3.223E+02	1.464E+03	1.861E+00
26000	2.441E+01	3.547E+02	8.193E+02	8.106E+02	3.232E+02	3.236E+02	1.481E+03	1.979E+00
27000	2.415E+01	3.556E+02	8.436E+02	8.349E+02	3.244E+02	3.247E+02	1.498E+03	2.090E+00
28000	2.392E+01	3.565E+02	8.676E+02	8.589E+02	3.255E+02	3.259E+02	1.515E+03	2.194E+00
29000	2.371E+01	3.574E+02	8.914E+02	8.827E+02	3.266E+02	3.269E+02	1.532E+03	2.292E+00
30000	2.352E+01	3.582E+02	9.150E+02	9.064E+02	3.277E+02	3.279E+02	1.550E+03	2.385E+00
32000	2.319E+01	3.597E+02	9.618E+02	9.531E+02	3.296E+02	3.299E+02	1.585E+03	2.555E+00
34000	2.291E+01	3.611E+02	1.008E+03	9.991E+02	3.314E+02	3.317E+02	1.621E+03	2.709E+00
36000	2.268E+01	3.624E+02	1.053E+03	1.045E+03	3.331E+02	3.334E+02	1.658E+03	2.849E+00
38000	2.248E+01	3.636E+02	1.099E+03	1.090E+03	3.347E+02	3.349E+02	1.695E+03	2.977E+00
40000	2.231E+01	3.647E+02	1.143E+03	1.135E+03	3.362E+02	3.364E+02	1.732E+03	3.095E+00
42000	2.217E+01	3.658E+02	1.188E+03	1.179E+03	3.376E+02	3.378E+02	1.769E+03	3.203E+00
44000	2.204E+01	3.669E+02	1.232E+03	1.223E+03	3.389E+02	3.391E+02	1.807E+03	3.304E+00
46000	2.193E+01	3.678E+02	1.276E+03	1.267E+03	3.401E+02	3.403E+02	1.845E+03	3.399E+00
48000	2.184E+01	3.688E+02	1.320E+03	1.311E+03	3.413E+02	3.414E+02	1.884E+03	3.487E+00
50000	2.175E+01	3.696E+02	1.363E+03	1.355E+03	3.424E+02	3.426E+02	1.922E+03	3.570E+00

Table 99: Internal thermodynamic properties of C_2^-

T(K)	Q_{int}	$\ln(Q_{int})$	E_{int}/RT	$C_{p,int}/R$
50	$2.033E+01$	$3.012E+00$	$9.834E-01$	$1.000E+00$
100	$4.033E+01$	$3.697E+00$	$9.920E-01$	$1.001E+00$
150	$6.033E+01$	$4.100E+00$	$9.949E-01$	$1.001E+00$
200	$8.034E+01$	$4.386E+00$	$9.965E-01$	$1.002E+00$
298.15	$1.197E+02$	$4.785E+00$	$9.999E-01$	$1.017E+00$
300	$1.204E+02$	$4.791E+00$	$1.000E+00$	$1.018E+00$
400	$1.607E+02$	$5.080E+00$	$1.011E+00$	$1.075E+00$
500	$2.018E+02$	$5.307E+00$	$1.033E+00$	$1.170E+00$
600	$2.443E+02$	$5.498E+00$	$1.064E+00$	$1.278E+00$
700	$2.887E+02$	$5.665E+00$	$1.102E+00$	$1.382E+00$
800	$3.353E+02$	$5.815E+00$	$1.143E+00$	$1.474E+00$
900	$3.846E+02$	$5.952E+00$	$1.185E+00$	$1.554E+00$
1000	$4.366E+02$	$6.079E+00$	$1.225E+00$	$1.621E+00$
2000	$1.129E+03$	$7.029E+00$	$1.518E+00$	$1.928E+00$
3000	$2.159E+03$	$7.677E+00$	$1.678E+00$	$2.079E+00$
4000	$3.562E+03$	$8.178E+00$	$1.811E+00$	$2.373E+00$
5000	$5.422E+03$	$8.598E+00$	$1.963E+00$	$2.770E+00$
6000	$7.868E+03$	$8.970E+00$	$2.125E+00$	$3.059E+00$
7000	$1.104E+04$	$9.309E+00$	$2.266E+00$	$3.138E+00$
8000	$1.505E+04$	$9.619E+00$	$2.371E+00$	$3.043E+00$
9000	$1.998E+04$	$9.902E+00$	$2.435E+00$	$2.851E+00$
10000	$2.587E+04$	$1.016E+01$	$2.466E+00$	$2.624E+00$
11000	$3.273E+04$	$1.040E+01$	$2.470E+00$	$2.395E+00$
12000	$4.055E+04$	$1.061E+01$	$2.454E+00$	$2.180E+00$
13000	$4.930E+04$	$1.081E+01$	$2.425E+00$	$1.983E+00$
14000	$5.893E+04$	$1.098E+01$	$2.387E+00$	$1.805E+00$
15000	$6.938E+04$	$1.115E+01$	$2.343E+00$	$1.646E+00$
16000	$8.059E+04$	$1.130E+01$	$2.295E+00$	$1.503E+00$
17000	$9.248E+04$	$1.143E+01$	$2.245E+00$	$1.375E+00$
18000	$1.050E+05$	$1.156E+01$	$2.193E+00$	$1.261E+00$
19000	$1.180E+05$	$1.168E+01$	$2.141E+00$	$1.158E+00$
20000	$1.316E+05$	$1.179E+01$	$2.090E+00$	$1.066E+00$
21000	$1.455E+05$	$1.189E+01$	$2.039E+00$	$9.837E-01$
22000	$1.598E+05$	$1.198E+01$	$1.989E+00$	$9.093E-01$
23000	$1.744E+05$	$1.207E+01$	$1.941E+00$	$8.422E-01$
24000	$1.892E+05$	$1.215E+01$	$1.894E+00$	$7.816E-01$
25000	$2.042E+05$	$1.223E+01$	$1.848E+00$	$7.267E-01$
26000	$2.194E+05$	$1.230E+01$	$1.804E+00$	$6.770E-01$
27000	$2.347E+05$	$1.237E+01$	$1.762E+00$	$6.318E-01$
28000	$2.500E+05$	$1.243E+01$	$1.720E+00$	$5.907E-01$
29000	$2.654E+05$	$1.249E+01$	$1.681E+00$	$5.532E-01$
30000	$2.808E+05$	$1.255E+01$	$1.643E+00$	$5.189E-01$
32000	$3.114E+05$	$1.265E+01$	$1.570E+00$	$4.588E-01$
34000	$3.418E+05$	$1.274E+01$	$1.504E+00$	$4.081E-01$
36000	$3.719E+05$	$1.283E+01$	$1.441E+00$	$3.650E-01$
38000	$4.014E+05$	$1.290E+01$	$1.384E+00$	$3.281E-01$
40000	$4.303E+05$	$1.297E+01$	$1.330E+00$	$2.964E-01$
42000	$4.586E+05$	$1.304E+01$	$1.280E+00$	$2.689E-01$
44000	$4.862E+05$	$1.309E+01$	$1.234E+00$	$2.449E-01$
46000	$5.131E+05$	$1.315E+01$	$1.190E+00$	$2.240E-01$
48000	$5.393E+05$	$1.320E+01$	$1.150E+00$	$2.055E-01$
50000	$5.648E+05$	$1.324E+01$	$1.112E+00$	$1.892E-01$

Table 100: Total thermodynamic properties of C_2^-

T [K]	C_p [J/mol/K]	S^0 [J/mol/K]	$H^0(T)-H^0(0)$ [KJ/mol]	$H^0(T)-H^0(298)$ [KJ/mol]	$-(G^0-H^0(0))/T$ [J/mol/K]	$-(G^0-H^0(298))/T$ [J/mol/K]	ΔH_f [KJ/mol]	$\mathrm{Log}(K_p)$
50	2.910E+01	1.446E+02	1.448E+00	-7.228E+00	1.157E+02	2.892E+02	-3.168E+02	3.321E+02
100	2.911E+01	1.648E+02	2.903E+00	-5.773E+00	1.358E+02	2.225E+02	-3.179E+02	1.664E+02
150	2.911E+01	1.766E+02	4.359E+00	-4.317E+00	1.475E+02	2.054E+02	-3.191E+02	1.110E+02
200	2.911E+01	1.850E+02	5.814E+00	-2.862E+00	1.559E+02	1.993E+02	-3.205E+02	8.318E+01
298.15	2.924E+01	1.966E+02	8.676E+00	0.000E+00	1.675E+02	1.966E+02	-3.239E+02	5.550E+01
300	2.925E+01	1.968E+02	8.730E+00	5.415E-02	1.677E+02	1.966E+02	-3.240E+02	5.515E+01
400	2.973E+01	2.052E+02	1.168E+01	3.000E+00	1.761E+02	1.978E+02	-3.272E+02	4.098E+01
500	3.051E+01	2.120E+02	1.469E+01	6.010E+00	1.826E+02	1.999E+02	-3.301E+02	3.240E+01
600	3.141E+01	2.176E+02	1.778E+01	9.106E+00	1.880E+02	2.024E+02	-3.328E+02	2.663E+01
700	3.227E+01	2.225E+02	2.097E+01	1.229E+01	1.926E+02	2.050E+02	-3.352E+02	2.248E+01
800	3.305E+01	2.269E+02	2.423E+01	1.556E+01	1.966E+02	2.074E+02	-3.376E+02	1.934E+01
900	3.371E+01	2.308E+02	2.757E+01	1.890E+01	2.002E+02	2.098E+02	-3.399E+02	1.689E+01
1000	3.426E+01	2.344E+02	3.097E+01	2.230E+01	2.034E+02	2.121E+02	-3.422E+02	1.491E+01
2000	3.681E+01	2.591E+02	6.681E+01	5.813E+01	2.257E+02	2.301E+02	-3.645E+02	5.746E+00
3000	3.807E+01	2.743E+02	1.042E+02	9.554E+01	2.395E+02	2.424E+02	-3.878E+02	2.486E+00
4000	4.052E+01	2.855E+02	1.434E+02	1.347E+02	2.497E+02	2.518E+02	-4.111E+02	7.514E-01
5000	4.382E+01	2.949E+02	1.856E+02	1.769E+02	2.578E+02	2.596E+02	-4.325E+02	-3.487E-01
6000	4.622E+01	3.031E+02	2.307E+02	2.220E+02	2.647E+02	2.661E+02	-4.516E+02	-1.118E+00
7000	4.688E+01	3.104E+02	2.774E+02	2.687E+02	2.707E+02	2.720E+02	-4.699E+02	-1.690E+00
8000	4.609E+01	3.166E+02	3.240E+02	3.153E+02	2.761E+02	2.772E+02	-4.886E+02	-2.137E+00
9000	4.449E+01	3.219E+02	3.693E+02	3.606E+02	2.809E+02	2.818E+02	-5.086E+02	-2.498E+00
10000	4.260E+01	3.265E+02	4.129E+02	4.042E+02	2.852E+02	2.861E+02	-5.299E+02	-2.799E+00
11000	4.070E+01	3.305E+02	4.545E+02	4.458E+02	2.891E+02	2.899E+02	-5.523E+02	-3.056E+00
12000	3.891E+01	3.339E+02	4.943E+02	4.856E+02	2.927E+02	2.935E+02	-5.756E+02	-3.279E+00
13000	3.727E+01	3.370E+02	5.324E+02	5.237E+02	2.960E+02	2.967E+02	-5.993E+02	-3.475E+00
14000	3.579E+01	3.397E+02	5.689E+02	5.602E+02	2.991E+02	2.997E+02	-6.233E+02	-3.651E+00
15000	3.447E+01	3.421E+02	6.040E+02	5.954E+02	3.019E+02	3.024E+02	-6.473E+02	-3.809E+00
16000	3.328E+01	3.443E+02	6.379E+02	6.292E+02	3.044E+02	3.050E+02	-6.713E+02	-3.952E+00
17000	3.222E+01	3.463E+02	6.706E+02	6.620E+02	3.068E+02	3.074E+02	-6.952E+02	-4.083E+00
18000	3.127E+01	3.481E+02	7.024E+02	6.937E+02	3.091E+02	3.096E+02	-7.190E+02	-4.204E+00
19000	3.042E+01	3.498E+02	7.332E+02	7.245E+02	3.112E+02	3.116E+02	-7.426E+02	-4.316E+00
20000	2.965E+01	3.513E+02	7.632E+02	7.545E+02	3.131E+02	3.136E+02	-7.661E+02	-4.419E+00
21000	2.896E+01	3.527E+02	7.925E+02	7.839E+02	3.150E+02	3.154E+02	-7.895E+02	-4.516E+00
22000	2.835E+01	3.541E+02	8.212E+02	8.125E+02	3.167E+02	3.171E+02	-8.127E+02	-4.606E+00
23000	2.779E+01	3.553E+02	8.492E+02	8.406E+02	3.184E+02	3.188E+02	-8.358E+02	-4.691E+00
24000	2.729E+01	3.565E+02	8.768E+02	8.681E+02	3.200E+02	3.203E+02	-8.588E+02	-4.772E+00
25000	2.683E+01	3.576E+02	9.038E+02	8.951E+02	3.214E+02	3.218E+02	-8.816E+02	-4.847E+00
26000	2.641E+01	3.586E+02	9.305E+02	9.218E+02	3.229E+02	3.232E+02	-9.044E+02	-4.919E+00
27000	2.604E+01	3.596E+02	9.567E+02	9.480E+02	3.242E+02	3.245E+02	-9.271E+02	-4.987E+00
28000	2.570E+01	3.606E+02	9.825E+02	9.739E+02	3.255E+02	3.258E+02	-9.497E+02	-5.052E+00
29000	2.539E+01	3.615E+02	1.008E+03	9.994E+02	3.267E+02	3.270E+02	-9.722E+02	-5.114E+00
30000	2.510E+01	3.623E+02	1.033E+03	1.025E+03	3.279E+02	3.282E+02	-9.947E+02	-5.173E+00
32000	2.460E+01	3.639E+02	1.083E+03	1.074E+03	3.301E+02	3.304E+02	-1.039E+03	-5.284E+00
34000	2.418E+01	3.654E+02	1.132E+03	1.123E+03	3.321E+02	3.324E+02	-1.084E+03	-5.385E+00
36000	2.382E+01	3.668E+02	1.180E+03	1.171E+03	3.340E+02	3.342E+02	-1.128E+03	-5.480E+00
38000	2.351E+01	3.681E+02	1.227E+03	1.218E+03	3.358E+02	3.360E+02	-1.172E+03	-5.568E+00
40000	2.325E+01	3.692E+02	1.274E+03	1.265E+03	3.374E+02	3.376E+02	-1.216E+03	-5.650E+00
42000	2.302E+01	3.704E+02	1.320E+03	1.311E+03	3.389E+02	3.392E+02	-1.260E+03	-5.727E+00
44000	2.282E+01	3.714E+02	1.366E+03	1.357E+03	3.404E+02	3.406E+02	-1.304E+03	-5.799E+00
46000	2.265E+01	3.725E+02	1.411E+03	1.403E+03	3.418E+02	3.420E+02	-1.347E+03	-5.867E+00
48000	2.250E+01	3.734E+02	1.457E+03	1.448E+03	3.431E+02	3.433E+02	-1.391E+03	-5.932E+00
50000	2.236E+01	3.743E+02	1.501E+03	1.493E+03	3.443E+02	3.445E+02	-1.434E+03	-5.994E+00

Table 101: Internal thermodynamic properties of C_3

T(K)	Q_{int}	$\ln(Q_{int})$	E_{int}/RT	$C_{p,int}/R$
50	$5.223E+01$	$3.956E+00$	$1.549E+00$	$2.276E+00$
100	$1.802E+02$	$5.194E+00$	$2.000E+00$	$2.526E+00$
150	$4.214E+02$	$6.043E+00$	$2.177E+00$	$2.529E+00$
200	$7.986E+02$	$6.683E+00$	$2.263E+00$	$2.513E+00$
298.15	$2.006E+03$	$7.604E+00$	$2.348E+00$	$2.549E+00$
300	$2.036E+03$	$7.619E+00$	$2.349E+00$	$2.550E+00$
400	$4.038E+03$	$8.303E+00$	$2.415E+00$	$2.683E+00$
500	$6.973E+03$	$8.850E+00$	$2.486E+00$	$2.858E+00$
600	$1.104E+04$	$9.310E+00$	$2.563E+00$	$3.038E+00$
700	$1.649E+04$	$9.711E+00$	$2.643E+00$	$3.203E+00$
800	$2.359E+04$	$1.007E+01$	$2.722E+00$	$3.345E+00$
900	$3.266E+04$	$1.039E+01$	$2.798E+00$	$3.465E+00$
1000	$4.402E+04$	$1.069E+01$	$2.870E+00$	$3.565E+00$
2000	$3.812E+05$	$1.285E+01$	$3.352E+00$	$4.004E+00$
3000	$1.567E+06$	$1.426E+01$	$3.627E+00$	$4.414E+00$
4000	$4.621E+06$	$1.535E+01$	$3.918E+00$	$5.222E+00$
5000	$1.150E+07$	$1.626E+01$	$4.272E+00$	$6.136E+00$
6000	$2.589E+07$	$1.707E+01$	$4.641E+00$	$6.756E+00$
7000	$5.429E+07$	$1.781E+01$	$4.961E+00$	$6.949E+00$
8000	$1.071E+08$	$1.849E+01$	$5.204E+00$	$6.817E+00$
9000	$1.997E+08$	$1.911E+01$	$5.368E+00$	$6.521E+00$
10000	$3.535E+08$	$1.968E+01$	$5.466E+00$	$6.170E+00$
11000	$5.966E+08$	$2.021E+01$	$5.514E+00$	$5.822E+00$
12000	$9.647E+08$	$2.069E+01$	$5.526E+00$	$5.496E+00$
13000	$1.501E+09$	$2.113E+01$	$5.512E+00$	$5.198E+00$
14000	$2.255E+09$	$2.154E+01$	$5.479E+00$	$4.924E+00$
15000	$3.287E+09$	$2.191E+01$	$5.434E+00$	$4.670E+00$
16000	$4.659E+09$	$2.226E+01$	$5.379E+00$	$4.434E+00$
17000	$6.443E+09$	$2.259E+01$	$5.317E+00$	$4.212E+00$
18000	$8.715E+09$	$2.289E+01$	$5.249E+00$	$4.003E+00$
19000	$1.155E+10$	$2.317E+01$	$5.178E+00$	$3.805E+00$
20000	$1.504E+10$	$2.343E+01$	$5.105E+00$	$3.618E+00$
21000	$1.926E+10$	$2.368E+01$	$5.030E+00$	$3.440E+00$
22000	$2.430E+10$	$2.391E+01$	$4.954E+00$	$3.272E+00$
23000	$3.023E+10$	$2.413E+01$	$4.877E+00$	$3.112E+00$
24000	$3.714E+10$	$2.434E+01$	$4.801E+00$	$2.962E+00$
25000	$4.511E+10$	$2.453E+01$	$4.724E+00$	$2.819E+00$
26000	$5.421E+10$	$2.472E+01$	$4.648E+00$	$2.685E+00$
27000	$6.452E+10$	$2.489E+01$	$4.573E+00$	$2.558E+00$
28000	$7.609E+10$	$2.506E+01$	$4.499E+00$	$2.438E+00$
29000	$8.899E+10$	$2.521E+01$	$4.426E+00$	$2.325E+00$
30000	$1.033E+11$	$2.536E+01$	$4.354E+00$	$2.218E+00$
32000	$1.362E+11$	$2.564E+01$	$4.214E+00$	$2.023E+00$
34000	$1.751E+11$	$2.589E+01$	$4.080E+00$	$1.849E+00$
36000	$2.203E+11$	$2.612E+01$	$3.952E+00$	$1.694E+00$
38000	$2.718E+11$	$2.633E+01$	$3.829E+00$	$1.557E+00$
40000	$3.299E+11$	$2.652E+01$	$3.713E+00$	$1.434E+00$
42000	$3.943E+11$	$2.670E+01$	$3.601E+00$	$1.323E+00$
44000	$4.651E+11$	$2.687E+01$	$3.496E+00$	$1.225E+00$
46000	$5.420E+11$	$2.702E+01$	$3.395E+00$	$1.136E+00$
48000	$6.250E+11$	$2.716E+01$	$3.299E+00$	$1.056E+00$
50000	$7.138E+11$	$2.729E+01$	$3.208E+00$	$9.837E-01$

Table 102: Total thermodynamic properties of C_3

T [K]	C_p [J/mol/K]	S^0 [J/mol/K]	$H^0(T)-H^0(0)$ [KJ/mol]	$H^0(T)-H^0(298)$ [KJ/mol]	$-(G^0-H^0(0))/T$ [J/mol/K]	$-(G^0-H^0(298))/T$ [J/mol/K]	ΔH_f [KJ/mol]	$\mathrm{Log}(K_p)$
50	3.971E+01	1.622E+02	1.683E+00	-1.034E+01	1.286E+02	3.689E+02	-4.498E+02	4.676E+02
100	4.179E+01	1.907E+02	3.742E+00	-8.276E+00	1.532E+02	2.734E+02	-4.500E+02	2.326E+02
150	4.181E+01	2.076E+02	5.833E+00	-6.184E+00	1.687E+02	2.489E+02	-4.503E+02	1.542E+02
200	4.168E+01	2.196E+02	7.920E+00	-4.098E+00	1.800E+02	2.401E+02	-4.510E+02	1.150E+02
298.15	4.198E+01	2.363E+02	1.202E+01	0.000E+00	1.960E+02	2.363E+02	-4.532E+02	7.612E+01
300	4.199E+01	2.366E+02	1.210E+01	7.810E-02	1.962E+02	2.363E+02	-4.532E+02	7.563E+01
400	4.309E+01	2.488E+02	1.634E+01	4.327E+00	2.079E+02	2.380E+02	-4.552E+02	5.586E+01
500	4.455E+01	2.586E+02	2.073E+01	8.708E+00	2.171E+02	2.411E+02	-4.566E+02	4.395E+01
600	4.605E+01	2.668E+02	2.526E+01	1.324E+01	2.247E+02	2.448E+02	-4.575E+02	3.599E+01
700	4.741E+01	2.740E+02	2.993E+01	1.791E+01	2.313E+02	2.484E+02	-4.582E+02	3.030E+01
800	4.860E+01	2.804E+02	3.473E+01	2.271E+01	2.370E+02	2.520E+02	-4.587E+02	2.602E+01
900	4.960E+01	2.862E+02	3.965E+01	2.763E+01	2.422E+02	2.555E+02	-4.592E+02	2.270E+01
1000	5.043E+01	2.915E+02	4.465E+01	3.263E+01	2.468E+02	2.589E+02	-4.595E+02	2.003E+01
2000	5.408E+01	3.279E+02	9.732E+01	8.530E+01	2.792E+02	2.852E+02	-4.629E+02	7.995E+00
3000	5.748E+01	3.503E+02	1.528E+02	1.408E+02	2.994E+02	3.034E+02	-4.673E+02	3.949E+00
4000	6.420E+01	3.677E+02	2.135E+02	2.014E+02	3.143E+02	3.174E+02	-4.692E+02	1.909E+00
5000	7.180E+01	3.829E+02	2.816E+02	2.695E+02	3.266E+02	3.290E+02	-4.652E+02	6.870E-01
6000	7.696E+01	3.965E+02	3.562E+02	3.442E+02	3.371E+02	3.391E+02	-4.559E+02	-1.159E-01
7000	7.856E+01	4.085E+02	4.343E+02	4.222E+02	3.465E+02	3.482E+02	-4.441E+02	-6.760E-01
8000	7.747E+01	4.189E+02	5.124E+02	5.004E+02	3.549E+02	3.564E+02	-4.327E+02	-1.085E+00
9000	7.500E+01	4.279E+02	5.888E+02	5.767E+02	3.625E+02	3.638E+02	-4.231E+02	-1.395E+00
10000	7.209E+01	4.357E+02	6.623E+02	6.503E+02	3.694E+02	3.706E+02	-4.157E+02	-1.639E+00
11000	6.919E+01	4.424E+02	7.329E+02	7.209E+02	3.758E+02	3.769E+02	-4.100E+02	-1.835E+00
12000	6.649E+01	4.483E+02	8.008E+02	7.887E+02	3.816E+02	3.826E+02	-4.056E+02	-1.996E+00
13000	6.400E+01	4.535E+02	8.660E+02	8.540E+02	3.869E+02	3.879E+02	-4.019E+02	-2.131E+00
14000	6.173E+01	4.582E+02	9.288E+02	9.168E+02	3.919E+02	3.927E+02	-3.986E+02	-2.246E+00
15000	5.962E+01	4.624E+02	9.895E+02	9.775E+02	3.964E+02	3.972E+02	-3.955E+02	-2.345E+00
16000	5.765E+01	4.662E+02	1.048E+03	1.036E+03	4.007E+02	4.014E+02	-3.925E+02	-2.431E+00
17000	5.581E+01	4.696E+02	1.105E+03	1.093E+03	4.046E+02	4.053E+02	-3.895E+02	-2.506E+00
18000	5.407E+01	4.728E+02	1.160E+03	1.148E+03	4.083E+02	4.090E+02	-3.867E+02	-2.572E+00
19000	5.242E+01	4.756E+02	1.213E+03	1.201E+03	4.118E+02	4.124E+02	-3.840E+02	-2.631E+00
20000	5.087E+01	4.783E+02	1.265E+03	1.253E+03	4.150E+02	4.156E+02	-3.814E+02	-2.684E+00
21000	4.939E+01	4.807E+02	1.315E+03	1.303E+03	4.181E+02	4.187E+02	-3.791E+02	-2.731E+00
22000	4.799E+01	4.830E+02	1.363E+03	1.351E+03	4.210E+02	4.216E+02	-3.770E+02	-2.774E+00
23000	4.666E+01	4.851E+02	1.411E+03	1.399E+03	4.238E+02	4.243E+02	-3.753E+02	-2.812E+00
24000	4.541E+01	4.871E+02	1.457E+03	1.445E+03	4.264E+02	4.269E+02	-3.738E+02	-2.848E+00
25000	4.423E+01	4.889E+02	1.502E+03	1.490E+03	4.288E+02	4.293E+02	-3.727E+02	-2.880E+00
26000	4.311E+01	4.906E+02	1.545E+03	1.533E+03	4.312E+02	4.316E+02	-3.720E+02	-2.910E+00
27000	4.205E+01	4.922E+02	1.588E+03	1.576E+03	4.334E+02	4.338E+02	-3.716E+02	-2.938E+00
28000	4.105E+01	4.937E+02	1.629E+03	1.617E+03	4.355E+02	4.359E+02	-3.716E+02	-2.964E+00
29000	4.012E+01	4.951E+02	1.670E+03	1.658E+03	4.376E+02	4.380E+02	-3.719E+02	-2.988E+00
30000	3.923E+01	4.965E+02	1.710E+03	1.698E+03	4.395E+02	4.399E+02	-3.726E+02	-3.010E+00
32000	3.760E+01	4.989E+02	1.786E+03	1.774E+03	4.431E+02	4.435E+02	-3.751E+02	-3.051E+00
34000	3.616E+01	5.012E+02	1.860E+03	1.848E+03	4.465E+02	4.468E+02	-3.789E+02	-3.087E+00
36000	3.488E+01	5.032E+02	1.931E+03	1.919E+03	4.496E+02	4.499E+02	-3.840E+02	-3.119E+00
38000	3.373E+01	5.051E+02	2.000E+03	1.988E+03	4.524E+02	4.528E+02	-3.902E+02	-3.149E+00
40000	3.271E+01	5.068E+02	2.066E+03	2.054E+03	4.551E+02	4.554E+02	-3.975E+02	-3.176E+00
42000	3.179E+01	5.084E+02	2.131E+03	2.119E+03	4.576E+02	4.579E+02	-4.058E+02	-3.201E+00
44000	3.097E+01	5.098E+02	2.193E+03	2.181E+03	4.600E+02	4.602E+02	-4.150E+02	-3.224E+00
46000	3.023E+01	5.112E+02	2.255E+03	2.243E+03	4.622E+02	4.624E+02	-4.250E+02	-3.246E+00
48000	2.957E+01	5.124E+02	2.314E+03	2.302E+03	4.642E+02	4.645E+02	-4.357E+02	-3.266E+00
50000	2.896E+01	5.136E+02	2.373E+03	2.361E+03	4.662E+02	4.664E+02	-4.471E+02	-3.285E+00

Table 103: Internal thermodynamic properties of CN

T(K)	Q_{int}	$\ln(Q_{int})$	E_{int}/RT	$C_{p,int}/R$
50	$3.743E+01$	$3.623E+00$	$9.819E-01$	$1.000E+00$
100	$7.420E+01$	$4.307E+00$	$9.912E-01$	$1.001E+00$
150	$1.110E+02$	$4.709E+00$	$9.943E-01$	$1.001E+00$
200	$1.478E+02$	$4.996E+00$	$9.960E-01$	$1.001E+00$
298.15	$2.200E+02$	$5.394E+00$	$9.982E-01$	$1.007E+00$
300	$2.214E+02$	$5.400E+00$	$9.983E-01$	$1.007E+00$
400	$2.952E+02$	$5.688E+00$	$1.004E+00$	$1.037E+00$
500	$3.697E+02$	$5.913E+00$	$1.016E+00$	$1.101E+00$
600	$4.457E+02$	$6.100E+00$	$1.037E+00$	$1.187E+00$
700	$5.241E+02$	$6.262E+00$	$1.065E+00$	$1.280E+00$
800	$6.055E+02$	$6.406E+00$	$1.098E+00$	$1.370E+00$
900	$6.904E+02$	$6.537E+00$	$1.133E+00$	$1.452E+00$
1000	$7.793E+02$	$6.658E+00$	$1.168E+00$	$1.524E+00$
2000	$1.935E+03$	$7.568E+00$	$1.476E+00$	$2.023E+00$
3000	$3.707E+03$	$8.218E+00$	$1.747E+00$	$2.552E+00$
4000	$6.350E+03$	$8.756E+00$	$1.999E+00$	$2.914E+00$
5000	$1.015E+04$	$9.225E+00$	$2.198E+00$	$3.045E+00$
6000	$1.535E+04$	$9.639E+00$	$2.341E+00$	$3.054E+00$
7000	$2.220E+04$	$1.001E+01$	$2.441E+00$	$3.032E+00$
8000	$3.091E+04$	$1.034E+01$	$2.514E+00$	$3.022E+00$
9000	$4.170E+04$	$1.064E+01$	$2.571E+00$	$3.032E+00$
10000	$5.482E+04$	$1.091E+01$	$2.618E+00$	$3.054E+00$
11000	$7.049E+04$	$1.116E+01$	$2.659E+00$	$3.074E+00$
12000	$8.898E+04$	$1.140E+01$	$2.694E+00$	$3.078E+00$
13000	$1.105E+05$	$1.161E+01$	$2.723E+00$	$3.056E+00$
14000	$1.353E+05$	$1.182E+01$	$2.745E+00$	$3.003E+00$
15000	$1.637E+05$	$1.201E+01$	$2.759E+00$	$2.920E+00$
16000	$1.956E+05$	$1.218E+01$	$2.766E+00$	$2.813E+00$
17000	$2.313E+05$	$1.235E+01$	$2.765E+00$	$2.687E+00$
18000	$2.709E+05$	$1.251E+01$	$2.757E+00$	$2.549E+00$
19000	$3.143E+05$	$1.266E+01$	$2.742E+00$	$2.404E+00$
20000	$3.616E+05$	$1.280E+01$	$2.722E+00$	$2.257E+00$
21000	$4.127E+05$	$1.293E+01$	$2.696E+00$	$2.112E+00$
22000	$4.675E+05$	$1.306E+01$	$2.666E+00$	$1.971E+00$
23000	$5.260E+05$	$1.317E+01$	$2.633E+00$	$1.837E+00$
24000	$5.879E+05$	$1.328E+01$	$2.597E+00$	$1.711E+00$
25000	$6.532E+05$	$1.339E+01$	$2.560E+00$	$1.593E+00$
26000	$7.216E+05$	$1.349E+01$	$2.520E+00$	$1.483E+00$
27000	$7.931E+05$	$1.358E+01$	$2.480E+00$	$1.381E+00$
28000	$8.673E+05$	$1.367E+01$	$2.439E+00$	$1.287E+00$
29000	$9.441E+05$	$1.376E+01$	$2.398E+00$	$1.200E+00$
30000	$1.023E+06$	$1.384E+01$	$2.356E+00$	$1.120E+00$
32000	$1.188E+06$	$1.399E+01$	$2.275E+00$	$9.793E-01$
34000	$1.361E+06$	$1.412E+01$	$2.195E+00$	$8.604E-01$
36000	$1.539E+06$	$1.425E+01$	$2.118E+00$	$7.598E-01$
38000	$1.722E+06$	$1.436E+01$	$2.044E+00$	$6.744E-01$
40000	$1.909E+06$	$1.446E+01$	$1.974E+00$	$6.015E-01$
42000	$2.099E+06$	$1.456E+01$	$1.907E+00$	$5.391E-01$
44000	$2.290E+06$	$1.464E+01$	$1.843E+00$	$4.854E-01$
46000	$2.483E+06$	$1.472E+01$	$1.783E+00$	$4.389E-01$
48000	$2.675E+06$	$1.480E+01$	$1.726E+00$	$3.984E-01$
50000	$2.867E+06$	$1.487E+01$	$1.673E+00$	$3.631E-01$

Table 104: Total thermodynamic properties of CN

T [K]	C_p [J/mol/K]	S^0 [J/mol/K]	$H^0(T)-H^0(0)$ [KJ/mol]	$H^0(T)-H^0(298)$ [KJ/mol]	$-(G^0-H^0(0))/T$ [J/mol/K]	$-(G^0-H^0(298))/T$ [J/mol/K]	ΔH_f [KJ/mol]	$\text{Log}(K_p)$
50	2.910E+01	1.507E+02	1.448E+00	-7.224E+00	1.217E+02	2.952E+02	4.065E+01	-4.186E+01
100	2.911E+01	1.708E+02	2.903E+00	-5.769E+00	1.418E+02	2.285E+02	4.064E+01	-2.063E+01
150	2.911E+01	1.826E+02	4.358E+00	-4.314E+00	1.536E+02	2.114E+02	4.058E+01	-1.355E+01
200	2.911E+01	1.910E+02	5.813E+00	-2.859E+00	1.619E+02	2.053E+02	4.037E+01	-1.003E+01
298.15	2.916E+01	2.026E+02	8.672E+00	0.000E+00	1.736E+02	2.026E+02	3.970E+01	-6.581E+00
300	2.916E+01	2.028E+02	8.726E+00	5.393E-02	1.737E+02	2.027E+02	3.968E+01	-6.538E+00
400	2.941E+01	2.112E+02	1.165E+01	2.980E+00	1.821E+02	2.038E+02	3.908E+01	-4.824E+00
500	2.994E+01	2.179E+02	1.462E+01	5.945E+00	1.886E+02	2.060E+02	3.866E+01	-3.808E+00
600	3.065E+01	2.234E+02	1.765E+01	8.974E+00	1.940E+02	2.084E+02	3.837E+01	-3.138E+00
700	3.143E+01	2.282E+02	2.075E+01	1.208E+01	1.985E+02	2.109E+02	3.817E+01	-2.662E+00
800	3.218E+01	2.324E+02	2.393E+01	1.526E+01	2.025E+02	2.133E+02	3.801E+01	-2.306E+00
900	3.286E+01	2.362E+02	2.718E+01	1.851E+01	2.060E+02	2.157E+02	3.790E+01	-2.031E+00
1000	3.346E+01	2.397E+02	3.050E+01	2.183E+01	2.092E+02	2.179E+02	3.780E+01	-1.811E+00
2000	3.761E+01	2.643E+02	6.612E+01	5.745E+01	2.312E+02	2.355E+02	3.741E+01	-8.301E-01
3000	4.201E+01	2.804E+02	1.059E+02	9.727E+01	2.450E+02	2.479E+02	3.896E+01	-5.006E-01
4000	4.502E+01	2.929E+02	1.496E+02	1.410E+02	2.555E+02	2.576E+02	4.316E+01	-3.236E-01
5000	4.610E+01	3.031E+02	1.953E+02	1.867E+02	2.640E+02	2.658E+02	4.859E+01	-2.044E-01
6000	4.618E+01	3.115E+02	2.415E+02	2.328E+02	2.713E+02	2.727E+02	5.396E+01	-1.153E-01
7000	4.600E+01	3.186E+02	2.876E+02	2.789E+02	2.775E+02	2.788E+02	5.869E+01	-4.533E-02
8000	4.591E+01	3.248E+02	3.335E+02	3.249E+02	2.831E+02	2.841E+02	6.268E+01	1.125E-02
9000	4.599E+01	3.302E+02	3.795E+02	3.708E+02	2.880E+02	2.890E+02	6.591E+01	5.790E-02
10000	4.618E+01	3.350E+02	4.256E+02	4.169E+02	2.925E+02	2.933E+02	6.821E+01	9.684E-02
11000	4.635E+01	3.394E+02	4.718E+02	4.632E+02	2.965E+02	2.973E+02	6.927E+01	1.295E-01
12000	4.638E+01	3.435E+02	5.182E+02	5.095E+02	3.003E+02	3.010E+02	6.873E+01	1.569E-01
13000	4.619E+01	3.472E+02	5.645E+02	5.558E+02	3.037E+02	3.044E+02	6.630E+01	1.796E-01
14000	4.575E+01	3.506E+02	6.105E+02	6.018E+02	3.070E+02	3.076E+02	6.194E+01	1.980E-01
15000	4.507E+01	3.537E+02	6.559E+02	6.473E+02	3.100E+02	3.106E+02	5.587E+01	2.127E-01
16000	4.418E+01	3.566E+02	7.006E+02	6.919E+02	3.128E+02	3.133E+02	4.853E+01	2.241E-01
17000	4.313E+01	3.592E+02	7.442E+02	7.356E+02	3.155E+02	3.160E+02	4.045E+01	2.327E-01
18000	4.198E+01	3.617E+02	7.868E+02	7.781E+02	3.180E+02	3.184E+02	3.218E+01	2.389E-01
19000	4.077E+01	3.639E+02	8.282E+02	8.195E+02	3.203E+02	3.208E+02	2.413E+01	2.432E-01
20000	3.955E+01	3.660E+02	8.683E+02	8.597E+02	3.226E+02	3.230E+02	1.661E+01	2.460E-01
21000	3.834E+01	3.679E+02	9.073E+02	8.986E+02	3.247E+02	3.251E+02	9.805E+00	2.477E-01
22000	3.718E+01	3.696E+02	9.450E+02	9.364E+02	3.267E+02	3.271E+02	3.799E+00	2.484E-01
23000	3.606E+01	3.712E+02	9.816E+02	9.730E+02	3.286E+02	3.289E+02	-1.407E+00	2.485E-01
24000	3.501E+01	3.728E+02	1.017E+03	1.008E+03	3.304E+02	3.307E+02	-5.853E+00	2.482E-01
25000	3.403E+01	3.742E+02	1.052E+03	1.043E+03	3.321E+02	3.324E+02	-9.608E+00	2.475E-01
26000	3.311E+01	3.755E+02	1.085E+03	1.077E+03	3.338E+02	3.341E+02	-1.275E+01	2.466E-01
27000	3.227E+01	3.767E+02	1.118E+03	1.109E+03	3.353E+02	3.356E+02	-1.537E+01	2.456E-01
28000	3.148E+01	3.779E+02	1.150E+03	1.141E+03	3.368E+02	3.371E+02	-1.753E+01	2.444E-01
29000	3.076E+01	3.790E+02	1.181E+03	1.172E+03	3.382E+02	3.386E+02	-1.931E+01	2.432E-01
30000	3.010E+01	3.800E+02	1.211E+03	1.203E+03	3.396E+02	3.399E+02	-2.077E+01	2.420E-01
32000	2.893E+01	3.819E+02	1.270E+03	1.262E+03	3.422E+02	3.425E+02	-2.293E+01	2.397E-01
34000	2.794E+01	3.836E+02	1.327E+03	1.318E+03	3.446E+02	3.449E+02	-2.435E+01	2.374E-01
36000	2.710E+01	3.852E+02	1.382E+03	1.374E+03	3.468E+02	3.471E+02	-2.528E+01	2.353E-01
38000	2.639E+01	3.866E+02	1.436E+03	1.427E+03	3.489E+02	3.491E+02	-2.586E+01	2.333E-01
40000	2.579E+01	3.880E+02	1.488E+03	1.479E+03	3.508E+02	3.510E+02	-2.623E+01	2.315E-01
42000	2.527E+01	3.892E+02	1.539E+03	1.530E+03	3.526E+02	3.528E+02	-2.644E+01	2.299E-01
44000	2.482E+01	3.904E+02	1.589E+03	1.580E+03	3.543E+02	3.545E+02	-2.656E+01	2.284E-01
46000	2.443E+01	3.915E+02	1.638E+03	1.630E+03	3.559E+02	3.561E+02	-2.662E+01	2.270E-01
48000	2.410E+01	3.925E+02	1.687E+03	1.678E+03	3.574E+02	3.576E+02	-2.664E+01	2.258E-01
50000	2.380E+01	3.935E+02	1.735E+03	1.726E+03	3.588E+02	3.590E+02	-2.664E+01	2.246E-01

Table 105: Internal thermodynamic properties of CN^+

T(K)	Q_{int}	$\ln(Q_{int})$	E_{int}/RT	$C_{p,int}/R$
50	$1.359E+02$	$4.912E+00$	$9.852E-01$	$1.000E+00$
100	$2.699E+02$	$5.598E+00$	$9.929E-01$	$1.001E+00$
150	$4.038E+02$	$6.001E+00$	$9.956E-01$	$1.001E+00$
200	$5.379E+02$	$6.288E+00$	$9.972E-01$	$1.004E+00$
298.15	$8.017E+02$	$6.687E+00$	$1.004E+00$	$1.040E+00$
300	$8.067E+02$	$6.693E+00$	$1.004E+00$	$1.041E+00$
400	$1.079E+03$	$6.984E+00$	$1.025E+00$	$1.144E+00$
500	$1.362E+03$	$7.217E+00$	$1.062E+00$	$1.282E+00$
600	$1.660E+03$	$7.414E+00$	$1.110E+00$	$1.419E+00$
700	$1.977E+03$	$7.589E+00$	$1.163E+00$	$1.540E+00$
800	$2.318E+03$	$7.748E+00$	$1.217E+00$	$1.639E+00$
900	$2.683E+03$	$7.895E+00$	$1.268E+00$	$1.719E+00$
1000	$3.074E+03$	$8.031E+00$	$1.317E+00$	$1.784E+00$
2000	$8.576E+03$	$9.057E+00$	$1.640E+00$	$2.082E+00$
3000	$1.727E+04$	$9.757E+00$	$1.812E+00$	$2.221E+00$
4000	$2.958E+04$	$1.029E+01$	$1.927E+00$	$2.316E+00$
5000	$4.591E+04$	$1.073E+01$	$2.012E+00$	$2.383E+00$
6000	$6.665E+04$	$1.111E+01$	$2.077E+00$	$2.411E+00$
7000	$9.213E+04$	$1.143E+01$	$2.123E+00$	$2.383E+00$
8000	$1.226E+05$	$1.172E+01$	$2.151E+00$	$2.298E+00$
9000	$1.580E+05$	$1.197E+01$	$2.160E+00$	$2.167E+00$
10000	$1.984E+05$	$1.220E+01$	$2.153E+00$	$2.008E+00$
11000	$2.433E+05$	$1.240E+01$	$2.132E+00$	$1.837E+00$
12000	$2.926E+05$	$1.259E+01$	$2.100E+00$	$1.668E+00$
13000	$3.456E+05$	$1.275E+01$	$2.061E+00$	$1.507E+00$
14000	$4.020E+05$	$1.290E+01$	$2.016E+00$	$1.359E+00$
15000	$4.612E+05$	$1.304E+01$	$1.968E+00$	$1.225E+00$
16000	$5.228E+05$	$1.317E+01$	$1.917E+00$	$1.105E+00$
17000	$5.864E+05$	$1.328E+01$	$1.866E+00$	$9.986E-01$
18000	$6.514E+05$	$1.339E+01$	$1.815E+00$	$9.045E-01$
19000	$7.177E+05$	$1.348E+01$	$1.765E+00$	$8.214E-01$
20000	$7.847E+05$	$1.357E+01$	$1.716E+00$	$7.479E-01$
21000	$8.522E+05$	$1.366E+01$	$1.669E+00$	$6.830E-01$
22000	$9.200E+05$	$1.373E+01$	$1.622E+00$	$6.254E-01$
23000	$9.879E+05$	$1.380E+01$	$1.578E+00$	$5.744E-01$
24000	$1.056E+06$	$1.387E+01$	$1.535E+00$	$5.289E-01$
25000	$1.123E+06$	$1.393E+01$	$1.494E+00$	$4.883E-01$
26000	$1.190E+06$	$1.399E+01$	$1.455E+00$	$4.519E-01$
27000	$1.256E+06$	$1.404E+01$	$1.417E+00$	$4.193E-01$
28000	$1.321E+06$	$1.409E+01$	$1.381E+00$	$3.900E-01$
29000	$1.386E+06$	$1.414E+01$	$1.346E+00$	$3.634E-01$
30000	$1.450E+06$	$1.419E+01$	$1.313E+00$	$3.395E-01$
32000	$1.575E+06$	$1.427E+01$	$1.251E+00$	$2.979E-01$
34000	$1.696E+06$	$1.434E+01$	$1.194E+00$	$2.633E-01$
36000	$1.813E+06$	$1.441E+01$	$1.141E+00$	$2.343E-01$
38000	$1.926E+06$	$1.447E+01$	$1.093E+00$	$2.098E-01$
40000	$2.035E+06$	$1.453E+01$	$1.048E+00$	$1.888E-01$
42000	$2.140E+06$	$1.458E+01$	$1.007E+00$	$1.708E-01$
44000	$2.240E+06$	$1.462E+01$	$9.684E-01$	$1.552E-01$
46000	$2.337E+06$	$1.466E+01$	$9.327E-01$	$1.417E-01$
48000	$2.430E+06$	$1.470E+01$	$8.995E-01$	$1.298E-01$
50000	$2.519E+06$	$1.474E+01$	$8.685E-01$	$1.193E-01$

Table 106: Total thermodynamic properties of CN^+

T [K]	C_p [J/mol/K]	S^0 [J/mol/K]	$H^0(T)-H^0(0)$ [KJ/mol]	$H^0(T)-H^0(298)$ [KJ/mol]	$-(G^0-H^0(0))/T$ [J/mol/K]	$-(G^0-H^0(298))/T$ [J/mol/K]	ΔH_f [KJ/mol]	$\mathrm{Log}(K_p)$
50	2.910E+01	1.614E+02	1.449E+00	-7.236E+00	1.324E+02	3.061E+02	1.354E+03	-1.414E+03
100	2.911E+01	1.816E+02	2.904E+00	-5.781E+00	1.526E+02	2.394E+02	1.355E+03	-7.065E+02
150	2.911E+01	1.934E+02	4.360E+00	-4.326E+00	1.643E+02	2.222E+02	1.356E+03	-4.706E+02
200	2.913E+01	2.018E+02	5.815E+00	-2.870E+00	1.727E+02	2.161E+02	1.356E+03	-3.525E+02
298.15	2.943E+01	2.134E+02	8.685E+00	0.000E+00	1.843E+02	2.134E+02	1.358E+03	-2.359E+02
300	2.944E+01	2.136E+02	8.740E+00	5.449E-02	1.845E+02	2.134E+02	1.358E+03	-2.344E+02
400	3.030E+01	2.222E+02	1.172E+01	3.037E+00	1.929E+02	2.146E+02	1.360E+03	-1.753E+02
500	3.144E+01	2.291E+02	1.481E+01	6.123E+00	1.995E+02	2.168E+02	1.361E+03	-1.397E+02
600	3.259E+01	2.349E+02	1.801E+01	9.326E+00	2.049E+02	2.194E+02	1.363E+03	-1.160E+02
700	3.359E+01	2.400E+02	2.132E+01	1.264E+01	2.096E+02	2.220E+02	1.365E+03	-9.905E+01
800	3.441E+01	2.446E+02	2.472E+01	1.604E+01	2.137E+02	2.245E+02	1.367E+03	-8.631E+01
900	3.508E+01	2.487E+02	2.820E+01	1.951E+01	2.173E+02	2.270E+02	1.370E+03	-7.638E+01
1000	3.562E+01	2.524E+02	3.173E+01	2.305E+01	2.206E+02	2.293E+02	1.372E+03	-6.842E+01
2000	3.810E+01	2.780E+02	6.884E+01	6.015E+01	2.436E+02	2.479E+02	1.394E+03	-3.237E+01
3000	3.925E+01	2.937E+02	1.076E+02	9.887E+01	2.578E+02	2.607E+02	1.415E+03	-2.016E+01
4000	4.004E+01	3.051E+02	1.472E+02	1.385E+02	2.683E+02	2.704E+02	1.436E+03	-1.396E+01
5000	4.060E+01	3.141E+02	1.876E+02	1.789E+02	2.766E+02	2.783E+02	1.457E+03	-1.018E+01
6000	4.083E+01	3.215E+02	2.283E+02	2.196E+02	2.835E+02	2.849E+02	1.478E+03	-7.630E+00
7000	4.060E+01	3.278E+02	2.691E+02	2.604E+02	2.894E+02	2.906E+02	1.498E+03	-5.781E+00
8000	3.989E+01	3.332E+02	3.094E+02	3.007E+02	2.945E+02	2.956E+02	1.517E+03	-4.375E+00
9000	3.880E+01	3.378E+02	3.487E+02	3.400E+02	2.991E+02	3.000E+02	1.534E+03	-3.268E+00
10000	3.748E+01	3.418E+02	3.869E+02	3.782E+02	3.031E+02	3.040E+02	1.549E+03	-2.374E+00
11000	3.606E+01	3.453E+02	4.236E+02	4.150E+02	3.068E+02	3.076E+02	1.562E+03	-1.635E+00
12000	3.465E+01	3.484E+02	4.590E+02	4.503E+02	3.102E+02	3.109E+02	1.571E+03	-1.015E+00
13000	3.332E+01	3.511E+02	4.930E+02	4.843E+02	3.132E+02	3.139E+02	1.577E+03	-4.880E-01
14000	3.208E+01	3.536E+02	5.257E+02	5.170E+02	3.160E+02	3.166E+02	1.580E+03	-3.495E-02
15000	3.097E+01	3.557E+02	5.572E+02	5.485E+02	3.186E+02	3.192E+02	1.581E+03	3.582E-01
16000	2.997E+01	3.577E+02	5.876E+02	5.790E+02	3.210E+02	3.215E+02	1.580E+03	7.022E-01
17000	2.909E+01	3.595E+02	6.172E+02	6.085E+02	3.232E+02	3.237E+02	1.579E+03	1.006E+00
18000	2.831E+01	3.611E+02	6.459E+02	6.372E+02	3.252E+02	3.257E+02	1.577E+03	1.275E+00
19000	2.761E+01	3.626E+02	6.738E+02	6.651E+02	3.272E+02	3.276E+02	1.577E+03	1.516E+00
20000	2.700E+01	3.641E+02	7.011E+02	6.924E+02	3.290E+02	3.294E+02	1.577E+03	1.732E+00
21000	2.646E+01	3.654E+02	7.278E+02	7.192E+02	3.307E+02	3.311E+02	1.579E+03	1.929E+00
22000	2.599E+01	3.666E+02	7.541E+02	7.454E+02	3.323E+02	3.327E+02	1.582E+03	2.107E+00
23000	2.556E+01	3.677E+02	7.798E+02	7.711E+02	3.338E+02	3.342E+02	1.587E+03	2.271E+00
24000	2.518E+01	3.688E+02	8.052E+02	7.965E+02	3.352E+02	3.356E+02	1.593E+03	2.421E+00
25000	2.485E+01	3.698E+02	8.302E+02	8.215E+02	3.366E+02	3.370E+02	1.601E+03	2.560E+00
26000	2.454E+01	3.708E+02	8.549E+02	8.462E+02	3.379E+02	3.382E+02	1.609E+03	2.689E+00
27000	2.427E+01	3.717E+02	8.793E+02	8.706E+02	3.391E+02	3.395E+02	1.619E+03	2.809E+00
28000	2.403E+01	3.726E+02	9.035E+02	8.948E+02	3.403E+02	3.406E+02	1.630E+03	2.922E+00
29000	2.381E+01	3.734E+02	9.274E+02	9.187E+02	3.414E+02	3.417E+02	1.642E+03	3.027E+00
30000	2.361E+01	3.742E+02	9.511E+02	9.424E+02	3.425E+02	3.428E+02	1.655E+03	3.126E+00
32000	2.326E+01	3.757E+02	9.980E+02	9.893E+02	3.446E+02	3.448E+02	1.682E+03	3.307E+00
34000	2.298E+01	3.771E+02	1.044E+03	1.036E+03	3.464E+02	3.467E+02	1.711E+03	3.470E+00
36000	2.273E+01	3.784E+02	1.090E+03	1.081E+03	3.482E+02	3.484E+02	1.743E+03	3.618E+00
38000	2.253E+01	3.797E+02	1.135E+03	1.126E+03	3.498E+02	3.500E+02	1.776E+03	3.752E+00
40000	2.236E+01	3.808E+02	1.180E+03	1.171E+03	3.513E+02	3.515E+02	1.809E+03	3.875E+00
42000	2.221E+01	3.819E+02	1.225E+03	1.216E+03	3.528E+02	3.530E+02	1.844E+03	3.989E+00
44000	2.208E+01	3.829E+02	1.269E+03	1.260E+03	3.541E+02	3.543E+02	1.880E+03	4.094E+00
46000	2.196E+01	3.839E+02	1.313E+03	1.304E+03	3.554E+02	3.556E+02	1.916E+03	4.192E+00
48000	2.186E+01	3.849E+02	1.357E+03	1.348E+03	3.566E+02	3.568E+02	1.953E+03	4.283E+00
50000	2.178E+01	3.857E+02	1.400E+03	1.392E+03	3.577E+02	3.579E+02	1.990E+03	4.369E+00

Table 107: Internal thermodynamic properties of CN^-

T(K)	Q_{int}	$\ln(Q_{int})$	E_{int}/RT	$C_{p,int}/R$
50	$1.842E+01$	$2.913E+00$	$9.816E-01$	$1.000E+00$
100	$3.650E+01$	$3.597E+00$	$9.910E-01$	$1.000E+00$
150	$5.458E+01$	$4.000E+00$	$9.942E-01$	$1.001E+00$
200	$7.267E+01$	$4.286E+00$	$9.959E-01$	$1.001E+00$
298.15	$1.082E+02$	$4.684E+00$	$9.979E-01$	$1.005E+00$
300	$1.089E+02$	$4.690E+00$	$9.980E-01$	$1.005E+00$
400	$1.451E+02$	$4.978E+00$	$1.002E+00$	$1.029E+00$
500	$1.817E+02$	$5.202E+00$	$1.012E+00$	$1.083E+00$
600	$2.188E+02$	$5.388E+00$	$1.030E+00$	$1.161E+00$
700	$2.570E+02$	$5.549E+00$	$1.055E+00$	$1.249E+00$
800	$2.964E+02$	$5.692E+00$	$1.085E+00$	$1.336E+00$
900	$3.375E+02$	$5.821E+00$	$1.118E+00$	$1.418E+00$
1000	$3.803E+02$	$5.941E+00$	$1.151E+00$	$1.490E+00$
2000	$9.283E+02$	$6.833E+00$	$1.433E+00$	$1.859E+00$
3000	$1.717E+03$	$7.448E+00$	$1.597E+00$	$1.975E+00$
4000	$2.760E+03$	$7.923E+00$	$1.700E+00$	$2.035E+00$
5000	$4.066E+03$	$8.310E+00$	$1.771E+00$	$2.077E+00$
6000	$5.644E+03$	$8.638E+00$	$1.825E+00$	$2.115E+00$
7000	$7.504E+03$	$8.923E+00$	$1.869E+00$	$2.151E+00$
8000	$9.655E+03$	$9.175E+00$	$1.907E+00$	$2.188E+00$
9000	$1.211E+04$	$9.402E+00$	$1.940E+00$	$2.227E+00$
10000	$1.488E+04$	$9.608E+00$	$1.971E+00$	$2.264E+00$
11000	$1.798E+04$	$9.797E+00$	$1.999E+00$	$2.297E+00$
12000	$2.142E+04$	$9.972E+00$	$2.025E+00$	$2.323E+00$
13000	$2.521E+04$	$1.014E+01$	$2.049E+00$	$2.336E+00$
14000	$2.937E+04$	$1.029E+01$	$2.069E+00$	$2.336E+00$
15000	$3.390E+04$	$1.043E+01$	$2.086E+00$	$2.320E+00$
16000	$3.880E+04$	$1.057E+01$	$2.100E+00$	$2.289E+00$
17000	$4.408E+04$	$1.069E+01$	$2.110E+00$	$2.244E+00$
18000	$4.974E+04$	$1.081E+01$	$2.116E+00$	$2.187E+00$
19000	$5.578E+04$	$1.093E+01$	$2.118E+00$	$2.120E+00$
20000	$6.218E+04$	$1.104E+01$	$2.116E+00$	$2.046E+00$
21000	$6.893E+04$	$1.114E+01$	$2.111E+00$	$1.966E+00$
22000	$7.603E+04$	$1.124E+01$	$2.103E+00$	$1.883E+00$
23000	$8.346E+04$	$1.133E+01$	$2.091E+00$	$1.799E+00$
24000	$9.120E+04$	$1.142E+01$	$2.077E+00$	$1.715E+00$
25000	$9.924E+04$	$1.151E+01$	$2.061E+00$	$1.632E+00$
26000	$1.076E+05$	$1.159E+01$	$2.043E+00$	$1.551E+00$
27000	$1.161E+05$	$1.166E+01$	$2.023E+00$	$1.472E+00$
28000	$1.250E+05$	$1.174E+01$	$2.002E+00$	$1.397E+00$
29000	$1.340E+05$	$1.181E+01$	$1.980E+00$	$1.325E+00$
30000	$1.433E+05$	$1.187E+01$	$1.957E+00$	$1.257E+00$
32000	$1.623E+05$	$1.200E+01$	$1.909E+00$	$1.131E+00$
34000	$1.819E+05$	$1.211E+01$	$1.860E+00$	$1.018E+00$
36000	$2.021E+05$	$1.222E+01$	$1.811E+00$	$9.189E-01$
38000	$2.226E+05$	$1.231E+01$	$1.761E+00$	$8.311E-01$
40000	$2.433E+05$	$1.240E+01$	$1.713E+00$	$7.538E-01$
42000	$2.642E+05$	$1.248E+01$	$1.665E+00$	$6.855E-01$
44000	$2.852E+05$	$1.256E+01$	$1.620E+00$	$6.252E-01$
46000	$3.062E+05$	$1.263E+01$	$1.575E+00$	$5.718E-01$
48000	$3.271E+05$	$1.270E+01$	$1.532E+00$	$5.245E-01$
50000	$3.479E+05$	$1.276E+01$	$1.491E+00$	$4.824E-01$

Table 108: Total thermodynamic properties of CN^-

T [K]	C_p [J/mol/K]	S^0 [J/mol/K]	$H^0(T)-H^0(0)$ [KJ/mol]	$H^0(T)-H^0(298)$ [KJ/mol]	$-(G^0-H^0(0))/T$ [J/mol/K]	$-(G^0-H^0(298))/T$ [J/mol/K]	ΔH_f [KJ/mol]	$\mathrm{Log}(K_p)$
50	2.910E+01	1.448E+02	1.447E+00	-7.224E+00	1.158E+02	2.892E+02	-3.330E+02	3.490E+02
100	2.911E+01	1.649E+02	2.903E+00	-5.769E+00	1.359E+02	2.226E+02	-3.341E+02	1.749E+02
150	2.911E+01	1.767E+02	4.358E+00	-4.313E+00	1.477E+02	2.055E+02	-3.352E+02	1.166E+02
200	2.911E+01	1.851E+02	5.813E+00	-2.858E+00	1.561E+02	1.994E+02	-3.364E+02	8.741E+01
298.15	2.914E+01	1.967E+02	8.671E+00	0.000E+00	1.677E+02	1.967E+02	-3.391E+02	5.838E+01
300	2.914E+01	1.969E+02	8.725E+00	5.388E-02	1.678E+02	1.967E+02	-3.392E+02	5.802E+01
400	2.934E+01	2.053E+02	1.165E+01	2.976E+00	1.762E+02	1.979E+02	-3.419E+02	4.320E+01
500	2.979E+01	2.119E+02	1.460E+01	5.931E+00	1.827E+02	2.001E+02	-3.444E+02	3.424E+01
600	3.044E+01	2.174E+02	1.761E+01	8.941E+00	1.881E+02	2.025E+02	-3.468E+02	2.822E+01
700	3.117E+01	2.222E+02	2.069E+01	1.202E+01	1.926E+02	2.050E+02	-3.491E+02	2.390E+01
800	3.190E+01	2.264E+02	2.385E+01	1.518E+01	1.966E+02	2.074E+02	-3.513E+02	2.063E+01
900	3.257E+01	2.302E+02	2.707E+01	1.840E+01	2.001E+02	2.097E+02	-3.536E+02	1.807E+01
1000	3.318E+01	2.336E+02	3.036E+01	2.169E+01	2.033E+02	2.119E+02	-3.558E+02	1.602E+01
2000	3.624E+01	2.578E+02	6.541E+01	5.674E+01	2.251E+02	2.294E+02	-3.775E+02	6.506E+00
3000	3.721E+01	2.727E+02	1.022E+02	9.353E+01	2.386E+02	2.415E+02	-3.998E+02	3.136E+00
4000	3.770E+01	2.835E+02	1.397E+02	1.310E+02	2.486E+02	2.507E+02	-4.226E+02	1.351E+00
5000	3.806E+01	2.919E+02	1.776E+02	1.689E+02	2.564E+02	2.581E+02	-4.457E+02	2.199E-01
6000	3.837E+01	2.989E+02	2.158E+02	2.071E+02	2.629E+02	2.644E+02	-4.691E+02	-5.753E-01
7000	3.867E+01	3.048E+02	2.543E+02	2.456E+02	2.685E+02	2.698E+02	-4.927E+02	-1.173E+00
8000	3.898E+01	3.100E+02	2.931E+02	2.844E+02	2.734E+02	2.745E+02	-5.166E+02	-1.643E+00
9000	3.930E+01	3.146E+02	3.323E+02	3.236E+02	2.777E+02	2.787E+02	-5.410E+02	-2.026E+00
10000	3.961E+01	3.188E+02	3.717E+02	3.631E+02	2.816E+02	2.825E+02	-5.661E+02	-2.347E+00
11000	3.989E+01	3.226E+02	4.115E+02	4.028E+02	2.852E+02	2.860E+02	-5.924E+02	-2.622E+00
12000	4.010E+01	3.261E+02	4.515E+02	4.428E+02	2.884E+02	2.892E+02	-6.201E+02	-2.861E+00
13000	4.021E+01	3.293E+02	4.916E+02	4.830E+02	2.914E+02	2.921E+02	-6.494E+02	-3.074E+00
14000	4.021E+01	3.322E+02	5.319E+02	5.232E+02	2.943E+02	2.949E+02	-6.803E+02	-3.264E+00
15000	4.008E+01	3.350E+02	5.720E+02	5.633E+02	2.969E+02	2.975E+02	-7.125E+02	-3.438E+00
16000	3.982E+01	3.376E+02	6.120E+02	6.033E+02	2.994E+02	2.999E+02	-7.453E+02	-3.596E+00
17000	3.945E+01	3.400E+02	6.516E+02	6.430E+02	3.017E+02	3.022E+02	-7.782E+02	-3.742E+00
18000	3.897E+01	3.422E+02	6.908E+02	6.822E+02	3.039E+02	3.044E+02	-8.106E+02	-3.878E+00
19000	3.841E+01	3.443E+02	7.295E+02	7.209E+02	3.059E+02	3.064E+02	-8.421E+02	-4.004E+00
20000	3.779E+01	3.463E+02	7.676E+02	7.590E+02	3.079E+02	3.083E+02	-8.724E+02	-4.122E+00
21000	3.713E+01	3.481E+02	8.051E+02	7.964E+02	3.098E+02	3.102E+02	-9.015E+02	-4.232E+00
22000	3.644E+01	3.498E+02	8.419E+02	8.332E+02	3.116E+02	3.120E+02	-9.293E+02	-4.336E+00
23000	3.574E+01	3.514E+02	8.780E+02	8.693E+02	3.133E+02	3.136E+02	-9.558E+02	-4.433E+00
24000	3.504E+01	3.529E+02	9.134E+02	9.047E+02	3.149E+02	3.152E+02	-9.811E+02	-4.525E+00
25000	3.435E+01	3.544E+02	9.481E+02	9.394E+02	3.164E+02	3.168E+02	-1.006E+03	-4.611E+00
26000	3.368E+01	3.557E+02	9.821E+02	9.734E+02	3.179E+02	3.182E+02	-1.029E+03	-4.693E+00
27000	3.303E+01	3.569E+02	1.015E+03	1.007E+03	3.193E+02	3.197E+02	-1.052E+03	-4.770E+00
28000	3.240E+01	3.581E+02	1.048E+03	1.040E+03	3.207E+02	3.210E+02	-1.074E+03	-4.844E+00
29000	3.180E+01	3.593E+02	1.080E+03	1.072E+03	3.220E+02	3.223E+02	-1.095E+03	-4.913E+00
30000	3.123E+01	3.603E+02	1.112E+03	1.103E+03	3.233E+02	3.236E+02	-1.117E+03	-4.980E+00
32000	3.019E+01	3.623E+02	1.173E+03	1.164E+03	3.257E+02	3.259E+02	-1.158E+03	-5.104E+00
34000	2.925E+01	3.641E+02	1.233E+03	1.224E+03	3.279E+02	3.281E+02	-1.198E+03	-5.217E+00
36000	2.843E+01	3.658E+02	1.290E+03	1.282E+03	3.299E+02	3.302E+02	-1.238E+03	-5.321E+00
38000	2.770E+01	3.673E+02	1.346E+03	1.338E+03	3.319E+02	3.321E+02	-1.278E+03	-5.417E+00
40000	2.705E+01	3.687E+02	1.401E+03	1.392E+03	3.337E+02	3.339E+02	-1.317E+03	-5.506E+00
42000	2.649E+01	3.700E+02	1.455E+03	1.446E+03	3.354E+02	3.356E+02	-1.356E+03	-5.589E+00
44000	2.598E+01	3.712E+02	1.507E+03	1.498E+03	3.370E+02	3.372E+02	-1.396E+03	-5.667E+00
46000	2.554E+01	3.724E+02	1.559E+03	1.550E+03	3.385E+02	3.387E+02	-1.435E+03	-5.740E+00
48000	2.515E+01	3.734E+02	1.609E+03	1.601E+03	3.399E+02	3.401E+02	-1.474E+03	-5.809E+00
50000	2.480E+01	3.745E+02	1.659E+03	1.650E+03	3.413E+02	3.414E+02	-1.514E+03	-5.873E+00

Table 109: Internal thermodynamic properties of CO

T(K)	Q_{int}	$\ln(Q_{int})$	E_{int}/RT	$C_{p,int}/R$
50	$1.842E+01$	$2.913E+00$	$9.816E-01$	$1.000E+00$
100	$3.650E+01$	$3.597E+00$	$9.910E-01$	$1.000E+00$
150	$5.458E+01$	$4.000E+00$	$9.942E-01$	$1.001E+00$
200	$7.267E+01$	$4.286E+00$	$9.959E-01$	$1.001E+00$
298.15	$1.082E+02$	$4.684E+00$	$9.979E-01$	$1.005E+00$
300	$1.089E+02$	$4.690E+00$	$9.980E-01$	$1.005E+00$
400	$1.451E+02$	$4.978E+00$	$1.002E+00$	$1.029E+00$
500	$1.817E+02$	$5.202E+00$	$1.012E+00$	$1.083E+00$
600	$2.188E+02$	$5.388E+00$	$1.030E+00$	$1.161E+00$
700	$2.570E+02$	$5.549E+00$	$1.055E+00$	$1.249E+00$
800	$2.964E+02$	$5.692E+00$	$1.085E+00$	$1.336E+00$
900	$3.375E+02$	$5.821E+00$	$1.118E+00$	$1.418E+00$
1000	$3.803E+02$	$5.941E+00$	$1.151E+00$	$1.490E+00$
2000	$9.283E+02$	$6.833E+00$	$1.433E+00$	$1.859E+00$
3000	$1.717E+03$	$7.448E+00$	$1.597E+00$	$1.975E+00$
4000	$2.760E+03$	$7.923E+00$	$1.700E+00$	$2.035E+00$
5000	$4.066E+03$	$8.310E+00$	$1.771E+00$	$2.079E+00$
6000	$5.645E+03$	$8.638E+00$	$1.827E+00$	$2.130E+00$
7000	$7.508E+03$	$8.924E+00$	$1.876E+00$	$2.221E+00$
8000	$9.678E+03$	$9.178E+00$	$1.929E+00$	$2.404E+00$
9000	$1.219E+04$	$9.409E+00$	$1.999E+00$	$2.732E+00$
10000	$1.512E+04$	$9.624E+00$	$2.095E+00$	$3.230E+00$
11000	$1.857E+04$	$9.829E+00$	$2.227E+00$	$3.872E+00$
12000	$2.270E+04$	$1.003E+01$	$2.393E+00$	$4.577E+00$
13000	$2.770E+04$	$1.023E+01$	$2.587E+00$	$5.231E+00$
14000	$3.381E+04$	$1.043E+01$	$2.795E+00$	$5.724E+00$
15000	$4.129E+04$	$1.063E+01$	$3.000E+00$	$5.992E+00$
16000	$5.042E+04$	$1.083E+01$	$3.189E+00$	$6.021E+00$
17000	$6.149E+04$	$1.103E+01$	$3.352E+00$	$5.847E+00$
18000	$7.476E+04$	$1.122E+01$	$3.482E+00$	$5.525E+00$
19000	$9.049E+04$	$1.141E+01$	$3.579E+00$	$5.116E+00$
20000	$1.089E+05$	$1.160E+01$	$3.645E+00$	$4.670E+00$
21000	$1.303E+05$	$1.178E+01$	$3.683E+00$	$4.223E+00$
22000	$1.547E+05$	$1.195E+01$	$3.698E+00$	$3.799E+00$
23000	$1.823E+05$	$1.211E+01$	$3.693E+00$	$3.410E+00$
24000	$2.132E+05$	$1.227E+01$	$3.674E+00$	$3.062E+00$
25000	$2.476E+05$	$1.242E+01$	$3.643E+00$	$2.754E+00$
26000	$2.854E+05$	$1.256E+01$	$3.604E+00$	$2.485E+00$
27000	$3.267E+05$	$1.270E+01$	$3.558E+00$	$2.250E+00$
28000	$3.715E+05$	$1.283E+01$	$3.508E+00$	$2.047E+00$
29000	$4.198E+05$	$1.295E+01$	$3.454E+00$	$1.870E+00$
30000	$4.715E+05$	$1.306E+01$	$3.399E+00$	$1.717E+00$
32000	$5.850E+05$	$1.328E+01$	$3.285E+00$	$1.468E+00$
34000	$7.116E+05$	$1.348E+01$	$3.173E+00$	$1.278E+00$
36000	$8.504E+05$	$1.365E+01$	$3.063E+00$	$1.131E+00$
38000	$1.001E+06$	$1.382E+01$	$2.958E+00$	$1.014E+00$
40000	$1.162E+06$	$1.397E+01$	$2.859E+00$	$9.206E-01$
42000	$1.333E+06$	$1.410E+01$	$2.765E+00$	$8.440E-01$
44000	$1.512E+06$	$1.423E+01$	$2.676E+00$	$7.802E-01$
46000	$1.700E+06$	$1.435E+01$	$2.592E+00$	$7.263E-01$
48000	$1.895E+06$	$1.445E+01$	$2.513E+00$	$6.799E-01$
50000	$2.097E+06$	$1.456E+01$	$2.439E+00$	$6.395E-01$

Table 110: Total thermodynamic properties of CO

T [K]	C_p [J/mol/K]	S^0 [J/mol/K]	$H^0(T)-H^0(0)$ [KJ/mol]	$H^0(T)-H^0(298)$ [KJ/mol]	$-(G^0-H^0(0))/T$ [J/mol/K]	$-(G^0-H^0(298))/T$ [J/mol/K]	ΔH_f [KJ/mol]	$\text{Log}(K_p)$
50	2.910E+01	1.457E+02	1.447E+00	-7.224E+00	1.167E+02	2.902E+02	-5.259E+02	5.494E+02
100	2.911E+01	1.659E+02	2.903E+00	-5.769E+00	1.368E+02	2.236E+02	-5.259E+02	2.747E+02
150	2.911E+01	1.777E+02	4.358E+00	-4.313E+00	1.486E+02	2.064E+02	-5.260E+02	1.831E+02
200	2.911E+01	1.860E+02	5.813E+00	-2.858E+00	1.570E+02	2.003E+02	-5.262E+02	1.373E+02
298.15	2.914E+01	1.977E+02	8.671E+00	0.000E+00	1.686E+02	1.977E+02	-5.269E+02	9.206E+01
300	2.914E+01	1.978E+02	8.725E+00	5.388E-02	1.688E+02	1.977E+02	-5.269E+02	9.150E+01
400	2.934E+01	2.062E+02	1.165E+01	2.976E+00	1.771E+02	1.988E+02	-5.275E+02	6.855E+01
500	2.979E+01	2.128E+02	1.460E+01	5.931E+00	1.836E+02	2.010E+02	-5.280E+02	5.476E+01
600	3.044E+01	2.183E+02	1.761E+01	8.941E+00	1.890E+02	2.034E+02	-5.284E+02	4.557E+01
700	3.117E+01	2.231E+02	2.069E+01	1.202E+01	1.935E+02	2.059E+02	-5.288E+02	3.899E+01
800	3.190E+01	2.273E+02	2.385E+01	1.518E+01	1.975E+02	2.083E+02	-5.290E+02	3.406E+01
900	3.257E+01	2.311E+02	2.707E+01	1.840E+01	2.010E+02	2.106E+02	-5.293E+02	3.022E+01
1000	3.318E+01	2.345E+02	3.036E+01	2.169E+01	2.042E+02	2.129E+02	-5.295E+02	2.715E+01
2000	3.624E+01	2.587E+02	6.541E+01	5.674E+01	2.260E+02	2.303E+02	-5.314E+02	1.330E+01
3000	3.721E+01	2.736E+02	1.022E+02	9.353E+01	2.396E+02	2.424E+02	-5.341E+02	8.664E+00
4000	3.770E+01	2.844E+02	1.397E+02	1.310E+02	2.495E+02	2.517E+02	-5.379E+02	6.332E+00
5000	3.807E+01	2.929E+02	1.776E+02	1.689E+02	2.573E+02	2.591E+02	-5.426E+02	4.921E+00
6000	3.850E+01	2.998E+02	2.158E+02	2.072E+02	2.639E+02	2.653E+02	-5.478E+02	3.973E+00
7000	3.926E+01	3.058E+02	2.547E+02	2.460E+02	2.694E+02	2.707E+02	-5.532E+02	3.288E+00
8000	4.077E+01	3.111E+02	2.946E+02	2.859E+02	2.743E+02	2.754E+02	-5.577E+02	2.770E+00
9000	4.350E+01	3.161E+02	3.366E+02	3.280E+02	2.787E+02	2.796E+02	-5.598E+02	2.364E+00
10000	4.764E+01	3.209E+02	3.821E+02	3.734E+02	2.827E+02	2.835E+02	-5.577E+02	2.040E+00
11000	5.298E+01	3.257E+02	4.323E+02	4.236E+02	2.864E+02	2.871E+02	-5.496E+02	1.776E+00
12000	5.885E+01	3.305E+02	4.882E+02	4.796E+02	2.898E+02	2.906E+02	-5.344E+02	1.562E+00
13000	6.428E+01	3.354E+02	5.499E+02	5.412E+02	2.931E+02	2.938E+02	-5.119E+02	1.386E+00
14000	6.838E+01	3.404E+02	6.163E+02	6.077E+02	2.964E+02	2.970E+02	-4.832E+02	1.243E+00
15000	7.060E+01	3.452E+02	6.860E+02	6.773E+02	2.994E+02	3.000E+02	-4.499E+02	1.127E+00
16000	7.085E+01	3.498E+02	7.569E+02	7.482E+02	3.024E+02	3.030E+02	-4.141E+02	1.033E+00
17000	6.940E+01	3.540E+02	8.271E+02	8.185E+02	3.054E+02	3.059E+02	-3.778E+02	9.567E-01
18000	6.672E+01	3.579E+02	8.953E+02	8.866E+02	3.082E+02	3.087E+02	-3.425E+02	8.952E-01
19000	6.332E+01	3.614E+02	9.603E+02	9.516E+02	3.109E+02	3.113E+02	-3.094E+02	8.454E-01
20000	5.961E+01	3.646E+02	1.022E+03	1.013E+03	3.135E+02	3.139E+02	-2.790E+02	8.050E-01
21000	5.590E+01	3.674E+02	1.080E+03	1.071E+03	3.160E+02	3.164E+02	-2.516E+02	7.720E-01
22000	5.237E+01	3.699E+02	1.134E+03	1.125E+03	3.184E+02	3.188E+02	-2.271E+02	7.450E-01
23000	4.914E+01	3.722E+02	1.184E+03	1.176E+03	3.207E+02	3.211E+02	-2.054E+02	7.226E-01
24000	4.624E+01	3.742E+02	1.232E+03	1.223E+03	3.229E+02	3.232E+02	-1.862E+02	7.041E-01
25000	4.368E+01	3.760E+02	1.277E+03	1.268E+03	3.250E+02	3.253E+02	-1.693E+02	6.886E-01
26000	4.144E+01	3.777E+02	1.320E+03	1.311E+03	3.269E+02	3.273E+02	-1.543E+02	6.756E-01
27000	3.949E+01	3.792E+02	1.360E+03	1.351E+03	3.289E+02	3.292E+02	-1.410E+02	6.647E-01
28000	3.780E+01	3.806E+02	1.399E+03	1.390E+03	3.307E+02	3.310E+02	-1.292E+02	6.553E-01
29000	3.634E+01	3.819E+02	1.436E+03	1.427E+03	3.324E+02	3.327E+02	-1.186E+02	6.474E-01
30000	3.506E+01	3.831E+02	1.471E+03	1.463E+03	3.341E+02	3.344E+02	-1.091E+02	6.405E-01
32000	3.300E+01	3.853E+02	1.539E+03	1.531E+03	3.372E+02	3.375E+02	-9.265E+01	6.296E-01
34000	3.141E+01	3.873E+02	1.604E+03	1.595E+03	3.401E+02	3.404E+02	-7.889E+01	6.213E-01
36000	3.019E+01	3.891E+02	1.665E+03	1.656E+03	3.428E+02	3.430E+02	-6.711E+01	6.151E-01
38000	2.922E+01	3.907E+02	1.725E+03	1.716E+03	3.453E+02	3.455E+02	-5.681E+01	6.104E-01
40000	2.844E+01	3.921E+02	1.782E+03	1.774E+03	3.476E+02	3.478E+02	-4.764E+01	6.068E-01
42000	2.780E+01	3.935E+02	1.838E+03	1.830E+03	3.497E+02	3.499E+02	-3.934E+01	6.041E-01
44000	2.727E+01	3.948E+02	1.894E+03	1.885E+03	3.518E+02	3.519E+02	-3.174E+01	6.021E-01
46000	2.682E+01	3.960E+02	1.948E+03	1.939E+03	3.536E+02	3.538E+02	-2.468E+01	6.006E-01
48000	2.644E+01	3.971E+02	2.001E+03	1.992E+03	3.554E+02	3.556E+02	-1.809E+01	5.996E-01
50000	2.610E+01	3.982E+02	2.053E+03	2.045E+03	3.571E+02	3.573E+02	-1.187E+01	5.989E-01

Table 111: Internal thermodynamic properties of CO^+

T(K)	Q_{int}	$\ln(Q_{int})$	E_{int}/RT	$C_{p,int}/R$
50	$3.600E+01$	$3.584E+00$	$9.812E-01$	$1.000E+00$
100	$7.133E+01$	$4.267E+00$	$9.908E-01$	$1.000E+00$
150	$1.067E+02$	$4.670E+00$	$9.940E-01$	$1.001E+00$
200	$1.420E+02$	$4.956E+00$	$9.957E-01$	$1.001E+00$
298.15	$2.114E+02$	$5.354E+00$	$9.978E-01$	$1.004E+00$
300	$2.128E+02$	$5.360E+00$	$9.978E-01$	$1.005E+00$
400	$2.836E+02$	$5.648E+00$	$1.002E+00$	$1.026E+00$
500	$3.550E+02$	$5.872E+00$	$1.011E+00$	$1.077E+00$
600	$4.274E+02$	$6.058E+00$	$1.028E+00$	$1.152E+00$
700	$5.017E+02$	$6.218E+00$	$1.052E+00$	$1.238E+00$
800	$5.784E+02$	$6.360E+00$	$1.081E+00$	$1.324E+00$
900	$6.581E+02$	$6.489E+00$	$1.112E+00$	$1.405E+00$
1000	$7.411E+02$	$6.608E+00$	$1.145E+00$	$1.478E+00$
2000	$1.800E+03$	$7.496E+00$	$1.426E+00$	$1.855E+00$
3000	$3.322E+03$	$8.108E+00$	$1.594E+00$	$1.993E+00$
4000	$5.344E+03$	$8.584E+00$	$1.712E+00$	$2.158E+00$
5000	$7.926E+03$	$8.978E+00$	$1.826E+00$	$2.424E+00$
6000	$1.118E+04$	$9.322E+00$	$1.954E+00$	$2.759E+00$
7000	$1.527E+04$	$9.633E+00$	$2.093E+00$	$3.094E+00$
8000	$2.038E+04$	$9.922E+00$	$2.236E+00$	$3.370E+00$
9000	$2.673E+04$	$1.019E+01$	$2.373E+00$	$3.548E+00$
10000	$3.455E+04$	$1.045E+01$	$2.495E+00$	$3.613E+00$
11000	$4.404E+04$	$1.069E+01$	$2.595E+00$	$3.573E+00$
12000	$5.539E+04$	$1.092E+01$	$2.672E+00$	$3.446E+00$
13000	$6.875E+04$	$1.114E+01$	$2.725E+00$	$3.259E+00$
14000	$8.423E+04$	$1.134E+01$	$2.755E+00$	$3.036E+00$
15000	$1.019E+05$	$1.153E+01$	$2.766E+00$	$2.799E+00$
16000	$1.218E+05$	$1.171E+01$	$2.760E+00$	$2.561E+00$
17000	$1.439E+05$	$1.188E+01$	$2.742E+00$	$2.332E+00$
18000	$1.682E+05$	$1.203E+01$	$2.713E+00$	$2.118E+00$
19000	$1.946E+05$	$1.218E+01$	$2.676E+00$	$1.922E+00$
20000	$2.230E+05$	$1.232E+01$	$2.634E+00$	$1.743E+00$
21000	$2.533E+05$	$1.244E+01$	$2.588E+00$	$1.583E+00$
22000	$2.854E+05$	$1.256E+01$	$2.539E+00$	$1.440E+00$
23000	$3.192E+05$	$1.267E+01$	$2.488E+00$	$1.312E+00$
24000	$3.544E+05$	$1.278E+01$	$2.437E+00$	$1.197E+00$
25000	$3.911E+05$	$1.288E+01$	$2.385E+00$	$1.096E+00$
26000	$4.290E+05$	$1.297E+01$	$2.334E+00$	$1.005E+00$
27000	$4.681E+05$	$1.306E+01$	$2.283E+00$	$9.236E-01$
28000	$5.082E+05$	$1.314E+01$	$2.233E+00$	$8.511E-01$
29000	$5.491E+05$	$1.322E+01$	$2.184E+00$	$7.860E-01$
30000	$5.908E+05$	$1.329E+01$	$2.137E+00$	$7.276E-01$
32000	$6.762E+05$	$1.342E+01$	$2.045E+00$	$6.276E-01$
34000	$7.635E+05$	$1.355E+01$	$1.960E+00$	$5.458E-01$
36000	$8.520E+05$	$1.366E+01$	$1.879E+00$	$4.783E-01$
38000	$9.412E+05$	$1.375E+01$	$1.804E+00$	$4.221E-01$
40000	$1.031E+06$	$1.385E+01$	$1.734E+00$	$3.749E-01$
42000	$1.120E+06$	$1.393E+01$	$1.668E+00$	$3.349E-01$
44000	$1.208E+06$	$1.400E+01$	$1.606E+00$	$3.009E-01$
46000	$1.296E+06$	$1.407E+01$	$1.549E+00$	$2.717E-01$
48000	$1.383E+06$	$1.414E+01$	$1.495E+00$	$2.464E-01$
50000	$1.468E+06$	$1.420E+01$	$1.445E+00$	$2.244E-01$

Table 112: Total thermodynamic properties of CO^+

T [K]	C_p [J/mol/K]	S^0 [J/mol/K]	$H^0(T)-H^0(0)$ [KJ/mol]	$H^0(T)-H^0(298)$ [KJ/mol]	$-(G^0-H^0(0))/T$ [J/mol/K]	$-(G^0-H^0(298))/T$ [J/mol/K]	ΔH_f [KJ/mol]	$\mathrm{Log}(K_p)$
50	2.910E+01	1.513E+02	1.447E+00	-7.224E+00	1.223E+02	2.957E+02	8.272E+02	-8.648E+02
100	2.911E+01	1.714E+02	2.902E+00	-5.769E+00	1.424E+02	2.291E+02	8.283E+02	-4.324E+02
150	2.911E+01	1.832E+02	4.358E+00	-4.313E+00	1.542E+02	2.120E+02	8.293E+02	-2.882E+02
200	2.911E+01	1.916E+02	5.813E+00	-2.858E+00	1.625E+02	2.059E+02	8.301E+02	-2.159E+02
298.15	2.914E+01	2.032E+02	8.671E+00	0.000E+00	1.742E+02	2.032E+02	8.315E+02	-1.445E+02
300	2.914E+01	2.034E+02	8.725E+00	5.394E-02	1.743E+02	2.032E+02	8.315E+02	-1.436E+02
400	2.932E+01	2.118E+02	1.165E+01	2.975E+00	1.827E+02	2.044E+02	8.329E+02	-1.074E+02
500	2.974E+01	2.184E+02	1.460E+01	5.926E+00	1.892E+02	2.065E+02	8.345E+02	-8.563E+01
600	3.036E+01	2.239E+02	1.760E+01	8.930E+00	1.945E+02	2.090E+02	8.362E+02	-7.108E+01
700	3.108E+01	2.286E+02	2.067E+01	1.200E+01	1.991E+02	2.115E+02	8.379E+02	-6.067E+01
800	3.180E+01	2.328E+02	2.382E+01	1.514E+01	2.030E+02	2.139E+02	8.397E+02	-5.285E+01
900	3.247E+01	2.366E+02	2.703E+01	1.836E+01	2.066E+02	2.162E+02	8.415E+02	-4.675E+01
1000	3.308E+01	2.400E+02	3.031E+01	2.164E+01	2.097E+02	2.184E+02	8.433E+02	-4.187E+01
2000	3.621E+01	2.642E+02	6.529E+01	5.662E+01	2.315E+02	2.358E+02	8.622E+02	-1.965E+01
3000	3.736E+01	2.791E+02	1.021E+02	9.345E+01	2.450E+02	2.479E+02	8.803E+02	-1.207E+01
4000	3.873E+01	2.900E+02	1.401E+02	1.314E+02	2.550E+02	2.571E+02	8.978E+02	-8.209E+00
5000	4.094E+01	2.989E+02	1.799E+02	1.712E+02	2.629E+02	2.646E+02	9.158E+02	-5.843E+00
6000	4.373E+01	3.066E+02	2.222E+02	2.135E+02	2.695E+02	2.710E+02	9.354E+02	-4.232E+00
7000	4.652E+01	3.135E+02	2.673E+02	2.586E+02	2.753E+02	2.766E+02	9.571E+02	-3.057E+00
8000	4.881E+01	3.199E+02	3.150E+02	3.064E+02	2.805E+02	2.816E+02	9.811E+02	-2.154E+00
9000	5.028E+01	3.257E+02	3.647E+02	3.560E+02	2.852E+02	2.862E+02	1.007E+03	-1.433E+00
10000	5.083E+01	3.311E+02	4.153E+02	4.066E+02	2.895E+02	2.904E+02	1.036E+03	-8.402E-01
11000	5.049E+01	3.359E+02	4.660E+02	4.574E+02	2.935E+02	2.943E+02	1.065E+03	-3.417E-01
12000	4.944E+01	3.402E+02	5.160E+02	5.074E+02	2.972E+02	2.980E+02	1.095E+03	8.542E-02
13000	4.788E+01	3.441E+02	5.647E+02	5.560E+02	3.007E+02	3.014E+02	1.125E+03	4.570E-01
14000	4.603E+01	3.476E+02	6.117E+02	6.030E+02	3.039E+02	3.046E+02	1.155E+03	7.842E-01
15000	4.405E+01	3.507E+02	6.567E+02	6.481E+02	3.070E+02	3.075E+02	1.185E+03	1.075E+00
16000	4.208E+01	3.535E+02	6.998E+02	6.911E+02	3.098E+02	3.103E+02	1.214E+03	1.336E+00
17000	4.017E+01	3.560E+02	7.409E+02	7.322E+02	3.124E+02	3.129E+02	1.242E+03	1.572E+00
18000	3.840E+01	3.583E+02	7.802E+02	7.715E+02	3.149E+02	3.154E+02	1.269E+03	1.786E+00
19000	3.676E+01	3.603E+02	8.178E+02	8.091E+02	3.172E+02	3.177E+02	1.295E+03	1.982E+00
20000	3.528E+01	3.621E+02	8.538E+02	8.451E+02	3.194E+02	3.199E+02	1.321E+03	2.161E+00
21000	3.395E+01	3.638E+02	8.884E+02	8.797E+02	3.215E+02	3.219E+02	1.346E+03	2.327E+00
22000	3.276E+01	3.654E+02	9.217E+02	9.130E+02	3.235E+02	3.239E+02	1.370E+03	2.481E+00
23000	3.169E+01	3.668E+02	9.539E+02	9.453E+02	3.253E+02	3.257E+02	1.394E+03	2.623E+00
24000	3.074E+01	3.681E+02	9.851E+02	9.765E+02	3.271E+02	3.274E+02	1.418E+03	2.756E+00
25000	2.989E+01	3.694E+02	1.016E+03	1.007E+03	3.288E+02	3.291E+02	1.441E+03	2.881E+00
26000	2.914E+01	3.705E+02	1.045E+03	1.036E+03	3.303E+02	3.307E+02	1.464E+03	2.998E+00
27000	2.847E+01	3.716E+02	1.074E+03	1.065E+03	3.319E+02	3.322E+02	1.486E+03	3.107E+00
28000	2.786E+01	3.726E+02	1.102E+03	1.093E+03	3.333E+02	3.336E+02	1.508E+03	3.211E+00
29000	2.732E+01	3.736E+02	1.130E+03	1.121E+03	3.347E+02	3.350E+02	1.530E+03	3.308E+00
30000	2.684E+01	3.745E+02	1.157E+03	1.148E+03	3.360E+02	3.363E+02	1.552E+03	3.401E+00
32000	2.600E+01	3.762E+02	1.209E+03	1.201E+03	3.384E+02	3.387E+02	1.595E+03	3.572E+00
34000	2.532E+01	3.778E+02	1.261E+03	1.252E+03	3.407E+02	3.410E+02	1.637E+03	3.727E+00
36000	2.476E+01	3.792E+02	1.311E+03	1.302E+03	3.428E+02	3.431E+02	1.679E+03	3.869E+00
38000	2.430E+01	3.806E+02	1.360E+03	1.351E+03	3.448E+02	3.450E+02	1.720E+03	3.999E+00
40000	2.390E+01	3.818E+02	1.408E+03	1.399E+03	3.466E+02	3.468E+02	1.762E+03	4.118E+00
42000	2.357E+01	3.829E+02	1.456E+03	1.447E+03	3.483E+02	3.485E+02	1.803E+03	4.229E+00
44000	2.329E+01	3.840E+02	1.502E+03	1.494E+03	3.499E+02	3.501E+02	1.844E+03	4.332E+00
46000	2.305E+01	3.851E+02	1.549E+03	1.540E+03	3.514E+02	3.516E+02	1.885E+03	4.428E+00
48000	2.284E+01	3.860E+02	1.594E+03	1.586E+03	3.528E+02	3.530E+02	1.926E+03	4.518E+00
50000	2.265E+01	3.870E+02	1.640E+03	1.631E+03	3.542E+02	3.543E+02	1.966E+03	4.603E+00

Table 113: Internal thermodynamic properties of CO_2

T(K)	Q_{int}	$\ln(Q_{int})$	E_{int}/RT	$C_{p,int}/R$
50	$4.455E+01$	$3.797E+00$	$9.962E-01$	$1.000E+00$
100	$8.894E+01$	$4.488E+00$	$9.994E-01$	$1.012E+00$
150	$1.338E+02$	$4.896E+00$	$1.020E+00$	$1.137E+00$
200	$1.807E+02$	$5.197E+00$	$1.079E+00$	$1.390E+00$
298.15	$2.877E+02$	$5.662E+00$	$1.276E+00$	$1.956E+00$
300	$2.900E+02$	$5.670E+00$	$1.280E+00$	$1.966E+00$
400	$4.327E+02$	$6.070E+00$	$1.515E+00$	$2.452E+00$
500	$6.219E+02$	$6.433E+00$	$1.743E+00$	$2.844E+00$
600	$8.708E+02$	$6.769E+00$	$1.954E+00$	$3.166E+00$
700	$1.194E+03$	$7.085E+00$	$2.147E+00$	$3.433E+00$
800	$1.609E+03$	$7.384E+00$	$2.322E+00$	$3.656E+00$
900	$2.135E+03$	$7.666E+00$	$2.481E+00$	$3.842E+00$
1000	$2.794E+03$	$7.935E+00$	$2.625E+00$	$3.996E+00$
2000	$2.375E+04$	$1.008E+01$	$3.524E+00$	$4.676E+00$
3000	$1.082E+05$	$1.159E+01$	$3.942E+00$	$4.848E+00$
4000	$3.485E+05$	$1.276E+01$	$4.179E+00$	$4.926E+00$
5000	$9.014E+05$	$1.371E+01$	$4.337E+00$	$5.029E+00$
6000	$2.011E+06$	$1.451E+01$	$4.468E+00$	$5.230E+00$
7000	$4.043E+06$	$1.521E+01$	$4.598E+00$	$5.543E+00$
8000	$7.538E+06$	$1.584E+01$	$4.739E+00$	$5.923E+00$
9000	$1.329E+07$	$1.640E+01$	$4.892E+00$	$6.287E+00$
10000	$2.243E+07$	$1.693E+01$	$5.046E+00$	$6.556E+00$
11000	$3.653E+07$	$1.741E+01$	$5.190E+00$	$6.679E+00$
12000	$5.770E+07$	$1.787E+01$	$5.314E+00$	$6.646E+00$
13000	$8.863E+07$	$1.830E+01$	$5.410E+00$	$6.477E+00$
14000	$1.327E+08$	$1.870E+01$	$5.477E+00$	$6.209E+00$
15000	$1.939E+08$	$1.908E+01$	$5.516E+00$	$5.883E+00$
16000	$2.770E+08$	$1.944E+01$	$5.527E+00$	$5.529E+00$
17000	$3.872E+08$	$1.977E+01$	$5.517E+00$	$5.172E+00$
18000	$5.303E+08$	$2.009E+01$	$5.488E+00$	$4.827E+00$
19000	$7.127E+08$	$2.038E+01$	$5.445E+00$	$4.504E+00$
20000	$9.410E+08$	$2.066E+01$	$5.390E+00$	$4.205E+00$
21000	$1.222E+09$	$2.092E+01$	$5.327E+00$	$3.932E+00$
22000	$1.564E+09$	$2.117E+01$	$5.258E+00$	$3.685E+00$
23000	$1.972E+09$	$2.140E+01$	$5.185E+00$	$3.462E+00$
24000	$2.455E+09$	$2.162E+01$	$5.109E+00$	$3.260E+00$
25000	$3.020E+09$	$2.183E+01$	$5.031E+00$	$3.077E+00$
26000	$3.673E+09$	$2.202E+01$	$4.953E+00$	$2.912E+00$
27000	$4.421E+09$	$2.221E+01$	$4.874E+00$	$2.761E+00$
28000	$5.271E+09$	$2.239E+01$	$4.796E+00$	$2.625E+00$
29000	$6.229E+09$	$2.255E+01$	$4.719E+00$	$2.500E+00$
30000	$7.300E+09$	$2.271E+01$	$4.643E+00$	$2.385E+00$
32000	$9.804E+09$	$2.301E+01$	$4.496E+00$	$2.182E+00$
34000	$1.282E+10$	$2.327E+01$	$4.354E+00$	$2.008E+00$
36000	$1.638E+10$	$2.352E+01$	$4.220E+00$	$1.857E+00$
38000	$2.051E+10$	$2.374E+01$	$4.092E+00$	$1.725E+00$
40000	$2.522E+10$	$2.395E+01$	$3.970E+00$	$1.608E+00$
42000	$3.052E+10$	$2.414E+01$	$3.855E+00$	$1.503E+00$
44000	$3.642E+10$	$2.432E+01$	$3.746E+00$	$1.409E+00$
46000	$4.293E+10$	$2.448E+01$	$3.643E+00$	$1.325E+00$
48000	$5.002E+10$	$2.464E+01$	$3.545E+00$	$1.248E+00$
50000	$5.770E+10$	$2.478E+01$	$3.451E+00$	$1.178E+00$

Table 114: Total thermodynamic properties of CO_2

T [K]	C_p [J/mol/K]	S^0 [J/mol/K]	$H^0(T)-H^0(0)$ [KJ/mol]	$H^0(T)-H^0(298)$ [KJ/mol]	$-(G^0-H^0(0))/T$ [J/mol/K]	$-(G^0-H^0(298))/T$ [J/mol/K]	ΔH_f [KJ/mol]	$\mathrm{Log}(K_p)$
50	2.910E+01	1.588E+02	1.454E+00	-7.907E+00	1.297E+02	3.169E+02	-8.060E+02	8.387E+02
100	2.920E+01	1.790E+02	2.910E+00	-6.451E+00	1.499E+02	2.435E+02	-8.067E+02	4.175E+02
150	3.024E+01	1.910E+02	4.390E+00	-4.970E+00	1.617E+02	2.241E+02	-8.075E+02	2.770E+02
200	3.234E+01	1.999E+02	5.952E+00	-3.409E+00	1.702E+02	2.170E+02	-8.083E+02	2.067E+02
298.15	3.705E+01	2.137E+02	9.360E+00	0.000E+00	1.823E+02	2.137E+02	-8.099E+02	1.371E+02
300	3.714E+01	2.140E+02	9.429E+00	6.860E-02	1.825E+02	2.137E+02	-8.099E+02	1.362E+02
400	4.117E+01	2.252E+02	1.335E+01	3.991E+00	1.918E+02	2.152E+02	-8.110E+02	1.010E+02
500	4.443E+01	2.348E+02	1.764E+01	8.277E+00	1.995E+02	2.182E+02	-8.117E+02	7.978E+01
600	4.711E+01	2.431E+02	2.222E+01	1.286E+01	2.061E+02	2.217E+02	-8.121E+02	6.564E+01
700	4.933E+01	2.506E+02	2.704E+01	1.768E+01	2.119E+02	2.253E+02	-8.123E+02	5.554E+01
800	5.119E+01	2.573E+02	3.207E+01	2.271E+01	2.172E+02	2.289E+02	-8.124E+02	4.797E+01
900	5.273E+01	2.634E+02	3.727E+01	2.791E+01	2.220E+02	2.324E+02	-8.124E+02	4.207E+01
1000	5.401E+01	2.690E+02	4.261E+01	3.325E+01	2.264E+02	2.358E+02	-8.123E+02	3.736E+01
2000	5.966E+01	3.087E+02	1.002E+02	9.081E+01	2.586E+02	2.633E+02	-8.100E+02	1.616E+01
3000	6.110E+01	3.332E+02	1.607E+02	1.513E+02	2.796E+02	2.828E+02	-8.084E+02	9.119E+00
4000	6.175E+01	3.509E+02	2.221E+02	2.128E+02	2.953E+02	2.977E+02	-8.087E+02	5.601E+00
5000	6.260E+01	3.647E+02	2.842E+02	2.749E+02	3.079E+02	3.098E+02	-8.103E+02	3.487E+00
6000	6.427E+01	3.763E+02	3.476E+02	3.382E+02	3.183E+02	3.199E+02	-8.123E+02	2.074E+00
7000	6.687E+01	3.864E+02	4.131E+02	4.037E+02	3.274E+02	3.287E+02	-8.131E+02	1.063E+00
8000	7.003E+01	3.955E+02	4.815E+02	4.722E+02	3.353E+02	3.365E+02	-8.113E+02	3.054E-01
9000	7.306E+01	4.039E+02	5.531E+02	5.438E+02	3.425E+02	3.435E+02	-8.057E+02	-2.814E-01
10000	7.530E+01	4.118E+02	6.274E+02	6.180E+02	3.490E+02	3.499E+02	-7.960E+02	-7.465E-01
11000	7.632E+01	4.190E+02	7.033E+02	6.940E+02	3.551E+02	3.559E+02	-7.826E+02	-1.122E+00
12000	7.604E+01	4.256E+02	7.796E+02	7.702E+02	3.607E+02	3.614E+02	-7.666E+02	-1.428E+00
13000	7.464E+01	4.317E+02	8.550E+02	8.456E+02	3.659E+02	3.666E+02	-7.492E+02	-1.682E+00
14000	7.241E+01	4.371E+02	9.286E+02	9.192E+02	3.708E+02	3.715E+02	-7.313E+02	-1.895E+00
15000	6.970E+01	4.420E+02	9.997E+02	9.903E+02	3.754E+02	3.760E+02	-7.137E+02	-2.074E+00
16000	6.676E+01	4.464E+02	1.068E+03	1.058E+03	3.797E+02	3.803E+02	-6.971E+02	-2.228E+00
17000	6.379E+01	4.504E+02	1.133E+03	1.124E+03	3.837E+02	3.843E+02	-6.818E+02	-2.360E+00
18000	6.092E+01	4.539E+02	1.196E+03	1.186E+03	3.875E+02	3.881E+02	-6.678E+02	-2.475E+00
19000	5.823E+01	4.572E+02	1.255E+03	1.246E+03	3.911E+02	3.916E+02	-6.552E+02	-2.577E+00
20000	5.575E+01	4.601E+02	1.312E+03	1.303E+03	3.945E+02	3.950E+02	-6.440E+02	-2.666E+00
21000	5.348E+01	4.628E+02	1.367E+03	1.357E+03	3.977E+02	3.981E+02	-6.341E+02	-2.745E+00
22000	5.143E+01	4.652E+02	1.419E+03	1.410E+03	4.007E+02	4.011E+02	-6.254E+02	-2.817E+00
23000	4.957E+01	4.674E+02	1.470E+03	1.460E+03	4.036E+02	4.039E+02	-6.178E+02	-2.881E+00
24000	4.789E+01	4.695E+02	1.518E+03	1.509E+03	4.062E+02	4.066E+02	-6.112E+02	-2.939E+00
25000	4.637E+01	4.714E+02	1.565E+03	1.556E+03	4.088E+02	4.092E+02	-6.056E+02	-2.992E+00
26000	4.499E+01	4.732E+02	1.611E+03	1.602E+03	4.113E+02	4.116E+02	-6.007E+02	-3.040E+00
27000	4.375E+01	4.749E+02	1.655E+03	1.646E+03	4.136E+02	4.139E+02	-5.966E+02	-3.085E+00
28000	4.261E+01	4.765E+02	1.699E+03	1.689E+03	4.158E+02	4.161E+02	-5.932E+02	-3.126E+00
29000	4.157E+01	4.779E+02	1.741E+03	1.731E+03	4.179E+02	4.182E+02	-5.904E+02	-3.164E+00
30000	4.062E+01	4.794E+02	1.782E+03	1.772E+03	4.199E+02	4.203E+02	-5.882E+02	-3.199E+00
32000	3.893E+01	4.819E+02	1.861E+03	1.852E+03	4.238E+02	4.240E+02	-5.853E+02	-3.263E+00
34000	3.748E+01	4.842E+02	1.938E+03	1.928E+03	4.272E+02	4.275E+02	-5.843E+02	-3.319E+00
36000	3.623E+01	4.863E+02	2.011E+03	2.002E+03	4.305E+02	4.307E+02	-5.848E+02	-3.369E+00
38000	3.513E+01	4.883E+02	2.083E+03	2.073E+03	4.334E+02	4.337E+02	-5.866E+02	-3.414E+00
40000	3.415E+01	4.900E+02	2.152E+03	2.143E+03	4.362E+02	4.365E+02	-5.897E+02	-3.454E+00
42000	3.328E+01	4.917E+02	2.219E+03	2.210E+03	4.388E+02	4.391E+02	-5.939E+02	-3.491E+00
44000	3.251E+01	4.932E+02	2.285E+03	2.276E+03	4.413E+02	4.415E+02	-5.991E+02	-3.525E+00
46000	3.180E+01	4.946E+02	2.349E+03	2.340E+03	4.436E+02	4.438E+02	-6.051E+02	-3.556E+00
48000	3.116E+01	4.960E+02	2.412E+03	2.403E+03	4.457E+02	4.459E+02	-6.120E+02	-3.585E+00
50000	3.058E+01	4.972E+02	2.474E+03	2.465E+03	4.478E+02	4.479E+02	-6.196E+02	-3.611E+00

Table 115: Internal thermodynamic properties of CO_2^+

T(K)	Q_{int}	$\ln(Q_{int})$	E_{int}/RT	$C_{p,int}/R$
50	$1.852E+02$	$5.222E+00$	$1.042E+00$	$1.209E+00$
100	$4.036E+02$	$6.000E+00$	$1.220E+00$	$1.523E+00$
150	$6.795E+02$	$6.521E+00$	$1.356E+00$	$1.748E+00$
200	$1.022E+03$	$6.930E+00$	$1.489E+00$	$2.025E+00$
298.15	$1.945E+03$	$7.573E+00$	$1.751E+00$	$2.533E+00$
300	$1.966E+03$	$7.584E+00$	$1.755E+00$	$2.541E+00$
400	$3.375E+03$	$8.124E+00$	$2.010E+00$	$2.998E+00$
500	$5.423E+03$	$8.598E+00$	$2.248E+00$	$3.388E+00$
600	$8.332E+03$	$9.028E+00$	$2.465E+00$	$3.702E+00$
700	$1.237E+04$	$9.423E+00$	$2.660E+00$	$3.947E+00$
800	$1.784E+04$	$9.789E+00$	$2.833E+00$	$4.136E+00$
900	$2.514E+04$	$1.013E+01$	$2.986E+00$	$4.283E+00$
1000	$3.468E+04$	$1.045E+01$	$3.122E+00$	$4.397E+00$
2000	$4.010E+05$	$1.290E+01$	$3.899E+00$	$4.829E+00$
3000	$2.090E+06$	$1.455E+01$	$4.228E+00$	$4.922E+00$
4000	$7.243E+06$	$1.580E+01$	$4.406E+00$	$4.957E+00$
5000	$1.961E+07$	$1.679E+01$	$4.519E+00$	$4.975E+00$
6000	$4.503E+07$	$1.762E+01$	$4.595E+00$	$4.977E+00$
7000	$9.182E+07$	$1.834E+01$	$4.648E+00$	$4.947E+00$
8000	$1.712E+08$	$1.896E+01$	$4.681E+00$	$4.875E+00$
9000	$2.975E+08$	$1.951E+01$	$4.697E+00$	$4.758E+00$
10000	$4.880E+08$	$2.001E+01$	$4.695E+00$	$4.605E+00$
11000	$7.629E+08$	$2.045E+01$	$4.679E+00$	$4.423E+00$
12000	$1.145E+09$	$2.086E+01$	$4.650E+00$	$4.224E+00$
13000	$1.658E+09$	$2.123E+01$	$4.609E+00$	$4.016E+00$
14000	$2.330E+09$	$2.157E+01$	$4.559E+00$	$3.807E+00$
15000	$3.185E+09$	$2.188E+01$	$4.502E+00$	$3.601E+00$
16000	$4.250E+09$	$2.217E+01$	$4.439E+00$	$3.400E+00$
17000	$5.551E+09$	$2.244E+01$	$4.373E+00$	$3.209E+00$
18000	$7.114E+09$	$2.269E+01$	$4.303E+00$	$3.026E+00$
19000	$8.960E+09$	$2.292E+01$	$4.231E+00$	$2.855E+00$
20000	$1.111E+10$	$2.313E+01$	$4.158E+00$	$2.693E+00$
21000	$1.359E+10$	$2.333E+01$	$4.085E+00$	$2.541E+00$
22000	$1.640E+10$	$2.352E+01$	$4.011E+00$	$2.400E+00$
23000	$1.957E+10$	$2.370E+01$	$3.938E+00$	$2.267E+00$
24000	$2.311E+10$	$2.386E+01$	$3.866E+00$	$2.144E+00$
25000	$2.702E+10$	$2.402E+01$	$3.795E+00$	$2.029E+00$
26000	$3.131E+10$	$2.417E+01$	$3.725E+00$	$1.922E+00$
27000	$3.599E+10$	$2.431E+01$	$3.656E+00$	$1.822E+00$
28000	$4.106E+10$	$2.444E+01$	$3.589E+00$	$1.729E+00$
29000	$4.652E+10$	$2.456E+01$	$3.523E+00$	$1.642E+00$
30000	$5.236E+10$	$2.468E+01$	$3.459E+00$	$1.560E+00$
32000	$6.520E+10$	$2.490E+01$	$3.336E+00$	$1.413E+00$
34000	$7.953E+10$	$2.510E+01$	$3.219E+00$	$1.285E+00$
36000	$9.530E+10$	$2.528E+01$	$3.108E+00$	$1.172E+00$
38000	$1.124E+11$	$2.545E+01$	$3.004E+00$	$1.072E+00$
40000	$1.308E+11$	$2.560E+01$	$2.905E+00$	$9.845E-01$
42000	$1.504E+11$	$2.574E+01$	$2.812E+00$	$9.064E-01$
44000	$1.711E+11$	$2.587E+01$	$2.723E+00$	$8.368E-01$
46000	$1.927E+11$	$2.598E+01$	$2.640E+00$	$7.746E-01$
48000	$2.153E+11$	$2.610E+01$	$2.561E+00$	$7.189E-01$
50000	$2.386E+11$	$2.620E+01$	$2.486E+00$	$6.687E-01$

Table 116: Total thermodynamic properties of CO_2^+

T [K]	C_p [J/mol/K]	S^0 [J/mol/K]	$H^0(T)-H^0(0)$ [KJ/mol]	$H^0(T)-H^0(298)$ [KJ/mol]	$-(G^0-H^0(0))/T$ [J/mol/K]	$-(G^0-H^0(298))/T$ [J/mol/K]	ΔH_f [KJ/mol]	$\mathrm{Log}(K_p)$
50	3.084E+01	1.710E+02	1.473E+00	-9.064E+00	1.416E+02	3.523E+02	5.243E+02	-5.513E+02
100	3.345E+01	1.934E+02	3.093E+00	-7.444E+00	1.624E+02	2.678E+02	5.248E+02	-2.773E+02
150	3.532E+01	2.073E+02	4.809E+00	-5.728E+00	1.752E+02	2.455E+02	5.253E+02	-1.859E+02
200	3.762E+01	2.178E+02	6.633E+00	-3.905E+00	1.846E+02	2.373E+02	5.258E+02	-1.402E+02
298.15	4.184E+01	2.336E+02	1.054E+01	0.000E+00	1.982E+02	2.336E+02	5.268E+02	-9.491E+01
300	4.192E+01	2.338E+02	1.062E+01	7.750E-02	1.984E+02	2.336E+02	5.268E+02	-9.434E+01
400	4.571E+01	2.464E+02	1.500E+01	4.463E+00	2.089E+02	2.353E+02	5.282E+02	-7.139E+01
500	4.895E+01	2.570E+02	1.974E+01	9.201E+00	2.175E+02	2.386E+02	5.300E+02	-5.757E+01
600	5.156E+01	2.661E+02	2.477E+01	1.423E+01	2.249E+02	2.424E+02	5.322E+02	-4.833E+01
700	5.360E+01	2.743E+02	3.003E+01	1.950E+01	2.313E+02	2.464E+02	5.345E+02	-4.169E+01
800	5.517E+01	2.815E+02	3.547E+01	2.494E+01	2.372E+02	2.503E+02	5.369E+02	-3.670E+01
900	5.639E+01	2.881E+02	4.105E+01	3.052E+01	2.425E+02	2.542E+02	5.394E+02	-3.280E+01
1000	5.735E+01	2.941E+02	4.674E+01	3.621E+01	2.473E+02	2.579E+02	5.419E+02	-2.966E+01
2000	6.094E+01	3.353E+02	1.064E+02	9.588E+01	2.821E+02	2.874E+02	5.671E+02	-1.525E+01
3000	6.171E+01	3.602E+02	1.678E+02	1.573E+02	3.043E+02	3.078E+02	5.904E+02	-1.022E+01
4000	6.200E+01	3.780E+02	2.297E+02	2.192E+02	3.206E+02	3.232E+02	6.113E+02	-7.611E+00
5000	6.216E+01	3.919E+02	2.918E+02	2.812E+02	3.335E+02	3.356E+02	6.304E+02	-5.991E+00
6000	6.216E+01	4.032E+02	3.540E+02	3.434E+02	3.442E+02	3.459E+02	6.481E+02	-4.878E+00
7000	6.192E+01	4.128E+02	4.160E+02	4.055E+02	3.533E+02	3.548E+02	6.646E+02	-4.063E+00
8000	6.132E+01	4.210E+02	4.777E+02	4.671E+02	3.613E+02	3.626E+02	6.804E+02	-3.436E+00
9000	6.035E+01	4.281E+02	5.385E+02	5.280E+02	3.683E+02	3.695E+02	6.960E+02	-2.937E+00
10000	5.907E+01	4.344E+02	5.983E+02	5.877E+02	3.746E+02	3.757E+02	7.120E+02	-2.528E+00
11000	5.756E+01	4.400E+02	6.566E+02	6.461E+02	3.803E+02	3.813E+02	7.286E+02	-2.186E+00
12000	5.591E+01	4.449E+02	7.133E+02	7.028E+02	3.855E+02	3.864E+02	7.458E+02	-1.895E+00
13000	5.418E+01	4.494E+02	7.684E+02	7.579E+02	3.902E+02	3.911E+02	7.637E+02	-1.642E+00
14000	5.244E+01	4.533E+02	8.217E+02	8.112E+02	3.946E+02	3.954E+02	7.821E+02	-1.420E+00
15000	5.072E+01	4.569E+02	8.733E+02	8.627E+02	3.986E+02	3.994E+02	8.009E+02	-1.224E+00
16000	4.906E+01	4.601E+02	9.232E+02	9.126E+02	4.024E+02	4.031E+02	8.200E+02	-1.047E+00
17000	4.747E+01	4.630E+02	9.714E+02	9.609E+02	4.059E+02	4.065E+02	8.391E+02	-8.880E-01
18000	4.595E+01	4.657E+02	1.018E+03	1.008E+03	4.091E+02	4.097E+02	8.582E+02	-7.432E-01
19000	4.452E+01	4.681E+02	1.063E+03	1.053E+03	4.122E+02	4.127E+02	8.773E+02	-6.107E-01
20000	4.318E+01	4.704E+02	1.107E+03	1.097E+03	4.150E+02	4.155E+02	8.961E+02	-4.888E-01
21000	4.192E+01	4.724E+02	1.150E+03	1.139E+03	4.177E+02	4.182E+02	9.147E+02	-3.762E-01
22000	4.074E+01	4.744E+02	1.191E+03	1.180E+03	4.202E+02	4.207E+02	9.331E+02	-2.718E-01
23000	3.964E+01	4.762E+02	1.231E+03	1.221E+03	4.226E+02	4.231E+02	9.512E+02	-1.745E-01
24000	3.861E+01	4.778E+02	1.270E+03	1.260E+03	4.249E+02	4.253E+02	9.690E+02	-8.368E-02
25000	3.766E+01	4.794E+02	1.308E+03	1.298E+03	4.270E+02	4.275E+02	9.865E+02	1.423E-03
26000	3.677E+01	4.808E+02	1.346E+03	1.335E+03	4.291E+02	4.295E+02	1.004E+03	8.138E-02
27000	3.593E+01	4.822E+02	1.382E+03	1.372E+03	4.310E+02	4.314E+02	1.020E+03	1.567E-01
28000	3.516E+01	4.835E+02	1.418E+03	1.407E+03	4.329E+02	4.333E+02	1.037E+03	2.278E-01
29000	3.444E+01	4.847E+02	1.452E+03	1.442E+03	4.346E+02	4.350E+02	1.053E+03	2.950E-01
30000	3.376E+01	4.859E+02	1.486E+03	1.476E+03	4.363E+02	4.367E+02	1.069E+03	3.587E-01
32000	3.254E+01	4.880E+02	1.553E+03	1.542E+03	4.395E+02	4.398E+02	1.101E+03	4.767E-01
34000	3.147E+01	4.900E+02	1.617E+03	1.606E+03	4.424E+02	4.427E+02	1.131E+03	5.838E-01
36000	3.053E+01	4.917E+02	1.679E+03	1.668E+03	4.451E+02	4.454E+02	1.160E+03	6.816E-01
38000	2.970E+01	4.934E+02	1.739E+03	1.728E+03	4.476E+02	4.479E+02	1.189E+03	7.712E-01
40000	2.897E+01	4.949E+02	1.798E+03	1.787E+03	4.499E+02	4.502E+02	1.217E+03	8.539E-01
42000	2.832E+01	4.963E+02	1.855E+03	1.844E+03	4.521E+02	4.524E+02	1.244E+03	9.304E-01
44000	2.774E+01	4.976E+02	1.911E+03	1.900E+03	4.541E+02	4.544E+02	1.271E+03	1.001E+00
46000	2.723E+01	4.988E+02	1.966E+03	1.955E+03	4.561E+02	4.563E+02	1.297E+03	1.068E+00
48000	2.676E+01	4.999E+02	2.020E+03	2.009E+03	4.579E+02	4.581E+02	1.322E+03	1.130E+00
50000	2.635E+01	5.010E+02	2.073E+03	2.062E+03	4.596E+02	4.598E+02	1.348E+03	1.188E+00

Table 117: Internal thermodynamic properties of e^-

T(K)	Q_{int}	$\ln(Q_{int})$	E_{int}/RT	$C_{p,int}/R$
50	$2.000E+00$	$6.931E-01$	$0.000E+00$	$0.000E+00$
100	$2.000E+00$	$6.931E-01$	$0.000E+00$	$0.000E+00$
150	$2.000E+00$	$6.931E-01$	$0.000E+00$	$0.000E+00$
200	$2.000E+00$	$6.931E-01$	$0.000E+00$	$0.000E+00$
298.15	$2.000E+00$	$6.931E-01$	$0.000E+00$	$0.000E+00$
300	$2.000E+00$	$6.931E-01$	$0.000E+00$	$0.000E+00$
400	$2.000E+00$	$6.931E-01$	$0.000E+00$	$0.000E+00$
500	$2.000E+00$	$6.931E-01$	$0.000E+00$	$0.000E+00$
600	$2.000E+00$	$6.931E-01$	$0.000E+00$	$0.000E+00$
700	$2.000E+00$	$6.931E-01$	$0.000E+00$	$0.000E+00$
800	$2.000E+00$	$6.931E-01$	$0.000E+00$	$0.000E+00$
900	$2.000E+00$	$6.931E-01$	$0.000E+00$	$0.000E+00$
1000	$2.000E+00$	$6.931E-01$	$0.000E+00$	$0.000E+00$
2000	$2.000E+00$	$6.931E-01$	$0.000E+00$	$0.000E+00$
3000	$2.000E+00$	$6.931E-01$	$0.000E+00$	$0.000E+00$
4000	$2.000E+00$	$6.931E-01$	$0.000E+00$	$0.000E+00$
5000	$2.000E+00$	$6.931E-01$	$0.000E+00$	$0.000E+00$
6000	$2.000E+00$	$6.931E-01$	$0.000E+00$	$0.000E+00$
7000	$2.000E+00$	$6.931E-01$	$0.000E+00$	$0.000E+00$
8000	$2.000E+00$	$6.931E-01$	$0.000E+00$	$0.000E+00$
9000	$2.000E+00$	$6.931E-01$	$0.000E+00$	$0.000E+00$
10000	$2.000E+00$	$6.931E-01$	$0.000E+00$	$0.000E+00$
11000	$2.000E+00$	$6.931E-01$	$0.000E+00$	$0.000E+00$
12000	$2.000E+00$	$6.931E-01$	$0.000E+00$	$0.000E+00$
13000	$2.000E+00$	$6.931E-01$	$0.000E+00$	$0.000E+00$
14000	$2.000E+00$	$6.931E-01$	$0.000E+00$	$0.000E+00$
15000	$2.000E+00$	$6.931E-01$	$0.000E+00$	$0.000E+00$
16000	$2.000E+00$	$6.931E-01$	$0.000E+00$	$0.000E+00$
17000	$2.000E+00$	$6.931E-01$	$0.000E+00$	$0.000E+00$
18000	$2.000E+00$	$6.931E-01$	$0.000E+00$	$0.000E+00$
19000	$2.000E+00$	$6.931E-01$	$0.000E+00$	$0.000E+00$
20000	$2.000E+00$	$6.931E-01$	$0.000E+00$	$0.000E+00$
21000	$2.000E+00$	$6.931E-01$	$0.000E+00$	$0.000E+00$
22000	$2.000E+00$	$6.931E-01$	$0.000E+00$	$0.000E+00$
23000	$2.000E+00$	$6.931E-01$	$0.000E+00$	$0.000E+00$
24000	$2.000E+00$	$6.931E-01$	$0.000E+00$	$0.000E+00$
25000	$2.000E+00$	$6.931E-01$	$0.000E+00$	$0.000E+00$
26000	$2.000E+00$	$6.931E-01$	$0.000E+00$	$0.000E+00$
27000	$2.000E+00$	$6.931E-01$	$0.000E+00$	$0.000E+00$
28000	$2.000E+00$	$6.931E-01$	$0.000E+00$	$0.000E+00$
29000	$2.000E+00$	$6.931E-01$	$0.000E+00$	$0.000E+00$
30000	$2.000E+00$	$6.931E-01$	$0.000E+00$	$0.000E+00$
32000	$2.000E+00$	$6.931E-01$	$0.000E+00$	$0.000E+00$
34000	$2.000E+00$	$6.931E-01$	$0.000E+00$	$0.000E+00$
36000	$2.000E+00$	$6.931E-01$	$0.000E+00$	$0.000E+00$
38000	$2.000E+00$	$6.931E-01$	$0.000E+00$	$0.000E+00$
40000	$2.000E+00$	$6.931E-01$	$0.000E+00$	$0.000E+00$
42000	$2.000E+00$	$6.931E-01$	$0.000E+00$	$0.000E+00$
44000	$2.000E+00$	$6.931E-01$	$0.000E+00$	$0.000E+00$
46000	$2.000E+00$	$6.931E-01$	$0.000E+00$	$0.000E+00$
48000	$2.000E+00$	$6.931E-01$	$0.000E+00$	$0.000E+00$
50000	$2.000E+00$	$6.931E-01$	$0.000E+00$	$0.000E+00$

Table 118: Total thermodynamic properties of e^-

T [K]	C_p [J/mol/K]	S^0 [J/mol/K]	$H^0(T)-H^0(0)$ [KJ/mol]	$H^0(T)-H^0(298)$ [KJ/mol]	$-(G^0-H^0(0))/T$ [J/mol/K]	$-(G^0-H^0(298))/T$ [J/mol/K]	ΔH_f [KJ/mol]	$\mathrm{Log}(K_p)$
50	2.079E+01	-1.614E+01	1.039E+00	-5.158E+00	-3.692E+01	8.703E+01	0.000E+00	0.000E+00
100	2.079E+01	-1.728E+00	2.079E+00	-4.119E+00	-2.252E+01	3.946E+01	0.000E+00	0.000E+00
150	2.079E+01	6.700E+00	3.118E+00	-3.079E+00	-1.409E+01	2.723E+01	0.000E+00	0.000E+00
200	2.079E+01	1.268E+01	4.157E+00	-2.040E+00	-8.107E+00	2.288E+01	0.000E+00	0.000E+00
298.15	2.079E+01	2.098E+01	6.197E+00	0.000E+00	1.928E-01	2.098E+01	0.000E+00	0.000E+00
300	2.079E+01	2.111E+01	6.236E+00	3.848E-02	3.213E-01	2.098E+01	0.000E+00	0.000E+00
400	2.079E+01	2.709E+01	8.315E+00	2.117E+00	6.301E+00	2.180E+01	0.000E+00	0.000E+00
500	2.079E+01	3.173E+01	1.039E+01	4.196E+00	1.094E+01	2.333E+01	0.000E+00	0.000E+00
600	2.079E+01	3.552E+01	1.247E+01	6.274E+00	1.473E+01	2.506E+01	0.000E+00	0.000E+00
700	2.079E+01	3.872E+01	1.455E+01	8.353E+00	1.793E+01	2.679E+01	0.000E+00	0.000E+00
800	2.079E+01	4.149E+01	1.663E+01	1.043E+01	2.071E+01	2.846E+01	0.000E+00	0.000E+00
900	2.079E+01	4.394E+01	1.871E+01	1.251E+01	2.316E+01	3.004E+01	0.000E+00	0.000E+00
1000	2.079E+01	4.613E+01	2.079E+01	1.459E+01	2.535E+01	3.155E+01	0.000E+00	0.000E+00
2000	2.079E+01	6.054E+01	4.157E+01	3.538E+01	3.976E+01	4.285E+01	0.000E+00	0.000E+00
3000	2.079E+01	6.897E+01	6.236E+01	5.616E+01	4.818E+01	5.025E+01	0.000E+00	0.000E+00
4000	2.079E+01	7.495E+01	8.314E+01	7.695E+01	5.416E+01	5.571E+01	0.000E+00	0.000E+00
5000	2.079E+01	7.959E+01	1.039E+02	9.773E+01	5.880E+01	6.004E+01	0.000E+00	0.000E+00
6000	2.079E+01	8.338E+01	1.247E+02	1.185E+02	6.259E+01	6.362E+01	0.000E+00	0.000E+00
7000	2.079E+01	8.658E+01	1.455E+02	1.393E+02	6.580E+01	6.668E+01	0.000E+00	0.000E+00
8000	2.079E+01	8.936E+01	1.663E+02	1.601E+02	6.857E+01	6.935E+01	0.000E+00	0.000E+00
9000	2.079E+01	9.181E+01	1.871E+02	1.809E+02	7.102E+01	7.171E+01	0.000E+00	0.000E+00
10000	2.079E+01	9.400E+01	2.079E+02	2.017E+02	7.321E+01	7.383E+01	0.000E+00	0.000E+00
11000	2.079E+01	9.598E+01	2.287E+02	2.224E+02	7.519E+01	7.575E+01	0.000E+00	0.000E+00
12000	2.079E+01	9.779E+01	2.494E+02	2.432E+02	7.700E+01	7.752E+01	0.000E+00	0.000E+00
13000	2.079E+01	9.945E+01	2.702E+02	2.640E+02	7.866E+01	7.914E+01	0.000E+00	0.000E+00
14000	2.079E+01	1.010E+02	2.910E+02	2.848E+02	8.020E+01	8.065E+01	0.000E+00	0.000E+00
15000	2.079E+01	1.024E+02	3.118E+02	3.056E+02	8.164E+01	8.205E+01	0.000E+00	0.000E+00
16000	2.079E+01	1.038E+02	3.326E+02	3.264E+02	8.298E+01	8.337E+01	0.000E+00	0.000E+00
17000	2.079E+01	1.050E+02	3.534E+02	3.472E+02	8.424E+01	8.460E+01	0.000E+00	0.000E+00
18000	2.079E+01	1.062E+02	3.741E+02	3.680E+02	8.543E+01	8.577E+01	0.000E+00	0.000E+00
19000	2.079E+01	1.073E+02	3.949E+02	3.887E+02	8.655E+01	8.688E+01	0.000E+00	0.000E+00
20000	2.079E+01	1.084E+02	4.157E+02	4.095E+02	8.762E+01	8.793E+01	0.000E+00	0.000E+00
21000	2.079E+01	1.094E+02	4.365E+02	4.303E+02	8.863E+01	8.893E+01	0.000E+00	0.000E+00
22000	2.079E+01	1.104E+02	4.573E+02	4.511E+02	8.960E+01	8.988E+01	0.000E+00	0.000E+00
23000	2.079E+01	1.113E+02	4.781E+02	4.719E+02	9.052E+01	9.079E+01	0.000E+00	0.000E+00
24000	2.079E+01	1.122E+02	4.989E+02	4.927E+02	9.141E+01	9.167E+01	0.000E+00	0.000E+00
25000	2.079E+01	1.130E+02	5.197E+02	5.135E+02	9.226E+01	9.250E+01	0.000E+00	0.000E+00
26000	2.079E+01	1.139E+02	5.404E+02	5.342E+02	9.307E+01	9.331E+01	0.000E+00	0.000E+00
27000	2.079E+01	1.146E+02	5.612E+02	5.550E+02	9.386E+01	9.408E+01	0.000E+00	0.000E+00
28000	2.079E+01	1.154E+02	5.820E+02	5.758E+02	9.461E+01	9.483E+01	0.000E+00	0.000E+00
29000	2.079E+01	1.161E+02	6.028E+02	5.966E+02	9.534E+01	9.555E+01	0.000E+00	0.000E+00
30000	2.079E+01	1.168E+02	6.236E+02	6.174E+02	9.605E+01	9.625E+01	0.000E+00	0.000E+00
32000	2.079E+01	1.182E+02	6.652E+02	6.590E+02	9.739E+01	9.758E+01	0.000E+00	0.000E+00
34000	2.079E+01	1.194E+02	7.067E+02	7.005E+02	9.865E+01	9.883E+01	0.000E+00	0.000E+00
36000	2.079E+01	1.206E+02	7.483E+02	7.421E+02	9.984E+01	1.000E+02	0.000E+00	0.000E+00
38000	2.079E+01	1.218E+02	7.899E+02	7.837E+02	1.010E+02	1.011E+02	0.000E+00	0.000E+00
40000	2.079E+01	1.228E+02	8.315E+02	8.252E+02	1.020E+02	1.022E+02	0.000E+00	0.000E+00
42000	2.079E+01	1.238E+02	8.730E+02	8.668E+02	1.030E+02	1.032E+02	0.000E+00	0.000E+00
44000	2.079E+01	1.248E+02	9.146E+02	9.084E+02	1.040E+02	1.042E+02	0.000E+00	0.000E+00
46000	2.079E+01	1.257E+02	9.562E+02	9.500E+02	1.049E+02	1.051E+02	0.000E+00	0.000E+00
48000	2.079E+01	1.266E+02	9.977E+02	9.915E+02	1.058E+02	1.059E+02	0.000E+00	0.000E+00
50000	2.079E+01	1.275E+02	1.039E+03	1.033E+03	1.067E+02	1.068E+02	0.000E+00	0.000E+00

Table 119: Internal thermodynamic properties of N ΔE=250 cm^{-1}

T(K)	Q_{int}	$\ln(Q_{int})$	E_{int}/RT	$C_{p,int}/R$
50	$4.000E+00$	$1.386E+00$	$7.081E-238$	$3.918E-235$
100	$4.000E+00$	$1.386E+00$	$4.948E-118$	$1.369E-115$
150	$4.000E+00$	$1.386E+00$	$3.688E-78$	$6.803E-76$
200	$4.000E+00$	$1.386E+00$	$2.925E-58$	$4.046E-56$
298.15	$4.000E+00$	$1.386E+00$	$1.171E-38$	$1.086E-36$
300	$4.000E+00$	$1.386E+00$	$2.062E-38$	$1.901E-36$
400	$4.000E+00$	$1.386E+00$	$1.590E-28$	$1.100E-26$
500	$4.000E+00$	$1.386E+00$	$1.294E-22$	$7.158E-21$
600	$4.000E+00$	$1.386E+00$	$1.090E-18$	$5.026E-17$
700	$4.000E+00$	$1.386E+00$	$6.779E-16$	$2.679E-14$
800	$4.000E+00$	$1.386E+00$	$8.291E-14$	$2.867E-12$
900	$4.000E+00$	$1.386E+00$	$3.437E-12$	$1.056E-10$
1000	$4.000E+00$	$1.386E+00$	$6.688E-11$	$1.850E-09$
2000	$4.000E+00$	$1.386E+00$	$3.404E-05$	$4.710E-04$
3000	$4.001E+00$	$1.387E+00$	$2.300E-03$	$2.130E-02$
4000	$4.010E+00$	$1.389E+00$	$1.759E-02$	$1.230E-01$
5000	$4.041E+00$	$1.397E+00$	$5.721E-02$	$3.217E-01$
6000	$4.105E+00$	$1.412E+00$	$1.217E-01$	$5.695E-01$
7000	$4.208E+00$	$1.437E+00$	$2.030E-01$	$8.058E-01$
8000	$4.348E+00$	$1.470E+00$	$2.907E-01$	$9.936E-01$
9000	$4.523E+00$	$1.509E+00$	$3.770E-01$	$1.139E+00$
10000	$4.726E+00$	$1.553E+00$	$4.612E-01$	$1.316E+00$
11000	$4.960E+00$	$1.601E+00$	$5.543E-01$	$1.712E+00$
12000	$5.232E+00$	$1.655E+00$	$6.845E-01$	$2.644E+00$
13000	$5.569E+00$	$1.717E+00$	$8.996E-01$	$4.501E+00$
14000	$6.025E+00$	$1.796E+00$	$1.258E+00$	$7.534E+00$
15000	$6.688E+00$	$1.900E+00$	$1.805E+00$	$1.149E+01$
16000	$7.685E+00$	$2.039E+00$	$2.537E+00$	$1.541E+01$
17000	$9.189E+00$	$2.218E+00$	$3.378E+00$	$1.795E+01$
18000	$1.142E+01$	$2.435E+00$	$4.208E+00$	$1.833E+01$
19000	$1.462E+01$	$2.682E+00$	$4.917E+00$	$1.677E+01$
20000	$1.908E+01$	$2.949E+00$	$5.447E+00$	$1.415E+01$
21000	$2.512E+01$	$3.224E+00$	$5.793E+00$	$1.131E+01$
22000	$3.305E+01$	$3.498E+00$	$5.985E+00$	$8.767E+00$
23000	$4.321E+01$	$3.766E+00$	$6.059E+00$	$6.690E+00$
24000	$5.592E+01$	$4.024E+00$	$6.050E+00$	$5.083E+00$
25000	$7.150E+01$	$4.270E+00$	$5.986E+00$	$3.872E+00$
26000	$9.026E+01$	$4.503E+00$	$5.886E+00$	$2.970E+00$
27000	$1.125E+02$	$4.723E+00$	$5.765E+00$	$2.298E+00$
28000	$1.384E+02$	$4.930E+00$	$5.632E+00$	$1.796E+00$
29000	$1.682E+02$	$5.125E+00$	$5.493E+00$	$1.419E+00$
30000	$2.021E+02$	$5.309E+00$	$5.352E+00$	$1.134E+00$
32000	$2.830E+02$	$5.646E+00$	$5.075E+00$	$7.455E-01$
34000	$3.819E+02$	$5.945E+00$	$4.813E+00$	$5.093E-01$
36000	$4.994E+02$	$6.213E+00$	$4.570E+00$	$3.599E-01$
38000	$6.355E+02$	$6.454E+00$	$4.345E+00$	$2.620E-01$
40000	$7.899E+02$	$6.672E+00$	$4.139E+00$	$1.958E-01$
42000	$9.622E+02$	$6.869E+00$	$3.950E+00$	$1.497E-01$
44000	$1.152E+03$	$7.049E+00$	$3.777E+00$	$1.168E-01$
46000	$1.357E+03$	$7.213E+00$	$3.617E+00$	$9.280E-02$
48000	$1.578E+03$	$7.364E+00$	$3.470E+00$	$7.490E-02$
50000	$1.813E+03$	$7.503E+00$	$3.334E+00$	$6.132E-02$

Table 120: Total thermodynamic properties of N ΔE=250 cm^{-1}

T [K]	C_p [J/mol/K]	S^0 [J/mol/K]	$H^0(T)-H^0(0)$ [KJ/mol]	$H^0(T)-H^0(298)$ [KJ/mol]	$-(G^0-H^0(0))/T$ [J/mol/K]	$-(G^0-H^0(298))/T$ [J/mol/K]	ΔH_f [KJ/mol]	$\mathrm{Log}(K_p)$
50	2.079E+01	1.162E+02	1.039E+00	-5.158E+00	9.540E+01	2.193E+02	4.711E+02	-4.897E+02
100	2.079E+01	1.306E+02	2.079E+00	-4.119E+00	1.098E+02	1.718E+02	4.714E+02	-2.436E+02
150	2.079E+01	1.390E+02	3.118E+00	-3.079E+00	1.182E+02	1.596E+02	4.717E+02	-1.615E+02
200	2.079E+01	1.450E+02	4.157E+00	-2.040E+00	1.242E+02	1.552E+02	4.720E+02	-1.204E+02
298.15	2.079E+01	1.533E+02	6.197E+00	0.000E+00	1.325E+02	1.533E+02	4.726E+02	-7.980E+01
300	2.079E+01	1.534E+02	6.236E+00	3.848E-02	1.327E+02	1.533E+02	4.727E+02	-7.929E+01
400	2.079E+01	1.594E+02	8.315E+00	2.117E+00	1.386E+02	1.541E+02	4.733E+02	-5.870E+01
500	2.079E+01	1.641E+02	1.039E+01	4.196E+00	1.433E+02	1.557E+02	4.739E+02	-4.634E+01
600	2.079E+01	1.678E+02	1.247E+01	6.274E+00	1.471E+02	1.574E+02	4.745E+02	-3.808E+01
700	2.079E+01	1.710E+02	1.455E+01	8.353E+00	1.503E+02	1.591E+02	4.750E+02	-3.218E+01
800	2.079E+01	1.738E+02	1.663E+01	1.043E+01	1.530E+02	1.608E+02	4.756E+02	-2.774E+01
900	2.079E+01	1.763E+02	1.871E+01	1.251E+01	1.555E+02	1.624E+02	4.761E+02	-2.429E+01
1000	2.079E+01	1.785E+02	2.079E+01	1.459E+01	1.577E+02	1.639E+02	4.765E+02	-2.153E+01
2000	2.079E+01	1.929E+02	4.157E+01	3.538E+01	1.721E+02	1.752E+02	4.799E+02	-9.044E+00
3000	2.096E+01	2.013E+02	6.242E+01	5.622E+01	1.805E+02	1.826E+02	4.825E+02	-4.856E+00
4000	2.181E+01	2.074E+02	8.373E+01	7.753E+01	1.865E+02	1.881E+02	4.852E+02	-2.751E+00
5000	2.346E+01	2.125E+02	1.063E+02	1.001E+02	1.912E+02	1.924E+02	4.889E+02	-1.480E+00
6000	2.552E+01	2.169E+02	1.308E+02	1.246E+02	1.951E+02	1.962E+02	4.943E+02	-6.242E-01
7000	2.749E+01	2.210E+02	1.573E+02	1.511E+02	1.985E+02	1.994E+02	5.016E+02	-5.416E-03
8000	2.905E+01	2.248E+02	1.856E+02	1.794E+02	2.016E+02	2.024E+02	5.102E+02	4.662E-01
9000	3.025E+01	2.283E+02	2.153E+02	2.091E+02	2.044E+02	2.051E+02	5.194E+02	8.395E-01
10000	3.173E+01	2.315E+02	2.462E+02	2.400E+02	2.069E+02	2.075E+02	5.285E+02	1.143E+00
11000	3.502E+01	2.347E+02	2.793E+02	2.731E+02	2.093E+02	2.099E+02	5.381E+02	1.397E+00
12000	4.277E+01	2.380E+02	3.177E+02	3.115E+02	2.116E+02	2.121E+02	5.507E+02	1.612E+00
13000	5.821E+01	2.420E+02	3.674E+02	3.613E+02	2.137E+02	2.142E+02	5.722E+02	1.799E+00
14000	8.342E+01	2.472E+02	4.375E+02	4.313E+02	2.159E+02	2.164E+02	6.117E+02	1.968E+00
15000	1.163E+02	2.540E+02	5.370E+02	5.308E+02	2.182E+02	2.187E+02	6.789E+02	2.128E+00
16000	1.489E+02	2.626E+02	6.700E+02	6.639E+02	2.207E+02	2.211E+02	7.785E+02	2.286E+00
17000	1.700E+02	2.724E+02	8.308E+02	8.246E+02	2.235E+02	2.238E+02	9.055E+02	2.447E+00
18000	1.732E+02	2.822E+02	1.004E+03	9.978E+02	2.265E+02	2.268E+02	1.045E+03	2.613E+00
19000	1.602E+02	2.913E+02	1.172E+03	1.166E+03	2.297E+02	2.300E+02	1.180E+03	2.783E+00
20000	1.384E+02	2.990E+02	1.322E+03	1.315E+03	2.329E+02	2.332E+02	1.299E+03	2.954E+00
21000	1.149E+02	3.052E+02	1.448E+03	1.442E+03	2.362E+02	2.365E+02	1.396E+03	3.121E+00
22000	9.368E+01	3.100E+02	1.552E+03	1.546E+03	2.395E+02	2.398E+02	1.471E+03	3.284E+00
23000	7.641E+01	3.138E+02	1.637E+03	1.630E+03	2.426E+02	2.429E+02	1.529E+03	3.438E+00
24000	6.305E+01	3.168E+02	1.706E+03	1.700E+03	2.457E+02	2.459E+02	1.574E+03	3.585E+00
25000	5.298E+01	3.191E+02	1.764E+03	1.758E+03	2.486E+02	2.488E+02	1.608E+03	3.724E+00
26000	4.548E+01	3.210E+02	1.813E+03	1.807E+03	2.513E+02	2.515E+02	1.634E+03	3.854E+00
27000	3.989E+01	3.226E+02	1.856E+03	1.849E+03	2.539E+02	2.542E+02	1.656E+03	3.977E+00
28000	3.572E+01	3.240E+02	1.893E+03	1.887E+03	2.564E+02	2.566E+02	1.673E+03	4.092E+00
29000	3.259E+01	3.252E+02	1.927E+03	1.921E+03	2.588E+02	2.590E+02	1.688E+03	4.200E+00
30000	3.021E+01	3.263E+02	1.959E+03	1.952E+03	2.610E+02	2.612E+02	1.701E+03	4.301E+00
32000	2.698E+01	3.281E+02	2.016E+03	2.009E+03	2.651E+02	2.653E+02	1.723E+03	4.488E+00
34000	2.502E+01	3.297E+02	2.067E+03	2.061E+03	2.689E+02	2.691E+02	1.743E+03	4.654E+00
36000	2.378E+01	3.311E+02	2.116E+03	2.110E+03	2.723E+02	2.725E+02	1.761E+03	4.804E+00
38000	2.296E+01	3.323E+02	2.163E+03	2.157E+03	2.754E+02	2.756E+02	1.778E+03	4.939E+00
40000	2.241E+01	3.335E+02	2.208E+03	2.202E+03	2.783E+02	2.784E+02	1.796E+03	5.062E+00
42000	2.203E+01	3.346E+02	2.253E+03	2.246E+03	2.809E+02	2.811E+02	1.813E+03	5.174E+00
44000	2.176E+01	3.356E+02	2.296E+03	2.290E+03	2.834E+02	2.836E+02	1.831E+03	5.277E+00
46000	2.156E+01	3.366E+02	2.340E+03	2.334E+03	2.857E+02	2.858E+02	1.848E+03	5.372E+00
48000	2.141E+01	3.375E+02	2.383E+03	2.376E+03	2.878E+02	2.880E+02	1.866E+03	5.460E+00
50000	2.130E+01	3.384E+02	2.425E+03	2.419E+03	2.898E+02	2.900E+02	1.884E+03	5.541E+00

Table 121: Internal thermodynamic properties of N ΔE=500 cm^{-1}

T(K)	Q_{int}	$\ln(Q_{int})$	E_{int}/RT	$C_{p,int}/R$
50	$4.000E+00$	$1.386E+00$	$7.081E-238$	$3.918E-235$
100	$4.000E+00$	$1.386E+00$	$4.948E-118$	$1.369E-115$
150	$4.000E+00$	$1.386E+00$	$3.688E-78$	$6.803E-76$
200	$4.000E+00$	$1.386E+00$	$2.925E-58$	$4.046E-56$
298.15	$4.000E+00$	$1.386E+00$	$1.171E-38$	$1.086E-36$
300	$4.000E+00$	$1.386E+00$	$2.062E-38$	$1.901E-36$
400	$4.000E+00$	$1.386E+00$	$1.590E-28$	$1.100E-26$
500	$4.000E+00$	$1.386E+00$	$1.294E-22$	$7.158E-21$
600	$4.000E+00$	$1.386E+00$	$1.090E-18$	$5.026E-17$
700	$4.000E+00$	$1.386E+00$	$6.779E-16$	$2.679E-14$
800	$4.000E+00$	$1.386E+00$	$8.291E-14$	$2.867E-12$
900	$4.000E+00$	$1.386E+00$	$3.437E-12$	$1.056E-10$
1000	$4.000E+00$	$1.386E+00$	$6.688E-11$	$1.850E-09$
2000	$4.000E+00$	$1.386E+00$	$3.404E-05$	$4.710E-04$
3000	$4.001E+00$	$1.387E+00$	$2.300E-03$	$2.130E-02$
4000	$4.010E+00$	$1.389E+00$	$1.759E-02$	$1.230E-01$
5000	$4.041E+00$	$1.397E+00$	$5.721E-02$	$3.217E-01$
6000	$4.105E+00$	$1.412E+00$	$1.217E-01$	$5.695E-01$
7000	$4.208E+00$	$1.437E+00$	$2.030E-01$	$8.057E-01$
8000	$4.348E+00$	$1.470E+00$	$2.905E-01$	$9.912E-01$
9000	$4.522E+00$	$1.509E+00$	$3.760E-01$	$1.120E+00$
10000	$4.725E+00$	$1.553E+00$	$4.556E-01$	$1.225E+00$
11000	$4.952E+00$	$1.600E+00$	$5.319E-01$	$1.385E+00$
12000	$5.205E+00$	$1.650E+00$	$6.156E-01$	$1.734E+00$
13000	$5.490E+00$	$1.703E+00$	$7.261E-01$	$2.445E+00$
14000	$5.826E+00$	$1.762E+00$	$8.898E-01$	$3.690E+00$
15000	$6.244E+00$	$1.832E+00$	$1.135E+00$	$5.550E+00$
16000	$6.789E+00$	$1.915E+00$	$1.483E+00$	$7.915E+00$
17000	$7.526E+00$	$2.018E+00$	$1.936E+00$	$1.043E+01$
18000	$8.532E+00$	$2.144E+00$	$2.470E+00$	$1.255E+01$
19000	$9.900E+00$	$2.293E+00$	$3.038E+00$	$1.382E+01$
20000	$1.173E+01$	$2.462E+00$	$3.587E+00$	$1.403E+01$
21000	$1.415E+01$	$2.650E+00$	$4.069E+00$	$1.328E+01$
22000	$1.726E+01$	$2.848E+00$	$4.459E+00$	$1.192E+01$
23000	$2.118E+01$	$3.053E+00$	$4.748E+00$	$1.028E+01$
24000	$2.604E+01$	$3.260E+00$	$4.944E+00$	$8.626E+00$
25000	$3.195E+01$	$3.464E+00$	$5.060E+00$	$7.118E+00$
26000	$3.901E+01$	$3.664E+00$	$5.114E+00$	$5.820E+00$
27000	$4.732E+01$	$3.857E+00$	$5.119E+00$	$4.740E+00$
28000	$5.698E+01$	$4.043E+00$	$5.089E+00$	$3.861E+00$
29000	$6.806E+01$	$4.220E+00$	$5.034E+00$	$3.154E+00$
30000	$8.064E+01$	$4.390E+00$	$4.962E+00$	$2.588E+00$
32000	$1.105E+02$	$4.705E+00$	$4.786E+00$	$1.773E+00$
34000	$1.468E+02$	$4.989E+00$	$4.592E+00$	$1.246E+00$
36000	$1.898E+02$	$5.246E+00$	$4.396E+00$	$8.983E-01$
38000	$2.395E+02$	$5.479E+00$	$4.206E+00$	$6.638E-01$
40000	$2.958E+02$	$5.690E+00$	$4.024E+00$	$5.016E-01$
42000	$3.585E+02$	$5.882E+00$	$3.854E+00$	$3.869E-01$
44000	$4.272E+02$	$6.057E+00$	$3.694E+00$	$3.040E-01$
46000	$5.018E+02$	$6.218E+00$	$3.545E+00$	$2.428E-01$
48000	$5.818E+02$	$6.366E+00$	$3.407E+00$	$1.968E-01$
50000	$6.669E+02$	$6.503E+00$	$3.277E+00$	$1.617E-01$

Table 122: Total thermodynamic properties of N ΔE=500 cm^{-1}

T [K]	C_p [J/mol/K]	S^0 [J/mol/K]	$H^0(T)-H^0(0)$ [KJ/mol]	$H^0(T)-H^0(298)$ [KJ/mol]	$-(G^0-H^0(0))/T$ [J/mol/K]	$-(G^0-H^0(298))/T$ [J/mol/K]	ΔH_f [KJ/mol]	$\mathrm{Log}(K_p)$
50	2.079E+01	1.162E+02	1.039E+00	-5.158E+00	9.540E+01	2.193E+02	4.711E+02	-4.897E+02
100	2.079E+01	1.306E+02	2.079E+00	-4.119E+00	1.098E+02	1.718E+02	4.714E+02	-2.436E+02
150	2.079E+01	1.390E+02	3.118E+00	-3.079E+00	1.182E+02	1.596E+02	4.717E+02	-1.615E+02
200	2.079E+01	1.450E+02	4.157E+00	-2.040E+00	1.242E+02	1.552E+02	4.720E+02	-1.204E+02
298.15	2.079E+01	1.533E+02	6.197E+00	0.000E+00	1.325E+02	1.533E+02	4.726E+02	-7.980E+01
300	2.079E+01	1.534E+02	6.236E+00	3.848E-02	1.327E+02	1.533E+02	4.727E+02	-7.929E+01
400	2.079E+01	1.594E+02	8.315E+00	2.117E+00	1.386E+02	1.541E+02	4.733E+02	-5.870E+01
500	2.079E+01	1.641E+02	1.039E+01	4.196E+00	1.433E+02	1.557E+02	4.739E+02	-4.634E+01
600	2.079E+01	1.678E+02	1.247E+01	6.274E+00	1.471E+02	1.574E+02	4.745E+02	-3.808E+01
700	2.079E+01	1.710E+02	1.455E+01	8.353E+00	1.503E+02	1.591E+02	4.750E+02	-3.218E+01
800	2.079E+01	1.738E+02	1.663E+01	1.043E+01	1.530E+02	1.608E+02	4.756E+02	-2.774E+01
900	2.079E+01	1.763E+02	1.871E+01	1.251E+01	1.555E+02	1.624E+02	4.761E+02	-2.429E+01
1000	2.079E+01	1.785E+02	2.079E+01	1.459E+01	1.577E+02	1.639E+02	4.765E+02	-2.153E+01
2000	2.079E+01	1.929E+02	4.157E+01	3.538E+01	1.721E+02	1.752E+02	4.799E+02	-9.044E+00
3000	2.096E+01	2.013E+02	6.242E+01	5.622E+01	1.805E+02	1.826E+02	4.825E+02	-4.856E+00
4000	2.181E+01	2.074E+02	8.373E+01	7.753E+01	1.865E+02	1.881E+02	4.852E+02	-2.751E+00
5000	2.346E+01	2.125E+02	1.063E+02	1.001E+02	1.912E+02	1.924E+02	4.889E+02	-1.480E+00
6000	2.552E+01	2.169E+02	1.308E+02	1.246E+02	1.951E+02	1.962E+02	4.943E+02	-6.242E-01
7000	2.748E+01	2.210E+02	1.573E+02	1.511E+02	1.985E+02	1.994E+02	5.015E+02	-5.417E-03
8000	2.903E+01	2.248E+02	1.856E+02	1.794E+02	2.016E+02	2.024E+02	5.101E+02	4.662E-01
9000	3.010E+01	2.283E+02	2.152E+02	2.090E+02	2.044E+02	2.051E+02	5.193E+02	8.394E-01
10000	3.097E+01	2.315E+02	2.457E+02	2.395E+02	2.069E+02	2.075E+02	5.281E+02	1.143E+00
11000	3.230E+01	2.345E+02	2.773E+02	2.711E+02	2.093E+02	2.098E+02	5.361E+02	1.396E+00
12000	3.520E+01	2.374E+02	3.109E+02	3.047E+02	2.115E+02	2.120E+02	5.439E+02	1.609E+00
13000	4.112E+01	2.404E+02	3.487E+02	3.425E+02	2.136E+02	2.141E+02	5.535E+02	1.793E+00
14000	5.147E+01	2.438E+02	3.946E+02	3.884E+02	2.157E+02	2.161E+02	5.688E+02	1.954E+00
15000	6.693E+01	2.479E+02	4.534E+02	4.472E+02	2.177E+02	2.181E+02	5.953E+02	2.098E+00
16000	8.659E+01	2.528E+02	5.299E+02	5.237E+02	2.197E+02	2.201E+02	6.384E+02	2.232E+00
17000	1.075E+02	2.587E+02	6.270E+02	6.208E+02	2.218E+02	2.222E+02	7.017E+02	2.360E+00
18000	1.252E+02	2.654E+02	7.437E+02	7.375E+02	2.241E+02	2.244E+02	7.850E+02	2.487E+00
19000	1.357E+02	2.725E+02	8.749E+02	8.687E+02	2.264E+02	2.267E+02	8.835E+02	2.614E+00
20000	1.374E+02	2.795E+02	1.012E+03	1.006E+03	2.289E+02	2.292E+02	9.895E+02	2.743E+00
21000	1.312E+02	2.861E+02	1.147E+03	1.141E+03	2.315E+02	2.318E+02	1.095E+03	2.872E+00
22000	1.199E+02	2.919E+02	1.273E+03	1.267E+03	2.341E+02	2.344E+02	1.192E+03	3.001E+00
23000	1.062E+02	2.970E+02	1.386E+03	1.380E+03	2.367E+02	2.370E+02	1.279E+03	3.129E+00
24000	9.251E+01	3.012E+02	1.485E+03	1.479E+03	2.393E+02	2.396E+02	1.353E+03	3.253E+00
25000	7.997E+01	3.047E+02	1.572E+03	1.565E+03	2.418E+02	2.421E+02	1.415E+03	3.374E+00
26000	6.917E+01	3.076E+02	1.646E+03	1.640E+03	2.443E+02	2.446E+02	1.467E+03	3.490E+00
27000	6.020E+01	3.101E+02	1.710E+03	1.704E+03	2.467E+02	2.469E+02	1.511E+03	3.601E+00
28000	5.289E+01	3.121E+02	1.767E+03	1.761E+03	2.490E+02	2.492E+02	1.547E+03	3.706E+00
29000	4.701E+01	3.139E+02	1.817E+03	1.810E+03	2.512E+02	2.514E+02	1.578E+03	3.807E+00
30000	4.231E+01	3.154E+02	1.861E+03	1.855E+03	2.533E+02	2.536E+02	1.604E+03	3.902E+00
32000	3.553E+01	3.179E+02	1.939E+03	1.932E+03	2.573E+02	2.575E+02	1.646E+03	4.079E+00
34000	3.114E+01	3.199E+02	2.005E+03	1.999E+03	2.609E+02	2.611E+02	1.680E+03	4.239E+00
36000	2.825E+01	3.216E+02	2.064E+03	2.058E+03	2.642E+02	2.644E+02	1.709E+03	4.383E+00
38000	2.630E+01	3.231E+02	2.119E+03	2.112E+03	2.673E+02	2.675E+02	1.734E+03	4.515E+00
40000	2.496E+01	3.244E+02	2.170E+03	2.164E+03	2.701E+02	2.703E+02	1.757E+03	4.635E+00
42000	2.400E+01	3.256E+02	2.219E+03	2.212E+03	2.727E+02	2.729E+02	1.779E+03	4.745E+00
44000	2.331E+01	3.267E+02	2.266E+03	2.260E+03	2.752E+02	2.753E+02	1.800E+03	4.846E+00
46000	2.280E+01	3.277E+02	2.312E+03	2.306E+03	2.774E+02	2.776E+02	1.821E+03	4.939E+00
48000	2.242E+01	3.286E+02	2.357E+03	2.351E+03	2.795E+02	2.797E+02	1.841E+03	5.026E+00
50000	2.213E+01	3.296E+02	2.402E+03	2.396E+03	2.815E+02	2.816E+02	1.861E+03	5.107E+00

Table 123: Internal thermodynamic properties of N ΔE=1000 cm^{-1}

T(K)	Q_{int}	$\ln(Q_{int})$	E_{int}/RT	$C_{p,int}/R$
50	$4.000E+00$	$1.386E+00$	$7.081E-238$	$3.918E-235$
100	$4.000E+00$	$1.386E+00$	$4.948E-118$	$1.369E-115$
150	$4.000E+00$	$1.386E+00$	$3.688E-78$	$6.803E-76$
200	$4.000E+00$	$1.386E+00$	$2.925E-58$	$4.046E-56$
298.15	$4.000E+00$	$1.386E+00$	$1.171E-38$	$1.086E-36$
300	$4.000E+00$	$1.386E+00$	$2.062E-38$	$1.901E-36$
400	$4.000E+00$	$1.386E+00$	$1.590E-28$	$1.100E-26$
500	$4.000E+00$	$1.386E+00$	$1.294E-22$	$7.158E-21$
600	$4.000E+00$	$1.386E+00$	$1.090E-18$	$5.026E-17$
700	$4.000E+00$	$1.386E+00$	$6.779E-16$	$2.679E-14$
800	$4.000E+00$	$1.386E+00$	$8.291E-14$	$2.867E-12$
900	$4.000E+00$	$1.386E+00$	$3.437E-12$	$1.056E-10$
1000	$4.000E+00$	$1.386E+00$	$6.688E-11$	$1.850E-09$
2000	$4.000E+00$	$1.386E+00$	$3.404E-05$	$4.710E-04$
3000	$4.001E+00$	$1.387E+00$	$2.300E-03$	$2.130E-02$
4000	$4.010E+00$	$1.389E+00$	$1.759E-02$	$1.230E-01$
5000	$4.041E+00$	$1.397E+00$	$5.721E-02$	$3.217E-01$
6000	$4.105E+00$	$1.412E+00$	$1.217E-01$	$5.695E-01$
7000	$4.208E+00$	$1.437E+00$	$2.030E-01$	$8.056E-01$
8000	$4.348E+00$	$1.470E+00$	$2.905E-01$	$9.903E-01$
9000	$4.522E+00$	$1.509E+00$	$3.756E-01$	$1.113E+00$
10000	$4.724E+00$	$1.553E+00$	$4.536E-01$	$1.192E+00$
11000	$4.949E+00$	$1.599E+00$	$5.239E-01$	$1.268E+00$
12000	$5.195E+00$	$1.648E+00$	$5.909E-01$	$1.406E+00$
13000	$5.462E+00$	$1.698E+00$	$6.633E-01$	$1.689E+00$
14000	$5.755E+00$	$1.750E+00$	$7.533E-01$	$2.202E+00$
15000	$6.086E+00$	$1.806E+00$	$8.751E-01$	$3.011E+00$
16000	$6.472E+00$	$1.868E+00$	$1.042E+00$	$4.136E+00$
17000	$6.939E+00$	$1.937E+00$	$1.264E+00$	$5.522E+00$
18000	$7.515E+00$	$2.017E+00$	$1.542E+00$	$7.034E+00$
19000	$8.239E+00$	$2.109E+00$	$1.870E+00$	$8.471E+00$
20000	$9.151E+00$	$2.214E+00$	$2.230E+00$	$9.625E+00$
21000	$1.030E+01$	$2.332E+00$	$2.601E+00$	$1.034E+01$
22000	$1.172E+01$	$2.461E+00$	$2.960E+00$	$1.055E+01$
23000	$1.346E+01$	$2.600E+00$	$3.286E+00$	$1.030E+01$
24000	$1.558E+01$	$2.746E+00$	$3.567E+00$	$9.699E+00$
25000	$1.811E+01$	$2.896E+00$	$3.796E+00$	$8.868E+00$
26000	$2.109E+01$	$3.049E+00$	$3.973E+00$	$7.931E+00$
27000	$2.457E+01$	$3.201E+00$	$4.102E+00$	$6.980E+00$
28000	$2.857E+01$	$3.352E+00$	$4.189E+00$	$6.075E+00$
29000	$3.312E+01$	$3.500E+00$	$4.239E+00$	$5.249E+00$
30000	$3.826E+01$	$3.644E+00$	$4.260E+00$	$4.518E+00$
32000	$5.035E+01$	$3.919E+00$	$4.238E+00$	$3.337E+00$
34000	$6.496E+01$	$4.174E+00$	$4.158E+00$	$2.477E+00$
36000	$8.214E+01$	$4.408E+00$	$4.047E+00$	$1.860E+00$
38000	$1.019E+02$	$4.624E+00$	$3.919E+00$	$1.418E+00$
40000	$1.241E+02$	$4.821E+00$	$3.786E+00$	$1.097E+00$
42000	$1.488E+02$	$5.003E+00$	$3.652E+00$	$8.621E-01$
44000	$1.759E+02$	$5.170E+00$	$3.521E+00$	$6.874E-01$
46000	$2.051E+02$	$5.323E+00$	$3.395E+00$	$5.557E-01$
48000	$2.364E+02$	$5.465E+00$	$3.274E+00$	$4.549E-01$
50000	$2.695E+02$	$5.597E+00$	$3.160E+00$	$3.768E-01$

Table 124: Total thermodynamic properties of N ΔE=1000 cm^{-1}

T [K]	C_p [J/mol/K]	S^0 [J/mol/K]	$H^0(T)-H^0(0)$ [KJ/mol]	$H^0(T)-H^0(298)$ [KJ/mol]	$-(G^0-H^0(0))/T$ [J/mol/K]	$-(G^0-H^0(298))/T$ [J/mol/K]	ΔH_f [KJ/mol]	$\mathrm{Log}(K_p)$
50	2.079E+01	1.162E+02	1.039E+00	-5.158E+00	9.540E+01	2.193E+02	4.711E+02	-4.897E+02
100	2.079E+01	1.306E+02	2.079E+00	-4.119E+00	1.098E+02	1.718E+02	4.714E+02	-2.436E+02
150	2.079E+01	1.390E+02	3.118E+00	-3.079E+00	1.182E+02	1.596E+02	4.717E+02	-1.615E+02
200	2.079E+01	1.450E+02	4.157E+00	-2.040E+00	1.242E+02	1.552E+02	4.720E+02	-1.204E+02
298.15	2.079E+01	1.533E+02	6.197E+00	0.000E+00	1.325E+02	1.533E+02	4.726E+02	-7.980E+01
300	2.079E+01	1.534E+02	6.236E+00	3.848E-02	1.327E+02	1.533E+02	4.727E+02	-7.929E+01
400	2.079E+01	1.594E+02	8.315E+00	2.117E+00	1.386E+02	1.541E+02	4.733E+02	-5.870E+01
500	2.079E+01	1.641E+02	1.039E+01	4.196E+00	1.433E+02	1.557E+02	4.739E+02	-4.634E+01
600	2.079E+01	1.678E+02	1.247E+01	6.274E+00	1.471E+02	1.574E+02	4.745E+02	-3.808E+01
700	2.079E+01	1.710E+02	1.455E+01	8.353E+00	1.503E+02	1.591E+02	4.750E+02	-3.218E+01
800	2.079E+01	1.738E+02	1.663E+01	1.043E+01	1.530E+02	1.608E+02	4.756E+02	-2.774E+01
900	2.079E+01	1.763E+02	1.871E+01	1.251E+01	1.555E+02	1.624E+02	4.761E+02	-2.429E+01
1000	2.079E+01	1.785E+02	2.079E+01	1.459E+01	1.577E+02	1.639E+02	4.765E+02	-2.153E+01
2000	2.079E+01	1.929E+02	4.157E+01	3.538E+01	1.721E+02	1.752E+02	4.799E+02	-9.044E+00
3000	2.096E+01	2.013E+02	6.242E+01	5.622E+01	1.805E+02	1.826E+02	4.825E+02	-4.856E+00
4000	2.181E+01	2.074E+02	8.373E+01	7.753E+01	1.865E+02	1.881E+02	4.852E+02	-2.751E+00
5000	2.346E+01	2.125E+02	1.063E+02	1.001E+02	1.912E+02	1.924E+02	4.889E+02	-1.480E+00
6000	2.552E+01	2.169E+02	1.308E+02	1.246E+02	1.951E+02	1.962E+02	4.943E+02	-6.242E-01
7000	2.748E+01	2.210E+02	1.573E+02	1.511E+02	1.985E+02	1.994E+02	5.015E+02	-5.417E-03
8000	2.902E+01	2.248E+02	1.856E+02	1.794E+02	2.016E+02	2.024E+02	5.101E+02	4.662E-01
9000	3.004E+01	2.283E+02	2.152E+02	2.090E+02	2.044E+02	2.051E+02	5.192E+02	8.394E-01
10000	3.069E+01	2.315E+02	2.456E+02	2.394E+02	2.069E+02	2.075E+02	5.279E+02	1.143E+00
11000	3.132E+01	2.344E+02	2.766E+02	2.704E+02	2.093E+02	2.098E+02	5.354E+02	1.396E+00
12000	3.248E+01	2.372E+02	3.084E+02	3.022E+02	2.115E+02	2.120E+02	5.414E+02	1.609E+00
13000	3.483E+01	2.399E+02	3.419E+02	3.357E+02	2.136E+02	2.141E+02	5.467E+02	1.791E+00
14000	3.909E+01	2.426E+02	3.787E+02	3.725E+02	2.156E+02	2.160E+02	5.529E+02	1.949E+00
15000	4.582E+01	2.455E+02	4.209E+02	4.147E+02	2.174E+02	2.179E+02	5.629E+02	2.087E+00
16000	5.517E+01	2.488E+02	4.712E+02	4.650E+02	2.193E+02	2.197E+02	5.797E+02	2.211E+00
17000	6.670E+01	2.524E+02	5.320E+02	5.258E+02	2.211E+02	2.215E+02	6.067E+02	2.325E+00
18000	7.927E+01	2.566E+02	6.050E+02	5.988E+02	2.230E+02	2.233E+02	6.462E+02	2.432E+00
19000	9.122E+01	2.612E+02	6.904E+02	6.841E+02	2.249E+02	2.252E+02	6.990E+02	2.534E+00
20000	1.008E+02	2.661E+02	7.866E+02	7.804E+02	2.268E+02	2.271E+02	7.639E+02	2.635E+00
21000	1.068E+02	2.712E+02	8.907E+02	8.845E+02	2.288E+02	2.291E+02	8.382E+02	2.734E+00
22000	1.085E+02	2.763E+02	9.987E+02	9.925E+02	2.309E+02	2.311E+02	9.180E+02	2.833E+00
23000	1.065E+02	2.811E+02	1.106E+03	1.100E+03	2.329E+02	2.332E+02	9.991E+02	2.932E+00
24000	1.014E+02	2.855E+02	1.211E+03	1.204E+03	2.350E+02	2.353E+02	1.078E+03	3.030E+00
25000	9.452E+01	2.895E+02	1.309E+03	1.302E+03	2.371E+02	2.374E+02	1.153E+03	3.127E+00
26000	8.673E+01	2.930E+02	1.399E+03	1.393E+03	2.392E+02	2.395E+02	1.221E+03	3.223E+00
27000	7.882E+01	2.962E+02	1.482E+03	1.476E+03	2.413E+02	2.415E+02	1.282E+03	3.316E+00
28000	7.129E+01	2.989E+02	1.557E+03	1.551E+03	2.433E+02	2.435E+02	1.337E+03	3.406E+00
29000	6.443E+01	3.013E+02	1.625E+03	1.619E+03	2.452E+02	2.454E+02	1.386E+03	3.494E+00
30000	5.835E+01	3.034E+02	1.686E+03	1.680E+03	2.471E+02	2.473E+02	1.429E+03	3.579E+00
32000	4.853E+01	3.068E+02	1.793E+03	1.786E+03	2.508E+02	2.510E+02	1.500E+03	3.738E+00
34000	4.138E+01	3.095E+02	1.882E+03	1.876E+03	2.542E+02	2.543E+02	1.557E+03	3.885E+00
36000	3.626E+01	3.117E+02	1.960E+03	1.953E+03	2.573E+02	2.575E+02	1.604E+03	4.020E+00
38000	3.257E+01	3.136E+02	2.028E+03	2.022E+03	2.602E+02	2.604E+02	1.644E+03	4.144E+00
40000	2.991E+01	3.152E+02	2.090E+03	2.084E+03	2.629E+02	2.631E+02	1.678E+03	4.258E+00
42000	2.795E+01	3.166E+02	2.148E+03	2.142E+03	2.654E+02	2.656E+02	1.709E+03	4.363E+00
44000	2.650E+01	3.179E+02	2.203E+03	2.196E+03	2.678E+02	2.679E+02	1.737E+03	4.461E+00
46000	2.541E+01	3.190E+02	2.254E+03	2.248E+03	2.700E+02	2.701E+02	1.763E+03	4.551E+00
48000	2.457E+01	3.201E+02	2.304E+03	2.298E+03	2.721E+02	2.722E+02	1.788E+03	4.635E+00
50000	2.392E+01	3.211E+02	2.353E+03	2.347E+03	2.740E+02	2.741E+02	1.812E+03	4.713E+00

Table 125: Internal thermodynamic properties of N^+ ΔE=250 cm^{-1}

T(K)	Q_{int}	$\ln(Q_{int})$	E_{int}/RT	$C_{p,int}/R$
50	$1.855E+00$	$6.178E-01$	$7.935E-01$	$1.038E+00$
100	$3.250E+00$	$1.179E+00$	$7.619E-01$	$4.742E-01$
150	$4.306E+00$	$1.460E+00$	$6.194E-01$	$2.328E-01$
200	$5.065E+00$	$1.622E+00$	$5.087E-01$	$1.335E-01$
298.15	$6.031E+00$	$1.797E+00$	$3.708E-01$	$5.995E-02$
300	$6.045E+00$	$1.799E+00$	$3.688E-01$	$5.920E-02$
400	$6.641E+00$	$1.893E+00$	$2.877E-01$	$3.298E-02$
500	$7.039E+00$	$1.952E+00$	$2.354E-01$	$2.092E-02$
600	$7.323E+00$	$1.991E+00$	$1.991E-01$	$1.443E-02$
700	$7.536E+00$	$2.020E+00$	$1.724E-01$	$1.054E-02$
800	$7.700E+00$	$2.041E+00$	$1.520E-01$	$8.037E-03$
900	$7.832E+00$	$2.058E+00$	$1.359E-01$	$6.328E-03$
1000	$7.939E+00$	$2.072E+00$	$1.229E-01$	$5.110E-03$
2000	$8.448E+00$	$2.134E+00$	$6.281E-02$	$2.424E-03$
3000	$8.630E+00$	$2.155E+00$	$4.481E-02$	$2.050E-02$
4000	$8.738E+00$	$2.168E+00$	$4.437E-02$	$6.980E-02$
5000	$8.835E+00$	$2.179E+00$	$5.571E-02$	$1.327E-01$
6000	$8.938E+00$	$2.190E+00$	$7.351E-02$	$1.905E-01$
7000	$9.054E+00$	$2.203E+00$	$9.363E-02$	$2.361E-01$
8000	$9.180E+00$	$2.217E+00$	$1.136E-01$	$2.695E-01$
9000	$9.314E+00$	$2.231E+00$	$1.324E-01$	$2.937E-01$
10000	$9.453E+00$	$2.246E+00$	$1.495E-01$	$3.118E-01$
11000	$9.596E+00$	$2.261E+00$	$1.649E-01$	$3.259E-01$
12000	$9.740E+00$	$2.276E+00$	$1.788E-01$	$3.379E-01$
13000	$9.886E+00$	$2.291E+00$	$1.915E-01$	$3.490E-01$
14000	$1.003E+01$	$2.306E+00$	$2.031E-01$	$3.603E-01$
15000	$1.018E+01$	$2.320E+00$	$2.140E-01$	$3.734E-01$
16000	$1.032E+01$	$2.334E+00$	$2.245E-01$	$3.912E-01$
17000	$1.047E+01$	$2.348E+00$	$2.351E-01$	$4.202E-01$
18000	$1.061E+01$	$2.362E+00$	$2.467E-01$	$4.735E-01$
19000	$1.076E+01$	$2.376E+00$	$2.610E-01$	$5.747E-01$
20000	$1.091E+01$	$2.389E+00$	$2.809E-01$	$7.638E-01$
21000	$1.107E+01$	$2.404E+00$	$3.112E-01$	$1.102E+00$
22000	$1.124E+01$	$2.419E+00$	$3.591E-01$	$1.673E+00$
23000	$1.144E+01$	$2.437E+00$	$4.346E-01$	$2.585E+00$
24000	$1.168E+01$	$2.458E+00$	$5.510E-01$	$3.959E+00$
25000	$1.198E+01$	$2.483E+00$	$7.242E-01$	$5.905E+00$
26000	$1.238E+01$	$2.516E+00$	$9.710E-01$	$8.482E+00$
27000	$1.292E+01$	$2.559E+00$	$1.306E+00$	$1.165E+01$
28000	$1.365E+01$	$2.614E+00$	$1.738E+00$	$1.520E+01$
29000	$1.464E+01$	$2.684E+00$	$2.265E+00$	$1.879E+01$
30000	$1.597E+01$	$2.771E+00$	$2.870E+00$	$2.194E+01$
32000	$2.004E+01$	$2.998E+00$	$4.190E+00$	$2.522E+01$
34000	$2.683E+01$	$3.289E+00$	$5.403E+00$	$2.369E+01$
36000	$3.754E+01$	$3.625E+00$	$6.300E+00$	$1.914E+01$
38000	$5.363E+01$	$3.982E+00$	$6.841E+00$	$1.409E+01$
40000	$7.674E+01$	$4.340E+00$	$7.093E+00$	$9.881E+00$
42000	$1.087E+02$	$4.688E+00$	$7.149E+00$	$6.812E+00$
44000	$1.514E+02$	$5.020E+00$	$7.082E+00$	$4.700E+00$
46000	$2.068E+02$	$5.332E+00$	$6.946E+00$	$3.277E+00$
48000	$2.769E+02$	$5.624E+00$	$6.772E+00$	$2.320E+00$
50000	$3.637E+02$	$5.896E+00$	$6.580E+00$	$1.671E+00$

Table 126: Total thermodynamic properties of N^+ ΔE=250 cm^{-1}

T [K]	C_p [J/mol/K]	S^0 [J/mol/K]	$H^0(T)$-$H^0(0)$ [KJ/mol]	$H^0(T)$-$H^0(298)$ [KJ/mol]	-(G^0-$H^0(0)$)/T [J/mol/K]	-(G^0-$H^0(298)$)/T [J/mol/K]	ΔH_f [KJ/mol]	Log(K_p)
50	2.942E+01	1.164E+02	1.369E+00	-5.747E+00	8.901E+01	2.313E+02	1.876E+03	-1.958E+03
100	2.473E+01	1.352E+02	2.712E+00	-4.404E+00	1.081E+02	1.792E+02	1.878E+03	-9.781E+02
150	2.272E+01	1.448E+02	3.890E+00	-3.226E+00	1.188E+02	1.663E+02	1.879E+03	-6.510E+02
200	2.190E+01	1.512E+02	5.003E+00	-2.113E+00	1.262E+02	1.618E+02	1.881E+03	-4.873E+02
298.15	2.129E+01	1.598E+02	7.117E+00	0.000E+00	1.359E+02	1.598E+02	1.884E+03	-3.255E+02
300	2.128E+01	1.599E+02	7.156E+00	3.939E-02	1.361E+02	1.598E+02	1.884E+03	-3.235E+02
400	2.106E+01	1.660E+02	9.271E+00	2.155E+00	1.428E+02	1.606E+02	1.886E+03	-2.415E+02
500	2.096E+01	1.707E+02	1.137E+01	4.255E+00	1.480E+02	1.622E+02	1.889E+03	-1.922E+02
600	2.091E+01	1.745E+02	1.346E+01	6.348E+00	1.521E+02	1.639E+02	1.892E+03	-1.592E+02
700	2.087E+01	1.777E+02	1.555E+01	8.437E+00	1.555E+02	1.657E+02	1.894E+03	-1.357E+02
800	2.085E+01	1.805E+02	1.764E+01	1.052E+01	1.585E+02	1.674E+02	1.897E+03	-1.180E+02
900	2.084E+01	1.830E+02	1.973E+01	1.261E+01	1.611E+02	1.690E+02	1.900E+03	-1.043E+02
1000	2.083E+01	1.852E+02	2.181E+01	1.469E+01	1.634E+02	1.705E+02	1.902E+03	-9.323E+01
2000	2.081E+01	1.996E+02	4.262E+01	3.550E+01	1.783E+02	1.818E+02	1.926E+03	-4.330E+01
3000	2.096E+01	2.081E+02	6.348E+01	5.636E+01	1.869E+02	1.893E+02	1.950E+03	-2.645E+01
4000	2.137E+01	2.141E+02	8.462E+01	7.750E+01	1.930E+02	1.948E+02	1.973E+03	-1.791E+01
5000	2.189E+01	2.190E+02	1.062E+02	9.913E+01	1.977E+02	1.991E+02	1.996E+03	-1.273E+01
6000	2.237E+01	2.230E+02	1.284E+02	1.213E+02	2.016E+02	2.028E+02	2.020E+03	-9.238E+00
7000	2.275E+01	2.265E+02	1.509E+02	1.438E+02	2.049E+02	2.059E+02	2.044E+03	-6.711E+00
8000	2.303E+01	2.295E+02	1.738E+02	1.667E+02	2.078E+02	2.087E+02	2.068E+03	-4.793E+00
9000	2.323E+01	2.323E+02	1.970E+02	1.899E+02	2.104E+02	2.112E+02	2.092E+03	-3.284E+00
10000	2.338E+01	2.347E+02	2.203E+02	2.132E+02	2.127E+02	2.134E+02	2.114E+03	-2.064E+00
11000	2.350E+01	2.369E+02	2.437E+02	2.366E+02	2.148E+02	2.154E+02	2.135E+03	-1.055E+00
12000	2.360E+01	2.390E+02	2.673E+02	2.602E+02	2.167E+02	2.173E+02	2.153E+03	-2.066E-01
13000	2.369E+01	2.409E+02	2.909E+02	2.838E+02	2.185E+02	2.191E+02	2.170E+03	5.171E-01
14000	2.378E+01	2.427E+02	3.146E+02	3.075E+02	2.202E+02	2.207E+02	2.184E+03	1.142E+00
15000	2.389E+01	2.443E+02	3.385E+02	3.314E+02	2.217E+02	2.222E+02	2.196E+03	1.687E+00
16000	2.404E+01	2.458E+02	3.624E+02	3.553E+02	2.232E+02	2.236E+02	2.207E+03	2.166E+00
17000	2.428E+01	2.473E+02	3.866E+02	3.795E+02	2.246E+02	2.250E+02	2.218E+03	2.591E+00
18000	2.472E+01	2.487E+02	4.111E+02	4.040E+02	2.259E+02	2.263E+02	2.230E+03	2.970E+00
19000	2.557E+01	2.501E+02	4.362E+02	4.291E+02	2.271E+02	2.275E+02	2.244E+03	3.312E+00
20000	2.714E+01	2.514E+02	4.624E+02	4.553E+02	2.283E+02	2.286E+02	2.259E+03	3.621E+00
21000	2.995E+01	2.528E+02	4.909E+02	4.837E+02	2.294E+02	2.298E+02	2.279E+03	3.903E+00
22000	3.469E+01	2.543E+02	5.230E+02	5.159E+02	2.305E+02	2.308E+02	2.303E+03	4.162E+00
23000	4.228E+01	2.560E+02	5.612E+02	5.541E+02	2.316E+02	2.319E+02	2.336E+03	4.402E+00
24000	5.371E+01	2.580E+02	6.088E+02	6.017E+02	2.326E+02	2.329E+02	2.379E+03	4.625E+00
25000	6.988E+01	2.605E+02	6.702E+02	6.631E+02	2.337E+02	2.340E+02	2.437E+03	4.834E+00
26000	9.131E+01	2.636E+02	7.504E+02	7.432E+02	2.348E+02	2.351E+02	2.516E+03	5.033E+00
27000	1.176E+02	2.676E+02	8.545E+02	8.473E+02	2.359E+02	2.362E+02	2.620E+03	5.224E+00
28000	1.472E+02	2.724E+02	9.867E+02	9.796E+02	2.371E+02	2.374E+02	2.752E+03	5.409E+00
29000	1.770E+02	2.781E+02	1.149E+03	1.142E+03	2.384E+02	2.387E+02	2.916E+03	5.591E+00
30000	2.032E+02	2.845E+02	1.340E+03	1.332E+03	2.399E+02	2.401E+02	3.109E+03	5.772E+00
32000	2.305E+02	2.987E+02	1.780E+03	1.773E+03	2.431E+02	2.433E+02	3.556E+03	6.133E+00
34000	2.177E+02	3.125E+02	2.234E+03	2.227E+03	2.468E+02	2.470E+02	4.020E+03	6.497E+00
36000	1.799E+02	3.239E+02	2.634E+03	2.627E+03	2.508E+02	2.510E+02	4.431E+03	6.858E+00
38000	1.379E+02	3.325E+02	2.951E+03	2.944E+03	2.549E+02	2.551E+02	4.760E+03	7.209E+00
40000	1.029E+02	3.387E+02	3.190E+03	3.183E+03	2.589E+02	2.591E+02	5.013E+03	7.545E+00
42000	7.743E+01	3.430E+02	3.369E+03	3.362E+03	2.628E+02	2.630E+02	5.207E+03	7.863E+00
44000	5.986E+01	3.462E+02	3.506E+03	3.498E+03	2.665E+02	2.667E+02	5.358E+03	8.162E+00
46000	4.803E+01	3.486E+02	3.613E+03	3.606E+03	2.701E+02	2.702E+02	5.481E+03	8.441E+00
48000	4.008E+01	3.505E+02	3.700E+03	3.693E+03	2.734E+02	2.735E+02	5.585E+03	8.703E+00
50000	3.468E+01	3.520E+02	3.775E+03	3.768E+03	2.765E+02	2.766E+02	5.677E+03	8.948E+00

Table 127: Internal thermodynamic properties of N^+ ΔE=500 cm^{-1}

T(K)	Q_{int}	$\ln(Q_{int})$	E_{int}/RT	$C_{p,int}/R$
50	$1.855E+00$	$6.178E-01$	$7.935E-01$	$1.038E+00$
100	$3.250E+00$	$1.179E+00$	$7.619E-01$	$4.742E-01$
150	$4.306E+00$	$1.460E+00$	$6.194E-01$	$2.328E-01$
200	$5.065E+00$	$1.622E+00$	$5.087E-01$	$1.335E-01$
298.15	$6.031E+00$	$1.797E+00$	$3.708E-01$	$5.995E-02$
300	$6.045E+00$	$1.799E+00$	$3.688E-01$	$5.920E-02$
400	$6.641E+00$	$1.893E+00$	$2.877E-01$	$3.298E-02$
500	$7.039E+00$	$1.952E+00$	$2.354E-01$	$2.092E-02$
600	$7.323E+00$	$1.991E+00$	$1.991E-01$	$1.443E-02$
700	$7.536E+00$	$2.020E+00$	$1.724E-01$	$1.054E-02$
800	$7.700E+00$	$2.041E+00$	$1.520E-01$	$8.037E-03$
900	$7.832E+00$	$2.058E+00$	$1.359E-01$	$6.328E-03$
1000	$7.939E+00$	$2.072E+00$	$1.229E-01$	$5.110E-03$
2000	$8.448E+00$	$2.134E+00$	$6.281E-02$	$2.424E-03$
3000	$8.630E+00$	$2.155E+00$	$4.481E-02$	$2.050E-02$
4000	$8.738E+00$	$2.168E+00$	$4.437E-02$	$6.980E-02$
5000	$8.835E+00$	$2.179E+00$	$5.571E-02$	$1.327E-01$
6000	$8.938E+00$	$2.190E+00$	$7.351E-02$	$1.905E-01$
7000	$9.054E+00$	$2.203E+00$	$9.363E-02$	$2.361E-01$
8000	$9.180E+00$	$2.217E+00$	$1.136E-01$	$2.695E-01$
9000	$9.314E+00$	$2.231E+00$	$1.324E-01$	$2.937E-01$
10000	$9.453E+00$	$2.246E+00$	$1.495E-01$	$3.118E-01$
11000	$9.596E+00$	$2.261E+00$	$1.649E-01$	$3.259E-01$
12000	$9.740E+00$	$2.276E+00$	$1.788E-01$	$3.379E-01$
13000	$9.886E+00$	$2.291E+00$	$1.915E-01$	$3.489E-01$
14000	$1.003E+01$	$2.306E+00$	$2.031E-01$	$3.600E-01$
15000	$1.018E+01$	$2.320E+00$	$2.140E-01$	$3.721E-01$
16000	$1.032E+01$	$2.334E+00$	$2.243E-01$	$3.866E-01$
17000	$1.047E+01$	$2.348E+00$	$2.344E-01$	$4.062E-01$
18000	$1.061E+01$	$2.362E+00$	$2.447E-01$	$4.357E-01$
19000	$1.075E+01$	$2.375E+00$	$2.559E-01$	$4.839E-01$
20000	$1.090E+01$	$2.389E+00$	$2.692E-01$	$5.652E-01$
21000	$1.105E+01$	$2.402E+00$	$2.862E-01$	$7.016E-01$
22000	$1.120E+01$	$2.416E+00$	$3.098E-01$	$9.243E-01$
23000	$1.137E+01$	$2.431E+00$	$3.436E-01$	$1.275E+00$
24000	$1.154E+01$	$2.446E+00$	$3.926E-01$	$1.803E+00$
25000	$1.175E+01$	$2.464E+00$	$4.634E-01$	$2.564E+00$
26000	$1.198E+01$	$2.484E+00$	$5.634E-01$	$3.615E+00$
27000	$1.227E+01$	$2.507E+00$	$7.009E-01$	$4.996E+00$
28000	$1.263E+01$	$2.536E+00$	$8.842E-01$	$6.724E+00$
29000	$1.308E+01$	$2.571E+00$	$1.120E+00$	$8.771E+00$
30000	$1.365E+01$	$2.614E+00$	$1.413E+00$	$1.105E+01$
32000	$1.530E+01$	$2.728E+00$	$2.162E+00$	$1.569E+01$
34000	$1.791E+01$	$2.885E+00$	$3.067E+00$	$1.907E+01$
36000	$2.192E+01$	$3.087E+00$	$3.995E+00$	$2.002E+01$
38000	$2.782E+01$	$3.326E+00$	$4.809E+00$	$1.857E+01$
40000	$3.620E+01$	$3.589E+00$	$5.429E+00$	$1.570E+01$
42000	$4.769E+01$	$3.865E+00$	$5.841E+00$	$1.248E+01$
44000	$6.296E+01$	$4.143E+00$	$6.075E+00$	$9.562E+00$
46000	$8.269E+01$	$4.415E+00$	$6.173E+00$	$7.200E+00$
48000	$1.076E+02$	$4.678E+00$	$6.176E+00$	$5.393E+00$
50000	$1.383E+02$	$4.929E+00$	$6.117E+00$	$4.050E+00$

Table 128: Total thermodynamic properties of N^+ ΔE=500 cm^{-1}

T [K]	C_p [J/mol/K]	S^0 [J/mol/K]	$H^0(T)-H^0(0)$ [KJ/mol]	$H^0(T)-H^0(298)$ [KJ/mol]	$-(G^0-H^0(0))/T$ [J/mol/K]	$-(G^0-H^0(298))/T$ [J/mol/K]	ΔH_f [KJ/mol]	$Log(K_p)$
50	2.942E+01	1.164E+02	1.369E+00	-5.747E+00	8.901E+01	2.313E+02	1.876E+03	-1.958E+03
100	2.473E+01	1.352E+02	2.712E+00	-4.404E+00	1.081E+02	1.792E+02	1.878E+03	-9.781E+02
150	2.272E+01	1.448E+02	3.890E+00	-3.226E+00	1.188E+02	1.663E+02	1.879E+03	-6.510E+02
200	2.190E+01	1.512E+02	5.003E+00	-2.113E+00	1.262E+02	1.618E+02	1.881E+03	-4.873E+02
298.15	2.129E+01	1.598E+02	7.117E+00	0.000E+00	1.359E+02	1.598E+02	1.884E+03	-3.255E+02
300	2.128E+01	1.599E+02	7.156E+00	3.939E-02	1.361E+02	1.598E+02	1.884E+03	-3.235E+02
400	2.106E+01	1.660E+02	9.271E+00	2.155E+00	1.428E+02	1.606E+02	1.886E+03	-2.415E+02
500	2.096E+01	1.707E+02	1.137E+01	4.255E+00	1.480E+02	1.622E+02	1.889E+03	-1.922E+02
600	2.091E+01	1.745E+02	1.346E+01	6.348E+00	1.521E+02	1.639E+02	1.892E+03	-1.592E+02
700	2.087E+01	1.777E+02	1.555E+01	8.437E+00	1.555E+02	1.657E+02	1.894E+03	-1.357E+02
800	2.085E+01	1.805E+02	1.764E+01	1.052E+01	1.585E+02	1.674E+02	1.897E+03	-1.180E+02
900	2.084E+01	1.830E+02	1.973E+01	1.261E+01	1.611E+02	1.690E+02	1.900E+03	-1.043E+02
1000	2.083E+01	1.852E+02	2.181E+01	1.469E+01	1.634E+02	1.705E+02	1.902E+03	-9.323E+01
2000	2.081E+01	1.996E+02	4.262E+01	3.550E+01	1.783E+02	1.818E+02	1.926E+03	-4.330E+01
3000	2.096E+01	2.081E+02	6.348E+01	5.636E+01	1.869E+02	1.893E+02	1.950E+03	-2.645E+01
4000	2.137E+01	2.141E+02	8.462E+01	7.750E+01	1.930E+02	1.948E+02	1.973E+03	-1.791E+01
5000	2.189E+01	2.190E+02	1.062E+02	9.913E+01	1.977E+02	1.991E+02	1.996E+03	-1.273E+01
6000	2.237E+01	2.230E+02	1.284E+02	1.213E+02	2.016E+02	2.028E+02	2.020E+03	-9.238E+00
7000	2.275E+01	2.265E+02	1.509E+02	1.438E+02	2.049E+02	2.059E+02	2.044E+03	-6.711E+00
8000	2.303E+01	2.295E+02	1.738E+02	1.667E+02	2.078E+02	2.087E+02	2.068E+03	-4.793E+00
9000	2.323E+01	2.323E+02	1.970E+02	1.899E+02	2.104E+02	2.112E+02	2.092E+03	-3.284E+00
10000	2.338E+01	2.347E+02	2.203E+02	2.132E+02	2.127E+02	2.134E+02	2.114E+03	-2.064E+00
11000	2.350E+01	2.369E+02	2.437E+02	2.366E+02	2.148E+02	2.154E+02	2.135E+03	-1.055E+00
12000	2.360E+01	2.390E+02	2.673E+02	2.602E+02	2.167E+02	2.173E+02	2.153E+03	-2.066E-01
13000	2.369E+01	2.409E+02	2.909E+02	2.838E+02	2.185E+02	2.191E+02	2.170E+03	5.171E-01
14000	2.378E+01	2.427E+02	3.146E+02	3.075E+02	2.202E+02	2.207E+02	2.184E+03	1.142E+00
15000	2.388E+01	2.443E+02	3.385E+02	3.314E+02	2.217E+02	2.222E+02	2.196E+03	1.687E+00
16000	2.400E+01	2.458E+02	3.624E+02	3.553E+02	2.232E+02	2.236E+02	2.207E+03	2.166E+00
17000	2.416E+01	2.473E+02	3.865E+02	3.794E+02	2.246E+02	2.250E+02	2.218E+03	2.591E+00
18000	2.441E+01	2.487E+02	4.108E+02	4.037E+02	2.259E+02	2.263E+02	2.230E+03	2.970E+00
19000	2.481E+01	2.500E+02	4.354E+02	4.282E+02	2.271E+02	2.275E+02	2.243E+03	3.312E+00
20000	2.549E+01	2.513E+02	4.605E+02	4.534E+02	2.283E+02	2.286E+02	2.257E+03	3.621E+00
21000	2.662E+01	2.526E+02	4.865E+02	4.794E+02	2.294E+02	2.297E+02	2.274E+03	3.903E+00
22000	2.847E+01	2.538E+02	5.140E+02	5.068E+02	2.305E+02	2.308E+02	2.294E+03	4.161E+00
23000	3.138E+01	2.552E+02	5.438E+02	5.367E+02	2.315E+02	2.318E+02	2.318E+03	4.399E+00
24000	3.577E+01	2.566E+02	5.772E+02	5.701E+02	2.325E+02	2.328E+02	2.347E+03	4.620E+00
25000	4.211E+01	2.582E+02	6.160E+02	6.089E+02	2.335E+02	2.338E+02	2.383E+03	4.825E+00
26000	5.084E+01	2.600E+02	6.622E+02	6.551E+02	2.345E+02	2.348E+02	2.428E+03	5.019E+00
27000	6.232E+01	2.621E+02	7.186E+02	7.115E+02	2.355E+02	2.358E+02	2.484E+03	5.201E+00
28000	7.669E+01	2.646E+02	7.879E+02	7.807E+02	2.365E+02	2.368E+02	2.554E+03	5.375E+00
29000	9.372E+01	2.676E+02	8.729E+02	8.657E+02	2.375E+02	2.378E+02	2.640E+03	5.542E+00
30000	1.127E+02	2.711E+02	9.759E+02	9.688E+02	2.386E+02	2.388E+02	2.746E+03	5.704E+00
32000	1.512E+02	2.796E+02	1.240E+03	1.233E+03	2.409E+02	2.411E+02	3.017E+03	6.016E+00
34000	1.794E+02	2.897E+02	1.574E+03	1.567E+03	2.434E+02	2.436E+02	3.360E+03	6.321E+00
36000	1.873E+02	3.003E+02	1.944E+03	1.937E+03	2.463E+02	2.465E+02	3.741E+03	6.624E+00
38000	1.752E+02	3.102E+02	2.309E+03	2.302E+03	2.494E+02	2.496E+02	4.118E+03	6.924E+00
40000	1.513E+02	3.186E+02	2.637E+03	2.630E+03	2.527E+02	2.528E+02	4.460E+03	7.219E+00
42000	1.245E+02	3.253E+02	2.913E+03	2.906E+03	2.560E+02	2.561E+02	4.750E+03	7.505E+00
44000	1.003E+02	3.305E+02	3.137E+03	3.130E+03	2.592E+02	2.594E+02	4.990E+03	7.781E+00
46000	8.065E+01	3.346E+02	3.317E+03	3.310E+03	2.624E+02	2.626E+02	5.186E+03	8.043E+00
48000	6.563E+01	3.376E+02	3.463E+03	3.456E+03	2.655E+02	2.657E+02	5.348E+03	8.293E+00
50000	5.446E+01	3.401E+02	3.582E+03	3.575E+03	2.684E+02	2.686E+02	5.484E+03	8.528E+00

Table 129: Internal thermodynamic properties of N^+ ΔE=1000 cm^{-1}

T(K)	Q_{int}	$\ln(Q_{int})$	E_{int}/RT	$C_{p,int}/R$
50	$1.855E+00$	$6.178E-01$	$7.935E-01$	$1.038E+00$
100	$3.250E+00$	$1.179E+00$	$7.619E-01$	$4.742E-01$
150	$4.306E+00$	$1.460E+00$	$6.194E-01$	$2.328E-01$
200	$5.065E+00$	$1.622E+00$	$5.087E-01$	$1.335E-01$
298.15	$6.031E+00$	$1.797E+00$	$3.708E-01$	$5.995E-02$
300	$6.045E+00$	$1.799E+00$	$3.688E-01$	$5.920E-02$
400	$6.641E+00$	$1.893E+00$	$2.877E-01$	$3.298E-02$
500	$7.039E+00$	$1.952E+00$	$2.354E-01$	$2.092E-02$
600	$7.323E+00$	$1.991E+00$	$1.991E-01$	$1.443E-02$
700	$7.536E+00$	$2.020E+00$	$1.724E-01$	$1.054E-02$
800	$7.700E+00$	$2.041E+00$	$1.520E-01$	$8.037E-03$
900	$7.832E+00$	$2.058E+00$	$1.359E-01$	$6.328E-03$
1000	$7.939E+00$	$2.072E+00$	$1.229E-01$	$5.110E-03$
2000	$8.448E+00$	$2.134E+00$	$6.281E-02$	$2.424E-03$
3000	$8.630E+00$	$2.155E+00$	$4.481E-02$	$2.050E-02$
4000	$8.738E+00$	$2.168E+00$	$4.437E-02$	$6.980E-02$
5000	$8.835E+00$	$2.179E+00$	$5.571E-02$	$1.327E-01$
6000	$8.938E+00$	$2.190E+00$	$7.351E-02$	$1.905E-01$
7000	$9.054E+00$	$2.203E+00$	$9.363E-02$	$2.361E-01$
8000	$9.180E+00$	$2.217E+00$	$1.136E-01$	$2.695E-01$
9000	$9.314E+00$	$2.231E+00$	$1.324E-01$	$2.937E-01$
10000	$9.453E+00$	$2.246E+00$	$1.495E-01$	$3.118E-01$
11000	$9.596E+00$	$2.261E+00$	$1.649E-01$	$3.259E-01$
12000	$9.740E+00$	$2.276E+00$	$1.788E-01$	$3.379E-01$
13000	$9.886E+00$	$2.291E+00$	$1.915E-01$	$3.489E-01$
14000	$1.003E+01$	$2.306E+00$	$2.031E-01$	$3.599E-01$
15000	$1.018E+01$	$2.320E+00$	$2.139E-01$	$3.717E-01$
16000	$1.032E+01$	$2.334E+00$	$2.242E-01$	$3.850E-01$
17000	$1.047E+01$	$2.348E+00$	$2.341E-01$	$4.013E-01$
18000	$1.061E+01$	$2.362E+00$	$2.440E-01$	$4.225E-01$
19000	$1.075E+01$	$2.375E+00$	$2.541E-01$	$4.522E-01$
20000	$1.090E+01$	$2.389E+00$	$2.650E-01$	$4.957E-01$
21000	$1.104E+01$	$2.402E+00$	$2.775E-01$	$5.616E-01$
22000	$1.119E+01$	$2.415E+00$	$2.925E-01$	$6.615E-01$
23000	$1.134E+01$	$2.428E+00$	$3.116E-01$	$8.111E-01$
24000	$1.150E+01$	$2.442E+00$	$3.367E-01$	$1.030E+00$
25000	$1.166E+01$	$2.457E+00$	$3.703E-01$	$1.340E+00$
26000	$1.185E+01$	$2.472E+00$	$4.154E-01$	$1.767E+00$
27000	$1.205E+01$	$2.489E+00$	$4.755E-01$	$2.335E+00$
28000	$1.227E+01$	$2.507E+00$	$5.544E-01$	$3.066E+00$
29000	$1.253E+01$	$2.528E+00$	$6.562E-01$	$3.975E+00$
30000	$1.284E+01$	$2.553E+00$	$7.844E-01$	$5.063E+00$
32000	$1.365E+01$	$2.614E+00$	$1.132E+00$	$7.708E+00$
34000	$1.482E+01$	$2.696E+00$	$1.605E+00$	$1.066E+01$
36000	$1.651E+01$	$2.804E+00$	$2.184E+00$	$1.330E+01$
38000	$1.889E+01$	$2.939E+00$	$2.820E+00$	$1.502E+01$
40000	$2.219E+01$	$3.100E+00$	$3.446E+00$	$1.546E+01$
42000	$2.662E+01$	$3.282E+00$	$4.005E+00$	$1.473E+01$
44000	$3.242E+01$	$3.479E+00$	$4.459E+00$	$1.319E+01$
46000	$3.984E+01$	$3.685E+00$	$4.799E+00$	$1.130E+01$
48000	$4.913E+01$	$3.894E+00$	$5.029E+00$	$9.389E+00$
50000	$6.051E+01$	$4.103E+00$	$5.168E+00$	$7.657E+00$

Table 130: Total thermodynamic properties of N^+ ΔE=1000 cm^{-1}

T [K]	C_p [J/mol/K]	S^0 [J/mol/K]	$H^0(T)-H^0(0)$ [KJ/mol]	$H^0(T)-H^0(298)$ [KJ/mol]	$-(G^0-H^0(0))/T$ [J/mol/K]	$-(G^0-H^0(298))/T$ [J/mol/K]	ΔH_f [KJ/mol]	$Log(K_p)$
50	2.942E+01	1.164E+02	1.369E+00	-5.747E+00	8.901E+01	2.313E+02	1.876E+03	-1.958E+03
100	2.473E+01	1.352E+02	2.712E+00	-4.404E+00	1.081E+02	1.792E+02	1.878E+03	-9.781E+02
150	2.272E+01	1.448E+02	3.890E+00	-3.226E+00	1.188E+02	1.663E+02	1.879E+03	-6.510E+02
200	2.190E+01	1.512E+02	5.003E+00	-2.113E+00	1.262E+02	1.618E+02	1.881E+03	-4.873E+02
298.15	2.129E+01	1.598E+02	7.117E+00	0.000E+00	1.359E+02	1.598E+02	1.884E+03	-3.255E+02
300	2.128E+01	1.599E+02	7.156E+00	3.939E-02	1.361E+02	1.598E+02	1.884E+03	-3.235E+02
400	2.106E+01	1.660E+02	9.271E+00	2.155E+00	1.428E+02	1.606E+02	1.886E+03	-2.415E+02
500	2.096E+01	1.707E+02	1.137E+01	4.255E+00	1.480E+02	1.622E+02	1.889E+03	-1.922E+02
600	2.091E+01	1.745E+02	1.346E+01	6.348E+00	1.521E+02	1.639E+02	1.892E+03	-1.592E+02
700	2.087E+01	1.777E+02	1.555E+01	8.437E+00	1.555E+02	1.657E+02	1.894E+03	-1.357E+02
800	2.085E+01	1.805E+02	1.764E+01	1.052E+01	1.585E+02	1.674E+02	1.897E+03	-1.180E+02
900	2.084E+01	1.830E+02	1.973E+01	1.261E+01	1.611E+02	1.690E+02	1.900E+03	-1.043E+02
1000	2.083E+01	1.852E+02	2.181E+01	1.469E+01	1.634E+02	1.705E+02	1.902E+03	-9.323E+01
2000	2.081E+01	1.996E+02	4.262E+01	3.550E+01	1.783E+02	1.818E+02	1.926E+03	-4.330E+01
3000	2.096E+01	2.081E+02	6.348E+01	5.636E+01	1.869E+02	1.893E+02	1.950E+03	-2.645E+01
4000	2.137E+01	2.141E+02	8.462E+01	7.750E+01	1.930E+02	1.948E+02	1.973E+03	-1.791E+01
5000	2.189E+01	2.190E+02	1.062E+02	9.913E+01	1.977E+02	1.991E+02	1.996E+03	-1.273E+01
6000	2.237E+01	2.230E+02	1.284E+02	1.213E+02	2.016E+02	2.028E+02	2.020E+03	-9.238E+00
7000	2.275E+01	2.265E+02	1.509E+02	1.438E+02	2.049E+02	2.059E+02	2.044E+03	-6.711E+00
8000	2.303E+01	2.295E+02	1.738E+02	1.667E+02	2.078E+02	2.087E+02	2.068E+03	-4.793E+00
9000	2.323E+01	2.323E+02	1.970E+02	1.899E+02	2.104E+02	2.112E+02	2.092E+03	-3.284E+00
10000	2.338E+01	2.347E+02	2.203E+02	2.132E+02	2.127E+02	2.134E+02	2.114E+03	-2.064E+00
11000	2.350E+01	2.369E+02	2.437E+02	2.366E+02	2.148E+02	2.154E+02	2.135E+03	-1.055E+00
12000	2.360E+01	2.390E+02	2.673E+02	2.602E+02	2.167E+02	2.173E+02	2.153E+03	-2.066E-01
13000	2.369E+01	2.409E+02	2.909E+02	2.838E+02	2.185E+02	2.191E+02	2.170E+03	5.171E-01
14000	2.378E+01	2.427E+02	3.146E+02	3.075E+02	2.202E+02	2.207E+02	2.184E+03	1.142E+00
15000	2.388E+01	2.443E+02	3.385E+02	3.314E+02	2.217E+02	2.222E+02	2.196E+03	1.687E+00
16000	2.399E+01	2.458E+02	3.624E+02	3.553E+02	2.232E+02	2.236E+02	2.207E+03	2.166E+00
17000	2.412E+01	2.473E+02	3.865E+02	3.793E+02	2.246E+02	2.250E+02	2.218E+03	2.591E+00
18000	2.430E+01	2.487E+02	4.107E+02	4.036E+02	2.259E+02	2.263E+02	2.230E+03	2.970E+00
19000	2.455E+01	2.500E+02	4.351E+02	4.280E+02	2.271E+02	2.275E+02	2.242E+03	3.312E+00
20000	2.491E+01	2.513E+02	4.598E+02	4.527E+02	2.283E+02	2.286E+02	2.257E+03	3.621E+00
21000	2.546E+01	2.525E+02	4.850E+02	4.778E+02	2.294E+02	2.297E+02	2.273E+03	3.902E+00
22000	2.629E+01	2.537E+02	5.108E+02	5.037E+02	2.305E+02	2.308E+02	2.291E+03	4.160E+00
23000	2.753E+01	2.549E+02	5.377E+02	5.305E+02	2.315E+02	2.318E+02	2.312E+03	4.398E+00
24000	2.935E+01	2.561E+02	5.660E+02	5.589E+02	2.325E+02	2.328E+02	2.336E+03	4.618E+00
25000	3.193E+01	2.573E+02	5.966E+02	5.895E+02	2.335E+02	2.338E+02	2.364E+03	4.822E+00
26000	3.548E+01	2.587E+02	6.302E+02	6.231E+02	2.344E+02	2.347E+02	2.396E+03	5.013E+00
27000	4.020E+01	2.601E+02	6.680E+02	6.609E+02	2.353E+02	2.356E+02	2.433E+03	5.193E+00
28000	4.628E+01	2.616E+02	7.111E+02	7.040E+02	2.363E+02	2.365E+02	2.477E+03	5.363E+00
29000	5.383E+01	2.634E+02	7.610E+02	7.539E+02	2.372E+02	2.374E+02	2.528E+03	5.524E+00
30000	6.288E+01	2.654E+02	8.192E+02	8.121E+02	2.381E+02	2.383E+02	2.589E+03	5.677E+00
32000	8.488E+01	2.701E+02	9.663E+02	9.592E+02	2.399E+02	2.401E+02	2.743E+03	5.967E+00
34000	1.094E+02	2.760E+02	1.160E+03	1.153E+03	2.419E+02	2.421E+02	2.946E+03	6.239E+00
36000	1.314E+02	2.829E+02	1.402E+03	1.395E+03	2.439E+02	2.441E+02	3.199E+03	6.501E+00
38000	1.456E+02	2.904E+02	1.681E+03	1.674E+03	2.462E+02	2.464E+02	3.490E+03	6.756E+00
40000	1.493E+02	2.980E+02	1.978E+03	1.970E+03	2.486E+02	2.488E+02	3.800E+03	7.006E+00
42000	1.432E+02	3.052E+02	2.272E+03	2.264E+03	2.511E+02	2.513E+02	4.109E+03	7.252E+00
44000	1.305E+02	3.116E+02	2.546E+03	2.539E+03	2.537E+02	2.539E+02	4.399E+03	7.492E+00
46000	1.147E+02	3.171E+02	2.792E+03	2.784E+03	2.564E+02	2.565E+02	4.660E+03	7.726E+00
48000	9.885E+01	3.216E+02	3.005E+03	2.998E+03	2.590E+02	2.591E+02	4.890E+03	7.952E+00
50000	8.445E+01	3.253E+02	3.188E+03	3.181E+03	2.616E+02	2.617E+02	5.090E+03	8.169E+00

Table 131: Internal thermodynamic properties of N^{2+} ΔE=250 cm^{-1}

T(K)	Q_{int}	$\ln(Q_{int})$	E_{int}/RT	$C_{p,int}/R$
50	$2.026E+00$	$7.063E-01$	$6.553E-02$	$3.245E-01$
100	$2.325E+00$	$8.439E-01$	$3.511E-01$	$7.576E-01$
150	$2.751E+00$	$1.012E+00$	$4.566E-01$	$5.553E-01$
200	$3.141E+00$	$1.144E+00$	$4.557E-01$	$3.641E-01$
298.15	$3.724E+00$	$1.315E+00$	$3.896E-01$	$1.761E-01$
300	$3.733E+00$	$1.317E+00$	$3.883E-01$	$1.740E-01$
400	$4.136E+00$	$1.420E+00$	$3.240E-01$	$9.827E-02$
500	$4.422E+00$	$1.487E+00$	$2.748E-01$	$6.239E-02$
600	$4.633E+00$	$1.533E+00$	$2.377E-01$	$4.291E-02$
700	$4.795E+00$	$1.568E+00$	$2.089E-01$	$3.124E-02$
800	$4.923E+00$	$1.594E+00$	$1.862E-01$	$2.373E-02$
900	$5.027E+00$	$1.615E+00$	$1.679E-01$	$1.862E-02$
1000	$5.112E+00$	$1.632E+00$	$1.528E-01$	$1.500E-02$
2000	$5.528E+00$	$1.710E+00$	$8.007E-02$	$3.634E-03$
3000	$5.679E+00$	$1.737E+00$	$5.418E-02$	$1.596E-03$
4000	$5.757E+00$	$1.750E+00$	$4.094E-02$	$8.932E-04$
5000	$5.804E+00$	$1.759E+00$	$3.289E-02$	$6.077E-04$
6000	$5.836E+00$	$1.764E+00$	$2.752E-02$	$8.129E-04$
7000	$5.859E+00$	$1.768E+00$	$2.380E-02$	$2.470E-03$
8000	$5.877E+00$	$1.771E+00$	$2.140E-02$	$7.479E-03$
9000	$5.891E+00$	$1.773E+00$	$2.038E-02$	$1.817E-02$
10000	$5.904E+00$	$1.776E+00$	$2.101E-02$	$3.655E-02$
11000	$5.917E+00$	$1.778E+00$	$2.359E-02$	$6.382E-02$
12000	$5.930E+00$	$1.780E+00$	$2.840E-02$	$1.002E-01$
13000	$5.945E+00$	$1.783E+00$	$3.560E-02$	$1.452E-01$
14000	$5.963E+00$	$1.786E+00$	$4.526E-02$	$1.976E-01$
15000	$5.984E+00$	$1.789E+00$	$5.733E-02$	$2.559E-01$
16000	$6.008E+00$	$1.793E+00$	$7.168E-02$	$3.184E-01$
17000	$6.038E+00$	$1.798E+00$	$8.810E-02$	$3.837E-01$
18000	$6.071E+00$	$1.804E+00$	$1.064E-01$	$4.501E-01$
19000	$6.109E+00$	$1.810E+00$	$1.262E-01$	$5.165E-01$
20000	$6.152E+00$	$1.817E+00$	$1.474E-01$	$5.817E-01$
21000	$6.200E+00$	$1.825E+00$	$1.696E-01$	$6.449E-01$
22000	$6.252E+00$	$1.833E+00$	$1.926E-01$	$7.055E-01$
23000	$6.309E+00$	$1.842E+00$	$2.161E-01$	$7.633E-01$
24000	$6.371E+00$	$1.852E+00$	$2.401E-01$	$8.183E-01$
25000	$6.437E+00$	$1.862E+00$	$2.643E-01$	$8.712E-01$
26000	$6.507E+00$	$1.873E+00$	$2.886E-01$	$9.236E-01$
27000	$6.581E+00$	$1.884E+00$	$3.131E-01$	$9.781E-01$
28000	$6.660E+00$	$1.896E+00$	$3.379E-01$	$1.039E+00$
29000	$6.742E+00$	$1.908E+00$	$3.633E-01$	$1.111E+00$
30000	$6.829E+00$	$1.921E+00$	$3.897E-01$	$1.205E+00$
32000	$7.015E+00$	$1.948E+00$	$4.491E-01$	$1.505E+00$
34000	$7.225E+00$	$1.978E+00$	$5.262E-01$	$2.075E+00$
36000	$7.467E+00$	$2.011E+00$	$6.384E-01$	$3.114E+00$
38000	$7.763E+00$	$2.049E+00$	$8.109E-01$	$4.857E+00$
40000	$8.143E+00$	$2.097E+00$	$1.076E+00$	$7.510E+00$
42000	$8.658E+00$	$2.159E+00$	$1.464E+00$	$1.112E+01$
44000	$9.378E+00$	$2.238E+00$	$1.999E+00$	$1.541E+01$
46000	$1.040E+01$	$2.342E+00$	$2.677E+00$	$1.971E+01$
48000	$1.185E+01$	$2.472E+00$	$3.462E+00$	$2.310E+01$
50000	$1.387E+01$	$2.630E+00$	$4.288E+00$	$2.481E+01$

Table 132: Total thermodynamic properties of N^{2+} ΔE=250 cm^{-1}

T [K]	C_p [J/mol/K]	S^0 [J/mol/K]	$H^0(T)$-$H^0(0)$ [KJ/mol]	$H^0(T)$-$H^0(298)$ [KJ/mol]	-(G^0-$H^0(0)$)/T [J/mol/K]	-(G^0-$H^0(298)$)/T [J/mol/K]	ΔH_f [KJ/mol]	Log(K_p)
50	2.348E+01	1.111E+02	1.067E+00	-6.097E+00	8.975E+01	2.330E+02	4.734E+03	-4.945E+03
100	2.709E+01	1.290E+02	2.370E+00	-4.793E+00	1.053E+02	1.769E+02	4.737E+03	-2.472E+03
150	2.540E+01	1.397E+02	3.687E+00	-3.476E+00	1.151E+02	1.629E+02	4.740E+03	-1.647E+03
200	2.381E+01	1.468E+02	4.915E+00	-2.248E+00	1.222E+02	1.580E+02	4.742E+03	-1.234E+03
298.15	2.225E+01	1.559E+02	7.163E+00	0.000E+00	1.319E+02	1.559E+02	4.747E+03	-8.263E+02
300	2.223E+01	1.561E+02	7.204E+00	4.113E-02	1.321E+02	1.559E+02	4.747E+03	-8.212E+02
400	2.160E+01	1.624E+02	9.392E+00	2.229E+00	1.389E+02	1.568E+02	4.752E+03	-6.145E+02
500	2.130E+01	1.672E+02	1.154E+01	4.372E+00	1.441E+02	1.584E+02	4.757E+03	-4.903E+02
600	2.114E+01	1.710E+02	1.366E+01	6.494E+00	1.483E+02	1.602E+02	4.762E+03	-4.074E+02
700	2.105E+01	1.743E+02	1.577E+01	8.603E+00	1.518E+02	1.620E+02	4.767E+03	-3.482E+02
800	2.098E+01	1.771E+02	1.787E+01	1.071E+01	1.548E+02	1.637E+02	4.771E+03	-3.037E+02
900	2.094E+01	1.796E+02	1.996E+01	1.280E+01	1.574E+02	1.653E+02	4.776E+03	-2.691E+02
1000	2.091E+01	1.818E+02	2.206E+01	1.489E+01	1.597E+02	1.669E+02	4.781E+03	-2.413E+02
2000	2.082E+01	1.962E+02	4.290E+01	3.574E+01	1.748E+02	1.783E+02	4.826E+03	-1.160E+02
3000	2.080E+01	2.047E+02	6.371E+01	5.655E+01	1.834E+02	1.858E+02	4.870E+03	-7.386E+01
4000	2.079E+01	2.106E+02	8.451E+01	7.734E+01	1.895E+02	1.913E+02	4.914E+03	-5.258E+01
5000	2.079E+01	2.153E+02	1.053E+02	9.814E+01	1.942E+02	1.957E+02	4.957E+03	-3.970E+01
6000	2.079E+01	2.191E+02	1.261E+02	1.189E+02	1.981E+02	1.992E+02	5.000E+03	-3.103E+01
7000	2.081E+01	2.223E+02	1.469E+02	1.397E+02	2.013E+02	2.023E+02	5.043E+03	-2.479E+01
8000	2.085E+01	2.251E+02	1.677E+02	1.606E+02	2.041E+02	2.050E+02	5.086E+03	-2.006E+01
9000	2.094E+01	2.275E+02	1.886E+02	1.814E+02	2.066E+02	2.074E+02	5.128E+03	-1.636E+01
10000	2.109E+01	2.297E+02	2.096E+02	2.024E+02	2.088E+02	2.095E+02	5.169E+03	-1.337E+01
11000	2.132E+01	2.318E+02	2.308E+02	2.236E+02	2.108E+02	2.114E+02	5.208E+03	-1.091E+01
12000	2.162E+01	2.336E+02	2.523E+02	2.451E+02	2.126E+02	2.132E+02	5.245E+03	-8.838E+00
13000	2.199E+01	2.354E+02	2.741E+02	2.669E+02	2.143E+02	2.148E+02	5.280E+03	-7.076E+00
14000	2.243E+01	2.370E+02	2.963E+02	2.891E+02	2.158E+02	2.164E+02	5.314E+03	-5.556E+00
15000	2.291E+01	2.386E+02	3.189E+02	3.118E+02	2.173E+02	2.178E+02	5.346E+03	-4.230E+00
16000	2.343E+01	2.401E+02	3.421E+02	3.349E+02	2.187E+02	2.191E+02	5.377E+03	-3.063E+00
17000	2.398E+01	2.415E+02	3.658E+02	3.587E+02	2.200E+02	2.204E+02	5.408E+03	-2.028E+00
18000	2.453E+01	2.429E+02	3.901E+02	3.829E+02	2.212E+02	2.216E+02	5.441E+03	-1.102E+00
19000	2.508E+01	2.442E+02	4.149E+02	4.077E+02	2.224E+02	2.228E+02	5.475E+03	-2.686E-01
20000	2.562E+01	2.455E+02	4.402E+02	4.331E+02	2.235E+02	2.239E+02	5.510E+03	4.863E-01
21000	2.615E+01	2.468E+02	4.661E+02	4.589E+02	2.246E+02	2.249E+02	5.548E+03	1.174E+00
22000	2.665E+01	2.480E+02	4.925E+02	4.854E+02	2.256E+02	2.260E+02	5.588E+03	1.803E+00
23000	2.713E+01	2.492E+02	5.194E+02	5.122E+02	2.266E+02	2.269E+02	5.630E+03	2.382E+00
24000	2.759E+01	2.504E+02	5.468E+02	5.396E+02	2.276E+02	2.279E+02	5.673E+03	2.917E+00
25000	2.803E+01	2.515E+02	5.746E+02	5.674E+02	2.285E+02	2.288E+02	5.719E+03	3.413E+00
26000	2.847E+01	2.526E+02	6.028E+02	5.957E+02	2.294E+02	2.297E+02	5.766E+03	3.874E+00
27000	2.892E+01	2.537E+02	6.315E+02	6.244E+02	2.303E+02	2.306E+02	5.815E+03	4.305E+00
28000	2.942E+01	2.548E+02	6.607E+02	6.535E+02	2.312E+02	2.314E+02	5.866E+03	4.708E+00
29000	3.003E+01	2.558E+02	6.904E+02	6.832E+02	2.320E+02	2.322E+02	5.918E+03	5.088E+00
30000	3.080E+01	2.568E+02	7.208E+02	7.136E+02	2.328E+02	2.331E+02	5.972E+03	5.444E+00
32000	3.330E+01	2.589E+02	7.846E+02	7.775E+02	2.344E+02	2.346E+02	6.084E+03	6.100E+00
34000	3.804E+01	2.611E+02	8.555E+02	8.483E+02	2.359E+02	2.361E+02	6.205E+03	6.690E+00
36000	4.668E+01	2.634E+02	9.394E+02	9.322E+02	2.373E+02	2.376E+02	6.342E+03	7.225E+00
38000	6.117E+01	2.663E+02	1.046E+03	1.039E+03	2.388E+02	2.390E+02	6.502E+03	7.715E+00
40000	8.323E+01	2.700E+02	1.189E+03	1.182E+03	2.403E+02	2.404E+02	6.701E+03	8.168E+00
42000	1.132E+02	2.747E+02	1.384E+03	1.377E+03	2.418E+02	2.419E+02	6.952E+03	8.593E+00
44000	1.489E+02	2.808E+02	1.646E+03	1.639E+03	2.434E+02	2.436E+02	7.271E+03	8.994E+00
46000	1.846E+02	2.882E+02	1.980E+03	1.973E+03	2.452E+02	2.453E+02	7.662E+03	9.379E+00
48000	2.128E+02	2.967E+02	2.379E+03	2.372E+03	2.472E+02	2.473E+02	8.120E+03	9.752E+00
50000	2.271E+02	3.058E+02	2.822E+03	2.815E+03	2.493E+02	2.495E+02	8.621E+03	1.012E+01

Table 133: Internal thermodynamic properties of N^{2+} ΔE=500 cm^{-1}

T(K)	Q_{int}	$\ln(Q_{int})$	E_{int}/RT	$C_{p,int}/R$
50	$2.026E+00$	$7.063E-01$	$6.553E-02$	$3.245E-01$
100	$2.325E+00$	$8.439E-01$	$3.511E-01$	$7.576E-01$
150	$2.751E+00$	$1.012E+00$	$4.566E-01$	$5.553E-01$
200	$3.141E+00$	$1.144E+00$	$4.557E-01$	$3.641E-01$
298.15	$3.724E+00$	$1.315E+00$	$3.896E-01$	$1.761E-01$
300	$3.733E+00$	$1.317E+00$	$3.883E-01$	$1.740E-01$
400	$4.136E+00$	$1.420E+00$	$3.240E-01$	$9.827E-02$
500	$4.422E+00$	$1.487E+00$	$2.748E-01$	$6.239E-02$
600	$4.633E+00$	$1.533E+00$	$2.377E-01$	$4.291E-02$
700	$4.795E+00$	$1.568E+00$	$2.089E-01$	$3.124E-02$
800	$4.923E+00$	$1.594E+00$	$1.862E-01$	$2.373E-02$
900	$5.027E+00$	$1.615E+00$	$1.679E-01$	$1.862E-02$
1000	$5.112E+00$	$1.632E+00$	$1.528E-01$	$1.500E-02$
2000	$5.528E+00$	$1.710E+00$	$8.007E-02$	$3.634E-03$
3000	$5.679E+00$	$1.737E+00$	$5.418E-02$	$1.596E-03$
4000	$5.757E+00$	$1.750E+00$	$4.094E-02$	$8.932E-04$
5000	$5.804E+00$	$1.759E+00$	$3.289E-02$	$6.077E-04$
6000	$5.836E+00$	$1.764E+00$	$2.752E-02$	$8.129E-04$
7000	$5.859E+00$	$1.768E+00$	$2.380E-02$	$2.470E-03$
8000	$5.877E+00$	$1.771E+00$	$2.140E-02$	$7.479E-03$
9000	$5.891E+00$	$1.773E+00$	$2.038E-02$	$1.817E-02$
10000	$5.904E+00$	$1.776E+00$	$2.101E-02$	$3.655E-02$
11000	$5.917E+00$	$1.778E+00$	$2.359E-02$	$6.382E-02$
12000	$5.930E+00$	$1.780E+00$	$2.840E-02$	$1.002E-01$
13000	$5.945E+00$	$1.783E+00$	$3.560E-02$	$1.452E-01$
14000	$5.963E+00$	$1.786E+00$	$4.526E-02$	$1.976E-01$
15000	$5.984E+00$	$1.789E+00$	$5.733E-02$	$2.559E-01$
16000	$6.008E+00$	$1.793E+00$	$7.168E-02$	$3.184E-01$
17000	$6.038E+00$	$1.798E+00$	$8.810E-02$	$3.837E-01$
18000	$6.071E+00$	$1.804E+00$	$1.064E-01$	$4.501E-01$
19000	$6.109E+00$	$1.810E+00$	$1.262E-01$	$5.165E-01$
20000	$6.152E+00$	$1.817E+00$	$1.474E-01$	$5.817E-01$
21000	$6.200E+00$	$1.825E+00$	$1.696E-01$	$6.448E-01$
22000	$6.252E+00$	$1.833E+00$	$1.925E-01$	$7.053E-01$
23000	$6.309E+00$	$1.842E+00$	$2.161E-01$	$7.625E-01$
24000	$6.371E+00$	$1.852E+00$	$2.400E-01$	$8.164E-01$
25000	$6.437E+00$	$1.862E+00$	$2.641E-01$	$8.670E-01$
26000	$6.507E+00$	$1.873E+00$	$2.882E-01$	$9.145E-01$
27000	$6.581E+00$	$1.884E+00$	$3.122E-01$	$9.598E-01$
28000	$6.659E+00$	$1.896E+00$	$3.361E-01$	$1.004E+00$
29000	$6.741E+00$	$1.908E+00$	$3.599E-01$	$1.049E+00$
30000	$6.826E+00$	$1.921E+00$	$3.837E-01$	$1.097E+00$
32000	$7.008E+00$	$1.947E+00$	$4.318E-01$	$1.218E+00$
34000	$7.205E+00$	$1.975E+00$	$4.832E-01$	$1.406E+00$
36000	$7.419E+00$	$2.004E+00$	$5.424E-01$	$1.719E+00$
38000	$7.654E+00$	$2.035E+00$	$6.168E-01$	$2.234E+00$
40000	$7.919E+00$	$2.069E+00$	$7.164E-01$	$3.041E+00$
42000	$8.227E+00$	$2.107E+00$	$8.536E-01$	$4.225E+00$
44000	$8.595E+00$	$2.151E+00$	$1.042E+00$	$5.842E+00$
46000	$9.050E+00$	$2.203E+00$	$1.294E+00$	$7.889E+00$
48000	$9.626E+00$	$2.264E+00$	$1.617E+00$	$1.026E+01$
50000	$1.036E+01$	$2.338E+00$	$2.013E+00$	$1.276E+01$

Table 134: Total thermodynamic properties of N^{2+} ΔE=500 cm^{-1}

T [K]	C_p [J/mol/K]	S^0 [J/mol/K]	$H^0(T)$-$H^0(0)$ [KJ/mol]	$H^0(T)$-$H^0(298)$ [KJ/mol]	-(G^0-$H^0(0)$)/T [J/mol/K]	-(G^0-$H^0(298)$)/T [J/mol/K]	ΔH_f [KJ/mol]	Log(K_p)
50	2.348E+01	1.111E+02	1.067E+00	-6.097E+00	8.975E+01	2.330E+02	4.734E+03	-4.945E+03
100	2.709E+01	1.290E+02	2.370E+00	-4.793E+00	1.053E+02	1.769E+02	4.737E+03	-2.472E+03
150	2.540E+01	1.397E+02	3.687E+00	-3.476E+00	1.151E+02	1.629E+02	4.740E+03	-1.647E+03
200	2.381E+01	1.468E+02	4.915E+00	-2.248E+00	1.222E+02	1.580E+02	4.742E+03	-1.234E+03
298.15	2.225E+01	1.559E+02	7.163E+00	0.000E+00	1.319E+02	1.559E+02	4.747E+03	-8.263E+02
300	2.223E+01	1.561E+02	7.204E+00	4.113E-02	1.321E+02	1.559E+02	4.747E+03	-8.212E+02
400	2.160E+01	1.624E+02	9.392E+00	2.229E+00	1.389E+02	1.568E+02	4.752E+03	-6.145E+02
500	2.130E+01	1.672E+02	1.154E+01	4.372E+00	1.441E+02	1.584E+02	4.757E+03	-4.903E+02
600	2.114E+01	1.710E+02	1.366E+01	6.494E+00	1.483E+02	1.602E+02	4.762E+03	-4.074E+02
700	2.105E+01	1.743E+02	1.577E+01	8.603E+00	1.518E+02	1.620E+02	4.767E+03	-3.482E+02
800	2.098E+01	1.771E+02	1.787E+01	1.071E+01	1.548E+02	1.637E+02	4.771E+03	-3.037E+02
900	2.094E+01	1.796E+02	1.996E+01	1.280E+01	1.574E+02	1.653E+02	4.776E+03	-2.691E+02
1000	2.091E+01	1.818E+02	2.206E+01	1.489E+01	1.597E+02	1.669E+02	4.781E+03	-2.413E+02
2000	2.082E+01	1.962E+02	4.290E+01	3.574E+01	1.748E+02	1.783E+02	4.826E+03	-1.160E+02
3000	2.080E+01	2.047E+02	6.371E+01	5.655E+01	1.834E+02	1.858E+02	4.870E+03	-7.386E+01
4000	2.079E+01	2.106E+02	8.451E+01	7.734E+01	1.895E+02	1.913E+02	4.914E+03	-5.258E+01
5000	2.079E+01	2.153E+02	1.053E+02	9.814E+01	1.942E+02	1.957E+02	4.957E+03	-3.970E+01
6000	2.079E+01	2.191E+02	1.261E+02	1.189E+02	1.981E+02	1.992E+02	5.000E+03	-3.103E+01
7000	2.081E+01	2.223E+02	1.469E+02	1.397E+02	2.013E+02	2.023E+02	5.043E+03	-2.479E+01
8000	2.085E+01	2.251E+02	1.677E+02	1.606E+02	2.041E+02	2.050E+02	5.086E+03	-2.006E+01
9000	2.094E+01	2.275E+02	1.886E+02	1.814E+02	2.066E+02	2.074E+02	5.128E+03	-1.636E+01
10000	2.109E+01	2.297E+02	2.096E+02	2.024E+02	2.088E+02	2.095E+02	5.169E+03	-1.337E+01
11000	2.132E+01	2.318E+02	2.308E+02	2.236E+02	2.108E+02	2.114E+02	5.208E+03	-1.091E+01
12000	2.162E+01	2.336E+02	2.523E+02	2.451E+02	2.126E+02	2.132E+02	5.245E+03	-8.838E+00
13000	2.199E+01	2.354E+02	2.741E+02	2.669E+02	2.143E+02	2.148E+02	5.280E+03	-7.076E+00
14000	2.243E+01	2.370E+02	2.963E+02	2.891E+02	2.158E+02	2.164E+02	5.314E+03	-5.556E+00
15000	2.291E+01	2.386E+02	3.189E+02	3.118E+02	2.173E+02	2.178E+02	5.346E+03	-4.230E+00
16000	2.343E+01	2.401E+02	3.421E+02	3.349E+02	2.187E+02	2.191E+02	5.377E+03	-3.063E+00
17000	2.398E+01	2.415E+02	3.658E+02	3.587E+02	2.200E+02	2.204E+02	5.408E+03	-2.028E+00
18000	2.453E+01	2.429E+02	3.901E+02	3.829E+02	2.212E+02	2.216E+02	5.441E+03	-1.102E+00
19000	2.508E+01	2.442E+02	4.149E+02	4.077E+02	2.224E+02	2.228E+02	5.475E+03	-2.686E-01
20000	2.562E+01	2.455E+02	4.402E+02	4.331E+02	2.235E+02	2.239E+02	5.510E+03	4.863E-01
21000	2.615E+01	2.468E+02	4.661E+02	4.589E+02	2.246E+02	2.249E+02	5.548E+03	1.174E+00
22000	2.665E+01	2.480E+02	4.925E+02	4.854E+02	2.256E+02	2.260E+02	5.588E+03	1.803E+00
23000	2.713E+01	2.492E+02	5.194E+02	5.122E+02	2.266E+02	2.269E+02	5.630E+03	2.382E+00
24000	2.757E+01	2.504E+02	5.468E+02	5.396E+02	2.276E+02	2.279E+02	5.673E+03	2.917E+00
25000	2.800E+01	2.515E+02	5.745E+02	5.674E+02	2.285E+02	2.288E+02	5.719E+03	3.413E+00
26000	2.839E+01	2.526E+02	6.027E+02	5.956E+02	2.294E+02	2.297E+02	5.766E+03	3.874E+00
27000	2.877E+01	2.537E+02	6.313E+02	6.242E+02	2.303E+02	2.306E+02	5.815E+03	4.305E+00
28000	2.914E+01	2.548E+02	6.603E+02	6.531E+02	2.312E+02	2.314E+02	5.866E+03	4.708E+00
29000	2.951E+01	2.558E+02	6.896E+02	6.824E+02	2.320E+02	2.322E+02	5.917E+03	5.087E+00
30000	2.991E+01	2.568E+02	7.193E+02	7.121E+02	2.328E+02	2.331E+02	5.970E+03	5.444E+00
32000	3.091E+01	2.588E+02	7.801E+02	7.729E+02	2.344E+02	2.346E+02	6.079E+03	6.100E+00
34000	3.247E+01	2.607E+02	8.433E+02	8.361E+02	2.359E+02	2.361E+02	6.193E+03	6.689E+00
36000	3.508E+01	2.626E+02	9.106E+02	9.035E+02	2.373E+02	2.375E+02	6.313E+03	7.222E+00
38000	3.936E+01	2.646E+02	9.847E+02	9.776E+02	2.387E+02	2.389E+02	6.441E+03	7.709E+00
40000	4.607E+01	2.668E+02	1.070E+03	1.062E+03	2.400E+02	2.402E+02	6.581E+03	8.156E+00
42000	5.591E+01	2.692E+02	1.171E+03	1.164E+03	2.414E+02	2.415E+02	6.739E+03	8.570E+00
44000	6.936E+01	2.721E+02	1.296E+03	1.289E+03	2.427E+02	2.428E+02	6.920E+03	8.956E+00
46000	8.638E+01	2.756E+02	1.451E+03	1.444E+03	2.440E+02	2.442E+02	7.133E+03	9.319E+00
48000	1.061E+02	2.797E+02	1.643E+03	1.636E+03	2.454E+02	2.456E+02	7.384E+03	9.662E+00
50000	1.269E+02	2.844E+02	1.876E+03	1.869E+03	2.469E+02	2.470E+02	7.675E+03	9.989E+00

Table 135: Internal thermodynamic properties of N^{2+} ΔE=1000 cm^{-1}

T(K)	Q_{int}	$\ln(Q_{int})$	E_{int}/RT	$C_{p,int}/R$
50	$2.026E+00$	$7.063E-01$	$6.553E-02$	$3.245E-01$
100	$2.325E+00$	$8.439E-01$	$3.511E-01$	$7.576E-01$
150	$2.751E+00$	$1.012E+00$	$4.566E-01$	$5.553E-01$
200	$3.141E+00$	$1.144E+00$	$4.557E-01$	$3.641E-01$
298.15	$3.724E+00$	$1.315E+00$	$3.896E-01$	$1.761E-01$
300	$3.733E+00$	$1.317E+00$	$3.883E-01$	$1.740E-01$
400	$4.136E+00$	$1.420E+00$	$3.240E-01$	$9.827E-02$
500	$4.422E+00$	$1.487E+00$	$2.748E-01$	$6.239E-02$
600	$4.633E+00$	$1.533E+00$	$2.377E-01$	$4.291E-02$
700	$4.795E+00$	$1.568E+00$	$2.089E-01$	$3.124E-02$
800	$4.923E+00$	$1.594E+00$	$1.862E-01$	$2.373E-02$
900	$5.027E+00$	$1.615E+00$	$1.679E-01$	$1.862E-02$
1000	$5.112E+00$	$1.632E+00$	$1.528E-01$	$1.500E-02$
2000	$5.528E+00$	$1.710E+00$	$8.007E-02$	$3.634E-03$
3000	$5.679E+00$	$1.737E+00$	$5.418E-02$	$1.596E-03$
4000	$5.757E+00$	$1.750E+00$	$4.094E-02$	$8.932E-04$
5000	$5.804E+00$	$1.759E+00$	$3.289E-02$	$6.077E-04$
6000	$5.836E+00$	$1.764E+00$	$2.752E-02$	$8.129E-04$
7000	$5.859E+00$	$1.768E+00$	$2.380E-02$	$2.470E-03$
8000	$5.877E+00$	$1.771E+00$	$2.140E-02$	$7.479E-03$
9000	$5.891E+00$	$1.773E+00$	$2.038E-02$	$1.817E-02$
10000	$5.904E+00$	$1.776E+00$	$2.101E-02$	$3.655E-02$
11000	$5.917E+00$	$1.778E+00$	$2.359E-02$	$6.382E-02$
12000	$5.930E+00$	$1.780E+00$	$2.840E-02$	$1.002E-01$
13000	$5.945E+00$	$1.783E+00$	$3.560E-02$	$1.452E-01$
14000	$5.963E+00$	$1.786E+00$	$4.526E-02$	$1.976E-01$
15000	$5.984E+00$	$1.789E+00$	$5.733E-02$	$2.559E-01$
16000	$6.008E+00$	$1.793E+00$	$7.168E-02$	$3.184E-01$
17000	$6.038E+00$	$1.798E+00$	$8.810E-02$	$3.837E-01$
18000	$6.071E+00$	$1.804E+00$	$1.064E-01$	$4.501E-01$
19000	$6.109E+00$	$1.810E+00$	$1.262E-01$	$5.165E-01$
20000	$6.152E+00$	$1.817E+00$	$1.474E-01$	$5.817E-01$
21000	$6.200E+00$	$1.825E+00$	$1.696E-01$	$6.448E-01$
22000	$6.252E+00$	$1.833E+00$	$1.925E-01$	$7.052E-01$
23000	$6.309E+00$	$1.842E+00$	$2.161E-01$	$7.623E-01$
24000	$6.371E+00$	$1.852E+00$	$2.400E-01$	$8.159E-01$
25000	$6.437E+00$	$1.862E+00$	$2.640E-01$	$8.659E-01$
26000	$6.507E+00$	$1.873E+00$	$2.881E-01$	$9.122E-01$
27000	$6.581E+00$	$1.884E+00$	$3.120E-01$	$9.552E-01$
28000	$6.659E+00$	$1.896E+00$	$3.357E-01$	$9.953E-01$
29000	$6.741E+00$	$1.908E+00$	$3.591E-01$	$1.033E+00$
30000	$6.826E+00$	$1.921E+00$	$3.822E-01$	$1.070E+00$
32000	$7.006E+00$	$1.947E+00$	$4.274E-01$	$1.144E+00$
34000	$7.200E+00$	$1.974E+00$	$4.721E-01$	$1.233E+00$
36000	$7.406E+00$	$2.002E+00$	$5.176E-01$	$1.357E+00$
38000	$7.626E+00$	$2.032E+00$	$5.663E-01$	$1.541E+00$
40000	$7.862E+00$	$2.062E+00$	$6.215E-01$	$1.819E+00$
42000	$8.116E+00$	$2.094E+00$	$6.876E-01$	$2.223E+00$
44000	$8.395E+00$	$2.128E+00$	$7.696E-01$	$2.789E+00$
46000	$8.707E+00$	$2.164E+00$	$8.730E-01$	$3.541E+00$
48000	$9.060E+00$	$2.204E+00$	$1.003E+00$	$4.491E+00$
50000	$9.469E+00$	$2.248E+00$	$1.165E+00$	$5.630E+00$

Table 136: Total thermodynamic properties of N^{2+} ΔE=1000 cm^{-1}

T [K]	C_p [J/mol/K]	S^0 [J/mol/K]	$H^0(T)$-$H^0(0)$ [KJ/mol]	$H^0(T)$-$H^0(298)$ [KJ/mol]	-(G^0-$H^0(0)$)/T [J/mol/K]	-(G^0-$H^0(298)$)/T [J/mol/K]	ΔH_f [KJ/mol]	Log(K_p)
50	2.348E+01	1.111E+02	1.067E+00	-6.097E+00	8.975E+01	2.330E+02	4.734E+03	-4.945E+03
100	2.709E+01	1.290E+02	2.370E+00	-4.793E+00	1.053E+02	1.769E+02	4.737E+03	-2.472E+03
150	2.540E+01	1.397E+02	3.687E+00	-3.476E+00	1.151E+02	1.629E+02	4.740E+03	-1.647E+03
200	2.381E+01	1.468E+02	4.915E+00	-2.248E+00	1.222E+02	1.580E+02	4.742E+03	-1.234E+03
298.15	2.225E+01	1.559E+02	7.163E+00	0.000E+00	1.319E+02	1.559E+02	4.747E+03	-8.263E+02
300	2.223E+01	1.561E+02	7.204E+00	4.113E-02	1.321E+02	1.559E+02	4.747E+03	-8.212E+02
400	2.160E+01	1.624E+02	9.392E+00	2.229E+00	1.389E+02	1.568E+02	4.752E+03	-6.145E+02
500	2.130E+01	1.672E+02	1.154E+01	4.372E+00	1.441E+02	1.584E+02	4.757E+03	-4.903E+02
600	2.114E+01	1.710E+02	1.366E+01	6.494E+00	1.483E+02	1.602E+02	4.762E+03	-4.074E+02
700	2.105E+01	1.743E+02	1.577E+01	8.603E+00	1.518E+02	1.620E+02	4.767E+03	-3.482E+02
800	2.098E+01	1.771E+02	1.787E+01	1.071E+01	1.548E+02	1.637E+02	4.771E+03	-3.037E+02
900	2.094E+01	1.796E+02	1.996E+01	1.280E+01	1.574E+02	1.653E+02	4.776E+03	-2.691E+02
1000	2.091E+01	1.818E+02	2.206E+01	1.489E+01	1.597E+02	1.669E+02	4.781E+03	-2.413E+02
2000	2.082E+01	1.962E+02	4.290E+01	3.574E+01	1.748E+02	1.783E+02	4.826E+03	-1.160E+02
3000	2.080E+01	2.047E+02	6.371E+01	5.655E+01	1.834E+02	1.858E+02	4.870E+03	-7.386E+01
4000	2.079E+01	2.106E+02	8.451E+01	7.734E+01	1.895E+02	1.913E+02	4.914E+03	-5.258E+01
5000	2.079E+01	2.153E+02	1.053E+02	9.814E+01	1.942E+02	1.957E+02	4.957E+03	-3.970E+01
6000	2.079E+01	2.191E+02	1.261E+02	1.189E+02	1.981E+02	1.992E+02	5.000E+03	-3.103E+01
7000	2.081E+01	2.223E+02	1.469E+02	1.397E+02	2.013E+02	2.023E+02	5.043E+03	-2.479E+01
8000	2.085E+01	2.251E+02	1.677E+02	1.606E+02	2.041E+02	2.050E+02	5.086E+03	-2.006E+01
9000	2.094E+01	2.275E+02	1.886E+02	1.814E+02	2.066E+02	2.074E+02	5.128E+03	-1.636E+01
10000	2.109E+01	2.297E+02	2.096E+02	2.024E+02	2.088E+02	2.095E+02	5.169E+03	-1.337E+01
11000	2.132E+01	2.318E+02	2.308E+02	2.236E+02	2.108E+02	2.114E+02	5.208E+03	-1.091E+01
12000	2.162E+01	2.336E+02	2.523E+02	2.451E+02	2.126E+02	2.132E+02	5.245E+03	-8.838E+00
13000	2.199E+01	2.354E+02	2.741E+02	2.669E+02	2.143E+02	2.148E+02	5.280E+03	-7.076E+00
14000	2.243E+01	2.370E+02	2.963E+02	2.891E+02	2.158E+02	2.164E+02	5.314E+03	-5.556E+00
15000	2.291E+01	2.386E+02	3.189E+02	3.118E+02	2.173E+02	2.178E+02	5.346E+03	-4.230E+00
16000	2.343E+01	2.401E+02	3.421E+02	3.349E+02	2.187E+02	2.191E+02	5.377E+03	-3.063E+00
17000	2.398E+01	2.415E+02	3.658E+02	3.587E+02	2.200E+02	2.204E+02	5.408E+03	-2.028E+00
18000	2.453E+01	2.429E+02	3.901E+02	3.829E+02	2.212E+02	2.216E+02	5.441E+03	-1.102E+00
19000	2.508E+01	2.442E+02	4.149E+02	4.077E+02	2.224E+02	2.228E+02	5.475E+03	-2.686E-01
20000	2.562E+01	2.455E+02	4.402E+02	4.331E+02	2.235E+02	2.239E+02	5.510E+03	4.863E-01
21000	2.615E+01	2.468E+02	4.661E+02	4.589E+02	2.246E+02	2.249E+02	5.548E+03	1.174E+00
22000	2.665E+01	2.480E+02	4.925E+02	4.854E+02	2.256E+02	2.260E+02	5.588E+03	1.803E+00
23000	2.712E+01	2.492E+02	5.194E+02	5.122E+02	2.266E+02	2.269E+02	5.629E+03	2.382E+00
24000	2.757E+01	2.504E+02	5.468E+02	5.396E+02	2.276E+02	2.279E+02	5.673E+03	2.917E+00
25000	2.798E+01	2.515E+02	5.745E+02	5.674E+02	2.285E+02	2.288E+02	5.719E+03	3.413E+00
26000	2.837E+01	2.526E+02	6.027E+02	5.955E+02	2.294E+02	2.297E+02	5.766E+03	3.874E+00
27000	2.873E+01	2.537E+02	6.313E+02	6.241E+02	2.303E+02	2.306E+02	5.815E+03	4.305E+00
28000	2.906E+01	2.548E+02	6.602E+02	6.530E+02	2.312E+02	2.314E+02	5.865E+03	4.708E+00
29000	2.938E+01	2.558E+02	6.894E+02	6.822E+02	2.320E+02	2.322E+02	5.917E+03	5.087E+00
30000	2.968E+01	2.568E+02	7.189E+02	7.118E+02	2.328E+02	2.331E+02	5.970E+03	5.444E+00
32000	3.030E+01	2.587E+02	7.789E+02	7.717E+02	2.344E+02	2.346E+02	6.078E+03	6.099E+00
34000	3.104E+01	2.606E+02	8.402E+02	8.330E+02	2.359E+02	2.361E+02	6.190E+03	6.688E+00
36000	3.207E+01	2.624E+02	9.032E+02	8.961E+02	2.373E+02	2.375E+02	6.306E+03	7.221E+00
38000	3.360E+01	2.641E+02	9.688E+02	9.616E+02	2.387E+02	2.388E+02	6.425E+03	7.707E+00
40000	3.591E+01	2.659E+02	1.038E+03	1.031E+03	2.400E+02	2.402E+02	6.550E+03	8.153E+00
42000	3.927E+01	2.678E+02	1.113E+03	1.106E+03	2.412E+02	2.414E+02	6.681E+03	8.565E+00
44000	4.397E+01	2.697E+02	1.196E+03	1.189E+03	2.425E+02	2.427E+02	6.821E+03	8.946E+00
46000	5.023E+01	2.718E+02	1.290E+03	1.283E+03	2.437E+02	2.439E+02	6.972E+03	9.302E+00
48000	5.813E+01	2.741E+02	1.398E+03	1.391E+03	2.449E+02	2.451E+02	7.138E+03	9.636E+00
50000	6.760E+01	2.766E+02	1.524E+03	1.516E+03	2.462E+02	2.463E+02	7.322E+03	9.950E+00

Table 137: Internal thermodynamic properties of N^{3+} ΔE=250 cm^{-1}

T(K)	Q_{int}	$\ln(Q_{int})$	E_{int}/RT	$C_{p,int}/R$
50	$1.000E+00$	$0.000E+00$	$0.000E+00$	$0.000E+00$
100	$1.000E+00$	$0.000E+00$	$0.000E+00$	$0.000E+00$
150	$1.000E+00$	$0.000E+00$	$1.690E-277$	$1.092E-274$
200	$1.000E+00$	$0.000E+00$	$1.726E-207$	$8.364E-205$
298.15	$1.000E+00$	$0.000E+00$	$2.126E-138$	$6.908E-136$
300	$1.000E+00$	$0.000E+00$	$1.567E-137$	$5.062E-135$
400	$1.000E+00$	$0.000E+00$	$1.372E-102$	$3.323E-100$
500	$1.000E+00$	$0.000E+00$	$1.204E-81$	$2.333E-79$
600	$1.000E+00$	$0.000E+00$	$1.067E-67$	$1.723E-65$
700	$1.000E+00$	$0.000E+00$	$9.560E-58$	$1.323E-55$
800	$1.000E+00$	$0.000E+00$	$2.734E-50$	$3.312E-48$
900	$1.000E+00$	$0.000E+00$	$1.699E-44$	$1.829E-42$
1000	$1.000E+00$	$0.000E+00$	$7.245E-40$	$7.020E-38$
2000	$1.000E+00$	$0.000E+00$	$3.974E-19$	$1.925E-17$
3000	$1.000E+00$	$8.460E-14$	$2.733E-12$	$8.826E-11$
4000	$1.000E+00$	$2.717E-10$	$6.582E-09$	$1.594E-07$
5000	$1.000E+00$	$3.453E-08$	$6.691E-07$	$1.297E-05$
6000	$1.000E+00$	$8.726E-07$	$1.409E-05$	$2.276E-04$
7000	$1.000E+00$	$8.765E-06$	$1.213E-04$	$1.679E-03$
8000	$1.000E+00$	$4.945E-05$	$5.989E-04$	$7.254E-03$
9000	$1.000E+00$	$1.899E-04$	$2.045E-03$	$2.201E-02$
10000	$1.001E+00$	$5.573E-04$	$5.399E-03$	$5.228E-02$
11000	$1.001E+00$	$1.344E-03$	$1.183E-02$	$1.041E-01$
12000	$1.003E+00$	$2.799E-03$	$2.257E-02$	$1.818E-01$
13000	$1.005E+00$	$5.203E-03$	$3.869E-02$	$2.871E-01$
14000	$1.009E+00$	$8.847E-03$	$6.099E-02$	$4.188E-01$
15000	$1.014E+00$	$1.400E-02$	$8.988E-02$	$5.734E-01$
16000	$1.021E+00$	$2.090E-02$	$1.254E-01$	$7.454E-01$
17000	$1.030E+00$	$2.973E-02$	$1.672E-01$	$9.282E-01$
18000	$1.041E+00$	$4.060E-02$	$2.147E-01$	$1.115E+00$
19000	$1.055E+00$	$5.359E-02$	$2.669E-01$	$1.298E+00$
20000	$1.071E+00$	$6.869E-02$	$3.229E-01$	$1.472E+00$
21000	$1.090E+00$	$8.585E-02$	$3.815E-01$	$1.633E+00$
22000	$1.111E+00$	$1.050E-01$	$4.416E-01$	$1.775E+00$
23000	$1.134E+00$	$1.260E-01$	$5.024E-01$	$1.898E+00$
24000	$1.160E+00$	$1.486E-01$	$5.627E-01$	$1.999E+00$
25000	$1.189E+00$	$1.728E-01$	$6.218E-01$	$2.080E+00$
26000	$1.219E+00$	$1.983E-01$	$6.792E-01$	$2.141E+00$
27000	$1.252E+00$	$2.250E-01$	$7.341E-01$	$2.182E+00$
28000	$1.287E+00$	$2.526E-01$	$7.863E-01$	$2.207E+00$
29000	$1.325E+00$	$2.811E-01$	$8.356E-01$	$2.218E+00$
30000	$1.364E+00$	$3.102E-01$	$8.816E-01$	$2.215E+00$
32000	$1.447E+00$	$3.698E-01$	$9.641E-01$	$2.181E+00$
34000	$1.538E+00$	$4.304E-01$	$1.034E+00$	$2.119E+00$
36000	$1.634E+00$	$4.912E-01$	$1.092E+00$	$2.044E+00$
38000	$1.736E+00$	$5.516E-01$	$1.140E+00$	$1.967E+00$
40000	$1.842E+00$	$6.111E-01$	$1.180E+00$	$1.901E+00$
42000	$1.953E+00$	$6.695E-01$	$1.213E+00$	$1.865E+00$
44000	$2.068E+00$	$7.266E-01$	$1.243E+00$	$1.890E+00$
46000	$2.187E+00$	$7.825E-01$	$1.273E+00$	$2.019E+00$
48000	$2.311E+00$	$8.375E-01$	$1.310E+00$	$2.320E+00$
50000	$2.440E+00$	$8.919E-01$	$1.361E+00$	$2.887E+00$

Table 138: Total thermodynamic properties of N^{3+} ΔE=250 cm^{-1}

T [K]	C_p [J/mol/K]	S^0 [J/mol/K]	$H^0(T)$-$H^0(0)$ [KJ/mol]	$H^0(T)$-$H^0(298)$ [KJ/mol]	-(G^0-$H^0(0)$)/T [J/mol/K]	-(G^0-$H^0(298)$)/T [J/mol/K]	ΔH_f [KJ/mol]	Log(K_p)
50	2.079E+01	1.047E+02	1.039E+00	-5.158E+00	8.387E+01	2.078E+02	9.314E+03	-9.730E+03
100	2.079E+01	1.191E+02	2.079E+00	-4.119E+00	9.828E+01	1.602E+02	9.317E+03	-4.865E+03
150	2.079E+01	1.275E+02	3.118E+00	-3.079E+00	1.067E+02	1.480E+02	9.320E+03	-3.242E+03
200	2.079E+01	1.335E+02	4.157E+00	-2.040E+00	1.127E+02	1.437E+02	9.324E+03	-2.431E+03
298.15	2.079E+01	1.418E+02	6.197E+00	0.000E+00	1.210E+02	1.418E+02	9.331E+03	-1.629E+03
300	2.079E+01	1.419E+02	6.236E+00	3.848E-02	1.211E+02	1.418E+02	9.331E+03	-1.619E+03
400	2.079E+01	1.479E+02	8.315E+00	2.117E+00	1.271E+02	1.426E+02	9.338E+03	-1.213E+03
500	2.079E+01	1.525E+02	1.039E+01	4.196E+00	1.317E+02	1.441E+02	9.344E+03	-9.686E+02
600	2.079E+01	1.563E+02	1.247E+01	6.274E+00	1.355E+02	1.458E+02	9.351E+03	-8.059E+02
700	2.079E+01	1.595E+02	1.455E+01	8.353E+00	1.387E+02	1.476E+02	9.358E+03	-6.895E+02
800	2.079E+01	1.623E+02	1.663E+01	1.043E+01	1.415E+02	1.492E+02	9.365E+03	-6.022E+02
900	2.079E+01	1.647E+02	1.871E+01	1.251E+01	1.439E+02	1.508E+02	9.372E+03	-5.343E+02
1000	2.079E+01	1.669E+02	2.079E+01	1.459E+01	1.461E+02	1.523E+02	9.378E+03	-4.799E+02
2000	2.079E+01	1.813E+02	4.157E+01	3.538E+01	1.606E+02	1.637E+02	9.444E+03	-2.343E+02
3000	2.079E+01	1.898E+02	6.236E+01	5.616E+01	1.690E+02	1.710E+02	9.509E+03	-1.518E+02
4000	2.079E+01	1.957E+02	8.314E+01	7.695E+01	1.750E+02	1.765E+02	9.573E+03	-1.103E+02
5000	2.079E+01	2.004E+02	1.039E+02	9.773E+01	1.796E+02	1.808E+02	9.638E+03	-8.521E+01
6000	2.079E+01	2.042E+02	1.247E+02	1.185E+02	1.834E+02	1.844E+02	9.702E+03	-6.838E+01
7000	2.080E+01	2.074E+02	1.455E+02	1.393E+02	1.866E+02	1.875E+02	9.766E+03	-5.628E+01
8000	2.085E+01	2.102E+02	1.663E+02	1.601E+02	1.894E+02	1.901E+02	9.829E+03	-4.714E+01
9000	2.097E+01	2.126E+02	1.872E+02	1.810E+02	1.918E+02	1.925E+02	9.892E+03	-3.999E+01
10000	2.122E+01	2.148E+02	2.083E+02	2.021E+02	1.940E+02	1.946E+02	9.954E+03	-3.423E+01
11000	2.165E+01	2.169E+02	2.297E+02	2.235E+02	1.960E+02	1.966E+02	1.001E+04	-2.949E+01
12000	2.230E+01	2.188E+02	2.517E+02	2.455E+02	1.978E+02	1.983E+02	1.007E+04	-2.552E+01
13000	2.317E+01	2.206E+02	2.744E+02	2.682E+02	1.995E+02	2.000E+02	1.013E+04	-2.213E+01
14000	2.427E+01	2.224E+02	2.981E+02	2.919E+02	2.011E+02	2.015E+02	1.018E+04	-1.922E+01
15000	2.555E+01	2.241E+02	3.230E+02	3.168E+02	2.026E+02	2.030E+02	1.024E+04	-1.668E+01
16000	2.698E+01	2.258E+02	3.493E+02	3.431E+02	2.039E+02	2.043E+02	1.030E+04	-1.445E+01
17000	2.850E+01	2.275E+02	3.770E+02	3.708E+02	2.053E+02	2.057E+02	1.035E+04	-1.246E+01
18000	3.005E+01	2.291E+02	4.063E+02	4.001E+02	2.066E+02	2.069E+02	1.041E+04	-1.069E+01
19000	3.158E+01	2.308E+02	4.371E+02	4.309E+02	2.078E+02	2.081E+02	1.047E+04	-9.096E+00
20000	3.303E+01	2.325E+02	4.694E+02	4.632E+02	2.090E+02	2.093E+02	1.053E+04	-7.653E+00
21000	3.436E+01	2.341E+02	5.031E+02	4.969E+02	2.101E+02	2.104E+02	1.060E+04	-6.339E+00
22000	3.555E+01	2.357E+02	5.381E+02	5.319E+02	2.113E+02	2.116E+02	1.067E+04	-5.137E+00
23000	3.656E+01	2.373E+02	5.741E+02	5.680E+02	2.124E+02	2.126E+02	1.074E+04	-4.032E+00
24000	3.741E+01	2.389E+02	6.112E+02	6.050E+02	2.134E+02	2.137E+02	1.082E+04	-3.012E+00
25000	3.808E+01	2.404E+02	6.489E+02	6.427E+02	2.145E+02	2.147E+02	1.089E+04	-2.067E+00
26000	3.858E+01	2.419E+02	6.873E+02	6.811E+02	2.155E+02	2.158E+02	1.097E+04	-1.189E+00
27000	3.893E+01	2.434E+02	7.260E+02	7.198E+02	2.165E+02	2.168E+02	1.105E+04	-3.700E-01
28000	3.914E+01	2.448E+02	7.651E+02	7.589E+02	2.175E+02	2.177E+02	1.113E+04	3.962E-01
29000	3.923E+01	2.462E+02	8.043E+02	7.981E+02	2.185E+02	2.187E+02	1.121E+04	1.115E+00
30000	3.921E+01	2.475E+02	8.435E+02	8.373E+02	2.194E+02	2.196E+02	1.130E+04	1.790E+00
32000	3.892E+01	2.501E+02	9.217E+02	9.155E+02	2.213E+02	2.214E+02	1.146E+04	3.029E+00
34000	3.841E+01	2.524E+02	9.990E+02	9.928E+02	2.230E+02	2.232E+02	1.163E+04	4.137E+00
36000	3.778E+01	2.546E+02	1.075E+03	1.069E+03	2.247E+02	2.249E+02	1.180E+04	5.137E+00
38000	3.714E+01	2.566E+02	1.150E+03	1.144E+03	2.263E+02	2.265E+02	1.198E+04	6.045E+00
40000	3.659E+01	2.585E+02	1.224E+03	1.218E+03	2.279E+02	2.281E+02	1.214E+04	6.874E+00
42000	3.630E+01	2.603E+02	1.297E+03	1.290E+03	2.294E+02	2.296E+02	1.232E+04	7.634E+00
44000	3.650E+01	2.620E+02	1.369E+03	1.363E+03	2.308E+02	2.310E+02	1.249E+04	8.335E+00
46000	3.757E+01	2.636E+02	1.443E+03	1.437E+03	2.322E+02	2.324E+02	1.266E+04	8.984E+00
48000	4.008E+01	2.652E+02	1.521E+03	1.514E+03	2.336E+02	2.337E+02	1.284E+04	9.587E+00
50000	4.479E+01	2.670E+02	1.605E+03	1.599E+03	2.349E+02	2.350E+02	1.302E+04	1.015E+01

Table 139: Internal thermodynamic properties of N^{3+} ΔE=500 cm^{-1}

T(K)	Q_{int}	$\ln(Q_{int})$	E_{int}/RT	$C_{p,int}/R$
50	$1.000E+00$	$0.000E+00$	$0.000E+00$	$0.000E+00$
100	$1.000E+00$	$0.000E+00$	$0.000E+00$	$0.000E+00$
150	$1.000E+00$	$0.000E+00$	$1.690E-277$	$1.092E-274$
200	$1.000E+00$	$0.000E+00$	$1.726E-207$	$8.364E-205$
298.15	$1.000E+00$	$0.000E+00$	$2.126E-138$	$6.908E-136$
300	$1.000E+00$	$0.000E+00$	$1.567E-137$	$5.062E-135$
400	$1.000E+00$	$0.000E+00$	$1.372E-102$	$3.323E-100$
500	$1.000E+00$	$0.000E+00$	$1.204E-81$	$2.333E-79$
600	$1.000E+00$	$0.000E+00$	$1.067E-67$	$1.723E-65$
700	$1.000E+00$	$0.000E+00$	$9.560E-58$	$1.323E-55$
800	$1.000E+00$	$0.000E+00$	$2.734E-50$	$3.312E-48$
900	$1.000E+00$	$0.000E+00$	$1.699E-44$	$1.829E-42$
1000	$1.000E+00$	$0.000E+00$	$7.245E-40$	$7.020E-38$
2000	$1.000E+00$	$0.000E+00$	$3.974E-19$	$1.925E-17$
3000	$1.000E+00$	$8.460E-14$	$2.733E-12$	$8.826E-11$
4000	$1.000E+00$	$2.717E-10$	$6.582E-09$	$1.594E-07$
5000	$1.000E+00$	$3.453E-08$	$6.691E-07$	$1.297E-05$
6000	$1.000E+00$	$8.726E-07$	$1.409E-05$	$2.276E-04$
7000	$1.000E+00$	$8.765E-06$	$1.213E-04$	$1.679E-03$
8000	$1.000E+00$	$4.945E-05$	$5.989E-04$	$7.254E-03$
9000	$1.000E+00$	$1.899E-04$	$2.045E-03$	$2.201E-02$
10000	$1.001E+00$	$5.573E-04$	$5.399E-03$	$5.228E-02$
11000	$1.001E+00$	$1.344E-03$	$1.183E-02$	$1.041E-01$
12000	$1.003E+00$	$2.799E-03$	$2.257E-02$	$1.818E-01$
13000	$1.005E+00$	$5.203E-03$	$3.869E-02$	$2.871E-01$
14000	$1.009E+00$	$8.847E-03$	$6.099E-02$	$4.188E-01$
15000	$1.014E+00$	$1.400E-02$	$8.988E-02$	$5.734E-01$
16000	$1.021E+00$	$2.090E-02$	$1.254E-01$	$7.454E-01$
17000	$1.030E+00$	$2.973E-02$	$1.672E-01$	$9.282E-01$
18000	$1.041E+00$	$4.060E-02$	$2.147E-01$	$1.115E+00$
19000	$1.055E+00$	$5.359E-02$	$2.669E-01$	$1.298E+00$
20000	$1.071E+00$	$6.869E-02$	$3.229E-01$	$1.472E+00$
21000	$1.090E+00$	$8.585E-02$	$3.815E-01$	$1.633E+00$
22000	$1.111E+00$	$1.050E-01$	$4.416E-01$	$1.775E+00$
23000	$1.134E+00$	$1.260E-01$	$5.024E-01$	$1.898E+00$
24000	$1.160E+00$	$1.486E-01$	$5.627E-01$	$1.999E+00$
25000	$1.189E+00$	$1.728E-01$	$6.218E-01$	$2.080E+00$
26000	$1.219E+00$	$1.983E-01$	$6.792E-01$	$2.141E+00$
27000	$1.252E+00$	$2.250E-01$	$7.341E-01$	$2.182E+00$
28000	$1.287E+00$	$2.526E-01$	$7.863E-01$	$2.207E+00$
29000	$1.325E+00$	$2.811E-01$	$8.356E-01$	$2.218E+00$
30000	$1.364E+00$	$3.102E-01$	$8.816E-01$	$2.215E+00$
32000	$1.447E+00$	$3.698E-01$	$9.641E-01$	$2.181E+00$
34000	$1.538E+00$	$4.304E-01$	$1.034E+00$	$2.119E+00$
36000	$1.634E+00$	$4.912E-01$	$1.092E+00$	$2.041E+00$
38000	$1.736E+00$	$5.516E-01$	$1.140E+00$	$1.959E+00$
40000	$1.842E+00$	$6.111E-01$	$1.179E+00$	$1.880E+00$
42000	$1.953E+00$	$6.694E-01$	$1.211E+00$	$1.813E+00$
44000	$2.067E+00$	$7.263E-01$	$1.237E+00$	$1.771E+00$
46000	$2.185E+00$	$7.818E-01$	$1.260E+00$	$1.772E+00$
48000	$2.307E+00$	$8.359E-01$	$1.282E+00$	$1.840E+00$
50000	$2.432E+00$	$8.887E-01$	$1.308E+00$	$2.012E+00$

Table 140: Total thermodynamic properties of N^{3+} ΔE=500 cm^{-1}

T [K]	C_p [J/mol/K]	S^0 [J/mol/K]	$H^0(T)-H^0(0)$ [KJ/mol]	$H^0(T)-H^0(298)$ [KJ/mol]	$-(G^0-H^0(0))/T$ [J/mol/K]	$-(G^0-H^0(298))/T$ [J/mol/K]	ΔH_f [KJ/mol]	$Log(K_p)$
50	2.079E+01	1.047E+02	1.039E+00	-5.158E+00	8.387E+01	2.078E+02	9.314E+03	-9.730E+03
100	2.079E+01	1.191E+02	2.079E+00	-4.119E+00	9.828E+01	1.602E+02	9.317E+03	-4.865E+03
150	2.079E+01	1.275E+02	3.118E+00	-3.079E+00	1.067E+02	1.480E+02	9.320E+03	-3.242E+03
200	2.079E+01	1.335E+02	4.157E+00	-2.040E+00	1.127E+02	1.437E+02	9.324E+03	-2.431E+03
298.15	2.079E+01	1.418E+02	6.197E+00	0.000E+00	1.210E+02	1.418E+02	9.331E+03	-1.629E+03
300	2.079E+01	1.419E+02	6.236E+00	3.848E-02	1.211E+02	1.418E+02	9.331E+03	-1.619E+03
400	2.079E+01	1.479E+02	8.315E+00	2.117E+00	1.271E+02	1.426E+02	9.338E+03	-1.213E+03
500	2.079E+01	1.525E+02	1.039E+01	4.196E+00	1.317E+02	1.441E+02	9.344E+03	-9.686E+02
600	2.079E+01	1.563E+02	1.247E+01	6.274E+00	1.355E+02	1.458E+02	9.351E+03	-8.059E+02
700	2.079E+01	1.595E+02	1.455E+01	8.353E+00	1.387E+02	1.476E+02	9.358E+03	-6.895E+02
800	2.079E+01	1.623E+02	1.663E+01	1.043E+01	1.415E+02	1.492E+02	9.365E+03	-6.022E+02
900	2.079E+01	1.647E+02	1.871E+01	1.251E+01	1.439E+02	1.508E+02	9.372E+03	-5.343E+02
1000	2.079E+01	1.669E+02	2.079E+01	1.459E+01	1.461E+02	1.523E+02	9.378E+03	-4.799E+02
2000	2.079E+01	1.813E+02	4.157E+01	3.538E+01	1.606E+02	1.637E+02	9.444E+03	-2.343E+02
3000	2.079E+01	1.898E+02	6.236E+01	5.616E+01	1.690E+02	1.710E+02	9.509E+03	-1.518E+02
4000	2.079E+01	1.957E+02	8.314E+01	7.695E+01	1.750E+02	1.765E+02	9.573E+03	-1.103E+02
5000	2.079E+01	2.004E+02	1.039E+02	9.773E+01	1.796E+02	1.808E+02	9.638E+03	-8.521E+01
6000	2.079E+01	2.042E+02	1.247E+02	1.185E+02	1.834E+02	1.844E+02	9.702E+03	-6.838E+01
7000	2.080E+01	2.074E+02	1.455E+02	1.393E+02	1.866E+02	1.875E+02	9.766E+03	-5.628E+01
8000	2.085E+01	2.102E+02	1.663E+02	1.601E+02	1.894E+02	1.901E+02	9.829E+03	-4.714E+01
9000	2.097E+01	2.126E+02	1.872E+02	1.810E+02	1.918E+02	1.925E+02	9.892E+03	-3.999E+01
10000	2.122E+01	2.148E+02	2.083E+02	2.021E+02	1.940E+02	1.946E+02	9.954E+03	-3.423E+01
11000	2.165E+01	2.169E+02	2.297E+02	2.235E+02	1.960E+02	1.966E+02	1.001E+04	-2.949E+01
12000	2.230E+01	2.188E+02	2.517E+02	2.455E+02	1.978E+02	1.983E+02	1.007E+04	-2.552E+01
13000	2.317E+01	2.206E+02	2.744E+02	2.682E+02	1.995E+02	2.000E+02	1.013E+04	-2.213E+01
14000	2.427E+01	2.224E+02	2.981E+02	2.919E+02	2.011E+02	2.015E+02	1.018E+04	-1.922E+01
15000	2.555E+01	2.241E+02	3.230E+02	3.168E+02	2.026E+02	2.030E+02	1.024E+04	-1.668E+01
16000	2.698E+01	2.258E+02	3.493E+02	3.431E+02	2.039E+02	2.043E+02	1.030E+04	-1.445E+01
17000	2.850E+01	2.275E+02	3.770E+02	3.708E+02	2.053E+02	2.057E+02	1.035E+04	-1.246E+01
18000	3.005E+01	2.291E+02	4.063E+02	4.001E+02	2.066E+02	2.069E+02	1.041E+04	-1.069E+01
19000	3.158E+01	2.308E+02	4.371E+02	4.309E+02	2.078E+02	2.081E+02	1.047E+04	-9.096E+00
20000	3.303E+01	2.325E+02	4.694E+02	4.632E+02	2.090E+02	2.093E+02	1.053E+04	-7.653E+00
21000	3.436E+01	2.341E+02	5.031E+02	4.969E+02	2.101E+02	2.104E+02	1.060E+04	-6.339E+00
22000	3.555E+01	2.357E+02	5.381E+02	5.319E+02	2.113E+02	2.116E+02	1.067E+04	-5.137E+00
23000	3.656E+01	2.373E+02	5.741E+02	5.680E+02	2.124E+02	2.126E+02	1.074E+04	-4.032E+00
24000	3.741E+01	2.389E+02	6.112E+02	6.050E+02	2.134E+02	2.137E+02	1.082E+04	-3.012E+00
25000	3.808E+01	2.404E+02	6.489E+02	6.427E+02	2.145E+02	2.147E+02	1.089E+04	-2.067E+00
26000	3.858E+01	2.419E+02	6.873E+02	6.811E+02	2.155E+02	2.158E+02	1.097E+04	-1.189E+00
27000	3.893E+01	2.434E+02	7.260E+02	7.198E+02	2.165E+02	2.168E+02	1.105E+04	-3.700E-01
28000	3.914E+01	2.448E+02	7.651E+02	7.589E+02	2.175E+02	2.177E+02	1.113E+04	3.962E-01
29000	3.923E+01	2.462E+02	8.043E+02	7.981E+02	2.185E+02	2.187E+02	1.121E+04	1.115E+00
30000	3.921E+01	2.475E+02	8.435E+02	8.373E+02	2.194E+02	2.196E+02	1.130E+04	1.790E+00
32000	3.892E+01	2.501E+02	9.217E+02	9.155E+02	2.213E+02	2.214E+02	1.146E+04	3.029E+00
34000	3.840E+01	2.524E+02	9.990E+02	9.928E+02	2.230E+02	2.232E+02	1.163E+04	4.137E+00
36000	3.776E+01	2.546E+02	1.075E+03	1.069E+03	2.247E+02	2.249E+02	1.180E+04	5.137E+00
38000	3.707E+01	2.566E+02	1.150E+03	1.144E+03	2.263E+02	2.265E+02	1.198E+04	6.045E+00
40000	3.641E+01	2.585E+02	1.224E+03	1.217E+03	2.279E+02	2.281E+02	1.214E+04	6.874E+00
42000	3.586E+01	2.602E+02	1.296E+03	1.290E+03	2.294E+02	2.296E+02	1.232E+04	7.634E+00
44000	3.551E+01	2.619E+02	1.367E+03	1.361E+03	2.308E+02	2.310E+02	1.248E+04	8.335E+00
46000	3.552E+01	2.635E+02	1.438E+03	1.432E+03	2.322E+02	2.324E+02	1.266E+04	8.984E+00
48000	3.609E+01	2.650E+02	1.510E+03	1.503E+03	2.336E+02	2.337E+02	1.283E+04	9.587E+00
50000	3.752E+01	2.665E+02	1.583E+03	1.577E+03	2.348E+02	2.350E+02	1.300E+04	1.015E+01

Table 141: Internal thermodynamic properties of N^{3+} ΔE=1000 cm^{-1}

T(K)	Q_{int}	$\ln(Q_{int})$	E_{int}/RT	$C_{p,int}/R$
50	$1.000E+00$	$0.000E+00$	$0.000E+00$	$0.000E+00$
100	$1.000E+00$	$0.000E+00$	$0.000E+00$	$0.000E+00$
150	$1.000E+00$	$0.000E+00$	$1.690E-277$	$1.092E-274$
200	$1.000E+00$	$0.000E+00$	$1.726E-207$	$8.364E-205$
298.15	$1.000E+00$	$0.000E+00$	$2.126E-138$	$6.908E-136$
300	$1.000E+00$	$0.000E+00$	$1.567E-137$	$5.062E-135$
400	$1.000E+00$	$0.000E+00$	$1.372E-102$	$3.323E-100$
500	$1.000E+00$	$0.000E+00$	$1.204E-81$	$2.333E-79$
600	$1.000E+00$	$0.000E+00$	$1.067E-67$	$1.723E-65$
700	$1.000E+00$	$0.000E+00$	$9.560E-58$	$1.323E-55$
800	$1.000E+00$	$0.000E+00$	$2.734E-50$	$3.312E-48$
900	$1.000E+00$	$0.000E+00$	$1.699E-44$	$1.829E-42$
1000	$1.000E+00$	$0.000E+00$	$7.245E-40$	$7.020E-38$
2000	$1.000E+00$	$0.000E+00$	$3.974E-19$	$1.925E-17$
3000	$1.000E+00$	$8.460E-14$	$2.733E-12$	$8.826E-11$
4000	$1.000E+00$	$2.717E-10$	$6.582E-09$	$1.594E-07$
5000	$1.000E+00$	$3.453E-08$	$6.691E-07$	$1.297E-05$
6000	$1.000E+00$	$8.726E-07$	$1.409E-05$	$2.276E-04$
7000	$1.000E+00$	$8.765E-06$	$1.213E-04$	$1.679E-03$
8000	$1.000E+00$	$4.945E-05$	$5.989E-04$	$7.254E-03$
9000	$1.000E+00$	$1.899E-04$	$2.045E-03$	$2.201E-02$
10000	$1.001E+00$	$5.573E-04$	$5.399E-03$	$5.228E-02$
11000	$1.001E+00$	$1.344E-03$	$1.183E-02$	$1.041E-01$
12000	$1.003E+00$	$2.799E-03$	$2.257E-02$	$1.818E-01$
13000	$1.005E+00$	$5.203E-03$	$3.869E-02$	$2.871E-01$
14000	$1.009E+00$	$8.847E-03$	$6.099E-02$	$4.188E-01$
15000	$1.014E+00$	$1.400E-02$	$8.988E-02$	$5.734E-01$
16000	$1.021E+00$	$2.090E-02$	$1.254E-01$	$7.454E-01$
17000	$1.030E+00$	$2.973E-02$	$1.672E-01$	$9.282E-01$
18000	$1.041E+00$	$4.060E-02$	$2.147E-01$	$1.115E+00$
19000	$1.055E+00$	$5.359E-02$	$2.669E-01$	$1.298E+00$
20000	$1.071E+00$	$6.869E-02$	$3.229E-01$	$1.472E+00$
21000	$1.090E+00$	$8.585E-02$	$3.815E-01$	$1.633E+00$
22000	$1.111E+00$	$1.050E-01$	$4.416E-01$	$1.775E+00$
23000	$1.134E+00$	$1.260E-01$	$5.024E-01$	$1.898E+00$
24000	$1.160E+00$	$1.486E-01$	$5.627E-01$	$1.999E+00$
25000	$1.189E+00$	$1.728E-01$	$6.218E-01$	$2.080E+00$
26000	$1.219E+00$	$1.983E-01$	$6.792E-01$	$2.141E+00$
27000	$1.252E+00$	$2.250E-01$	$7.341E-01$	$2.182E+00$
28000	$1.287E+00$	$2.526E-01$	$7.863E-01$	$2.207E+00$
29000	$1.325E+00$	$2.811E-01$	$8.356E-01$	$2.218E+00$
30000	$1.364E+00$	$3.102E-01$	$8.816E-01$	$2.215E+00$
32000	$1.447E+00$	$3.698E-01$	$9.641E-01$	$2.181E+00$
34000	$1.538E+00$	$4.304E-01$	$1.034E+00$	$2.118E+00$
36000	$1.634E+00$	$4.912E-01$	$1.092E+00$	$2.040E+00$
38000	$1.736E+00$	$5.516E-01$	$1.140E+00$	$1.956E+00$
40000	$1.842E+00$	$6.110E-01$	$1.178E+00$	$1.871E+00$
42000	$1.953E+00$	$6.693E-01$	$1.210E+00$	$1.793E+00$
44000	$2.067E+00$	$7.262E-01$	$1.234E+00$	$1.726E+00$
46000	$2.185E+00$	$7.815E-01$	$1.255E+00$	$1.678E+00$
48000	$2.305E+00$	$8.353E-01$	$1.272E+00$	$1.658E+00$
50000	$2.429E+00$	$8.875E-01$	$1.288E+00$	$1.679E+00$

Table 142: Total thermodynamic properties of N^{3+} ΔE=1000 cm^{-1}

T [K]	C_p [J/mol/K]	S^0 [J/mol/K]	$H^0(T)$-$H^0(0)$ [KJ/mol]	$H^0(T)$-$H^0(298)$ [KJ/mol]	-(G^0-$H^0(0)$)/T [J/mol/K]	-(G^0-$H^0(298)$)/T [J/mol/K]	ΔH_f [KJ/mol]	Log(K_p)
50	2.079E+01	1.047E+02	1.039E+00	-5.158E+00	8.387E+01	2.078E+02	9.314E+03	-9.730E+03
100	2.079E+01	1.191E+02	2.079E+00	-4.119E+00	9.828E+01	1.602E+02	9.317E+03	-4.865E+03
150	2.079E+01	1.275E+02	3.118E+00	-3.079E+00	1.067E+02	1.480E+02	9.320E+03	-3.242E+03
200	2.079E+01	1.335E+02	4.157E+00	-2.040E+00	1.127E+02	1.437E+02	9.324E+03	-2.431E+03
298.15	2.079E+01	1.418E+02	6.197E+00	0.000E+00	1.210E+02	1.418E+02	9.331E+03	-1.629E+03
300	2.079E+01	1.419E+02	6.236E+00	3.848E-02	1.211E+02	1.418E+02	9.331E+03	-1.619E+03
400	2.079E+01	1.479E+02	8.315E+00	2.117E+00	1.271E+02	1.426E+02	9.338E+03	-1.213E+03
500	2.079E+01	1.525E+02	1.039E+01	4.196E+00	1.317E+02	1.441E+02	9.344E+03	-9.686E+02
600	2.079E+01	1.563E+02	1.247E+01	6.274E+00	1.355E+02	1.458E+02	9.351E+03	-8.059E+02
700	2.079E+01	1.595E+02	1.455E+01	8.353E+00	1.387E+02	1.476E+02	9.358E+03	-6.895E+02
800	2.079E+01	1.623E+02	1.663E+01	1.043E+01	1.415E+02	1.492E+02	9.365E+03	-6.022E+02
900	2.079E+01	1.647E+02	1.871E+01	1.251E+01	1.439E+02	1.508E+02	9.372E+03	-5.343E+02
1000	2.079E+01	1.669E+02	2.079E+01	1.459E+01	1.461E+02	1.523E+02	9.378E+03	-4.799E+02
2000	2.079E+01	1.813E+02	4.157E+01	3.538E+01	1.606E+02	1.637E+02	9.444E+03	-2.343E+02
3000	2.079E+01	1.898E+02	6.236E+01	5.616E+01	1.690E+02	1.710E+02	9.509E+03	-1.518E+02
4000	2.079E+01	1.957E+02	8.314E+01	7.695E+01	1.750E+02	1.765E+02	9.573E+03	-1.103E+02
5000	2.079E+01	2.004E+02	1.039E+02	9.773E+01	1.796E+02	1.808E+02	9.638E+03	-8.521E+01
6000	2.079E+01	2.042E+02	1.247E+02	1.185E+02	1.834E+02	1.844E+02	9.702E+03	-6.838E+01
7000	2.080E+01	2.074E+02	1.455E+02	1.393E+02	1.866E+02	1.875E+02	9.766E+03	-5.628E+01
8000	2.085E+01	2.102E+02	1.663E+02	1.601E+02	1.894E+02	1.901E+02	9.829E+03	-4.714E+01
9000	2.097E+01	2.126E+02	1.872E+02	1.810E+02	1.918E+02	1.925E+02	9.892E+03	-3.999E+01
10000	2.122E+01	2.148E+02	2.083E+02	2.021E+02	1.940E+02	1.946E+02	9.954E+03	-3.423E+01
11000	2.165E+01	2.169E+02	2.297E+02	2.235E+02	1.960E+02	1.966E+02	1.001E+04	-2.949E+01
12000	2.230E+01	2.188E+02	2.517E+02	2.455E+02	1.978E+02	1.983E+02	1.007E+04	-2.552E+01
13000	2.317E+01	2.206E+02	2.744E+02	2.682E+02	1.995E+02	2.000E+02	1.013E+04	-2.213E+01
14000	2.427E+01	2.224E+02	2.981E+02	2.919E+02	2.011E+02	2.015E+02	1.018E+04	-1.922E+01
15000	2.555E+01	2.241E+02	3.230E+02	3.168E+02	2.026E+02	2.030E+02	1.024E+04	-1.668E+01
16000	2.698E+01	2.258E+02	3.493E+02	3.431E+02	2.039E+02	2.043E+02	1.030E+04	-1.445E+01
17000	2.850E+01	2.275E+02	3.770E+02	3.708E+02	2.053E+02	2.057E+02	1.035E+04	-1.246E+01
18000	3.005E+01	2.291E+02	4.063E+02	4.001E+02	2.066E+02	2.069E+02	1.041E+04	-1.069E+01
19000	3.158E+01	2.308E+02	4.371E+02	4.309E+02	2.078E+02	2.081E+02	1.047E+04	-9.096E+00
20000	3.303E+01	2.325E+02	4.694E+02	4.632E+02	2.090E+02	2.093E+02	1.053E+04	-7.653E+00
21000	3.436E+01	2.341E+02	5.031E+02	4.969E+02	2.101E+02	2.104E+02	1.060E+04	-6.339E+00
22000	3.555E+01	2.357E+02	5.381E+02	5.319E+02	2.113E+02	2.116E+02	1.067E+04	-5.137E+00
23000	3.656E+01	2.373E+02	5.741E+02	5.680E+02	2.124E+02	2.126E+02	1.074E+04	-4.032E+00
24000	3.741E+01	2.389E+02	6.112E+02	6.050E+02	2.134E+02	2.137E+02	1.082E+04	-3.012E+00
25000	3.808E+01	2.404E+02	6.489E+02	6.427E+02	2.145E+02	2.147E+02	1.089E+04	-2.067E+00
26000	3.858E+01	2.419E+02	6.873E+02	6.811E+02	2.155E+02	2.158E+02	1.097E+04	-1.189E+00
27000	3.893E+01	2.434E+02	7.260E+02	7.198E+02	2.165E+02	2.168E+02	1.105E+04	-3.700E-01
28000	3.914E+01	2.448E+02	7.651E+02	7.589E+02	2.175E+02	2.177E+02	1.113E+04	3.962E-01
29000	3.923E+01	2.462E+02	8.043E+02	7.981E+02	2.185E+02	2.187E+02	1.121E+04	1.115E+00
30000	3.920E+01	2.475E+02	8.435E+02	8.373E+02	2.194E+02	2.196E+02	1.130E+04	1.790E+00
32000	3.892E+01	2.501E+02	9.217E+02	9.155E+02	2.213E+02	2.214E+02	1.146E+04	3.029E+00
34000	3.840E+01	2.524E+02	9.990E+02	9.928E+02	2.230E+02	2.232E+02	1.163E+04	4.137E+00
36000	3.775E+01	2.546E+02	1.075E+03	1.069E+03	2.247E+02	2.249E+02	1.180E+04	5.137E+00
38000	3.705E+01	2.566E+02	1.150E+03	1.144E+03	2.263E+02	2.265E+02	1.197E+04	6.045E+00
40000	3.635E+01	2.585E+02	1.223E+03	1.217E+03	2.279E+02	2.281E+02	1.214E+04	6.874E+00
42000	3.569E+01	2.602E+02	1.295E+03	1.289E+03	2.294E+02	2.296E+02	1.231E+04	7.634E+00
44000	3.514E+01	2.619E+02	1.366E+03	1.360E+03	2.308E+02	2.310E+02	1.248E+04	8.335E+00
46000	3.474E+01	2.634E+02	1.436E+03	1.430E+03	2.322E+02	2.324E+02	1.265E+04	8.984E+00
48000	3.457E+01	2.649E+02	1.505E+03	1.499E+03	2.336E+02	2.337E+02	1.282E+04	9.586E+00
50000	3.475E+01	2.663E+02	1.575E+03	1.568E+03	2.348E+02	2.350E+02	1.299E+04	1.015E+01

Table 143: Internal thermodynamic properties of N^{4+} ΔE=250 cm^{-1}

T(K)	Q_{int}	$\ln(Q_{int})$	E_{int}/RT	$C_{p,int}/R$
50	$2.000E+00$	$6.931E-01$	$0.000E+00$	$0.000E+00$
100	$2.000E+00$	$6.931E-01$	$0.000E+00$	$0.000E+00$
150	$2.000E+00$	$6.931E-01$	$0.000E+00$	$0.000E+00$
200	$2.000E+00$	$6.931E-01$	$2.075E-249$	$1.204E-246$
298.15	$2.000E+00$	$6.931E-01$	$1.191E-166$	$4.636E-164$
300	$2.000E+00$	$6.931E-01$	$1.304E-165$	$5.045E-163$
400	$2.000E+00$	$6.931E-01$	$9.501E-124$	$2.756E-121$
500	$2.000E+00$	$6.931E-01$	$1.184E-98$	$2.746E-96$
600	$2.000E+00$	$6.931E-01$	$6.151E-82$	$1.189E-79$
700	$2.000E+00$	$6.931E-01$	$5.228E-70$	$8.665E-68$
800	$2.000E+00$	$6.931E-01$	$4.546E-61$	$6.593E-59$
900	$2.000E+00$	$6.931E-01$	$4.021E-54$	$5.184E-52$
1000	$2.000E+00$	$6.931E-01$	$1.435E-48$	$1.665E-46$
2000	$2.000E+00$	$6.931E-01$	$1.117E-23$	$6.482E-22$
3000	$2.000E+00$	$6.931E-01$	$1.860E-15$	$7.195E-14$
4000	$2.000E+00$	$6.931E-01$	$2.205E-11$	$6.395E-10$
5000	$2.000E+00$	$6.931E-01$	$5.831E-09$	$1.353E-07$
6000	$2.000E+00$	$6.931E-01$	$2.323E-07$	$4.492E-06$
7000	$2.000E+00$	$6.931E-01$	$3.153E-06$	$5.226E-05$
8000	$2.000E+00$	$6.931E-01$	$2.190E-05$	$3.176E-04$
9000	$2.000E+00$	$6.932E-01$	$9.752E-05$	$1.257E-03$
10000	$2.000E+00$	$6.932E-01$	$3.185E-04$	$3.695E-03$
11000	$2.000E+00$	$6.932E-01$	$8.313E-04$	$8.767E-03$
12000	$2.000E+00$	$6.933E-01$	$1.835E-03$	$1.774E-02$
13000	$2.001E+00$	$6.935E-01$	$3.563E-03$	$3.178E-02$
14000	$2.002E+00$	$6.939E-01$	$6.256E-03$	$5.180E-02$
15000	$2.003E+00$	$6.945E-01$	$1.014E-02$	$7.832E-02$
16000	$2.004E+00$	$6.953E-01$	$1.540E-02$	$1.114E-01$
17000	$2.007E+00$	$6.964E-01$	$2.218E-02$	$1.509E-01$
18000	$2.010E+00$	$6.979E-01$	$3.056E-02$	$1.960E-01$
19000	$2.013E+00$	$6.998E-01$	$4.057E-02$	$2.461E-01$
20000	$2.018E+00$	$7.022E-01$	$5.217E-02$	$2.999E-01$
21000	$2.024E+00$	$7.050E-01$	$6.531E-02$	$3.565E-01$
22000	$2.031E+00$	$7.084E-01$	$7.987E-02$	$4.148E-01$
23000	$2.039E+00$	$7.123E-01$	$9.571E-02$	$4.736E-01$
24000	$2.048E+00$	$7.167E-01$	$1.127E-01$	$5.320E-01$
25000	$2.058E+00$	$7.217E-01$	$1.306E-01$	$5.890E-01$
26000	$2.069E+00$	$7.272E-01$	$1.493E-01$	$6.439E-01$
27000	$2.082E+00$	$7.332E-01$	$1.686E-01$	$6.960E-01$
28000	$2.095E+00$	$7.397E-01$	$1.883E-01$	$7.448E-01$
29000	$2.110E+00$	$7.466E-01$	$2.083E-01$	$7.899E-01$
30000	$2.126E+00$	$7.540E-01$	$2.284E-01$	$8.311E-01$
32000	$2.160E+00$	$7.700E-01$	$2.683E-01$	$9.011E-01$
34000	$2.198E+00$	$7.875E-01$	$3.072E-01$	$9.546E-01$
36000	$2.239E+00$	$8.061E-01$	$3.443E-01$	$9.926E-01$
38000	$2.283E+00$	$8.256E-01$	$3.791E-01$	$1.017E+00$
40000	$2.330E+00$	$8.459E-01$	$4.113E-01$	$1.029E+00$
42000	$2.379E+00$	$8.667E-01$	$4.409E-01$	$1.032E+00$
44000	$2.430E+00$	$8.879E-01$	$4.677E-01$	$1.029E+00$
46000	$2.482E+00$	$9.092E-01$	$4.919E-01$	$1.021E+00$
48000	$2.536E+00$	$9.306E-01$	$5.137E-01$	$1.010E+00$
50000	$2.591E+00$	$9.520E-01$	$5.334E-01$	$9.998E-01$

Table 144: Total thermodynamic properties of N^{4+} ΔE=250 cm^{-1}

T [K]	C_p [J/mol/K]	S^0 [J/mol/K]	$H^0(T)-H^0(0)$ [KJ/mol]	$H^0(T)-H^0(298)$ [KJ/mol]	$-(G^0-H^0(0))/T$ [J/mol/K]	$-(G^0-H^0(298))/T$ [J/mol/K]	ΔH_f [KJ/mol]	$Log(K_p)$
50	2.079E+01	1.104E+02	1.039E+00	-5.158E+00	8.964E+01	2.136E+02	1.679E+04	-1.754E+04
100	2.079E+01	1.248E+02	2.079E+00	-4.119E+00	1.040E+02	1.660E+02	1.679E+04	-8.770E+03
150	2.079E+01	1.333E+02	3.118E+00	-3.079E+00	1.125E+02	1.538E+02	1.680E+04	-5.846E+03
200	2.079E+01	1.392E+02	4.157E+00	-2.040E+00	1.185E+02	1.494E+02	1.680E+04	-4.383E+03
298.15	2.079E+01	1.475E+02	6.197E+00	0.000E+00	1.268E+02	1.475E+02	1.681E+04	-2.938E+03
300	2.079E+01	1.477E+02	6.236E+00	3.848E-02	1.269E+02	1.475E+02	1.681E+04	-2.920E+03
400	2.079E+01	1.537E+02	8.315E+00	2.117E+00	1.329E+02	1.483E+02	1.682E+04	-2.188E+03
500	2.079E+01	1.583E+02	1.039E+01	4.196E+00	1.375E+02	1.499E+02	1.683E+04	-1.749E+03
600	2.079E+01	1.621E+02	1.247E+01	6.274E+00	1.413E+02	1.516E+02	1.684E+04	-1.456E+03
700	2.079E+01	1.653E+02	1.455E+01	8.353E+00	1.445E+02	1.533E+02	1.685E+04	-1.246E+03
800	2.079E+01	1.681E+02	1.663E+01	1.043E+01	1.473E+02	1.550E+02	1.686E+04	-1.089E+03
900	2.079E+01	1.705E+02	1.871E+01	1.251E+01	1.497E+02	1.566E+02	1.686E+04	-9.666E+02
1000	2.079E+01	1.727E+02	2.079E+01	1.459E+01	1.519E+02	1.581E+02	1.687E+04	-8.687E+02
2000	2.079E+01	1.871E+02	4.157E+01	3.538E+01	1.663E+02	1.694E+02	1.696E+04	-4.271E+02
3000	2.079E+01	1.955E+02	6.236E+01	5.616E+01	1.747E+02	1.768E+02	1.705E+04	-2.791E+02
4000	2.079E+01	2.015E+02	8.314E+01	7.695E+01	1.807E+02	1.823E+02	1.713E+04	-2.048E+02
5000	2.079E+01	2.062E+02	1.039E+02	9.773E+01	1.854E+02	1.866E+02	1.722E+04	-1.599E+02
6000	2.079E+01	2.099E+02	1.247E+02	1.185E+02	1.892E+02	1.902E+02	1.730E+04	-1.299E+02
7000	2.079E+01	2.131E+02	1.455E+02	1.393E+02	1.923E+02	1.932E+02	1.739E+04	-1.083E+02
8000	2.079E+01	2.159E+02	1.663E+02	1.601E+02	1.951E+02	1.959E+02	1.747E+04	-9.206E+01
9000	2.080E+01	2.184E+02	1.871E+02	1.809E+02	1.976E+02	1.983E+02	1.755E+04	-7.936E+01
10000	2.082E+01	2.206E+02	2.079E+02	2.017E+02	1.998E+02	2.004E+02	1.764E+04	-6.915E+01
11000	2.086E+01	2.225E+02	2.287E+02	2.225E+02	2.018E+02	2.023E+02	1.772E+04	-6.076E+01
12000	2.093E+01	2.244E+02	2.496E+02	2.434E+02	2.036E+02	2.041E+02	1.780E+04	-5.373E+01
13000	2.105E+01	2.260E+02	2.706E+02	2.644E+02	2.052E+02	2.057E+02	1.787E+04	-4.776E+01
14000	2.122E+01	2.276E+02	2.917E+02	2.855E+02	2.068E+02	2.072E+02	1.794E+04	-4.262E+01
15000	2.144E+01	2.291E+02	3.131E+02	3.069E+02	2.082E+02	2.086E+02	1.802E+04	-3.815E+01
16000	2.171E+01	2.305E+02	3.346E+02	3.284E+02	2.096E+02	2.099E+02	1.809E+04	-3.422E+01
17000	2.204E+01	2.318E+02	3.565E+02	3.503E+02	2.108E+02	2.112E+02	1.816E+04	-3.074E+01
18000	2.242E+01	2.331E+02	3.787E+02	3.725E+02	2.120E+02	2.124E+02	1.823E+04	-2.764E+01
19000	2.283E+01	2.343E+02	4.014E+02	3.951E+02	2.132E+02	2.135E+02	1.830E+04	-2.484E+01
20000	2.328E+01	2.355E+02	4.244E+02	4.182E+02	2.142E+02	2.146E+02	1.838E+04	-2.232E+01
21000	2.375E+01	2.366E+02	4.479E+02	4.417E+02	2.153E+02	2.156E+02	1.846E+04	-2.003E+01
22000	2.423E+01	2.377E+02	4.719E+02	4.657E+02	2.163E+02	2.166E+02	1.854E+04	-1.794E+01
23000	2.472E+01	2.388E+02	4.964E+02	4.902E+02	2.172E+02	2.175E+02	1.862E+04	-1.602E+01
24000	2.521E+01	2.399E+02	5.214E+02	5.152E+02	2.182E+02	2.184E+02	1.870E+04	-1.426E+01
25000	2.568E+01	2.409E+02	5.468E+02	5.406E+02	2.191E+02	2.193E+02	1.878E+04	-1.263E+01
26000	2.614E+01	2.419E+02	5.727E+02	5.665E+02	2.199E+02	2.202E+02	1.887E+04	-1.112E+01
27000	2.657E+01	2.429E+02	5.991E+02	5.929E+02	2.208E+02	2.210E+02	1.896E+04	-9.708E+00
28000	2.698E+01	2.439E+02	6.259E+02	6.196E+02	2.216E+02	2.218E+02	1.905E+04	-8.395E+00
29000	2.735E+01	2.449E+02	6.530E+02	6.468E+02	2.223E+02	2.226E+02	1.914E+04	-7.167E+00
30000	2.770E+01	2.458E+02	6.805E+02	6.744E+02	2.231E+02	2.233E+02	1.923E+04	-6.015E+00
32000	2.828E+01	2.476E+02	7.365E+02	7.304E+02	2.246E+02	2.248E+02	1.942E+04	-3.912E+00
34000	2.872E+01	2.493E+02	7.936E+02	7.874E+02	2.260E+02	2.262E+02	1.961E+04	-2.039E+00
36000	2.904E+01	2.510E+02	8.514E+02	8.452E+02	2.273E+02	2.275E+02	1.980E+04	-3.569E-01
38000	2.924E+01	2.526E+02	9.096E+02	9.035E+02	2.286E+02	2.288E+02	2.000E+04	1.163E+00
40000	2.934E+01	2.541E+02	9.682E+02	9.620E+02	2.298E+02	2.300E+02	2.020E+04	2.544E+00
42000	2.937E+01	2.555E+02	1.027E+03	1.021E+03	2.310E+02	2.312E+02	2.039E+04	3.806E+00
44000	2.934E+01	2.569E+02	1.086E+03	1.080E+03	2.322E+02	2.323E+02	2.059E+04	4.964E+00
46000	2.927E+01	2.582E+02	1.144E+03	1.138E+03	2.333E+02	2.334E+02	2.079E+04	6.032E+00
48000	2.918E+01	2.594E+02	1.203E+03	1.197E+03	2.343E+02	2.345E+02	2.099E+04	7.021E+00
50000	2.910E+01	2.606E+02	1.261E+03	1.255E+03	2.354E+02	2.355E+02	2.119E+04	7.939E+00

Table 145: Internal thermodynamic properties of N^{4+} ΔE=500 cm^{-1}

T(K)	Q_{int}	$\ln(Q_{int})$	E_{int}/RT	$C_{p,int}/R$
50	$2.000E+00$	$6.931E-01$	$0.000E+00$	$0.000E+00$
100	$2.000E+00$	$6.931E-01$	$0.000E+00$	$0.000E+00$
150	$2.000E+00$	$6.931E-01$	$0.000E+00$	$0.000E+00$
200	$2.000E+00$	$6.931E-01$	$2.075E-249$	$1.204E-246$
298.15	$2.000E+00$	$6.931E-01$	$1.191E-166$	$4.636E-164$
300	$2.000E+00$	$6.931E-01$	$1.304E-165$	$5.045E-163$
400	$2.000E+00$	$6.931E-01$	$9.501E-124$	$2.756E-121$
500	$2.000E+00$	$6.931E-01$	$1.184E-98$	$2.746E-96$
600	$2.000E+00$	$6.931E-01$	$6.151E-82$	$1.189E-79$
700	$2.000E+00$	$6.931E-01$	$5.228E-70$	$8.665E-68$
800	$2.000E+00$	$6.931E-01$	$4.546E-61$	$6.593E-59$
900	$2.000E+00$	$6.931E-01$	$4.021E-54$	$5.184E-52$
1000	$2.000E+00$	$6.931E-01$	$1.435E-48$	$1.665E-46$
2000	$2.000E+00$	$6.931E-01$	$1.117E-23$	$6.482E-22$
3000	$2.000E+00$	$6.931E-01$	$1.860E-15$	$7.195E-14$
4000	$2.000E+00$	$6.931E-01$	$2.205E-11$	$6.395E-10$
5000	$2.000E+00$	$6.931E-01$	$5.831E-09$	$1.353E-07$
6000	$2.000E+00$	$6.931E-01$	$2.323E-07$	$4.492E-06$
7000	$2.000E+00$	$6.931E-01$	$3.153E-06$	$5.226E-05$
8000	$2.000E+00$	$6.931E-01$	$2.190E-05$	$3.176E-04$
9000	$2.000E+00$	$6.932E-01$	$9.752E-05$	$1.257E-03$
10000	$2.000E+00$	$6.932E-01$	$3.185E-04$	$3.695E-03$
11000	$2.000E+00$	$6.932E-01$	$8.313E-04$	$8.767E-03$
12000	$2.000E+00$	$6.933E-01$	$1.835E-03$	$1.774E-02$
13000	$2.001E+00$	$6.935E-01$	$3.563E-03$	$3.178E-02$
14000	$2.002E+00$	$6.939E-01$	$6.256E-03$	$5.180E-02$
15000	$2.003E+00$	$6.945E-01$	$1.014E-02$	$7.832E-02$
16000	$2.004E+00$	$6.953E-01$	$1.540E-02$	$1.114E-01$
17000	$2.007E+00$	$6.964E-01$	$2.218E-02$	$1.509E-01$
18000	$2.010E+00$	$6.979E-01$	$3.056E-02$	$1.960E-01$
19000	$2.013E+00$	$6.998E-01$	$4.057E-02$	$2.461E-01$
20000	$2.018E+00$	$7.022E-01$	$5.217E-02$	$2.999E-01$
21000	$2.024E+00$	$7.050E-01$	$6.531E-02$	$3.565E-01$
22000	$2.031E+00$	$7.084E-01$	$7.987E-02$	$4.148E-01$
23000	$2.039E+00$	$7.123E-01$	$9.571E-02$	$4.736E-01$
24000	$2.048E+00$	$7.167E-01$	$1.127E-01$	$5.320E-01$
25000	$2.058E+00$	$7.217E-01$	$1.306E-01$	$5.890E-01$
26000	$2.069E+00$	$7.272E-01$	$1.493E-01$	$6.439E-01$
27000	$2.082E+00$	$7.332E-01$	$1.686E-01$	$6.960E-01$
28000	$2.095E+00$	$7.397E-01$	$1.883E-01$	$7.448E-01$
29000	$2.110E+00$	$7.466E-01$	$2.083E-01$	$7.899E-01$
30000	$2.126E+00$	$7.540E-01$	$2.284E-01$	$8.311E-01$
32000	$2.160E+00$	$7.700E-01$	$2.683E-01$	$9.011E-01$
34000	$2.198E+00$	$7.875E-01$	$3.072E-01$	$9.546E-01$
36000	$2.239E+00$	$8.061E-01$	$3.443E-01$	$9.926E-01$
38000	$2.283E+00$	$8.256E-01$	$3.791E-01$	$1.017E+00$
40000	$2.330E+00$	$8.459E-01$	$4.113E-01$	$1.029E+00$
42000	$2.379E+00$	$8.667E-01$	$4.409E-01$	$1.032E+00$
44000	$2.430E+00$	$8.878E-01$	$4.677E-01$	$1.029E+00$
46000	$2.482E+00$	$9.092E-01$	$4.919E-01$	$1.020E+00$
48000	$2.536E+00$	$9.306E-01$	$5.137E-01$	$1.009E+00$
50000	$2.591E+00$	$9.520E-01$	$5.333E-01$	$9.978E-01$

Table 146: Total thermodynamic properties of N^{4+} ΔE=500 cm^{-1}

T [K]	C_p [J/mol/K]	S^0 [J/mol/K]	$H^0(T)-H^0(0)$ [KJ/mol]	$H^0(T)-H^0(298)$ [KJ/mol]	$-(G^0-H^0(0))/T$ [J/mol/K]	$-(G^0-H^0(298))/T$ [J/mol/K]	ΔH_f [KJ/mol]	$Log(K_p)$
50	2.079E+01	1.104E+02	1.039E+00	-5.158E+00	8.964E+01	2.136E+02	1.679E+04	-1.754E+04
100	2.079E+01	1.248E+02	2.079E+00	-4.119E+00	1.040E+02	1.660E+02	1.679E+04	-8.770E+03
150	2.079E+01	1.333E+02	3.118E+00	-3.079E+00	1.125E+02	1.538E+02	1.680E+04	-5.846E+03
200	2.079E+01	1.392E+02	4.157E+00	-2.040E+00	1.185E+02	1.494E+02	1.680E+04	-4.383E+03
298.15	2.079E+01	1.475E+02	6.197E+00	0.000E+00	1.268E+02	1.475E+02	1.681E+04	-2.938E+03
300	2.079E+01	1.477E+02	6.236E+00	3.848E-02	1.269E+02	1.475E+02	1.681E+04	-2.920E+03
400	2.079E+01	1.537E+02	8.315E+00	2.117E+00	1.329E+02	1.483E+02	1.682E+04	-2.188E+03
500	2.079E+01	1.583E+02	1.039E+01	4.196E+00	1.375E+02	1.499E+02	1.683E+04	-1.749E+03
600	2.079E+01	1.621E+02	1.247E+01	6.274E+00	1.413E+02	1.516E+02	1.684E+04	-1.456E+03
700	2.079E+01	1.653E+02	1.455E+01	8.353E+00	1.445E+02	1.533E+02	1.685E+04	-1.246E+03
800	2.079E+01	1.681E+02	1.663E+01	1.043E+01	1.473E+02	1.550E+02	1.686E+04	-1.089E+03
900	2.079E+01	1.705E+02	1.871E+01	1.251E+01	1.497E+02	1.566E+02	1.686E+04	-9.666E+02
1000	2.079E+01	1.727E+02	2.079E+01	1.459E+01	1.519E+02	1.581E+02	1.687E+04	-8.687E+02
2000	2.079E+01	1.871E+02	4.157E+01	3.538E+01	1.663E+02	1.694E+02	1.696E+04	-4.271E+02
3000	2.079E+01	1.955E+02	6.236E+01	5.616E+01	1.747E+02	1.768E+02	1.705E+04	-2.791E+02
4000	2.079E+01	2.015E+02	8.314E+01	7.695E+01	1.807E+02	1.823E+02	1.713E+04	-2.048E+02
5000	2.079E+01	2.062E+02	1.039E+02	9.773E+01	1.854E+02	1.866E+02	1.722E+04	-1.599E+02
6000	2.079E+01	2.099E+02	1.247E+02	1.185E+02	1.892E+02	1.902E+02	1.730E+04	-1.299E+02
7000	2.079E+01	2.131E+02	1.455E+02	1.393E+02	1.923E+02	1.932E+02	1.739E+04	-1.083E+02
8000	2.079E+01	2.159E+02	1.663E+02	1.601E+02	1.951E+02	1.959E+02	1.747E+04	-9.206E+01
9000	2.080E+01	2.184E+02	1.871E+02	1.809E+02	1.976E+02	1.983E+02	1.755E+04	-7.936E+01
10000	2.082E+01	2.206E+02	2.079E+02	2.017E+02	1.998E+02	2.004E+02	1.764E+04	-6.915E+01
11000	2.086E+01	2.225E+02	2.287E+02	2.225E+02	2.018E+02	2.023E+02	1.772E+04	-6.076E+01
12000	2.093E+01	2.244E+02	2.496E+02	2.434E+02	2.036E+02	2.041E+02	1.780E+04	-5.373E+01
13000	2.105E+01	2.260E+02	2.706E+02	2.644E+02	2.052E+02	2.057E+02	1.787E+04	-4.776E+01
14000	2.122E+01	2.276E+02	2.917E+02	2.855E+02	2.068E+02	2.072E+02	1.794E+04	-4.262E+01
15000	2.144E+01	2.291E+02	3.131E+02	3.069E+02	2.082E+02	2.086E+02	1.802E+04	-3.815E+01
16000	2.171E+01	2.305E+02	3.346E+02	3.284E+02	2.096E+02	2.099E+02	1.809E+04	-3.422E+01
17000	2.204E+01	2.318E+02	3.565E+02	3.503E+02	2.108E+02	2.112E+02	1.816E+04	-3.074E+01
18000	2.242E+01	2.331E+02	3.787E+02	3.725E+02	2.120E+02	2.124E+02	1.823E+04	-2.764E+01
19000	2.283E+01	2.343E+02	4.014E+02	3.951E+02	2.132E+02	2.135E+02	1.830E+04	-2.484E+01
20000	2.328E+01	2.355E+02	4.244E+02	4.182E+02	2.142E+02	2.146E+02	1.838E+04	-2.232E+01
21000	2.375E+01	2.366E+02	4.479E+02	4.417E+02	2.153E+02	2.156E+02	1.846E+04	-2.003E+01
22000	2.423E+01	2.377E+02	4.719E+02	4.657E+02	2.163E+02	2.166E+02	1.854E+04	-1.794E+01
23000	2.472E+01	2.388E+02	4.964E+02	4.902E+02	2.172E+02	2.175E+02	1.862E+04	-1.602E+01
24000	2.521E+01	2.399E+02	5.214E+02	5.152E+02	2.182E+02	2.184E+02	1.870E+04	-1.426E+01
25000	2.568E+01	2.409E+02	5.468E+02	5.406E+02	2.191E+02	2.193E+02	1.878E+04	-1.263E+01
26000	2.614E+01	2.419E+02	5.727E+02	5.665E+02	2.199E+02	2.202E+02	1.887E+04	-1.112E+01
27000	2.657E+01	2.429E+02	5.991E+02	5.929E+02	2.208E+02	2.210E+02	1.896E+04	-9.708E+00
28000	2.698E+01	2.439E+02	6.259E+02	6.196E+02	2.216E+02	2.218E+02	1.905E+04	-8.395E+00
29000	2.735E+01	2.449E+02	6.530E+02	6.468E+02	2.223E+02	2.226E+02	1.914E+04	-7.167E+00
30000	2.770E+01	2.458E+02	6.805E+02	6.744E+02	2.231E+02	2.233E+02	1.923E+04	-6.015E+00
32000	2.828E+01	2.476E+02	7.365E+02	7.304E+02	2.246E+02	2.248E+02	1.942E+04	-3.912E+00
34000	2.872E+01	2.493E+02	7.936E+02	7.874E+02	2.260E+02	2.262E+02	1.961E+04	-2.039E+00
36000	2.904E+01	2.510E+02	8.514E+02	8.452E+02	2.273E+02	2.275E+02	1.980E+04	-3.569E-01
38000	2.924E+01	2.526E+02	9.096E+02	9.035E+02	2.286E+02	2.288E+02	2.000E+04	1.163E+00
40000	2.934E+01	2.541E+02	9.682E+02	9.620E+02	2.298E+02	2.300E+02	2.020E+04	2.544E+00
42000	2.937E+01	2.555E+02	1.027E+03	1.021E+03	2.310E+02	2.312E+02	2.039E+04	3.806E+00
44000	2.934E+01	2.569E+02	1.086E+03	1.080E+03	2.322E+02	2.323E+02	2.059E+04	4.964E+00
46000	2.927E+01	2.582E+02	1.144E+03	1.138E+03	2.333E+02	2.334E+02	2.079E+04	6.032E+00
48000	2.918E+01	2.594E+02	1.203E+03	1.197E+03	2.343E+02	2.345E+02	2.099E+04	7.021E+00
50000	2.908E+01	2.606E+02	1.261E+03	1.255E+03	2.354E+02	2.355E+02	2.119E+04	7.939E+00

Table 147: Internal thermodynamic properties of N^{4+} ΔE=1000 cm^{-1}

T(K)	Q_{int}	$\ln(Q_{int})$	E_{int}/RT	$C_{p,int}/R$
50	$2.000E+00$	$6.931E-01$	$0.000E+00$	$0.000E+00$
100	$2.000E+00$	$6.931E-01$	$0.000E+00$	$0.000E+00$
150	$2.000E+00$	$6.931E-01$	$0.000E+00$	$0.000E+00$
200	$2.000E+00$	$6.931E-01$	$2.075E-249$	$1.204E-246$
298.15	$2.000E+00$	$6.931E-01$	$1.191E-166$	$4.636E-164$
300	$2.000E+00$	$6.931E-01$	$1.304E-165$	$5.045E-163$
400	$2.000E+00$	$6.931E-01$	$9.501E-124$	$2.756E-121$
500	$2.000E+00$	$6.931E-01$	$1.184E-98$	$2.746E-96$
600	$2.000E+00$	$6.931E-01$	$6.151E-82$	$1.189E-79$
700	$2.000E+00$	$6.931E-01$	$5.228E-70$	$8.665E-68$
800	$2.000E+00$	$6.931E-01$	$4.546E-61$	$6.593E-59$
900	$2.000E+00$	$6.931E-01$	$4.021E-54$	$5.184E-52$
1000	$2.000E+00$	$6.931E-01$	$1.435E-48$	$1.665E-46$
2000	$2.000E+00$	$6.931E-01$	$1.117E-23$	$6.482E-22$
3000	$2.000E+00$	$6.931E-01$	$1.860E-15$	$7.195E-14$
4000	$2.000E+00$	$6.931E-01$	$2.205E-11$	$6.395E-10$
5000	$2.000E+00$	$6.931E-01$	$5.831E-09$	$1.353E-07$
6000	$2.000E+00$	$6.931E-01$	$2.323E-07$	$4.492E-06$
7000	$2.000E+00$	$6.931E-01$	$3.153E-06$	$5.226E-05$
8000	$2.000E+00$	$6.931E-01$	$2.190E-05$	$3.176E-04$
9000	$2.000E+00$	$6.932E-01$	$9.752E-05$	$1.257E-03$
10000	$2.000E+00$	$6.932E-01$	$3.185E-04$	$3.695E-03$
11000	$2.000E+00$	$6.932E-01$	$8.313E-04$	$8.767E-03$
12000	$2.000E+00$	$6.933E-01$	$1.835E-03$	$1.774E-02$
13000	$2.001E+00$	$6.935E-01$	$3.563E-03$	$3.178E-02$
14000	$2.002E+00$	$6.939E-01$	$6.256E-03$	$5.180E-02$
15000	$2.003E+00$	$6.945E-01$	$1.014E-02$	$7.832E-02$
16000	$2.004E+00$	$6.953E-01$	$1.540E-02$	$1.114E-01$
17000	$2.007E+00$	$6.964E-01$	$2.218E-02$	$1.509E-01$
18000	$2.010E+00$	$6.979E-01$	$3.056E-02$	$1.960E-01$
19000	$2.013E+00$	$6.998E-01$	$4.057E-02$	$2.461E-01$
20000	$2.018E+00$	$7.022E-01$	$5.217E-02$	$2.999E-01$
21000	$2.024E+00$	$7.050E-01$	$6.531E-02$	$3.565E-01$
22000	$2.031E+00$	$7.084E-01$	$7.987E-02$	$4.148E-01$
23000	$2.039E+00$	$7.123E-01$	$9.571E-02$	$4.736E-01$
24000	$2.048E+00$	$7.167E-01$	$1.127E-01$	$5.320E-01$
25000	$2.058E+00$	$7.217E-01$	$1.306E-01$	$5.890E-01$
26000	$2.069E+00$	$7.272E-01$	$1.493E-01$	$6.439E-01$
27000	$2.082E+00$	$7.332E-01$	$1.686E-01$	$6.960E-01$
28000	$2.095E+00$	$7.397E-01$	$1.883E-01$	$7.448E-01$
29000	$2.110E+00$	$7.466E-01$	$2.083E-01$	$7.899E-01$
30000	$2.126E+00$	$7.540E-01$	$2.284E-01$	$8.311E-01$
32000	$2.160E+00$	$7.700E-01$	$2.683E-01$	$9.011E-01$
34000	$2.198E+00$	$7.875E-01$	$3.072E-01$	$9.546E-01$
36000	$2.239E+00$	$8.061E-01$	$3.443E-01$	$9.926E-01$
38000	$2.283E+00$	$8.256E-01$	$3.791E-01$	$1.017E+00$
40000	$2.330E+00$	$8.459E-01$	$4.113E-01$	$1.029E+00$
42000	$2.379E+00$	$8.667E-01$	$4.409E-01$	$1.032E+00$
44000	$2.430E+00$	$8.878E-01$	$4.677E-01$	$1.029E+00$
46000	$2.482E+00$	$9.092E-01$	$4.919E-01$	$1.020E+00$
48000	$2.536E+00$	$9.306E-01$	$5.137E-01$	$1.009E+00$
50000	$2.591E+00$	$9.520E-01$	$5.333E-01$	$9.971E-01$

Table 148: Total thermodynamic properties of N^{4+} ΔE=1000 cm^{-1}

T [K]	C_p [J/mol/K]	S^0 [J/mol/K]	$H^0(T)-H^0(0)$ [KJ/mol]	$H^0(T)-H^0(298)$ [KJ/mol]	$-(G^0-H^0(0))/T$ [J/mol/K]	$-(G^0-H^0(298))/T$ [J/mol/K]	ΔH_f [KJ/mol]	$Log(K_p)$
50	2.079E+01	1.104E+02	1.039E+00	-5.158E+00	8.964E+01	2.136E+02	1.679E+04	-1.754E+04
100	2.079E+01	1.248E+02	2.079E+00	-4.119E+00	1.040E+02	1.660E+02	1.679E+04	-8.770E+03
150	2.079E+01	1.333E+02	3.118E+00	-3.079E+00	1.125E+02	1.538E+02	1.680E+04	-5.846E+03
200	2.079E+01	1.392E+02	4.157E+00	-2.040E+00	1.185E+02	1.494E+02	1.680E+04	-4.383E+03
298.15	2.079E+01	1.475E+02	6.197E+00	0.000E+00	1.268E+02	1.475E+02	1.681E+04	-2.938E+03
300	2.079E+01	1.477E+02	6.236E+00	3.848E-02	1.269E+02	1.475E+02	1.681E+04	-2.920E+03
400	2.079E+01	1.537E+02	8.315E+00	2.117E+00	1.329E+02	1.483E+02	1.682E+04	-2.188E+03
500	2.079E+01	1.583E+02	1.039E+01	4.196E+00	1.375E+02	1.499E+02	1.683E+04	-1.749E+03
600	2.079E+01	1.621E+02	1.247E+01	6.274E+00	1.413E+02	1.516E+02	1.684E+04	-1.456E+03
700	2.079E+01	1.653E+02	1.455E+01	8.353E+00	1.445E+02	1.533E+02	1.685E+04	-1.246E+03
800	2.079E+01	1.681E+02	1.663E+01	1.043E+01	1.473E+02	1.550E+02	1.686E+04	-1.089E+03
900	2.079E+01	1.705E+02	1.871E+01	1.251E+01	1.497E+02	1.566E+02	1.686E+04	-9.666E+02
1000	2.079E+01	1.727E+02	2.079E+01	1.459E+01	1.519E+02	1.581E+02	1.687E+04	-8.687E+02
2000	2.079E+01	1.871E+02	4.157E+01	3.538E+01	1.663E+02	1.694E+02	1.696E+04	-4.271E+02
3000	2.079E+01	1.955E+02	6.236E+01	5.616E+01	1.747E+02	1.768E+02	1.705E+04	-2.791E+02
4000	2.079E+01	2.015E+02	8.314E+01	7.695E+01	1.807E+02	1.823E+02	1.713E+04	-2.048E+02
5000	2.079E+01	2.062E+02	1.039E+02	9.773E+01	1.854E+02	1.866E+02	1.722E+04	-1.599E+02
6000	2.079E+01	2.099E+02	1.247E+02	1.185E+02	1.892E+02	1.902E+02	1.730E+04	-1.299E+02
7000	2.079E+01	2.131E+02	1.455E+02	1.393E+02	1.923E+02	1.932E+02	1.739E+04	-1.083E+02
8000	2.079E+01	2.159E+02	1.663E+02	1.601E+02	1.951E+02	1.959E+02	1.747E+04	-9.206E+01
9000	2.080E+01	2.184E+02	1.871E+02	1.809E+02	1.976E+02	1.983E+02	1.755E+04	-7.936E+01
10000	2.082E+01	2.206E+02	2.079E+02	2.017E+02	1.998E+02	2.004E+02	1.764E+04	-6.915E+01
11000	2.086E+01	2.225E+02	2.287E+02	2.225E+02	2.018E+02	2.023E+02	1.772E+04	-6.076E+01
12000	2.093E+01	2.244E+02	2.496E+02	2.434E+02	2.036E+02	2.041E+02	1.780E+04	-5.373E+01
13000	2.105E+01	2.260E+02	2.706E+02	2.644E+02	2.052E+02	2.057E+02	1.787E+04	-4.776E+01
14000	2.122E+01	2.276E+02	2.917E+02	2.855E+02	2.068E+02	2.072E+02	1.794E+04	-4.262E+01
15000	2.144E+01	2.291E+02	3.131E+02	3.069E+02	2.082E+02	2.086E+02	1.802E+04	-3.815E+01
16000	2.171E+01	2.305E+02	3.346E+02	3.284E+02	2.096E+02	2.099E+02	1.809E+04	-3.422E+01
17000	2.204E+01	2.318E+02	3.565E+02	3.503E+02	2.108E+02	2.112E+02	1.816E+04	-3.074E+01
18000	2.242E+01	2.331E+02	3.787E+02	3.725E+02	2.120E+02	2.124E+02	1.823E+04	-2.764E+01
19000	2.283E+01	2.343E+02	4.014E+02	3.951E+02	2.132E+02	2.135E+02	1.830E+04	-2.484E+01
20000	2.328E+01	2.355E+02	4.244E+02	4.182E+02	2.142E+02	2.146E+02	1.838E+04	-2.232E+01
21000	2.375E+01	2.366E+02	4.479E+02	4.417E+02	2.153E+02	2.156E+02	1.846E+04	-2.003E+01
22000	2.423E+01	2.377E+02	4.719E+02	4.657E+02	2.163E+02	2.166E+02	1.854E+04	-1.794E+01
23000	2.472E+01	2.388E+02	4.964E+02	4.902E+02	2.172E+02	2.175E+02	1.862E+04	-1.602E+01
24000	2.521E+01	2.399E+02	5.214E+02	5.152E+02	2.182E+02	2.184E+02	1.870E+04	-1.426E+01
25000	2.568E+01	2.409E+02	5.468E+02	5.406E+02	2.191E+02	2.193E+02	1.878E+04	-1.263E+01
26000	2.614E+01	2.419E+02	5.727E+02	5.665E+02	2.199E+02	2.202E+02	1.887E+04	-1.112E+01
27000	2.657E+01	2.429E+02	5.991E+02	5.929E+02	2.208E+02	2.210E+02	1.896E+04	-9.708E+00
28000	2.698E+01	2.439E+02	6.259E+02	6.196E+02	2.216E+02	2.218E+02	1.905E+04	-8.395E+00
29000	2.735E+01	2.449E+02	6.530E+02	6.468E+02	2.223E+02	2.226E+02	1.914E+04	-7.167E+00
30000	2.770E+01	2.458E+02	6.805E+02	6.744E+02	2.231E+02	2.233E+02	1.923E+04	-6.015E+00
32000	2.828E+01	2.476E+02	7.365E+02	7.304E+02	2.246E+02	2.248E+02	1.942E+04	-3.912E+00
34000	2.872E+01	2.493E+02	7.936E+02	7.874E+02	2.260E+02	2.262E+02	1.961E+04	-2.039E+00
36000	2.904E+01	2.510E+02	8.514E+02	8.452E+02	2.273E+02	2.275E+02	1.980E+04	-3.569E-01
38000	2.924E+01	2.526E+02	9.096E+02	9.035E+02	2.286E+02	2.288E+02	2.000E+04	1.163E+00
40000	2.934E+01	2.541E+02	9.682E+02	9.620E+02	2.298E+02	2.300E+02	2.020E+04	2.544E+00
42000	2.937E+01	2.555E+02	1.027E+03	1.021E+03	2.310E+02	2.312E+02	2.039E+04	3.806E+00
44000	2.934E+01	2.569E+02	1.086E+03	1.080E+03	2.322E+02	2.323E+02	2.059E+04	4.964E+00
46000	2.927E+01	2.582E+02	1.144E+03	1.138E+03	2.333E+02	2.334E+02	2.079E+04	6.032E+00
48000	2.918E+01	2.594E+02	1.203E+03	1.197E+03	2.343E+02	2.345E+02	2.099E+04	7.021E+00
50000	2.908E+01	2.606E+02	1.261E+03	1.255E+03	2.354E+02	2.355E+02	2.119E+04	7.939E+00

Table 149: Internal thermodynamic properties of N^-

T(K)	Q_{int}	$\ln(Q_{int})$	E_{int}/RT	$C_{p,int}/R$
50	$5.565E+00$	$1.716E+00$	$1.944E-01$	$3.418E-01$
100	$6.486E+00$	$1.870E+00$	$2.241E-01$	$1.741E-01$
150	$7.061E+00$	$1.955E+00$	$1.919E-01$	$9.248E-02$
200	$7.430E+00$	$2.006E+00$	$1.619E-01$	$5.602E-02$
298.15	$7.861E+00$	$2.062E+00$	$1.214E-01$	$2.683E-02$
300	$7.867E+00$	$2.063E+00$	$1.208E-01$	$2.652E-02$
400	$8.115E+00$	$2.094E+00$	$9.564E-02$	$1.533E-02$
500	$8.274E+00$	$2.113E+00$	$7.899E-02$	$9.957E-03$
600	$8.385E+00$	$2.126E+00$	$6.721E-02$	$6.979E-03$
700	$8.467E+00$	$2.136E+00$	$5.847E-02$	$5.160E-03$
800	$8.529E+00$	$2.143E+00$	$5.172E-02$	$3.970E-03$
900	$8.579E+00$	$2.149E+00$	$4.637E-02$	$3.152E-03$
1000	$8.619E+00$	$2.154E+00$	$4.202E-02$	$2.581E-03$
2000	$8.806E+00$	$2.175E+00$	$2.351E-02$	$1.504E-02$
3000	$8.897E+00$	$2.186E+00$	$3.095E-02$	$8.472E-02$
4000	$9.004E+00$	$2.198E+00$	$5.549E-02$	$1.717E-01$
5000	$9.146E+00$	$2.213E+00$	$8.567E-02$	$2.361E-01$
6000	$9.314E+00$	$2.231E+00$	$1.141E-01$	$2.717E-01$
7000	$9.496E+00$	$2.251E+00$	$1.378E-01$	$2.853E-01$
8000	$9.685E+00$	$2.271E+00$	$1.563E-01$	$2.847E-01$
9000	$9.873E+00$	$2.290E+00$	$1.701E-01$	$2.759E-01$
10000	$1.006E+01$	$2.308E+00$	$1.801E-01$	$2.626E-01$
11000	$1.023E+01$	$2.326E+00$	$1.869E-01$	$2.473E-01$
12000	$1.040E+01$	$2.342E+00$	$1.913E-01$	$2.314E-01$
13000	$1.057E+01$	$2.358E+00$	$1.937E-01$	$2.158E-01$
14000	$1.072E+01$	$2.372E+00$	$1.948E-01$	$2.009E-01$
15000	$1.086E+01$	$2.386E+00$	$1.947E-01$	$1.869E-01$
16000	$1.100E+01$	$2.398E+00$	$1.938E-01$	$1.740E-01$
17000	$1.113E+01$	$2.410E+00$	$1.923E-01$	$1.620E-01$
18000	$1.125E+01$	$2.421E+00$	$1.903E-01$	$1.510E-01$
19000	$1.137E+01$	$2.431E+00$	$1.880E-01$	$1.409E-01$
20000	$1.148E+01$	$2.441E+00$	$1.854E-01$	$1.317E-01$
21000	$1.158E+01$	$2.449E+00$	$1.826E-01$	$1.233E-01$
22000	$1.168E+01$	$2.458E+00$	$1.797E-01$	$1.155E-01$
23000	$1.177E+01$	$2.466E+00$	$1.768E-01$	$1.085E-01$
24000	$1.186E+01$	$2.473E+00$	$1.738E-01$	$1.020E-01$
25000	$1.195E+01$	$2.480E+00$	$1.708E-01$	$9.600E-02$
26000	$1.202E+01$	$2.487E+00$	$1.678E-01$	$9.052E-02$
27000	$1.210E+01$	$2.493E+00$	$1.649E-01$	$8.547E-02$
28000	$1.217E+01$	$2.499E+00$	$1.620E-01$	$8.081E-02$
29000	$1.224E+01$	$2.505E+00$	$1.591E-01$	$7.651E-02$
30000	$1.231E+01$	$2.510E+00$	$1.563E-01$	$7.253E-02$
32000	$1.243E+01$	$2.520E+00$	$1.508E-01$	$6.542E-02$
34000	$1.254E+01$	$2.529E+00$	$1.456E-01$	$5.928E-02$
36000	$1.264E+01$	$2.537E+00$	$1.406E-01$	$5.394E-02$
38000	$1.274E+01$	$2.545E+00$	$1.360E-01$	$4.928E-02$
40000	$1.283E+01$	$2.552E+00$	$1.315E-01$	$4.519E-02$
42000	$1.291E+01$	$2.558E+00$	$1.273E-01$	$4.158E-02$
44000	$1.298E+01$	$2.564E+00$	$1.233E-01$	$3.838E-02$
46000	$1.305E+01$	$2.569E+00$	$1.196E-01$	$3.553E-02$
48000	$1.312E+01$	$2.574E+00$	$1.160E-01$	$3.298E-02$
50000	$1.318E+01$	$2.579E+00$	$1.127E-01$	$3.069E-02$

Table 150: Total thermodynamic properties of N^-

T [K]	C_p [J/mol/K]	S^0 [J/mol/K]	$H^0(T)-H^0(0)$ [KJ/mol]	$H^0(T)-H^0(298)$ [KJ/mol]	$-(G^0-H^0(0))/T$ [J/mol/K]	$-(G^0-H^0(298))/T$ [J/mol/K]	ΔH_f [KJ/mol]	$\mathrm{Log}(K_p)$
50	2.363E+01	1.205E+02	1.120E+00	-5.378E+00	9.815E+01	2.281E+02	4.769E+02	-4.947E+02
100	2.223E+01	1.365E+02	2.265E+00	-4.233E+00	1.138E+02	1.788E+02	4.763E+02	-2.458E+02
150	2.155E+01	1.453E+02	3.357E+00	-3.141E+00	1.230E+02	1.663E+02	4.756E+02	-1.629E+02
200	2.125E+01	1.515E+02	4.426E+00	-2.072E+00	1.294E+02	1.619E+02	4.749E+02	-1.215E+02
298.15	2.101E+01	1.599E+02	6.498E+00	0.000E+00	1.381E+02	1.599E+02	4.735E+02	-8.071E+01
300	2.101E+01	1.601E+02	6.537E+00	3.891E-02	1.383E+02	1.599E+02	4.735E+02	-8.019E+01
400	2.091E+01	1.661E+02	8.633E+00	2.134E+00	1.445E+02	1.608E+02	4.721E+02	-5.961E+01
500	2.087E+01	1.708E+02	1.072E+01	4.223E+00	1.493E+02	1.623E+02	4.706E+02	-4.730E+01
600	2.084E+01	1.746E+02	1.281E+01	6.309E+00	1.532E+02	1.640E+02	4.691E+02	-3.912E+01
700	2.083E+01	1.778E+02	1.489E+01	8.392E+00	1.565E+02	1.658E+02	4.676E+02	-3.329E+01
800	2.082E+01	1.805E+02	1.697E+01	1.047E+01	1.593E+02	1.674E+02	4.661E+02	-2.894E+01
900	2.081E+01	1.830E+02	1.905E+01	1.256E+01	1.618E+02	1.691E+02	4.645E+02	-2.556E+01
1000	2.081E+01	1.852E+02	2.114E+01	1.464E+01	1.641E+02	1.706E+02	4.629E+02	-2.287E+01
2000	2.091E+01	1.996E+02	4.196E+01	3.547E+01	1.786E+02	1.819E+02	4.456E+02	-1.096E+01
3000	2.149E+01	2.082E+02	6.313E+01	5.663E+01	1.872E+02	1.893E+02	4.276E+02	-7.144E+00
4000	2.221E+01	2.145E+02	8.499E+01	7.849E+01	1.932E+02	1.949E+02	4.101E+02	-5.317E+00
5000	2.275E+01	2.195E+02	1.075E+02	1.010E+02	1.980E+02	1.993E+02	3.929E+02	-4.267E+00
6000	2.305E+01	2.237E+02	1.304E+02	1.239E+02	2.019E+02	2.030E+02	3.760E+02	-3.597E+00
7000	2.316E+01	2.272E+02	1.535E+02	1.470E+02	2.053E+02	2.062E+02	3.590E+02	-3.139E+00
8000	2.315E+01	2.303E+02	1.767E+02	1.702E+02	2.082E+02	2.091E+02	3.417E+02	-2.812E+00
9000	2.308E+01	2.331E+02	1.998E+02	1.933E+02	2.109E+02	2.116E+02	3.236E+02	-2.571E+00
10000	2.297E+01	2.355E+02	2.228E+02	2.163E+02	2.132E+02	2.138E+02	3.041E+02	-2.388E+00
11000	2.284E+01	2.377E+02	2.457E+02	2.392E+02	2.153E+02	2.159E+02	2.827E+02	-2.248E+00
12000	2.271E+01	2.397E+02	2.685E+02	2.620E+02	2.173E+02	2.178E+02	2.589E+02	-2.141E+00
13000	2.258E+01	2.415E+02	2.912E+02	2.847E+02	2.191E+02	2.196E+02	2.325E+02	-2.059E+00
14000	2.246E+01	2.431E+02	3.137E+02	3.072E+02	2.207E+02	2.212E+02	2.037E+02	-1.996E+00
15000	2.234E+01	2.447E+02	3.361E+02	3.296E+02	2.223E+02	2.227E+02	1.730E+02	-1.949E+00
16000	2.223E+01	2.461E+02	3.584E+02	3.519E+02	2.237E+02	2.241E+02	1.411E+02	-1.915E+00
17000	2.213E+01	2.475E+02	3.806E+02	3.741E+02	2.251E+02	2.255E+02	1.087E+02	-1.891E+00
18000	2.204E+01	2.487E+02	4.026E+02	3.961E+02	2.263E+02	2.267E+02	7.649E+01	-1.875E+00
19000	2.196E+01	2.499E+02	4.246E+02	4.181E+02	2.276E+02	2.279E+02	4.511E+01	-1.865E+00
20000	2.188E+01	2.510E+02	4.466E+02	4.401E+02	2.287E+02	2.290E+02	1.493E+01	-1.861E+00
21000	2.181E+01	2.521E+02	4.684E+02	4.619E+02	2.298E+02	2.301E+02	-1.382E+01	-1.861E+00
22000	2.175E+01	2.531E+02	4.902E+02	4.837E+02	2.308E+02	2.311E+02	-4.105E+01	-1.864E+00
23000	2.169E+01	2.541E+02	5.119E+02	5.054E+02	2.318E+02	2.321E+02	-6.675E+01	-1.870E+00
24000	2.163E+01	2.550E+02	5.335E+02	5.271E+02	2.328E+02	2.330E+02	-9.100E+01	-1.877E+00
25000	2.158E+01	2.559E+02	5.552E+02	5.487E+02	2.337E+02	2.339E+02	-1.139E+02	-1.886E+00
26000	2.154E+01	2.567E+02	5.767E+02	5.702E+02	2.346E+02	2.348E+02	-1.355E+02	-1.896E+00
27000	2.150E+01	2.575E+02	5.982E+02	5.917E+02	2.354E+02	2.356E+02	-1.560E+02	-1.907E+00
28000	2.146E+01	2.583E+02	6.197E+02	6.132E+02	2.362E+02	2.364E+02	-1.755E+02	-1.919E+00
29000	2.142E+01	2.591E+02	6.412E+02	6.347E+02	2.370E+02	2.372E+02	-1.941E+02	-1.930E+00
30000	2.139E+01	2.598E+02	6.626E+02	6.561E+02	2.377E+02	2.379E+02	-2.119E+02	-1.943E+00
32000	2.133E+01	2.612E+02	7.053E+02	6.988E+02	2.391E+02	2.393E+02	-2.455E+02	-1.968E+00
34000	2.128E+01	2.625E+02	7.479E+02	7.414E+02	2.405E+02	2.407E+02	-2.769E+02	-1.993E+00
36000	2.123E+01	2.637E+02	7.904E+02	7.839E+02	2.417E+02	2.419E+02	-3.065E+02	-2.018E+00
38000	2.120E+01	2.648E+02	8.328E+02	8.263E+02	2.429E+02	2.431E+02	-3.348E+02	-2.042E+00
40000	2.116E+01	2.659E+02	8.752E+02	8.687E+02	2.440E+02	2.442E+02	-3.620E+02	-2.066E+00
42000	2.113E+01	2.669E+02	9.175E+02	9.110E+02	2.451E+02	2.453E+02	-3.882E+02	-2.089E+00
44000	2.111E+01	2.679E+02	9.597E+02	9.532E+02	2.461E+02	2.463E+02	-4.138E+02	-2.112E+00
46000	2.108E+01	2.689E+02	1.002E+03	9.954E+02	2.471E+02	2.472E+02	-4.388E+02	-2.134E+00
48000	2.106E+01	2.698E+02	1.044E+03	1.038E+03	2.480E+02	2.482E+02	-4.632E+02	-2.155E+00
50000	2.104E+01	2.706E+02	1.086E+03	1.080E+03	2.489E+02	2.490E+02	-4.873E+02	-2.176E+00

Table 151: Internal thermodynamic properties of N_2

T(K)	Q_{int}	$\ln(Q_{int})$	E_{int}/RT	$C_{p,int}/R$
50	$8.903E+00$	$2.186E+00$	$9.809E-01$	$1.000E+00$
100	$1.764E+01$	$2.870E+00$	$9.906E-01$	$1.000E+00$
150	$2.638E+01$	$3.272E+00$	$9.939E-01$	$1.001E+00$
200	$3.512E+01$	$3.559E+00$	$9.956E-01$	$1.001E+00$
298.15	$5.228E+01$	$3.957E+00$	$9.976E-01$	$1.003E+00$
300	$5.260E+01$	$3.963E+00$	$9.976E-01$	$1.003E+00$
400	$7.011E+01$	$4.250E+00$	$1.000E+00$	$1.018E+00$
500	$8.770E+01$	$4.474E+00$	$1.007E+00$	$1.058E+00$
600	$1.055E+02$	$4.659E+00$	$1.021E+00$	$1.121E+00$
700	$1.236E+02$	$4.817E+00$	$1.041E+00$	$1.199E+00$
800	$1.423E+02$	$4.958E+00$	$1.066E+00$	$1.281E+00$
900	$1.616E+02$	$5.085E+00$	$1.094E+00$	$1.360E+00$
1000	$1.816E+02$	$5.202E+00$	$1.124E+00$	$1.433E+00$
2000	$4.331E+02$	$6.071E+00$	$1.397E+00$	$1.827E+00$
3000	$7.900E+02$	$6.672E+00$	$1.565E+00$	$1.954E+00$
4000	$1.259E+03$	$7.138E+00$	$1.671E+00$	$2.017E+00$
5000	$1.843E+03$	$7.519E+00$	$1.744E+00$	$2.061E+00$
6000	$2.546E+03$	$7.842E+00$	$1.801E+00$	$2.106E+00$
7000	$3.372E+03$	$8.123E+00$	$1.849E+00$	$2.177E+00$
8000	$4.330E+03$	$8.373E+00$	$1.897E+00$	$2.312E+00$
9000	$5.432E+03$	$8.600E+00$	$1.956E+00$	$2.553E+00$
10000	$6.701E+03$	$8.810E+00$	$2.033E+00$	$2.925E+00$
11000	$8.171E+03$	$9.008E+00$	$2.136E+00$	$3.422E+00$
12000	$9.893E+03$	$9.200E+00$	$2.267E+00$	$3.997E+00$
13000	$1.193E+04$	$9.387E+00$	$2.422E+00$	$4.578E+00$
14000	$1.437E+04$	$9.573E+00$	$2.595E+00$	$5.080E+00$
15000	$1.729E+04$	$9.758E+00$	$2.774E+00$	$5.438E+00$
16000	$2.080E+04$	$9.942E+00$	$2.947E+00$	$5.617E+00$
17000	$2.498E+04$	$1.013E+01$	$3.105E+00$	$5.617E+00$
18000	$2.995E+04$	$1.031E+01$	$3.241E+00$	$5.464E+00$
19000	$3.580E+04$	$1.049E+01$	$3.351E+00$	$5.197E+00$
20000	$4.261E+04$	$1.066E+01$	$3.435E+00$	$4.858E+00$
21000	$5.046E+04$	$1.083E+01$	$3.494E+00$	$4.481E+00$
22000	$5.942E+04$	$1.099E+01$	$3.530E+00$	$4.096E+00$
23000	$6.954E+04$	$1.115E+01$	$3.546E+00$	$3.721E+00$
24000	$8.088E+04$	$1.130E+01$	$3.546E+00$	$3.366E+00$
25000	$9.345E+04$	$1.145E+01$	$3.532E+00$	$3.040E+00$
26000	$1.073E+05$	$1.158E+01$	$3.508E+00$	$2.743E+00$
27000	$1.224E+05$	$1.172E+01$	$3.474E+00$	$2.477E+00$
28000	$1.388E+05$	$1.184E+01$	$3.434E+00$	$2.239E+00$
29000	$1.564E+05$	$1.196E+01$	$3.389E+00$	$2.028E+00$
30000	$1.754E+05$	$1.207E+01$	$3.341E+00$	$1.841E+00$
32000	$2.168E+05$	$1.229E+01$	$3.237E+00$	$1.527E+00$
34000	$2.630E+05$	$1.248E+01$	$3.129E+00$	$1.280E+00$
36000	$3.135E+05$	$1.266E+01$	$3.020E+00$	$1.084E+00$
38000	$3.681E+05$	$1.282E+01$	$2.914E+00$	$9.278E-01$
40000	$4.263E+05$	$1.296E+01$	$2.812E+00$	$8.013E-01$
42000	$4.878E+05$	$1.310E+01$	$2.713E+00$	$6.980E-01$
44000	$5.523E+05$	$1.322E+01$	$2.620E+00$	$6.129E-01$
46000	$6.193E+05$	$1.334E+01$	$2.531E+00$	$5.421E-01$
48000	$6.885E+05$	$1.344E+01$	$2.447E+00$	$4.826E-01$
50000	$7.595E+05$	$1.354E+01$	$2.367E+00$	$4.323E-01$

Table 152: Total thermodynamic properties of N_2

T [K]	C_p [J/mol/K]	S^0 [J/mol/K]	$H^0(T)-H^0(0)$ [KJ/mol]	$H^0(T)-H^0(298)$ [KJ/mol]	$-(G^0-H^0(0))/T$ [J/mol/K]	$-(G^0-H^0(298))/T$ [J/mol/K]	ΔH_f [KJ/mol]	$\mathrm{Log}(K_p)$
50	2.910E+01	1.396E+02	1.447E+00	-7.223E+00	1.107E+02	2.841E+02	0.000E+00	0.000E+00
100	2.910E+01	1.598E+02	2.902E+00	-5.768E+00	1.308E+02	2.175E+02	0.000E+00	0.000E+00
150	2.911E+01	1.716E+02	4.358E+00	-4.313E+00	1.426E+02	2.004E+02	0.000E+00	0.000E+00
200	2.911E+01	1.800E+02	5.813E+00	-2.857E+00	1.509E+02	1.943E+02	0.000E+00	0.000E+00
298.15	2.912E+01	1.916E+02	8.670E+00	0.000E+00	1.625E+02	1.916E+02	0.000E+00	0.000E+00
300	2.913E+01	1.918E+02	8.724E+00	5.391E-02	1.627E+02	1.916E+02	0.000E+00	0.000E+00
400	2.925E+01	2.002E+02	1.164E+01	2.971E+00	1.711E+02	1.928E+02	0.000E+00	0.000E+00
500	2.958E+01	2.067E+02	1.458E+01	5.911E+00	1.776E+02	1.949E+02	0.000E+00	0.000E+00
600	3.011E+01	2.122E+02	1.756E+01	8.894E+00	1.829E+02	1.974E+02	0.000E+00	0.000E+00
700	3.075E+01	2.169E+02	2.061E+01	1.194E+01	1.874E+02	1.998E+02	0.000E+00	0.000E+00
800	3.143E+01	2.210E+02	2.372E+01	1.505E+01	1.914E+02	2.022E+02	0.000E+00	0.000E+00
900	3.209E+01	2.248E+02	2.689E+01	1.822E+01	1.949E+02	2.045E+02	0.000E+00	0.000E+00
1000	3.270E+01	2.282E+02	3.013E+01	2.146E+01	1.980E+02	2.067E+02	0.000E+00	0.000E+00
2000	3.597E+01	2.521E+02	6.481E+01	5.614E+01	2.197E+02	2.240E+02	0.000E+00	0.000E+00
3000	3.703E+01	2.669E+02	1.014E+02	9.272E+01	2.331E+02	2.360E+02	0.000E+00	0.000E+00
4000	3.756E+01	2.776E+02	1.387E+02	1.300E+02	2.429E+02	2.451E+02	0.000E+00	0.000E+00
5000	3.792E+01	2.861E+02	1.764E+02	1.678E+02	2.508E+02	2.525E+02	0.000E+00	0.000E+00
6000	3.830E+01	2.930E+02	2.146E+02	2.059E+02	2.572E+02	2.587E+02	0.000E+00	0.000E+00
7000	3.888E+01	2.989E+02	2.531E+02	2.444E+02	2.628E+02	2.640E+02	0.000E+00	0.000E+00
8000	4.001E+01	3.042E+02	2.925E+02	2.838E+02	2.676E+02	2.687E+02	0.000E+00	0.000E+00
9000	4.201E+01	3.090E+02	3.334E+02	3.248E+02	2.720E+02	2.729E+02	0.000E+00	0.000E+00
10000	4.511E+01	3.136E+02	3.769E+02	3.682E+02	2.759E+02	2.768E+02	0.000E+00	0.000E+00
11000	4.924E+01	3.181E+02	4.240E+02	4.153E+02	2.795E+02	2.803E+02	0.000E+00	0.000E+00
12000	5.402E+01	3.226E+02	4.756E+02	4.669E+02	2.829E+02	2.836E+02	0.000E+00	0.000E+00
13000	5.885E+01	3.271E+02	5.320E+02	5.234E+02	2.861E+02	2.868E+02	0.000E+00	0.000E+00
14000	6.302E+01	3.316E+02	5.931E+02	5.844E+02	2.892E+02	2.899E+02	0.000E+00	0.000E+00
15000	6.600E+01	3.361E+02	6.577E+02	6.490E+02	2.922E+02	2.928E+02	0.000E+00	0.000E+00
16000	6.749E+01	3.404E+02	7.246E+02	7.159E+02	2.951E+02	2.956E+02	0.000E+00	0.000E+00
17000	6.749E+01	3.445E+02	7.922E+02	7.835E+02	2.979E+02	2.984E+02	0.000E+00	0.000E+00
18000	6.622E+01	3.483E+02	8.591E+02	8.505E+02	3.006E+02	3.011E+02	0.000E+00	0.000E+00
19000	6.400E+01	3.518E+02	9.243E+02	9.156E+02	3.032E+02	3.036E+02	0.000E+00	0.000E+00
20000	6.118E+01	3.550E+02	9.869E+02	9.783E+02	3.057E+02	3.061E+02	0.000E+00	0.000E+00
21000	5.805E+01	3.579E+02	1.047E+03	1.038E+03	3.081E+02	3.085E+02	0.000E+00	0.000E+00
22000	5.484E+01	3.606E+02	1.103E+03	1.094E+03	3.104E+02	3.108E+02	0.000E+00	0.000E+00
23000	5.172E+01	3.629E+02	1.156E+03	1.148E+03	3.127E+02	3.131E+02	0.000E+00	0.000E+00
24000	4.878E+01	3.651E+02	1.206E+03	1.198E+03	3.148E+02	3.152E+02	0.000E+00	0.000E+00
25000	4.606E+01	3.670E+02	1.254E+03	1.245E+03	3.169E+02	3.172E+02	0.000E+00	0.000E+00
26000	4.360E+01	3.688E+02	1.299E+03	1.290E+03	3.188E+02	3.192E+02	0.000E+00	0.000E+00
27000	4.138E+01	3.704E+02	1.341E+03	1.332E+03	3.207E+02	3.210E+02	0.000E+00	0.000E+00
28000	3.941E+01	3.718E+02	1.382E+03	1.373E+03	3.225E+02	3.228E+02	0.000E+00	0.000E+00
29000	3.765E+01	3.732E+02	1.420E+03	1.411E+03	3.242E+02	3.245E+02	0.000E+00	0.000E+00
30000	3.609E+01	3.744E+02	1.457E+03	1.448E+03	3.259E+02	3.262E+02	0.000E+00	0.000E+00
32000	3.348E+01	3.767E+02	1.526E+03	1.518E+03	3.290E+02	3.293E+02	0.000E+00	0.000E+00
34000	3.143E+01	3.786E+02	1.591E+03	1.582E+03	3.319E+02	3.321E+02	0.000E+00	0.000E+00
36000	2.980E+01	3.804E+02	1.652E+03	1.644E+03	3.345E+02	3.347E+02	0.000E+00	0.000E+00
38000	2.850E+01	3.820E+02	1.711E+03	1.702E+03	3.370E+02	3.372E+02	0.000E+00	0.000E+00
40000	2.745E+01	3.834E+02	1.767E+03	1.758E+03	3.392E+02	3.395E+02	0.000E+00	0.000E+00
42000	2.659E+01	3.847E+02	1.821E+03	1.812E+03	3.414E+02	3.416E+02	0.000E+00	0.000E+00
44000	2.588E+01	3.859E+02	1.873E+03	1.864E+03	3.434E+02	3.436E+02	0.000E+00	0.000E+00
46000	2.529E+01	3.871E+02	1.924E+03	1.916E+03	3.453E+02	3.454E+02	0.000E+00	0.000E+00
48000	2.480E+01	3.881E+02	1.974E+03	1.966E+03	3.470E+02	3.472E+02	0.000E+00	0.000E+00
50000	2.438E+01	3.892E+02	2.023E+03	2.015E+03	3.487E+02	3.489E+02	0.000E+00	0.000E+00

Table 153: Internal thermodynamic properties of N_2^+

T(K)	Q_{int}	$\ln(Q_{int})$	E_{int}/RT	$C_{p,int}/R$
50	$1.842E+01$	$2.913E+00$	$9.816E-01$	$1.000E+00$
100	$3.650E+01$	$3.597E+00$	$9.910E-01$	$1.000E+00$
150	$5.459E+01$	$4.000E+00$	$9.942E-01$	$1.001E+00$
200	$7.268E+01$	$4.286E+00$	$9.959E-01$	$1.001E+00$
298.15	$1.082E+02$	$4.684E+00$	$9.979E-01$	$1.004E+00$
300	$1.089E+02$	$4.690E+00$	$9.979E-01$	$1.005E+00$
400	$1.451E+02$	$4.978E+00$	$1.002E+00$	$1.027E+00$
500	$1.817E+02$	$5.202E+00$	$1.011E+00$	$1.078E+00$
600	$2.188E+02$	$5.388E+00$	$1.029E+00$	$1.154E+00$
700	$2.568E+02$	$5.548E+00$	$1.053E+00$	$1.240E+00$
800	$2.961E+02$	$5.691E+00$	$1.082E+00$	$1.327E+00$
900	$3.370E+02$	$5.820E+00$	$1.113E+00$	$1.409E+00$
1000	$3.795E+02$	$5.939E+00$	$1.147E+00$	$1.482E+00$
2000	$9.265E+02$	$6.831E+00$	$1.452E+00$	$2.013E+00$
3000	$1.760E+03$	$7.473E+00$	$1.732E+00$	$2.564E+00$
4000	$3.005E+03$	$8.008E+00$	$1.992E+00$	$2.940E+00$
5000	$4.799E+03$	$8.476E+00$	$2.200E+00$	$3.097E+00$
6000	$7.271E+03$	$8.892E+00$	$2.355E+00$	$3.145E+00$
7000	$1.055E+04$	$9.264E+00$	$2.469E+00$	$3.161E+00$
8000	$1.475E+04$	$9.599E+00$	$2.556E+00$	$3.170E+00$
9000	$2.002E+04$	$9.904E+00$	$2.624E+00$	$3.170E+00$
10000	$2.647E+04$	$1.018E+01$	$2.678E+00$	$3.145E+00$
11000	$3.424E+04$	$1.044E+01$	$2.718E+00$	$3.088E+00$
12000	$4.343E+04$	$1.068E+01$	$2.745E+00$	$2.994E+00$
13000	$5.413E+04$	$1.090E+01$	$2.760E+00$	$2.867E+00$
14000	$6.643E+04$	$1.110E+01$	$2.762E+00$	$2.716E+00$
15000	$8.035E+04$	$1.129E+01$	$2.753E+00$	$2.549E+00$
16000	$9.593E+04$	$1.147E+01$	$2.735E+00$	$2.376E+00$
17000	$1.131E+05$	$1.164E+01$	$2.709E+00$	$2.202E+00$
18000	$1.320E+05$	$1.179E+01$	$2.676E+00$	$2.033E+00$
19000	$1.524E+05$	$1.193E+01$	$2.638E+00$	$1.873E+00$
20000	$1.743E+05$	$1.207E+01$	$2.596E+00$	$1.724E+00$
21000	$1.976E+05$	$1.219E+01$	$2.551E+00$	$1.585E+00$
22000	$2.222E+05$	$1.231E+01$	$2.504E+00$	$1.458E+00$
23000	$2.481E+05$	$1.242E+01$	$2.456E+00$	$1.342E+00$
24000	$2.752E+05$	$1.253E+01$	$2.408E+00$	$1.237E+00$
25000	$3.033E+05$	$1.262E+01$	$2.359E+00$	$1.141E+00$
26000	$3.324E+05$	$1.271E+01$	$2.310E+00$	$1.054E+00$
27000	$3.624E+05$	$1.280E+01$	$2.262E+00$	$9.756E-01$
28000	$3.931E+05$	$1.288E+01$	$2.215E+00$	$9.045E-01$
29000	$4.245E+05$	$1.296E+01$	$2.169E+00$	$8.400E-01$
30000	$4.566E+05$	$1.303E+01$	$2.123E+00$	$7.815E-01$
32000	$5.222E+05$	$1.317E+01$	$2.036E+00$	$6.799E-01$
34000	$5.893E+05$	$1.329E+01$	$1.954E+00$	$5.956E-01$
36000	$6.575E+05$	$1.340E+01$	$1.876E+00$	$5.252E-01$
38000	$7.263E+05$	$1.350E+01$	$1.804E+00$	$4.659E-01$
40000	$7.953E+05$	$1.359E+01$	$1.736E+00$	$4.157E-01$
42000	$8.642E+05$	$1.367E+01$	$1.672E+00$	$3.729E-01$
44000	$9.328E+05$	$1.375E+01$	$1.612E+00$	$3.361E-01$
46000	$1.001E+06$	$1.382E+01$	$1.556E+00$	$3.044E-01$
48000	$1.068E+06$	$1.388E+01$	$1.503E+00$	$2.768E-01$
50000	$1.135E+06$	$1.394E+01$	$1.453E+00$	$2.527E-01$

Table 154: Total thermodynamic properties of N_2^+

T [K]	C_p [J/mol/K]	S^0 [J/mol/K]	$H^0(T)-H^0(0)$ [KJ/mol]	$H^0(T)-H^0(298)$ [KJ/mol]	$-(G^0-H^0(0))/T$ [J/mol/K]	$-(G^0-H^0(298))/T$ [J/mol/K]	ΔH_f [KJ/mol]	$\mathrm{Log}(K_p)$
50	2.910E+01	1.457E+02	1.447E+00	-7.224E+00	1.167E+02	2.902E+02	1.504E+03	-1.572E+03
100	2.911E+01	1.659E+02	2.903E+00	-5.769E+00	1.368E+02	2.236E+02	1.505E+03	-7.861E+02
150	2.911E+01	1.777E+02	4.358E+00	-4.313E+00	1.486E+02	2.064E+02	1.506E+03	-5.239E+02
200	2.911E+01	1.860E+02	5.813E+00	-2.858E+00	1.570E+02	2.003E+02	1.508E+03	-3.927E+02
298.15	2.914E+01	1.977E+02	8.671E+00	0.000E+00	1.686E+02	1.977E+02	1.510E+03	-2.631E+02
300	2.914E+01	1.978E+02	8.725E+00	5.387E-02	1.688E+02	1.977E+02	1.510E+03	-2.614E+02
400	2.932E+01	2.062E+02	1.165E+01	2.975E+00	1.771E+02	1.988E+02	1.512E+03	-1.957E+02
500	2.975E+01	2.128E+02	1.460E+01	5.927E+00	1.836E+02	2.010E+02	1.514E+03	-1.562E+02
600	3.038E+01	2.183E+02	1.760E+01	8.932E+00	1.890E+02	2.034E+02	1.516E+03	-1.298E+02
700	3.110E+01	2.230E+02	2.068E+01	1.201E+01	1.935E+02	2.059E+02	1.518E+03	-1.109E+02
800	3.182E+01	2.272E+02	2.382E+01	1.515E+01	1.975E+02	2.083E+02	1.520E+03	-9.676E+01
900	3.250E+01	2.310E+02	2.704E+01	1.837E+01	2.010E+02	2.106E+02	1.522E+03	-8.572E+01
1000	3.311E+01	2.345E+02	3.032E+01	2.165E+01	2.042E+02	2.128E+02	1.524E+03	-7.688E+01
2000	3.752E+01	2.589E+02	6.572E+01	5.705E+01	2.260E+02	2.303E+02	1.546E+03	-3.685E+01
3000	4.211E+01	2.749E+02	1.056E+02	9.689E+01	2.398E+02	2.427E+02	1.570E+03	-2.331E+01
4000	4.523E+01	2.875E+02	1.494E+02	1.407E+02	2.502E+02	2.524E+02	1.597E+03	-1.642E+01
5000	4.653E+01	2.978E+02	1.954E+02	1.867E+02	2.587E+02	2.604E+02	1.626E+03	-1.222E+01
6000	4.693E+01	3.063E+02	2.422E+02	2.335E+02	2.660E+02	2.674E+02	1.656E+03	-9.362E+00
7000	4.707E+01	3.136E+02	2.892E+02	2.805E+02	2.723E+02	2.735E+02	1.685E+03	-7.286E+00
8000	4.715E+01	3.199E+02	3.363E+02	3.276E+02	2.778E+02	2.789E+02	1.713E+03	-5.702E+00
9000	4.714E+01	3.254E+02	3.835E+02	3.748E+02	2.828E+02	2.838E+02	1.740E+03	-4.449E+00
10000	4.694E+01	3.304E+02	4.305E+02	4.219E+02	2.873E+02	2.882E+02	1.765E+03	-3.432E+00
11000	4.646E+01	3.348E+02	4.772E+02	4.686E+02	2.914E+02	2.922E+02	1.785E+03	-2.589E+00
12000	4.568E+01	3.388E+02	5.233E+02	5.147E+02	2.952E+02	2.959E+02	1.800E+03	-1.879E+00
13000	4.462E+01	3.425E+02	5.685E+02	5.598E+02	2.987E+02	2.994E+02	1.810E+03	-1.275E+00
14000	4.337E+01	3.457E+02	6.125E+02	6.039E+02	3.020E+02	3.026E+02	1.814E+03	-7.547E-01
15000	4.198E+01	3.487E+02	6.552E+02	6.465E+02	3.050E+02	3.056E+02	1.813E+03	-3.035E-01
16000	4.054E+01	3.513E+02	6.965E+02	6.878E+02	3.078E+02	3.083E+02	1.808E+03	9.048E-02
17000	3.909E+01	3.537E+02	7.363E+02	7.276E+02	3.104E+02	3.109E+02	1.801E+03	4.370E-01
18000	3.769E+01	3.559E+02	7.747E+02	7.660E+02	3.129E+02	3.134E+02	1.793E+03	7.438E-01
19000	3.636E+01	3.579E+02	8.117E+02	8.030E+02	3.152E+02	3.157E+02	1.786E+03	1.017E+00
20000	3.512E+01	3.598E+02	8.474E+02	8.388E+02	3.174E+02	3.178E+02	1.780E+03	1.262E+00
21000	3.397E+01	3.615E+02	8.820E+02	8.733E+02	3.195E+02	3.199E+02	1.775E+03	1.483E+00
22000	3.291E+01	3.630E+02	9.154E+02	9.067E+02	3.214E+02	3.218E+02	1.773E+03	1.684E+00
23000	3.195E+01	3.644E+02	9.478E+02	9.391E+02	3.232E+02	3.236E+02	1.773E+03	1.867E+00
24000	3.107E+01	3.658E+02	9.793E+02	9.706E+02	3.250E+02	3.254E+02	1.775E+03	2.034E+00
25000	3.027E+01	3.671E+02	1.010E+03	1.001E+03	3.266E+02	3.270E+02	1.779E+03	2.189E+00
26000	2.955E+01	3.682E+02	1.040E+03	1.031E+03	3.282E+02	3.286E+02	1.785E+03	2.332E+00
27000	2.890E+01	3.693E+02	1.069E+03	1.060E+03	3.297E+02	3.301E+02	1.792E+03	2.465E+00
28000	2.831E+01	3.704E+02	1.098E+03	1.089E+03	3.312E+02	3.315E+02	1.802E+03	2.590E+00
29000	2.777E+01	3.714E+02	1.126E+03	1.117E+03	3.325E+02	3.328E+02	1.812E+03	2.706E+00
30000	2.728E+01	3.723E+02	1.153E+03	1.145E+03	3.338E+02	3.341E+02	1.823E+03	2.815E+00
32000	2.644E+01	3.740E+02	1.207E+03	1.198E+03	3.363E+02	3.366E+02	1.849E+03	3.015E+00
34000	2.574E+01	3.756E+02	1.259E+03	1.250E+03	3.386E+02	3.388E+02	1.878E+03	3.193E+00
36000	2.515E+01	3.771E+02	1.310E+03	1.301E+03	3.407E+02	3.409E+02	1.909E+03	3.355E+00
38000	2.466E+01	3.784E+02	1.360E+03	1.351E+03	3.426E+02	3.428E+02	1.942E+03	3.502E+00
40000	2.424E+01	3.796E+02	1.409E+03	1.400E+03	3.444E+02	3.446E+02	1.977E+03	3.637E+00
42000	2.389E+01	3.808E+02	1.457E+03	1.448E+03	3.461E+02	3.463E+02	2.013E+03	3.761E+00
44000	2.358E+01	3.819E+02	1.504E+03	1.496E+03	3.477E+02	3.479E+02	2.049E+03	3.876E+00
46000	2.332E+01	3.830E+02	1.551E+03	1.542E+03	3.492E+02	3.494E+02	2.086E+03	3.982E+00
48000	2.309E+01	3.840E+02	1.598E+03	1.589E+03	3.507E+02	3.509E+02	2.124E+03	4.082E+00
50000	2.289E+01	3.849E+02	1.644E+03	1.635E+03	3.520E+02	3.522E+02	2.163E+03	4.175E+00

Table 155: Internal thermodynamic properties of N_2^-

T(K)	Q_{int}	$\ln(Q_{int})$	E_{int}/RT	$C_{p,int}/R$
50	$4.192E+01$	$3.736E+00$	$9.839E-01$	$1.000E+00$
100	$8.318E+01$	$4.421E+00$	$9.921E-01$	$1.000E+00$
150	$1.244E+02$	$4.824E+00$	$9.950E-01$	$1.001E+00$
200	$1.657E+02$	$5.110E+00$	$9.965E-01$	$1.001E+00$
298.15	$2.468E+02$	$5.509E+00$	$9.988E-01$	$1.009E+00$
300	$2.483E+02$	$5.515E+00$	$9.989E-01$	$1.009E+00$
400	$3.312E+02$	$5.803E+00$	$1.005E+00$	$1.047E+00$
500	$4.151E+02$	$6.029E+00$	$1.020E+00$	$1.120E+00$
600	$5.010E+02$	$6.217E+00$	$1.045E+00$	$1.213E+00$
700	$5.899E+02$	$6.380E+00$	$1.076E+00$	$1.310E+00$
800	$6.826E+02$	$6.526E+00$	$1.111E+00$	$1.401E+00$
900	$7.796E+02$	$6.659E+00$	$1.148E+00$	$1.482E+00$
1000	$8.815E+02$	$6.782E+00$	$1.185E+00$	$1.553E+00$
2000	$2.209E+03$	$7.700E+00$	$1.472E+00$	$1.886E+00$
3000	$4.146E+03$	$8.330E+00$	$1.629E+00$	$1.986E+00$
4000	$6.718E+03$	$8.813E+00$	$1.725E+00$	$2.038E+00$
5000	$9.947E+03$	$9.205E+00$	$1.792E+00$	$2.076E+00$
6000	$1.385E+04$	$9.536E+00$	$1.842E+00$	$2.110E+00$
7000	$1.846E+04$	$9.823E+00$	$1.882E+00$	$2.140E+00$
8000	$2.379E+04$	$1.008E+01$	$1.916E+00$	$2.166E+00$
9000	$2.986E+04$	$1.030E+01$	$1.945E+00$	$2.182E+00$
10000	$3.670E+04$	$1.051E+01$	$1.969E+00$	$2.183E+00$
11000	$4.432E+04$	$1.070E+01$	$1.988E+00$	$2.166E+00$
12000	$5.272E+04$	$1.087E+01$	$2.001E+00$	$2.130E+00$
13000	$6.190E+04$	$1.103E+01$	$2.009E+00$	$2.077E+00$
14000	$7.184E+04$	$1.118E+01$	$2.012E+00$	$2.010E+00$
15000	$8.254E+04$	$1.132E+01$	$2.009E+00$	$1.932E+00$
16000	$9.394E+04$	$1.145E+01$	$2.001E+00$	$1.848E+00$
17000	$1.060E+05$	$1.157E+01$	$1.990E+00$	$1.760E+00$
18000	$1.187E+05$	$1.168E+01$	$1.975E+00$	$1.673E+00$
19000	$1.321E+05$	$1.179E+01$	$1.957E+00$	$1.587E+00$
20000	$1.459E+05$	$1.189E+01$	$1.936E+00$	$1.505E+00$
21000	$1.603E+05$	$1.198E+01$	$1.914E+00$	$1.427E+00$
22000	$1.751E+05$	$1.207E+01$	$1.890E+00$	$1.355E+00$
23000	$1.904E+05$	$1.216E+01$	$1.865E+00$	$1.288E+00$
24000	$2.060E+05$	$1.224E+01$	$1.840E+00$	$1.226E+00$
25000	$2.219E+05$	$1.231E+01$	$1.814E+00$	$1.169E+00$
26000	$2.382E+05$	$1.238E+01$	$1.788E+00$	$1.117E+00$
27000	$2.547E+05$	$1.245E+01$	$1.762E+00$	$1.070E+00$
28000	$2.714E+05$	$1.251E+01$	$1.737E+00$	$1.027E+00$
29000	$2.884E+05$	$1.257E+01$	$1.712E+00$	$9.875E-01$
30000	$3.055E+05$	$1.263E+01$	$1.687E+00$	$9.519E-01$
32000	$3.401E+05$	$1.274E+01$	$1.639E+00$	$8.897E-01$
34000	$3.751E+05$	$1.283E+01$	$1.593E+00$	$8.375E-01$
36000	$4.103E+05$	$1.292E+01$	$1.550E+00$	$7.933E-01$
38000	$4.457E+05$	$1.301E+01$	$1.509E+00$	$7.552E-01$
40000	$4.811E+05$	$1.308E+01$	$1.471E+00$	$7.220E-01$
42000	$5.164E+05$	$1.315E+01$	$1.434E+00$	$6.925E-01$
44000	$5.516E+05$	$1.322E+01$	$1.400E+00$	$6.660E-01$
46000	$5.866E+05$	$1.328E+01$	$1.368E+00$	$6.418E-01$
48000	$6.214E+05$	$1.334E+01$	$1.337E+00$	$6.195E-01$
50000	$6.558E+05$	$1.339E+01$	$1.308E+00$	$5.986E-01$

Table 156: Total thermodynamic properties of N_2^-

T [K]	C_p [J/mol/K]	S^0 [J/mol/K]	$H^0(T)-H^0(0)$ [KJ/mol]	$H^0(T)-H^0(298)$ [KJ/mol]	$-(G^0-H^0(0))/T$ [J/mol/K]	$-(G^0-H^0(298))/T$ [J/mol/K]	ΔH_f [KJ/mol]	$\mathrm{Log}(K_p)$
50	2.910E+01	1.526E+02	1.448E+00	-7.225E+00	1.236E+02	2.971E+02	3.292E+01	-3.288E+01
100	2.911E+01	1.727E+02	2.904E+00	-5.770E+00	1.437E+02	2.304E+02	3.189E+01	-1.589E+01
150	2.911E+01	1.845E+02	4.359E+00	-4.314E+00	1.555E+02	2.133E+02	3.085E+01	-1.042E+01
200	2.911E+01	1.929E+02	5.814E+00	-2.859E+00	1.638E+02	2.072E+02	2.981E+01	-7.773E+00
298.15	2.917E+01	2.045E+02	8.673E+00	0.000E+00	1.754E+02	2.045E+02	2.777E+01	-5.286E+00
300	2.918E+01	2.047E+02	8.727E+00	5.401E-02	1.756E+02	2.045E+02	2.773E+01	-5.256E+00
400	2.949E+01	2.131E+02	1.166E+01	2.985E+00	1.840E+02	2.057E+02	2.566E+01	-4.090E+00
500	3.010E+01	2.198E+02	1.463E+01	5.962E+00	1.905E+02	2.078E+02	2.362E+01	-3.444E+00
600	3.087E+01	2.253E+02	1.768E+01	9.010E+00	1.959E+02	2.103E+02	2.161E+01	-3.049E+00
700	3.168E+01	2.302E+02	2.081E+01	1.214E+01	2.004E+02	2.128E+02	1.962E+01	-2.792E+00
800	3.244E+01	2.344E+02	2.402E+01	1.534E+01	2.044E+02	2.152E+02	1.763E+01	-2.618E+00
900	3.311E+01	2.383E+02	2.730E+01	1.862E+01	2.080E+02	2.176E+02	1.566E+01	-2.497E+00
1000	3.370E+01	2.418E+02	3.064E+01	2.196E+01	2.112E+02	2.198E+02	1.368E+01	-2.412E+00
2000	3.646E+01	2.662E+02	6.604E+01	5.737E+01	2.332E+02	2.376E+02	-6.376E+00	-2.256E+00
3000	3.730E+01	2.812E+02	1.030E+02	9.431E+01	2.469E+02	2.498E+02	-2.680E+01	-2.388E+00
4000	3.773E+01	2.920E+02	1.405E+02	1.318E+02	2.569E+02	2.590E+02	-4.737E+01	-2.545E+00
5000	3.805E+01	3.005E+02	1.784E+02	1.697E+02	2.648E+02	2.665E+02	-6.801E+01	-2.694E+00
6000	3.833E+01	3.074E+02	2.166E+02	2.079E+02	2.713E+02	2.728E+02	-8.871E+01	-2.829E+00
7000	3.858E+01	3.134E+02	2.551E+02	2.464E+02	2.769E+02	2.781E+02	-1.096E+02	-2.952E+00
8000	3.879E+01	3.185E+02	2.938E+02	2.851E+02	2.818E+02	2.829E+02	-1.311E+02	-3.064E+00
9000	3.892E+01	3.231E+02	3.326E+02	3.239E+02	2.861E+02	2.871E+02	-1.539E+02	-3.167E+00
10000	3.893E+01	3.272E+02	3.716E+02	3.629E+02	2.900E+02	2.909E+02	-1.792E+02	-3.263E+00
11000	3.879E+01	3.309E+02	4.104E+02	4.018E+02	2.936E+02	2.944E+02	-2.082E+02	-3.354E+00
12000	3.849E+01	3.343E+02	4.491E+02	4.404E+02	2.968E+02	2.976E+02	-2.420E+02	-3.443E+00
13000	3.805E+01	3.373E+02	4.874E+02	4.787E+02	2.998E+02	3.005E+02	-2.809E+02	-3.530E+00
14000	3.749E+01	3.401E+02	5.252E+02	5.165E+02	3.026E+02	3.032E+02	-3.249E+02	-3.617E+00
15000	3.685E+01	3.427E+02	5.623E+02	5.537E+02	3.052E+02	3.058E+02	-3.732E+02	-3.704E+00
16000	3.615E+01	3.451E+02	5.988E+02	5.902E+02	3.076E+02	3.082E+02	-4.244E+02	-3.790E+00
17000	3.542E+01	3.472E+02	6.346E+02	6.260E+02	3.099E+02	3.104E+02	-4.770E+02	-3.877E+00
18000	3.469E+01	3.492E+02	6.697E+02	6.610E+02	3.120E+02	3.125E+02	-5.296E+02	-3.962E+00
19000	3.398E+01	3.511E+02	7.040E+02	6.954E+02	3.140E+02	3.145E+02	-5.813E+02	-4.047E+00
20000	3.330E+01	3.528E+02	7.377E+02	7.290E+02	3.159E+02	3.164E+02	-6.310E+02	-4.131E+00
21000	3.265E+01	3.544E+02	7.706E+02	7.620E+02	3.177E+02	3.181E+02	-6.785E+02	-4.212E+00
22000	3.205E+01	3.559E+02	8.030E+02	7.943E+02	3.194E+02	3.198E+02	-7.234E+02	-4.291E+00
23000	3.149E+01	3.573E+02	8.348E+02	8.261E+02	3.210E+02	3.214E+02	-7.656E+02	-4.368E+00
24000	3.098E+01	3.587E+02	8.660E+02	8.573E+02	3.226E+02	3.229E+02	-8.054E+02	-4.442E+00
25000	3.050E+01	3.599E+02	8.967E+02	8.880E+02	3.241E+02	3.244E+02	-8.429E+02	-4.514E+00
26000	3.007E+01	3.611E+02	9.270E+02	9.183E+02	3.254E+02	3.258E+02	-8.782E+02	-4.583E+00
27000	2.968E+01	3.622E+02	9.569E+02	9.482E+02	3.268E+02	3.271E+02	-9.116E+02	-4.650E+00
28000	2.932E+01	3.633E+02	9.864E+02	9.777E+02	3.281E+02	3.284E+02	-9.432E+02	-4.714E+00
29000	2.900E+01	3.643E+02	1.016E+03	1.007E+03	3.293E+02	3.296E+02	-9.734E+02	-4.776E+00
30000	2.870E+01	3.653E+02	1.044E+03	1.036E+03	3.305E+02	3.308E+02	-1.002E+03	-4.835E+00
32000	2.818E+01	3.671E+02	1.101E+03	1.093E+03	3.327E+02	3.330E+02	-1.056E+03	-4.947E+00
34000	2.775E+01	3.688E+02	1.157E+03	1.148E+03	3.348E+02	3.351E+02	-1.107E+03	-5.051E+00
36000	2.738E+01	3.704E+02	1.212E+03	1.204E+03	3.367E+02	3.370E+02	-1.154E+03	-5.147E+00
38000	2.707E+01	3.719E+02	1.267E+03	1.258E+03	3.386E+02	3.388E+02	-1.200E+03	-5.237E+00
40000	2.679E+01	3.733E+02	1.321E+03	1.312E+03	3.402E+02	3.405E+02	-1.244E+03	-5.321E+00
42000	2.654E+01	3.746E+02	1.374E+03	1.365E+03	3.419E+02	3.421E+02	-1.286E+03	-5.400E+00
44000	2.632E+01	3.758E+02	1.427E+03	1.418E+03	3.434E+02	3.436E+02	-1.327E+03	-5.473E+00
46000	2.612E+01	3.770E+02	1.479E+03	1.470E+03	3.448E+02	3.450E+02	-1.367E+03	-5.543E+00
48000	2.594E+01	3.781E+02	1.531E+03	1.523E+03	3.462E+02	3.464E+02	-1.407E+03	-5.609E+00
50000	2.576E+01	3.791E+02	1.583E+03	1.574E+03	3.475E+02	3.476E+02	-1.446E+03	-5.671E+00

Table 157: Internal thermodynamic properties of N_3

T(K)	Q_{int}	$\ln(Q_{int})$	E_{int}/RT	$C_{p,int}/R$
50	$9.116E+01$	$4.513E+00$	$1.228E+00$	$1.426E+00$
100	$2.190E+02$	$5.389E+00$	$1.270E+00$	$1.213E+00$
150	$3.642E+02$	$5.898E+00$	$1.241E+00$	$1.191E+00$
200	$5.203E+02$	$6.254E+00$	$1.246E+00$	$1.350E+00$
298.15	$8.709E+02$	$6.769E+00$	$1.360E+00$	$1.851E+00$
300	$8.782E+02$	$6.778E+00$	$1.363E+00$	$1.861E+00$
400	$1.333E+03$	$7.195E+00$	$1.551E+00$	$2.358E+00$
500	$1.926E+03$	$7.563E+00$	$1.756E+00$	$2.782E+00$
600	$2.701E+03$	$7.901E+00$	$1.958E+00$	$3.136E+00$
700	$3.705E+03$	$8.217E+00$	$2.147E+00$	$3.427E+00$
800	$4.993E+03$	$8.516E+00$	$2.323E+00$	$3.667E+00$
900	$6.626E+03$	$8.799E+00$	$2.483E+00$	$3.862E+00$
1000	$8.674E+03$	$9.068E+00$	$2.630E+00$	$4.022E+00$
2000	$7.431E+04$	$1.122E+01$	$3.540E+00$	$4.696E+00$
3000	$3.409E+05$	$1.274E+01$	$3.957E+00$	$4.859E+00$
4000	$1.102E+06$	$1.391E+01$	$4.191E+00$	$4.915E+00$
5000	$2.855E+06$	$1.486E+01$	$4.337E+00$	$4.918E+00$
6000	$6.352E+06$	$1.566E+01$	$4.430E+00$	$4.856E+00$
7000	$1.263E+07$	$1.635E+01$	$4.482E+00$	$4.724E+00$
8000	$2.301E+07$	$1.695E+01$	$4.501E+00$	$4.530E+00$
9000	$3.909E+07$	$1.748E+01$	$4.491E+00$	$4.295E+00$
10000	$6.265E+07$	$1.795E+01$	$4.459E+00$	$4.038E+00$
11000	$9.560E+07$	$1.838E+01$	$4.408E+00$	$3.775E+00$
12000	$1.399E+08$	$1.876E+01$	$4.345E+00$	$3.519E+00$
13000	$1.976E+08$	$1.910E+01$	$4.272E+00$	$3.274E+00$
14000	$2.704E+08$	$1.942E+01$	$4.192E+00$	$3.044E+00$
15000	$3.600E+08$	$1.970E+01$	$4.109E+00$	$2.832E+00$
16000	$4.681E+08$	$1.996E+01$	$4.023E+00$	$2.637E+00$
17000	$5.958E+08$	$2.021E+01$	$3.936E+00$	$2.458E+00$
18000	$7.443E+08$	$2.043E+01$	$3.849E+00$	$2.294E+00$
19000	$9.143E+08$	$2.063E+01$	$3.763E+00$	$2.144E+00$
20000	$1.107E+09$	$2.082E+01$	$3.679E+00$	$2.008E+00$
21000	$1.322E+09$	$2.100E+01$	$3.596E+00$	$1.883E+00$
22000	$1.559E+09$	$2.117E+01$	$3.516E+00$	$1.769E+00$
23000	$1.820E+09$	$2.132E+01$	$3.437E+00$	$1.664E+00$
24000	$2.103E+09$	$2.147E+01$	$3.361E+00$	$1.568E+00$
25000	$2.409E+09$	$2.160E+01$	$3.288E+00$	$1.479E+00$
26000	$2.737E+09$	$2.173E+01$	$3.217E+00$	$1.398E+00$
27000	$3.086E+09$	$2.185E+01$	$3.148E+00$	$1.323E+00$
28000	$3.456E+09$	$2.196E+01$	$3.082E+00$	$1.253E+00$
29000	$3.846E+09$	$2.207E+01$	$3.017E+00$	$1.189E+00$
30000	$4.256E+09$	$2.217E+01$	$2.955E+00$	$1.129E+00$
32000	$5.131E+09$	$2.236E+01$	$2.838E+00$	$1.022E+00$
34000	$6.074E+09$	$2.253E+01$	$2.728E+00$	$9.290E-01$
36000	$7.078E+09$	$2.268E+01$	$2.626E+00$	$8.478E-01$
38000	$8.137E+09$	$2.282E+01$	$2.530E+00$	$7.766E-01$
40000	$9.243E+09$	$2.295E+01$	$2.441E+00$	$7.138E-01$
42000	$1.039E+10$	$2.306E+01$	$2.358E+00$	$6.582E-01$
44000	$1.157E+10$	$2.317E+01$	$2.279E+00$	$6.086E-01$
46000	$1.279E+10$	$2.327E+01$	$2.206E+00$	$5.644E-01$
48000	$1.402E+10$	$2.336E+01$	$2.136E+00$	$5.247E-01$
50000	$1.528E+10$	$2.345E+01$	$2.071E+00$	$4.890E-01$

Table 158: Total thermodynamic properties of N_3

T [K]	C_p [J/mol/K]	S^0 [J/mol/K]	$H^0(T)-H^0(0)$ [KJ/mol]	$H^0(T)-H^0(298)$ [KJ/mol]	$-(G^0-H^0(0))/T$ [J/mol/K]	$-(G^0-H^0(298))/T$ [J/mol/K]	ΔH_f [KJ/mol]	$\mathrm{Log}(K_p)$
50	3.265E+01	1.661E+02	1.550E+00	-8.019E+00	1.351E+02	3.265E+02	4.136E+02	-4.343E+02
100	3.087E+01	1.881E+02	3.134E+00	-6.435E+00	1.568E+02	2.525E+02	4.130E+02	-2.184E+02
150	3.069E+01	2.006E+02	4.666E+00	-4.903E+00	1.694E+02	2.332E+02	4.124E+02	-1.466E+02
200	3.201E+01	2.095E+02	6.229E+00	-3.341E+00	1.784E+02	2.262E+02	4.117E+02	-1.107E+02
298.15	3.617E+01	2.231E+02	9.569E+00	0.000E+00	1.910E+02	2.231E+02	4.108E+02	-7.533E+01
300	3.626E+01	2.233E+02	9.636E+00	6.698E-02	1.912E+02	2.231E+02	4.108E+02	-7.488E+01
400	4.039E+01	2.343E+02	1.347E+01	3.904E+00	2.006E+02	2.246E+02	4.102E+02	-5.702E+01
500	4.392E+01	2.437E+02	1.769E+01	8.125E+00	2.083E+02	2.275E+02	4.100E+02	-4.630E+01
600	4.686E+01	2.520E+02	2.224E+01	1.267E+01	2.149E+02	2.309E+02	4.101E+02	-3.916E+01
700	4.928E+01	2.594E+02	2.705E+01	1.748E+01	2.208E+02	2.344E+02	4.104E+02	-3.406E+01
800	5.127E+01	2.661E+02	3.208E+01	2.251E+01	2.260E+02	2.380E+02	4.107E+02	-3.023E+01
900	5.290E+01	2.722E+02	3.729E+01	2.772E+01	2.308E+02	2.414E+02	4.112E+02	-2.725E+01
1000	5.423E+01	2.779E+02	4.265E+01	3.308E+01	2.352E+02	2.448E+02	4.117E+02	-2.486E+01
2000	5.984E+01	3.177E+02	1.004E+02	9.086E+01	2.675E+02	2.723E+02	4.174E+02	-1.406E+01
3000	6.118E+01	3.423E+02	1.611E+02	1.515E+02	2.886E+02	2.918E+02	4.232E+02	-1.040E+01
4000	6.165E+01	3.600E+02	2.225E+02	2.130E+02	3.043E+02	3.067E+02	4.287E+02	-8.548E+00
5000	6.167E+01	3.737E+02	2.842E+02	2.747E+02	3.169E+02	3.188E+02	4.338E+02	-7.422E+00
6000	6.116E+01	3.849E+02	3.457E+02	3.361E+02	3.273E+02	3.289E+02	4.381E+02	-6.663E+00
7000	6.006E+01	3.943E+02	4.064E+02	3.968E+02	3.362E+02	3.376E+02	4.409E+02	-6.116E+00
8000	5.845E+01	4.022E+02	4.656E+02	4.561E+02	3.440E+02	3.452E+02	4.411E+02	-5.705E+00
9000	5.649E+01	4.090E+02	5.231E+02	5.136E+02	3.509E+02	3.519E+02	4.372E+02	-5.386E+00
10000	5.436E+01	4.148E+02	5.786E+02	5.690E+02	3.570E+02	3.579E+02	4.274E+02	-5.134E+00
11000	5.218E+01	4.199E+02	6.318E+02	6.223E+02	3.625E+02	3.633E+02	4.101E+02	-4.935E+00
12000	5.004E+01	4.244E+02	6.830E+02	6.734E+02	3.674E+02	3.682E+02	3.838E+02	-4.777E+00
13000	4.801E+01	4.283E+02	7.320E+02	7.224E+02	3.720E+02	3.727E+02	3.481E+02	-4.655E+00
14000	4.610E+01	4.318E+02	7.790E+02	7.694E+02	3.761E+02	3.768E+02	3.036E+02	-4.561E+00
15000	4.433E+01	4.349E+02	8.242E+02	8.146E+02	3.799E+02	3.806E+02	2.519E+02	-4.491E+00
16000	4.271E+01	4.377E+02	8.677E+02	8.581E+02	3.835E+02	3.841E+02	1.951E+02	-4.442E+00
17000	4.122E+01	4.402E+02	9.097E+02	9.001E+02	3.867E+02	3.873E+02	1.356E+02	-4.411E+00
18000	3.986E+01	4.426E+02	9.502E+02	9.406E+02	3.898E+02	3.903E+02	7.571E+01	-4.393E+00
19000	3.862E+01	4.447E+02	9.894E+02	9.799E+02	3.926E+02	3.931E+02	1.718E+01	-4.385E+00
20000	3.748E+01	4.466E+02	1.028E+03	1.018E+03	3.953E+02	3.957E+02	-3.872E+01	-4.387E+00
21000	3.644E+01	4.484E+02	1.064E+03	1.055E+03	3.978E+02	3.982E+02	-9.120E+01	-4.395E+00
22000	3.549E+01	4.501E+02	1.100E+03	1.091E+03	4.001E+02	4.005E+02	-1.399E+02	-4.408E+00
23000	3.462E+01	4.517E+02	1.135E+03	1.126E+03	4.023E+02	4.027E+02	-1.848E+02	-4.425E+00
24000	3.382E+01	4.531E+02	1.170E+03	1.160E+03	4.044E+02	4.048E+02	-2.259E+02	-4.444E+00
25000	3.309E+01	4.545E+02	1.203E+03	1.194E+03	4.064E+02	4.068E+02	-2.636E+02	-4.465E+00
26000	3.241E+01	4.558E+02	1.236E+03	1.226E+03	4.082E+02	4.086E+02	-2.980E+02	-4.488E+00
27000	3.178E+01	4.570E+02	1.268E+03	1.258E+03	4.100E+02	4.104E+02	-3.296E+02	-4.511E+00
28000	3.120E+01	4.581E+02	1.299E+03	1.290E+03	4.117E+02	4.121E+02	-3.587E+02	-4.535E+00
29000	3.067E+01	4.592E+02	1.330E+03	1.321E+03	4.133E+02	4.137E+02	-3.855E+02	-4.559E+00
30000	3.017E+01	4.602E+02	1.361E+03	1.351E+03	4.149E+02	4.152E+02	-4.104E+02	-4.583E+00
32000	2.928E+01	4.622E+02	1.420E+03	1.411E+03	4.178E+02	4.181E+02	-4.552E+02	-4.630E+00
34000	2.851E+01	4.639E+02	1.478E+03	1.468E+03	4.204E+02	4.207E+02	-4.946E+02	-4.676E+00
36000	2.784E+01	4.655E+02	1.534E+03	1.525E+03	4.229E+02	4.232E+02	-5.301E+02	-4.719E+00
38000	2.724E+01	4.670E+02	1.589E+03	1.580E+03	4.252E+02	4.254E+02	-5.624E+02	-4.761E+00
40000	2.672E+01	4.684E+02	1.643E+03	1.634E+03	4.273E+02	4.276E+02	-5.923E+02	-4.801E+00
42000	2.626E+01	4.697E+02	1.696E+03	1.687E+03	4.293E+02	4.295E+02	-6.203E+02	-4.838E+00
44000	2.585E+01	4.709E+02	1.748E+03	1.739E+03	4.312E+02	4.314E+02	-6.469E+02	-4.874E+00
46000	2.548E+01	4.721E+02	1.800E+03	1.790E+03	4.329E+02	4.331E+02	-6.723E+02	-4.908E+00
48000	2.515E+01	4.731E+02	1.850E+03	1.841E+03	4.346E+02	4.348E+02	-6.968E+02	-4.941E+00
50000	2.485E+01	4.741E+02	1.900E+03	1.891E+03	4.361E+02	4.363E+02	-7.206E+02	-4.971E+00

Table 159: Internal thermodynamic properties of NO

T(K)	Q_{int}	$\ln(Q_{int})$	E_{int}/RT	$C_{p,int}/R$
50	$8.492E+01$	$4.442E+00$	$9.840E-01$	$1.000E+00$
100	$1.685E+02$	$5.127E+00$	$9.920E-01$	$1.000E+00$
150	$2.521E+02$	$5.530E+00$	$9.947E-01$	$1.000E+00$
200	$3.356E+02$	$5.816E+00$	$9.961E-01$	$1.000E+00$
298.15	$4.998E+02$	$6.214E+00$	$9.985E-01$	$1.010E+00$
300	$5.029E+02$	$6.220E+00$	$9.985E-01$	$1.010E+00$
400	$6.708E+02$	$6.508E+00$	$1.006E+00$	$1.054E+00$
500	$8.410E+02$	$6.735E+00$	$1.023E+00$	$1.135E+00$
600	$1.016E+03$	$6.923E+00$	$1.050E+00$	$1.234E+00$
700	$1.197E+03$	$7.088E+00$	$1.083E+00$	$1.334E+00$
800	$1.387E+03$	$7.235E+00$	$1.121E+00$	$1.426E+00$
900	$1.586E+03$	$7.369E+00$	$1.159E+00$	$1.506E+00$
1000	$1.796E+03$	$7.493E+00$	$1.197E+00$	$1.576E+00$
2000	$4.546E+03$	$8.422E+00$	$1.487E+00$	$1.899E+00$
3000	$8.581E+03$	$9.057E+00$	$1.643E+00$	$1.999E+00$
4000	$1.396E+04$	$9.544E+00$	$1.739E+00$	$2.056E+00$
5000	$2.074E+04$	$9.940E+00$	$1.808E+00$	$2.111E+00$
6000	$2.899E+04$	$1.027E+01$	$1.865E+00$	$2.192E+00$
7000	$3.880E+04$	$1.057E+01$	$1.920E+00$	$2.317E+00$
8000	$5.033E+04$	$1.083E+01$	$1.979E+00$	$2.479E+00$
9000	$6.378E+04$	$1.106E+01$	$2.045E+00$	$2.655E+00$
10000	$7.940E+04$	$1.128E+01$	$2.114E+00$	$2.812E+00$
11000	$9.743E+04$	$1.149E+01$	$2.183E+00$	$2.924E+00$
12000	$1.181E+05$	$1.168E+01$	$2.247E+00$	$2.978E+00$
13000	$1.417E+05$	$1.186E+01$	$2.304E+00$	$2.971E+00$
14000	$1.684E+05$	$1.203E+01$	$2.349E+00$	$2.909E+00$
15000	$1.983E+05$	$1.220E+01$	$2.383E+00$	$2.805E+00$
16000	$2.315E+05$	$1.235E+01$	$2.406E+00$	$2.670E+00$
17000	$2.679E+05$	$1.250E+01$	$2.417E+00$	$2.518E+00$
18000	$3.076E+05$	$1.264E+01$	$2.418E+00$	$2.357E+00$
19000	$3.505E+05$	$1.277E+01$	$2.410E+00$	$2.194E+00$
20000	$3.965E+05$	$1.289E+01$	$2.396E+00$	$2.036E+00$
21000	$4.455E+05$	$1.301E+01$	$2.375E+00$	$1.884E+00$
22000	$4.972E+05$	$1.312E+01$	$2.349E+00$	$1.742E+00$
23000	$5.516E+05$	$1.322E+01$	$2.320E+00$	$1.609E+00$
24000	$6.084E+05$	$1.332E+01$	$2.288E+00$	$1.487E+00$
25000	$6.675E+05$	$1.341E+01$	$2.253E+00$	$1.375E+00$
26000	$7.287E+05$	$1.350E+01$	$2.218E+00$	$1.272E+00$
27000	$7.918E+05$	$1.358E+01$	$2.181E+00$	$1.178E+00$
28000	$8.565E+05$	$1.366E+01$	$2.143E+00$	$1.093E+00$
29000	$9.228E+05$	$1.374E+01$	$2.106E+00$	$1.016E+00$
30000	$9.905E+05$	$1.381E+01$	$2.068E+00$	$9.450E-01$
32000	$1.129E+06$	$1.394E+01$	$1.994E+00$	$8.220E-01$
34000	$1.272E+06$	$1.406E+01$	$1.922E+00$	$7.195E-01$
36000	$1.416E+06$	$1.416E+01$	$1.853E+00$	$6.337E-01$
38000	$1.563E+06$	$1.426E+01$	$1.787E+00$	$5.615E-01$
40000	$1.710E+06$	$1.435E+01$	$1.724E+00$	$5.003E-01$
42000	$1.858E+06$	$1.443E+01$	$1.664E+00$	$4.481E-01$
44000	$2.004E+06$	$1.451E+01$	$1.608E+00$	$4.033E-01$
46000	$2.150E+06$	$1.458E+01$	$1.555E+00$	$3.647E-01$
48000	$2.295E+06$	$1.465E+01$	$1.504E+00$	$3.312E-01$
50000	$2.438E+06$	$1.471E+01$	$1.457E+00$	$3.020E-01$

Table 160: Total thermodynamic properties of NO

T [K]	C_p [J/mol/K]	S^0 [J/mol/K]	$H^0(T)-H^0(0)$ [KJ/mol]	$H^0(T)-H^0(298)$ [KJ/mol]	$-(G^0-H^0(0))/T$ [J/mol/K]	$-(G^0-H^0(298))/T$ [J/mol/K]	ΔH_f [KJ/mol]	$\mathrm{Log}(K_p)$
50	2.910E+01	1.593E+02	1.448E+00	-7.224E+00	1.303E+02	3.038E+02	8.979E+01	-9.313E+01
100	2.910E+01	1.794E+02	2.904E+00	-5.769E+00	1.504E+02	2.371E+02	8.979E+01	-4.623E+01
150	2.910E+01	1.912E+02	4.359E+00	-4.314E+00	1.622E+02	2.200E+02	8.979E+01	-3.059E+01
200	2.910E+01	1.996E+02	5.814E+00	-2.859E+00	1.706E+02	2.139E+02	8.979E+01	-2.278E+01
298.15	2.918E+01	2.112E+02	8.673E+00	0.000E+00	1.822E+02	2.112E+02	8.978E+01	-1.506E+01
300	2.919E+01	2.114E+02	8.727E+00	5.401E-02	1.823E+02	2.112E+02	8.978E+01	-1.496E+01
400	2.955E+01	2.199E+02	1.166E+01	2.988E+00	1.907E+02	2.124E+02	8.977E+01	-1.105E+01
500	3.022E+01	2.265E+02	1.465E+01	5.975E+00	1.972E+02	2.146E+02	8.976E+01	-8.709E+00
600	3.104E+01	2.321E+02	1.771E+01	9.037E+00	2.026E+02	2.171E+02	8.975E+01	-7.146E+00
700	3.187E+01	2.370E+02	2.086E+01	1.218E+01	2.072E+02	2.196E+02	8.975E+01	-6.030E+00
800	3.264E+01	2.413E+02	2.408E+01	1.541E+01	2.112E+02	2.220E+02	8.975E+01	-5.193E+00
900	3.331E+01	2.452E+02	2.738E+01	1.871E+01	2.147E+02	2.244E+02	8.976E+01	-4.542E+00
1000	3.389E+01	2.487E+02	3.074E+01	2.207E+01	2.179E+02	2.266E+02	8.977E+01	-4.021E+00
2000	3.658E+01	2.732E+02	6.629E+01	5.762E+01	2.401E+02	2.444E+02	8.973E+01	-1.676E+00
3000	3.741E+01	2.882E+02	1.033E+02	9.467E+01	2.538E+02	2.567E+02	8.902E+01	-8.970E-01
4000	3.788E+01	2.991E+02	1.410E+02	1.323E+02	2.638E+02	2.660E+02	8.756E+01	-5.122E-01
5000	3.834E+01	3.076E+02	1.791E+02	1.704E+02	2.718E+02	2.735E+02	8.559E+01	-2.858E-01
6000	3.901E+01	3.146E+02	2.177E+02	2.091E+02	2.783E+02	2.798E+02	8.341E+01	-1.386E-01
7000	4.005E+01	3.207E+02	2.572E+02	2.486E+02	2.839E+02	2.852E+02	8.149E+01	-3.603E-02
8000	4.140E+01	3.261E+02	2.979E+02	2.893E+02	2.889E+02	2.900E+02	8.032E+01	3.939E-02
9000	4.286E+01	3.311E+02	3.401E+02	3.314E+02	2.933E+02	2.943E+02	8.011E+01	9.752E-02
10000	4.416E+01	3.357E+02	3.836E+02	3.749E+02	2.973E+02	2.982E+02	8.066E+01	1.442E-01
11000	4.510E+01	3.399E+02	4.283E+02	4.196E+02	3.010E+02	3.018E+02	8.134E+01	1.826E-01
12000	4.555E+01	3.439E+02	4.736E+02	4.650E+02	3.044E+02	3.051E+02	8.133E+01	2.148E-01
13000	4.549E+01	3.475E+02	5.192E+02	5.105E+02	3.076E+02	3.082E+02	7.994E+01	2.419E-01
14000	4.498E+01	3.509E+02	5.645E+02	5.558E+02	3.106E+02	3.112E+02	7.678E+01	2.644E-01
15000	4.411E+01	3.539E+02	6.090E+02	6.004E+02	3.134E+02	3.139E+02	7.184E+01	2.830E-01
16000	4.299E+01	3.568E+02	6.526E+02	6.439E+02	3.160E+02	3.165E+02	6.542E+01	2.979E-01
17000	4.172E+01	3.593E+02	6.950E+02	6.863E+02	3.185E+02	3.190E+02	5.799E+01	3.098E-01
18000	4.038E+01	3.617E+02	7.360E+02	7.274E+02	3.208E+02	3.213E+02	5.007E+01	3.191E-01
19000	3.903E+01	3.638E+02	7.757E+02	7.670E+02	3.230E+02	3.235E+02	4.211E+01	3.261E-01
20000	3.771E+01	3.658E+02	8.141E+02	8.054E+02	3.251E+02	3.255E+02	3.446E+01	3.314E-01
21000	3.645E+01	3.676E+02	8.512E+02	8.425E+02	3.271E+02	3.275E+02	2.734E+01	3.352E-01
22000	3.527E+01	3.693E+02	8.870E+02	8.784E+02	3.290E+02	3.294E+02	2.087E+01	3.379E-01
23000	3.416E+01	3.708E+02	9.217E+02	9.130E+02	3.307E+02	3.311E+02	1.510E+01	3.398E-01
24000	3.315E+01	3.722E+02	9.554E+02	9.467E+02	3.324E+02	3.328E+02	9.999E+00	3.410E-01
25000	3.222E+01	3.736E+02	9.880E+02	9.794E+02	3.341E+02	3.344E+02	5.541E+00	3.417E-01
26000	3.136E+01	3.748E+02	1.020E+03	1.011E+03	3.356E+02	3.359E+02	1.661E+00	3.419E-01
27000	3.059E+01	3.760E+02	1.051E+03	1.042E+03	3.371E+02	3.374E+02	-1.706E+00	3.419E-01
28000	2.988E+01	3.771E+02	1.081E+03	1.072E+03	3.385E+02	3.388E+02	-4.627E+00	3.417E-01
29000	2.923E+01	3.781E+02	1.111E+03	1.102E+03	3.398E+02	3.401E+02	-7.161E+00	3.413E-01
30000	2.864E+01	3.791E+02	1.140E+03	1.131E+03	3.411E+02	3.414E+02	-9.364E+00	3.408E-01
32000	2.762E+01	3.809E+02	1.196E+03	1.187E+03	3.436E+02	3.438E+02	-1.297E+01	3.396E-01
34000	2.677E+01	3.826E+02	1.250E+03	1.241E+03	3.458E+02	3.461E+02	-1.575E+01	3.382E-01
36000	2.605E+01	3.841E+02	1.303E+03	1.294E+03	3.479E+02	3.481E+02	-1.795E+01	3.368E-01
38000	2.545E+01	3.855E+02	1.354E+03	1.346E+03	3.498E+02	3.501E+02	-1.972E+01	3.354E-01
40000	2.495E+01	3.868E+02	1.405E+03	1.396E+03	3.516E+02	3.519E+02	-2.118E+01	3.340E-01
42000	2.451E+01	3.880E+02	1.454E+03	1.446E+03	3.534E+02	3.536E+02	-2.241E+01	3.326E-01
44000	2.414E+01	3.891E+02	1.503E+03	1.494E+03	3.550E+02	3.551E+02	-2.347E+01	3.313E-01
46000	2.382E+01	3.902E+02	1.551E+03	1.542E+03	3.565E+02	3.566E+02	-2.440E+01	3.301E-01
48000	2.354E+01	3.912E+02	1.598E+03	1.590E+03	3.579E+02	3.581E+02	-2.524E+01	3.289E-01
50000	2.330E+01	3.921E+02	1.645E+03	1.636E+03	3.592E+02	3.594E+02	-2.600E+01	3.278E-01

Table 161: Internal thermodynamic properties of NO^+

T(K)	Q_{int}	$\ln(Q_{int})$	E_{int}/RT	$C_{p,int}/R$
50	$1.782E+01$	$2.880E+00$	$9.810E-01$	$1.000E+00$
100	$3.531E+01$	$3.564E+00$	$9.906E-01$	$1.000E+00$
150	$5.280E+01$	$3.966E+00$	$9.939E-01$	$1.001E+00$
200	$7.029E+01$	$4.253E+00$	$9.956E-01$	$1.001E+00$
298.15	$1.046E+02$	$4.651E+00$	$9.975E-01$	$1.003E+00$
300	$1.053E+02$	$4.657E+00$	$9.976E-01$	$1.003E+00$
400	$1.403E+02$	$4.944E+00$	$1.000E+00$	$1.017E+00$
500	$1.755E+02$	$5.168E+00$	$1.007E+00$	$1.056E+00$
600	$2.111E+02$	$5.353E+00$	$1.020E+00$	$1.119E+00$
700	$2.474E+02$	$5.511E+00$	$1.040E+00$	$1.196E+00$
800	$2.847E+02$	$5.652E+00$	$1.064E+00$	$1.277E+00$
900	$3.233E+02$	$5.779E+00$	$1.092E+00$	$1.356E+00$
1000	$3.633E+02$	$5.895E+00$	$1.122E+00$	$1.429E+00$
2000	$8.651E+02$	$6.763E+00$	$1.396E+00$	$1.827E+00$
3000	$1.577E+03$	$7.363E+00$	$1.564E+00$	$1.957E+00$
4000	$2.513E+03$	$7.829E+00$	$1.671E+00$	$2.022E+00$
5000	$3.680E+03$	$8.211E+00$	$1.746E+00$	$2.069E+00$
6000	$5.086E+03$	$8.534E+00$	$1.804E+00$	$2.115E+00$
7000	$6.741E+03$	$8.816E+00$	$1.853E+00$	$2.188E+00$
8000	$8.661E+03$	$9.067E+00$	$1.902E+00$	$2.326E+00$
9000	$1.087E+04$	$9.294E+00$	$1.962E+00$	$2.572E+00$
10000	$1.342E+04$	$9.505E+00$	$2.041E+00$	$2.950E+00$
11000	$1.638E+04$	$9.704E+00$	$2.145E+00$	$3.445E+00$
12000	$1.985E+04$	$9.896E+00$	$2.276E+00$	$4.002E+00$
13000	$2.396E+04$	$1.008E+01$	$2.430E+00$	$4.539E+00$
14000	$2.886E+04$	$1.027E+01$	$2.597E+00$	$4.973E+00$
15000	$3.472E+04$	$1.046E+01$	$2.766E+00$	$5.246E+00$
16000	$4.172E+04$	$1.064E+01$	$2.924E+00$	$5.337E+00$
17000	$5.003E+04$	$1.082E+01$	$3.065E+00$	$5.257E+00$
18000	$5.981E+04$	$1.100E+01$	$3.181E+00$	$5.043E+00$
19000	$7.121E+04$	$1.117E+01$	$3.271E+00$	$4.735E+00$
20000	$8.437E+04$	$1.134E+01$	$3.336E+00$	$4.375E+00$
21000	$9.939E+04$	$1.151E+01$	$3.376E+00$	$3.995E+00$
22000	$1.164E+05$	$1.166E+01$	$3.396E+00$	$3.619E+00$
23000	$1.353E+05$	$1.182E+01$	$3.398E+00$	$3.260E+00$
24000	$1.563E+05$	$1.196E+01$	$3.385E+00$	$2.928E+00$
25000	$1.794E+05$	$1.210E+01$	$3.360E+00$	$2.627E+00$
26000	$2.046E+05$	$1.223E+01$	$3.327E+00$	$2.356E+00$
27000	$2.318E+05$	$1.235E+01$	$3.286E+00$	$2.115E+00$
28000	$2.610E+05$	$1.247E+01$	$3.241E+00$	$1.902E+00$
29000	$2.922E+05$	$1.259E+01$	$3.191E+00$	$1.713E+00$
30000	$3.253E+05$	$1.269E+01$	$3.139E+00$	$1.547E+00$
32000	$3.969E+05$	$1.289E+01$	$3.031E+00$	$1.272E+00$
34000	$4.754E+05$	$1.307E+01$	$2.921E+00$	$1.057E+00$
36000	$5.601E+05$	$1.324E+01$	$2.812E+00$	$8.878E-01$
38000	$6.502E+05$	$1.339E+01$	$2.707E+00$	$7.535E-01$
40000	$7.452E+05$	$1.352E+01$	$2.607E+00$	$6.457E-01$
42000	$8.442E+05$	$1.365E+01$	$2.511E+00$	$5.583E-01$
44000	$9.469E+05$	$1.376E+01$	$2.421E+00$	$4.867E-01$
46000	$1.052E+06$	$1.387E+01$	$2.335E+00$	$4.275E-01$
48000	$1.160E+06$	$1.396E+01$	$2.255E+00$	$3.781E-01$
50000	$1.270E+06$	$1.405E+01$	$2.179E+00$	$3.365E-01$

Table 162: Total thermodynamic properties of NO^+

T [K]	C_p [J/mol/K]	S^0 [J/mol/K]	$H^0(T)-H^0(0)$ [KJ/mol]	$H^0(T)-H^0(298)$ [KJ/mol]	$-(G^0-H^0(0))/T$ [J/mol/K]	$-(G^0-H^0(298))/T$ [J/mol/K]	ΔH_f [KJ/mol]	$\mathrm{Log}(K_p)$
50	2.910E+01	1.463E+02	1.447E+00	-7.223E+00	1.173E+02	2.907E+02	9.847E+02	-1.030E+03
100	2.910E+01	1.664E+02	2.902E+00	-5.768E+00	1.374E+02	2.241E+02	9.857E+02	-5.150E+02
150	2.911E+01	1.782E+02	4.358E+00	-4.313E+00	1.492E+02	2.070E+02	9.868E+02	-3.433E+02
200	2.911E+01	1.866E+02	5.813E+00	-2.857E+00	1.576E+02	2.009E+02	9.878E+02	-2.573E+02
298.15	2.912E+01	1.982E+02	8.670E+00	0.000E+00	1.692E+02	1.982E+02	9.898E+02	-1.723E+02
300	2.912E+01	1.984E+02	8.724E+00	5.390E-02	1.693E+02	1.982E+02	9.899E+02	-1.713E+02
400	2.924E+01	2.068E+02	1.164E+01	2.971E+00	1.777E+02	1.994E+02	9.919E+02	-1.281E+02
500	2.957E+01	2.134E+02	1.458E+01	5.910E+00	1.842E+02	2.016E+02	9.940E+02	-1.022E+02
600	3.009E+01	2.188E+02	1.756E+01	8.892E+00	1.895E+02	2.040E+02	9.959E+02	-8.488E+01
700	3.073E+01	2.235E+02	2.060E+01	1.193E+01	1.941E+02	2.064E+02	9.979E+02	-7.248E+01
800	3.140E+01	2.276E+02	2.371E+01	1.504E+01	1.980E+02	2.088E+02	9.999E+02	-6.316E+01
900	3.206E+01	2.314E+02	2.688E+01	1.821E+01	2.015E+02	2.111E+02	1.002E+03	-5.590E+01
1000	3.267E+01	2.348E+02	3.012E+01	2.145E+01	2.047E+02	2.133E+02	1.004E+03	-5.008E+01
2000	3.597E+01	2.587E+02	6.478E+01	5.611E+01	2.263E+02	2.306E+02	1.024E+03	-2.366E+01
3000	3.706E+01	2.735E+02	1.014E+02	9.270E+01	2.397E+02	2.426E+02	1.043E+03	-1.468E+01
4000	3.760E+01	2.842E+02	1.387E+02	1.301E+02	2.496E+02	2.517E+02	1.062E+03	-1.010E+01
5000	3.799E+01	2.927E+02	1.765E+02	1.679E+02	2.574E+02	2.591E+02	1.081E+03	-7.303E+00
6000	3.837E+01	2.996E+02	2.147E+02	2.060E+02	2.639E+02	2.653E+02	1.099E+03	-5.407E+00
7000	3.898E+01	3.056E+02	2.533E+02	2.447E+02	2.694E+02	2.706E+02	1.117E+03	-4.029E+00
8000	4.012E+01	3.109E+02	2.928E+02	2.842E+02	2.742E+02	2.753E+02	1.135E+03	-2.979E+00
9000	4.217E+01	3.157E+02	3.339E+02	3.252E+02	2.786E+02	2.796E+02	1.155E+03	-2.149E+00
10000	4.531E+01	3.203E+02	3.775E+02	3.689E+02	2.825E+02	2.834E+02	1.176E+03	-1.473E+00
11000	4.943E+01	3.248E+02	4.248E+02	4.162E+02	2.862E+02	2.870E+02	1.200E+03	-9.089E-01
12000	5.406E+01	3.293E+02	4.766E+02	4.679E+02	2.896E+02	2.903E+02	1.228E+03	-4.287E-01
13000	5.852E+01	3.338E+02	5.329E+02	5.242E+02	2.928E+02	2.935E+02	1.258E+03	-1.288E-02
14000	6.213E+01	3.383E+02	5.933E+02	5.847E+02	2.959E+02	2.965E+02	1.290E+03	3.526E-01
15000	6.440E+01	3.426E+02	6.567E+02	6.480E+02	2.989E+02	2.994E+02	1.325E+03	6.778E-01
16000	6.516E+01	3.468E+02	7.216E+02	7.130E+02	3.017E+02	3.023E+02	1.361E+03	9.700E-01
17000	6.450E+01	3.508E+02	7.866E+02	7.779E+02	3.045E+02	3.050E+02	1.397E+03	1.235E+00
18000	6.272E+01	3.544E+02	8.502E+02	8.416E+02	3.072E+02	3.077E+02	1.432E+03	1.476E+00
19000	6.016E+01	3.577E+02	9.117E+02	9.031E+02	3.098E+02	3.102E+02	1.467E+03	1.698E+00
20000	5.717E+01	3.608E+02	9.704E+02	9.618E+02	3.122E+02	3.127E+02	1.500E+03	1.901E+00
21000	5.401E+01	3.635E+02	1.026E+03	1.017E+03	3.146E+02	3.150E+02	1.533E+03	2.090E+00
22000	5.087E+01	3.659E+02	1.078E+03	1.070E+03	3.169E+02	3.173E+02	1.563E+03	2.265E+00
23000	4.789E+01	3.681E+02	1.128E+03	1.119E+03	3.191E+02	3.194E+02	1.593E+03	2.428E+00
24000	4.513E+01	3.701E+02	1.174E+03	1.166E+03	3.211E+02	3.215E+02	1.622E+03	2.580E+00
25000	4.263E+01	3.719E+02	1.218E+03	1.210E+03	3.231E+02	3.235E+02	1.649E+03	2.722E+00
26000	4.038E+01	3.735E+02	1.260E+03	1.251E+03	3.251E+02	3.254E+02	1.676E+03	2.856E+00
27000	3.837E+01	3.750E+02	1.299E+03	1.290E+03	3.269E+02	3.272E+02	1.702E+03	2.982E+00
28000	3.660E+01	3.763E+02	1.336E+03	1.328E+03	3.286E+02	3.289E+02	1.727E+03	3.100E+00
29000	3.503E+01	3.776E+02	1.372E+03	1.364E+03	3.303E+02	3.306E+02	1.751E+03	3.212E+00
30000	3.365E+01	3.788E+02	1.407E+03	1.398E+03	3.319E+02	3.322E+02	1.775E+03	3.318E+00
32000	3.136E+01	3.809E+02	1.472E+03	1.463E+03	3.349E+02	3.351E+02	1.822E+03	3.513E+00
34000	2.957E+01	3.827E+02	1.532E+03	1.524E+03	3.376E+02	3.379E+02	1.867E+03	3.690E+00
36000	2.817E+01	3.844E+02	1.590E+03	1.581E+03	3.402E+02	3.404E+02	1.911E+03	3.852E+00
38000	2.705E+01	3.858E+02	1.645E+03	1.636E+03	3.426E+02	3.428E+02	1.955E+03	3.999E+00
40000	2.616E+01	3.872E+02	1.698E+03	1.690E+03	3.448E+02	3.450E+02	1.998E+03	4.135E+00
42000	2.543E+01	3.885E+02	1.750E+03	1.741E+03	3.468E+02	3.470E+02	2.040E+03	4.261E+00
44000	2.483E+01	3.896E+02	1.800E+03	1.792E+03	3.487E+02	3.489E+02	2.082E+03	4.377E+00
46000	2.434E+01	3.907E+02	1.849E+03	1.841E+03	3.505E+02	3.507E+02	2.124E+03	4.486E+00
48000	2.393E+01	3.918E+02	1.898E+03	1.889E+03	3.522E+02	3.524E+02	2.166E+03	4.587E+00
50000	2.358E+01	3.927E+02	1.945E+03	1.936E+03	3.538E+02	3.540E+02	2.207E+03	4.682E+00

Table 163: Internal thermodynamic properties of NO_2

T(K)	Q_{int}	$\ln(Q_{int})$	E_{int}/RT	$C_{p,int}/R$
50	$3.053E+02$	$5.721E+00$	$1.496E+00$	$1.500E+00$
100	$8.619E+02$	$6.759E+00$	$1.498E+00$	$1.502E+00$
150	$1.584E+03$	$7.367E+00$	$1.504E+00$	$1.540E+00$
200	$2.447E+03$	$7.802E+00$	$1.524E+00$	$1.642E+00$
298.15	$4.563E+03$	$8.426E+00$	$1.613E+00$	$1.966E+00$
300	$4.609E+03$	$8.436E+00$	$1.615E+00$	$1.973E+00$
400	$7.470E+03$	$8.919E+00$	$1.754E+00$	$2.364E+00$
500	$1.124E+04$	$9.327E+00$	$1.914E+00$	$2.737E+00$
600	$1.616E+04$	$9.690E+00$	$2.078E+00$	$3.055E+00$
700	$2.253E+04$	$1.002E+01$	$2.237E+00$	$3.312E+00$
800	$3.068E+04$	$1.033E+01$	$2.385E+00$	$3.516E+00$
900	$4.095E+04$	$1.062E+01$	$2.520E+00$	$3.677E+00$
1000	$5.374E+04$	$1.089E+01$	$2.642E+00$	$3.805E+00$
2000	$4.382E+05$	$1.299E+01$	$3.384E+00$	$4.315E+00$
3000	$1.858E+06$	$1.444E+01$	$3.734E+00$	$4.555E+00$
4000	$5.628E+06$	$1.554E+01$	$3.972E+00$	$4.818E+00$
5000	$1.395E+07$	$1.645E+01$	$4.164E+00$	$5.028E+00$
6000	$3.023E+07$	$1.722E+01$	$4.318E+00$	$5.126E+00$
7000	$5.936E+07$	$1.790E+01$	$4.433E+00$	$5.104E+00$
8000	$1.079E+08$	$1.850E+01$	$4.510E+00$	$4.980E+00$
9000	$1.840E+08$	$1.903E+01$	$4.552E+00$	$4.777E+00$
10000	$2.975E+08$	$1.951E+01$	$4.562E+00$	$4.524E+00$
11000	$4.593E+08$	$1.995E+01$	$4.546E+00$	$4.245E+00$
12000	$6.811E+08$	$2.034E+01$	$4.509E+00$	$3.957E+00$
13000	$9.752E+08$	$2.070E+01$	$4.455E+00$	$3.674E+00$
14000	$1.354E+09$	$2.103E+01$	$4.390E+00$	$3.405E+00$
15000	$1.828E+09$	$2.133E+01$	$4.316E+00$	$3.154E+00$
16000	$2.409E+09$	$2.160E+01$	$4.236E+00$	$2.923E+00$
17000	$3.106E+09$	$2.186E+01$	$4.152E+00$	$2.713E+00$
18000	$3.929E+09$	$2.209E+01$	$4.067E+00$	$2.523E+00$
19000	$4.884E+09$	$2.231E+01$	$3.981E+00$	$2.351E+00$
20000	$5.977E+09$	$2.251E+01$	$3.896E+00$	$2.197E+00$
21000	$7.214E+09$	$2.270E+01$	$3.811E+00$	$2.058E+00$
22000	$8.596E+09$	$2.287E+01$	$3.729E+00$	$1.933E+00$
23000	$1.013E+10$	$2.304E+01$	$3.648E+00$	$1.820E+00$
24000	$1.181E+10$	$2.319E+01$	$3.570E+00$	$1.719E+00$
25000	$1.364E+10$	$2.334E+01$	$3.494E+00$	$1.627E+00$
26000	$1.562E+10$	$2.347E+01$	$3.421E+00$	$1.544E+00$
27000	$1.775E+10$	$2.360E+01$	$3.350E+00$	$1.468E+00$
28000	$2.003E+10$	$2.372E+01$	$3.281E+00$	$1.400E+00$
29000	$2.244E+10$	$2.383E+01$	$3.215E+00$	$1.337E+00$
30000	$2.500E+10$	$2.394E+01$	$3.152E+00$	$1.280E+00$
32000	$3.052E+10$	$2.414E+01$	$3.031E+00$	$1.179E+00$
34000	$3.656E+10$	$2.432E+01$	$2.920E+00$	$1.094E+00$
36000	$4.307E+10$	$2.449E+01$	$2.816E+00$	$1.021E+00$
38000	$5.002E+10$	$2.464E+01$	$2.720E+00$	$9.588E-01$
40000	$5.738E+10$	$2.477E+01$	$2.631E+00$	$9.045E-01$
42000	$6.510E+10$	$2.490E+01$	$2.547E+00$	$8.569E-01$
44000	$7.316E+10$	$2.502E+01$	$2.470E+00$	$8.151E-01$
46000	$8.152E+10$	$2.512E+01$	$2.397E+00$	$7.779E-01$
48000	$9.014E+10$	$2.522E+01$	$2.329E+00$	$7.448E-01$
50000	$9.900E+10$	$2.532E+01$	$2.265E+00$	$7.151E-01$

Table 164: Total thermodynamic properties of NO_2

T [K]	C_p [J/mol/K]	S^0 [J/mol/K]	$H^0(T)-H^0(0)$ [KJ/mol]	$H^0(T)-H^0(298)$ [KJ/mol]	$-(G^0-H^0(0))/T$ [J/mol/K]	$-(G^0-H^0(298))/T$ [J/mol/K]	ΔH_f [KJ/mol]	$\text{Log}(K_p)$
50	3.326E+01	1.795E+02	1.661E+00	-8.536E+00	1.463E+02	3.502E+02	3.543E+01	-3.928E+01
100	3.328E+01	2.026E+02	3.324E+00	-6.873E+00	1.693E+02	2.713E+02	3.491E+01	-2.088E+01
150	3.359E+01	2.161E+02	4.994E+00	-5.203E+00	1.828E+02	2.508E+02	3.440E+01	-1.484E+01
200	3.444E+01	2.259E+02	6.692E+00	-3.505E+00	1.924E+02	2.434E+02	3.391E+01	-1.187E+01
298.15	3.713E+01	2.401E+02	1.020E+01	0.000E+00	2.059E+02	2.401E+02	3.312E+01	-8.984E+00
300	3.719E+01	2.403E+02	1.027E+01	6.900E-02	2.061E+02	2.401E+02	3.311E+01	-8.949E+00
400	4.045E+01	2.514E+02	1.415E+01	3.949E+00	2.161E+02	2.416E+02	3.256E+01	-7.519E+00
500	4.355E+01	2.608E+02	1.835E+01	8.152E+00	2.241E+02	2.445E+02	3.223E+01	-6.673E+00
600	4.619E+01	2.690E+02	2.284E+01	1.264E+01	2.309E+02	2.479E+02	3.207E+01	-6.114E+00
700	4.833E+01	2.763E+02	2.757E+01	1.737E+01	2.369E+02	2.515E+02	3.202E+01	-5.715E+00
800	5.002E+01	2.829E+02	3.249E+01	2.229E+01	2.422E+02	2.550E+02	3.205E+01	-5.417E+00
900	5.136E+01	2.888E+02	3.756E+01	2.736E+01	2.471E+02	2.584E+02	3.213E+01	-5.184E+00
1000	5.242E+01	2.943E+02	4.275E+01	3.256E+01	2.515E+02	2.617E+02	3.224E+01	-4.997E+00
2000	5.666E+01	3.323E+02	9.785E+01	8.766E+01	2.834E+02	2.885E+02	3.350E+01	-4.141E+00
3000	5.866E+01	3.557E+02	1.555E+02	1.453E+02	3.038E+02	3.072E+02	3.392E+01	-3.848E+00
4000	6.085E+01	3.728E+02	2.153E+02	2.051E+02	3.190E+02	3.216E+02	3.410E+01	-3.700E+00
5000	6.259E+01	3.866E+02	2.770E+02	2.668E+02	3.312E+02	3.332E+02	3.462E+01	-3.610E+00
6000	6.341E+01	3.981E+02	3.401E+02	3.299E+02	3.414E+02	3.431E+02	3.512E+01	-3.549E+00
7000	6.323E+01	4.079E+02	4.035E+02	3.933E+02	3.502E+02	3.517E+02	3.495E+01	-3.506E+00
8000	6.219E+01	4.163E+02	4.663E+02	4.561E+02	3.580E+02	3.593E+02	3.365E+01	-3.474E+00
9000	6.051E+01	4.235E+02	5.277E+02	5.175E+02	3.649E+02	3.660E+02	3.084E+01	-3.450E+00
10000	5.841E+01	4.298E+02	5.872E+02	5.770E+02	3.711E+02	3.721E+02	2.609E+01	-3.433E+00
11000	5.608E+01	4.352E+02	6.444E+02	6.342E+02	3.766E+02	3.776E+02	1.889E+01	-3.423E+00
12000	5.368E+01	4.400E+02	6.993E+02	6.891E+02	3.817E+02	3.826E+02	8.819E+00	-3.417E+00
13000	5.133E+01	4.442E+02	7.518E+02	7.416E+02	3.864E+02	3.872E+02	-4.346E+00	-3.416E+00
14000	4.909E+01	4.479E+02	8.020E+02	7.918E+02	3.906E+02	3.914E+02	-2.048E+01	-3.420E+00
15000	4.701E+01	4.512E+02	8.500E+02	8.398E+02	3.946E+02	3.953E+02	-3.914E+01	-3.427E+00
16000	4.509E+01	4.542E+02	8.961E+02	8.859E+02	3.982E+02	3.989E+02	-5.964E+01	-3.438E+00
17000	4.334E+01	4.569E+02	9.403E+02	9.301E+02	4.016E+02	4.022E+02	-8.122E+01	-3.451E+00
18000	4.176E+01	4.593E+02	9.828E+02	9.726E+02	4.047E+02	4.053E+02	-1.032E+02	-3.467E+00
19000	4.034E+01	4.616E+02	1.024E+03	1.014E+03	4.077E+02	4.082E+02	-1.248E+02	-3.484E+00
20000	3.905E+01	4.636E+02	1.064E+03	1.053E+03	4.104E+02	4.109E+02	-1.459E+02	-3.503E+00
21000	3.790E+01	4.655E+02	1.102E+03	1.092E+03	4.130E+02	4.135E+02	-1.660E+02	-3.522E+00
22000	3.686E+01	4.672E+02	1.139E+03	1.129E+03	4.154E+02	4.159E+02	-1.851E+02	-3.542E+00
23000	3.592E+01	4.688E+02	1.176E+03	1.166E+03	4.177E+02	4.181E+02	-2.030E+02	-3.562E+00
24000	3.508E+01	4.703E+02	1.211E+03	1.201E+03	4.199E+02	4.203E+02	-2.199E+02	-3.582E+00
25000	3.431E+01	4.718E+02	1.246E+03	1.236E+03	4.219E+02	4.223E+02	-2.358E+02	-3.602E+00
26000	3.362E+01	4.731E+02	1.280E+03	1.270E+03	4.239E+02	4.242E+02	-2.507E+02	-3.621E+00
27000	3.299E+01	4.743E+02	1.313E+03	1.303E+03	4.257E+02	4.261E+02	-2.649E+02	-3.640E+00
28000	3.242E+01	4.755E+02	1.346E+03	1.336E+03	4.275E+02	4.278E+02	-2.783E+02	-3.659E+00
29000	3.190E+01	4.767E+02	1.378E+03	1.368E+03	4.291E+02	4.295E+02	-2.910E+02	-3.678E+00
30000	3.143E+01	4.777E+02	1.410E+03	1.400E+03	4.307E+02	4.311E+02	-3.032E+02	-3.695E+00
32000	3.059E+01	4.797E+02	1.472E+03	1.462E+03	4.337E+02	4.341E+02	-3.261E+02	-3.730E+00
34000	2.988E+01	4.816E+02	1.532E+03	1.522E+03	4.365E+02	4.368E+02	-3.476E+02	-3.762E+00
36000	2.928E+01	4.833E+02	1.591E+03	1.581E+03	4.391E+02	4.393E+02	-3.678E+02	-3.792E+00
38000	2.876E+01	4.848E+02	1.649E+03	1.639E+03	4.414E+02	4.417E+02	-3.872E+02	-3.821E+00
40000	2.831E+01	4.863E+02	1.706E+03	1.696E+03	4.436E+02	4.439E+02	-4.059E+02	-3.849E+00
42000	2.791E+01	4.877E+02	1.763E+03	1.752E+03	4.457E+02	4.459E+02	-4.240E+02	-3.874E+00
44000	2.756E+01	4.889E+02	1.818E+03	1.808E+03	4.476E+02	4.479E+02	-4.418E+02	-3.899E+00
46000	2.725E+01	4.902E+02	1.873E+03	1.863E+03	4.494E+02	4.497E+02	-4.591E+02	-3.922E+00
48000	2.698E+01	4.913E+02	1.927E+03	1.917E+03	4.512E+02	4.514E+02	-4.762E+02	-3.944E+00
50000	2.673E+01	4.924E+02	1.981E+03	1.971E+03	4.528E+02	4.530E+02	-4.931E+02	-3.965E+00

Table 165: Internal thermodynamic properties of N_2 O

T(K)	Q_{int}	$\ln(Q_{int})$	E_{int}/RT	$C_{p,int}/R$
50	$8.327E+01$	$4.422E+00$	$9.960E-01$	$1.000E+00$
100	$1.663E+02$	$5.114E+00$	$1.002E+00$	$1.030E+00$
150	$2.509E+02$	$5.525E+00$	$1.039E+00$	$1.227E+00$
200	$3.419E+02$	$5.835E+00$	$1.124E+00$	$1.542E+00$
298.15	$5.592E+02$	$6.326E+00$	$1.364E+00$	$2.145E+00$
300	$5.639E+02$	$6.335E+00$	$1.369E+00$	$2.155E+00$
400	$8.665E+02$	$6.764E+00$	$1.628E+00$	$2.633E+00$
500	$1.279E+03$	$7.154E+00$	$1.868E+00$	$3.012E+00$
600	$1.834E+03$	$7.514E+00$	$2.085E+00$	$3.320E+00$
700	$2.567E+03$	$7.850E+00$	$2.280E+00$	$3.574E+00$
800	$3.521E+03$	$8.167E+00$	$2.456E+00$	$3.783E+00$
900	$4.746E+03$	$8.465E+00$	$2.613E+00$	$3.956E+00$
1000	$6.297E+03$	$8.748E+00$	$2.755E+00$	$4.099E+00$
2000	$5.794E+04$	$1.097E+01$	$3.615E+00$	$4.661E+00$
3000	$2.699E+05$	$1.251E+01$	$3.935E+00$	$4.385E+00$
4000	$8.454E+05$	$1.365E+01$	$3.968E+00$	$3.728E+00$
5000	$2.028E+06$	$1.452E+01$	$3.854E+00$	$3.092E+00$
6000	$4.036E+06$	$1.521E+01$	$3.689E+00$	$2.677E+00$
7000	$7.041E+06$	$1.577E+01$	$3.531E+00$	$2.530E+00$
8000	$1.119E+07$	$1.623E+01$	$3.408E+00$	$2.605E+00$
9000	$1.663E+07$	$1.663E+01$	$3.330E+00$	$2.806E+00$
10000	$2.356E+07$	$1.698E+01$	$3.289E+00$	$3.031E+00$
11000	$3.221E+07$	$1.729E+01$	$3.274E+00$	$3.201E+00$
12000	$4.281E+07$	$1.757E+01$	$3.271E+00$	$3.276E+00$
13000	$5.563E+07$	$1.783E+01$	$3.271E+00$	$3.251E+00$
14000	$7.088E+07$	$1.808E+01$	$3.267E+00$	$3.144E+00$
15000	$8.877E+07$	$1.830E+01$	$3.253E+00$	$2.978E+00$
16000	$1.094E+08$	$1.851E+01$	$3.230E+00$	$2.780E+00$
17000	$1.330E+08$	$1.871E+01$	$3.197E+00$	$2.568E+00$
18000	$1.595E+08$	$1.889E+01$	$3.156E+00$	$2.358E+00$
19000	$1.889E+08$	$1.906E+01$	$3.109E+00$	$2.157E+00$
20000	$2.213E+08$	$1.921E+01$	$3.057E+00$	$1.971E+00$
21000	$2.565E+08$	$1.936E+01$	$3.001E+00$	$1.802E+00$
22000	$2.945E+08$	$1.950E+01$	$2.943E+00$	$1.650E+00$
23000	$3.353E+08$	$1.963E+01$	$2.884E+00$	$1.514E+00$
24000	$3.786E+08$	$1.975E+01$	$2.824E+00$	$1.393E+00$
25000	$4.243E+08$	$1.987E+01$	$2.764E+00$	$1.286E+00$
26000	$4.723E+08$	$1.997E+01$	$2.706E+00$	$1.190E+00$
27000	$5.226E+08$	$2.007E+01$	$2.648E+00$	$1.106E+00$
28000	$5.748E+08$	$2.017E+01$	$2.592E+00$	$1.031E+00$
29000	$6.289E+08$	$2.026E+01$	$2.537E+00$	$9.638E-01$
30000	$6.848E+08$	$2.034E+01$	$2.483E+00$	$9.039E-01$
32000	$8.011E+08$	$2.050E+01$	$2.381E+00$	$8.018E-01$
34000	$9.229E+08$	$2.064E+01$	$2.286E+00$	$7.185E-01$
36000	$1.049E+09$	$2.077E+01$	$2.197E+00$	$6.497E-01$
38000	$1.179E+09$	$2.089E+01$	$2.114E+00$	$5.921E-01$
40000	$1.311E+09$	$2.099E+01$	$2.036E+00$	$5.432E-01$
42000	$1.445E+09$	$2.109E+01$	$1.964E+00$	$5.012E-01$
44000	$1.581E+09$	$2.118E+01$	$1.897E+00$	$4.647E-01$
46000	$1.718E+09$	$2.126E+01$	$1.834E+00$	$4.328E-01$
48000	$1.855E+09$	$2.134E+01$	$1.775E+00$	$4.046E-01$
50000	$1.992E+09$	$2.141E+01$	$1.720E+00$	$3.795E-01$

Table 166: Total thermodynamic properties of N_2 O

T [K]	C_p [J/mol/K]	S^0 [J/mol/K]	$H^0(T)-H^0(0)$ [KJ/mol]	$H^0(T)-H^0(298)$ [KJ/mol]	$-(G^0-H^0(0))/T$ [J/mol/K]	$-(G^0-H^0(298))/T$ [J/mol/K]	ΔH_f [KJ/mol]	$\mathrm{Log}(K_p)$
50	2.910E+01	1.640E+02	1.453E+00	-8.126E+00	1.349E+02	3.265E+02	8.476E+01	-9.128E+01
100	2.935E+01	1.842E+02	2.911E+00	-6.668E+00	1.551E+02	2.509E+02	8.404E+01	-4.715E+01
150	3.098E+01	1.963E+02	4.413E+00	-5.166E+00	1.669E+02	2.308E+02	8.336E+01	-3.257E+01
200	3.361E+01	2.056E+02	6.026E+00	-3.553E+00	1.755E+02	2.234E+02	8.278E+01	-2.534E+01
298.15	3.862E+01	2.200E+02	9.579E+00	0.000E+00	1.879E+02	2.200E+02	8.205E+01	-1.825E+01
300	3.870E+01	2.202E+02	9.651E+00	7.154E-02	1.881E+02	2.200E+02	8.204E+01	-1.816E+01
400	4.268E+01	2.319E+02	1.373E+01	4.149E+00	1.976E+02	2.216E+02	8.171E+01	-1.460E+01
500	4.583E+01	2.418E+02	1.816E+01	8.580E+00	2.055E+02	2.247E+02	8.167E+01	-1.246E+01
600	4.839E+01	2.504E+02	2.288E+01	1.329E+01	2.123E+02	2.282E+02	8.183E+01	-1.104E+01
700	5.050E+01	2.580E+02	2.782E+01	1.824E+01	2.183E+02	2.320E+02	8.210E+01	-1.002E+01
800	5.224E+01	2.649E+02	3.296E+01	2.338E+01	2.237E+02	2.357E+02	8.247E+01	-9.256E+00
900	5.368E+01	2.711E+02	3.826E+01	2.868E+01	2.286E+02	2.393E+02	8.288E+01	-8.656E+00
1000	5.487E+01	2.769E+02	4.369E+01	3.411E+01	2.332E+02	2.427E+02	8.334E+01	-8.174E+00
2000	5.954E+01	3.169E+02	1.017E+02	9.211E+01	2.660E+02	2.708E+02	8.841E+01	-5.946E+00
3000	5.725E+01	3.407E+02	1.605E+02	1.509E+02	2.872E+02	2.904E+02	9.119E+01	-5.162E+00
4000	5.178E+01	3.565E+02	2.151E+02	2.056E+02	3.027E+02	3.051E+02	8.803E+01	-4.769E+00
5000	4.649E+01	3.675E+02	2.642E+02	2.546E+02	3.146E+02	3.165E+02	7.811E+01	-4.550E+00
6000	4.304E+01	3.756E+02	3.087E+02	2.992E+02	3.241E+02	3.257E+02	6.283E+01	-4.426E+00
7000	4.182E+01	3.821E+02	3.510E+02	3.414E+02	3.320E+02	3.333E+02	4.438E+01	-4.358E+00
8000	4.244E+01	3.877E+02	3.930E+02	3.834E+02	3.386E+02	3.398E+02	2.481E+01	-4.326E+00
9000	4.412E+01	3.928E+02	4.362E+02	4.266E+02	3.443E+02	3.454E+02	5.244E+00	-4.315E+00
10000	4.599E+01	3.976E+02	4.813E+02	4.717E+02	3.494E+02	3.504E+02	-1.441E+01	-4.317E+00
11000	4.740E+01	4.020E+02	5.280E+02	5.185E+02	3.540E+02	3.549E+02	-3.520E+01	-4.329E+00
12000	4.802E+01	4.062E+02	5.758E+02	5.662E+02	3.582E+02	3.590E+02	-5.860E+01	-4.347E+00
13000	4.782E+01	4.100E+02	6.238E+02	6.142E+02	3.620E+02	3.628E+02	-8.579E+01	-4.371E+00
14000	4.692E+01	4.135E+02	6.712E+02	6.617E+02	3.656E+02	3.663E+02	-1.173E+02	-4.400E+00
15000	4.555E+01	4.167E+02	7.175E+02	7.079E+02	3.689E+02	3.695E+02	-1.528E+02	-4.433E+00
16000	4.390E+01	4.196E+02	7.622E+02	7.527E+02	3.720E+02	3.726E+02	-1.915E+02	-4.471E+00
17000	4.214E+01	4.222E+02	8.053E+02	7.957E+02	3.748E+02	3.754E+02	-2.321E+02	-4.511E+00
18000	4.039E+01	4.246E+02	8.465E+02	8.370E+02	3.775E+02	3.781E+02	-2.733E+02	-4.554E+00
19000	3.872E+01	4.267E+02	8.861E+02	8.765E+02	3.801E+02	3.806E+02	-3.140E+02	-4.599E+00
20000	3.717E+01	4.287E+02	9.240E+02	9.144E+02	3.825E+02	3.829E+02	-3.534E+02	-4.645E+00
21000	3.577E+01	4.304E+02	9.605E+02	9.509E+02	3.847E+02	3.851E+02	-3.909E+02	-4.691E+00
22000	3.450E+01	4.321E+02	9.956E+02	9.860E+02	3.868E+02	3.872E+02	-4.264E+02	-4.737E+00
23000	3.337E+01	4.336E+02	1.030E+03	1.020E+03	3.888E+02	3.892E+02	-4.596E+02	-4.783E+00
24000	3.237E+01	4.350E+02	1.062E+03	1.053E+03	3.907E+02	3.911E+02	-4.906E+02	-4.828E+00
25000	3.148E+01	4.363E+02	1.094E+03	1.085E+03	3.925E+02	3.929E+02	-5.195E+02	-4.872E+00
26000	3.068E+01	4.375E+02	1.125E+03	1.116E+03	3.942E+02	3.946E+02	-5.465E+02	-4.915E+00
27000	2.998E+01	4.386E+02	1.156E+03	1.146E+03	3.958E+02	3.962E+02	-5.717E+02	-4.956E+00
28000	2.936E+01	4.397E+02	1.185E+03	1.176E+03	3.974E+02	3.977E+02	-5.954E+02	-4.997E+00
29000	2.880E+01	4.407E+02	1.214E+03	1.205E+03	3.989E+02	3.992E+02	-6.176E+02	-5.036E+00
30000	2.830E+01	4.417E+02	1.243E+03	1.233E+03	4.003E+02	4.006E+02	-6.387E+02	-5.073E+00
32000	2.745E+01	4.435E+02	1.299E+03	1.289E+03	4.029E+02	4.032E+02	-6.775E+02	-5.145E+00
34000	2.676E+01	4.451E+02	1.353E+03	1.343E+03	4.054E+02	4.056E+02	-7.129E+02	-5.212E+00
36000	2.619E+01	4.467E+02	1.406E+03	1.396E+03	4.076E+02	4.079E+02	-7.455E+02	-5.274E+00
38000	2.571E+01	4.481E+02	1.458E+03	1.448E+03	4.097E+02	4.100E+02	-7.760E+02	-5.332E+00
40000	2.530E+01	4.494E+02	1.509E+03	1.499E+03	4.117E+02	4.119E+02	-8.049E+02	-5.386E+00
42000	2.495E+01	4.506E+02	1.559E+03	1.549E+03	4.135E+02	4.137E+02	-8.323E+02	-5.437E+00
44000	2.465E+01	4.518E+02	1.609E+03	1.599E+03	4.152E+02	4.154E+02	-8.586E+02	-5.485E+00
46000	2.439E+01	4.528E+02	1.658E+03	1.648E+03	4.168E+02	4.170E+02	-8.840E+02	-5.530E+00
48000	2.415E+01	4.539E+02	1.706E+03	1.696E+03	4.183E+02	4.185E+02	-9.088E+02	-5.572E+00
50000	2.394E+01	4.549E+02	1.754E+03	1.745E+03	4.198E+02	4.200E+02	-9.328E+02	-5.612E+00

Table 167: Internal thermodynamic properties of N_2 O^+

T(K)	Q_{int}	$\ln(Q_{int})$	E_{int}/RT	$C_{p,int}/R$
50	$1.733E+02$	$5.155E+00$	$1.079E+00$	$1.308E+00$
100	$3.898E+02$	$5.966E+00$	$1.262E+00$	$1.525E+00$
150	$6.656E+02$	$6.501E+00$	$1.385E+00$	$1.759E+00$
200	$1.009E+03$	$6.917E+00$	$1.516E+00$	$2.061E+00$
298.15	$1.944E+03$	$7.572E+00$	$1.785E+00$	$2.583E+00$
300	$1.965E+03$	$7.583E+00$	$1.790E+00$	$2.592E+00$
400	$3.408E+03$	$8.134E+00$	$2.046E+00$	$3.023E+00$
500	$5.519E+03$	$8.616E+00$	$2.278E+00$	$3.382E+00$
600	$8.519E+03$	$9.050E+00$	$2.487E+00$	$3.674E+00$
700	$1.268E+04$	$9.448E+00$	$2.674E+00$	$3.907E+00$
800	$1.832E+04$	$9.816E+00$	$2.840E+00$	$4.091E+00$
900	$2.583E+04$	$1.016E+01$	$2.988E+00$	$4.237E+00$
1000	$3.563E+04$	$1.048E+01$	$3.119E+00$	$4.354E+00$
2000	$4.082E+05$	$1.292E+01$	$3.877E+00$	$4.759E+00$
3000	$2.088E+06$	$1.455E+01$	$4.134E+00$	$4.434E+00$
4000	$6.880E+06$	$1.574E+01$	$4.124E+00$	$3.734E+00$
5000	$1.702E+07$	$1.665E+01$	$3.973E+00$	$3.018E+00$
6000	$3.449E+07$	$1.736E+01$	$3.762E+00$	$2.423E+00$
7000	$6.056E+07$	$1.792E+01$	$3.537E+00$	$1.963E+00$
8000	$9.573E+07$	$1.838E+01$	$3.317E+00$	$1.614E+00$
9000	$1.398E+08$	$1.876E+01$	$3.113E+00$	$1.349E+00$
10000	$1.922E+08$	$1.907E+01$	$2.926E+00$	$1.145E+00$
11000	$2.519E+08$	$1.934E+01$	$2.756E+00$	$9.870E-01$
12000	$3.181E+08$	$1.958E+01$	$2.603E+00$	$8.616E-01$
13000	$3.896E+08$	$1.978E+01$	$2.465E+00$	$7.609E-01$
14000	$4.655E+08$	$1.996E+01$	$2.341E+00$	$6.786E-01$
15000	$5.450E+08$	$2.012E+01$	$2.228E+00$	$6.106E-01$
16000	$6.272E+08$	$2.026E+01$	$2.125E+00$	$5.535E-01$
17000	$7.113E+08$	$2.038E+01$	$2.031E+00$	$5.050E-01$
18000	$7.969E+08$	$2.050E+01$	$1.945E+00$	$4.633E-01$
19000	$8.834E+08$	$2.060E+01$	$1.866E+00$	$4.272E-01$
20000	$9.703E+08$	$2.069E+01$	$1.793E+00$	$3.957E-01$
21000	$1.057E+09$	$2.078E+01$	$1.726E+00$	$3.678E-01$
22000	$1.144E+09$	$2.086E+01$	$1.664E+00$	$3.431E-01$
23000	$1.230E+09$	$2.093E+01$	$1.606E+00$	$3.210E-01$
24000	$1.316E+09$	$2.100E+01$	$1.552E+00$	$3.011E-01$
25000	$1.400E+09$	$2.106E+01$	$1.501E+00$	$2.832E-01$
26000	$1.484E+09$	$2.112E+01$	$1.454E+00$	$2.669E-01$
27000	$1.566E+09$	$2.117E+01$	$1.410E+00$	$2.521E-01$
28000	$1.647E+09$	$2.122E+01$	$1.368E+00$	$2.385E-01$
29000	$1.727E+09$	$2.127E+01$	$1.329E+00$	$2.261E-01$
30000	$1.806E+09$	$2.131E+01$	$1.292E+00$	$2.147E-01$
32000	$1.958E+09$	$2.140E+01$	$1.224E+00$	$1.943E-01$
34000	$2.105E+09$	$2.147E+01$	$1.163E+00$	$1.768E-01$
36000	$2.246E+09$	$2.153E+01$	$1.108E+00$	$1.617E-01$
38000	$2.382E+09$	$2.159E+01$	$1.058E+00$	$1.484E-01$
40000	$2.512E+09$	$2.164E+01$	$1.012E+00$	$1.367E-01$
42000	$2.636E+09$	$2.169E+01$	$9.700E-01$	$1.264E-01$
44000	$2.755E+09$	$2.174E+01$	$9.315E-01$	$1.172E-01$
46000	$2.870E+09$	$2.178E+01$	$8.959E-01$	$1.090E-01$
48000	$2.979E+09$	$2.181E+01$	$8.629E-01$	$1.016E-01$
50000	$3.084E+09$	$2.185E+01$	$8.323E-01$	$9.494E-02$

Table 168: Total thermodynamic properties of N_2 O^+

T [K]	C_p [J/mol/K]	S^0 [J/mol/K]	$H^0(T)-H^0(0)$ [KJ/mol]	$H^0(T)-H^0(298)$ [KJ/mol]	$-(G^0-H^0(0))/T$ [J/mol/K]	$-(G^0-H^0(298))/T$ [J/mol/K]	ΔH_f [KJ/mol]	$\mathrm{Log}(K_p)$
50	3.166E+01	1.708E+02	1.488E+00	-9.134E+00	1.410E+02	3.534E+02	1.329E+03	-1.392E+03
100	3.347E+01	1.934E+02	3.128E+00	-7.494E+00	1.622E+02	2.684E+02	1.330E+03	-6.975E+02
150	3.541E+01	2.073E+02	4.845E+00	-5.777E+00	1.750E+02	2.458E+02	1.330E+03	-4.659E+02
200	3.793E+01	2.179E+02	6.678E+00	-3.944E+00	1.845E+02	2.376E+02	1.331E+03	-3.501E+02
298.15	4.226E+01	2.338E+02	1.062E+01	0.000E+00	1.982E+02	2.338E+02	1.333E+03	-2.356E+02
300	4.234E+01	2.341E+02	1.070E+01	7.800E-02	1.984E+02	2.339E+02	1.333E+03	-2.341E+02
400	4.592E+01	2.468E+02	1.512E+01	4.497E+00	2.090E+02	2.356E+02	1.335E+03	-1.761E+02
500	4.890E+01	2.574E+02	1.986E+01	9.243E+00	2.177E+02	2.389E+02	1.337E+03	-1.412E+02
600	5.133E+01	2.665E+02	2.488E+01	1.426E+01	2.251E+02	2.428E+02	1.340E+03	-1.179E+02
700	5.327E+01	2.746E+02	3.011E+01	1.949E+01	2.316E+02	2.467E+02	1.342E+03	-1.012E+02
800	5.480E+01	2.818E+02	3.552E+01	2.490E+01	2.374E+02	2.507E+02	1.345E+03	-8.865E+01
900	5.602E+01	2.883E+02	4.106E+01	3.044E+01	2.427E+02	2.545E+02	1.348E+03	-7.889E+01
1000	5.698E+01	2.943E+02	4.672E+01	3.609E+01	2.476E+02	2.582E+02	1.351E+03	-7.105E+01
2000	6.036E+01	3.353E+02	1.060E+02	9.543E+01	2.822E+02	2.876E+02	1.378E+03	-3.550E+01
3000	5.765E+01	3.594E+02	1.655E+02	1.548E+02	3.042E+02	3.078E+02	1.402E+03	-2.341E+01
4000	5.183E+01	3.752E+02	2.203E+02	2.097E+02	3.201E+02	3.228E+02	1.420E+03	-1.727E+01
5000	4.588E+01	3.861E+02	2.691E+02	2.585E+02	3.323E+02	3.344E+02	1.431E+03	-1.355E+01
6000	4.094E+01	3.940E+02	3.124E+02	3.018E+02	3.420E+02	3.438E+02	1.435E+03	-1.105E+01
7000	3.711E+01	4.001E+02	3.514E+02	3.407E+02	3.499E+02	3.514E+02	1.434E+03	-9.267E+00
8000	3.421E+01	4.048E+02	3.869E+02	3.763E+02	3.564E+02	3.578E+02	1.429E+03	-7.931E+00
9000	3.200E+01	4.087E+02	4.200E+02	4.094E+02	3.620E+02	3.632E+02	1.420E+03	-6.898E+00
10000	3.031E+01	4.120E+02	4.511E+02	4.405E+02	3.669E+02	3.679E+02	1.407E+03	-6.077E+00
11000	2.899E+01	4.148E+02	4.807E+02	4.701E+02	3.711E+02	3.721E+02	1.390E+03	-5.413E+00
12000	2.795E+01	4.173E+02	5.092E+02	4.986E+02	3.749E+02	3.757E+02	1.368E+03	-4.867E+00
13000	2.711E+01	4.195E+02	5.367E+02	5.261E+02	3.782E+02	3.790E+02	1.341E+03	-4.413E+00
14000	2.643E+01	4.215E+02	5.635E+02	5.529E+02	3.812E+02	3.820E+02	1.310E+03	-4.033E+00
15000	2.586E+01	4.233E+02	5.896E+02	5.790E+02	3.840E+02	3.847E+02	1.275E+03	-3.711E+00
16000	2.539E+01	4.249E+02	6.152E+02	6.046E+02	3.865E+02	3.871E+02	1.238E+03	-3.438E+00
17000	2.498E+01	4.265E+02	6.404E+02	6.298E+02	3.888E+02	3.894E+02	1.200E+03	-3.204E+00
18000	2.464E+01	4.279E+02	6.652E+02	6.546E+02	3.909E+02	3.915E+02	1.163E+03	-3.002E+00
19000	2.434E+01	4.292E+02	6.897E+02	6.791E+02	3.929E+02	3.935E+02	1.128E+03	-2.827E+00
20000	2.408E+01	4.304E+02	7.139E+02	7.033E+02	3.948E+02	3.953E+02	1.096E+03	-2.674E+00
21000	2.384E+01	4.316E+02	7.379E+02	7.272E+02	3.965E+02	3.970E+02	1.067E+03	-2.540E+00
22000	2.364E+01	4.327E+02	7.616E+02	7.510E+02	3.981E+02	3.986E+02	1.041E+03	-2.421E+00
23000	2.345E+01	4.338E+02	7.851E+02	7.745E+02	3.996E+02	4.001E+02	1.018E+03	-2.314E+00
24000	2.329E+01	4.348E+02	8.085E+02	7.979E+02	4.011E+02	4.015E+02	9.980E+02	-2.219E+00
25000	2.314E+01	4.357E+02	8.317E+02	8.211E+02	4.024E+02	4.029E+02	9.812E+02	-2.133E+00
26000	2.301E+01	4.366E+02	8.548E+02	8.442E+02	4.037E+02	4.041E+02	9.670E+02	-2.054E+00
27000	2.288E+01	4.375E+02	8.778E+02	8.671E+02	4.050E+02	4.054E+02	9.552E+02	-1.983E+00
28000	2.277E+01	4.383E+02	9.006E+02	8.900E+02	4.061E+02	4.065E+02	9.455E+02	-1.917E+00
29000	2.267E+01	4.391E+02	9.233E+02	9.127E+02	4.073E+02	4.076E+02	9.376E+02	-1.857E+00
30000	2.257E+01	4.399E+02	9.459E+02	9.353E+02	4.083E+02	4.087E+02	9.315E+02	-1.801E+00
32000	2.240E+01	4.413E+02	9.909E+02	9.803E+02	4.104E+02	4.107E+02	9.234E+02	-1.700E+00
34000	2.226E+01	4.427E+02	1.036E+03	1.025E+03	4.122E+02	4.125E+02	9.201E+02	-1.611E+00
36000	2.213E+01	4.439E+02	1.080E+03	1.069E+03	4.139E+02	4.142E+02	9.205E+02	-1.533E+00
38000	2.202E+01	4.451E+02	1.124E+03	1.113E+03	4.156E+02	4.158E+02	9.238E+02	-1.462E+00
40000	2.192E+01	4.463E+02	1.168E+03	1.157E+03	4.171E+02	4.173E+02	9.295E+02	-1.399E+00
42000	2.184E+01	4.473E+02	1.212E+03	1.201E+03	4.185E+02	4.187E+02	9.372E+02	-1.341E+00
44000	2.176E+01	4.484E+02	1.255E+03	1.245E+03	4.198E+02	4.201E+02	9.464E+02	-1.288E+00
46000	2.169E+01	4.493E+02	1.299E+03	1.288E+03	4.211E+02	4.213E+02	9.570E+02	-1.238E+00
48000	2.163E+01	4.502E+02	1.342E+03	1.332E+03	4.223E+02	4.225E+02	9.686E+02	-1.193E+00
50000	2.158E+01	4.511E+02	1.385E+03	1.375E+03	4.234E+02	4.236E+02	9.812E+02	-1.150E+00

Table 169: Internal thermodynamic properties of NCO

T(K)	Q_{int}	$\ln(Q_{int})$	E_{int}/RT	$C_{p,int}/R$
50	$1.907E+02$	$5.251E+00$	$1.163E+00$	$1.428E+00$
100	$4.490E+02$	$6.107E+00$	$1.283E+00$	$1.358E+00$
150	$7.604E+02$	$6.634E+00$	$1.322E+00$	$1.490E+00$
200	$1.123E+03$	$7.024E+00$	$1.399E+00$	$1.778E+00$
298.15	$2.042E+03$	$7.622E+00$	$1.617E+00$	$2.324E+00$
300	$2.063E+03$	$7.632E+00$	$1.621E+00$	$2.333E+00$
400	$3.397E+03$	$8.131E+00$	$1.857E+00$	$2.781E+00$
500	$5.267E+03$	$8.569E+00$	$2.080E+00$	$3.153E+00$
600	$7.840E+03$	$8.967E+00$	$2.286E+00$	$3.462E+00$
700	$1.131E+04$	$9.334E+00$	$2.472E+00$	$3.715E+00$
800	$1.591E+04$	$9.675E+00$	$2.641E+00$	$3.920E+00$
900	$2.191E+04$	$9.995E+00$	$2.792E+00$	$4.085E+00$
1000	$2.962E+04$	$1.030E+01$	$2.929E+00$	$4.219E+00$
2000	$3.030E+05$	$1.262E+01$	$3.748E+00$	$4.764E+00$
3000	$1.496E+06$	$1.422E+01$	$4.112E+00$	$4.891E+00$
4000	$5.031E+06$	$1.543E+01$	$4.313E+00$	$4.935E+00$
5000	$1.336E+07$	$1.641E+01$	$4.438E+00$	$4.926E+00$
6000	$3.023E+07$	$1.722E+01$	$4.514E+00$	$4.850E+00$
7000	$6.082E+07$	$1.792E+01$	$4.552E+00$	$4.703E+00$
8000	$1.118E+08$	$1.853E+01$	$4.559E+00$	$4.503E+00$
9000	$1.911E+08$	$1.907E+01$	$4.540E+00$	$4.270E+00$
10000	$3.077E+08$	$1.954E+01$	$4.501E+00$	$4.022E+00$
11000	$4.714E+08$	$1.997E+01$	$4.446E+00$	$3.773E+00$
12000	$6.921E+08$	$2.036E+01$	$4.380E+00$	$3.531E+00$
13000	$9.798E+08$	$2.070E+01$	$4.305E+00$	$3.299E+00$
14000	$1.344E+09$	$2.102E+01$	$4.226E+00$	$3.081E+00$
15000	$1.794E+09$	$2.131E+01$	$4.142E+00$	$2.877E+00$
16000	$2.338E+09$	$2.157E+01$	$4.057E+00$	$2.687E+00$
17000	$2.982E+09$	$2.182E+01$	$3.971E+00$	$2.511E+00$
18000	$3.732E+09$	$2.204E+01$	$3.886E+00$	$2.348E+00$
19000	$4.595E+09$	$2.225E+01$	$3.801E+00$	$2.197E+00$
20000	$5.572E+09$	$2.244E+01$	$3.717E+00$	$2.058E+00$
21000	$6.666E+09$	$2.262E+01$	$3.635E+00$	$1.930E+00$
22000	$7.880E+09$	$2.279E+01$	$3.555E+00$	$1.811E+00$
23000	$9.213E+09$	$2.294E+01$	$3.476E+00$	$1.701E+00$
24000	$1.066E+10$	$2.309E+01$	$3.400E+00$	$1.600E+00$
25000	$1.223E+10$	$2.323E+01$	$3.326E+00$	$1.507E+00$
26000	$1.392E+10$	$2.336E+01$	$3.255E+00$	$1.421E+00$
27000	$1.572E+10$	$2.348E+01$	$3.185E+00$	$1.341E+00$
28000	$1.763E+10$	$2.359E+01$	$3.118E+00$	$1.267E+00$
29000	$1.964E+10$	$2.370E+01$	$3.053E+00$	$1.198E+00$
30000	$2.176E+10$	$2.380E+01$	$2.990E+00$	$1.135E+00$
32000	$2.629E+10$	$2.399E+01$	$2.871E+00$	$1.021E+00$
34000	$3.118E+10$	$2.416E+01$	$2.759E+00$	$9.219E-01$
36000	$3.640E+10$	$2.432E+01$	$2.654E+00$	$8.360E-01$
38000	$4.191E+10$	$2.446E+01$	$2.557E+00$	$7.609E-01$
40000	$4.767E+10$	$2.459E+01$	$2.465E+00$	$6.950E-01$
42000	$5.365E+10$	$2.471E+01$	$2.379E+00$	$6.370E-01$
44000	$5.982E+10$	$2.481E+01$	$2.299E+00$	$5.856E-01$
46000	$6.614E+10$	$2.492E+01$	$2.224E+00$	$5.400E-01$
48000	$7.260E+10$	$2.501E+01$	$2.153E+00$	$4.994E-01$
50000	$7.916E+10$	$2.509E+01$	$2.086E+00$	$4.630E-01$

Table 170: Total thermodynamic properties of NCO

T [K]	C_p [J/mol/K]	S^0 [J/mol/K]	$H^0(T)-H^0(0)$ [KJ/mol]	$H^0(T)-H^0(298)$ [KJ/mol]	$-(G^0-H^0(0))/T$ [J/mol/K]	$-(G^0-H^0(298))/T$ [J/mol/K]	ΔH_f [KJ/mol]	$\text{Log}(K_p)$
50	3.266E+01	1.717E+02	1.523E+00	-8.683E+00	1.412E+02	3.454E+02	-2.858E+02	2.962E+02
100	3.208E+01	1.942E+02	3.145E+00	-7.061E+00	1.628E+02	2.648E+02	-2.863E+02	1.469E+02
150	3.318E+01	2.073E+02	4.767E+00	-5.439E+00	1.756E+02	2.436E+02	-2.870E+02	9.696E+01
200	3.557E+01	2.172E+02	6.484E+00	-3.722E+00	1.848E+02	2.358E+02	-2.876E+02	7.195E+01
298.15	4.011E+01	2.323E+02	1.021E+01	0.000E+00	1.981E+02	2.323E+02	-2.889E+02	4.717E+01
300	4.019E+01	2.325E+02	1.028E+01	7.430E-02	1.983E+02	2.323E+02	-2.889E+02	4.686E+01
400	4.391E+01	2.446E+02	1.449E+01	4.285E+00	2.084E+02	2.339E+02	-2.897E+02	3.427E+01
500	4.700E+01	2.548E+02	1.904E+01	8.835E+00	2.167E+02	2.371E+02	-2.901E+02	2.670E+01
600	4.957E+01	2.636E+02	2.387E+01	1.367E+01	2.238E+02	2.408E+02	-2.901E+02	2.164E+01
700	5.167E+01	2.714E+02	2.894E+01	1.873E+01	2.300E+02	2.446E+02	-2.900E+02	1.804E+01
800	5.338E+01	2.784E+02	3.419E+01	2.399E+01	2.357E+02	2.484E+02	-2.898E+02	1.533E+01
900	5.475E+01	2.848E+02	3.960E+01	2.940E+01	2.408E+02	2.521E+02	-2.894E+02	1.323E+01
1000	5.587E+01	2.906E+02	4.514E+01	3.493E+01	2.454E+02	2.557E+02	-2.890E+02	1.155E+01
2000	6.040E+01	3.311E+02	1.039E+02	9.369E+01	2.792E+02	2.843E+02	-2.845E+02	4.051E+00
3000	6.146E+01	3.559E+02	1.649E+02	1.547E+02	3.009E+02	3.043E+02	-2.812E+02	1.587E+00
4000	6.182E+01	3.736E+02	2.266E+02	2.164E+02	3.170E+02	3.195E+02	-2.795E+02	3.669E-01
5000	6.174E+01	3.874E+02	2.884E+02	2.782E+02	3.297E+02	3.318E+02	-2.791E+02	-3.624E-01
6000	6.111E+01	3.986E+02	3.499E+02	3.397E+02	3.403E+02	3.420E+02	-2.803E+02	-8.490E-01
7000	5.989E+01	4.079E+02	4.104E+02	4.002E+02	3.493E+02	3.508E+02	-2.832E+02	-1.199E+00
8000	5.823E+01	4.159E+02	4.695E+02	4.593E+02	3.571E+02	3.584E+02	-2.883E+02	-1.465E+00
9000	5.629E+01	4.226E+02	5.268E+02	5.166E+02	3.641E+02	3.652E+02	-2.956E+02	-1.677E+00
10000	5.423E+01	4.284E+02	5.821E+02	5.719E+02	3.702E+02	3.712E+02	-3.053E+02	-1.851E+00
11000	5.216E+01	4.335E+02	6.353E+02	6.250E+02	3.757E+02	3.767E+02	-3.178E+02	-1.999E+00
12000	5.014E+01	4.379E+02	6.864E+02	6.762E+02	3.807E+02	3.816E+02	-3.332E+02	-2.127E+00
13000	4.822E+01	4.419E+02	7.356E+02	7.254E+02	3.853E+02	3.861E+02	-3.514E+02	-2.242E+00
14000	4.641E+01	4.454E+02	7.829E+02	7.727E+02	3.895E+02	3.902E+02	-3.724E+02	-2.346E+00
15000	4.471E+01	4.485E+02	8.284E+02	8.182E+02	3.933E+02	3.940E+02	-3.956E+02	-2.441E+00
16000	4.313E+01	4.514E+02	8.723E+02	8.621E+02	3.968E+02	3.975E+02	-4.202E+02	-2.530E+00
17000	4.166E+01	4.539E+02	9.147E+02	9.045E+02	4.001E+02	4.007E+02	-4.455E+02	-2.613E+00
18000	4.031E+01	4.563E+02	9.557E+02	9.455E+02	4.032E+02	4.038E+02	-4.709E+02	-2.691E+00
19000	3.905E+01	4.584E+02	9.954E+02	9.852E+02	4.060E+02	4.066E+02	-4.957E+02	-2.765E+00
20000	3.790E+01	4.604E+02	1.034E+03	1.024E+03	4.087E+02	4.092E+02	-5.196E+02	-2.834E+00
21000	3.683E+01	4.622E+02	1.071E+03	1.061E+03	4.112E+02	4.117E+02	-5.424E+02	-2.901E+00
22000	3.584E+01	4.639E+02	1.108E+03	1.097E+03	4.136E+02	4.140E+02	-5.639E+02	-2.963E+00
23000	3.493E+01	4.655E+02	1.143E+03	1.133E+03	4.158E+02	4.162E+02	-5.842E+02	-3.022E+00
24000	3.409E+01	4.669E+02	1.177E+03	1.167E+03	4.179E+02	4.183E+02	-6.033E+02	-3.079E+00
25000	3.332E+01	4.683E+02	1.211E+03	1.201E+03	4.199E+02	4.203E+02	-6.213E+02	-3.132E+00
26000	3.260E+01	4.696E+02	1.244E+03	1.234E+03	4.218E+02	4.222E+02	-6.383E+02	-3.182E+00
27000	3.193E+01	4.708E+02	1.276E+03	1.266E+03	4.236E+02	4.239E+02	-6.545E+02	-3.231E+00
28000	3.132E+01	4.720E+02	1.308E+03	1.298E+03	4.253E+02	4.256E+02	-6.698E+02	-3.276E+00
29000	3.075E+01	4.731E+02	1.339E+03	1.329E+03	4.269E+02	4.272E+02	-6.845E+02	-3.320E+00
30000	3.022E+01	4.741E+02	1.370E+03	1.359E+03	4.285E+02	4.288E+02	-6.986E+02	-3.361E+00
32000	2.927E+01	4.760E+02	1.429E+03	1.419E+03	4.314E+02	4.317E+02	-7.254E+02	-3.439E+00
34000	2.845E+01	4.778E+02	1.487E+03	1.476E+03	4.341E+02	4.344E+02	-7.507E+02	-3.510E+00
36000	2.774E+01	4.794E+02	1.543E+03	1.533E+03	4.365E+02	4.368E+02	-7.749E+02	-3.575E+00
38000	2.711E+01	4.809E+02	1.598E+03	1.587E+03	4.388E+02	4.391E+02	-7.983E+02	-3.635E+00
40000	2.657E+01	4.822E+02	1.651E+03	1.641E+03	4.410E+02	4.412E+02	-8.210E+02	-3.690E+00
42000	2.608E+01	4.835E+02	1.704E+03	1.694E+03	4.429E+02	4.432E+02	-8.433E+02	-3.742E+00
44000	2.566E+01	4.847E+02	1.756E+03	1.746E+03	4.448E+02	4.451E+02	-8.652E+02	-3.790E+00
46000	2.528E+01	4.859E+02	1.807E+03	1.796E+03	4.466E+02	4.468E+02	-8.869E+02	-3.836E+00
48000	2.494E+01	4.869E+02	1.857E+03	1.847E+03	4.482E+02	4.485E+02	-9.084E+02	-3.878E+00
50000	2.464E+01	4.879E+02	1.906E+03	1.896E+03	4.498E+02	4.500E+02	-9.298E+02	-3.918E+00

Table 171: Internal thermodynamic properties of O ΔE=250 cm^{-1}

T(K)	Q_{int}	$\ln(Q_{int})$	E_{int}/RT	$C_{p,int}/R$
50	$5.033E+00$	$1.616E+00$	$3.033E-02$	$1.412E-01$
100	$5.345E+00$	$1.676E+00$	$1.543E-01$	$3.510E-01$
150	$5.770E+00$	$1.753E+00$	$2.157E-01$	$3.094E-01$
200	$6.155E+00$	$1.817E+00$	$2.296E-01$	$2.345E-01$
298.15	$6.731E+00$	$1.907E+00$	$2.131E-01$	$1.354E-01$
300	$6.740E+00$	$1.908E+00$	$2.126E-01$	$1.341E-01$
400	$7.139E+00$	$1.966E+00$	$1.860E-01$	$8.380E-02$
500	$7.422E+00$	$2.005E+00$	$1.626E-01$	$5.667E-02$
600	$7.632E+00$	$2.032E+00$	$1.435E-01$	$4.069E-02$
700	$7.794E+00$	$2.053E+00$	$1.280E-01$	$3.056E-02$
800	$7.921E+00$	$2.070E+00$	$1.154E-01$	$2.376E-02$
900	$8.025E+00$	$2.083E+00$	$1.049E-01$	$1.899E-02$
1000	$8.110E+00$	$2.093E+00$	$9.616E-02$	$1.552E-02$
2000	$8.526E+00$	$2.143E+00$	$5.211E-02$	$4.855E-03$
3000	$8.680E+00$	$2.161E+00$	$3.775E-02$	$1.818E-02$
4000	$8.772E+00$	$2.172E+00$	$3.779E-02$	$6.207E-02$
5000	$8.855E+00$	$2.181E+00$	$4.854E-02$	$1.218E-01$
6000	$8.947E+00$	$2.191E+00$	$6.563E-02$	$1.788E-01$
7000	$9.051E+00$	$2.203E+00$	$8.518E-02$	$2.240E-01$
8000	$9.166E+00$	$2.216E+00$	$1.047E-01$	$2.580E-01$
9000	$9.290E+00$	$2.229E+00$	$1.236E-01$	$2.946E-01$
10000	$9.422E+00$	$2.243E+00$	$1.441E-01$	$3.760E-01$
11000	$9.564E+00$	$2.258E+00$	$1.736E-01$	$5.954E-01$
12000	$9.730E+00$	$2.275E+00$	$2.275E-01$	$1.112E+00$
13000	$9.945E+00$	$2.297E+00$	$3.310E-01$	$2.135E+00$
14000	$1.025E+01$	$2.328E+00$	$5.168E-01$	$3.860E+00$
15000	$1.073E+01$	$2.373E+00$	$8.183E-01$	$6.334E+00$
16000	$1.146E+01$	$2.439E+00$	$1.255E+00$	$9.309E+00$
17000	$1.257E+01$	$2.531E+00$	$1.816E+00$	$1.220E+01$
18000	$1.420E+01$	$2.653E+00$	$2.456E+00$	$1.429E+01$
19000	$1.650E+01$	$2.803E+00$	$3.106E+00$	$1.510E+01$
20000	$1.965E+01$	$2.978E+00$	$3.698E+00$	$1.460E+01$
21000	$2.383E+01$	$3.171E+00$	$4.185E+00$	$1.316E+01$
22000	$2.921E+01$	$3.374E+00$	$4.552E+00$	$1.128E+01$
23000	$3.597E+01$	$3.583E+00$	$4.801E+00$	$9.334E+00$
24000	$4.428E+01$	$3.790E+00$	$4.953E+00$	$7.562E+00$
25000	$5.429E+01$	$3.994E+00$	$5.026E+00$	$6.057E+00$
26000	$6.615E+01$	$4.192E+00$	$5.041E+00$	$4.830E+00$
27000	$7.998E+01$	$4.382E+00$	$5.014E+00$	$3.853E+00$
28000	$9.589E+01$	$4.563E+00$	$4.959E+00$	$3.084E+00$
29000	$1.140E+02$	$4.736E+00$	$4.883E+00$	$2.482E+00$
30000	$1.343E+02$	$4.900E+00$	$4.795E+00$	$2.011E+00$
32000	$1.819E+02$	$5.203E+00$	$4.599E+00$	$1.350E+00$
34000	$2.389E+02$	$5.476E+00$	$4.394E+00$	$9.338E-01$
36000	$3.054E+02$	$5.721E+00$	$4.194E+00$	$6.648E-01$
38000	$3.811E+02$	$5.943E+00$	$4.003E+00$	$4.860E-01$
40000	$4.658E+02$	$6.144E+00$	$3.824E+00$	$3.639E-01$
42000	$5.591E+02$	$6.326E+00$	$3.657E+00$	$2.784E-01$
44000	$6.604E+02$	$6.493E+00$	$3.502E+00$	$2.171E-01$
46000	$7.692E+02$	$6.645E+00$	$3.358E+00$	$1.723E-01$
48000	$8.848E+02$	$6.785E+00$	$3.225E+00$	$1.388E-01$
50000	$1.007E+03$	$6.914E+00$	$3.101E+00$	$1.134E-01$

Table 172: Total thermodynamic properties of O ΔE=250 cm^{-1}

T [K]	C_p [J/mol/K]	S^0 [J/mol/K]	$H^0(T)-H^0(0)$ [KJ/mol]	$H^0(T)-H^0(298)$ [KJ/mol]	$-(G^0-H^0(0))/T$ [J/mol/K]	$-(G^0-H^0(298))/T$ [J/mol/K]	ΔH_f [KJ/mol]	$\mathrm{Log}(K_p)$
50	2.196E+01	1.200E+02	1.052E+00	-5.674E+00	9.897E+01	2.335E+02	2.471E+02	-2.559E+02
100	2.370E+01	1.359E+02	2.207E+00	-4.519E+00	1.139E+02	1.811E+02	2.476E+02	-1.267E+02
150	2.336E+01	1.455E+02	3.387E+00	-3.339E+00	1.229E+02	1.678E+02	2.480E+02	-8.360E+01
200	2.274E+01	1.522E+02	4.539E+00	-2.187E+00	1.295E+02	1.631E+02	2.484E+02	-6.199E+01
298.15	2.191E+01	1.611E+02	6.726E+00	0.000E+00	1.385E+02	1.611E+02	2.492E+02	-4.060E+01
300	2.190E+01	1.612E+02	6.766E+00	4.060E-02	1.386E+02	1.611E+02	2.492E+02	-4.033E+01
400	2.148E+01	1.674E+02	8.933E+00	2.208E+00	1.451E+02	1.619E+02	2.499E+02	-2.947E+01
500	2.126E+01	1.722E+02	1.107E+01	4.343E+00	1.501E+02	1.635E+02	2.505E+02	-2.294E+01
600	2.112E+01	1.761E+02	1.319E+01	6.462E+00	1.541E+02	1.653E+02	2.510E+02	-1.857E+01
700	2.104E+01	1.793E+02	1.530E+01	8.570E+00	1.575E+02	1.671E+02	2.515E+02	-1.545E+01
800	2.098E+01	1.821E+02	1.740E+01	1.067E+01	1.604E+02	1.688E+02	2.519E+02	-1.310E+01
900	2.094E+01	1.846E+02	1.949E+01	1.277E+01	1.629E+02	1.704E+02	2.523E+02	-1.127E+01
1000	2.091E+01	1.868E+02	2.159E+01	1.486E+01	1.652E+02	1.719E+02	2.527E+02	-9.806E+00
2000	2.083E+01	2.012E+02	4.244E+01	3.571E+01	1.800E+02	1.834E+02	2.553E+02	-3.176E+00
3000	2.094E+01	2.097E+02	6.330E+01	5.657E+01	1.886E+02	1.908E+02	2.567E+02	-9.478E-01
4000	2.130E+01	2.158E+02	8.440E+01	7.768E+01	1.947E+02	1.963E+02	2.573E+02	1.709E-01
5000	2.180E+01	2.206E+02	1.060E+02	9.922E+01	1.994E+02	2.007E+02	2.577E+02	8.435E-01
6000	2.227E+01	2.246E+02	1.280E+02	1.213E+02	2.033E+02	2.044E+02	2.580E+02	1.292E+00
7000	2.265E+01	2.281E+02	1.505E+02	1.437E+02	2.066E+02	2.075E+02	2.583E+02	1.613E+00
8000	2.293E+01	2.311E+02	1.733E+02	1.665E+02	2.094E+02	2.103E+02	2.589E+02	1.855E+00
9000	2.324E+01	2.338E+02	1.963E+02	1.896E+02	2.120E+02	2.128E+02	2.601E+02	2.043E+00
10000	2.391E+01	2.363E+02	2.198E+02	2.131E+02	2.143E+02	2.150E+02	2.624E+02	2.194E+00
11000	2.574E+01	2.387E+02	2.445E+02	2.378E+02	2.164E+02	2.170E+02	2.666E+02	2.320E+00
12000	3.003E+01	2.411E+02	2.721E+02	2.654E+02	2.184E+02	2.189E+02	2.746E+02	2.427E+00
13000	3.854E+01	2.438E+02	3.060E+02	2.993E+02	2.202E+02	2.207E+02	2.898E+02	2.521E+00
14000	5.288E+01	2.471E+02	3.512E+02	3.444E+02	2.220E+02	2.225E+02	3.170E+02	2.607E+00
15000	7.345E+01	2.514E+02	4.139E+02	4.071E+02	2.238E+02	2.243E+02	3.625E+02	2.691E+00
16000	9.818E+01	2.569E+02	4.995E+02	4.928E+02	2.257E+02	2.261E+02	4.316E+02	2.777E+00
17000	1.222E+02	2.636E+02	6.100E+02	6.033E+02	2.277E+02	2.281E+02	5.261E+02	2.869E+00
18000	1.396E+02	2.711E+02	7.417E+02	7.350E+02	2.299E+02	2.303E+02	6.423E+02	2.968E+00
19000	1.463E+02	2.789E+02	8.856E+02	8.789E+02	2.323E+02	2.327E+02	7.712E+02	3.075E+00
20000	1.422E+02	2.864E+02	1.031E+03	1.024E+03	2.348E+02	2.352E+02	9.015E+02	3.190E+00
21000	1.302E+02	2.930E+02	1.167E+03	1.161E+03	2.374E+02	2.378E+02	1.024E+03	3.310E+00
22000	1.146E+02	2.987E+02	1.290E+03	1.283E+03	2.401E+02	2.404E+02	1.132E+03	3.432E+00
23000	9.839E+01	3.035E+02	1.396E+03	1.390E+03	2.428E+02	2.431E+02	1.225E+03	3.554E+00
24000	8.366E+01	3.073E+02	1.487E+03	1.480E+03	2.454E+02	2.457E+02	1.302E+03	3.673E+00
25000	7.114E+01	3.105E+02	1.564E+03	1.558E+03	2.479E+02	2.482E+02	1.366E+03	3.789E+00
26000	6.094E+01	3.131E+02	1.630E+03	1.624E+03	2.504E+02	2.506E+02	1.418E+03	3.901E+00
27000	5.282E+01	3.152E+02	1.687E+03	1.680E+03	2.527E+02	2.530E+02	1.462E+03	4.009E+00
28000	4.643E+01	3.170E+02	1.736E+03	1.730E+03	2.550E+02	2.552E+02	1.499E+03	4.111E+00
29000	4.143E+01	3.186E+02	1.780E+03	1.774E+03	2.572E+02	2.574E+02	1.530E+03	4.208E+00
30000	3.751E+01	3.199E+02	1.820E+03	1.813E+03	2.592E+02	2.595E+02	1.556E+03	4.301E+00
32000	3.201E+01	3.221E+02	1.889E+03	1.882E+03	2.631E+02	2.633E+02	1.600E+03	4.473E+00
34000	2.855E+01	3.240E+02	1.949E+03	1.942E+03	2.666E+02	2.668E+02	1.636E+03	4.628E+00
36000	2.631E+01	3.255E+02	2.004E+03	1.997E+03	2.699E+02	2.701E+02	1.666E+03	4.769E+00
38000	2.483E+01	3.269E+02	2.055E+03	2.048E+03	2.728E+02	2.730E+02	1.693E+03	4.897E+00
40000	2.381E+01	3.281E+02	2.103E+03	2.097E+03	2.756E+02	2.757E+02	1.718E+03	5.014E+00
42000	2.310E+01	3.293E+02	2.150E+03	2.144E+03	2.781E+02	2.782E+02	1.741E+03	5.122E+00
44000	2.259E+01	3.304E+02	2.196E+03	2.189E+03	2.804E+02	2.806E+02	1.763E+03	5.221E+00
46000	2.222E+01	3.314E+02	2.241E+03	2.234E+03	2.826E+02	2.828E+02	1.785E+03	5.313E+00
48000	2.194E+01	3.323E+02	2.285E+03	2.278E+03	2.847E+02	2.848E+02	1.806E+03	5.397E+00
50000	2.173E+01	3.332E+02	2.328E+03	2.322E+03	2.866E+02	2.867E+02	1.826E+03	5.476E+00

Table 173: Internal thermodynamic properties of O ΔE=500 cm^{-1}

T(K)	Q_{int}	$\ln(Q_{int})$	E_{int}/RT	$C_{p,int}/R$
50	$5.033E+00$	$1.616E+00$	$3.033E-02$	$1.412E-01$
100	$5.345E+00$	$1.676E+00$	$1.543E-01$	$3.510E-01$
150	$5.770E+00$	$1.753E+00$	$2.157E-01$	$3.094E-01$
200	$6.155E+00$	$1.817E+00$	$2.296E-01$	$2.345E-01$
298.15	$6.731E+00$	$1.907E+00$	$2.131E-01$	$1.354E-01$
300	$6.740E+00$	$1.908E+00$	$2.126E-01$	$1.341E-01$
400	$7.139E+00$	$1.966E+00$	$1.860E-01$	$8.380E-02$
500	$7.422E+00$	$2.005E+00$	$1.626E-01$	$5.667E-02$
600	$7.632E+00$	$2.032E+00$	$1.435E-01$	$4.069E-02$
700	$7.794E+00$	$2.053E+00$	$1.280E-01$	$3.056E-02$
800	$7.921E+00$	$2.070E+00$	$1.154E-01$	$2.376E-02$
900	$8.025E+00$	$2.083E+00$	$1.049E-01$	$1.899E-02$
1000	$8.110E+00$	$2.093E+00$	$9.616E-02$	$1.552E-02$
2000	$8.526E+00$	$2.143E+00$	$5.211E-02$	$4.855E-03$
3000	$8.680E+00$	$2.161E+00$	$3.775E-02$	$1.818E-02$
4000	$8.772E+00$	$2.172E+00$	$3.779E-02$	$6.207E-02$
5000	$8.855E+00$	$2.181E+00$	$4.854E-02$	$1.218E-01$
6000	$8.947E+00$	$2.191E+00$	$6.563E-02$	$1.788E-01$
7000	$9.051E+00$	$2.203E+00$	$8.517E-02$	$2.239E-01$
8000	$9.166E+00$	$2.216E+00$	$1.046E-01$	$2.562E-01$
9000	$9.290E+00$	$2.229E+00$	$1.229E-01$	$2.825E-01$
10000	$9.420E+00$	$2.243E+00$	$1.406E-01$	$3.208E-01$
11000	$9.555E+00$	$2.257E+00$	$1.604E-01$	$4.083E-01$
12000	$9.700E+00$	$2.272E+00$	$1.883E-01$	$6.068E-01$
13000	$9.864E+00$	$2.289E+00$	$2.341E-01$	$1.001E+00$
14000	$1.006E+01$	$2.309E+00$	$3.113E-01$	$1.685E+00$
15000	$1.032E+01$	$2.334E+00$	$4.356E-01$	$2.731E+00$
16000	$1.067E+01$	$2.368E+00$	$6.217E-01$	$4.156E+00$
17000	$1.117E+01$	$2.413E+00$	$8.792E-01$	$5.879E+00$
18000	$1.185E+01$	$2.472E+00$	$1.208E+00$	$7.709E+00$
19000	$1.278E+01$	$2.548E+00$	$1.595E+00$	$9.378E+00$
20000	$1.401E+01$	$2.640E+00$	$2.018E+00$	$1.062E+01$
21000	$1.563E+01$	$2.749E+00$	$2.446E+00$	$1.127E+01$
22000	$1.768E+01$	$2.872E+00$	$2.850E+00$	$1.130E+01$
23000	$2.023E+01$	$3.007E+00$	$3.207E+00$	$1.079E+01$
24000	$2.334E+01$	$3.150E+00$	$3.506E+00$	$9.926E+00$
25000	$2.706E+01$	$3.298E+00$	$3.742E+00$	$8.866E+00$
26000	$3.145E+01$	$3.449E+00$	$3.918E+00$	$7.753E+00$
27000	$3.656E+01$	$3.599E+00$	$4.040E+00$	$6.681E+00$
28000	$4.241E+01$	$3.747E+00$	$4.117E+00$	$5.703E+00$
29000	$4.903E+01$	$3.893E+00$	$4.156E+00$	$4.842E+00$
30000	$5.647E+01$	$4.034E+00$	$4.166E+00$	$4.101E+00$
32000	$7.382E+01$	$4.302E+00$	$4.124E+00$	$2.947E+00$
34000	$9.453E+01$	$4.549E+00$	$4.030E+00$	$2.140E+00$
36000	$1.186E+02$	$4.776E+00$	$3.908E+00$	$1.577E+00$
38000	$1.460E+02$	$4.984E+00$	$3.774E+00$	$1.184E+00$
40000	$1.766E+02$	$5.174E+00$	$3.638E+00$	$9.038E-01$
42000	$2.102E+02$	$5.348E+00$	$3.502E+00$	$7.020E-01$
44000	$2.466E+02$	$5.508E+00$	$3.371E+00$	$5.540E-01$
46000	$2.857E+02$	$5.655E+00$	$3.246E+00$	$4.438E-01$
48000	$3.272E+02$	$5.791E+00$	$3.128E+00$	$3.603E-01$
50000	$3.709E+02$	$5.916E+00$	$3.016E+00$	$2.962E-01$

Table 174: Total thermodynamic properties of O ΔE=500 cm^{-1}

T [K]	C_p [J/mol/K]	S^0 [J/mol/K]	$H^0(T)-H^0(0)$ [KJ/mol]	$H^0(T)-H^0(298)$ [KJ/mol]	$-(G^0-H^0(0))/T$ [J/mol/K]	$-(G^0-H^0(298))/T$ [J/mol/K]	ΔH_f [KJ/mol]	$\mathrm{Log}(K_p)$
50	2.196E+01	1.200E+02	1.052E+00	-5.674E+00	9.897E+01	2.335E+02	2.471E+02	-2.559E+02
100	2.370E+01	1.359E+02	2.207E+00	-4.519E+00	1.139E+02	1.811E+02	2.476E+02	-1.267E+02
150	2.336E+01	1.455E+02	3.387E+00	-3.339E+00	1.229E+02	1.678E+02	2.480E+02	-8.360E+01
200	2.274E+01	1.522E+02	4.539E+00	-2.187E+00	1.295E+02	1.631E+02	2.484E+02	-6.199E+01
298.15	2.191E+01	1.611E+02	6.726E+00	0.000E+00	1.385E+02	1.611E+02	2.492E+02	-4.060E+01
300	2.190E+01	1.612E+02	6.766E+00	4.056E-02	1.386E+02	1.611E+02	2.492E+02	-4.033E+01
400	2.148E+01	1.674E+02	8.933E+00	2.208E+00	1.451E+02	1.619E+02	2.499E+02	-2.947E+01
500	2.126E+01	1.722E+02	1.107E+01	4.343E+00	1.501E+02	1.635E+02	2.505E+02	-2.294E+01
600	2.112E+01	1.761E+02	1.319E+01	6.462E+00	1.541E+02	1.653E+02	2.510E+02	-1.857E+01
700	2.104E+01	1.793E+02	1.530E+01	8.570E+00	1.575E+02	1.671E+02	2.515E+02	-1.545E+01
800	2.098E+01	1.821E+02	1.740E+01	1.067E+01	1.604E+02	1.688E+02	2.519E+02	-1.310E+01
900	2.094E+01	1.846E+02	1.949E+01	1.277E+01	1.629E+02	1.704E+02	2.523E+02	-1.127E+01
1000	2.091E+01	1.868E+02	2.159E+01	1.486E+01	1.652E+02	1.719E+02	2.527E+02	-9.806E+00
2000	2.083E+01	2.012E+02	4.244E+01	3.571E+01	1.800E+02	1.834E+02	2.553E+02	-3.176E+00
3000	2.094E+01	2.097E+02	6.330E+01	5.658E+01	1.886E+02	1.908E+02	2.567E+02	-9.478E-01
4000	2.130E+01	2.158E+02	8.440E+01	7.768E+01	1.947E+02	1.964E+02	2.573E+02	1.709E-01
5000	2.180E+01	2.206E+02	1.060E+02	9.922E+01	1.994E+02	2.007E+02	2.577E+02	8.435E-01
6000	2.227E+01	2.246E+02	1.280E+02	1.213E+02	2.033E+02	2.044E+02	2.580E+02	1.292E+00
7000	2.265E+01	2.281E+02	1.505E+02	1.437E+02	2.066E+02	2.075E+02	2.583E+02	1.613E+00
8000	2.292E+01	2.311E+02	1.732E+02	1.665E+02	2.094E+02	2.103E+02	2.589E+02	1.855E+00
9000	2.314E+01	2.338E+02	1.963E+02	1.896E+02	2.120E+02	2.128E+02	2.601E+02	2.043E+00
10000	2.345E+01	2.363E+02	2.196E+02	2.128E+02	2.143E+02	2.150E+02	2.621E+02	2.194E+00
11000	2.418E+01	2.385E+02	2.433E+02	2.366E+02	2.164E+02	2.170E+02	2.654E+02	2.319E+00
12000	2.583E+01	2.407E+02	2.682E+02	2.615E+02	2.183E+02	2.189E+02	2.707E+02	2.425E+00
13000	2.911E+01	2.429E+02	2.955E+02	2.888E+02	2.202E+02	2.207E+02	2.793E+02	2.517E+00
14000	3.479E+01	2.452E+02	3.272E+02	3.205E+02	2.218E+02	2.223E+02	2.931E+02	2.599E+00
15000	4.349E+01	2.479E+02	3.661E+02	3.594E+02	2.235E+02	2.239E+02	3.148E+02	2.675E+00
16000	5.534E+01	2.511E+02	4.153E+02	4.086E+02	2.251E+02	2.255E+02	3.474E+02	2.746E+00
17000	6.967E+01	2.548E+02	4.776E+02	4.709E+02	2.268E+02	2.272E+02	3.938E+02	2.817E+00
18000	8.488E+01	2.593E+02	5.549E+02	5.482E+02	2.284E+02	2.288E+02	4.556E+02	2.889E+00
19000	9.876E+01	2.642E+02	6.470E+02	6.402E+02	2.302E+02	2.305E+02	5.325E+02	2.964E+00
20000	1.091E+02	2.696E+02	7.513E+02	7.445E+02	2.320E+02	2.324E+02	6.221E+02	3.044E+00
21000	1.145E+02	2.751E+02	8.635E+02	8.568E+02	2.339E+02	2.343E+02	7.200E+02	3.127E+00
22000	1.147E+02	2.804E+02	9.785E+02	9.718E+02	2.359E+02	2.362E+02	8.209E+02	3.214E+00
23000	1.105E+02	2.854E+02	1.092E+03	1.085E+03	2.380E+02	2.383E+02	9.200E+02	3.304E+00
24000	1.033E+02	2.900E+02	1.199E+03	1.192E+03	2.401E+02	2.403E+02	1.014E+03	3.395E+00
25000	9.451E+01	2.940E+02	1.298E+03	1.291E+03	2.421E+02	2.424E+02	1.099E+03	3.487E+00
26000	8.525E+01	2.976E+02	1.387E+03	1.381E+03	2.442E+02	2.445E+02	1.176E+03	3.579E+00
27000	7.633E+01	3.006E+02	1.468E+03	1.462E+03	2.462E+02	2.465E+02	1.243E+03	3.668E+00
28000	6.820E+01	3.032E+02	1.540E+03	1.534E+03	2.482E+02	2.485E+02	1.302E+03	3.756E+00
29000	6.104E+01	3.055E+02	1.605E+03	1.598E+03	2.502E+02	2.504E+02	1.354E+03	3.842E+00
30000	5.489E+01	3.075E+02	1.663E+03	1.656E+03	2.520E+02	2.523E+02	1.399E+03	3.925E+00
32000	4.529E+01	3.107E+02	1.762E+03	1.756E+03	2.556E+02	2.558E+02	1.474E+03	4.081E+00
34000	3.858E+01	3.132E+02	1.846E+03	1.839E+03	2.589E+02	2.591E+02	1.533E+03	4.226E+00
36000	3.390E+01	3.153E+02	1.918E+03	1.911E+03	2.620E+02	2.622E+02	1.580E+03	4.358E+00
38000	3.063E+01	3.170E+02	1.982E+03	1.976E+03	2.649E+02	2.650E+02	1.621E+03	4.481E+00
40000	2.830E+01	3.185E+02	2.041E+03	2.034E+03	2.675E+02	2.677E+02	1.656E+03	4.593E+00
42000	2.662E+01	3.199E+02	2.096E+03	2.089E+03	2.700E+02	2.701E+02	1.687E+03	4.697E+00
44000	2.539E+01	3.211E+02	2.148E+03	2.141E+03	2.723E+02	2.724E+02	1.715E+03	4.793E+00
46000	2.448E+01	3.222E+02	2.198E+03	2.191E+03	2.744E+02	2.746E+02	1.742E+03	4.882E+00
48000	2.378E+01	3.232E+02	2.246E+03	2.239E+03	2.764E+02	2.766E+02	1.767E+03	4.965E+00
50000	2.325E+01	3.242E+02	2.293E+03	2.286E+03	2.783E+02	2.784E+02	1.791E+03	5.043E+00

Table 175: Internal thermodynamic properties of O ΔE=1000 cm^{-1}

T(K)	Q_{int}	$\ln(Q_{int})$	E_{int}/RT	$C_{p,int}/R$
50	$5.033E+00$	$1.616E+00$	$3.033E-02$	$1.412E-01$
100	$5.345E+00$	$1.676E+00$	$1.543E-01$	$3.510E-01$
150	$5.770E+00$	$1.753E+00$	$2.157E-01$	$3.094E-01$
200	$6.155E+00$	$1.817E+00$	$2.296E-01$	$2.345E-01$
298.15	$6.731E+00$	$1.907E+00$	$2.131E-01$	$1.354E-01$
300	$6.740E+00$	$1.908E+00$	$2.126E-01$	$1.341E-01$
400	$7.139E+00$	$1.966E+00$	$1.860E-01$	$8.380E-02$
500	$7.422E+00$	$2.005E+00$	$1.626E-01$	$5.667E-02$
600	$7.632E+00$	$2.032E+00$	$1.435E-01$	$4.069E-02$
700	$7.794E+00$	$2.053E+00$	$1.280E-01$	$3.056E-02$
800	$7.921E+00$	$2.070E+00$	$1.154E-01$	$2.376E-02$
900	$8.025E+00$	$2.083E+00$	$1.049E-01$	$1.899E-02$
1000	$8.110E+00$	$2.093E+00$	$9.616E-02$	$1.552E-02$
2000	$8.526E+00$	$2.143E+00$	$5.211E-02$	$4.855E-03$
3000	$8.680E+00$	$2.161E+00$	$3.775E-02$	$1.818E-02$
4000	$8.772E+00$	$2.172E+00$	$3.779E-02$	$6.207E-02$
5000	$8.855E+00$	$2.181E+00$	$4.854E-02$	$1.218E-01$
6000	$8.947E+00$	$2.191E+00$	$6.563E-02$	$1.788E-01$
7000	$9.051E+00$	$2.203E+00$	$8.517E-02$	$2.238E-01$
8000	$9.166E+00$	$2.216E+00$	$1.046E-01$	$2.556E-01$
9000	$9.290E+00$	$2.229E+00$	$1.227E-01$	$2.782E-01$
10000	$9.419E+00$	$2.243E+00$	$1.393E-01$	$3.013E-01$
11000	$9.552E+00$	$2.257E+00$	$1.557E-01$	$3.422E-01$
12000	$9.690E+00$	$2.271E+00$	$1.744E-01$	$4.282E-01$
13000	$9.835E+00$	$2.286E+00$	$1.997E-01$	$5.956E-01$
14000	$9.995E+00$	$2.302E+00$	$2.375E-01$	$8.854E-01$
15000	$1.018E+01$	$2.320E+00$	$2.947E-01$	$1.336E+00$
16000	$1.040E+01$	$2.342E+00$	$3.787E-01$	$1.972E+00$
17000	$1.068E+01$	$2.368E+00$	$4.958E-01$	$2.796E+00$
18000	$1.103E+01$	$2.401E+00$	$6.502E-01$	$3.777E+00$
19000	$1.148E+01$	$2.441E+00$	$8.428E-01$	$4.849E+00$
20000	$1.206E+01$	$2.490E+00$	$1.070E+00$	$5.919E+00$
21000	$1.278E+01$	$2.548E+00$	$1.325E+00$	$6.883E+00$
22000	$1.368E+01$	$2.616E+00$	$1.595E+00$	$7.647E+00$
23000	$1.477E+01$	$2.693E+00$	$1.871E+00$	$8.149E+00$
24000	$1.609E+01$	$2.778E+00$	$2.138E+00$	$8.367E+00$
25000	$1.764E+01$	$2.870E+00$	$2.387E+00$	$8.317E+00$
26000	$1.946E+01$	$2.968E+00$	$2.610E+00$	$8.043E+00$
27000	$2.156E+01$	$3.071E+00$	$2.804E+00$	$7.603E+00$
28000	$2.394E+01$	$3.176E+00$	$2.965E+00$	$7.056E+00$
29000	$2.663E+01$	$3.282E+00$	$3.096E+00$	$6.456E+00$
30000	$2.963E+01$	$3.389E+00$	$3.198E+00$	$5.843E+00$
32000	$3.659E+01$	$3.600E+00$	$3.326E+00$	$4.683E+00$
34000	$4.485E+01$	$3.803E+00$	$3.376E+00$	$3.697E+00$
36000	$5.440E+01$	$3.996E+00$	$3.371E+00$	$2.907E+00$
38000	$6.521E+01$	$4.178E+00$	$3.330E+00$	$2.293E+00$
40000	$7.724E+01$	$4.347E+00$	$3.266E+00$	$1.820E+00$
42000	$9.042E+01$	$4.504E+00$	$3.188E+00$	$1.458E+00$
44000	$1.047E+02$	$4.651E+00$	$3.103E+00$	$1.180E+00$
46000	$1.199E+02$	$4.787E+00$	$3.014E+00$	$9.644E-01$
48000	$1.361E+02$	$4.913E+00$	$2.925E+00$	$7.961E-01$
50000	$1.530E+02$	$5.031E+00$	$2.837E+00$	$6.635E-01$

Table 176: Total thermodynamic properties of O ΔE=1000 cm^{-1}

T [K]	C_p [J/mol/K]	S^0 [J/mol/K]	$H^0(T)-H^0(0)$ [KJ/mol]	$H^0(T)-H^0(298)$ [KJ/mol]	$-(G^0-H^0(0))/T$ [J/mol/K]	$-(G^0-H^0(298))/T$ [J/mol/K]	ΔH_f [KJ/mol]	$\mathrm{Log}(K_p)$
50	2.196E+01	1.200E+02	1.052E+00	-5.674E+00	9.897E+01	2.335E+02	2.471E+02	-2.559E+02
100	2.370E+01	1.359E+02	2.207E+00	-4.519E+00	1.139E+02	1.811E+02	2.476E+02	-1.267E+02
150	2.336E+01	1.455E+02	3.387E+00	-3.339E+00	1.229E+02	1.678E+02	2.480E+02	-8.360E+01
200	2.274E+01	1.522E+02	4.539E+00	-2.187E+00	1.295E+02	1.631E+02	2.484E+02	-6.199E+01
298.15	2.191E+01	1.611E+02	6.726E+00	0.000E+00	1.385E+02	1.611E+02	2.492E+02	-4.060E+01
300	2.190E+01	1.612E+02	6.766E+00	4.060E-02	1.386E+02	1.611E+02	2.492E+02	-4.033E+01
400	2.148E+01	1.674E+02	8.933E+00	2.208E+00	1.451E+02	1.619E+02	2.499E+02	-2.947E+01
500	2.126E+01	1.722E+02	1.107E+01	4.343E+00	1.501E+02	1.635E+02	2.505E+02	-2.294E+01
600	2.112E+01	1.761E+02	1.319E+01	6.462E+00	1.541E+02	1.653E+02	2.510E+02	-1.857E+01
700	2.104E+01	1.793E+02	1.530E+01	8.570E+00	1.575E+02	1.671E+02	2.515E+02	-1.545E+01
800	2.098E+01	1.821E+02	1.740E+01	1.067E+01	1.604E+02	1.688E+02	2.519E+02	-1.310E+01
900	2.094E+01	1.846E+02	1.949E+01	1.277E+01	1.629E+02	1.704E+02	2.523E+02	-1.127E+01
1000	2.091E+01	1.868E+02	2.159E+01	1.486E+01	1.652E+02	1.719E+02	2.527E+02	-9.806E+00
2000	2.083E+01	2.012E+02	4.244E+01	3.571E+01	1.800E+02	1.834E+02	2.553E+02	-3.176E+00
3000	2.094E+01	2.097E+02	6.330E+01	5.657E+01	1.886E+02	1.908E+02	2.567E+02	-9.478E-01
4000	2.130E+01	2.158E+02	8.440E+01	7.768E+01	1.947E+02	1.963E+02	2.573E+02	1.709E-01
5000	2.180E+01	2.206E+02	1.060E+02	9.922E+01	1.994E+02	2.007E+02	2.577E+02	8.435E-01
6000	2.227E+01	2.246E+02	1.280E+02	1.213E+02	2.033E+02	2.044E+02	2.580E+02	1.292E+00
7000	2.265E+01	2.281E+02	1.505E+02	1.437E+02	2.066E+02	2.075E+02	2.583E+02	1.613E+00
8000	2.291E+01	2.311E+02	1.732E+02	1.665E+02	2.094E+02	2.103E+02	2.589E+02	1.855E+00
9000	2.310E+01	2.338E+02	1.963E+02	1.895E+02	2.120E+02	2.128E+02	2.600E+02	2.043E+00
10000	2.329E+01	2.363E+02	2.194E+02	2.127E+02	2.143E+02	2.150E+02	2.620E+02	2.194E+00
11000	2.363E+01	2.385E+02	2.429E+02	2.362E+02	2.164E+02	2.170E+02	2.650E+02	2.319E+00
12000	2.435E+01	2.406E+02	2.668E+02	2.601E+02	2.183E+02	2.189E+02	2.693E+02	2.425E+00
13000	2.574E+01	2.426E+02	2.918E+02	2.851E+02	2.201E+02	2.206E+02	2.756E+02	2.516E+00
14000	2.815E+01	2.446E+02	3.186E+02	3.119E+02	2.218E+02	2.223E+02	2.845E+02	2.596E+00
15000	3.189E+01	2.466E+02	3.486E+02	3.418E+02	2.234E+02	2.238E+02	2.972E+02	2.668E+00
16000	3.719E+01	2.488E+02	3.829E+02	3.762E+02	2.249E+02	2.253E+02	3.151E+02	2.735E+00
17000	4.404E+01	2.513E+02	4.234E+02	4.167E+02	2.264E+02	2.268E+02	3.396E+02	2.798E+00
18000	5.219E+01	2.540E+02	4.715E+02	4.647E+02	2.278E+02	2.282E+02	3.721E+02	2.858E+00
19000	6.110E+01	2.571E+02	5.281E+02	5.214E+02	2.293E+02	2.297E+02	4.136E+02	2.918E+00
20000	7.000E+01	2.605E+02	5.937E+02	5.869E+02	2.308E+02	2.311E+02	4.645E+02	2.978E+00
21000	7.801E+01	2.641E+02	6.678E+02	6.610E+02	2.323E+02	2.326E+02	5.243E+02	3.039E+00
22000	8.437E+01	2.679E+02	7.491E+02	7.424E+02	2.338E+02	2.341E+02	5.915E+02	3.103E+00
23000	8.854E+01	2.717E+02	8.358E+02	8.291E+02	2.354E+02	2.357E+02	6.643E+02	3.167E+00
24000	9.036E+01	2.755E+02	9.254E+02	9.187E+02	2.370E+02	2.372E+02	7.403E+02	3.234E+00
25000	8.994E+01	2.792E+02	1.016E+03	1.009E+03	2.386E+02	2.388E+02	8.172E+02	3.301E+00
26000	8.766E+01	2.827E+02	1.105E+03	1.098E+03	2.402E+02	2.405E+02	8.929E+02	3.370E+00
27000	8.400E+01	2.859E+02	1.191E+03	1.184E+03	2.418E+02	2.421E+02	9.657E+02	3.439E+00
28000	7.946E+01	2.889E+02	1.272E+03	1.266E+03	2.435E+02	2.437E+02	1.034E+03	3.508E+00
29000	7.447E+01	2.916E+02	1.349E+03	1.343E+03	2.451E+02	2.453E+02	1.099E+03	3.577E+00
30000	6.937E+01	2.941E+02	1.421E+03	1.415E+03	2.467E+02	2.469E+02	1.158E+03	3.645E+00
32000	5.972E+01	2.982E+02	1.550E+03	1.544E+03	2.498E+02	2.500E+02	1.262E+03	3.776E+00
34000	5.152E+01	3.016E+02	1.661E+03	1.654E+03	2.527E+02	2.529E+02	1.348E+03	3.902E+00
36000	4.496E+01	3.043E+02	1.757E+03	1.751E+03	2.555E+02	2.557E+02	1.420E+03	4.020E+00
38000	3.985E+01	3.066E+02	1.842E+03	1.835E+03	2.581E+02	2.583E+02	1.480E+03	4.130E+00
40000	3.592E+01	3.086E+02	1.918E+03	1.911E+03	2.606E+02	2.608E+02	1.532E+03	4.234E+00
42000	3.291E+01	3.102E+02	1.986E+03	1.980E+03	2.629E+02	2.631E+02	1.577E+03	4.331E+00
44000	3.060E+01	3.117E+02	2.050E+03	2.043E+03	2.651E+02	2.653E+02	1.617E+03	4.421E+00
46000	2.880E+01	3.130E+02	2.109E+03	2.102E+03	2.672E+02	2.673E+02	1.653E+03	4.505E+00
48000	2.741E+01	3.142E+02	2.165E+03	2.158E+03	2.691E+02	2.693E+02	1.686E+03	4.584E+00
50000	2.630E+01	3.153E+02	2.219E+03	2.212E+03	2.709E+02	2.711E+02	1.716E+03	4.658E+00

Table 177: Internal thermodynamic properties of O^+ ΔE=250 cm^{-1}

T(K)	Q_{int}	$\ln(Q_{int})$	E_{int}/RT	$C_{p,int}/R$
50	$4.000E+00$	$1.386E+00$	$0.000E+00$	$0.000E+00$
100	$4.000E+00$	$1.386E+00$	$2.672E-165$	$1.031E-162$
150	$4.000E+00$	$1.386E+00$	$1.265E-109$	$3.255E-107$
200	$4.000E+00$	$1.386E+00$	$8.006E-82$	$1.544E-79$
298.15	$4.000E+00$	$1.386E+00$	$2.041E-54$	$2.641E-52$
300	$4.000E+00$	$1.386E+00$	$4.505E-54$	$5.794E-52$
400	$4.000E+00$	$1.386E+00$	$3.105E-40$	$2.995E-38$
500	$4.000E+00$	$1.386E+00$	$5.931E-32$	$4.577E-30$
600	$4.000E+00$	$1.386E+00$	$1.902E-26$	$1.223E-24$
700	$4.000E+00$	$1.386E+00$	$1.592E-22$	$8.774E-21$
800	$4.000E+00$	$1.386E+00$	$1.368E-19$	$6.597E-18$
900	$4.000E+00$	$1.386E+00$	$2.583E-17$	$1.107E-15$
1000	$4.000E+00$	$1.386E+00$	$1.691E-15$	$6.525E-14$
2000	$4.000E+00$	$1.386E+00$	$2.019E-07$	$3.896E-06$
3000	$4.000E+00$	$1.386E+00$	$8.363E-05$	$1.076E-03$
4000	$4.001E+00$	$1.386E+00$	$1.571E-03$	$1.520E-02$
5000	$4.005E+00$	$1.387E+00$	$8.736E-03$	$6.793E-02$
6000	$4.016E+00$	$1.390E+00$	$2.669E-02$	$1.738E-01$
7000	$4.042E+00$	$1.397E+00$	$5.809E-02$	$3.253E-01$
8000	$4.085E+00$	$1.407E+00$	$1.024E-01$	$5.013E-01$
9000	$4.147E+00$	$1.422E+00$	$1.566E-01$	$6.786E-01$
10000	$4.229E+00$	$1.442E+00$	$2.170E-01$	$8.383E-01$
11000	$4.330E+00$	$1.466E+00$	$2.797E-01$	$9.686E-01$
12000	$4.448E+00$	$1.493E+00$	$3.413E-01$	$1.065E+00$
13000	$4.582E+00$	$1.522E+00$	$3.996E-01$	$1.127E+00$
14000	$4.729E+00$	$1.554E+00$	$4.529E-01$	$1.160E+00$
15000	$4.888E+00$	$1.587E+00$	$5.005E-01$	$1.168E+00$
16000	$5.055E+00$	$1.620E+00$	$5.419E-01$	$1.157E+00$
17000	$5.229E+00$	$1.654E+00$	$5.775E-01$	$1.133E+00$
18000	$5.410E+00$	$1.688E+00$	$6.075E-01$	$1.101E+00$
19000	$5.594E+00$	$1.722E+00$	$6.326E-01$	$1.067E+00$
20000	$5.782E+00$	$1.755E+00$	$6.535E-01$	$1.037E+00$
21000	$5.972E+00$	$1.787E+00$	$6.712E-01$	$1.018E+00$
22000	$6.163E+00$	$1.819E+00$	$6.870E-01$	$1.023E+00$
23000	$6.357E+00$	$1.850E+00$	$7.024E-01$	$1.069E+00$
24000	$6.552E+00$	$1.880E+00$	$7.197E-01$	$1.177E+00$
25000	$6.750E+00$	$1.910E+00$	$7.416E-01$	$1.379E+00$
26000	$6.953E+00$	$1.939E+00$	$7.721E-01$	$1.713E+00$
27000	$7.164E+00$	$1.969E+00$	$8.158E-01$	$2.224E+00$
28000	$7.388E+00$	$2.000E+00$	$8.785E-01$	$2.963E+00$
29000	$7.630E+00$	$2.032E+00$	$9.670E-01$	$3.979E+00$
30000	$7.900E+00$	$2.067E+00$	$1.089E+00$	$5.313E+00$
32000	$8.568E+00$	$2.148E+00$	$1.461E+00$	$8.982E+00$
34000	$9.514E+00$	$2.253E+00$	$2.038E+00$	$1.366E+01$
36000	$1.092E+01$	$2.390E+00$	$2.815E+00$	$1.828E+01$
38000	$1.302E+01$	$2.567E+00$	$3.720E+00$	$2.136E+01$
40000	$1.613E+01$	$2.781E+00$	$4.627E+00$	$2.196E+01$
42000	$2.062E+01$	$3.026E+00$	$5.420E+00$	$2.025E+01$
44000	$2.693E+01$	$3.293E+00$	$6.028E+00$	$1.721E+01$
46000	$3.555E+01$	$3.571E+00$	$6.440E+00$	$1.382E+01$
48000	$4.702E+01$	$3.851E+00$	$6.681E+00$	$1.072E+01$
50000	$6.193E+01$	$4.126E+00$	$6.789E+00$	$8.166E+00$

Table 178: Total thermodynamic properties of O^+ ΔE=250 cm^{-1}

T [K]	C_p [J/mol/K]	S^0 [J/mol/K]	$H^0(T)$-$H^0(0)$ [KJ/mol]	$H^0(T)$-$H^0(298)$ [KJ/mol]	-(G^0-$H^0(0)$)/T [J/mol/K]	-(G^0-$H^0(298)$)/T [J/mol/K]	ΔH_f [KJ/mol]	Log(K_p)
50	2.079E+01	1.178E+02	1.039E+00	-5.158E+00	9.706E+01	2.210E+02	1.562E+03	-1.630E+03
100	2.079E+01	1.322E+02	2.079E+00	-4.119E+00	1.115E+02	1.734E+02	1.563E+03	-8.143E+02
150	2.079E+01	1.407E+02	3.118E+00	-3.079E+00	1.199E+02	1.612E+02	1.565E+03	-5.420E+02
200	2.079E+01	1.467E+02	4.157E+00	-2.040E+00	1.259E+02	1.569E+02	1.566E+03	-4.058E+02
298.15	2.079E+01	1.550E+02	6.197E+00	0.000E+00	1.342E+02	1.550E+02	1.569E+03	-2.710E+02
300	2.079E+01	1.551E+02	6.236E+00	3.848E-02	1.343E+02	1.550E+02	1.569E+03	-2.693E+02
400	2.079E+01	1.611E+02	8.315E+00	2.117E+00	1.403E+02	1.558E+02	1.572E+03	-2.010E+02
500	2.079E+01	1.657E+02	1.039E+01	4.196E+00	1.449E+02	1.573E+02	1.574E+03	-1.599E+02
600	2.079E+01	1.695E+02	1.247E+01	6.274E+00	1.487E+02	1.590E+02	1.577E+03	-1.325E+02
700	2.079E+01	1.727E+02	1.455E+01	8.353E+00	1.519E+02	1.608E+02	1.579E+03	-1.128E+02
800	2.079E+01	1.755E+02	1.663E+01	1.043E+01	1.547E+02	1.624E+02	1.582E+03	-9.810E+01
900	2.079E+01	1.779E+02	1.871E+01	1.251E+01	1.571E+02	1.640E+02	1.584E+03	-8.662E+01
1000	2.079E+01	1.801E+02	2.079E+01	1.459E+01	1.593E+02	1.655E+02	1.587E+03	-7.742E+01
2000	2.079E+01	1.945E+02	4.157E+01	3.538E+01	1.737E+02	1.768E+02	1.610E+03	-3.574E+01
3000	2.080E+01	2.029E+02	6.236E+01	5.616E+01	1.822E+02	1.842E+02	1.632E+03	-2.164E+01
4000	2.091E+01	2.089E+02	8.320E+01	7.700E+01	1.882E+02	1.897E+02	1.653E+03	-1.450E+01
5000	2.135E+01	2.137E+02	1.043E+02	9.810E+01	1.928E+02	1.940E+02	1.674E+03	-1.016E+01
6000	2.223E+01	2.176E+02	1.260E+02	1.198E+02	1.966E+02	1.976E+02	1.695E+03	-7.224E+00
7000	2.349E+01	2.211E+02	1.489E+02	1.427E+02	1.999E+02	2.008E+02	1.716E+03	-5.104E+00
8000	2.495E+01	2.244E+02	1.731E+02	1.669E+02	2.027E+02	2.035E+02	1.739E+03	-3.493E+00
9000	2.643E+01	2.274E+02	1.988E+02	1.926E+02	2.053E+02	2.060E+02	1.764E+03	-2.223E+00
10000	2.776E+01	2.302E+02	2.259E+02	2.197E+02	2.077E+02	2.083E+02	1.790E+03	-1.193E+00
11000	2.884E+01	2.329E+02	2.542E+02	2.480E+02	2.098E+02	2.104E+02	1.819E+03	-3.360E-01
12000	2.964E+01	2.355E+02	2.835E+02	2.773E+02	2.119E+02	2.124E+02	1.849E+03	3.895E-01
13000	3.016E+01	2.379E+02	3.134E+02	3.072E+02	2.138E+02	2.142E+02	1.881E+03	1.014E+00
14000	3.043E+01	2.401E+02	3.437E+02	3.375E+02	2.156E+02	2.160E+02	1.914E+03	1.558E+00
15000	3.050E+01	2.422E+02	3.742E+02	3.680E+02	2.173E+02	2.177E+02	1.949E+03	2.039E+00
16000	3.041E+01	2.442E+02	4.047E+02	3.985E+02	2.189E+02	2.193E+02	1.983E+03	2.467E+00
17000	3.021E+01	2.460E+02	4.350E+02	4.288E+02	2.204E+02	2.208E+02	2.018E+03	2.851E+00
18000	2.994E+01	2.478E+02	4.651E+02	4.589E+02	2.219E+02	2.223E+02	2.054E+03	3.198E+00
19000	2.966E+01	2.494E+02	4.949E+02	4.887E+02	2.233E+02	2.237E+02	2.089E+03	3.514E+00
20000	2.940E+01	2.509E+02	5.244E+02	5.182E+02	2.247E+02	2.250E+02	2.125E+03	3.804E+00
21000	2.925E+01	2.523E+02	5.537E+02	5.475E+02	2.259E+02	2.262E+02	2.161E+03	4.071E+00
22000	2.929E+01	2.537E+02	5.830E+02	5.768E+02	2.272E+02	2.275E+02	2.196E+03	4.317E+00
23000	2.967E+01	2.550E+02	6.124E+02	6.062E+02	2.283E+02	2.286E+02	2.233E+03	4.545E+00
24000	3.057E+01	2.563E+02	6.425E+02	6.363E+02	2.295E+02	2.298E+02	2.270E+03	4.758E+00
25000	3.225E+01	2.575E+02	6.738E+02	6.676E+02	2.306E+02	2.308E+02	2.309E+03	4.958E+00
26000	3.503E+01	2.589E+02	7.074E+02	7.011E+02	2.317E+02	2.319E+02	2.350E+03	5.145E+00
27000	3.928E+01	2.602E+02	7.444E+02	7.382E+02	2.327E+02	2.329E+02	2.395E+03	5.321E+00
28000	4.542E+01	2.618E+02	7.865E+02	7.803E+02	2.337E+02	2.339E+02	2.445E+03	5.488E+00
29000	5.387E+01	2.635E+02	8.360E+02	8.298E+02	2.347E+02	2.349E+02	2.502E+03	5.647E+00
30000	6.496E+01	2.655E+02	8.951E+02	8.890E+02	2.357E+02	2.359E+02	2.569E+03	5.800E+00
32000	9.547E+01	2.706E+02	1.054E+03	1.048E+03	2.377E+02	2.379E+02	2.744E+03	6.088E+00
34000	1.344E+02	2.776E+02	1.283E+03	1.277E+03	2.398E+02	2.400E+02	2.990E+03	6.362E+00
36000	1.727E+02	2.864E+02	1.591E+03	1.585E+03	2.422E+02	2.423E+02	3.316E+03	6.631E+00
38000	1.983E+02	2.965E+02	1.965E+03	1.959E+03	2.448E+02	2.449E+02	3.707E+03	6.898E+00
40000	2.033E+02	3.069E+02	2.370E+03	2.364E+03	2.476E+02	2.478E+02	4.130E+03	7.167E+00
42000	1.892E+02	3.165E+02	2.766E+03	2.759E+03	2.507E+02	2.508E+02	4.543E+03	7.437E+00
44000	1.638E+02	3.248E+02	3.120E+03	3.114E+03	2.538E+02	2.540E+02	4.915E+03	7.704E+00
46000	1.357E+02	3.314E+02	3.419E+03	3.413E+03	2.571E+02	2.572E+02	5.233E+03	7.966E+00
48000	1.099E+02	3.366E+02	3.664E+03	3.658E+03	2.603E+02	2.604E+02	5.496E+03	8.220E+00
50000	8.868E+01	3.407E+02	3.862E+03	3.856E+03	2.634E+02	2.636E+02	5.713E+03	8.464E+00

Table 179: Internal thermodynamic properties of O^+ ΔE=500 cm^{-1}

T(K)	Q_{int}	$\ln(Q_{int})$	E_{int}/RT	$C_{p,int}/R$
50	$4.000E+00$	$1.386E+00$	$0.000E+00$	$0.000E+00$
100	$4.000E+00$	$1.386E+00$	$2.672E-165$	$1.031E-162$
150	$4.000E+00$	$1.386E+00$	$1.265E-109$	$3.255E-107$
200	$4.000E+00$	$1.386E+00$	$8.006E-82$	$1.544E-79$
298.15	$4.000E+00$	$1.386E+00$	$2.041E-54$	$2.641E-52$
300	$4.000E+00$	$1.386E+00$	$4.505E-54$	$5.794E-52$
400	$4.000E+00$	$1.386E+00$	$3.105E-40$	$2.995E-38$
500	$4.000E+00$	$1.386E+00$	$5.931E-32$	$4.577E-30$
600	$4.000E+00$	$1.386E+00$	$1.902E-26$	$1.223E-24$
700	$4.000E+00$	$1.386E+00$	$1.592E-22$	$8.774E-21$
800	$4.000E+00$	$1.386E+00$	$1.368E-19$	$6.597E-18$
900	$4.000E+00$	$1.386E+00$	$2.583E-17$	$1.107E-15$
1000	$4.000E+00$	$1.386E+00$	$1.691E-15$	$6.525E-14$
2000	$4.000E+00$	$1.386E+00$	$2.019E-07$	$3.896E-06$
3000	$4.000E+00$	$1.386E+00$	$8.363E-05$	$1.076E-03$
4000	$4.001E+00$	$1.386E+00$	$1.571E-03$	$1.520E-02$
5000	$4.005E+00$	$1.387E+00$	$8.736E-03$	$6.793E-02$
6000	$4.016E+00$	$1.390E+00$	$2.669E-02$	$1.738E-01$
7000	$4.042E+00$	$1.397E+00$	$5.809E-02$	$3.253E-01$
8000	$4.085E+00$	$1.407E+00$	$1.024E-01$	$5.013E-01$
9000	$4.147E+00$	$1.422E+00$	$1.566E-01$	$6.786E-01$
10000	$4.229E+00$	$1.442E+00$	$2.170E-01$	$8.383E-01$
11000	$4.330E+00$	$1.466E+00$	$2.797E-01$	$9.686E-01$
12000	$4.448E+00$	$1.493E+00$	$3.413E-01$	$1.065E+00$
13000	$4.582E+00$	$1.522E+00$	$3.996E-01$	$1.127E+00$
14000	$4.729E+00$	$1.554E+00$	$4.529E-01$	$1.160E+00$
15000	$4.888E+00$	$1.587E+00$	$5.005E-01$	$1.168E+00$
16000	$5.055E+00$	$1.620E+00$	$5.419E-01$	$1.157E+00$
17000	$5.229E+00$	$1.654E+00$	$5.775E-01$	$1.133E+00$
18000	$5.410E+00$	$1.688E+00$	$6.075E-01$	$1.101E+00$
19000	$5.594E+00$	$1.722E+00$	$6.325E-01$	$1.066E+00$
20000	$5.782E+00$	$1.755E+00$	$6.534E-01$	$1.034E+00$
21000	$5.972E+00$	$1.787E+00$	$6.709E-01$	$1.011E+00$
22000	$6.163E+00$	$1.819E+00$	$6.862E-01$	$1.009E+00$
23000	$6.356E+00$	$1.849E+00$	$7.008E-01$	$1.040E+00$
24000	$6.551E+00$	$1.880E+00$	$7.165E-01$	$1.125E+00$
25000	$6.748E+00$	$1.909E+00$	$7.357E-01$	$1.288E+00$
26000	$6.948E+00$	$1.939E+00$	$7.618E-01$	$1.561E+00$
27000	$7.156E+00$	$1.968E+00$	$7.987E-01$	$1.983E+00$
28000	$7.373E+00$	$1.998E+00$	$8.513E-01$	$2.596E+00$
29000	$7.606E+00$	$2.029E+00$	$9.253E-01$	$3.445E+00$
30000	$7.861E+00$	$2.062E+00$	$1.027E+00$	$4.567E+00$
32000	$8.477E+00$	$2.137E+00$	$1.340E+00$	$7.710E+00$
34000	$9.323E+00$	$2.232E+00$	$1.834E+00$	$1.187E+01$
36000	$1.055E+01$	$2.356E+00$	$2.516E+00$	$1.628E+01$
38000	$1.235E+01$	$2.513E+00$	$3.337E+00$	$1.970E+01$
40000	$1.498E+01$	$2.707E+00$	$4.200E+00$	$2.109E+01$
42000	$1.875E+01$	$2.931E+00$	$4.992E+00$	$2.027E+01$
44000	$2.402E+01$	$3.179E+00$	$5.637E+00$	$1.787E+01$
46000	$3.120E+01$	$3.440E+00$	$6.103E+00$	$1.482E+01$
48000	$4.073E+01$	$3.707E+00$	$6.402E+00$	$1.179E+01$
50000	$5.309E+01$	$3.972E+00$	$6.564E+00$	$9.167E+00$

Table 180: Total thermodynamic properties of O^+ ΔE=500 cm^{-1}

T [K]	C_p [J/mol/K]	S^0 [J/mol/K]	$H^0(T)-H^0(0)$ [KJ/mol]	$H^0(T)-H^0(298)$ [KJ/mol]	$-(G^0-H^0(0))/T$ [J/mol/K]	$-(G^0-H^0(298))/T$ [J/mol/K]	ΔH_f [KJ/mol]	$Log(K_p)$
50	2.079E+01	1.178E+02	1.039E+00	-5.158E+00	9.706E+01	2.210E+02	1.562E+03	-1.630E+03
100	2.079E+01	1.322E+02	2.079E+00	-4.119E+00	1.115E+02	1.734E+02	1.563E+03	-8.143E+02
150	2.079E+01	1.407E+02	3.118E+00	-3.079E+00	1.199E+02	1.612E+02	1.565E+03	-5.420E+02
200	2.079E+01	1.467E+02	4.157E+00	-2.040E+00	1.259E+02	1.569E+02	1.566E+03	-4.058E+02
298.15	2.079E+01	1.550E+02	6.197E+00	0.000E+00	1.342E+02	1.550E+02	1.569E+03	-2.710E+02
300	2.079E+01	1.551E+02	6.236E+00	3.848E-02	1.343E+02	1.550E+02	1.569E+03	-2.693E+02
400	2.079E+01	1.611E+02	8.315E+00	2.117E+00	1.403E+02	1.558E+02	1.572E+03	-2.010E+02
500	2.079E+01	1.657E+02	1.039E+01	4.196E+00	1.449E+02	1.573E+02	1.574E+03	-1.599E+02
600	2.079E+01	1.695E+02	1.247E+01	6.274E+00	1.487E+02	1.590E+02	1.577E+03	-1.325E+02
700	2.079E+01	1.727E+02	1.455E+01	8.353E+00	1.519E+02	1.608E+02	1.579E+03	-1.128E+02
800	2.079E+01	1.755E+02	1.663E+01	1.043E+01	1.547E+02	1.624E+02	1.582E+03	-9.810E+01
900	2.079E+01	1.779E+02	1.871E+01	1.251E+01	1.571E+02	1.640E+02	1.584E+03	-8.662E+01
1000	2.079E+01	1.801E+02	2.079E+01	1.459E+01	1.593E+02	1.655E+02	1.587E+03	-7.742E+01
2000	2.079E+01	1.945E+02	4.157E+01	3.538E+01	1.737E+02	1.768E+02	1.610E+03	-3.574E+01
3000	2.080E+01	2.029E+02	6.236E+01	5.616E+01	1.822E+02	1.842E+02	1.632E+03	-2.164E+01
4000	2.091E+01	2.089E+02	8.320E+01	7.700E+01	1.882E+02	1.897E+02	1.653E+03	-1.450E+01
5000	2.135E+01	2.137E+02	1.043E+02	9.810E+01	1.928E+02	1.940E+02	1.674E+03	-1.016E+01
6000	2.223E+01	2.176E+02	1.260E+02	1.198E+02	1.966E+02	1.976E+02	1.695E+03	-7.224E+00
7000	2.349E+01	2.211E+02	1.489E+02	1.427E+02	1.999E+02	2.008E+02	1.716E+03	-5.104E+00
8000	2.495E+01	2.244E+02	1.731E+02	1.669E+02	2.027E+02	2.035E+02	1.739E+03	-3.493E+00
9000	2.643E+01	2.274E+02	1.988E+02	1.926E+02	2.053E+02	2.060E+02	1.764E+03	-2.223E+00
10000	2.776E+01	2.302E+02	2.259E+02	2.197E+02	2.077E+02	2.083E+02	1.790E+03	-1.193E+00
11000	2.884E+01	2.329E+02	2.542E+02	2.480E+02	2.098E+02	2.104E+02	1.819E+03	-3.360E-01
12000	2.964E+01	2.355E+02	2.835E+02	2.773E+02	2.119E+02	2.124E+02	1.849E+03	3.895E-01
13000	3.016E+01	2.379E+02	3.134E+02	3.072E+02	2.138E+02	2.142E+02	1.881E+03	1.014E+00
14000	3.043E+01	2.401E+02	3.437E+02	3.375E+02	2.156E+02	2.160E+02	1.914E+03	1.558E+00
15000	3.050E+01	2.422E+02	3.742E+02	3.680E+02	2.173E+02	2.177E+02	1.949E+03	2.039E+00
16000	3.041E+01	2.442E+02	4.047E+02	3.985E+02	2.189E+02	2.193E+02	1.983E+03	2.467E+00
17000	3.021E+01	2.460E+02	4.350E+02	4.288E+02	2.204E+02	2.208E+02	2.018E+03	2.851E+00
18000	2.994E+01	2.478E+02	4.651E+02	4.589E+02	2.219E+02	2.223E+02	2.054E+03	3.198E+00
19000	2.965E+01	2.494E+02	4.949E+02	4.887E+02	2.233E+02	2.237E+02	2.089E+03	3.514E+00
20000	2.938E+01	2.509E+02	5.244E+02	5.182E+02	2.247E+02	2.250E+02	2.125E+03	3.804E+00
21000	2.920E+01	2.523E+02	5.536E+02	5.475E+02	2.259E+02	2.262E+02	2.160E+03	4.071E+00
22000	2.918E+01	2.537E+02	5.828E+02	5.766E+02	2.272E+02	2.275E+02	2.196E+03	4.317E+00
23000	2.944E+01	2.550E+02	6.121E+02	6.059E+02	2.283E+02	2.286E+02	2.233E+03	4.545E+00
24000	3.014E+01	2.562E+02	6.418E+02	6.356E+02	2.295E+02	2.298E+02	2.270E+03	4.758E+00
25000	3.149E+01	2.575E+02	6.726E+02	6.664E+02	2.306E+02	2.308E+02	2.308E+03	4.958E+00
26000	3.376E+01	2.588E+02	7.051E+02	6.989E+02	2.316E+02	2.319E+02	2.348E+03	5.145E+00
27000	3.727E+01	2.601E+02	7.405E+02	7.343E+02	2.327E+02	2.329E+02	2.391E+03	5.321E+00
28000	4.237E+01	2.615E+02	7.802E+02	7.740E+02	2.337E+02	2.339E+02	2.438E+03	5.488E+00
29000	4.943E+01	2.631E+02	8.259E+02	8.197E+02	2.347E+02	2.349E+02	2.492E+03	5.646E+00
30000	5.876E+01	2.650E+02	8.798E+02	8.736E+02	2.357E+02	2.358E+02	2.554E+03	5.798E+00
32000	8.489E+01	2.696E+02	1.022E+03	1.016E+03	2.376E+02	2.378E+02	2.712E+03	6.083E+00
34000	1.195E+02	2.757E+02	1.225E+03	1.219E+03	2.397E+02	2.398E+02	2.933E+03	6.354E+00
36000	1.562E+02	2.836E+02	1.501E+03	1.495E+03	2.419E+02	2.421E+02	3.226E+03	6.616E+00
38000	1.846E+02	2.929E+02	1.844E+03	1.838E+03	2.443E+02	2.445E+02	3.586E+03	6.875E+00
40000	1.961E+02	3.027E+02	2.228E+03	2.222E+03	2.470E+02	2.471E+02	3.988E+03	7.135E+00
42000	1.893E+02	3.122E+02	2.616E+03	2.610E+03	2.499E+02	2.500E+02	4.394E+03	7.396E+00
44000	1.694E+02	3.205E+02	2.977E+03	2.970E+03	2.529E+02	2.530E+02	4.772E+03	7.655E+00
46000	1.440E+02	3.275E+02	3.290E+03	3.284E+03	2.560E+02	2.561E+02	5.104E+03	7.910E+00
48000	1.188E+02	3.331E+02	3.553E+03	3.547E+03	2.591E+02	2.592E+02	5.385E+03	8.158E+00
50000	9.701E+01	3.375E+02	3.768E+03	3.762E+03	2.621E+02	2.623E+02	5.619E+03	8.397E+00

Table 181: Internal thermodynamic properties of O^+ ΔE=1000 cm^{-1}

T(K)	Q_{int}	$\ln(Q_{int})$	E_{int}/RT	$C_{p,int}/R$
50	$4.000E+00$	$1.386E+00$	$0.000E+00$	$0.000E+00$
100	$4.000E+00$	$1.386E+00$	$2.672E-165$	$1.031E-162$
150	$4.000E+00$	$1.386E+00$	$1.265E-109$	$3.255E-107$
200	$4.000E+00$	$1.386E+00$	$8.006E-82$	$1.544E-79$
298.15	$4.000E+00$	$1.386E+00$	$2.041E-54$	$2.641E-52$
300	$4.000E+00$	$1.386E+00$	$4.505E-54$	$5.794E-52$
400	$4.000E+00$	$1.386E+00$	$3.105E-40$	$2.995E-38$
500	$4.000E+00$	$1.386E+00$	$5.931E-32$	$4.577E-30$
600	$4.000E+00$	$1.386E+00$	$1.902E-26$	$1.223E-24$
700	$4.000E+00$	$1.386E+00$	$1.592E-22$	$8.774E-21$
800	$4.000E+00$	$1.386E+00$	$1.368E-19$	$6.597E-18$
900	$4.000E+00$	$1.386E+00$	$2.583E-17$	$1.107E-15$
1000	$4.000E+00$	$1.386E+00$	$1.691E-15$	$6.525E-14$
2000	$4.000E+00$	$1.386E+00$	$2.019E-07$	$3.896E-06$
3000	$4.000E+00$	$1.386E+00$	$8.363E-05$	$1.076E-03$
4000	$4.001E+00$	$1.386E+00$	$1.571E-03$	$1.520E-02$
5000	$4.005E+00$	$1.387E+00$	$8.736E-03$	$6.793E-02$
6000	$4.016E+00$	$1.390E+00$	$2.669E-02$	$1.738E-01$
7000	$4.042E+00$	$1.397E+00$	$5.809E-02$	$3.253E-01$
8000	$4.085E+00$	$1.407E+00$	$1.024E-01$	$5.013E-01$
9000	$4.147E+00$	$1.422E+00$	$1.566E-01$	$6.786E-01$
10000	$4.229E+00$	$1.442E+00$	$2.170E-01$	$8.383E-01$
11000	$4.330E+00$	$1.466E+00$	$2.797E-01$	$9.686E-01$
12000	$4.448E+00$	$1.493E+00$	$3.413E-01$	$1.065E+00$
13000	$4.582E+00$	$1.522E+00$	$3.996E-01$	$1.127E+00$
14000	$4.729E+00$	$1.554E+00$	$4.529E-01$	$1.160E+00$
15000	$4.888E+00$	$1.587E+00$	$5.005E-01$	$1.168E+00$
16000	$5.055E+00$	$1.620E+00$	$5.419E-01$	$1.157E+00$
17000	$5.229E+00$	$1.654E+00$	$5.775E-01$	$1.133E+00$
18000	$5.410E+00$	$1.688E+00$	$6.074E-01$	$1.100E+00$
19000	$5.594E+00$	$1.722E+00$	$6.324E-01$	$1.063E+00$
20000	$5.782E+00$	$1.755E+00$	$6.529E-01$	$1.025E+00$
21000	$5.971E+00$	$1.787E+00$	$6.698E-01$	$9.916E-01$
22000	$6.162E+00$	$1.818E+00$	$6.839E-01$	$9.672E-01$
23000	$6.354E+00$	$1.849E+00$	$6.959E-01$	$9.580E-01$
24000	$6.547E+00$	$1.879E+00$	$7.070E-01$	$9.722E-01$
25000	$6.740E+00$	$1.908E+00$	$7.185E-01$	$1.020E+00$
26000	$6.934E+00$	$1.936E+00$	$7.317E-01$	$1.115E+00$
27000	$7.131E+00$	$1.964E+00$	$7.486E-01$	$1.271E+00$
28000	$7.330E+00$	$1.992E+00$	$7.712E-01$	$1.509E+00$
29000	$7.535E+00$	$2.020E+00$	$8.022E-01$	$1.847E+00$
30000	$7.748E+00$	$2.047E+00$	$8.443E-01$	$2.307E+00$
32000	$8.213E+00$	$2.106E+00$	$9.748E-01$	$3.664E+00$
34000	$8.765E+00$	$2.171E+00$	$1.189E+00$	$5.676E+00$
36000	$9.462E+00$	$2.247E+00$	$1.508E+00$	$8.281E+00$
38000	$1.038E+01$	$2.340E+00$	$1.941E+00$	$1.119E+01$
40000	$1.162E+01$	$2.453E+00$	$2.473E+00$	$1.388E+01$
42000	$1.330E+01$	$2.587E+00$	$3.066E+00$	$1.582E+01$
44000	$1.555E+01$	$2.744E+00$	$3.669E+00$	$1.663E+01$
46000	$1.854E+01$	$2.920E+00$	$4.228E+00$	$1.628E+01$
48000	$2.242E+01$	$3.110E+00$	$4.707E+00$	$1.502E+01$
50000	$2.739E+01$	$3.310E+00$	$5.085E+00$	$1.325E+01$

Table 182: Total thermodynamic properties of O^+ ΔE=1000 cm^{-1}

T [K]	C_p [J/mol/K]	S^0 [J/mol/K]	$H^0(T)$-$H^0(0)$ [KJ/mol]	$H^0(T)$-$H^0(298)$ [KJ/mol]	-(G^0-$H^0(0)$)/T [J/mol/K]	-(G^0-$H^0(298)$)/T [J/mol/K]	ΔH_f [KJ/mol]	Log(K_p)
50	2.079E+01	1.178E+02	1.039E+00	-5.158E+00	9.706E+01	2.210E+02	1.562E+03	-1.630E+03
100	2.079E+01	1.322E+02	2.079E+00	-4.119E+00	1.115E+02	1.734E+02	1.563E+03	-8.143E+02
150	2.079E+01	1.407E+02	3.118E+00	-3.079E+00	1.199E+02	1.612E+02	1.565E+03	-5.420E+02
200	2.079E+01	1.467E+02	4.157E+00	-2.040E+00	1.259E+02	1.569E+02	1.566E+03	-4.058E+02
298.15	2.079E+01	1.550E+02	6.197E+00	0.000E+00	1.342E+02	1.550E+02	1.569E+03	-2.710E+02
300	2.079E+01	1.551E+02	6.236E+00	3.848E-02	1.343E+02	1.550E+02	1.569E+03	-2.693E+02
400	2.079E+01	1.611E+02	8.315E+00	2.117E+00	1.403E+02	1.558E+02	1.572E+03	-2.010E+02
500	2.079E+01	1.657E+02	1.039E+01	4.196E+00	1.449E+02	1.573E+02	1.574E+03	-1.599E+02
600	2.079E+01	1.695E+02	1.247E+01	6.274E+00	1.487E+02	1.590E+02	1.577E+03	-1.325E+02
700	2.079E+01	1.727E+02	1.455E+01	8.353E+00	1.519E+02	1.608E+02	1.579E+03	-1.128E+02
800	2.079E+01	1.755E+02	1.663E+01	1.043E+01	1.547E+02	1.624E+02	1.582E+03	-9.810E+01
900	2.079E+01	1.779E+02	1.871E+01	1.251E+01	1.571E+02	1.640E+02	1.584E+03	-8.662E+01
1000	2.079E+01	1.801E+02	2.079E+01	1.459E+01	1.593E+02	1.655E+02	1.587E+03	-7.742E+01
2000	2.079E+01	1.945E+02	4.157E+01	3.538E+01	1.737E+02	1.768E+02	1.610E+03	-3.574E+01
3000	2.080E+01	2.029E+02	6.236E+01	5.616E+01	1.822E+02	1.842E+02	1.632E+03	-2.164E+01
4000	2.091E+01	2.089E+02	8.320E+01	7.700E+01	1.882E+02	1.897E+02	1.653E+03	-1.450E+01
5000	2.135E+01	2.137E+02	1.043E+02	9.810E+01	1.928E+02	1.940E+02	1.674E+03	-1.016E+01
6000	2.223E+01	2.176E+02	1.260E+02	1.198E+02	1.966E+02	1.976E+02	1.695E+03	-7.224E+00
7000	2.349E+01	2.211E+02	1.489E+02	1.427E+02	1.999E+02	2.008E+02	1.716E+03	-5.104E+00
8000	2.495E+01	2.244E+02	1.731E+02	1.669E+02	2.027E+02	2.035E+02	1.739E+03	-3.493E+00
9000	2.643E+01	2.274E+02	1.988E+02	1.926E+02	2.053E+02	2.060E+02	1.764E+03	-2.223E+00
10000	2.776E+01	2.302E+02	2.259E+02	2.197E+02	2.077E+02	2.083E+02	1.790E+03	-1.193E+00
11000	2.884E+01	2.329E+02	2.542E+02	2.480E+02	2.098E+02	2.104E+02	1.819E+03	-3.360E-01
12000	2.964E+01	2.355E+02	2.835E+02	2.773E+02	2.119E+02	2.124E+02	1.849E+03	3.895E-01
13000	3.016E+01	2.379E+02	3.134E+02	3.072E+02	2.138E+02	2.142E+02	1.881E+03	1.014E+00
14000	3.043E+01	2.401E+02	3.437E+02	3.375E+02	2.156E+02	2.160E+02	1.914E+03	1.558E+00
15000	3.050E+01	2.422E+02	3.742E+02	3.680E+02	2.173E+02	2.177E+02	1.949E+03	2.039E+00
16000	3.041E+01	2.442E+02	4.047E+02	3.985E+02	2.189E+02	2.193E+02	1.983E+03	2.467E+00
17000	3.020E+01	2.460E+02	4.350E+02	4.288E+02	2.204E+02	2.208E+02	2.018E+03	2.851E+00
18000	2.993E+01	2.478E+02	4.651E+02	4.589E+02	2.219E+02	2.223E+02	2.054E+03	3.198E+00
19000	2.962E+01	2.494E+02	4.948E+02	4.886E+02	2.233E+02	2.237E+02	2.089E+03	3.514E+00
20000	2.931E+01	2.509E+02	5.243E+02	5.181E+02	2.247E+02	2.250E+02	2.125E+03	3.804E+00
21000	2.903E+01	2.523E+02	5.535E+02	5.473E+02	2.259E+02	2.262E+02	2.160E+03	4.071E+00
22000	2.883E+01	2.537E+02	5.824E+02	5.762E+02	2.272E+02	2.274E+02	2.196E+03	4.317E+00
23000	2.875E+01	2.549E+02	6.112E+02	6.050E+02	2.283E+02	2.286E+02	2.232E+03	4.545E+00
24000	2.887E+01	2.561E+02	6.400E+02	6.338E+02	2.295E+02	2.297E+02	2.268E+03	4.758E+00
25000	2.927E+01	2.573E+02	6.690E+02	6.628E+02	2.306E+02	2.308E+02	2.304E+03	4.957E+00
26000	3.005E+01	2.585E+02	6.986E+02	6.924E+02	2.316E+02	2.319E+02	2.341E+03	5.144E+00
27000	3.136E+01	2.596E+02	7.293E+02	7.231E+02	2.326E+02	2.329E+02	2.380E+03	5.319E+00
28000	3.333E+01	2.608E+02	7.616E+02	7.554E+02	2.336E+02	2.338E+02	2.420E+03	5.485E+00
29000	3.615E+01	2.620E+02	7.962E+02	7.900E+02	2.346E+02	2.348E+02	2.462E+03	5.642E+00
30000	3.997E+01	2.633E+02	8.342E+02	8.280E+02	2.355E+02	2.357E+02	2.508E+03	5.791E+00
32000	5.125E+01	2.662E+02	9.245E+02	9.183E+02	2.373E+02	2.375E+02	2.615E+03	6.070E+00
34000	6.798E+01	2.698E+02	1.043E+03	1.037E+03	2.392E+02	2.393E+02	2.750E+03	6.327E+00
36000	8.964E+01	2.743E+02	1.200E+03	1.194E+03	2.410E+02	2.412E+02	2.924E+03	6.569E+00
38000	1.138E+02	2.798E+02	1.403E+03	1.397E+03	2.429E+02	2.430E+02	3.145E+03	6.800E+00
40000	1.362E+02	2.862E+02	1.654E+03	1.648E+03	2.449E+02	2.450E+02	3.413E+03	7.025E+00
42000	1.523E+02	2.933E+02	1.944E+03	1.938E+03	2.470E+02	2.472E+02	3.721E+03	7.246E+00
44000	1.590E+02	3.006E+02	2.257E+03	2.250E+03	2.493E+02	2.494E+02	4.052E+03	7.466E+00
46000	1.561E+02	3.076E+02	2.573E+03	2.567E+03	2.517E+02	2.518E+02	4.387E+03	7.684E+00
48000	1.457E+02	3.141E+02	2.876E+03	2.870E+03	2.541E+02	2.543E+02	4.708E+03	7.899E+00
50000	1.310E+02	3.197E+02	3.153E+03	3.147E+03	2.566E+02	2.568E+02	5.004E+03	8.110E+00

Table 183: Internal thermodynamic properties of O^{2+} ΔE=250 cm^{-1}

T(K)	Q_{int}	$\ln(Q_{int})$	E_{int}/RT	$C_{p,int}/R$
50	$1.116E+00$	$1.093E-01$	$3.416E-01$	$1.030E+00$
100	$1.647E+00$	$4.992E-01$	$7.434E-01$	$1.112E+00$
150	$2.275E+00$	$8.218E-01$	$8.245E-01$	$8.497E-01$
200	$2.877E+00$	$1.057E+00$	$7.983E-01$	$6.011E-01$
298.15	$3.873E+00$	$1.354E+00$	$6.801E-01$	$3.155E-01$
300	$3.890E+00$	$1.358E+00$	$6.778E-01$	$3.120E-01$
400	$4.654E+00$	$1.538E+00$	$5.682E-01$	$1.825E-01$
500	$5.233E+00$	$1.655E+00$	$4.839E-01$	$1.179E-01$
600	$5.682E+00$	$1.737E+00$	$4.196E-01$	$8.189E-02$
700	$6.038E+00$	$1.798E+00$	$3.697E-01$	$5.999E-02$
800	$6.326E+00$	$1.845E+00$	$3.300E-01$	$4.575E-02$
900	$6.564E+00$	$1.882E+00$	$2.979E-01$	$3.600E-02$
1000	$6.764E+00$	$1.912E+00$	$2.713E-01$	$2.905E-02$
2000	$7.775E+00$	$2.051E+00$	$1.428E-01$	$7.148E-03$
3000	$8.157E+00$	$2.099E+00$	$9.715E-02$	$6.521E-03$
4000	$8.361E+00$	$2.124E+00$	$7.612E-02$	$2.297E-02$
5000	$8.496E+00$	$2.140E+00$	$6.878E-02$	$5.856E-02$
6000	$8.604E+00$	$2.152E+00$	$7.087E-02$	$1.049E-01$
7000	$8.703E+00$	$2.164E+00$	$7.915E-02$	$1.523E-01$
8000	$8.802E+00$	$2.175E+00$	$9.102E-02$	$1.948E-01$
9000	$8.904E+00$	$2.186E+00$	$1.046E-01$	$2.300E-01$
10000	$9.009E+00$	$2.198E+00$	$1.186E-01$	$2.583E-01$
11000	$9.117E+00$	$2.210E+00$	$1.323E-01$	$2.806E-01$
12000	$9.228E+00$	$2.222E+00$	$1.455E-01$	$2.983E-01$
13000	$9.341E+00$	$2.234E+00$	$1.578E-01$	$3.127E-01$
14000	$9.455E+00$	$2.247E+00$	$1.693E-01$	$3.248E-01$
15000	$9.569E+00$	$2.259E+00$	$1.800E-01$	$3.352E-01$
16000	$9.684E+00$	$2.271E+00$	$1.900E-01$	$3.447E-01$
17000	$9.799E+00$	$2.282E+00$	$1.994E-01$	$3.536E-01$
18000	$9.914E+00$	$2.294E+00$	$2.082E-01$	$3.624E-01$
19000	$1.003E+01$	$2.305E+00$	$2.165E-01$	$3.713E-01$
20000	$1.014E+01$	$2.317E+00$	$2.245E-01$	$3.805E-01$
21000	$1.026E+01$	$2.328E+00$	$2.322E-01$	$3.904E-01$
22000	$1.037E+01$	$2.339E+00$	$2.396E-01$	$4.009E-01$
23000	$1.048E+01$	$2.350E+00$	$2.469E-01$	$4.122E-01$
24000	$1.059E+01$	$2.360E+00$	$2.540E-01$	$4.245E-01$
25000	$1.071E+01$	$2.371E+00$	$2.611E-01$	$4.377E-01$
26000	$1.082E+01$	$2.381E+00$	$2.681E-01$	$4.522E-01$
27000	$1.093E+01$	$2.391E+00$	$2.753E-01$	$4.683E-01$
28000	$1.104E+01$	$2.402E+00$	$2.825E-01$	$4.867E-01$
29000	$1.115E+01$	$2.412E+00$	$2.899E-01$	$5.086E-01$
30000	$1.126E+01$	$2.422E+00$	$2.976E-01$	$5.359E-01$
32000	$1.149E+01$	$2.441E+00$	$3.149E-01$	$6.206E-01$
34000	$1.172E+01$	$2.461E+00$	$3.372E-01$	$7.861E-01$
36000	$1.196E+01$	$2.481E+00$	$3.703E-01$	$1.118E+00$
38000	$1.221E+01$	$2.503E+00$	$4.247E-01$	$1.756E+00$
40000	$1.251E+01$	$2.526E+00$	$5.174E-01$	$2.907E+00$
42000	$1.287E+01$	$2.555E+00$	$6.733E-01$	$4.827E+00$
44000	$1.335E+01$	$2.592E+00$	$9.246E-01$	$7.760E+00$
46000	$1.403E+01$	$2.641E+00$	$1.306E+00$	$1.182E+01$
48000	$1.499E+01$	$2.707E+00$	$1.845E+00$	$1.679E+01$
50000	$1.638E+01$	$2.796E+00$	$2.548E+00$	$2.202E+01$

Table 184: Total thermodynamic properties of O^{2+} ΔE=250 cm^{-1}

T [K]	C_p [J/mol/K]	S^0 [J/mol/K]	$H^0(T)-H^0(0)$ [KJ/mol]	$H^0(T)-H^0(298)$ [KJ/mol]	$-(G^0-H^0(0))/T$ [J/mol/K]	$-(G^0-H^0(298))/T$ [J/mol/K]	ΔH_f [KJ/mol]	$Log(K_p)$
50	2.935E+01	1.101E+02	1.181E+00	-6.702E+00	8.644E+01	2.441E+02	4.955E+03	-5.176E+03
100	3.003E+01	1.311E+02	2.697E+00	-5.187E+00	1.041E+02	1.829E+02	4.958E+03	-2.588E+03
150	2.785E+01	1.428E+02	4.146E+00	-3.737E+00	1.152E+02	1.678E+02	4.961E+03	-1.724E+03
200	2.578E+01	1.506E+02	5.485E+00	-2.399E+00	1.231E+02	1.626E+02	4.964E+03	-1.292E+03
298.15	2.341E+01	1.603E+02	7.883E+00	0.000E+00	1.339E+02	1.603E+02	4.969E+03	-8.653E+02
300	2.338E+01	1.605E+02	7.926E+00	4.325E-02	1.341E+02	1.603E+02	4.969E+03	-8.599E+02
400	2.230E+01	1.671E+02	1.020E+01	2.321E+00	1.415E+02	1.612E+02	4.974E+03	-6.435E+02
500	2.177E+01	1.720E+02	1.240E+01	4.521E+00	1.472E+02	1.629E+02	4.978E+03	-5.136E+02
600	2.147E+01	1.759E+02	1.456E+01	6.682E+00	1.516E+02	1.648E+02	4.983E+03	-4.268E+02
700	2.129E+01	1.792E+02	1.670E+01	8.819E+00	1.553E+02	1.666E+02	4.988E+03	-3.648E+02
800	2.117E+01	1.820E+02	1.882E+01	1.094E+01	1.585E+02	1.684E+02	4.993E+03	-3.183E+02
900	2.109E+01	1.845E+02	2.094E+01	1.305E+01	1.613E+02	1.700E+02	4.997E+03	-2.821E+02
1000	2.103E+01	1.867E+02	2.304E+01	1.516E+01	1.637E+02	1.716E+02	5.002E+03	-2.530E+02
2000	2.085E+01	2.012E+02	4.395E+01	3.606E+01	1.793E+02	1.832E+02	5.046E+03	-1.220E+02
3000	2.084E+01	2.097E+02	6.478E+01	5.690E+01	1.881E+02	1.907E+02	5.089E+03	-7.788E+01
4000	2.098E+01	2.157E+02	8.568E+01	7.779E+01	1.943E+02	1.962E+02	5.131E+03	-5.564E+01
5000	2.127E+01	2.204E+02	1.068E+02	9.891E+01	1.991E+02	2.006E+02	5.172E+03	-4.219E+01
6000	2.166E+01	2.243E+02	1.282E+02	1.204E+02	2.029E+02	2.042E+02	5.214E+03	-3.315E+01
7000	2.205E+01	2.277E+02	1.501E+02	1.422E+02	2.062E+02	2.074E+02	5.255E+03	-2.664E+01
8000	2.241E+01	2.307E+02	1.723E+02	1.645E+02	2.091E+02	2.101E+02	5.296E+03	-2.173E+01
9000	2.270E+01	2.333E+02	1.949E+02	1.870E+02	2.117E+02	2.125E+02	5.339E+03	-1.787E+01
10000	2.293E+01	2.357E+02	2.177E+02	2.098E+02	2.139E+02	2.147E+02	5.382E+03	-1.476E+01
11000	2.312E+01	2.379E+02	2.408E+02	2.329E+02	2.160E+02	2.167E+02	5.426E+03	-1.219E+01
12000	2.327E+01	2.399E+02	2.639E+02	2.561E+02	2.179E+02	2.186E+02	5.471E+03	-1.004E+01
13000	2.339E+01	2.418E+02	2.873E+02	2.794E+02	2.197E+02	2.203E+02	5.517E+03	-8.197E+00
14000	2.349E+01	2.435E+02	3.107E+02	3.028E+02	2.213E+02	2.219E+02	5.564E+03	-6.607E+00
15000	2.357E+01	2.452E+02	3.342E+02	3.264E+02	2.229E+02	2.234E+02	5.612E+03	-5.217E+00
16000	2.365E+01	2.467E+02	3.579E+02	3.500E+02	2.243E+02	2.248E+02	5.661E+03	-3.990E+00
17000	2.373E+01	2.481E+02	3.816E+02	3.737E+02	2.257E+02	2.261E+02	5.710E+03	-2.899E+00
18000	2.380E+01	2.495E+02	4.053E+02	3.974E+02	2.270E+02	2.274E+02	5.760E+03	-1.920E+00
19000	2.387E+01	2.508E+02	4.291E+02	4.213E+02	2.282E+02	2.286E+02	5.810E+03	-1.036E+00
20000	2.395E+01	2.520E+02	4.531E+02	4.452E+02	2.293E+02	2.297E+02	5.861E+03	-2.341E-01
21000	2.403E+01	2.532E+02	4.771E+02	4.692E+02	2.304E+02	2.308E+02	5.912E+03	4.979E-01
22000	2.412E+01	2.543E+02	5.011E+02	4.932E+02	2.315E+02	2.319E+02	5.964E+03	1.169E+00
23000	2.421E+01	2.553E+02	5.253E+02	5.174E+02	2.325E+02	2.329E+02	6.016E+03	1.788E+00
24000	2.432E+01	2.564E+02	5.495E+02	5.417E+02	2.335E+02	2.338E+02	6.068E+03	2.359E+00
25000	2.443E+01	2.574E+02	5.739E+02	5.660E+02	2.344E+02	2.347E+02	6.121E+03	2.890E+00
26000	2.455E+01	2.583E+02	5.984E+02	5.905E+02	2.353E+02	2.356E+02	6.173E+03	3.384E+00
27000	2.468E+01	2.593E+02	6.230E+02	6.151E+02	2.362E+02	2.365E+02	6.226E+03	3.845E+00
28000	2.483E+01	2.602E+02	6.478E+02	6.399E+02	2.370E+02	2.373E+02	6.280E+03	4.277E+00
29000	2.502E+01	2.610E+02	6.727E+02	6.648E+02	2.378E+02	2.381E+02	6.334E+03	4.683E+00
30000	2.524E+01	2.619E+02	6.978E+02	6.899E+02	2.386E+02	2.389E+02	6.388E+03	5.064E+00
32000	2.595E+01	2.636E+02	7.489E+02	7.410E+02	2.401E+02	2.404E+02	6.497E+03	5.765E+00
34000	2.732E+01	2.651E+02	8.020E+02	7.942E+02	2.416E+02	2.418E+02	6.608E+03	6.394E+00
36000	3.008E+01	2.668E+02	8.591E+02	8.512E+02	2.429E+02	2.431E+02	6.724E+03	6.963E+00
38000	3.539E+01	2.685E+02	9.240E+02	9.162E+02	2.442E+02	2.444E+02	6.848E+03	7.481E+00
40000	4.496E+01	2.706E+02	1.004E+03	9.956E+02	2.455E+02	2.457E+02	6.987E+03	7.957E+00
42000	6.092E+01	2.731E+02	1.108E+03	1.100E+03	2.467E+02	2.469E+02	7.151E+03	8.396E+00
44000	8.531E+01	2.765E+02	1.253E+03	1.245E+03	2.480E+02	2.482E+02	7.355E+03	8.806E+00
46000	1.190E+02	2.810E+02	1.456E+03	1.448E+03	2.493E+02	2.495E+02	7.618E+03	9.191E+00
48000	1.604E+02	2.869E+02	1.734E+03	1.726E+03	2.508E+02	2.509E+02	7.956E+03	9.559E+00
50000	2.039E+02	2.943E+02	2.099E+03	2.091E+03	2.524E+02	2.525E+02	8.381E+03	9.915E+00

Table 185: Internal thermodynamic properties of O^{2+} ΔE=500 cm^{-1}

T(K)	Q_{int}	$\ln(Q_{int})$	E_{int}/RT	$C_{p,int}/R$
50	$1.116E+00$	$1.093E-01$	$3.416E-01$	$1.030E+00$
100	$1.647E+00$	$4.992E-01$	$7.434E-01$	$1.112E+00$
150	$2.275E+00$	$8.218E-01$	$8.245E-01$	$8.497E-01$
200	$2.877E+00$	$1.057E+00$	$7.983E-01$	$6.011E-01$
298.15	$3.873E+00$	$1.354E+00$	$6.801E-01$	$3.155E-01$
300	$3.890E+00$	$1.358E+00$	$6.778E-01$	$3.120E-01$
400	$4.654E+00$	$1.538E+00$	$5.682E-01$	$1.825E-01$
500	$5.233E+00$	$1.655E+00$	$4.839E-01$	$1.179E-01$
600	$5.682E+00$	$1.737E+00$	$4.196E-01$	$8.189E-02$
700	$6.038E+00$	$1.798E+00$	$3.697E-01$	$5.999E-02$
800	$6.326E+00$	$1.845E+00$	$3.300E-01$	$4.575E-02$
900	$6.564E+00$	$1.882E+00$	$2.979E-01$	$3.600E-02$
1000	$6.764E+00$	$1.912E+00$	$2.713E-01$	$2.905E-02$
2000	$7.775E+00$	$2.051E+00$	$1.428E-01$	$7.148E-03$
3000	$8.157E+00$	$2.099E+00$	$9.715E-02$	$6.521E-03$
4000	$8.361E+00$	$2.124E+00$	$7.612E-02$	$2.297E-02$
5000	$8.496E+00$	$2.140E+00$	$6.878E-02$	$5.856E-02$
6000	$8.604E+00$	$2.152E+00$	$7.087E-02$	$1.049E-01$
7000	$8.703E+00$	$2.164E+00$	$7.915E-02$	$1.523E-01$
8000	$8.802E+00$	$2.175E+00$	$9.102E-02$	$1.948E-01$
9000	$8.904E+00$	$2.186E+00$	$1.046E-01$	$2.300E-01$
10000	$9.009E+00$	$2.198E+00$	$1.186E-01$	$2.583E-01$
11000	$9.117E+00$	$2.210E+00$	$1.323E-01$	$2.806E-01$
12000	$9.228E+00$	$2.222E+00$	$1.455E-01$	$2.983E-01$
13000	$9.341E+00$	$2.234E+00$	$1.578E-01$	$3.127E-01$
14000	$9.455E+00$	$2.247E+00$	$1.693E-01$	$3.248E-01$
15000	$9.569E+00$	$2.259E+00$	$1.800E-01$	$3.352E-01$
16000	$9.684E+00$	$2.271E+00$	$1.900E-01$	$3.447E-01$
17000	$9.799E+00$	$2.282E+00$	$1.994E-01$	$3.536E-01$
18000	$9.914E+00$	$2.294E+00$	$2.082E-01$	$3.624E-01$
19000	$1.003E+01$	$2.305E+00$	$2.165E-01$	$3.713E-01$
20000	$1.014E+01$	$2.317E+00$	$2.245E-01$	$3.805E-01$
21000	$1.026E+01$	$2.328E+00$	$2.322E-01$	$3.904E-01$
22000	$1.037E+01$	$2.339E+00$	$2.396E-01$	$4.009E-01$
23000	$1.048E+01$	$2.350E+00$	$2.469E-01$	$4.122E-01$
24000	$1.059E+01$	$2.360E+00$	$2.540E-01$	$4.244E-01$
25000	$1.071E+01$	$2.371E+00$	$2.611E-01$	$4.374E-01$
26000	$1.082E+01$	$2.381E+00$	$2.681E-01$	$4.514E-01$
27000	$1.093E+01$	$2.391E+00$	$2.752E-01$	$4.665E-01$
28000	$1.104E+01$	$2.402E+00$	$2.823E-01$	$4.829E-01$
29000	$1.115E+01$	$2.412E+00$	$2.895E-01$	$5.010E-01$
30000	$1.126E+01$	$2.422E+00$	$2.969E-01$	$5.214E-01$
32000	$1.149E+01$	$2.441E+00$	$3.125E-01$	$5.736E-01$
34000	$1.171E+01$	$2.461E+00$	$3.300E-01$	$6.551E-01$
36000	$1.194E+01$	$2.480E+00$	$3.516E-01$	$7.952E-01$
38000	$1.218E+01$	$2.500E+00$	$3.809E-01$	$1.043E+00$
40000	$1.243E+01$	$2.520E+00$	$4.238E-01$	$1.475E+00$
42000	$1.271E+01$	$2.543E+00$	$4.895E-01$	$2.190E+00$
44000	$1.303E+01$	$2.568E+00$	$5.905E-01$	$3.312E+00$
46000	$1.342E+01$	$2.597E+00$	$7.426E-01$	$4.963E+00$
48000	$1.391E+01$	$2.633E+00$	$9.635E-01$	$7.230E+00$
50000	$1.456E+01$	$2.678E+00$	$1.270E+00$	$1.011E+01$

Table 186: Total thermodynamic properties of O^{2+} ΔE=500 cm^{-1}

T [K]	C_p [J/mol/K]	S^0 [J/mol/K]	$H^0(T)$-$H^0(0)$ [KJ/mol]	$H^0(T)$-$H^0(298)$ [KJ/mol]	-(G^0-$H^0(0)$)/T [J/mol/K]	-(G^0-$H^0(298)$)/T [J/mol/K]	ΔH_f [KJ/mol]	Log(K_p)
50	2.935E+01	1.101E+02	1.181E+00	-6.702E+00	8.644E+01	2.441E+02	4.955E+03	-5.176E+03
100	3.003E+01	1.311E+02	2.697E+00	-5.187E+00	1.041E+02	1.829E+02	4.958E+03	-2.588E+03
150	2.785E+01	1.428E+02	4.146E+00	-3.737E+00	1.152E+02	1.678E+02	4.961E+03	-1.724E+03
200	2.578E+01	1.506E+02	5.485E+00	-2.399E+00	1.231E+02	1.626E+02	4.964E+03	-1.292E+03
298.15	2.341E+01	1.603E+02	7.883E+00	0.000E+00	1.339E+02	1.603E+02	4.969E+03	-8.653E+02
300	2.338E+01	1.605E+02	7.926E+00	4.325E-02	1.341E+02	1.603E+02	4.969E+03	-8.599E+02
400	2.230E+01	1.671E+02	1.020E+01	2.321E+00	1.415E+02	1.612E+02	4.974E+03	-6.435E+02
500	2.177E+01	1.720E+02	1.240E+01	4.521E+00	1.472E+02	1.629E+02	4.978E+03	-5.136E+02
600	2.147E+01	1.759E+02	1.456E+01	6.682E+00	1.516E+02	1.648E+02	4.983E+03	-4.268E+02
700	2.129E+01	1.792E+02	1.670E+01	8.819E+00	1.553E+02	1.666E+02	4.988E+03	-3.648E+02
800	2.117E+01	1.820E+02	1.882E+01	1.094E+01	1.585E+02	1.684E+02	4.993E+03	-3.183E+02
900	2.109E+01	1.845E+02	2.094E+01	1.305E+01	1.613E+02	1.700E+02	4.997E+03	-2.821E+02
1000	2.103E+01	1.867E+02	2.304E+01	1.516E+01	1.637E+02	1.716E+02	5.002E+03	-2.530E+02
2000	2.085E+01	2.012E+02	4.395E+01	3.606E+01	1.793E+02	1.832E+02	5.046E+03	-1.220E+02
3000	2.084E+01	2.097E+02	6.478E+01	5.690E+01	1.881E+02	1.907E+02	5.089E+03	-7.788E+01
4000	2.098E+01	2.157E+02	8.568E+01	7.779E+01	1.943E+02	1.962E+02	5.131E+03	-5.564E+01
5000	2.127E+01	2.204E+02	1.068E+02	9.891E+01	1.991E+02	2.006E+02	5.172E+03	-4.219E+01
6000	2.166E+01	2.243E+02	1.282E+02	1.204E+02	2.029E+02	2.042E+02	5.214E+03	-3.315E+01
7000	2.205E+01	2.277E+02	1.501E+02	1.422E+02	2.062E+02	2.074E+02	5.255E+03	-2.664E+01
8000	2.241E+01	2.307E+02	1.723E+02	1.645E+02	2.091E+02	2.101E+02	5.296E+03	-2.173E+01
9000	2.270E+01	2.333E+02	1.949E+02	1.870E+02	2.117E+02	2.125E+02	5.339E+03	-1.787E+01
10000	2.293E+01	2.357E+02	2.177E+02	2.098E+02	2.139E+02	2.147E+02	5.382E+03	-1.476E+01
11000	2.312E+01	2.379E+02	2.408E+02	2.329E+02	2.160E+02	2.167E+02	5.426E+03	-1.219E+01
12000	2.327E+01	2.399E+02	2.639E+02	2.561E+02	2.179E+02	2.186E+02	5.471E+03	-1.004E+01
13000	2.339E+01	2.418E+02	2.873E+02	2.794E+02	2.197E+02	2.203E+02	5.517E+03	-8.197E+00
14000	2.349E+01	2.435E+02	3.107E+02	3.028E+02	2.213E+02	2.219E+02	5.564E+03	-6.607E+00
15000	2.357E+01	2.452E+02	3.342E+02	3.264E+02	2.229E+02	2.234E+02	5.612E+03	-5.217E+00
16000	2.365E+01	2.467E+02	3.579E+02	3.500E+02	2.243E+02	2.248E+02	5.661E+03	-3.990E+00
17000	2.373E+01	2.481E+02	3.816E+02	3.737E+02	2.257E+02	2.261E+02	5.710E+03	-2.899E+00
18000	2.380E+01	2.495E+02	4.053E+02	3.974E+02	2.270E+02	2.274E+02	5.760E+03	-1.920E+00
19000	2.387E+01	2.508E+02	4.291E+02	4.213E+02	2.282E+02	2.286E+02	5.810E+03	-1.036E+00
20000	2.395E+01	2.520E+02	4.531E+02	4.452E+02	2.293E+02	2.297E+02	5.861E+03	-2.341E-01
21000	2.403E+01	2.532E+02	4.771E+02	4.692E+02	2.304E+02	2.308E+02	5.912E+03	4.979E-01
22000	2.412E+01	2.543E+02	5.011E+02	4.932E+02	2.315E+02	2.319E+02	5.964E+03	1.169E+00
23000	2.421E+01	2.553E+02	5.253E+02	5.174E+02	2.325E+02	2.329E+02	6.016E+03	1.788E+00
24000	2.432E+01	2.564E+02	5.495E+02	5.417E+02	2.335E+02	2.338E+02	6.068E+03	2.359E+00
25000	2.442E+01	2.574E+02	5.739E+02	5.660E+02	2.344E+02	2.347E+02	6.121E+03	2.890E+00
26000	2.454E+01	2.583E+02	5.984E+02	5.905E+02	2.353E+02	2.356E+02	6.173E+03	3.384E+00
27000	2.466E+01	2.593E+02	6.230E+02	6.151E+02	2.362E+02	2.365E+02	6.226E+03	3.845E+00
28000	2.480E+01	2.602E+02	6.477E+02	6.399E+02	2.370E+02	2.373E+02	6.280E+03	4.277E+00
29000	2.495E+01	2.610E+02	6.726E+02	6.647E+02	2.378E+02	2.381E+02	6.334E+03	4.683E+00
30000	2.512E+01	2.619E+02	6.976E+02	6.898E+02	2.386E+02	2.389E+02	6.387E+03	5.064E+00
32000	2.556E+01	2.635E+02	7.483E+02	7.404E+02	2.401E+02	2.404E+02	6.496E+03	5.765E+00
34000	2.623E+01	2.651E+02	8.000E+02	7.921E+02	2.416E+02	2.418E+02	6.606E+03	6.394E+00
36000	2.740E+01	2.666E+02	8.535E+02	8.457E+02	2.429E+02	2.431E+02	6.718E+03	6.963E+00
38000	2.946E+01	2.681E+02	9.102E+02	9.023E+02	2.442E+02	2.444E+02	6.834E+03	7.480E+00
40000	3.305E+01	2.698E+02	9.724E+02	9.645E+02	2.454E+02	2.456E+02	6.956E+03	7.954E+00
42000	3.899E+01	2.715E+02	1.044E+03	1.036E+03	2.466E+02	2.468E+02	7.087E+03	8.390E+00
44000	4.832E+01	2.735E+02	1.131E+03	1.123E+03	2.478E+02	2.480E+02	7.233E+03	8.795E+00
46000	6.205E+01	2.759E+02	1.240E+03	1.232E+03	2.490E+02	2.492E+02	7.402E+03	9.172E+00
48000	8.090E+01	2.790E+02	1.382E+03	1.374E+03	2.502E+02	2.503E+02	7.604E+03	9.527E+00
50000	1.049E+02	2.827E+02	1.567E+03	1.559E+03	2.514E+02	2.515E+02	7.850E+03	9.863E+00

Table 187: Internal thermodynamic properties of O^{2+} ΔE=1000 cm^{-1}

T(K)	Q_{int}	$\ln(Q_{int})$	E_{int}/RT	$C_{p,int}/R$
50	$1.116E+00$	$1.093E-01$	$3.416E-01$	$1.030E+00$
100	$1.647E+00$	$4.992E-01$	$7.434E-01$	$1.112E+00$
150	$2.275E+00$	$8.218E-01$	$8.245E-01$	$8.497E-01$
200	$2.877E+00$	$1.057E+00$	$7.983E-01$	$6.011E-01$
298.15	$3.873E+00$	$1.354E+00$	$6.801E-01$	$3.155E-01$
300	$3.890E+00$	$1.358E+00$	$6.778E-01$	$3.120E-01$
400	$4.654E+00$	$1.538E+00$	$5.682E-01$	$1.825E-01$
500	$5.233E+00$	$1.655E+00$	$4.839E-01$	$1.179E-01$
600	$5.682E+00$	$1.737E+00$	$4.196E-01$	$8.189E-02$
700	$6.038E+00$	$1.798E+00$	$3.697E-01$	$5.999E-02$
800	$6.326E+00$	$1.845E+00$	$3.300E-01$	$4.575E-02$
900	$6.564E+00$	$1.882E+00$	$2.979E-01$	$3.600E-02$
1000	$6.764E+00$	$1.912E+00$	$2.713E-01$	$2.905E-02$
2000	$7.775E+00$	$2.051E+00$	$1.428E-01$	$7.148E-03$
3000	$8.157E+00$	$2.099E+00$	$9.715E-02$	$6.521E-03$
4000	$8.361E+00$	$2.124E+00$	$7.612E-02$	$2.297E-02$
5000	$8.496E+00$	$2.140E+00$	$6.878E-02$	$5.856E-02$
6000	$8.604E+00$	$2.152E+00$	$7.087E-02$	$1.049E-01$
7000	$8.703E+00$	$2.164E+00$	$7.915E-02$	$1.523E-01$
8000	$8.802E+00$	$2.175E+00$	$9.102E-02$	$1.948E-01$
9000	$8.904E+00$	$2.186E+00$	$1.046E-01$	$2.300E-01$
10000	$9.009E+00$	$2.198E+00$	$1.186E-01$	$2.583E-01$
11000	$9.117E+00$	$2.210E+00$	$1.323E-01$	$2.806E-01$
12000	$9.228E+00$	$2.222E+00$	$1.455E-01$	$2.983E-01$
13000	$9.341E+00$	$2.234E+00$	$1.578E-01$	$3.127E-01$
14000	$9.455E+00$	$2.247E+00$	$1.693E-01$	$3.248E-01$
15000	$9.569E+00$	$2.259E+00$	$1.800E-01$	$3.352E-01$
16000	$9.684E+00$	$2.271E+00$	$1.900E-01$	$3.447E-01$
17000	$9.799E+00$	$2.282E+00$	$1.994E-01$	$3.536E-01$
18000	$9.914E+00$	$2.294E+00$	$2.082E-01$	$3.624E-01$
19000	$1.003E+01$	$2.305E+00$	$2.165E-01$	$3.713E-01$
20000	$1.014E+01$	$2.317E+00$	$2.245E-01$	$3.805E-01$
21000	$1.026E+01$	$2.328E+00$	$2.322E-01$	$3.904E-01$
22000	$1.037E+01$	$2.339E+00$	$2.396E-01$	$4.009E-01$
23000	$1.048E+01$	$2.350E+00$	$2.469E-01$	$4.122E-01$
24000	$1.059E+01$	$2.360E+00$	$2.540E-01$	$4.243E-01$
25000	$1.071E+01$	$2.371E+00$	$2.611E-01$	$4.373E-01$
26000	$1.082E+01$	$2.381E+00$	$2.681E-01$	$4.512E-01$
27000	$1.093E+01$	$2.391E+00$	$2.752E-01$	$4.660E-01$
28000	$1.104E+01$	$2.402E+00$	$2.822E-01$	$4.817E-01$
29000	$1.115E+01$	$2.412E+00$	$2.894E-01$	$4.985E-01$
30000	$1.126E+01$	$2.422E+00$	$2.967E-01$	$5.166E-01$
32000	$1.149E+01$	$2.441E+00$	$3.117E-01$	$5.581E-01$
34000	$1.171E+01$	$2.461E+00$	$3.277E-01$	$6.118E-01$
36000	$1.194E+01$	$2.480E+00$	$3.454E-01$	$6.884E-01$
38000	$1.217E+01$	$2.499E+00$	$3.664E-01$	$8.064E-01$
40000	$1.241E+01$	$2.518E+00$	$3.927E-01$	$9.940E-01$
42000	$1.266E+01$	$2.538E+00$	$4.279E-01$	$1.291E+00$
44000	$1.293E+01$	$2.559E+00$	$4.767E-01$	$1.746E+00$
46000	$1.322E+01$	$2.582E+00$	$5.456E-01$	$2.418E+00$
48000	$1.356E+01$	$2.607E+00$	$6.423E-01$	$3.366E+00$
50000	$1.396E+01$	$2.636E+00$	$7.756E-01$	$4.637E+00$

Table 188: Total thermodynamic properties of O^{2+} ΔE=1000 cm^{-1}

T [K]	C_p [J/mol/K]	S^0 [J/mol/K]	$H^0(T)-H^0(0)$ [KJ/mol]	$H^0(T)-H^0(298)$ [KJ/mol]	$-(G^0-H^0(0))/T$ [J/mol/K]	$-(G^0-H^0(298))/T$ [J/mol/K]	ΔH_f [KJ/mol]	$Log(K_p)$
50	2.935E+01	1.101E+02	1.181E+00	-6.702E+00	8.644E+01	2.441E+02	4.955E+03	-5.176E+03
100	3.003E+01	1.311E+02	2.697E+00	-5.187E+00	1.041E+02	1.829E+02	4.958E+03	-2.588E+03
150	2.785E+01	1.428E+02	4.146E+00	-3.737E+00	1.152E+02	1.678E+02	4.961E+03	-1.724E+03
200	2.578E+01	1.506E+02	5.485E+00	-2.399E+00	1.231E+02	1.626E+02	4.964E+03	-1.292E+03
298.15	2.341E+01	1.603E+02	7.883E+00	0.000E+00	1.339E+02	1.603E+02	4.969E+03	-8.653E+02
300	2.338E+01	1.605E+02	7.926E+00	4.325E-02	1.341E+02	1.603E+02	4.969E+03	-8.599E+02
400	2.230E+01	1.671E+02	1.020E+01	2.321E+00	1.415E+02	1.612E+02	4.974E+03	-6.435E+02
500	2.177E+01	1.720E+02	1.240E+01	4.521E+00	1.472E+02	1.629E+02	4.978E+03	-5.136E+02
600	2.147E+01	1.759E+02	1.456E+01	6.682E+00	1.516E+02	1.648E+02	4.983E+03	-4.268E+02
700	2.129E+01	1.792E+02	1.670E+01	8.819E+00	1.553E+02	1.666E+02	4.988E+03	-3.648E+02
800	2.117E+01	1.820E+02	1.882E+01	1.094E+01	1.585E+02	1.684E+02	4.993E+03	-3.183E+02
900	2.109E+01	1.845E+02	2.094E+01	1.305E+01	1.613E+02	1.700E+02	4.997E+03	-2.821E+02
1000	2.103E+01	1.867E+02	2.304E+01	1.516E+01	1.637E+02	1.716E+02	5.002E+03	-2.530E+02
2000	2.085E+01	2.012E+02	4.395E+01	3.606E+01	1.793E+02	1.832E+02	5.046E+03	-1.220E+02
3000	2.084E+01	2.097E+02	6.478E+01	5.690E+01	1.881E+02	1.907E+02	5.089E+03	-7.788E+01
4000	2.098E+01	2.157E+02	8.568E+01	7.779E+01	1.943E+02	1.962E+02	5.131E+03	-5.564E+01
5000	2.127E+01	2.204E+02	1.068E+02	9.891E+01	1.991E+02	2.006E+02	5.172E+03	-4.219E+01
6000	2.166E+01	2.243E+02	1.282E+02	1.204E+02	2.029E+02	2.042E+02	5.214E+03	-3.315E+01
7000	2.205E+01	2.277E+02	1.501E+02	1.422E+02	2.062E+02	2.074E+02	5.255E+03	-2.664E+01
8000	2.241E+01	2.307E+02	1.723E+02	1.645E+02	2.091E+02	2.101E+02	5.296E+03	-2.173E+01
9000	2.270E+01	2.333E+02	1.949E+02	1.870E+02	2.117E+02	2.125E+02	5.339E+03	-1.787E+01
10000	2.293E+01	2.357E+02	2.177E+02	2.098E+02	2.139E+02	2.147E+02	5.382E+03	-1.476E+01
11000	2.312E+01	2.379E+02	2.408E+02	2.329E+02	2.160E+02	2.167E+02	5.426E+03	-1.219E+01
12000	2.327E+01	2.399E+02	2.639E+02	2.561E+02	2.179E+02	2.186E+02	5.471E+03	-1.004E+01
13000	2.339E+01	2.418E+02	2.873E+02	2.794E+02	2.197E+02	2.203E+02	5.517E+03	-8.197E+00
14000	2.349E+01	2.435E+02	3.107E+02	3.028E+02	2.213E+02	2.219E+02	5.564E+03	-6.607E+00
15000	2.357E+01	2.452E+02	3.342E+02	3.264E+02	2.229E+02	2.234E+02	5.612E+03	-5.217E+00
16000	2.365E+01	2.467E+02	3.579E+02	3.500E+02	2.243E+02	2.248E+02	5.661E+03	-3.990E+00
17000	2.373E+01	2.481E+02	3.816E+02	3.737E+02	2.257E+02	2.261E+02	5.710E+03	-2.899E+00
18000	2.380E+01	2.495E+02	4.053E+02	3.974E+02	2.270E+02	2.274E+02	5.760E+03	-1.920E+00
19000	2.387E+01	2.508E+02	4.291E+02	4.213E+02	2.282E+02	2.286E+02	5.810E+03	-1.036E+00
20000	2.395E+01	2.520E+02	4.531E+02	4.452E+02	2.293E+02	2.297E+02	5.861E+03	-2.341E-01
21000	2.403E+01	2.532E+02	4.771E+02	4.692E+02	2.304E+02	2.308E+02	5.912E+03	4.979E-01
22000	2.412E+01	2.543E+02	5.011E+02	4.932E+02	2.315E+02	2.319E+02	5.964E+03	1.169E+00
23000	2.421E+01	2.553E+02	5.253E+02	5.174E+02	2.325E+02	2.329E+02	6.016E+03	1.788E+00
24000	2.431E+01	2.564E+02	5.495E+02	5.417E+02	2.335E+02	2.338E+02	6.068E+03	2.359E+00
25000	2.442E+01	2.574E+02	5.739E+02	5.660E+02	2.344E+02	2.347E+02	6.121E+03	2.890E+00
26000	2.454E+01	2.583E+02	5.984E+02	5.905E+02	2.353E+02	2.356E+02	6.173E+03	3.384E+00
27000	2.466E+01	2.593E+02	6.230E+02	6.151E+02	2.362E+02	2.365E+02	6.226E+03	3.845E+00
28000	2.479E+01	2.602E+02	6.477E+02	6.398E+02	2.370E+02	2.373E+02	6.280E+03	4.277E+00
29000	2.493E+01	2.610E+02	6.726E+02	6.647E+02	2.378E+02	2.381E+02	6.333E+03	4.683E+00
30000	2.508E+01	2.619E+02	6.976E+02	6.897E+02	2.386E+02	2.389E+02	6.387E+03	5.064E+00
32000	2.543E+01	2.635E+02	7.481E+02	7.402E+02	2.401E+02	2.404E+02	6.496E+03	5.765E+00
34000	2.587E+01	2.651E+02	7.994E+02	7.915E+02	2.416E+02	2.418E+02	6.606E+03	6.394E+00
36000	2.651E+01	2.666E+02	8.517E+02	8.438E+02	2.429E+02	2.431E+02	6.717E+03	6.963E+00
38000	2.749E+01	2.680E+02	9.056E+02	8.978E+02	2.442E+02	2.444E+02	6.830E+03	7.480E+00
40000	2.905E+01	2.695E+02	9.620E+02	9.542E+02	2.454E+02	2.456E+02	6.945E+03	7.953E+00
42000	3.152E+01	2.709E+02	1.022E+03	1.015E+03	2.466E+02	2.468E+02	7.065E+03	8.389E+00
44000	3.530E+01	2.725E+02	1.089E+03	1.081E+03	2.477E+02	2.479E+02	7.191E+03	8.791E+00
46000	4.089E+01	2.742E+02	1.165E+03	1.157E+03	2.488E+02	2.490E+02	7.327E+03	9.166E+00
48000	4.877E+01	2.761E+02	1.254E+03	1.246E+03	2.499E+02	2.501E+02	7.476E+03	9.516E+00
50000	5.934E+01	2.783E+02	1.362E+03	1.354E+03	2.510E+02	2.512E+02	7.644E+03	9.845E+00

Table 189: Internal thermodynamic properties of O^{3+} ΔE=250 cm^{-1}

T(K)	Q_{int}	$\ln(Q_{int})$	E_{int}/RT	$C_{p,int}/R$
50	$2.000E+00$	$6.932E-01$	$3.289E-04$	$3.658E-03$
100	$2.015E+00$	$7.008E-01$	$4.244E-02$	$2.342E-01$
150	$2.098E+00$	$7.411E-01$	$1.735E-01$	$6.130E-01$
200	$2.248E+00$	$8.101E-01$	$3.068E-01$	$7.589E-01$
298.15	$2.620E+00$	$9.630E-01$	$4.411E-01$	$6.281E-01$
300	$2.627E+00$	$9.657E-01$	$4.422E-01$	$6.242E-01$
400	$2.996E+00$	$1.097E+00$	$4.622E-01$	$4.289E-01$
500	$3.315E+00$	$1.199E+00$	$4.413E-01$	$2.960E-01$
600	$3.583E+00$	$1.276E+00$	$4.095E-01$	$2.118E-01$
700	$3.807E+00$	$1.337E+00$	$3.771E-01$	$1.574E-01$
800	$3.996E+00$	$1.385E+00$	$3.472E-01$	$1.208E-01$
900	$4.156E+00$	$1.425E+00$	$3.206E-01$	$9.531E-02$
1000	$4.294E+00$	$1.457E+00$	$2.971E-01$	$7.695E-02$
2000	$5.029E+00$	$1.615E+00$	$1.675E-01$	$1.852E-02$
3000	$5.323E+00$	$1.672E+00$	$1.157E-01$	$8.059E-03$
4000	$5.481E+00$	$1.701E+00$	$8.829E-02$	$4.479E-03$
5000	$5.579E+00$	$1.719E+00$	$7.135E-02$	$2.846E-03$
6000	$5.646E+00$	$1.731E+00$	$5.985E-02$	$1.988E-03$
7000	$5.695E+00$	$1.740E+00$	$5.155E-02$	$1.630E-03$
8000	$5.731E+00$	$1.746E+00$	$4.533E-02$	$2.009E-03$
9000	$5.760E+00$	$1.751E+00$	$4.060E-02$	$3.850E-03$
10000	$5.784E+00$	$1.755E+00$	$3.712E-02$	$8.239E-03$
11000	$5.804E+00$	$1.759E+00$	$3.483E-02$	$1.638E-02$
12000	$5.821E+00$	$1.762E+00$	$3.379E-02$	$2.935E-02$
13000	$5.837E+00$	$1.764E+00$	$3.413E-02$	$4.789E-02$
14000	$5.852E+00$	$1.767E+00$	$3.595E-02$	$7.232E-02$
15000	$5.867E+00$	$1.769E+00$	$3.935E-02$	$1.026E-01$
16000	$5.883E+00$	$1.772E+00$	$4.440E-02$	$1.384E-01$
17000	$5.900E+00$	$1.775E+00$	$5.110E-02$	$1.790E-01$
18000	$5.919E+00$	$1.778E+00$	$5.943E-02$	$2.238E-01$
19000	$5.939E+00$	$1.782E+00$	$6.933E-02$	$2.718E-01$
20000	$5.962E+00$	$1.785E+00$	$8.071E-02$	$3.223E-01$
21000	$5.987E+00$	$1.790E+00$	$9.345E-02$	$3.745E-01$
22000	$6.015E+00$	$1.794E+00$	$1.074E-01$	$4.274E-01$
23000	$6.046E+00$	$1.799E+00$	$1.225E-01$	$4.806E-01$
24000	$6.080E+00$	$1.805E+00$	$1.385E-01$	$5.333E-01$
25000	$6.116E+00$	$1.811E+00$	$1.553E-01$	$5.851E-01$
26000	$6.156E+00$	$1.817E+00$	$1.729E-01$	$6.354E-01$
27000	$6.198E+00$	$1.824E+00$	$1.909E-01$	$6.840E-01$
28000	$6.243E+00$	$1.832E+00$	$2.093E-01$	$7.306E-01$
29000	$6.292E+00$	$1.839E+00$	$2.281E-01$	$7.750E-01$
30000	$6.342E+00$	$1.847E+00$	$2.470E-01$	$8.170E-01$
32000	$6.452E+00$	$1.864E+00$	$2.851E-01$	$8.934E-01$
34000	$6.572E+00$	$1.883E+00$	$3.229E-01$	$9.597E-01$
36000	$6.702E+00$	$1.902E+00$	$3.599E-01$	$1.016E+00$
38000	$6.840E+00$	$1.923E+00$	$3.957E-01$	$1.064E+00$
40000	$6.986E+00$	$1.944E+00$	$4.301E-01$	$1.104E+00$
42000	$7.140E+00$	$1.966E+00$	$4.631E-01$	$1.139E+00$
44000	$7.301E+00$	$1.988E+00$	$4.945E-01$	$1.171E+00$
46000	$7.468E+00$	$2.011E+00$	$5.247E-01$	$1.207E+00$
48000	$7.642E+00$	$2.034E+00$	$5.540E-01$	$1.252E+00$
50000	$7.821E+00$	$2.057E+00$	$5.831E-01$	$1.317E+00$

Table 190: Total thermodynamic properties of O^{3+} ΔE=250 cm^{-1}

T [K]	C_p [J/mol/K]	S^0 [J/mol/K]	$H^0(T)-H^0(0)$ [KJ/mol]	$H^0(T)-H^0(298)$ [KJ/mol]	$-(G^0-H^0(0))/T$ [J/mol/K]	$-(G^0-H^0(298))/T$ [J/mol/K]	ΔH_f [KJ/mol]	$Log(K_p)$
50	2.082E+01	1.121E+02	1.040E+00	-6.252E+00	9.130E+01	2.371E+02	1.026E+04	-1.072E+04
100	2.273E+01	1.269E+02	2.114E+00	-5.177E+00	1.058E+02	1.787E+02	1.026E+04	-5.358E+03
150	2.588E+01	1.368E+02	3.334E+00	-3.957E+00	1.145E+02	1.631E+02	1.026E+04	-3.571E+03
200	2.710E+01	1.444E+02	4.667E+00	-2.623E+00	1.211E+02	1.575E+02	1.027E+04	-2.677E+03
298.15	2.601E+01	1.551E+02	7.291E+00	0.000E+00	1.307E+02	1.551E+02	1.028E+04	-1.794E+03
300	2.598E+01	1.553E+02	7.339E+00	4.808E-02	1.308E+02	1.551E+02	1.028E+04	-1.783E+03
400	2.435E+01	1.625E+02	9.852E+00	2.561E+00	1.379E+02	1.561E+02	1.028E+04	-1.336E+03
500	2.325E+01	1.678E+02	1.223E+01	4.937E+00	1.434E+02	1.579E+02	1.029E+04	-1.067E+03
600	2.255E+01	1.720E+02	1.452E+01	7.224E+00	1.478E+02	1.599E+02	1.030E+04	-8.878E+02
700	2.209E+01	1.754E+02	1.675E+01	9.454E+00	1.515E+02	1.619E+02	1.030E+04	-7.597E+02
800	2.179E+01	1.783E+02	1.894E+01	1.165E+01	1.547E+02	1.638E+02	1.031E+04	-6.636E+02
900	2.158E+01	1.809E+02	2.111E+01	1.381E+01	1.575E+02	1.656E+02	1.032E+04	-5.887E+02
1000	2.143E+01	1.832E+02	2.326E+01	1.596E+01	1.599E+02	1.672E+02	1.032E+04	-5.288E+02
2000	2.094E+01	1.978E+02	4.436E+01	3.707E+01	1.756E+02	1.793E+02	1.039E+04	-2.585E+02
3000	2.085E+01	2.063E+02	6.525E+01	5.795E+01	1.845E+02	1.870E+02	1.045E+04	-1.678E+02
4000	2.082E+01	2.123E+02	8.608E+01	7.879E+01	1.908E+02	1.926E+02	1.052E+04	-1.222E+02
5000	2.081E+01	2.169E+02	1.069E+02	9.961E+01	1.956E+02	1.970E+02	1.058E+04	-9.469E+01
6000	2.080E+01	2.207E+02	1.277E+02	1.204E+02	1.994E+02	2.007E+02	1.064E+04	-7.622E+01
7000	2.080E+01	2.239E+02	1.485E+02	1.412E+02	2.027E+02	2.038E+02	1.070E+04	-6.295E+01
8000	2.080E+01	2.267E+02	1.693E+02	1.620E+02	2.055E+02	2.064E+02	1.076E+04	-5.295E+01
9000	2.082E+01	2.292E+02	1.901E+02	1.828E+02	2.080E+02	2.088E+02	1.082E+04	-4.512E+01
10000	2.086E+01	2.313E+02	2.109E+02	2.037E+02	2.103E+02	2.110E+02	1.088E+04	-3.882E+01
11000	2.092E+01	2.333E+02	2.318E+02	2.245E+02	2.123E+02	2.129E+02	1.095E+04	-3.364E+01
12000	2.103E+01	2.352E+02	2.528E+02	2.455E+02	2.141E+02	2.147E+02	1.101E+04	-2.929E+01
13000	2.118E+01	2.369E+02	2.739E+02	2.666E+02	2.158E+02	2.163E+02	1.108E+04	-2.559E+01
14000	2.139E+01	2.384E+02	2.952E+02	2.879E+02	2.173E+02	2.179E+02	1.114E+04	-2.241E+01
15000	2.164E+01	2.399E+02	3.167E+02	3.094E+02	2.188E+02	2.193E+02	1.121E+04	-1.963E+01
16000	2.194E+01	2.413E+02	3.385E+02	3.312E+02	2.202E+02	2.206E+02	1.128E+04	-1.718E+01
17000	2.227E+01	2.427E+02	3.606E+02	3.533E+02	2.214E+02	2.219E+02	1.134E+04	-1.501E+01
18000	2.265E+01	2.439E+02	3.831E+02	3.758E+02	2.227E+02	2.231E+02	1.141E+04	-1.307E+01
19000	2.305E+01	2.452E+02	4.059E+02	3.986E+02	2.238E+02	2.242E+02	1.148E+04	-1.132E+01
20000	2.347E+01	2.464E+02	4.291E+02	4.219E+02	2.249E+02	2.253E+02	1.156E+04	-9.735E+00
21000	2.390E+01	2.475E+02	4.528E+02	4.455E+02	2.260E+02	2.263E+02	1.163E+04	-8.293E+00
22000	2.434E+01	2.487E+02	4.769E+02	4.697E+02	2.270E+02	2.273E+02	1.170E+04	-6.975E+00
23000	2.478E+01	2.497E+02	5.015E+02	4.942E+02	2.279E+02	2.283E+02	1.177E+04	-5.763E+00
24000	2.522E+01	2.508E+02	5.265E+02	5.192E+02	2.289E+02	2.292E+02	1.185E+04	-4.646E+00
25000	2.565E+01	2.518E+02	5.520E+02	5.447E+02	2.298E+02	2.301E+02	1.192E+04	-3.612E+00
26000	2.607E+01	2.529E+02	5.778E+02	5.705E+02	2.306E+02	2.309E+02	1.200E+04	-2.651E+00
27000	2.647E+01	2.538E+02	6.041E+02	5.968E+02	2.315E+02	2.318E+02	1.207E+04	-1.756E+00
28000	2.686E+01	2.548E+02	6.308E+02	6.235E+02	2.323E+02	2.326E+02	1.215E+04	-9.190E-01
29000	2.723E+01	2.558E+02	6.578E+02	6.505E+02	2.331E+02	2.333E+02	1.222E+04	-1.353E-01
30000	2.758E+01	2.567E+02	6.852E+02	6.779E+02	2.339E+02	2.341E+02	1.230E+04	6.009E-01
32000	2.821E+01	2.585E+02	7.410E+02	7.337E+02	2.353E+02	2.356E+02	1.246E+04	1.948E+00
34000	2.877E+01	2.602E+02	7.980E+02	7.907E+02	2.368E+02	2.370E+02	1.261E+04	3.151E+00
36000	2.924E+01	2.619E+02	8.560E+02	8.487E+02	2.381E+02	2.383E+02	1.277E+04	4.234E+00
38000	2.963E+01	2.635E+02	9.149E+02	9.076E+02	2.394E+02	2.396E+02	1.293E+04	5.215E+00
40000	2.996E+01	2.650E+02	9.745E+02	9.672E+02	2.406E+02	2.408E+02	1.309E+04	6.109E+00
42000	3.025E+01	2.665E+02	1.035E+03	1.027E+03	2.418E+02	2.420E+02	1.325E+04	6.928E+00
44000	3.052E+01	2.679E+02	1.096E+03	1.088E+03	2.430E+02	2.432E+02	1.341E+04	7.682E+00
46000	3.082E+01	2.692E+02	1.157E+03	1.150E+03	2.441E+02	2.443E+02	1.358E+04	8.379E+00
48000	3.120E+01	2.706E+02	1.219E+03	1.212E+03	2.452E+02	2.453E+02	1.374E+04	9.025E+00
50000	3.174E+01	2.719E+02	1.282E+03	1.274E+03	2.462E+02	2.464E+02	1.390E+04	9.626E+00

Table 191: Internal thermodynamic properties of O^{3+} ΔE=500 cm^{-1}

T(K)	Q_{int}	$\ln(Q_{int})$	E_{int}/RT	$C_{p,int}/R$
50	$2.000E+00$	$6.932E-01$	$3.289E-04$	$3.658E-03$
100	$2.015E+00$	$7.008E-01$	$4.244E-02$	$2.342E-01$
150	$2.098E+00$	$7.411E-01$	$1.735E-01$	$6.130E-01$
200	$2.248E+00$	$8.101E-01$	$3.068E-01$	$7.589E-01$
298.15	$2.620E+00$	$9.630E-01$	$4.411E-01$	$6.281E-01$
300	$2.627E+00$	$9.657E-01$	$4.422E-01$	$6.242E-01$
400	$2.996E+00$	$1.097E+00$	$4.622E-01$	$4.289E-01$
500	$3.315E+00$	$1.199E+00$	$4.413E-01$	$2.960E-01$
600	$3.583E+00$	$1.276E+00$	$4.095E-01$	$2.118E-01$
700	$3.807E+00$	$1.337E+00$	$3.771E-01$	$1.574E-01$
800	$3.996E+00$	$1.385E+00$	$3.472E-01$	$1.208E-01$
900	$4.156E+00$	$1.425E+00$	$3.206E-01$	$9.531E-02$
1000	$4.294E+00$	$1.457E+00$	$2.971E-01$	$7.695E-02$
2000	$5.029E+00$	$1.615E+00$	$1.675E-01$	$1.852E-02$
3000	$5.323E+00$	$1.672E+00$	$1.157E-01$	$8.059E-03$
4000	$5.481E+00$	$1.701E+00$	$8.829E-02$	$4.479E-03$
5000	$5.579E+00$	$1.719E+00$	$7.135E-02$	$2.846E-03$
6000	$5.646E+00$	$1.731E+00$	$5.985E-02$	$1.988E-03$
7000	$5.695E+00$	$1.740E+00$	$5.155E-02$	$1.630E-03$
8000	$5.731E+00$	$1.746E+00$	$4.533E-02$	$2.009E-03$
9000	$5.760E+00$	$1.751E+00$	$4.060E-02$	$3.850E-03$
10000	$5.784E+00$	$1.755E+00$	$3.712E-02$	$8.239E-03$
11000	$5.804E+00$	$1.759E+00$	$3.483E-02$	$1.638E-02$
12000	$5.821E+00$	$1.762E+00$	$3.379E-02$	$2.935E-02$
13000	$5.837E+00$	$1.764E+00$	$3.413E-02$	$4.789E-02$
14000	$5.852E+00$	$1.767E+00$	$3.595E-02$	$7.232E-02$
15000	$5.867E+00$	$1.769E+00$	$3.935E-02$	$1.026E-01$
16000	$5.883E+00$	$1.772E+00$	$4.440E-02$	$1.384E-01$
17000	$5.900E+00$	$1.775E+00$	$5.110E-02$	$1.790E-01$
18000	$5.919E+00$	$1.778E+00$	$5.943E-02$	$2.238E-01$
19000	$5.939E+00$	$1.782E+00$	$6.933E-02$	$2.718E-01$
20000	$5.962E+00$	$1.785E+00$	$8.071E-02$	$3.223E-01$
21000	$5.987E+00$	$1.790E+00$	$9.345E-02$	$3.745E-01$
22000	$6.015E+00$	$1.794E+00$	$1.074E-01$	$4.274E-01$
23000	$6.046E+00$	$1.799E+00$	$1.225E-01$	$4.806E-01$
24000	$6.080E+00$	$1.805E+00$	$1.385E-01$	$5.333E-01$
25000	$6.116E+00$	$1.811E+00$	$1.553E-01$	$5.851E-01$
26000	$6.156E+00$	$1.817E+00$	$1.729E-01$	$6.354E-01$
27000	$6.198E+00$	$1.824E+00$	$1.909E-01$	$6.840E-01$
28000	$6.243E+00$	$1.832E+00$	$2.093E-01$	$7.306E-01$
29000	$6.292E+00$	$1.839E+00$	$2.281E-01$	$7.750E-01$
30000	$6.342E+00$	$1.847E+00$	$2.470E-01$	$8.170E-01$
32000	$6.452E+00$	$1.864E+00$	$2.851E-01$	$8.934E-01$
34000	$6.572E+00$	$1.883E+00$	$3.229E-01$	$9.597E-01$
36000	$6.702E+00$	$1.902E+00$	$3.599E-01$	$1.016E+00$
38000	$6.840E+00$	$1.923E+00$	$3.957E-01$	$1.064E+00$
40000	$6.986E+00$	$1.944E+00$	$4.301E-01$	$1.103E+00$
42000	$7.140E+00$	$1.966E+00$	$4.630E-01$	$1.137E+00$
44000	$7.301E+00$	$1.988E+00$	$4.943E-01$	$1.167E+00$
46000	$7.468E+00$	$2.011E+00$	$5.242E-01$	$1.198E+00$
48000	$7.641E+00$	$2.034E+00$	$5.530E-01$	$1.234E+00$
50000	$7.820E+00$	$2.057E+00$	$5.812E-01$	$1.284E+00$

Table 192: Total thermodynamic properties of O^{3+} ΔE=500 cm^{-1}

T [K]	C_p [J/mol/K]	S^0 [J/mol/K]	$H^0(T)-H^0(0)$ [KJ/mol]	$H^0(T)-H^0(298)$ [KJ/mol]	$-(G^0-H^0(0))/T$ [J/mol/K]	$-(G^0-H^0(298))/T$ [J/mol/K]	ΔH_f [KJ/mol]	$Log(K_p)$
50	2.082E+01	1.121E+02	1.040E+00	-6.252E+00	9.130E+01	2.371E+02	1.026E+04	-1.072E+04
100	2.273E+01	1.269E+02	2.114E+00	-5.177E+00	1.058E+02	1.787E+02	1.026E+04	-5.358E+03
150	2.588E+01	1.368E+02	3.334E+00	-3.957E+00	1.145E+02	1.631E+02	1.026E+04	-3.571E+03
200	2.710E+01	1.444E+02	4.667E+00	-2.623E+00	1.211E+02	1.575E+02	1.027E+04	-2.677E+03
298.15	2.601E+01	1.551E+02	7.291E+00	0.000E+00	1.307E+02	1.551E+02	1.028E+04	-1.794E+03
300	2.598E+01	1.553E+02	7.339E+00	4.808E-02	1.308E+02	1.551E+02	1.028E+04	-1.783E+03
400	2.435E+01	1.625E+02	9.852E+00	2.561E+00	1.379E+02	1.561E+02	1.028E+04	-1.336E+03
500	2.325E+01	1.678E+02	1.223E+01	4.937E+00	1.434E+02	1.579E+02	1.029E+04	-1.067E+03
600	2.255E+01	1.720E+02	1.452E+01	7.224E+00	1.478E+02	1.599E+02	1.030E+04	-8.878E+02
700	2.209E+01	1.754E+02	1.675E+01	9.454E+00	1.515E+02	1.619E+02	1.030E+04	-7.597E+02
800	2.179E+01	1.783E+02	1.894E+01	1.165E+01	1.547E+02	1.638E+02	1.031E+04	-6.636E+02
900	2.158E+01	1.809E+02	2.111E+01	1.381E+01	1.575E+02	1.656E+02	1.032E+04	-5.887E+02
1000	2.143E+01	1.832E+02	2.326E+01	1.596E+01	1.599E+02	1.672E+02	1.032E+04	-5.288E+02
2000	2.094E+01	1.978E+02	4.436E+01	3.707E+01	1.756E+02	1.793E+02	1.039E+04	-2.585E+02
3000	2.085E+01	2.063E+02	6.525E+01	5.795E+01	1.845E+02	1.870E+02	1.045E+04	-1.678E+02
4000	2.082E+01	2.123E+02	8.608E+01	7.879E+01	1.908E+02	1.926E+02	1.052E+04	-1.222E+02
5000	2.081E+01	2.169E+02	1.069E+02	9.961E+01	1.956E+02	1.970E+02	1.058E+04	-9.469E+01
6000	2.080E+01	2.207E+02	1.277E+02	1.204E+02	1.994E+02	2.007E+02	1.064E+04	-7.622E+01
7000	2.080E+01	2.239E+02	1.485E+02	1.412E+02	2.027E+02	2.038E+02	1.070E+04	-6.295E+01
8000	2.080E+01	2.267E+02	1.693E+02	1.620E+02	2.055E+02	2.064E+02	1.076E+04	-5.295E+01
9000	2.082E+01	2.292E+02	1.901E+02	1.828E+02	2.080E+02	2.088E+02	1.082E+04	-4.512E+01
10000	2.086E+01	2.313E+02	2.109E+02	2.037E+02	2.103E+02	2.110E+02	1.088E+04	-3.882E+01
11000	2.092E+01	2.333E+02	2.318E+02	2.245E+02	2.123E+02	2.129E+02	1.095E+04	-3.364E+01
12000	2.103E+01	2.352E+02	2.528E+02	2.455E+02	2.141E+02	2.147E+02	1.101E+04	-2.929E+01
13000	2.118E+01	2.369E+02	2.739E+02	2.666E+02	2.158E+02	2.163E+02	1.108E+04	-2.559E+01
14000	2.139E+01	2.384E+02	2.952E+02	2.879E+02	2.173E+02	2.179E+02	1.114E+04	-2.241E+01
15000	2.164E+01	2.399E+02	3.167E+02	3.094E+02	2.188E+02	2.193E+02	1.121E+04	-1.963E+01
16000	2.194E+01	2.413E+02	3.385E+02	3.312E+02	2.202E+02	2.206E+02	1.128E+04	-1.718E+01
17000	2.227E+01	2.427E+02	3.606E+02	3.533E+02	2.214E+02	2.219E+02	1.134E+04	-1.501E+01
18000	2.265E+01	2.439E+02	3.831E+02	3.758E+02	2.227E+02	2.231E+02	1.141E+04	-1.307E+01
19000	2.305E+01	2.452E+02	4.059E+02	3.986E+02	2.238E+02	2.242E+02	1.148E+04	-1.132E+01
20000	2.347E+01	2.464E+02	4.291E+02	4.219E+02	2.249E+02	2.253E+02	1.156E+04	-9.735E+00
21000	2.390E+01	2.475E+02	4.528E+02	4.455E+02	2.260E+02	2.263E+02	1.163E+04	-8.293E+00
22000	2.434E+01	2.487E+02	4.769E+02	4.697E+02	2.270E+02	2.273E+02	1.170E+04	-6.975E+00
23000	2.478E+01	2.497E+02	5.015E+02	4.942E+02	2.279E+02	2.283E+02	1.177E+04	-5.763E+00
24000	2.522E+01	2.508E+02	5.265E+02	5.192E+02	2.289E+02	2.292E+02	1.185E+04	-4.646E+00
25000	2.565E+01	2.518E+02	5.520E+02	5.447E+02	2.298E+02	2.301E+02	1.192E+04	-3.612E+00
26000	2.607E+01	2.529E+02	5.778E+02	5.705E+02	2.306E+02	2.309E+02	1.200E+04	-2.651E+00
27000	2.647E+01	2.538E+02	6.041E+02	5.968E+02	2.315E+02	2.318E+02	1.207E+04	-1.756E+00
28000	2.686E+01	2.548E+02	6.308E+02	6.235E+02	2.323E+02	2.326E+02	1.215E+04	-9.190E-01
29000	2.723E+01	2.558E+02	6.578E+02	6.505E+02	2.331E+02	2.333E+02	1.222E+04	-1.353E-01
30000	2.758E+01	2.567E+02	6.852E+02	6.779E+02	2.339E+02	2.341E+02	1.230E+04	6.009E-01
32000	2.821E+01	2.585E+02	7.410E+02	7.337E+02	2.353E+02	2.356E+02	1.246E+04	1.948E+00
34000	2.877E+01	2.602E+02	7.980E+02	7.907E+02	2.368E+02	2.370E+02	1.261E+04	3.151E+00
36000	2.923E+01	2.619E+02	8.560E+02	8.487E+02	2.381E+02	2.383E+02	1.277E+04	4.234E+00
38000	2.963E+01	2.635E+02	9.149E+02	9.076E+02	2.394E+02	2.396E+02	1.293E+04	5.215E+00
40000	2.996E+01	2.650E+02	9.745E+02	9.672E+02	2.406E+02	2.408E+02	1.309E+04	6.109E+00
42000	3.024E+01	2.665E+02	1.035E+03	1.027E+03	2.418E+02	2.420E+02	1.325E+04	6.928E+00
44000	3.049E+01	2.679E+02	1.095E+03	1.088E+03	2.430E+02	2.432E+02	1.341E+04	7.682E+00
46000	3.075E+01	2.692E+02	1.157E+03	1.149E+03	2.441E+02	2.443E+02	1.358E+04	8.379E+00
48000	3.105E+01	2.706E+02	1.218E+03	1.211E+03	2.452E+02	2.453E+02	1.374E+04	9.025E+00
50000	3.146E+01	2.718E+02	1.281E+03	1.274E+03	2.462E+02	2.464E+02	1.390E+04	9.626E+00

Table 193: Internal thermodynamic properties of O^{3+} ΔE=1000 cm^{-1}

T(K)	Q_{int}	$\ln(Q_{int})$	E_{int}/RT	$C_{p,int}/R$
50	$2.000E+00$	$6.932E-01$	$3.289E-04$	$3.658E-03$
100	$2.015E+00$	$7.008E-01$	$4.244E-02$	$2.342E-01$
150	$2.098E+00$	$7.411E-01$	$1.735E-01$	$6.130E-01$
200	$2.248E+00$	$8.101E-01$	$3.068E-01$	$7.589E-01$
298.15	$2.620E+00$	$9.630E-01$	$4.411E-01$	$6.281E-01$
300	$2.627E+00$	$9.657E-01$	$4.422E-01$	$6.242E-01$
400	$2.996E+00$	$1.097E+00$	$4.622E-01$	$4.289E-01$
500	$3.315E+00$	$1.199E+00$	$4.413E-01$	$2.960E-01$
600	$3.583E+00$	$1.276E+00$	$4.095E-01$	$2.118E-01$
700	$3.807E+00$	$1.337E+00$	$3.771E-01$	$1.574E-01$
800	$3.996E+00$	$1.385E+00$	$3.472E-01$	$1.208E-01$
900	$4.156E+00$	$1.425E+00$	$3.206E-01$	$9.531E-02$
1000	$4.294E+00$	$1.457E+00$	$2.971E-01$	$7.695E-02$
2000	$5.029E+00$	$1.615E+00$	$1.675E-01$	$1.852E-02$
3000	$5.323E+00$	$1.672E+00$	$1.157E-01$	$8.059E-03$
4000	$5.481E+00$	$1.701E+00$	$8.829E-02$	$4.479E-03$
5000	$5.579E+00$	$1.719E+00$	$7.135E-02$	$2.846E-03$
6000	$5.646E+00$	$1.731E+00$	$5.985E-02$	$1.988E-03$
7000	$5.695E+00$	$1.740E+00$	$5.155E-02$	$1.630E-03$
8000	$5.731E+00$	$1.746E+00$	$4.533E-02$	$2.009E-03$
9000	$5.760E+00$	$1.751E+00$	$4.060E-02$	$3.850E-03$
10000	$5.784E+00$	$1.755E+00$	$3.712E-02$	$8.239E-03$
11000	$5.804E+00$	$1.759E+00$	$3.483E-02$	$1.638E-02$
12000	$5.821E+00$	$1.762E+00$	$3.379E-02$	$2.935E-02$
13000	$5.837E+00$	$1.764E+00$	$3.413E-02$	$4.789E-02$
14000	$5.852E+00$	$1.767E+00$	$3.595E-02$	$7.232E-02$
15000	$5.867E+00$	$1.769E+00$	$3.935E-02$	$1.026E-01$
16000	$5.883E+00$	$1.772E+00$	$4.440E-02$	$1.384E-01$
17000	$5.900E+00$	$1.775E+00$	$5.110E-02$	$1.790E-01$
18000	$5.919E+00$	$1.778E+00$	$5.943E-02$	$2.238E-01$
19000	$5.939E+00$	$1.782E+00$	$6.933E-02$	$2.718E-01$
20000	$5.962E+00$	$1.785E+00$	$8.071E-02$	$3.223E-01$
21000	$5.987E+00$	$1.790E+00$	$9.345E-02$	$3.745E-01$
22000	$6.015E+00$	$1.794E+00$	$1.074E-01$	$4.274E-01$
23000	$6.046E+00$	$1.799E+00$	$1.225E-01$	$4.806E-01$
24000	$6.080E+00$	$1.805E+00$	$1.385E-01$	$5.333E-01$
25000	$6.116E+00$	$1.811E+00$	$1.553E-01$	$5.851E-01$
26000	$6.156E+00$	$1.817E+00$	$1.729E-01$	$6.354E-01$
27000	$6.198E+00$	$1.824E+00$	$1.909E-01$	$6.840E-01$
28000	$6.243E+00$	$1.832E+00$	$2.093E-01$	$7.306E-01$
29000	$6.292E+00$	$1.839E+00$	$2.281E-01$	$7.750E-01$
30000	$6.342E+00$	$1.847E+00$	$2.470E-01$	$8.170E-01$
32000	$6.452E+00$	$1.864E+00$	$2.851E-01$	$8.934E-01$
34000	$6.572E+00$	$1.883E+00$	$3.229E-01$	$9.597E-01$
36000	$6.702E+00$	$1.902E+00$	$3.599E-01$	$1.016E+00$
38000	$6.840E+00$	$1.923E+00$	$3.957E-01$	$1.063E+00$
40000	$6.986E+00$	$1.944E+00$	$4.301E-01$	$1.102E+00$
42000	$7.140E+00$	$1.966E+00$	$4.629E-01$	$1.134E+00$
44000	$7.301E+00$	$1.988E+00$	$4.940E-01$	$1.161E+00$
46000	$7.468E+00$	$2.011E+00$	$5.235E-01$	$1.184E+00$
48000	$7.641E+00$	$2.033E+00$	$5.515E-01$	$1.206E+00$
50000	$7.819E+00$	$2.057E+00$	$5.782E-01$	$1.231E+00$

Table 194: Total thermodynamic properties of O^{3+} ΔE=1000 cm^{-1}

T [K]	C_p [J/mol/K]	S^0 [J/mol/K]	$H^0(T)-H^0(0)$ [KJ/mol]	$H^0(T)-H^0(298)$ [KJ/mol]	$-(G^0-H^0(0))/T$ [J/mol/K]	$-(G^0-H^0(298))/T$ [J/mol/K]	ΔH_f [KJ/mol]	$Log(K_p)$
50	2.082E+01	1.121E+02	1.040E+00	-6.252E+00	9.130E+01	2.371E+02	1.026E+04	-1.072E+04
100	2.273E+01	1.269E+02	2.114E+00	-5.177E+00	1.058E+02	1.787E+02	1.026E+04	-5.358E+03
150	2.588E+01	1.368E+02	3.334E+00	-3.957E+00	1.145E+02	1.631E+02	1.026E+04	-3.571E+03
200	2.710E+01	1.444E+02	4.667E+00	-2.623E+00	1.211E+02	1.575E+02	1.027E+04	-2.677E+03
298.15	2.601E+01	1.551E+02	7.291E+00	0.000E+00	1.307E+02	1.551E+02	1.028E+04	-1.794E+03
300	2.598E+01	1.553E+02	7.339E+00	4.808E-02	1.308E+02	1.551E+02	1.028E+04	-1.783E+03
400	2.435E+01	1.625E+02	9.852E+00	2.561E+00	1.379E+02	1.561E+02	1.028E+04	-1.336E+03
500	2.325E+01	1.678E+02	1.223E+01	4.937E+00	1.434E+02	1.579E+02	1.029E+04	-1.067E+03
600	2.255E+01	1.720E+02	1.452E+01	7.224E+00	1.478E+02	1.599E+02	1.030E+04	-8.878E+02
700	2.209E+01	1.754E+02	1.675E+01	9.454E+00	1.515E+02	1.619E+02	1.030E+04	-7.597E+02
800	2.179E+01	1.783E+02	1.894E+01	1.165E+01	1.547E+02	1.638E+02	1.031E+04	-6.636E+02
900	2.158E+01	1.809E+02	2.111E+01	1.381E+01	1.575E+02	1.656E+02	1.032E+04	-5.887E+02
1000	2.143E+01	1.832E+02	2.326E+01	1.596E+01	1.599E+02	1.672E+02	1.032E+04	-5.288E+02
2000	2.094E+01	1.978E+02	4.436E+01	3.707E+01	1.756E+02	1.793E+02	1.039E+04	-2.585E+02
3000	2.085E+01	2.063E+02	6.525E+01	5.795E+01	1.845E+02	1.870E+02	1.045E+04	-1.678E+02
4000	2.082E+01	2.123E+02	8.608E+01	7.879E+01	1.908E+02	1.926E+02	1.052E+04	-1.222E+02
5000	2.081E+01	2.169E+02	1.069E+02	9.961E+01	1.956E+02	1.970E+02	1.058E+04	-9.469E+01
6000	2.080E+01	2.207E+02	1.277E+02	1.204E+02	1.994E+02	2.007E+02	1.064E+04	-7.622E+01
7000	2.080E+01	2.239E+02	1.485E+02	1.412E+02	2.027E+02	2.038E+02	1.070E+04	-6.295E+01
8000	2.080E+01	2.267E+02	1.693E+02	1.620E+02	2.055E+02	2.064E+02	1.076E+04	-5.295E+01
9000	2.082E+01	2.292E+02	1.901E+02	1.828E+02	2.080E+02	2.088E+02	1.082E+04	-4.512E+01
10000	2.086E+01	2.313E+02	2.109E+02	2.037E+02	2.103E+02	2.110E+02	1.088E+04	-3.882E+01
11000	2.092E+01	2.333E+02	2.318E+02	2.245E+02	2.123E+02	2.129E+02	1.095E+04	-3.364E+01
12000	2.103E+01	2.352E+02	2.528E+02	2.455E+02	2.141E+02	2.147E+02	1.101E+04	-2.929E+01
13000	2.118E+01	2.369E+02	2.739E+02	2.666E+02	2.158E+02	2.163E+02	1.108E+04	-2.559E+01
14000	2.139E+01	2.384E+02	2.952E+02	2.879E+02	2.173E+02	2.179E+02	1.114E+04	-2.241E+01
15000	2.164E+01	2.399E+02	3.167E+02	3.094E+02	2.188E+02	2.193E+02	1.121E+04	-1.963E+01
16000	2.194E+01	2.413E+02	3.385E+02	3.312E+02	2.202E+02	2.206E+02	1.128E+04	-1.718E+01
17000	2.227E+01	2.427E+02	3.606E+02	3.533E+02	2.214E+02	2.219E+02	1.134E+04	-1.501E+01
18000	2.265E+01	2.439E+02	3.831E+02	3.758E+02	2.227E+02	2.231E+02	1.141E+04	-1.307E+01
19000	2.305E+01	2.452E+02	4.059E+02	3.986E+02	2.238E+02	2.242E+02	1.148E+04	-1.132E+01
20000	2.347E+01	2.464E+02	4.291E+02	4.219E+02	2.249E+02	2.253E+02	1.156E+04	-9.735E+00
21000	2.390E+01	2.475E+02	4.528E+02	4.455E+02	2.260E+02	2.263E+02	1.163E+04	-8.293E+00
22000	2.434E+01	2.487E+02	4.769E+02	4.697E+02	2.270E+02	2.273E+02	1.170E+04	-6.975E+00
23000	2.478E+01	2.497E+02	5.015E+02	4.942E+02	2.279E+02	2.283E+02	1.177E+04	-5.763E+00
24000	2.522E+01	2.508E+02	5.265E+02	5.192E+02	2.289E+02	2.292E+02	1.185E+04	-4.646E+00
25000	2.565E+01	2.518E+02	5.520E+02	5.447E+02	2.298E+02	2.301E+02	1.192E+04	-3.612E+00
26000	2.607E+01	2.529E+02	5.778E+02	5.705E+02	2.306E+02	2.309E+02	1.200E+04	-2.651E+00
27000	2.647E+01	2.538E+02	6.041E+02	5.968E+02	2.315E+02	2.318E+02	1.207E+04	-1.756E+00
28000	2.686E+01	2.548E+02	6.308E+02	6.235E+02	2.323E+02	2.326E+02	1.215E+04	-9.190E-01
29000	2.723E+01	2.558E+02	6.578E+02	6.505E+02	2.331E+02	2.333E+02	1.222E+04	-1.353E-01
30000	2.758E+01	2.567E+02	6.852E+02	6.779E+02	2.339E+02	2.341E+02	1.230E+04	6.009E-01
32000	2.821E+01	2.585E+02	7.410E+02	7.337E+02	2.353E+02	2.356E+02	1.246E+04	1.948E+00
34000	2.877E+01	2.602E+02	7.980E+02	7.907E+02	2.368E+02	2.370E+02	1.261E+04	3.151E+00
36000	2.923E+01	2.619E+02	8.560E+02	8.487E+02	2.381E+02	2.383E+02	1.277E+04	4.234E+00
38000	2.963E+01	2.635E+02	9.149E+02	9.076E+02	2.394E+02	2.396E+02	1.293E+04	5.215E+00
40000	2.995E+01	2.650E+02	9.745E+02	9.672E+02	2.406E+02	2.408E+02	1.309E+04	6.109E+00
42000	3.022E+01	2.665E+02	1.035E+03	1.027E+03	2.418E+02	2.420E+02	1.325E+04	6.928E+00
44000	3.044E+01	2.679E+02	1.095E+03	1.088E+03	2.430E+02	2.432E+02	1.341E+04	7.682E+00
46000	3.063E+01	2.692E+02	1.156E+03	1.149E+03	2.441E+02	2.443E+02	1.358E+04	8.379E+00
48000	3.082E+01	2.706E+02	1.218E+03	1.210E+03	2.452E+02	2.453E+02	1.374E+04	9.025E+00
50000	3.102E+01	2.718E+02	1.280E+03	1.272E+03	2.462E+02	2.464E+02	1.390E+04	9.626E+00

Table 195: Internal thermodynamic properties of O^{4+} ΔE=250 cm^{-1}

T(K)	Q_{int}	$\ln(Q_{int})$	E_{int}/RT	$C_{p,int}/R$
50	$1.000E+00$	$0.000E+00$	$0.000E+00$	$0.000E+00$
100	$1.000E+00$	$0.000E+00$	$0.000E+00$	$0.000E+00$
150	$1.000E+00$	$0.000E+00$	$0.000E+00$	$0.000E+00$
200	$1.000E+00$	$0.000E+00$	$3.735E-254$	$2.209E-251$
298.15	$1.000E+00$	$0.000E+00$	$9.772E-170$	$3.880E-167$
300	$1.000E+00$	$0.000E+00$	$1.123E-168$	$4.433E-166$
400	$1.000E+00$	$0.000E+00$	$5.936E-126$	$1.757E-123$
500	$1.000E+00$	$0.000E+00$	$2.474E-100$	$5.861E-98$
600	$1.000E+00$	$0.000E+00$	$2.901E-83$	$5.727E-81$
700	$1.000E+00$	$0.000E+00$	$4.427E-71$	$7.493E-69$
800	$1.000E+00$	$0.000E+00$	$5.986E-62$	$8.866E-60$
900	$1.000E+00$	$0.000E+00$	$7.474E-55$	$9.841E-53$
1000	$1.000E+00$	$0.000E+00$	$3.518E-49$	$4.169E-47$
2000	$1.000E+00$	$0.000E+00$	$9.610E-24$	$5.696E-22$
3000	$1.000E+00$	$0.000E+00$	$2.440E-15$	$9.641E-14$
4000	$1.000E+00$	$1.206E-12$	$3.573E-11$	$1.059E-09$
5000	$1.000E+00$	$4.526E-10$	$1.073E-08$	$2.545E-07$
6000	$1.000E+00$	$2.355E-08$	$4.654E-07$	$9.196E-06$
7000	$1.000E+00$	$3.963E-07$	$6.712E-06$	$1.137E-04$
8000	$1.000E+00$	$3.292E-06$	$4.879E-05$	$7.232E-04$
9000	$1.000E+00$	$1.709E-05$	$2.251E-04$	$2.966E-03$
10000	$1.000E+00$	$6.380E-05$	$7.564E-04$	$8.968E-03$
11000	$1.000E+00$	$1.875E-04$	$2.020E-03$	$2.177E-02$
12000	$1.000E+00$	$4.602E-04$	$4.546E-03$	$4.490E-02$
13000	$1.001E+00$	$9.839E-04$	$8.970E-03$	$8.174E-02$
14000	$1.002E+00$	$1.887E-03$	$1.597E-02$	$1.350E-01$
15000	$1.003E+00$	$3.316E-03$	$2.618E-02$	$2.063E-01$
16000	$1.005E+00$	$5.430E-03$	$4.014E-02$	$2.961E-01$
17000	$1.008E+00$	$8.386E-03$	$5.827E-02$	$4.034E-01$
18000	$1.012E+00$	$1.233E-02$	$8.080E-02$	$5.265E-01$
19000	$1.018E+00$	$1.740E-02$	$1.078E-01$	$6.624E-01$
20000	$1.024E+00$	$2.371E-02$	$1.391E-01$	$8.077E-01$
21000	$1.032E+00$	$3.134E-02$	$1.745E-01$	$9.587E-01$
22000	$1.041E+00$	$4.035E-02$	$2.137E-01$	$1.112E+00$
23000	$1.052E+00$	$5.077E-02$	$2.560E-01$	$1.263E+00$
24000	$1.065E+00$	$6.261E-02$	$3.010E-01$	$1.408E+00$
25000	$1.079E+00$	$7.584E-02$	$3.481E-01$	$1.546E+00$
26000	$1.095E+00$	$9.044E-02$	$3.966E-01$	$1.673E+00$
27000	$1.112E+00$	$1.063E-01$	$4.461E-01$	$1.789E+00$
28000	$1.131E+00$	$1.235E-01$	$4.959E-01$	$1.891E+00$
29000	$1.152E+00$	$1.417E-01$	$5.456E-01$	$1.980E+00$
30000	$1.175E+00$	$1.611E-01$	$5.947E-01$	$2.054E+00$
32000	$1.224E+00$	$2.025E-01$	$6.896E-01$	$2.164E+00$
34000	$1.280E+00$	$2.470E-01$	$7.784E-01$	$2.225E+00$
36000	$1.342E+00$	$2.938E-01$	$8.595E-01$	$2.247E+00$
38000	$1.408E+00$	$3.423E-01$	$9.324E-01$	$2.237E+00$
40000	$1.480E+00$	$3.918E-01$	$9.969E-01$	$2.205E+00$
42000	$1.556E+00$	$4.418E-01$	$1.053E+00$	$2.158E+00$
44000	$1.636E+00$	$4.920E-01$	$1.102E+00$	$2.100E+00$
46000	$1.719E+00$	$5.419E-01$	$1.144E+00$	$2.038E+00$
48000	$1.807E+00$	$5.914E-01$	$1.180E+00$	$1.973E+00$
50000	$1.897E+00$	$6.402E-01$	$1.211E+00$	$1.909E+00$

Table 196: Total thermodynamic properties of O^{4+} ΔE=250 cm^{-1}

T [K]	C_p [J/mol/K]	S^0 [J/mol/K]	$H^0(T)-H^0(0)$ [KJ/mol]	$H^0(T)-H^0(298)$ [KJ/mol]	$-(G^0-H^0(0))/T$ [J/mol/K]	$-(G^0-H^0(298))/T$ [J/mol/K]	ΔH_f [KJ/mol]	$Log(K_p)$
50	2.079E+01	1.063E+02	1.039E+00	-5.158E+00	8.553E+01	2.095E+02	1.773E+04	-1.852E+04
100	2.079E+01	1.207E+02	2.079E+00	-4.119E+00	9.994E+01	1.619E+02	1.773E+04	-9.261E+03
150	2.079E+01	1.292E+02	3.118E+00	-3.079E+00	1.084E+02	1.497E+02	1.774E+04	-6.173E+03
200	2.079E+01	1.351E+02	4.157E+00	-2.040E+00	1.143E+02	1.453E+02	1.774E+04	-4.629E+03
298.15	2.079E+01	1.434E+02	6.197E+00	0.000E+00	1.227E+02	1.434E+02	1.775E+04	-3.103E+03
300	2.079E+01	1.436E+02	6.236E+00	3.848E-02	1.228E+02	1.434E+02	1.775E+04	-3.084E+03
400	2.079E+01	1.495E+02	8.315E+00	2.117E+00	1.288E+02	1.442E+02	1.776E+04	-2.311E+03
500	2.079E+01	1.542E+02	1.039E+01	4.196E+00	1.334E+02	1.458E+02	1.777E+04	-1.847E+03
600	2.079E+01	1.580E+02	1.247E+01	6.274E+00	1.372E+02	1.475E+02	1.778E+04	-1.538E+03
700	2.079E+01	1.612E+02	1.455E+01	8.353E+00	1.404E+02	1.492E+02	1.779E+04	-1.317E+03
800	2.079E+01	1.639E+02	1.663E+01	1.043E+01	1.432E+02	1.509E+02	1.780E+04	-1.151E+03
900	2.079E+01	1.664E+02	1.871E+01	1.251E+01	1.456E+02	1.525E+02	1.780E+04	-1.022E+03
1000	2.079E+01	1.686E+02	2.079E+01	1.459E+01	1.478E+02	1.540E+02	1.781E+04	-9.183E+02
2000	2.079E+01	1.830E+02	4.157E+01	3.538E+01	1.622E+02	1.653E+02	1.790E+04	-4.522E+02
3000	2.079E+01	1.914E+02	6.236E+01	5.616E+01	1.706E+02	1.727E+02	1.798E+04	-2.961E+02
4000	2.079E+01	1.974E+02	8.314E+01	7.695E+01	1.766E+02	1.782E+02	1.807E+04	-2.177E+02
5000	2.079E+01	2.020E+02	1.039E+02	9.773E+01	1.813E+02	1.825E+02	1.815E+04	-1.704E+02
6000	2.079E+01	2.058E+02	1.247E+02	1.185E+02	1.850E+02	1.861E+02	1.823E+04	-1.387E+02
7000	2.079E+01	2.090E+02	1.455E+02	1.393E+02	1.882E+02	1.891E+02	1.831E+04	-1.160E+02
8000	2.079E+01	2.118E+02	1.663E+02	1.601E+02	1.910E+02	1.918E+02	1.839E+04	-9.889E+01
9000	2.081E+01	2.143E+02	1.871E+02	1.809E+02	1.935E+02	1.942E+02	1.848E+04	-8.552E+01
10000	2.086E+01	2.165E+02	2.079E+02	2.017E+02	1.957E+02	1.963E+02	1.856E+04	-7.477E+01
11000	2.097E+01	2.184E+02	2.288E+02	2.226E+02	1.977E+02	1.982E+02	1.864E+04	-6.594E+01
12000	2.116E+01	2.203E+02	2.499E+02	2.437E+02	1.995E+02	2.000E+02	1.873E+04	-5.855E+01
13000	2.147E+01	2.220E+02	2.712E+02	2.650E+02	2.011E+02	2.016E+02	1.881E+04	-5.226E+01
14000	2.191E+01	2.236E+02	2.929E+02	2.867E+02	2.027E+02	2.031E+02	1.890E+04	-4.685E+01
15000	2.250E+01	2.251E+02	3.151E+02	3.089E+02	2.041E+02	2.045E+02	1.899E+04	-4.214E+01
16000	2.325E+01	2.266E+02	3.379E+02	3.317E+02	2.055E+02	2.059E+02	1.908E+04	-3.800E+01
17000	2.414E+01	2.280E+02	3.616E+02	3.554E+02	2.068E+02	2.071E+02	1.917E+04	-3.433E+01
18000	2.516E+01	2.294E+02	3.862E+02	3.801E+02	2.080E+02	2.083E+02	1.926E+04	-3.105E+01
19000	2.629E+01	2.308E+02	4.120E+02	4.058E+02	2.092E+02	2.095E+02	1.936E+04	-2.810E+01
20000	2.750E+01	2.322E+02	4.389E+02	4.327E+02	2.103E+02	2.106E+02	1.945E+04	-2.543E+01
21000	2.876E+01	2.336E+02	4.670E+02	4.608E+02	2.113E+02	2.116E+02	1.955E+04	-2.301E+01
22000	3.003E+01	2.349E+02	4.964E+02	4.902E+02	2.124E+02	2.127E+02	1.964E+04	-2.079E+01
23000	3.128E+01	2.363E+02	5.270E+02	5.208E+02	2.134E+02	2.137E+02	1.974E+04	-1.876E+01
24000	3.250E+01	2.377E+02	5.589E+02	5.527E+02	2.144E+02	2.146E+02	1.985E+04	-1.689E+01
25000	3.364E+01	2.390E+02	5.920E+02	5.858E+02	2.153E+02	2.156E+02	1.995E+04	-1.515E+01
26000	3.470E+01	2.404E+02	6.262E+02	6.200E+02	2.163E+02	2.165E+02	2.005E+04	-1.355E+01
27000	3.566E+01	2.417E+02	6.614E+02	6.552E+02	2.172E+02	2.174E+02	2.016E+04	-1.205E+01
28000	3.651E+01	2.430E+02	6.975E+02	6.913E+02	2.181E+02	2.183E+02	2.026E+04	-1.065E+01
29000	3.725E+01	2.443E+02	7.344E+02	7.282E+02	2.190E+02	2.192E+02	2.037E+04	-9.346E+00
30000	3.787E+01	2.456E+02	7.719E+02	7.657E+02	2.198E+02	2.200E+02	2.048E+04	-8.120E+00
32000	3.878E+01	2.480E+02	8.486E+02	8.424E+02	2.215E+02	2.217E+02	2.070E+04	-5.880E+00
34000	3.929E+01	2.504E+02	9.268E+02	9.206E+02	2.232E+02	2.233E+02	2.092E+04	-3.882E+00
36000	3.947E+01	2.527E+02	1.006E+03	9.994E+02	2.247E+02	2.249E+02	2.114E+04	-2.087E+00
38000	3.939E+01	2.548E+02	1.084E+03	1.078E+03	2.263E+02	2.264E+02	2.136E+04	-4.650E-01
40000	3.912E+01	2.568E+02	1.163E+03	1.157E+03	2.277E+02	2.279E+02	2.158E+04	1.010E+00
42000	3.873E+01	2.587E+02	1.241E+03	1.235E+03	2.292E+02	2.293E+02	2.180E+04	2.359E+00
44000	3.825E+01	2.605E+02	1.318E+03	1.312E+03	2.306E+02	2.307E+02	2.202E+04	3.598E+00
46000	3.773E+01	2.622E+02	1.394E+03	1.388E+03	2.319E+02	2.320E+02	2.224E+04	4.740E+00
48000	3.719E+01	2.638E+02	1.469E+03	1.463E+03	2.332E+02	2.333E+02	2.246E+04	5.797E+00
50000	3.666E+01	2.653E+02	1.543E+03	1.536E+03	2.344E+02	2.346E+02	2.268E+04	6.779E+00

Table 197: Internal thermodynamic properties of O^{4+} ΔE=500 cm^{-1}

T(K)	Q_{int}	$\ln(Q_{int})$	E_{int}/RT	$C_{p,int}/R$
50	$1.000E+00$	$0.000E+00$	$0.000E+00$	$0.000E+00$
100	$1.000E+00$	$0.000E+00$	$0.000E+00$	$0.000E+00$
150	$1.000E+00$	$0.000E+00$	$0.000E+00$	$0.000E+00$
200	$1.000E+00$	$0.000E+00$	$3.735E-254$	$2.209E-251$
298.15	$1.000E+00$	$0.000E+00$	$9.772E-170$	$3.880E-167$
300	$1.000E+00$	$0.000E+00$	$1.123E-168$	$4.433E-166$
400	$1.000E+00$	$0.000E+00$	$5.936E-126$	$1.757E-123$
500	$1.000E+00$	$0.000E+00$	$2.474E-100$	$5.861E-98$
600	$1.000E+00$	$0.000E+00$	$2.901E-83$	$5.727E-81$
700	$1.000E+00$	$0.000E+00$	$4.427E-71$	$7.493E-69$
800	$1.000E+00$	$0.000E+00$	$5.986E-62$	$8.866E-60$
900	$1.000E+00$	$0.000E+00$	$7.474E-55$	$9.841E-53$
1000	$1.000E+00$	$0.000E+00$	$3.518E-49$	$4.169E-47$
2000	$1.000E+00$	$0.000E+00$	$9.610E-24$	$5.696E-22$
3000	$1.000E+00$	$0.000E+00$	$2.440E-15$	$9.641E-14$
4000	$1.000E+00$	$1.206E-12$	$3.573E-11$	$1.059E-09$
5000	$1.000E+00$	$4.526E-10$	$1.073E-08$	$2.545E-07$
6000	$1.000E+00$	$2.355E-08$	$4.654E-07$	$9.196E-06$
7000	$1.000E+00$	$3.963E-07$	$6.712E-06$	$1.137E-04$
8000	$1.000E+00$	$3.292E-06$	$4.879E-05$	$7.232E-04$
9000	$1.000E+00$	$1.709E-05$	$2.251E-04$	$2.966E-03$
10000	$1.000E+00$	$6.380E-05$	$7.564E-04$	$8.968E-03$
11000	$1.000E+00$	$1.875E-04$	$2.020E-03$	$2.177E-02$
12000	$1.000E+00$	$4.602E-04$	$4.546E-03$	$4.490E-02$
13000	$1.001E+00$	$9.839E-04$	$8.970E-03$	$8.174E-02$
14000	$1.002E+00$	$1.887E-03$	$1.597E-02$	$1.350E-01$
15000	$1.003E+00$	$3.316E-03$	$2.618E-02$	$2.063E-01$
16000	$1.005E+00$	$5.430E-03$	$4.014E-02$	$2.961E-01$
17000	$1.008E+00$	$8.386E-03$	$5.827E-02$	$4.034E-01$
18000	$1.012E+00$	$1.233E-02$	$8.080E-02$	$5.265E-01$
19000	$1.018E+00$	$1.740E-02$	$1.078E-01$	$6.624E-01$
20000	$1.024E+00$	$2.371E-02$	$1.391E-01$	$8.077E-01$
21000	$1.032E+00$	$3.134E-02$	$1.745E-01$	$9.587E-01$
22000	$1.041E+00$	$4.035E-02$	$2.137E-01$	$1.112E+00$
23000	$1.052E+00$	$5.077E-02$	$2.560E-01$	$1.263E+00$
24000	$1.065E+00$	$6.261E-02$	$3.010E-01$	$1.408E+00$
25000	$1.079E+00$	$7.584E-02$	$3.481E-01$	$1.546E+00$
26000	$1.095E+00$	$9.044E-02$	$3.966E-01$	$1.673E+00$
27000	$1.112E+00$	$1.063E-01$	$4.461E-01$	$1.789E+00$
28000	$1.131E+00$	$1.235E-01$	$4.959E-01$	$1.891E+00$
29000	$1.152E+00$	$1.417E-01$	$5.456E-01$	$1.980E+00$
30000	$1.175E+00$	$1.611E-01$	$5.947E-01$	$2.054E+00$
32000	$1.224E+00$	$2.025E-01$	$6.896E-01$	$2.164E+00$
34000	$1.280E+00$	$2.470E-01$	$7.784E-01$	$2.225E+00$
36000	$1.342E+00$	$2.938E-01$	$8.595E-01$	$2.247E+00$
38000	$1.408E+00$	$3.423E-01$	$9.324E-01$	$2.237E+00$
40000	$1.480E+00$	$3.918E-01$	$9.969E-01$	$2.205E+00$
42000	$1.556E+00$	$4.418E-01$	$1.053E+00$	$2.158E+00$
44000	$1.636E+00$	$4.920E-01$	$1.102E+00$	$2.100E+00$
46000	$1.719E+00$	$5.419E-01$	$1.144E+00$	$2.038E+00$
48000	$1.807E+00$	$5.914E-01$	$1.180E+00$	$1.973E+00$
50000	$1.897E+00$	$6.402E-01$	$1.211E+00$	$1.908E+00$

Table 198: Total thermodynamic properties of O^{4+} ΔE=500 cm^{-1}

T [K]	C_p [J/mol/K]	S^0 [J/mol/K]	$H^0(T)-H^0(0)$ [KJ/mol]	$H^0(T)-H^0(298)$ [KJ/mol]	$-(G^0-H^0(0))/T$ [J/mol/K]	$-(G^0-H^0(298))/T$ [J/mol/K]	ΔH_f [KJ/mol]	$Log(K_p)$
50	2.079E+01	1.063E+02	1.039E+00	-5.158E+00	8.553E+01	2.095E+02	1.773E+04	-1.852E+04
100	2.079E+01	1.207E+02	2.079E+00	-4.119E+00	9.994E+01	1.619E+02	1.773E+04	-9.261E+03
150	2.079E+01	1.292E+02	3.118E+00	-3.079E+00	1.084E+02	1.497E+02	1.774E+04	-6.173E+03
200	2.079E+01	1.351E+02	4.157E+00	-2.040E+00	1.143E+02	1.453E+02	1.774E+04	-4.629E+03
298.15	2.079E+01	1.434E+02	6.197E+00	0.000E+00	1.227E+02	1.434E+02	1.775E+04	-3.103E+03
300	2.079E+01	1.436E+02	6.236E+00	3.848E-02	1.228E+02	1.434E+02	1.775E+04	-3.084E+03
400	2.079E+01	1.495E+02	8.315E+00	2.117E+00	1.288E+02	1.442E+02	1.776E+04	-2.311E+03
500	2.079E+01	1.542E+02	1.039E+01	4.196E+00	1.334E+02	1.458E+02	1.777E+04	-1.847E+03
600	2.079E+01	1.580E+02	1.247E+01	6.274E+00	1.372E+02	1.475E+02	1.778E+04	-1.538E+03
700	2.079E+01	1.612E+02	1.455E+01	8.353E+00	1.404E+02	1.492E+02	1.779E+04	-1.317E+03
800	2.079E+01	1.639E+02	1.663E+01	1.043E+01	1.432E+02	1.509E+02	1.780E+04	-1.151E+03
900	2.079E+01	1.664E+02	1.871E+01	1.251E+01	1.456E+02	1.525E+02	1.780E+04	-1.022E+03
1000	2.079E+01	1.686E+02	2.079E+01	1.459E+01	1.478E+02	1.540E+02	1.781E+04	-9.183E+02
2000	2.079E+01	1.830E+02	4.157E+01	3.538E+01	1.622E+02	1.653E+02	1.790E+04	-4.522E+02
3000	2.079E+01	1.914E+02	6.236E+01	5.616E+01	1.706E+02	1.727E+02	1.798E+04	-2.961E+02
4000	2.079E+01	1.974E+02	8.314E+01	7.695E+01	1.766E+02	1.782E+02	1.807E+04	-2.177E+02
5000	2.079E+01	2.020E+02	1.039E+02	9.773E+01	1.813E+02	1.825E+02	1.815E+04	-1.704E+02
6000	2.079E+01	2.058E+02	1.247E+02	1.185E+02	1.850E+02	1.861E+02	1.823E+04	-1.387E+02
7000	2.079E+01	2.090E+02	1.455E+02	1.393E+02	1.882E+02	1.891E+02	1.831E+04	-1.160E+02
8000	2.079E+01	2.118E+02	1.663E+02	1.601E+02	1.910E+02	1.918E+02	1.839E+04	-9.889E+01
9000	2.081E+01	2.143E+02	1.871E+02	1.809E+02	1.935E+02	1.942E+02	1.848E+04	-8.552E+01
10000	2.086E+01	2.165E+02	2.079E+02	2.017E+02	1.957E+02	1.963E+02	1.856E+04	-7.477E+01
11000	2.097E+01	2.184E+02	2.288E+02	2.226E+02	1.977E+02	1.982E+02	1.864E+04	-6.594E+01
12000	2.116E+01	2.203E+02	2.499E+02	2.437E+02	1.995E+02	2.000E+02	1.873E+04	-5.855E+01
13000	2.147E+01	2.220E+02	2.712E+02	2.650E+02	2.011E+02	2.016E+02	1.881E+04	-5.226E+01
14000	2.191E+01	2.236E+02	2.929E+02	2.867E+02	2.027E+02	2.031E+02	1.890E+04	-4.685E+01
15000	2.250E+01	2.251E+02	3.151E+02	3.089E+02	2.041E+02	2.045E+02	1.899E+04	-4.214E+01
16000	2.325E+01	2.266E+02	3.379E+02	3.317E+02	2.055E+02	2.059E+02	1.908E+04	-3.800E+01
17000	2.414E+01	2.280E+02	3.616E+02	3.554E+02	2.068E+02	2.071E+02	1.917E+04	-3.433E+01
18000	2.516E+01	2.294E+02	3.862E+02	3.801E+02	2.080E+02	2.083E+02	1.926E+04	-3.105E+01
19000	2.629E+01	2.308E+02	4.120E+02	4.058E+02	2.092E+02	2.095E+02	1.936E+04	-2.810E+01
20000	2.750E+01	2.322E+02	4.389E+02	4.327E+02	2.103E+02	2.106E+02	1.945E+04	-2.543E+01
21000	2.876E+01	2.336E+02	4.670E+02	4.608E+02	2.113E+02	2.116E+02	1.955E+04	-2.301E+01
22000	3.003E+01	2.349E+02	4.964E+02	4.902E+02	2.124E+02	2.127E+02	1.964E+04	-2.079E+01
23000	3.128E+01	2.363E+02	5.270E+02	5.208E+02	2.134E+02	2.137E+02	1.974E+04	-1.876E+01
24000	3.250E+01	2.377E+02	5.589E+02	5.527E+02	2.144E+02	2.146E+02	1.985E+04	-1.689E+01
25000	3.364E+01	2.390E+02	5.920E+02	5.858E+02	2.153E+02	2.156E+02	1.995E+04	-1.515E+01
26000	3.470E+01	2.404E+02	6.262E+02	6.200E+02	2.163E+02	2.165E+02	2.005E+04	-1.355E+01
27000	3.566E+01	2.417E+02	6.614E+02	6.552E+02	2.172E+02	2.174E+02	2.016E+04	-1.205E+01
28000	3.651E+01	2.430E+02	6.975E+02	6.913E+02	2.181E+02	2.183E+02	2.026E+04	-1.065E+01
29000	3.725E+01	2.443E+02	7.344E+02	7.282E+02	2.190E+02	2.192E+02	2.037E+04	-9.346E+00
30000	3.787E+01	2.456E+02	7.719E+02	7.657E+02	2.198E+02	2.200E+02	2.048E+04	-8.120E+00
32000	3.878E+01	2.480E+02	8.486E+02	8.424E+02	2.215E+02	2.217E+02	2.070E+04	-5.880E+00
34000	3.929E+01	2.504E+02	9.268E+02	9.206E+02	2.232E+02	2.233E+02	2.092E+04	-3.882E+00
36000	3.947E+01	2.527E+02	1.006E+03	9.994E+02	2.247E+02	2.249E+02	2.114E+04	-2.087E+00
38000	3.939E+01	2.548E+02	1.084E+03	1.078E+03	2.263E+02	2.264E+02	2.136E+04	-4.650E-01
40000	3.912E+01	2.568E+02	1.163E+03	1.157E+03	2.277E+02	2.279E+02	2.158E+04	1.010E+00
42000	3.873E+01	2.587E+02	1.241E+03	1.235E+03	2.292E+02	2.293E+02	2.180E+04	2.359E+00
44000	3.825E+01	2.605E+02	1.318E+03	1.312E+03	2.306E+02	2.307E+02	2.202E+04	3.598E+00
46000	3.773E+01	2.622E+02	1.394E+03	1.388E+03	2.319E+02	2.320E+02	2.224E+04	4.740E+00
48000	3.719E+01	2.638E+02	1.469E+03	1.463E+03	2.332E+02	2.333E+02	2.246E+04	5.797E+00
50000	3.665E+01	2.653E+02	1.543E+03	1.536E+03	2.344E+02	2.346E+02	2.268E+04	6.779E+00

Table 199: Internal thermodynamic properties of O^{4+} ΔE=1000 cm^{-1}

T(K)	Q_{int}	$\ln(Q_{int})$	E_{int}/RT	$C_{p,int}/R$
50	$1.000E+00$	$0.000E+00$	$0.000E+00$	$0.000E+00$
100	$1.000E+00$	$0.000E+00$	$0.000E+00$	$0.000E+00$
150	$1.000E+00$	$0.000E+00$	$0.000E+00$	$0.000E+00$
200	$1.000E+00$	$0.000E+00$	$3.735E-254$	$2.209E-251$
298.15	$1.000E+00$	$0.000E+00$	$9.772E-170$	$3.880E-167$
300	$1.000E+00$	$0.000E+00$	$1.123E-168$	$4.433E-166$
400	$1.000E+00$	$0.000E+00$	$5.936E-126$	$1.757E-123$
500	$1.000E+00$	$0.000E+00$	$2.474E-100$	$5.861E-98$
600	$1.000E+00$	$0.000E+00$	$2.901E-83$	$5.727E-81$
700	$1.000E+00$	$0.000E+00$	$4.427E-71$	$7.493E-69$
800	$1.000E+00$	$0.000E+00$	$5.986E-62$	$8.866E-60$
900	$1.000E+00$	$0.000E+00$	$7.474E-55$	$9.841E-53$
1000	$1.000E+00$	$0.000E+00$	$3.518E-49$	$4.169E-47$
2000	$1.000E+00$	$0.000E+00$	$9.610E-24$	$5.696E-22$
3000	$1.000E+00$	$0.000E+00$	$2.440E-15$	$9.641E-14$
4000	$1.000E+00$	$1.206E-12$	$3.573E-11$	$1.059E-09$
5000	$1.000E+00$	$4.526E-10$	$1.073E-08$	$2.545E-07$
6000	$1.000E+00$	$2.355E-08$	$4.654E-07$	$9.196E-06$
7000	$1.000E+00$	$3.963E-07$	$6.712E-06$	$1.137E-04$
8000	$1.000E+00$	$3.292E-06$	$4.879E-05$	$7.232E-04$
9000	$1.000E+00$	$1.709E-05$	$2.251E-04$	$2.966E-03$
10000	$1.000E+00$	$6.380E-05$	$7.564E-04$	$8.968E-03$
11000	$1.000E+00$	$1.875E-04$	$2.020E-03$	$2.177E-02$
12000	$1.000E+00$	$4.602E-04$	$4.546E-03$	$4.490E-02$
13000	$1.001E+00$	$9.839E-04$	$8.970E-03$	$8.174E-02$
14000	$1.002E+00$	$1.887E-03$	$1.597E-02$	$1.350E-01$
15000	$1.003E+00$	$3.316E-03$	$2.618E-02$	$2.063E-01$
16000	$1.005E+00$	$5.430E-03$	$4.014E-02$	$2.961E-01$
17000	$1.008E+00$	$8.386E-03$	$5.827E-02$	$4.034E-01$
18000	$1.012E+00$	$1.233E-02$	$8.080E-02$	$5.265E-01$
19000	$1.018E+00$	$1.740E-02$	$1.078E-01$	$6.624E-01$
20000	$1.024E+00$	$2.371E-02$	$1.391E-01$	$8.077E-01$
21000	$1.032E+00$	$3.134E-02$	$1.745E-01$	$9.587E-01$
22000	$1.041E+00$	$4.035E-02$	$2.137E-01$	$1.112E+00$
23000	$1.052E+00$	$5.077E-02$	$2.560E-01$	$1.263E+00$
24000	$1.065E+00$	$6.261E-02$	$3.010E-01$	$1.408E+00$
25000	$1.079E+00$	$7.584E-02$	$3.481E-01$	$1.546E+00$
26000	$1.095E+00$	$9.044E-02$	$3.966E-01$	$1.673E+00$
27000	$1.112E+00$	$1.063E-01$	$4.461E-01$	$1.789E+00$
28000	$1.131E+00$	$1.235E-01$	$4.959E-01$	$1.891E+00$
29000	$1.152E+00$	$1.417E-01$	$5.456E-01$	$1.980E+00$
30000	$1.175E+00$	$1.611E-01$	$5.947E-01$	$2.054E+00$
32000	$1.224E+00$	$2.025E-01$	$6.896E-01$	$2.164E+00$
34000	$1.280E+00$	$2.470E-01$	$7.784E-01$	$2.225E+00$
36000	$1.342E+00$	$2.938E-01$	$8.595E-01$	$2.247E+00$
38000	$1.408E+00$	$3.423E-01$	$9.324E-01$	$2.237E+00$
40000	$1.480E+00$	$3.918E-01$	$9.969E-01$	$2.205E+00$
42000	$1.556E+00$	$4.418E-01$	$1.053E+00$	$2.158E+00$
44000	$1.636E+00$	$4.920E-01$	$1.102E+00$	$2.100E+00$
46000	$1.719E+00$	$5.419E-01$	$1.144E+00$	$2.038E+00$
48000	$1.807E+00$	$5.914E-01$	$1.180E+00$	$1.973E+00$
50000	$1.897E+00$	$6.402E-01$	$1.211E+00$	$1.907E+00$

Table 200: Total thermodynamic properties of O^{4+} ΔE=1000 cm^{-1}

T [K]	C_p [J/mol/K]	S^0 [J/mol/K]	$H^0(T)-H^0(0)$ [KJ/mol]	$H^0(T)-H^0(298)$ [KJ/mol]	$-(G^0-H^0(0))/T$ [J/mol/K]	$-(G^0-H^0(298))/T$ [J/mol/K]	ΔH_f [KJ/mol]	$Log(K_p)$
50	2.079E+01	1.063E+02	1.039E+00	-5.158E+00	8.553E+01	2.095E+02	1.773E+04	-1.852E+04
100	2.079E+01	1.207E+02	2.079E+00	-4.119E+00	9.994E+01	1.619E+02	1.773E+04	-9.261E+03
150	2.079E+01	1.292E+02	3.118E+00	-3.079E+00	1.084E+02	1.497E+02	1.774E+04	-6.173E+03
200	2.079E+01	1.351E+02	4.157E+00	-2.040E+00	1.143E+02	1.453E+02	1.774E+04	-4.629E+03
298.15	2.079E+01	1.434E+02	6.197E+00	0.000E+00	1.227E+02	1.434E+02	1.775E+04	-3.103E+03
300	2.079E+01	1.436E+02	6.236E+00	3.848E-02	1.228E+02	1.434E+02	1.775E+04	-3.084E+03
400	2.079E+01	1.495E+02	8.315E+00	2.117E+00	1.288E+02	1.442E+02	1.776E+04	-2.311E+03
500	2.079E+01	1.542E+02	1.039E+01	4.196E+00	1.334E+02	1.458E+02	1.777E+04	-1.847E+03
600	2.079E+01	1.580E+02	1.247E+01	6.274E+00	1.372E+02	1.475E+02	1.778E+04	-1.538E+03
700	2.079E+01	1.612E+02	1.455E+01	8.353E+00	1.404E+02	1.492E+02	1.779E+04	-1.317E+03
800	2.079E+01	1.639E+02	1.663E+01	1.043E+01	1.432E+02	1.509E+02	1.780E+04	-1.151E+03
900	2.079E+01	1.664E+02	1.871E+01	1.251E+01	1.456E+02	1.525E+02	1.780E+04	-1.022E+03
1000	2.079E+01	1.686E+02	2.079E+01	1.459E+01	1.478E+02	1.540E+02	1.781E+04	-9.183E+02
2000	2.079E+01	1.830E+02	4.157E+01	3.538E+01	1.622E+02	1.653E+02	1.790E+04	-4.522E+02
3000	2.079E+01	1.914E+02	6.236E+01	5.616E+01	1.706E+02	1.727E+02	1.798E+04	-2.961E+02
4000	2.079E+01	1.974E+02	8.314E+01	7.695E+01	1.766E+02	1.782E+02	1.807E+04	-2.177E+02
5000	2.079E+01	2.020E+02	1.039E+02	9.773E+01	1.813E+02	1.825E+02	1.815E+04	-1.704E+02
6000	2.079E+01	2.058E+02	1.247E+02	1.185E+02	1.850E+02	1.861E+02	1.823E+04	-1.387E+02
7000	2.079E+01	2.090E+02	1.455E+02	1.393E+02	1.882E+02	1.891E+02	1.831E+04	-1.160E+02
8000	2.079E+01	2.118E+02	1.663E+02	1.601E+02	1.910E+02	1.918E+02	1.839E+04	-9.889E+01
9000	2.081E+01	2.143E+02	1.871E+02	1.809E+02	1.935E+02	1.942E+02	1.848E+04	-8.552E+01
10000	2.086E+01	2.165E+02	2.079E+02	2.017E+02	1.957E+02	1.963E+02	1.856E+04	-7.477E+01
11000	2.097E+01	2.184E+02	2.288E+02	2.226E+02	1.977E+02	1.982E+02	1.864E+04	-6.594E+01
12000	2.116E+01	2.203E+02	2.499E+02	2.437E+02	1.995E+02	2.000E+02	1.873E+04	-5.855E+01
13000	2.147E+01	2.220E+02	2.712E+02	2.650E+02	2.011E+02	2.016E+02	1.881E+04	-5.226E+01
14000	2.191E+01	2.236E+02	2.929E+02	2.867E+02	2.027E+02	2.031E+02	1.890E+04	-4.685E+01
15000	2.250E+01	2.251E+02	3.151E+02	3.089E+02	2.041E+02	2.045E+02	1.899E+04	-4.214E+01
16000	2.325E+01	2.266E+02	3.379E+02	3.317E+02	2.055E+02	2.059E+02	1.908E+04	-3.800E+01
17000	2.414E+01	2.280E+02	3.616E+02	3.554E+02	2.068E+02	2.071E+02	1.917E+04	-3.433E+01
18000	2.516E+01	2.294E+02	3.862E+02	3.801E+02	2.080E+02	2.083E+02	1.926E+04	-3.105E+01
19000	2.629E+01	2.308E+02	4.120E+02	4.058E+02	2.092E+02	2.095E+02	1.936E+04	-2.810E+01
20000	2.750E+01	2.322E+02	4.389E+02	4.327E+02	2.103E+02	2.106E+02	1.945E+04	-2.543E+01
21000	2.876E+01	2.336E+02	4.670E+02	4.608E+02	2.113E+02	2.116E+02	1.955E+04	-2.301E+01
22000	3.003E+01	2.349E+02	4.964E+02	4.902E+02	2.124E+02	2.127E+02	1.964E+04	-2.079E+01
23000	3.128E+01	2.363E+02	5.270E+02	5.208E+02	2.134E+02	2.137E+02	1.974E+04	-1.876E+01
24000	3.250E+01	2.377E+02	5.589E+02	5.527E+02	2.144E+02	2.146E+02	1.985E+04	-1.689E+01
25000	3.364E+01	2.390E+02	5.920E+02	5.858E+02	2.153E+02	2.156E+02	1.995E+04	-1.515E+01
26000	3.470E+01	2.404E+02	6.262E+02	6.200E+02	2.163E+02	2.165E+02	2.005E+04	-1.355E+01
27000	3.566E+01	2.417E+02	6.614E+02	6.552E+02	2.172E+02	2.174E+02	2.016E+04	-1.205E+01
28000	3.651E+01	2.430E+02	6.975E+02	6.913E+02	2.181E+02	2.183E+02	2.026E+04	-1.065E+01
29000	3.725E+01	2.443E+02	7.344E+02	7.282E+02	2.190E+02	2.192E+02	2.037E+04	-9.346E+00
30000	3.787E+01	2.456E+02	7.719E+02	7.657E+02	2.198E+02	2.200E+02	2.048E+04	-8.120E+00
32000	3.878E+01	2.480E+02	8.486E+02	8.424E+02	2.215E+02	2.217E+02	2.070E+04	-5.880E+00
34000	3.929E+01	2.504E+02	9.268E+02	9.206E+02	2.232E+02	2.233E+02	2.092E+04	-3.882E+00
36000	3.947E+01	2.527E+02	1.006E+03	9.994E+02	2.247E+02	2.249E+02	2.114E+04	-2.087E+00
38000	3.939E+01	2.548E+02	1.084E+03	1.078E+03	2.263E+02	2.264E+02	2.136E+04	-4.650E-01
40000	3.912E+01	2.568E+02	1.163E+03	1.157E+03	2.277E+02	2.279E+02	2.158E+04	1.010E+00
42000	3.873E+01	2.587E+02	1.241E+03	1.235E+03	2.292E+02	2.293E+02	2.180E+04	2.359E+00
44000	3.825E+01	2.605E+02	1.318E+03	1.312E+03	2.306E+02	2.307E+02	2.202E+04	3.598E+00
46000	3.773E+01	2.622E+02	1.394E+03	1.388E+03	2.319E+02	2.320E+02	2.224E+04	4.740E+00
48000	3.719E+01	2.638E+02	1.469E+03	1.463E+03	2.332E+02	2.333E+02	2.246E+04	5.797E+00
50000	3.665E+01	2.653E+02	1.543E+03	1.536E+03	2.344E+02	2.346E+02	2.268E+04	6.779E+00

Table 201: Internal thermodynamic properties of O^-

T(K)	Q_{int}	$\ln(Q_{int})$	E_{int}/RT	$C_{p,int}/R$
50	$4.012E+00$	$1.389E+00$	$1.555E-02$	$7.902E-02$
100	$4.157E+00$	$1.425E+00$	$9.594E-02$	$2.352E-01$
150	$4.366E+00$	$1.474E+00$	$1.424E-01$	$2.215E-01$
200	$4.559E+00$	$1.517E+00$	$1.563E-01$	$1.747E-01$
298.15	$4.851E+00$	$1.579E+00$	$1.499E-01$	$1.056E-01$
300	$4.855E+00$	$1.580E+00$	$1.496E-01$	$1.047E-01$
400	$5.058E+00$	$1.621E+00$	$1.332E-01$	$6.710E-02$
500	$5.202E+00$	$1.649E+00$	$1.177E-01$	$4.612E-02$
600	$5.308E+00$	$1.669E+00$	$1.046E-01$	$3.348E-02$
700	$5.390E+00$	$1.685E+00$	$9.385E-02$	$2.535E-02$
800	$5.455E+00$	$1.696E+00$	$8.492E-02$	$1.983E-02$
900	$5.507E+00$	$1.706E+00$	$7.746E-02$	$1.593E-02$
1000	$5.550E+00$	$1.714E+00$	$7.116E-02$	$1.307E-02$
2000	$5.761E+00$	$1.751E+00$	$3.905E-02$	$4.714E-03$
3000	$5.840E+00$	$1.765E+00$	$3.019E-02$	$2.820E-02$
4000	$5.895E+00$	$1.774E+00$	$3.811E-02$	$1.033E-01$
5000	$5.958E+00$	$1.785E+00$	$6.130E-02$	$2.062E-01$
6000	$6.042E+00$	$1.799E+00$	$9.372E-02$	$3.022E-01$
7000	$6.146E+00$	$1.816E+00$	$1.289E-01$	$3.734E-01$
8000	$6.267E+00$	$1.835E+00$	$1.625E-01$	$4.168E-01$
9000	$6.399E+00$	$1.856E+00$	$1.920E-01$	$4.364E-01$
10000	$6.539E+00$	$1.878E+00$	$2.167E-01$	$4.385E-01$
11000	$6.682E+00$	$1.899E+00$	$2.365E-01$	$4.289E-01$
12000	$6.825E+00$	$1.921E+00$	$2.519E-01$	$4.121E-01$
13000	$6.968E+00$	$1.941E+00$	$2.634E-01$	$3.912E-01$
14000	$7.107E+00$	$1.961E+00$	$2.717E-01$	$3.684E-01$
15000	$7.243E+00$	$1.980E+00$	$2.774E-01$	$3.452E-01$
16000	$7.375E+00$	$1.998E+00$	$2.809E-01$	$3.225E-01$
17000	$7.502E+00$	$2.015E+00$	$2.827E-01$	$3.008E-01$
18000	$7.624E+00$	$2.031E+00$	$2.831E-01$	$2.803E-01$
19000	$7.742E+00$	$2.047E+00$	$2.825E-01$	$2.612E-01$
20000	$7.855E+00$	$2.061E+00$	$2.810E-01$	$2.434E-01$
21000	$7.963E+00$	$2.075E+00$	$2.788E-01$	$2.271E-01$
22000	$8.066E+00$	$2.088E+00$	$2.761E-01$	$2.121E-01$
23000	$8.165E+00$	$2.100E+00$	$2.730E-01$	$1.983E-01$
24000	$8.260E+00$	$2.111E+00$	$2.696E-01$	$1.856E-01$
25000	$8.351E+00$	$2.122E+00$	$2.660E-01$	$1.740E-01$
26000	$8.438E+00$	$2.133E+00$	$2.623E-01$	$1.633E-01$
27000	$8.521E+00$	$2.143E+00$	$2.584E-01$	$1.535E-01$
28000	$8.601E+00$	$2.152E+00$	$2.545E-01$	$1.445E-01$
29000	$8.678E+00$	$2.161E+00$	$2.506E-01$	$1.362E-01$
30000	$8.751E+00$	$2.169E+00$	$2.466E-01$	$1.285E-01$
32000	$8.889E+00$	$2.185E+00$	$2.388E-01$	$1.149E-01$
34000	$9.017E+00$	$2.199E+00$	$2.312E-01$	$1.033E-01$
36000	$9.135E+00$	$2.212E+00$	$2.238E-01$	$9.322E-02$
38000	$9.244E+00$	$2.224E+00$	$2.167E-01$	$8.453E-02$
40000	$9.346E+00$	$2.235E+00$	$2.099E-01$	$7.696E-02$
42000	$9.441E+00$	$2.245E+00$	$2.034E-01$	$7.033E-02$
44000	$9.529E+00$	$2.254E+00$	$1.972E-01$	$6.451E-02$
46000	$9.612E+00$	$2.263E+00$	$1.913E-01$	$5.936E-02$
48000	$9.689E+00$	$2.271E+00$	$1.857E-01$	$5.479E-02$
50000	$9.762E+00$	$2.278E+00$	$1.804E-01$	$5.072E-02$

Table 202: Total thermodynamic properties of O^-

T [K]	C_p [J/mol/K]	S^0 [J/mol/K]	$H^0(T)-H^0(0)$ [KJ/mol]	$H^0(T)-H^0(298)$ [KJ/mol]	$-(G^0-H^0(0))/T$ [J/mol/K]	$-(G^0-H^0(298))/T$ [J/mol/K]	ΔH_f [KJ/mol]	$\mathrm{Log}(K_p)$
50	2.144E+01	1.180E+02	1.046E+00	-5.523E+00	9.708E+01	2.285E+02	9.094E+01	-9.200E+01
100	2.274E+01	1.334E+02	2.158E+00	-4.411E+00	1.118E+02	1.775E+02	9.029E+01	-4.463E+01
150	2.263E+01	1.426E+02	3.296E+00	-3.273E+00	1.206E+02	1.644E+02	8.966E+01	-2.896E+01
200	2.224E+01	1.491E+02	4.417E+00	-2.152E+00	1.270E+02	1.598E+02	8.901E+01	-2.118E+01
298.15	2.166E+01	1.578E+02	6.569E+00	0.000E+00	1.358E+02	1.578E+02	8.769E+01	-1.357E+01
300	2.166E+01	1.579E+02	6.609E+00	4.011E-02	1.359E+02	1.578E+02	8.767E+01	-1.348E+01
400	2.134E+01	1.641E+02	8.758E+00	2.189E+00	1.422E+02	1.587E+02	8.625E+01	-9.692E+00
500	2.117E+01	1.689E+02	1.088E+01	4.314E+00	1.471E+02	1.602E+02	8.477E+01	-7.457E+00
600	2.107E+01	1.727E+02	1.299E+01	6.425E+00	1.511E+02	1.620E+02	8.322E+01	-5.994E+00
700	2.100E+01	1.760E+02	1.510E+01	8.528E+00	1.544E+02	1.638E+02	8.162E+01	-4.968E+00
800	2.095E+01	1.788E+02	1.719E+01	1.062E+01	1.573E+02	1.655E+02	7.997E+01	-4.214E+00
900	2.092E+01	1.812E+02	1.929E+01	1.272E+01	1.598E+02	1.671E+02	7.828E+01	-3.640E+00
1000	2.089E+01	1.834E+02	2.138E+01	1.481E+01	1.621E+02	1.686E+02	7.656E+01	-3.190E+00
2000	2.083E+01	1.979E+02	4.222E+01	3.565E+01	1.768E+02	1.801E+02	5.837E+01	-1.371E+00
3000	2.102E+01	2.063E+02	6.311E+01	5.654E+01	1.853E+02	1.875E+02	3.900E+01	-9.354E-01
4000	2.164E+01	2.125E+02	8.441E+01	7.784E+01	1.914E+02	1.930E+02	1.906E+01	-8.048E-01
5000	2.250E+01	2.174E+02	1.065E+02	9.991E+01	1.961E+02	1.974E+02	-8.574E-01	-7.792E-01
6000	2.330E+01	2.216E+02	1.294E+02	1.228E+02	2.000E+02	2.011E+02	-2.050E+01	-7.968E-01
7000	2.389E+01	2.252E+02	1.530E+02	1.464E+02	2.033E+02	2.043E+02	-3.981E+01	-8.337E-01
8000	2.425E+01	2.284E+02	1.771E+02	1.705E+02	2.063E+02	2.071E+02	-5.870E+01	-8.793E-01
9000	2.441E+01	2.313E+02	2.014E+02	1.949E+02	2.089E+02	2.096E+02	-7.701E+01	-9.283E-01
10000	2.443E+01	2.339E+02	2.259E+02	2.193E+02	2.113E+02	2.119E+02	-9.461E+01	-9.779E-01
11000	2.435E+01	2.362E+02	2.503E+02	2.437E+02	2.134E+02	2.140E+02	-1.115E+02	-1.027E+00
12000	2.421E+01	2.383E+02	2.746E+02	2.680E+02	2.154E+02	2.160E+02	-1.275E+02	-1.074E+00
13000	2.404E+01	2.402E+02	2.987E+02	2.921E+02	2.173E+02	2.178E+02	-1.429E+02	-1.119E+00
14000	2.385E+01	2.420E+02	3.226E+02	3.161E+02	2.190E+02	2.194E+02	-1.577E+02	-1.162E+00
15000	2.366E+01	2.437E+02	3.464E+02	3.398E+02	2.206E+02	2.210E+02	-1.719E+02	-1.203E+00
16000	2.347E+01	2.452E+02	3.699E+02	3.634E+02	2.221E+02	2.225E+02	-1.857E+02	-1.242E+00
17000	2.329E+01	2.466E+02	3.933E+02	3.868E+02	2.234E+02	2.238E+02	-1.991E+02	-1.279E+00
18000	2.312E+01	2.479E+02	4.165E+02	4.100E+02	2.248E+02	2.251E+02	-2.121E+02	-1.314E+00
19000	2.296E+01	2.492E+02	4.396E+02	4.330E+02	2.260E+02	2.264E+02	-2.250E+02	-1.347E+00
20000	2.281E+01	2.503E+02	4.624E+02	4.559E+02	2.272E+02	2.275E+02	-2.376E+02	-1.379E+00
21000	2.268E+01	2.514E+02	4.852E+02	4.786E+02	2.283E+02	2.287E+02	-2.500E+02	-1.410E+00
22000	2.255E+01	2.525E+02	5.078E+02	5.012E+02	2.294E+02	2.297E+02	-2.623E+02	-1.438E+00
23000	2.243E+01	2.535E+02	5.303E+02	5.237E+02	2.304E+02	2.307E+02	-2.744E+02	-1.466E+00
24000	2.233E+01	2.544E+02	5.527E+02	5.461E+02	2.314E+02	2.317E+02	-2.864E+02	-1.493E+00
25000	2.223E+01	2.554E+02	5.750E+02	5.684E+02	2.324E+02	2.326E+02	-2.984E+02	-1.518E+00
26000	2.214E+01	2.562E+02	5.971E+02	5.906E+02	2.333E+02	2.335E+02	-3.102E+02	-1.543E+00
27000	2.206E+01	2.571E+02	6.192E+02	6.127E+02	2.341E+02	2.344E+02	-3.220E+02	-1.566E+00
28000	2.199E+01	2.579E+02	6.413E+02	6.347E+02	2.350E+02	2.352E+02	-3.338E+02	-1.589E+00
29000	2.192E+01	2.586E+02	6.632E+02	6.566E+02	2.358E+02	2.360E+02	-3.454E+02	-1.611E+00
30000	2.186E+01	2.594E+02	6.851E+02	6.785E+02	2.365E+02	2.368E+02	-3.570E+02	-1.632E+00
32000	2.174E+01	2.608E+02	7.287E+02	7.221E+02	2.380E+02	2.382E+02	-3.801E+02	-1.672E+00
34000	2.164E+01	2.621E+02	7.721E+02	7.655E+02	2.394E+02	2.396E+02	-4.030E+02	-1.709E+00
36000	2.156E+01	2.633E+02	8.153E+02	8.087E+02	2.407E+02	2.409E+02	-4.258E+02	-1.745E+00
38000	2.149E+01	2.645E+02	8.583E+02	8.518E+02	2.419E+02	2.421E+02	-4.485E+02	-1.778E+00
40000	2.143E+01	2.656E+02	9.012E+02	8.947E+02	2.431E+02	2.432E+02	-4.710E+02	-1.810E+00
42000	2.137E+01	2.666E+02	9.440E+02	9.375E+02	2.442E+02	2.443E+02	-4.935E+02	-1.840E+00
44000	2.132E+01	2.676E+02	9.867E+02	9.802E+02	2.452E+02	2.454E+02	-5.158E+02	-1.868E+00
46000	2.128E+01	2.686E+02	1.029E+03	1.023E+03	2.462E+02	2.463E+02	-5.381E+02	-1.895E+00
48000	2.124E+01	2.695E+02	1.072E+03	1.065E+03	2.472E+02	2.473E+02	-5.603E+02	-1.921E+00
50000	2.121E+01	2.704E+02	1.114E+03	1.108E+03	2.481E+02	2.482E+02	-5.824E+02	-1.946E+00

Table 203: Internal thermodynamic properties of O_2

T(K)	Q_{int}	$\ln(Q_{int})$	E_{int}/RT	$C_{p,int}/R$
50	$3.697E+01$	$3.610E+00$	$9.864E-01$	$1.000E+00$
100	$7.345E+01$	$4.297E+00$	$9.935E-01$	$1.001E+00$
150	$1.099E+02$	$4.700E+00$	$9.959E-01$	$1.001E+00$
200	$1.464E+02$	$4.987E+00$	$9.974E-01$	$1.003E+00$
298.15	$2.182E+02$	$5.386E+00$	$1.003E+00$	$1.033E+00$
300	$2.196E+02$	$5.392E+00$	$1.003E+00$	$1.034E+00$
400	$2.937E+02$	$5.682E+00$	$1.021E+00$	$1.121E+00$
500	$3.699E+02$	$5.913E+00$	$1.052E+00$	$1.240E+00$
600	$4.498E+02$	$6.109E+00$	$1.094E+00$	$1.360E+00$
700	$5.342E+02$	$6.281E+00$	$1.140E+00$	$1.467E+00$
800	$6.239E+02$	$6.436E+00$	$1.186E+00$	$1.558E+00$
900	$7.194E+02$	$6.578E+00$	$1.232E+00$	$1.633E+00$
1000	$8.209E+02$	$6.710E+00$	$1.275E+00$	$1.695E+00$
2000	$2.207E+03$	$7.699E+00$	$1.583E+00$	$2.046E+00$
3000	$4.362E+03$	$8.381E+00$	$1.783E+00$	$2.313E+00$
4000	$7.452E+03$	$8.916E+00$	$1.942E+00$	$2.518E+00$
5000	$1.166E+04$	$9.364E+00$	$2.074E+00$	$2.673E+00$
6000	$1.719E+04$	$9.752E+00$	$2.184E+00$	$2.792E+00$
7000	$2.425E+04$	$1.010E+01$	$2.276E+00$	$2.846E+00$
8000	$3.302E+04$	$1.040E+01$	$2.346E+00$	$2.813E+00$
9000	$4.365E+04$	$1.068E+01$	$2.392E+00$	$2.696E+00$
10000	$5.624E+04$	$1.094E+01$	$2.414E+00$	$2.520E+00$
11000	$7.080E+04$	$1.117E+01$	$2.414E+00$	$2.315E+00$
12000	$8.730E+04$	$1.138E+01$	$2.397E+00$	$2.104E+00$
13000	$1.057E+05$	$1.157E+01$	$2.367E+00$	$1.903E+00$
14000	$1.257E+05$	$1.174E+01$	$2.327E+00$	$1.719E+00$
15000	$1.474E+05$	$1.190E+01$	$2.281E+00$	$1.554E+00$
16000	$1.705E+05$	$1.205E+01$	$2.231E+00$	$1.410E+00$
17000	$1.949E+05$	$1.218E+01$	$2.179E+00$	$1.284E+00$
18000	$2.204E+05$	$1.230E+01$	$2.126E+00$	$1.175E+00$
19000	$2.469E+05$	$1.242E+01$	$2.073E+00$	$1.080E+00$
20000	$2.743E+05$	$1.252E+01$	$2.022E+00$	$9.966E-01$
21000	$3.023E+05$	$1.262E+01$	$1.971E+00$	$9.241E-01$
22000	$3.310E+05$	$1.271E+01$	$1.922E+00$	$8.604E-01$
23000	$3.601E+05$	$1.279E+01$	$1.875E+00$	$8.042E-01$
24000	$3.897E+05$	$1.287E+01$	$1.829E+00$	$7.542E-01$
25000	$4.195E+05$	$1.295E+01$	$1.785E+00$	$7.096E-01$
26000	$4.495E+05$	$1.302E+01$	$1.743E+00$	$6.696E-01$
27000	$4.797E+05$	$1.308E+01$	$1.702E+00$	$6.335E-01$
28000	$5.100E+05$	$1.314E+01$	$1.664E+00$	$6.008E-01$
29000	$5.403E+05$	$1.320E+01$	$1.626E+00$	$5.710E-01$
30000	$5.706E+05$	$1.325E+01$	$1.591E+00$	$5.437E-01$
32000	$6.309E+05$	$1.335E+01$	$1.524E+00$	$4.955E-01$
34000	$6.907E+05$	$1.345E+01$	$1.462E+00$	$4.543E-01$
36000	$7.497E+05$	$1.353E+01$	$1.405E+00$	$4.186E-01$
38000	$8.077E+05$	$1.360E+01$	$1.352E+00$	$3.874E-01$
40000	$8.646E+05$	$1.367E+01$	$1.303E+00$	$3.598E-01$
42000	$9.204E+05$	$1.373E+01$	$1.258E+00$	$3.352E-01$
44000	$9.748E+05$	$1.379E+01$	$1.215E+00$	$3.132E-01$
46000	$1.028E+06$	$1.384E+01$	$1.176E+00$	$2.933E-01$
48000	$1.080E+06$	$1.389E+01$	$1.139E+00$	$2.754E-01$
50000	$1.131E+06$	$1.394E+01$	$1.104E+00$	$2.591E-01$

Table 204: Total thermodynamic properties of O_2

T [K]	C_p [J/mol/K]	S^0 [J/mol/K]	$H^0(T)-H^0(0)$ [KJ/mol]	$H^0(T)-H^0(298)$ [KJ/mol]	$-(G^0-H^0(0))/T$ [J/mol/K]	$-(G^0-H^0(298))/T$ [J/mol/K]	ΔH_f [KJ/mol]	$\mathrm{Log}(K_p)$
50	2.910E+01	1.532E+02	1.449E+00	-7.234E+00	1.242E+02	2.979E+02	0.000E+00	0.000E+00
100	2.911E+01	1.733E+02	2.905E+00	-5.779E+00	1.443E+02	2.311E+02	0.000E+00	0.000E+00
150	2.911E+01	1.852E+02	4.360E+00	-4.323E+00	1.561E+02	2.140E+02	0.000E+00	0.000E+00
200	2.913E+01	1.935E+02	5.816E+00	-2.868E+00	1.644E+02	2.079E+02	0.000E+00	0.000E+00
298.15	2.938E+01	2.052E+02	8.683E+00	0.000E+00	1.761E+02	2.052E+02	0.000E+00	0.000E+00
300	2.939E+01	2.054E+02	8.738E+00	5.441E-02	1.762E+02	2.052E+02	0.000E+00	0.000E+00
400	3.011E+01	2.139E+02	1.171E+01	3.026E+00	1.847E+02	2.064E+02	0.000E+00	0.000E+00
500	3.109E+01	2.207E+02	1.477E+01	6.085E+00	1.912E+02	2.086E+02	0.000E+00	0.000E+00
600	3.209E+01	2.265E+02	1.793E+01	9.245E+00	1.966E+02	2.111E+02	0.000E+00	0.000E+00
700	3.298E+01	2.315E+02	2.118E+01	1.250E+01	2.013E+02	2.137E+02	0.000E+00	0.000E+00
800	3.374E+01	2.360E+02	2.452E+01	1.584E+01	2.053E+02	2.162E+02	0.000E+00	0.000E+00
900	3.436E+01	2.400E+02	2.793E+01	1.924E+01	2.089E+02	2.186E+02	0.000E+00	0.000E+00
1000	3.488E+01	2.436E+02	3.139E+01	2.270E+01	2.122E+02	2.209E+02	0.000E+00	0.000E+00
2000	3.780E+01	2.688E+02	6.789E+01	5.920E+01	2.349E+02	2.392E+02	0.000E+00	0.000E+00
3000	4.002E+01	2.846E+02	1.068E+02	9.814E+01	2.490E+02	2.519E+02	0.000E+00	0.000E+00
4000	4.172E+01	2.963E+02	1.477E+02	1.391E+02	2.594E+02	2.616E+02	0.000E+00	0.000E+00
5000	4.302E+01	3.058E+02	1.901E+02	1.814E+02	2.678E+02	2.695E+02	0.000E+00	0.000E+00
6000	4.400E+01	3.137E+02	2.337E+02	2.250E+02	2.748E+02	2.762E+02	0.000E+00	0.000E+00
7000	4.445E+01	3.206E+02	2.779E+02	2.693E+02	2.808E+02	2.821E+02	0.000E+00	0.000E+00
8000	4.418E+01	3.265E+02	3.223E+02	3.136E+02	2.862E+02	2.873E+02	0.000E+00	0.000E+00
9000	4.320E+01	3.316E+02	3.661E+02	3.574E+02	2.909E+02	2.919E+02	0.000E+00	0.000E+00
10000	4.174E+01	3.361E+02	4.086E+02	3.999E+02	2.952E+02	2.961E+02	0.000E+00	0.000E+00
11000	4.003E+01	3.400E+02	4.495E+02	4.408E+02	2.991E+02	2.999E+02	0.000E+00	0.000E+00
12000	3.828E+01	3.434E+02	4.886E+02	4.799E+02	3.027E+02	3.034E+02	0.000E+00	0.000E+00
13000	3.661E+01	3.464E+02	5.261E+02	5.174E+02	3.059E+02	3.066E+02	0.000E+00	0.000E+00
14000	3.508E+01	3.491E+02	5.619E+02	5.532E+02	3.089E+02	3.096E+02	0.000E+00	0.000E+00
15000	3.371E+01	3.514E+02	5.963E+02	5.876E+02	3.117E+02	3.123E+02	0.000E+00	0.000E+00
16000	3.251E+01	3.536E+02	6.294E+02	6.207E+02	3.142E+02	3.148E+02	0.000E+00	0.000E+00
17000	3.146E+01	3.555E+02	6.613E+02	6.527E+02	3.166E+02	3.171E+02	0.000E+00	0.000E+00
18000	3.055E+01	3.573E+02	6.923E+02	6.837E+02	3.188E+02	3.193E+02	0.000E+00	0.000E+00
19000	2.976E+01	3.589E+02	7.225E+02	7.138E+02	3.209E+02	3.214E+02	0.000E+00	0.000E+00
20000	2.907E+01	3.604E+02	7.519E+02	7.432E+02	3.228E+02	3.233E+02	0.000E+00	0.000E+00
21000	2.847E+01	3.618E+02	7.807E+02	7.720E+02	3.246E+02	3.251E+02	0.000E+00	0.000E+00
22000	2.794E+01	3.631E+02	8.089E+02	8.002E+02	3.264E+02	3.268E+02	0.000E+00	0.000E+00
23000	2.747E+01	3.644E+02	8.366E+02	8.279E+02	3.280E+02	3.284E+02	0.000E+00	0.000E+00
24000	2.706E+01	3.655E+02	8.638E+02	8.551E+02	3.295E+02	3.299E+02	0.000E+00	0.000E+00
25000	2.669E+01	3.666E+02	8.907E+02	8.820E+02	3.310E+02	3.314E+02	0.000E+00	0.000E+00
26000	2.635E+01	3.677E+02	9.172E+02	9.085E+02	3.324E+02	3.327E+02	0.000E+00	0.000E+00
27000	2.605E+01	3.687E+02	9.434E+02	9.347E+02	3.337E+02	3.340E+02	0.000E+00	0.000E+00
28000	2.578E+01	3.696E+02	9.693E+02	9.606E+02	3.350E+02	3.353E+02	0.000E+00	0.000E+00
29000	2.553E+01	3.705E+02	9.950E+02	9.863E+02	3.362E+02	3.365E+02	0.000E+00	0.000E+00
30000	2.531E+01	3.714E+02	1.020E+03	1.012E+03	3.374E+02	3.376E+02	0.000E+00	0.000E+00
32000	2.491E+01	3.730E+02	1.071E+03	1.062E+03	3.395E+02	3.398E+02	0.000E+00	0.000E+00
34000	2.456E+01	3.745E+02	1.120E+03	1.111E+03	3.415E+02	3.418E+02	0.000E+00	0.000E+00
36000	2.427E+01	3.759E+02	1.169E+03	1.160E+03	3.434E+02	3.436E+02	0.000E+00	0.000E+00
38000	2.401E+01	3.772E+02	1.217E+03	1.208E+03	3.451E+02	3.454E+02	0.000E+00	0.000E+00
40000	2.378E+01	3.784E+02	1.265E+03	1.256E+03	3.468E+02	3.470E+02	0.000E+00	0.000E+00
42000	2.357E+01	3.796E+02	1.312E+03	1.304E+03	3.483E+02	3.485E+02	0.000E+00	0.000E+00
44000	2.339E+01	3.807E+02	1.359E+03	1.351E+03	3.498E+02	3.500E+02	0.000E+00	0.000E+00
46000	2.323E+01	3.817E+02	1.406E+03	1.397E+03	3.511E+02	3.513E+02	0.000E+00	0.000E+00
48000	2.308E+01	3.827E+02	1.452E+03	1.444E+03	3.524E+02	3.526E+02	0.000E+00	0.000E+00
50000	2.294E+01	3.836E+02	1.498E+03	1.490E+03	3.536E+02	3.538E+02	0.000E+00	0.000E+00

Table 205: Internal thermodynamic properties of O_2^+

T(K)	Q_{int}	$\ln(Q_{int})$	E_{int}/RT	$C_{p,int}/R$
50	$4.202E+01$	$3.738E+00$	$9.839E-01$	$1.000E+00$
100	$8.336E+01$	$4.423E+00$	$9.922E-01$	$1.001E+00$
150	$1.247E+02$	$4.826E+00$	$9.950E-01$	$1.001E+00$
200	$1.661E+02$	$5.113E+00$	$9.965E-01$	$1.001E+00$
298.15	$2.474E+02$	$5.511E+00$	$9.992E-01$	$1.011E+00$
300	$2.489E+02$	$5.517E+00$	$9.992E-01$	$1.012E+00$
400	$3.321E+02$	$5.805E+00$	$1.007E+00$	$1.057E+00$
500	$4.165E+02$	$6.032E+00$	$1.025E+00$	$1.138E+00$
600	$5.032E+02$	$6.221E+00$	$1.052E+00$	$1.238E+00$
700	$5.933E+02$	$6.386E+00$	$1.086E+00$	$1.339E+00$
800	$6.875E+02$	$6.533E+00$	$1.123E+00$	$1.432E+00$
900	$7.865E+02$	$6.668E+00$	$1.162E+00$	$1.514E+00$
1000	$8.908E+02$	$6.792E+00$	$1.201E+00$	$1.584E+00$
2000	$2.264E+03$	$7.725E+00$	$1.495E+00$	$1.916E+00$
3000	$4.291E+03$	$8.364E+00$	$1.656E+00$	$2.027E+00$
4000	$7.013E+03$	$8.856E+00$	$1.758E+00$	$2.102E+00$
5000	$1.047E+04$	$9.257E+00$	$1.836E+00$	$2.204E+00$
6000	$1.473E+04$	$9.598E+00$	$1.911E+00$	$2.379E+00$
7000	$1.990E+04$	$9.899E+00$	$1.995E+00$	$2.633E+00$
8000	$2.614E+04$	$1.017E+01$	$2.093E+00$	$2.916E+00$
9000	$3.365E+04$	$1.042E+01$	$2.198E+00$	$3.159E+00$
10000	$4.265E+04$	$1.066E+01$	$2.303E+00$	$3.307E+00$
11000	$5.336E+04$	$1.088E+01$	$2.396E+00$	$3.340E+00$
12000	$6.595E+04$	$1.110E+01$	$2.473E+00$	$3.268E+00$
13000	$8.058E+04$	$1.130E+01$	$2.528E+00$	$3.117E+00$
14000	$9.732E+04$	$1.149E+01$	$2.564E+00$	$2.917E+00$
15000	$1.162E+05$	$1.166E+01$	$2.580E+00$	$2.694E+00$
16000	$1.373E+05$	$1.183E+01$	$2.580E+00$	$2.466E+00$
17000	$1.605E+05$	$1.199E+01$	$2.566E+00$	$2.245E+00$
18000	$1.857E+05$	$1.213E+01$	$2.543E+00$	$2.038E+00$
19000	$2.129E+05$	$1.227E+01$	$2.511E+00$	$1.849E+00$
20000	$2.420E+05$	$1.240E+01$	$2.474E+00$	$1.677E+00$
21000	$2.727E+05$	$1.252E+01$	$2.432E+00$	$1.524E+00$
22000	$3.051E+05$	$1.263E+01$	$2.388E+00$	$1.387E+00$
23000	$3.389E+05$	$1.273E+01$	$2.341E+00$	$1.265E+00$
24000	$3.740E+05$	$1.283E+01$	$2.294E+00$	$1.156E+00$
25000	$4.104E+05$	$1.292E+01$	$2.247E+00$	$1.060E+00$
26000	$4.477E+05$	$1.301E+01$	$2.199E+00$	$9.742E-01$
27000	$4.861E+05$	$1.309E+01$	$2.153E+00$	$8.976E-01$
28000	$5.252E+05$	$1.317E+01$	$2.106E+00$	$8.292E-01$
29000	$5.651E+05$	$1.324E+01$	$2.061E+00$	$7.678E-01$
30000	$6.055E+05$	$1.331E+01$	$2.017E+00$	$7.127E-01$
32000	$6.878E+05$	$1.344E+01$	$1.933E+00$	$6.183E-01$
34000	$7.715E+05$	$1.356E+01$	$1.853E+00$	$5.409E-01$
36000	$8.558E+05$	$1.366E+01$	$1.778E+00$	$4.769E-01$
38000	$9.404E+05$	$1.375E+01$	$1.708E+00$	$4.234E-01$
40000	$1.025E+06$	$1.384E+01$	$1.643E+00$	$3.782E-01$
42000	$1.109E+06$	$1.392E+01$	$1.582E+00$	$3.398E-01$
44000	$1.192E+06$	$1.399E+01$	$1.525E+00$	$3.070E-01$
46000	$1.274E+06$	$1.406E+01$	$1.471E+00$	$2.786E-01$
48000	$1.355E+06$	$1.412E+01$	$1.421E+00$	$2.539E-01$
50000	$1.434E+06$	$1.418E+01$	$1.374E+00$	$2.324E-01$

Table 206: Total thermodynamic properties of O_2^+

T [K]	C_p [J/mol/K]	S^0 [J/mol/K]	$H^0(T)-H^0(0)$ [KJ/mol]	$H^0(T)-H^0(298)$ [KJ/mol]	$-(G^0-H^0(0))/T$ [J/mol/K]	$-(G^0-H^0(298))/T$ [J/mol/K]	ΔH_f [KJ/mol]	$\mathrm{Log}(K_p)$
50	2.910E+01	1.542E+02	1.448E+00	-7.226E+00	1.253E+02	2.987E+02	1.166E+03	-1.218E+03
100	2.911E+01	1.744E+02	2.904E+00	-5.771E+00	1.454E+02	2.321E+02	1.167E+03	-6.094E+02
150	2.911E+01	1.862E+02	4.359E+00	-4.315E+00	1.571E+02	2.150E+02	1.168E+03	-4.062E+02
200	2.911E+01	1.946E+02	5.814E+00	-2.860E+00	1.655E+02	2.089E+02	1.169E+03	-3.045E+02
298.15	2.920E+01	2.062E+02	8.674E+00	0.000E+00	1.771E+02	2.062E+02	1.171E+03	-2.039E+02
300	2.920E+01	2.064E+02	8.728E+00	5.405E-02	1.773E+02	2.062E+02	1.171E+03	-2.027E+02
400	2.957E+01	2.148E+02	1.166E+01	2.990E+00	1.857E+02	2.074E+02	1.173E+03	-1.517E+02
500	3.025E+01	2.215E+02	1.465E+01	5.979E+00	1.922E+02	2.095E+02	1.175E+03	-1.210E+02
600	3.108E+01	2.271E+02	1.772E+01	9.045E+00	1.976E+02	2.120E+02	1.177E+03	-1.006E+02
700	3.192E+01	2.319E+02	2.087E+01	1.220E+01	2.021E+02	2.145E+02	1.179E+03	-8.592E+01
800	3.269E+01	2.363E+02	2.410E+01	1.543E+01	2.061E+02	2.170E+02	1.181E+03	-7.491E+01
900	3.337E+01	2.402E+02	2.741E+01	1.873E+01	2.097E+02	2.193E+02	1.183E+03	-6.634E+01
1000	3.395E+01	2.437E+02	3.077E+01	2.210E+01	2.129E+02	2.216E+02	1.185E+03	-5.947E+01
2000	3.672E+01	2.683E+02	6.643E+01	5.775E+01	2.351E+02	2.394E+02	1.205E+03	-2.833E+01
3000	3.764E+01	2.834E+02	1.037E+02	9.499E+01	2.488E+02	2.517E+02	1.224E+03	-1.777E+01
4000	3.827E+01	2.943E+02	1.416E+02	1.329E+02	2.589E+02	2.611E+02	1.242E+03	-1.240E+01
5000	3.911E+01	3.029E+02	1.803E+02	1.716E+02	2.669E+02	2.686E+02	1.259E+03	-9.141E+00
6000	4.057E+01	3.102E+02	2.201E+02	2.114E+02	2.735E+02	2.749E+02	1.276E+03	-6.936E+00
7000	4.267E+01	3.166E+02	2.616E+02	2.529E+02	2.792E+02	2.804E+02	1.294E+03	-5.339E+00
8000	4.503E+01	3.224E+02	3.055E+02	2.968E+02	2.842E+02	2.853E+02	1.314E+03	-4.123E+00
9000	4.705E+01	3.279E+02	3.516E+02	3.429E+02	2.888E+02	2.898E+02	1.337E+03	-3.162E+00
10000	4.829E+01	3.329E+02	3.993E+02	3.906E+02	2.929E+02	2.938E+02	1.363E+03	-2.379E+00
11000	4.856E+01	3.375E+02	4.478E+02	4.391E+02	2.968E+02	2.976E+02	1.392E+03	-1.725E+00
12000	4.795E+01	3.417E+02	4.961E+02	4.875E+02	3.004E+02	3.011E+02	1.422E+03	-1.169E+00
13000	4.670E+01	3.455E+02	5.435E+02	5.348E+02	3.037E+02	3.044E+02	1.452E+03	-6.879E-01
14000	4.504E+01	3.489E+02	5.894E+02	5.807E+02	3.068E+02	3.074E+02	1.483E+03	-2.668E-01
15000	4.318E+01	3.519E+02	6.335E+02	6.249E+02	3.097E+02	3.103E+02	1.514E+03	1.058E-01
16000	4.129E+01	3.547E+02	6.758E+02	6.671E+02	3.124E+02	3.130E+02	1.544E+03	4.384E-01
17000	3.945E+01	3.571E+02	7.161E+02	7.075E+02	3.150E+02	3.155E+02	1.573E+03	7.376E-01
18000	3.773E+01	3.593E+02	7.547E+02	7.460E+02	3.174E+02	3.179E+02	1.601E+03	1.008E+00
19000	3.616E+01	3.613E+02	7.916E+02	7.830E+02	3.197E+02	3.201E+02	1.629E+03	1.255E+00
20000	3.473E+01	3.631E+02	8.271E+02	8.184E+02	3.218E+02	3.222E+02	1.655E+03	1.481E+00
21000	3.345E+01	3.648E+02	8.611E+02	8.525E+02	3.238E+02	3.242E+02	1.682E+03	1.688E+00
22000	3.232E+01	3.663E+02	8.940E+02	8.854E+02	3.257E+02	3.261E+02	1.707E+03	1.880E+00
23000	3.130E+01	3.678E+02	9.258E+02	9.171E+02	3.275E+02	3.279E+02	1.732E+03	2.057E+00
24000	3.040E+01	3.691E+02	9.567E+02	9.480E+02	3.292E+02	3.296E+02	1.756E+03	2.222E+00
25000	2.960E+01	3.703E+02	9.867E+02	9.780E+02	3.308E+02	3.312E+02	1.780E+03	2.376E+00
26000	2.889E+01	3.714E+02	1.016E+03	1.007E+03	3.324E+02	3.327E+02	1.804E+03	2.520E+00
27000	2.825E+01	3.725E+02	1.044E+03	1.036E+03	3.338E+02	3.341E+02	1.827E+03	2.655E+00
28000	2.768E+01	3.735E+02	1.072E+03	1.064E+03	3.352E+02	3.355E+02	1.850E+03	2.782E+00
29000	2.717E+01	3.745E+02	1.100E+03	1.091E+03	3.366E+02	3.369E+02	1.872E+03	2.902E+00
30000	2.671E+01	3.754E+02	1.127E+03	1.118E+03	3.378E+02	3.381E+02	1.894E+03	3.015E+00
32000	2.593E+01	3.771E+02	1.179E+03	1.171E+03	3.402E+02	3.405E+02	1.938E+03	3.224E+00
34000	2.528E+01	3.786E+02	1.231E+03	1.222E+03	3.425E+02	3.427E+02	1.982E+03	3.412E+00
36000	2.475E+01	3.801E+02	1.281E+03	1.272E+03	3.445E+02	3.448E+02	2.025E+03	3.583E+00
38000	2.431E+01	3.814E+02	1.330E+03	1.321E+03	3.464E+02	3.466E+02	2.067E+03	3.739E+00
40000	2.393E+01	3.826E+02	1.378E+03	1.369E+03	3.482E+02	3.484E+02	2.109E+03	3.882E+00
42000	2.361E+01	3.838E+02	1.425E+03	1.417E+03	3.499E+02	3.501E+02	2.151E+03	4.015E+00
44000	2.334E+01	3.849E+02	1.472E+03	1.464E+03	3.514E+02	3.516E+02	2.192E+03	4.137E+00
46000	2.310E+01	3.859E+02	1.519E+03	1.510E+03	3.529E+02	3.531E+02	2.234E+03	4.252E+00
48000	2.290E+01	3.869E+02	1.565E+03	1.556E+03	3.543E+02	3.545E+02	2.275E+03	4.358E+00
50000	2.272E+01	3.878E+02	1.610E+03	1.602E+03	3.556E+02	3.558E+02	2.316E+03	4.458E+00

Table 207: Internal thermodynamic properties of O_2^-

T(K)	Q_{int}	$\ln(Q_{int})$	E_{int}/RT	$C_{p,int}/R$
50	$6.109E+01$	$4.112E+00$	$9.892E-01$	$1.000E+00$
100	$1.215E+02$	$4.800E+00$	$9.950E-01$	$1.001E+00$
150	$1.820E+02$	$5.204E+00$	$9.974E-01$	$1.005E+00$
200	$2.426E+02$	$5.492E+00$	$1.002E+00$	$1.029E+00$
298.15	$3.635E+02$	$5.896E+00$	$1.029E+00$	$1.157E+00$
300	$3.658E+02$	$5.902E+00$	$1.030E+00$	$1.160E+00$
400	$4.954E+02$	$6.205E+00$	$1.085E+00$	$1.336E+00$
500	$6.355E+02$	$6.454E+00$	$1.151E+00$	$1.491E+00$
600	$7.886E+02$	$6.670E+00$	$1.218E+00$	$1.611E+00$
700	$9.560E+02$	$6.863E+00$	$1.281E+00$	$1.701E+00$
800	$1.139E+03$	$7.038E+00$	$1.338E+00$	$1.770E+00$
900	$1.337E+03$	$7.198E+00$	$1.389E+00$	$1.823E+00$
1000	$1.551E+03$	$7.347E+00$	$1.434E+00$	$1.864E+00$
2000	$4.622E+03$	$8.439E+00$	$1.705E+00$	$2.050E+00$
3000	$9.483E+03$	$9.157E+00$	$1.837E+00$	$2.148E+00$
4000	$1.630E+04$	$9.699E+00$	$1.928E+00$	$2.263E+00$
5000	$2.528E+04$	$1.014E+01$	$2.008E+00$	$2.379E+00$
6000	$3.667E+04$	$1.051E+01$	$2.074E+00$	$2.420E+00$
7000	$5.068E+04$	$1.083E+01$	$2.120E+00$	$2.346E+00$
8000	$6.737E+04$	$1.112E+01$	$2.138E+00$	$2.178E+00$
9000	$8.664E+04$	$1.137E+01$	$2.131E+00$	$1.960E+00$
10000	$1.083E+05$	$1.159E+01$	$2.102E+00$	$1.730E+00$
11000	$1.321E+05$	$1.179E+01$	$2.058E+00$	$1.511E+00$
12000	$1.576E+05$	$1.197E+01$	$2.004E+00$	$1.314E+00$
13000	$1.846E+05$	$1.213E+01$	$1.944E+00$	$1.142E+00$
14000	$2.128E+05$	$1.227E+01$	$1.882E+00$	$9.949E-01$
15000	$2.417E+05$	$1.240E+01$	$1.818E+00$	$8.699E-01$
16000	$2.713E+05$	$1.251E+01$	$1.756E+00$	$7.640E-01$
17000	$3.012E+05$	$1.262E+01$	$1.695E+00$	$6.742E-01$
18000	$3.313E+05$	$1.271E+01$	$1.636E+00$	$5.979E-01$
19000	$3.614E+05$	$1.280E+01$	$1.579E+00$	$5.329E-01$
20000	$3.913E+05$	$1.288E+01$	$1.526E+00$	$4.771E-01$
21000	$4.210E+05$	$1.295E+01$	$1.475E+00$	$4.292E-01$
22000	$4.504E+05$	$1.302E+01$	$1.426E+00$	$3.877E-01$
23000	$4.794E+05$	$1.308E+01$	$1.380E+00$	$3.517E-01$
24000	$5.079E+05$	$1.314E+01$	$1.337E+00$	$3.202E-01$
25000	$5.360E+05$	$1.319E+01$	$1.295E+00$	$2.927E-01$
26000	$5.635E+05$	$1.324E+01$	$1.256E+00$	$2.684E-01$
27000	$5.904E+05$	$1.329E+01$	$1.219E+00$	$2.469E-01$
28000	$6.168E+05$	$1.333E+01$	$1.184E+00$	$2.278E-01$
29000	$6.426E+05$	$1.337E+01$	$1.151E+00$	$2.107E-01$
30000	$6.678E+05$	$1.341E+01$	$1.119E+00$	$1.955E-01$
32000	$7.165E+05$	$1.348E+01$	$1.061E+00$	$1.695E-01$
34000	$7.628E+05$	$1.354E+01$	$1.008E+00$	$1.483E-01$
36000	$8.069E+05$	$1.360E+01$	$9.595E-01$	$1.307E-01$
38000	$8.489E+05$	$1.365E+01$	$9.155E-01$	$1.160E-01$
40000	$8.888E+05$	$1.370E+01$	$8.752E-01$	$1.037E-01$
42000	$9.267E+05$	$1.374E+01$	$8.382E-01$	$9.318E-02$
44000	$9.628E+05$	$1.378E+01$	$8.041E-01$	$8.418E-02$
46000	$9.971E+05$	$1.381E+01$	$7.726E-01$	$7.641E-02$
48000	$1.030E+06$	$1.384E+01$	$7.435E-01$	$6.966E-02$
50000	$1.061E+06$	$1.387E+01$	$7.164E-01$	$6.375E-02$

Table 208: Total thermodynamic properties of O_2^-

T [K]	C_p [J/mol/K]	S^0 [J/mol/K]	$H^0(T)-H^0(0)$ [KJ/mol]	$H^0(T)-H^0(298)$ [KJ/mol]	$-(G^0-H^0(0))/T$ [J/mol/K]	$-(G^0-H^0(298))/T$ [J/mol/K]	ΔH_f [KJ/mol]	$\mathrm{Log}(K_p)$
50	2.911E+01	1.574E+02	1.450E+00	-7.298E+00	1.284E+02	3.033E+02	-4.455E+01	4.760E+01
100	2.911E+01	1.776E+02	2.906E+00	-5.843E+00	1.485E+02	2.360E+02	-4.559E+01	2.412E+01
150	2.914E+01	1.894E+02	4.362E+00	-4.387E+00	1.603E+02	2.186E+02	-4.663E+01	1.611E+01
200	2.934E+01	1.978E+02	5.823E+00	-2.926E+00	1.687E+02	2.124E+02	-4.766E+01	1.201E+01
298.15	3.041E+01	2.097E+02	8.749E+00	0.000E+00	1.803E+02	2.097E+02	-4.965E+01	7.835E+00
300	3.043E+01	2.098E+02	8.805E+00	5.632E-02	1.805E+02	2.097E+02	-4.968E+01	7.781E+00
400	3.189E+01	2.188E+02	1.192E+01	3.173E+00	1.890E+02	2.109E+02	-5.162E+01	5.580E+00
500	3.318E+01	2.261E+02	1.518E+01	6.429E+00	1.957E+02	2.132E+02	-5.350E+01	4.209E+00
600	3.418E+01	2.322E+02	1.855E+01	9.799E+00	2.013E+02	2.159E+02	-5.537E+01	3.263E+00
700	3.493E+01	2.375E+02	2.200E+01	1.326E+01	2.061E+02	2.186E+02	-5.724E+01	2.563E+00
800	3.550E+01	2.422E+02	2.553E+01	1.678E+01	2.103E+02	2.213E+02	-5.914E+01	2.021E+00
900	3.594E+01	2.464E+02	2.910E+01	2.035E+01	2.141E+02	2.238E+02	-6.105E+01	1.585E+00
1000	3.628E+01	2.502E+02	3.271E+01	2.396E+01	2.175E+02	2.263E+02	-6.298E+01	1.225E+00
2000	3.783E+01	2.760E+02	6.993E+01	6.118E+01	2.410E+02	2.454E+02	-8.305E+01	-6.191E-01
3000	3.865E+01	2.915E+02	1.082E+02	9.943E+01	2.554E+02	2.583E+02	-1.045E+02	-1.422E+00
4000	3.960E+01	3.027E+02	1.473E+02	1.385E+02	2.659E+02	2.681E+02	-1.271E+02	-1.921E+00
5000	4.056E+01	3.117E+02	1.874E+02	1.786E+02	2.742E+02	2.759E+02	-1.502E+02	-2.281E+00
6000	4.090E+01	3.191E+02	2.282E+02	2.194E+02	2.811E+02	2.825E+02	-1.737E+02	-2.562E+00
7000	4.029E+01	3.254E+02	2.689E+02	2.601E+02	2.870E+02	2.882E+02	-1.981E+02	-2.792E+00
8000	3.890E+01	3.307E+02	3.085E+02	2.998E+02	2.921E+02	2.932E+02	-2.236E+02	-2.988E+00
9000	3.709E+01	3.352E+02	3.465E+02	3.378E+02	2.966E+02	2.976E+02	-2.501E+02	-3.159E+00
10000	3.517E+01	3.390E+02	3.827E+02	3.739E+02	3.007E+02	3.016E+02	-2.773E+02	-3.312E+00
11000	3.335E+01	3.422E+02	4.169E+02	4.082E+02	3.043E+02	3.051E+02	-3.047E+02	-3.450E+00
12000	3.171E+01	3.451E+02	4.494E+02	4.407E+02	3.076E+02	3.083E+02	-3.322E+02	-3.576E+00
13000	3.028E+01	3.475E+02	4.804E+02	4.716E+02	3.106E+02	3.113E+02	-3.594E+02	-3.692E+00
14000	2.906E+01	3.497E+02	5.101E+02	5.013E+02	3.133E+02	3.139E+02	-3.864E+02	-3.799E+00
15000	2.802E+01	3.517E+02	5.386E+02	5.298E+02	3.158E+02	3.164E+02	-4.130E+02	-3.898E+00
16000	2.714E+01	3.535E+02	5.661E+02	5.574E+02	3.181E+02	3.186E+02	-4.393E+02	-3.990E+00
17000	2.639E+01	3.551E+02	5.929E+02	5.841E+02	3.202E+02	3.208E+02	-4.653E+02	-4.077E+00
18000	2.576E+01	3.566E+02	6.190E+02	6.102E+02	3.222E+02	3.227E+02	-4.910E+02	-4.159E+00
19000	2.522E+01	3.580E+02	6.445E+02	6.357E+02	3.241E+02	3.245E+02	-5.165E+02	-4.236E+00
20000	2.475E+01	3.593E+02	6.694E+02	6.607E+02	3.258E+02	3.262E+02	-5.417E+02	-4.309E+00
21000	2.436E+01	3.604E+02	6.940E+02	6.852E+02	3.274E+02	3.278E+02	-5.667E+02	-4.377E+00
22000	2.401E+01	3.616E+02	7.181E+02	7.094E+02	3.289E+02	3.293E+02	-5.915E+02	-4.443E+00
23000	2.371E+01	3.626E+02	7.420E+02	7.333E+02	3.304E+02	3.308E+02	-6.161E+02	-4.505E+00
24000	2.345E+01	3.636E+02	7.656E+02	7.568E+02	3.317E+02	3.321E+02	-6.406E+02	-4.565E+00
25000	2.322E+01	3.646E+02	7.889E+02	7.802E+02	3.330E+02	3.334E+02	-6.650E+02	-4.622E+00
26000	2.302E+01	3.655E+02	8.120E+02	8.033E+02	3.343E+02	3.346E+02	-6.891E+02	-4.676E+00
27000	2.284E+01	3.664E+02	8.350E+02	8.262E+02	3.354E+02	3.358E+02	-7.132E+02	-4.728E+00
28000	2.268E+01	3.672E+02	8.577E+02	8.490E+02	3.366E+02	3.369E+02	-7.371E+02	-4.778E+00
29000	2.254E+01	3.680E+02	8.803E+02	8.716E+02	3.376E+02	3.379E+02	-7.610E+02	-4.826E+00
30000	2.241E+01	3.688E+02	9.028E+02	8.940E+02	3.387E+02	3.389E+02	-7.847E+02	-4.873E+00
32000	2.220E+01	3.702E+02	9.474E+02	9.386E+02	3.406E+02	3.409E+02	-8.319E+02	-4.961E+00
34000	2.202E+01	3.715E+02	9.916E+02	9.829E+02	3.424E+02	3.426E+02	-8.787E+02	-5.043E+00
36000	2.187E+01	3.728E+02	1.036E+03	1.027E+03	3.440E+02	3.443E+02	-9.252E+02	-5.120E+00
38000	2.175E+01	3.740E+02	1.079E+03	1.070E+03	3.456E+02	3.458E+02	-9.714E+02	-5.192E+00
40000	2.165E+01	3.751E+02	1.122E+03	1.114E+03	3.470E+02	3.472E+02	-1.017E+03	-5.260E+00
42000	2.156E+01	3.761E+02	1.166E+03	1.157E+03	3.484E+02	3.486E+02	-1.063E+03	-5.325E+00
44000	2.149E+01	3.771E+02	1.209E+03	1.200E+03	3.497E+02	3.499E+02	-1.109E+03	-5.386E+00
46000	2.142E+01	3.781E+02	1.252E+03	1.243E+03	3.509E+02	3.511E+02	-1.154E+03	-5.445E+00
48000	2.136E+01	3.790E+02	1.294E+03	1.286E+03	3.520E+02	3.522E+02	-1.199E+03	-5.500E+00
50000	2.132E+01	3.799E+02	1.337E+03	1.328E+03	3.531E+02	3.533E+02	-1.244E+03	-5.553E+00

Table 209: Internal thermodynamic properties of O_3

T(K)	Q_{int}	$\ln(Q_{int})$	E_{int}/RT	$C_{p,int}/R$
50	$2.302E+02$	$5.439E+00$	$1.496E+00$	$1.500E+00$
100	$6.498E+02$	$6.477E+00$	$1.498E+00$	$1.504E+00$
150	$1.194E+03$	$7.085E+00$	$1.507E+00$	$1.562E+00$
200	$1.850E+03$	$7.523E+00$	$1.539E+00$	$1.723E+00$
298.15	$3.500E+03$	$8.160E+00$	$1.680E+00$	$2.234E+00$
300	$3.536E+03$	$8.171E+00$	$1.683E+00$	$2.245E+00$
400	$5.901E+03$	$8.683E+00$	$1.892E+00$	$2.778E+00$
500	$9.218E+03$	$9.129E+00$	$2.113E+00$	$3.198E+00$
600	$1.381E+04$	$9.533E+00$	$2.321E+00$	$3.506E+00$
700	$2.003E+04$	$9.905E+00$	$2.507E+00$	$3.729E+00$
800	$2.830E+04$	$1.025E+01$	$2.671E+00$	$3.893E+00$
900	$3.909E+04$	$1.057E+01$	$2.814E+00$	$4.016E+00$
1000	$5.293E+04$	$1.088E+01$	$2.939E+00$	$4.110E+00$
2000	$5.264E+05$	$1.317E+01$	$3.677E+00$	$4.861E+00$
3000	$2.676E+06$	$1.480E+01$	$4.461E+00$	$7.257E+00$
4000	$1.084E+07$	$1.620E+01$	$5.218E+00$	$7.082E+00$
5000	$3.571E+07$	$1.739E+01$	$5.385E+00$	$5.015E+00$
6000	$9.393E+07$	$1.836E+01$	$5.184E+00$	$3.464E+00$
7000	$2.041E+08$	$1.913E+01$	$4.867E+00$	$2.549E+00$
8000	$3.825E+08$	$1.976E+01$	$4.540E+00$	$2.000E+00$
9000	$6.414E+08$	$2.028E+01$	$4.237E+00$	$1.647E+00$
10000	$9.880E+08$	$2.071E+01$	$3.965E+00$	$1.404E+00$
11000	$1.425E+09$	$2.108E+01$	$3.724E+00$	$1.227E+00$
12000	$1.952E+09$	$2.139E+01$	$3.510E+00$	$1.090E+00$
13000	$2.566E+09$	$2.167E+01$	$3.319E+00$	$9.813E-01$
14000	$3.261E+09$	$2.191E+01$	$3.149E+00$	$8.920E-01$
15000	$4.030E+09$	$2.212E+01$	$2.996E+00$	$8.170E-01$
16000	$4.868E+09$	$2.231E+01$	$2.858E+00$	$7.529E-01$
17000	$5.767E+09$	$2.248E+01$	$2.732E+00$	$6.973E-01$
18000	$6.719E+09$	$2.263E+01$	$2.618E+00$	$6.485E-01$
19000	$7.719E+09$	$2.277E+01$	$2.513E+00$	$6.052E-01$
20000	$8.759E+09$	$2.289E+01$	$2.417E+00$	$5.666E-01$
21000	$9.834E+09$	$2.301E+01$	$2.328E+00$	$5.319E-01$
22000	$1.094E+10$	$2.312E+01$	$2.245E+00$	$5.006E-01$
23000	$1.206E+10$	$2.321E+01$	$2.169E+00$	$4.720E-01$
24000	$1.321E+10$	$2.330E+01$	$2.098E+00$	$4.460E-01$
25000	$1.437E+10$	$2.339E+01$	$2.031E+00$	$4.222E-01$
26000	$1.555E+10$	$2.347E+01$	$1.969E+00$	$4.003E-01$
27000	$1.673E+10$	$2.354E+01$	$1.910E+00$	$3.801E-01$
28000	$1.791E+10$	$2.361E+01$	$1.855E+00$	$3.614E-01$
29000	$1.910E+10$	$2.367E+01$	$1.803E+00$	$3.441E-01$
30000	$2.029E+10$	$2.373E+01$	$1.755E+00$	$3.280E-01$
32000	$2.265E+10$	$2.384E+01$	$1.664E+00$	$2.991E-01$
34000	$2.500E+10$	$2.394E+01$	$1.583E+00$	$2.739E-01$
36000	$2.731E+10$	$2.403E+01$	$1.510E+00$	$2.517E-01$
38000	$2.957E+10$	$2.411E+01$	$1.443E+00$	$2.321E-01$
40000	$3.180E+10$	$2.418E+01$	$1.382E+00$	$2.147E-01$
42000	$3.397E+10$	$2.425E+01$	$1.326E+00$	$1.992E-01$
44000	$3.609E+10$	$2.431E+01$	$1.275E+00$	$1.853E-01$
46000	$3.815E+10$	$2.436E+01$	$1.227E+00$	$1.728E-01$
48000	$4.016E+10$	$2.442E+01$	$1.183E+00$	$1.615E-01$
50000	$4.211E+10$	$2.446E+01$	$1.142E+00$	$1.513E-01$

Table 210: Total thermodynamic properties of O_3

T [K]	C_p [J/mol/K]	S^0 [J/mol/K]	$H^0(T)-H^0(0)$ [KJ/mol]	$H^0(T)-H^0(298)$ [KJ/mol]	$-(G^0-H^0(0))/T$ [J/mol/K]	$-(G^0-H^0(298))/T$ [J/mol/K]	ΔH_f [KJ/mol]	$\mathrm{Log}(K_p)$
50	3.326E+01	1.777E+02	1.661E+00	-8.700E+00	1.445E+02	3.517E+02	1.451E+02	-1.543E+02
100	3.329E+01	2.007E+02	3.325E+00	-7.037E+00	1.675E+02	2.711E+02	1.446E+02	-7.861E+01
150	3.377E+01	2.143E+02	4.998E+00	-5.363E+00	1.810E+02	2.501E+02	1.441E+02	-5.348E+01
200	3.511E+01	2.242E+02	6.716E+00	-3.644E+00	1.906E+02	2.424E+02	1.436E+02	-4.096E+01
298.15	3.936E+01	2.389E+02	1.036E+01	0.000E+00	2.042E+02	2.389E+02	1.429E+02	-2.864E+01
300	3.945E+01	2.392E+02	1.043E+01	7.340E-02	2.044E+02	2.389E+02	1.429E+02	-2.848E+01
400	4.388E+01	2.512E+02	1.461E+01	4.246E+00	2.147E+02	2.406E+02	1.427E+02	-2.227E+01
500	4.738E+01	2.614E+02	1.918E+01	8.818E+00	2.230E+02	2.437E+02	1.426E+02	-1.854E+01
600	4.994E+01	2.702E+02	2.405E+01	1.369E+01	2.302E+02	2.474E+02	1.428E+02	-1.606E+01
700	5.179E+01	2.781E+02	2.914E+01	1.878E+01	2.364E+02	2.512E+02	1.430E+02	-1.428E+01
800	5.316E+01	2.851E+02	3.439E+01	2.403E+01	2.421E+02	2.551E+02	1.432E+02	-1.295E+01
900	5.418E+01	2.914E+02	3.976E+01	2.940E+01	2.472E+02	2.587E+02	1.435E+02	-1.191E+01
1000	5.496E+01	2.972E+02	4.522E+01	3.486E+01	2.519E+02	2.623E+02	1.437E+02	-1.107E+01
2000	6.120E+01	3.368E+02	1.027E+02	9.236E+01	2.854E+02	2.906E+02	1.465E+02	-7.295E+00
3000	8.113E+01	3.653E+02	1.736E+02	1.633E+02	3.074E+02	3.109E+02	1.590E+02	-5.985E+00
4000	7.967E+01	3.892E+02	2.567E+02	2.463E+02	3.250E+02	3.276E+02	1.807E+02	-5.249E+00
5000	6.248E+01	4.051E+02	3.278E+02	3.174E+02	3.396E+02	3.416E+02	1.882E+02	-4.764E+00
6000	4.959E+01	4.153E+02	3.833E+02	3.729E+02	3.514E+02	3.531E+02	1.784E+02	-4.442E+00
7000	4.198E+01	4.223E+02	4.288E+02	4.184E+02	3.610E+02	3.625E+02	1.574E+02	-4.232E+00
8000	3.741E+01	4.276E+02	4.683E+02	4.579E+02	3.690E+02	3.703E+02	1.304E+02	-4.097E+00
9000	3.448E+01	4.318E+02	5.041E+02	4.938E+02	3.758E+02	3.769E+02	1.006E+02	-4.013E+00
10000	3.246E+01	4.353E+02	5.375E+02	5.272E+02	3.816E+02	3.826E+02	7.028E+01	-3.963E+00
11000	3.098E+01	4.384E+02	5.692E+02	5.589E+02	3.866E+02	3.875E+02	4.062E+01	-3.936E+00
12000	2.985E+01	4.410E+02	5.996E+02	5.893E+02	3.910E+02	3.919E+02	1.228E+01	-3.925E+00
13000	2.895E+01	4.433E+02	6.290E+02	6.186E+02	3.950E+02	3.958E+02	-1.449E+01	-3.926E+00
14000	2.820E+01	4.455E+02	6.576E+02	6.472E+02	3.985E+02	3.992E+02	-3.968E+01	-3.933E+00
15000	2.758E+01	4.474E+02	6.855E+02	6.751E+02	4.017E+02	4.024E+02	-6.336E+01	-3.946E+00
16000	2.705E+01	4.491E+02	7.128E+02	7.024E+02	4.046E+02	4.052E+02	-8.570E+01	-3.962E+00
17000	2.658E+01	4.508E+02	7.396E+02	7.292E+02	4.073E+02	4.079E+02	-1.068E+02	-3.981E+00
18000	2.618E+01	4.523E+02	7.659E+02	7.556E+02	4.097E+02	4.103E+02	-1.270E+02	-4.001E+00
19000	2.582E+01	4.537E+02	7.919E+02	7.816E+02	4.120E+02	4.126E+02	-1.462E+02	-4.022E+00
20000	2.550E+01	4.550E+02	8.176E+02	8.072E+02	4.141E+02	4.146E+02	-1.647E+02	-4.043E+00
21000	2.521E+01	4.562E+02	8.429E+02	8.326E+02	4.161E+02	4.166E+02	-1.824E+02	-4.065E+00
22000	2.495E+01	4.574E+02	8.680E+02	8.576E+02	4.179E+02	4.184E+02	-1.997E+02	-4.086E+00
23000	2.471E+01	4.585E+02	8.928E+02	8.825E+02	4.197E+02	4.201E+02	-2.164E+02	-4.108E+00
24000	2.450E+01	4.596E+02	9.174E+02	9.071E+02	4.213E+02	4.218E+02	-2.327E+02	-4.129E+00
25000	2.430E+01	4.606E+02	9.418E+02	9.315E+02	4.229E+02	4.233E+02	-2.486E+02	-4.150E+00
26000	2.411E+01	4.615E+02	9.660E+02	9.557E+02	4.244E+02	4.247E+02	-2.642E+02	-4.170E+00
27000	2.395E+01	4.624E+02	9.901E+02	9.797E+02	4.257E+02	4.261E+02	-2.794E+02	-4.191E+00
28000	2.379E+01	4.633E+02	1.014E+03	1.004E+03	4.271E+02	4.274E+02	-2.944E+02	-4.210E+00
29000	2.365E+01	4.641E+02	1.038E+03	1.027E+03	4.283E+02	4.287E+02	-3.092E+02	-4.230E+00
30000	2.351E+01	4.649E+02	1.061E+03	1.051E+03	4.295E+02	4.299E+02	-3.238E+02	-4.249E+00
32000	2.327E+01	4.664E+02	1.108E+03	1.098E+03	4.318E+02	4.321E+02	-3.523E+02	-4.286E+00
34000	2.306E+01	4.678E+02	1.154E+03	1.144E+03	4.339E+02	4.342E+02	-3.801E+02	-4.321E+00
36000	2.288E+01	4.691E+02	1.200E+03	1.190E+03	4.358E+02	4.361E+02	-4.074E+02	-4.354E+00
38000	2.272E+01	4.704E+02	1.246E+03	1.236E+03	4.376E+02	4.379E+02	-4.342E+02	-4.387E+00
40000	2.257E+01	4.715E+02	1.291E+03	1.281E+03	4.392E+02	4.395E+02	-4.606E+02	-4.417E+00
42000	2.244E+01	4.726E+02	1.336E+03	1.326E+03	4.408E+02	4.411E+02	-4.866E+02	-4.447E+00
44000	2.233E+01	4.737E+02	1.381E+03	1.371E+03	4.423E+02	4.425E+02	-5.123E+02	-4.475E+00
46000	2.222E+01	4.747E+02	1.426E+03	1.415E+03	4.437E+02	4.439E+02	-5.377E+02	-4.502E+00
48000	2.213E+01	4.756E+02	1.470E+03	1.460E+03	4.450E+02	4.452E+02	-5.628E+02	-4.528E+00
50000	2.204E+01	4.765E+02	1.514E+03	1.504E+03	4.462E+02	4.464E+02	-5.876E+02	-4.553E+00

Table 211: Internal thermodynamic properties of O_3^-

T(K)	Q_{int}	$\ln(Q_{int})$	E_{int}/RT	$C_{p,int}/R$
50	$5.000E-01$	$-6.931E-01$	$2.119E-06$	$3.354E-05$
100	$5.002E-01$	$-6.928E-01$	$2.948E-03$	$2.360E-02$
150	$5.027E-01$	$-6.877E-01$	$2.976E-02$	$1.668E-01$
200	$5.111E-01$	$-6.712E-01$	$9.476E-02$	$4.272E-01$
298.15	$5.506E-01$	$-5.967E-01$	$3.055E-01$	$1.043E+00$
300	$5.517E-01$	$-5.948E-01$	$3.101E-01$	$1.054E+00$
400	$6.245E-01$	$-4.707E-01$	$5.654E-01$	$1.582E+00$
500	$7.276E-01$	$-3.180E-01$	$8.084E-01$	$1.956E+00$
600	$8.597E-01$	$-1.512E-01$	$1.022E+00$	$2.212E+00$
700	$1.021E+00$	$2.052E-02$	$1.206E+00$	$2.390E+00$
800	$1.212E+00$	$1.920E-01$	$1.362E+00$	$2.516E+00$
900	$1.434E+00$	$3.603E-01$	$1.496E+00$	$2.608E+00$
1000	$1.689E+00$	$5.240E-01$	$1.611E+00$	$2.677E+00$
2000	$6.470E+00$	$1.867E+00$	$2.219E+00$	$2.892E+00$
3000	$1.668E+01$	$2.814E+00$	$2.433E+00$	$2.801E+00$
4000	$3.401E+01$	$3.527E+00$	$2.511E+00$	$2.714E+00$
5000	$5.985E+01$	$4.092E+00$	$2.555E+00$	$2.772E+00$
6000	$9.575E+01$	$4.562E+00$	$2.600E+00$	$2.873E+00$
7000	$1.434E+02$	$4.966E+00$	$2.642E+00$	$2.889E+00$
8000	$2.045E+02$	$5.321E+00$	$2.667E+00$	$2.777E+00$
9000	$2.800E+02$	$5.635E+00$	$2.668E+00$	$2.568E+00$
10000	$3.706E+02$	$5.915E+00$	$2.646E+00$	$2.310E+00$
11000	$4.760E+02$	$6.165E+00$	$2.603E+00$	$2.042E+00$
12000	$5.956E+02$	$6.390E+00$	$2.545E+00$	$1.789E+00$
13000	$7.283E+02$	$6.591E+00$	$2.478E+00$	$1.562E+00$
14000	$8.728E+02$	$6.772E+00$	$2.406E+00$	$1.364E+00$
15000	$1.028E+03$	$6.935E+00$	$2.330E+00$	$1.194E+00$
16000	$1.192E+03$	$7.083E+00$	$2.255E+00$	$1.048E+00$
17000	$1.363E+03$	$7.218E+00$	$2.180E+00$	$9.247E-01$
18000	$1.541E+03$	$7.340E+00$	$2.107E+00$	$8.194E-01$
19000	$1.724E+03$	$7.452E+00$	$2.037E+00$	$7.295E-01$
20000	$1.910E+03$	$7.555E+00$	$1.970E+00$	$6.525E-01$
21000	$2.099E+03$	$7.649E+00$	$1.905E+00$	$5.863E-01$
22000	$2.291E+03$	$7.737E+00$	$1.844E+00$	$5.292E-01$
23000	$2.483E+03$	$7.817E+00$	$1.786E+00$	$4.795E-01$
24000	$2.676E+03$	$7.892E+00$	$1.730E+00$	$4.363E-01$
25000	$2.869E+03$	$7.962E+00$	$1.678E+00$	$3.984E-01$
26000	$3.061E+03$	$8.027E+00$	$1.628E+00$	$3.650E-01$
27000	$3.252E+03$	$8.087E+00$	$1.581E+00$	$3.355E-01$
28000	$3.442E+03$	$8.144E+00$	$1.536E+00$	$3.094E-01$
29000	$3.630E+03$	$8.197E+00$	$1.493E+00$	$2.861E-01$
30000	$3.815E+03$	$8.247E+00$	$1.452E+00$	$2.653E-01$
32000	$4.180E+03$	$8.338E+00$	$1.377E+00$	$2.298E-01$
34000	$4.535E+03$	$8.420E+00$	$1.309E+00$	$2.009E-01$
36000	$4.878E+03$	$8.493E+00$	$1.247E+00$	$1.770E-01$
38000	$5.210E+03$	$8.558E+00$	$1.190E+00$	$1.571E-01$
40000	$5.531E+03$	$8.618E+00$	$1.138E+00$	$1.403E-01$
42000	$5.839E+03$	$8.672E+00$	$1.090E+00$	$1.261E-01$
44000	$6.137E+03$	$8.722E+00$	$1.046E+00$	$1.139E-01$
46000	$6.423E+03$	$8.768E+00$	$1.005E+00$	$1.034E-01$
48000	$6.698E+03$	$8.810E+00$	$9.672E-01$	$9.421E-02$
50000	$6.963E+03$	$8.848E+00$	$9.321E-01$	$8.622E-02$

Table 212: Total thermodynamic properties of O_3^-

T [K]	C_p [J/mol/K]	S^0 [J/mol/K]	$H^0(T)-H^0(0)$ [KJ/mol]	$H^0(T)-H^0(298)$ [KJ/mol]	$-(G^0-H^0(0))/T$ [J/mol/K]	$-(G^0-H^0(298))/T$ [J/mol/K]	ΔH_f [KJ/mol]	$\mathrm{Log}(K_p)$
50	2.079E+01	1.143E+02	1.039E+00	-5.915E+00	9.347E+01	2.326E+02	-5.949E+01	5.695E+01
100	2.098E+01	1.287E+02	2.081E+00	-4.874E+00	1.079E+02	1.774E+02	-6.167E+01	2.544E+01
150	2.217E+01	1.374E+02	3.155E+00	-3.800E+00	1.163E+02	1.627E+02	-6.381E+01	1.454E+01
200	2.434E+01	1.440E+02	4.315E+00	-2.640E+00	1.225E+02	1.572E+02	-6.588E+01	8.903E+00
298.15	2.946E+01	1.547E+02	6.955E+00	0.000E+00	1.314E+02	1.547E+02	-6.958E+01	3.098E+00
300	2.955E+01	1.549E+02	7.009E+00	5.458E-02	1.315E+02	1.547E+02	-6.965E+01	3.023E+00
400	3.394E+01	1.640E+02	1.020E+01	3.240E+00	1.385E+02	1.559E+02	-7.300E+01	-7.563E-02
500	3.705E+01	1.720E+02	1.375E+01	6.799E+00	1.444E+02	1.584E+02	-7.610E+01	-2.020E+00
600	3.918E+01	1.789E+02	1.757E+01	1.062E+01	1.496E+02	1.612E+02	-7.910E+01	-3.370E+00
700	4.066E+01	1.851E+02	2.157E+01	1.461E+01	1.543E+02	1.642E+02	-8.207E+01	-4.371E+00
800	4.171E+01	1.906E+02	2.569E+01	1.873E+01	1.585E+02	1.672E+02	-8.503E+01	-5.150E+00
900	4.247E+01	1.955E+02	2.990E+01	2.295E+01	1.623E+02	1.700E+02	-8.801E+01	-5.777E+00
1000	4.304E+01	2.000E+02	3.418E+01	2.722E+01	1.659E+02	1.728E+02	-9.100E+01	-6.296E+00
2000	4.483E+01	2.307E+02	7.848E+01	7.152E+01	1.914E+02	1.949E+02	-1.222E+02	-8.983E+00
3000	4.408E+01	2.488E+02	1.230E+02	1.161E+02	2.077E+02	2.101E+02	-1.569E+02	-1.017E+01
4000	4.335E+01	2.613E+02	1.667E+02	1.597E+02	2.196E+02	2.214E+02	-1.954E+02	-1.093E+01
5000	4.383E+01	2.710E+02	2.102E+02	2.032E+02	2.290E+02	2.304E+02	-2.363E+02	-1.149E+01
6000	4.467E+01	2.791E+02	2.544E+02	2.475E+02	2.367E+02	2.378E+02	-2.781E+02	-1.194E+01
7000	4.480E+01	2.860E+02	2.993E+02	2.923E+02	2.432E+02	2.442E+02	-3.205E+02	-1.231E+01
8000	4.388E+01	2.919E+02	3.437E+02	3.367E+02	2.490E+02	2.498E+02	-3.634E+02	-1.263E+01
9000	4.214E+01	2.970E+02	3.868E+02	3.798E+02	2.540E+02	2.548E+02	-4.067E+02	-1.290E+01
10000	3.999E+01	3.013E+02	4.278E+02	4.209E+02	2.586E+02	2.592E+02	-4.502E+02	-1.315E+01
11000	3.777E+01	3.050E+02	4.667E+02	4.598E+02	2.626E+02	2.632E+02	-4.935E+02	-1.338E+01
12000	3.566E+01	3.082E+02	5.034E+02	4.964E+02	2.663E+02	2.669E+02	-5.363E+02	-1.358E+01
13000	3.378E+01	3.110E+02	5.381E+02	5.311E+02	2.696E+02	2.701E+02	-5.785E+02	-1.377E+01
14000	3.213E+01	3.134E+02	5.710E+02	5.641E+02	2.727E+02	2.732E+02	-6.201E+02	-1.394E+01
15000	3.071E+01	3.156E+02	6.024E+02	5.955E+02	2.755E+02	2.759E+02	-6.611E+02	-1.410E+01
16000	2.950E+01	3.176E+02	6.325E+02	6.256E+02	2.780E+02	2.785E+02	-7.014E+02	-1.425E+01
17000	2.848E+01	3.193E+02	6.615E+02	6.545E+02	2.804E+02	2.808E+02	-7.412E+02	-1.438E+01
18000	2.760E+01	3.209E+02	6.895E+02	6.826E+02	2.826E+02	2.830E+02	-7.804E+02	-1.451E+01
19000	2.685E+01	3.224E+02	7.168E+02	7.098E+02	2.847E+02	2.850E+02	-8.192E+02	-1.464E+01
20000	2.621E+01	3.238E+02	7.433E+02	7.363E+02	2.866E+02	2.869E+02	-8.576E+02	-1.475E+01
21000	2.566E+01	3.250E+02	7.692E+02	7.622E+02	2.884E+02	2.887E+02	-8.956E+02	-1.486E+01
22000	2.519E+01	3.262E+02	7.946E+02	7.877E+02	2.901E+02	2.904E+02	-9.333E+02	-1.496E+01
23000	2.477E+01	3.273E+02	8.196E+02	8.126E+02	2.917E+02	2.920E+02	-9.706E+02	-1.506E+01
24000	2.441E+01	3.284E+02	8.442E+02	8.372E+02	2.932E+02	2.935E+02	-1.008E+03	-1.515E+01
25000	2.410E+01	3.294E+02	8.684E+02	8.615E+02	2.946E+02	2.949E+02	-1.045E+03	-1.524E+01
26000	2.382E+01	3.303E+02	8.924E+02	8.854E+02	2.960E+02	2.962E+02	-1.081E+03	-1.533E+01
27000	2.358E+01	3.312E+02	9.161E+02	9.091E+02	2.972E+02	2.975E+02	-1.118E+03	-1.541E+01
28000	2.336E+01	3.320E+02	9.395E+02	9.326E+02	2.985E+02	2.987E+02	-1.154E+03	-1.549E+01
29000	2.316E+01	3.329E+02	9.628E+02	9.559E+02	2.996E+02	2.999E+02	-1.190E+03	-1.557E+01
30000	2.299E+01	3.336E+02	9.859E+02	9.789E+02	3.008E+02	3.010E+02	-1.226E+03	-1.564E+01
32000	2.270E+01	3.351E+02	1.032E+03	1.025E+03	3.029E+02	3.031E+02	-1.297E+03	-1.578E+01
34000	2.246E+01	3.365E+02	1.077E+03	1.070E+03	3.048E+02	3.050E+02	-1.367E+03	-1.590E+01
36000	2.226E+01	3.378E+02	1.121E+03	1.114E+03	3.066E+02	3.068E+02	-1.438E+03	-1.602E+01
38000	2.209E+01	3.389E+02	1.166E+03	1.159E+03	3.083E+02	3.085E+02	-1.507E+03	-1.614E+01
40000	2.195E+01	3.401E+02	1.210E+03	1.203E+03	3.098E+02	3.100E+02	-1.576E+03	-1.624E+01
42000	2.184E+01	3.411E+02	1.254E+03	1.247E+03	3.113E+02	3.115E+02	-1.645E+03	-1.634E+01
44000	2.173E+01	3.422E+02	1.297E+03	1.290E+03	3.127E+02	3.128E+02	-1.714E+03	-1.644E+01
46000	2.165E+01	3.431E+02	1.340E+03	1.334E+03	3.140E+02	3.141E+02	-1.782E+03	-1.653E+01
48000	2.157E+01	3.441E+02	1.384E+03	1.377E+03	3.152E+02	3.154E+02	-1.850E+03	-1.661E+01
50000	2.150E+01	3.449E+02	1.427E+03	1.420E+03	3.164E+02	3.165E+02	-1.917E+03	-1.669E+01

Tables of fitting coefficients for C_p/R

Table 213: Fitting coefficients for C_p/R of Ar ΔE=250 cm^{-1}

T interval (K)	a_1	a_2	a_3	a_4	a_5	a_6	a_7
50 - 2000	7.257133320E - 15	-1.988956360E - 11	2.500000010E+00	-1.990200930E - 06	4.618502380E - 05	7.466441090E - 03	-3.174136300E - 01
2000 - 10000	7.812378090E - 04	-1.205414500E - 01	9.888953670E+00	-2.301609154E+02	3.846276931E+03	-3.277786980E+04	1.116867020E+05
10000 - 15000	-7.668330695E+01	4.006927186E+03	-8.703988560E+04	1.005467840E+06	-6.506678340E+06	2.232447700E+07	-3.162933960E+07
15000 - 25000	1.600209389E+03	-4.828230550E+04	5.992728700E+05	-3.919821110E+06	1.427028120E+07	-2.745246310E+07	2.182804910E+07
25000 - 35000	5.239570633E+01	-8.423839272E+02	5.682230702E+03	-2.044790110E+04	4.126713420E+04	-4.405849140E+04	1.933324610E+04
35000 - 50000	-2.452843018E+02	3.544855426E+03	-2.125911340E+04	6.776944900E+04	-1.210954070E+05	1.150307590E+05	-4.538649880E+04
Residuals: min=2.357E - 12, max=1.204E - 02, mean=5.680E - 04.							

Table 214: Fitting coefficients for C_p/R of Ar ΔE=500 cm^{-1}

T interval (K)	a_1	a_2	a_3	a_4	a_5	a_6	a_7
50 - 2000	4.165245930E - 15	-1.164197930E - 11	2.500000010E+00	-1.215129670E - 06	3.172185980E - 05	4.261091670E - 03	-1.875642700E - 01
2000 - 10000	3.259748920E - 04	-5.034028010E - 02	5.589073190E+00	-9.634930505E+01	1.612701945E+03	-1.377007260E+04	4.702921800E+04
10000 - 15000	-2.022930953E+01	1.043607112E+03	-2.234389900E+04	2.538790770E+05	-1.610574410E+06	5.389841250E+06	-7.387023910E+06
15000 - 25000	-5.108800064E+02	1.766477530E+04	-2.494627800E+05	1.841327590E+06	-7.493923480E+06	1.596436370E+07	-1.393118020E+07
25000 - 35000	4.363271246E+01	-6.946253068E+02	4.924863017E+03	-1.974085070E+04	4.677568000E+04	-6.133952980E+04	3.437462650E+04
35000 - 50000	7.518922140E+00	-7.304720628E+01	2.828416846E+02	-5.043389208E+02	3.457737605E+02	1.028968776E+02	-1.823414376E+02
Residuals: min=1.151E - 13, max=1.926E - 02, mean=6.794E - 04.							

Table 215: Fitting coefficients for C_p/R of Ar ΔE=1000 cm^{-1}

T interval (K)	a_1	a_2	a_3	a_4	a_5	a_6	a_7
50 - 2000	3.276516920E - 15	-9.192362370E - 12	2.500000010E+00	-1.040174320E - 06	3.818374420E - 05	2.560684420E - 03	-1.310031100E - 01
2000 - 10000	1.595424650E - 04	-2.467356640E - 02	4.016739570E+00	-4.740986190E+01	7.956315473E+02	-6.814975365E+03	2.336331960E+04
10000 - 15000	-5.180724380E+00	2.659591663E+02	-5.652582112E+03	6.358831340E+04	-3.971163850E+05	1.296317640E+06	-1.703989590E+06
15000 - 25000	-5.218994271E+02	1.620336780E+04	-2.066555540E+05	1.384294570E+06	-5.133673970E+06	9.999720640E+06	-8.002506120E+06
25000 - 35000	-3.085952784E+02	6.019764023E+03	-4.832365340E+04	2.055123210E+05	-4.896492470E+05	6.206690080E+05	-3.272859290E+05
35000 - 50000	3.026715366E+01	-3.724137505E+02	1.958318737E+03	-5.569193060E+03	9.028222176E+03	-7.876465197E+03	2.882939675E+03
Residuals: min=3.849E - 12, max=1.236E - 02, mean=2.592E - 04.							

Table 216: Fitting coefficients for C_p/R of Ar^+ ΔE=250 cm^{-1}

T interval (K)	a_1	a_2	a_3	a_4	a_5	a_6	a_7
50 - 2000	-2.024059320E - 07	6.833332210E - 04	1.839911630E+00	2.123521763E+02	-1.881298930E+04	6.771022450E+05	-8.575786110E+06
2000 - 10000	-3.446154050E - 05	8.408663490E - 03	2.210158390E+00	5.770793860E+00	-6.635591961E+01	4.078756349E+02	-1.034680758E+03
10000 - 15000	1.920173600E - 01	-1.004136741E+01	2.214604504E+02	-2.548345042E+03	1.670385480E+04	-5.850430950E+04	8.560522880E+04
15000 - 25000	-1.365105718E+02	4.451307895E+03	-6.012780670E+04	4.302911520E+05	-1.717745980E+06	3.618430490E+06	-3.129947360E+06
25000 - 35000	-5.003738060E+03	1.123777810E+05	-1.035621410E+06	5.015600790E+06	-1.347322370E+07	1.905280560E+07	-1.109379100E+07
35000 - 50000	-7.310343128E+02	1.091463040E+04	-6.614971380E+04	2.102743370E+05	-3.716139780E+05	3.472816250E+05	-1.343392720E+05
Residuals: min=3.648E - 09, max=7.143E - 03, mean=4.819E - 04.							

Table 217: Fitting coefficients for C_p/R of Ar^+ ΔE=500 cm^{-1}

T interval (K)	a_1	a_2	a_3	a_4	a_5	a_6	a_7
50 - 2000	-2.024059150E - 07	6.833331660E - 04	1.839911680E+00	2.123521601E+02	-1.881298710E+04	6.771021140E+05	-8.575783400E+06
2000 - 10000	-3.445339090E - 05	8.407510270E - 03	2.210221800E+00	5.769070600E+00	-6.633170053E+01	4.077101113E+02	-1.034258510E+03
10000 - 15000	8.291889140E - 02	-4.335648550E+00	9.714061762E+01	-1.103478006E+03	7.254057896E+03	-2.551711640E+04	3.757075560E+04
15000 - 25000	-3.159809804E+01	1.018610790E+03	-1.356287150E+04	9.532136740E+04	-3.714459340E+05	7.566586080E+05	-6.229946900E+05
25000 - 35000	-5.060553229E+03	1.009973180E+05	-8.318388920E+05	3.616549560E+06	-8.750400550E+06	1.117288180E+07	-5.884163120E+06
35000 - 50000	-2.319455760E+03	3.149774750E+04	-1.768958500E+05	5.274553550E+05	-8.820342780E+05	7.850668070E+05	-2.907264110E+05
Residuals: min=2.249E - 08, max=6.460E - 03, mean=2.288E - 04.							

Table 218: Fitting coefficients for C_p/R of Ar^+ ΔE=1000 cm^{-1}

T interval (K)	a_1	a_2	a_3	a_4	a_5	a_6	a_7
50 - 2000	-2.024059380E - 07	6.833332390E - 04	1.839911610E+00	2.123521818E+02	-1.881299010E+04	6.771022910E+05	-8.575787080E+06
2000 - 10000	-3.445339660E - 05	8.407511080E - 03	2.210221760E+00	5.769071850E+00	-6.633171896E+01	4.077102489E+02	-1.034258917E+03
10000 - 15000	3.362314620E - 02	-1.780351600E+00	4.195336972E+01	-4.676410497E+02	3.130828529E+03	-1.124265080E+04	1.695055360E+04
15000 - 25000	-7.210465110E+00	2.296713600E+02	-3.005765274E+03	2.064046090E+04	-7.759694800E+04	1.492133300E+05	-1.108793790E+05
25000 - 35000	8.489213390E+02	-1.936836230E+04	1.824250030E+05	-9.069095000E+05	2.506464410E+06	-3.645771510E+06	2.178667940E+06
35000 - 50000	6.947124946E+02	-1.217190050E+04	8.367234690E+04	-2.936844060E+05	5.618323180E+05	-5.599344230E+05	2.283838860E+05
Residuals: min=3.201E - 08, max=6.460E - 03, mean=1.651E - 04.							

Table 219: Fitting coefficients for C_p/R of Ar^{2+} ΔE=250 cm^{-1}

T interval (K)	a_1	a_2	a_3	a_4	a_5	a_6	a_7
50 - 2000	-2.658816260E - 07	8.196786160E - 04	2.120042990E+00	8.386427424E+01	-6.713448830E+03	2.344549620E+05	-2.979848150E+06
2000 - 10000	-3.976301380E - 04	6.200391430E - 02	-9.998353300E - 01	9.022672404E+01	-1.007891124E+03	5.390606447E+03	-1.131952570E+04
10000 - 15000	5.218988100E - 03	-2.994438000E - 01	9.151125440E+00	-6.689172640E+01	3.849867183E+02	-1.226967693E+03	1.703788892E+03
15000 - 25000	1.521660350E+00	-5.095013083E+01	7.129776911E+02	-5.275832140E+03	2.204328110E+04	-4.920153940E+04	4.593316840E+04
25000 - 35000	-5.565828074E+02	1.189446550E+04	-1.056852630E+05	4.994245270E+05	-1.322251260E+06	1.856329210E+06	-1.076458590E+06
35000 - 50000	-1.825762850E+04	2.715764820E+05	-1.669958620E+06	5.431366200E+06	-9.852414110E+06	9.452659440E+06	-3.748960240E+06
Residuals: min=6.828E - 09, max=3.489E - 03, mean=1.881E - 04.							

Table 220: Fitting coefficients for C_p/R of Ar^{2+} ΔE=500 cm^{-1}

T interval (K)	a_1	a_2	a_3	a_4	a_5	a_6	a_7
50 - 2000	-2.658816370E - 07	8.196786500E - 04	2.120042960E+00	8.386428447E+01	-6.713450229E+03	2.344550430E+05	-2.979849840E+06
2000 - 10000	-3.976300520E - 04	6.200390220E - 02	-9.998346700E - 01	9.022670581E+01	-1.007890857E+03	5.390604478E+03	-1.131951990E+04
10000 - 15000	6.089246020E - 03	-3.435432500E - 01	1.007917785E+01	-7.727269777E+01	4.500768514E+02	-1.443857090E+03	2.003812069E+03
15000 - 25000	5.508753600E - 01	-1.846200560E+01	2.603641221E+02	-1.914443636E+03	8.001316761E+03	-1.789974570E+04	1.682560690E+04
25000 - 35000	-1.186292900E+02	2.511398059E+03	-2.205872550E+04	1.027765000E+05	-2.671569760E+05	3.659050310E+05	-2.048091060E+05
35000 - 50000	-3.301906721E+03	4.299042790E+04	-2.263255700E+05	6.111897490E+05	-8.807071900E+05	6.269483440E+05	-1.633992210E+05
Residuals: min=1.642E - 08, max=3.616E - 03, mean=1.614E - 04.							

Table 221: Fitting coefficients for C_p/R of Ar^{2+} ΔE=1000 cm^{-1}

T interval (K)	a_1	a_2	a_3	a_4	a_5	a_6	a_7
50 - 2000	-2.658816300E - 07	8.196786290E - 04	2.120042980E+00	8.386427799E+01	-6.713449342E+03	2.344549910E+05	-2.979848770E+06
2000 - 10000	-3.976301600E - 04	6.200391760E - 02	-9.998355200E - 01	9.022672961E+01	-1.007891210E+03	5.390607118E+03	-1.131952770E+04
10000 - 15000	6.000734550E - 03	-3.392027200E - 01	9.990818450E+00	-7.631695430E+01	4.442832714E+02	-1.425195696E+03	1.978858165E+03
15000 - 25000	1.955304300E - 01	-6.564578270E+00	9.452765267E+01	-6.821427906E+02	2.850319132E+03	-6.409849176E+03	6.133779582E+03
25000 - 35000	-2.543451791E+01	5.344266523E+02	-4.643631298E+03	2.133330790E+04	-5.429547780E+04	7.198456620E+04	-3.812565220E+04
35000 - 50000	1.839442123E+03	-2.801336710E+04	1.767569270E+05	-5.906069620E+05	1.100352020E+06	-1.081801270E+06	4.379711660E+05
Residuals: min=2.009E - 08, max=1.294E - 03, mean=3.146E - 05.							

Table 222: Fitting coefficients for C_p/R of Ar^{3+} ΔE=250 cm^{-1}

T interval (K)	a_1	a_2	a_3	a_4	a_5	a_6	a_7
50 - 2000	4.873620830E - 11	-1.664363570E - 07	2.500168390E+00	-6.508119390E - 02	1.071858782E+01	-7.621490400E+02	1.925815820E+04
2000 - 10000	6.247035060E - 04	-1.134403600E - 01	1.062136954E+01	-2.861853724E+02	4.997686006E+03	-3.782784340E+04	1.048514210E+05
10000 - 15000	3.399638650E - 02	-1.416324740E+00	2.171111424E+01	-6.892932692E+01	-2.109626998E+02	1.986485065E+03	-3.673979128E+03
15000 - 25000	2.080575450E - 02	-1.319820080E+00	2.727375356E+01	-1.829586195E+02	6.911550824E+02	-1.341624773E+03	1.105010498E+03
25000 - 35000	-7.778300570E+00	1.205838121E+02	-6.472245145E+02	1.004617157E+03	3.093950315E+03	-1.301907450E+04	1.315246340E+04
35000 - 50000	-1.924627653E+03	3.167520730E+04	-2.160212000E+05	7.812969230E+05	-1.579600700E+06	1.690915450E+06	-7.473798560E+05
Residuals: min=1.437E - 08, max=1.896E - 03, mean=1.167E - 04.							

Table 223: Fitting coefficients for C_p/R of Ar^{3+} ΔE=500 cm^{-1}

T interval (K)	a_1	a_2	a_3	a_4	a_5	a_6	a_7
50 - 2000	4.872511780E - 11	-1.664015320E - 07	2.500168360E+00	-6.507180190E - 02	1.071735609E+01	-7.620792338E+02	1.925674410E+04
2000 - 10000	6.247036220E - 04	-1.134403700E - 01	1.062137050E+01	-2.861854002E+02	4.997686428E+03	-3.782784660E+04	1.048514300E+05
10000 - 15000	3.402544720E - 02	-1.417750820E+00	2.174016453E+01	-6.924376668E+01	-2.090553441E+02	1.980337298E+03	-3.665752987E+03
15000 - 25000	9.131342460E - 03	-9.405730600E - 01	2.215890689E+01	-1.462961084E+02	5.438311779E+02	-1.026898871E+03	8.257077399E+02
25000 - 35000	7.470105940E+00	-1.658948398E+02	1.543866712E+03	-7.645273075E+03	2.136930110E+04	-3.193563560E+04	1.998348200E+04
35000 - 50000	-1.336510013E+03	2.032200760E+04	-1.284917900E+05	4.321806950E+05	-8.147081290E+05	8.148783310E+05	-3.369808860E+05
Residuals: min=3.827E - 09, max=7.606E - 04, mean=4.444E - 05.							

Table 224: Fitting coefficients for C_p/R of Ar^{3+} ΔE=1000 cm^{-1}

T interval (K)	a_1	a_2	a_3	a_4	a_5	a_6	a_7
50 - 2000	4.873470210E - 11	-1.664314630E - 07	2.500168380E+00	-6.507993660E - 02	1.071843142E+01	-7.621405585E+02	1.925799220E+04
2000 - 10000	6.247035030E - 04	-1.134403600E - 01	1.062136952E+01	-2.861853723E+02	4.997686006E+03	-3.782784340E+04	1.048514210E+05
10000 - 15000	3.408093110E - 02	-1.420474710E+00	2.179567649E+01	-6.984489134E+01	-2.054073703E+02	1.968573931E+03	-3.650005706E+03
15000 - 25000	4.915197070E - 03	-8.031629600E - 01	2.029982132E+01	-1.329300414E+02	4.899664599E+02	-9.115159348E+02	7.230516200E+02
25000 - 35000	2.165725590E+00	-4.904294937E+01	4.687380569E+02	-2.354550973E+03	6.675161021E+03	-1.008455670E+04	6.382512588E+03
35000 - 50000	-2.860675319E+02	4.302061866E+03	-2.685018940E+04	8.893615410E+04	-1.645023880E+05	1.605921560E+05	-6.426373360E+04
Residuals: min=1.475E - 08, max=2.884E - 04, mean=2.474E - 05.							

Table 225: Fitting coefficients for C_p/R of Ar^{4+} ΔE=250 cm^{-1}

T interval (K)	a_1	a_2	a_3	a_4	a_5	a_6	a_7
50 - 2000	4.770080660E - 07	-1.041303030E - 03	2.356945670E+00	7.096317569E+02	-1.090357590E+05	6.087830880E+06	-1.176476950E+08
2000 - 10000	-3.068893150E - 04	6.017473050E - 02	-6.305916700E - 01	7.245926807E+01	-6.879910981E+02	2.881109293E+03	-3.955909964E+03
10000 - 15000	-4.156878280E - 03	1.762483400E - 01	-9.513452000E - 01	4.748458899E+01	-3.400782686E+02	1.218124354E+03	-1.695845155E+03
15000 - 25000	4.690235730E - 03	-2.078922200E - 01	6.213956720E+00	-2.552206396E+01	8.559665056E+01	-1.206348999E+02	7.019150036E+01
25000 - 35000	1.186685870E+00	-2.539301520E+01	2.297560275E+02	-1.083565125E+03	2.902177880E+03	-4.119142585E+03	2.435021012E+03
35000 - 50000	2.587494934E+01	-5.123955749E+02	4.100508555E+03	-1.711986910E+04	3.966922660E+04	-4.854809830E+04	2.461115970E+04
Residuals: min=5.530E - 09, max=4.339E - 02, mean=4.441E - 04.							

Table 226: Fitting coefficients for C_p/R of Ar^{4+} ΔE=500 cm^{-1}

T interval (K)	a_1	a_2	a_3	a_4	a_5	a_6	a_7
50 - 2000	4.770081710E - 07	-1.041303360E - 03	2.356946200E+00	7.096316648E+02	-1.090357470E+05	6.087830170E+06	-1.176476810E+08
2000 - 10000	-3.068888650E - 04	6.017466610E - 02	-6.305880500E - 01	7.245916608E+01	-6.879895709E+02	2.881097739E+03	-3.955875288E+03
10000 - 15000	-4.083543210E - 03	1.726375500E - 01	-8.775396500E - 01	4.668295007E+01	-3.351985470E+02	1.202340350E+03	-1.674649751E+03
15000 - 25000	4.714375450E - 03	-2.086436800E - 01	6.223645440E+00	-2.558830173E+01	8.584985713E+01	-1.211481131E+02	7.062241718E+01
25000 - 35000	8.254486200E - 01	-1.728735477E+01	1.541475492E+02	-7.081823601E+02	1.855646076E+03	-2.565271504E+03	1.474751487E+03
35000 - 50000	3.011081724E+01	-4.945928826E+02	3.403958804E+03	-1.254123580E+04	2.615981960E+04	-2.926599720E+04	1.373335480E+04
Residuals: min=6.461E - 10, max=4.339E - 02, mean=4.391E - 04.							

Table 227: Fitting coefficients for C_p/R of Ar^{4+} ΔE=1000 cm^{-1}

T interval (K)	a_1	a_2	a_3	a_4	a_5	a_6	a_7
50 - 2000	4.770080560E - 07	-1.041303000E - 03	2.356945660E+00	7.096317583E+02	-1.090357590E+05	6.087830860E+06	-1.176476950E+08
2000 - 10000	-3.068889070E - 04	6.017467230E - 02	-6.305884100E - 01	7.245917625E+01	-6.879897259E+02	2.881098931E+03	-3.955878922E+03
10000 - 15000	-3.328968490E - 03	1.356062800E - 01	-1.231270700E - 01	3.851650319E+01	-2.856570802E+02	1.042642173E+03	-1.460938270E+03
15000 - 25000	4.704144360E - 03	-2.083256600E - 01	6.219551120E+00	-2.556035465E+01	8.574318540E+01	-1.209322301E+02	7.044142963E+01
25000 - 35000	-1.839731000E - 01	3.506279790E+00	-2.409041332E+01	1.056925786E+02	-2.327063225E+02	2.903788008E+02	-1.513838005E+02
35000 - 50000	1.088544905E+01	-1.799803108E+02	1.247632866E+03	-4.614102594E+03	9.665149628E+03	-1.083554120E+04	5.088183719E+03
Residuals: min=5.565E - 10, max=4.339E - 02, mean=4.390E - 04.							

Table 228: Fitting coefficients for C_p/R of C ΔE=250 cm^{-1}

T interval (K)	a_1	a_2	a_3	a_4	a_5	a_6	a_7
50 - 2000	5.518787840E - 08	7.300026140E - 06	2.494540650E+00	1.342068460E+00	-1.105745390E+02	-6.468787891E+02	2.977489430E+05
2000 - 10000	3.422518100E - 03	-5.322491500E - 01	3.558209777E+01	-1.063197209E+03	1.892231110E+04	-1.738558040E+05	6.447536620E+05
10000 - 15000	1.059311508E+02	-5.443350075E+03	1.157450170E+05	-1.301340890E+06	8.143463020E+06	-2.683442270E+07	3.633392070E+07
15000 - 25000	1.626990440E+01	-9.994191085E+02	1.833622600E+04	-1.554463490E+05	6.845016930E+05	-1.527927420E+06	1.371951580E+06
25000 - 35000	-2.263638070E+00	9.874024760E+01	-1.143219623E+03	6.181268736E+03	-1.757426340E+04	2.566591670E+04	-1.524304490E+04
35000 - 50000	-2.192408234E+01	3.223171887E+02	-1.952170766E+03	6.278812946E+03	-1.128376120E+04	1.076547520E+04	-4.262112647E+03
Residuals: min=8.309E - 08, max=5.180E - 03, mean=3.978E - 04.							

Table 229: Fitting coefficients for C_p/R of C ΔE=500 cm^{-1}

T interval (K)	a_1	a_2	a_3	a_4	a_5	a_6	a_7
50 - 2000	5.518799730E - 08	7.299639980E - 06	2.494541010E+00	1.341950340E+00	-1.105582423E+02	-6.478383965E+02	2.977689240E+05
2000 - 10000	1.261144440E - 03	-1.886988700E - 01	1.375299936E+01	-3.532993573E+02	6.436765857E+03	-6.088154440E+04	2.321031540E+05
10000 - 15000	1.470230900E+01	-7.164515500E+02	1.429307470E+04	-1.484041500E+05	8.386782760E+05	-2.415185600E+06	2.733929100E+06
15000 - 25000	1.647856397E+02	-4.970955851E+03	6.129196850E+04	-3.959271670E+05	1.418084120E+06	-2.678038270E+06	2.088133690E+06
25000 - 35000	-7.828350590E+00	2.023751059E+02	-1.875552502E+03	8.746978827E+03	-2.220874460E+04	2.952737540E+04	-1.616731340E+04
35000 - 50000	5.123155100E+00	-5.871433298E+01	2.943118632E+02	-7.926466467E+02	1.231821515E+03	-1.033733253E+03	3.648660777E+02
Residuals: min=1.836E - 08, max=2.116E - 03, mean=1.222E - 04.							

Table 230: Fitting coefficients for C_p/R of C ΔE=1000 cm^{-1}

T interval (K)	a_1	a_2	a_3	a_4	a_5	a_6	a_7
50 - 2000	5.518791450E - 08	7.299909740E - 06	2.494540760E+00	1.342033490E+00	-1.105697435E+02	-6.471600273E+02	2.977547620E+05
2000 - 10000	4.661839100E - 04	-6.252067190E - 02	5.748753380E+00	-9.347017788E+01	1.875999151E+03	-1.970007100E+04	8.200333950E+04
10000 - 15000	8.503852500E - 01	-3.276093856E+01	4.186314994E+02	-8.161782967E+02	-2.452506230E+04	1.985086280E+05	-4.461507200E+05
15000 - 25000	-2.287706272E+01	8.977716029E+02	-1.393340990E+04	1.100920120E+05	-4.685584650E+05	1.025611400E+06	-9.081621530E+05
25000 - 35000	-3.812850063E+01	7.265411917E+02	-5.628104332E+03	2.306899640E+04	-5.299842650E+04	6.489227920E+04	-3.311953700E+04
35000 - 50000	4.266720480E+00	-4.032308742E+01	1.705134500E+02	-3.847834293E+02	5.045264246E+02	-3.561153597E+02	1.050008205E+02
Residuals: min=5.819E - 09, max=1.124E - 03, mean=9.105E - 05.							

Table 231: Fitting coefficients for C_p/R of C^+ ΔE=250 cm^{-1}

T interval (K)	a_1	a_2	a_3	a_4	a_5	a_6	a_7
50 - 2000	5.395141740E - 08	2.646497920E - 04	2.353176380E+00	3.395795403E+01	-3.651803824E+03	1.807538110E+05	-3.323565310E+06
2000 - 10000	-9.574770380E - 05	1.587935540E - 02	1.451292280E+00	3.510215303E+01	-6.188820332E+02	5.267351293E+03	-1.528909040E+04
10000 - 15000	1.363470900E - 01	-7.315376130E+00	1.671037377E+02	-1.986918428E+03	1.350509230E+04	-4.852032920E+04	7.236948310E+04
15000 - 25000	-3.175836574E+01	1.060348610E+03	-1.468757130E+04	1.079470320E+05	-4.427678980E+05	9.579347090E+05	-8.486814650E+05
25000 - 35000	-2.316013662E+03	4.803659440E+04	-4.113946520E+05	1.860717310E+06	-4.685886020E+06	6.231771280E+06	-3.421789650E+06
35000 - 50000	-5.726371972E+02	7.396003446E+03	-3.905361560E+04	1.085343980E+05	-1.677776790E+05	1.368777340E+05	-4.602248200E+04
Residuals: min=1.470E - 09, max=1.760E - 03, mean=9.744E - 05.							

Table 232: Fitting coefficients for C_p/R of C^+ ΔE=500 cm^{-1}

T interval (K)	a_1	a_2	a_3	a_4	a_5	a_6	a_7
50 - 2000	5.395139430E - 08	2.646498660E - 04	2.353176310E+00	3.395797674E+01	-3.651806964E+03	1.807539970E+05	-3.323569190E+06
2000 - 10000	-9.579622430E - 05	1.588664910E - 02	1.450858980E+00	3.511515559E+01	-6.190900219E+02	5.269036427E+03	-1.529451100E+04
10000 - 15000	5.171404950E - 02	-2.815210870E+00	6.727109484E+01	-8.036524302E+02	5.598146763E+03	-2.025953950E+04	3.013301650E+04
15000 - 25000	-7.431093700E+00	2.470493986E+02	-3.399524877E+03	2.477100690E+04	-1.001462720E+05	2.119143150E+05	-1.810988060E+05
25000 - 35000	-5.146937348E+01	3.255652320E+02	4.107991910E+03	-5.226439720E+04	2.221501070E+05	-4.206299660E+05	3.006578240E+05
35000 - 50000	5.102140419E+02	-8.048616038E+03	5.130041640E+04	-1.698308280E+05	3.098396780E+05	-2.967526700E+05	1.169789580E+05
Residuals: min=7.687E - 09, max=1.760E - 03, mean=5.286E - 05.							

Table 233: Fitting coefficients for C_p/R of C^+ ΔE=1000 cm^{-1}

T interval (K)	a_1	a_2	a_3	a_4	a_5	a_6	a_7
50 - 2000	5.395140840E - 08	2.646498210E - 04	2.353176350E+00	3.395796307E+01	-3.651805102E+03	1.807538880E+05	-3.323566940E+06
2000 - 10000	-9.579624410E - 05	1.588665190E - 02	1.450858830E+00	3.511515994E+01	-6.190900861E+02	5.269036906E+03	-1.529451240E+04
10000 - 15000	1.637927710E - 02	-9.528605700E - 01	2.629195270E+01	-3.215858887E+02	2.399014620E+03	-8.897463264E+03	1.325004590E+04
15000 - 25000	-1.701917870E+00	5.691950591E+01	-7.844297439E+02	5.724371918E+03	-2.291051660E+04	4.747257640E+04	-3.890528210E+04
25000 - 35000	9.926271530E+01	-2.152706893E+03	1.932288370E+04	-9.158813430E+04	2.410034840E+05	-3.323134600E+05	1.872493140E+05
35000 - 50000	3.033973828E+02	-3.892095037E+03	2.011006850E+04	-5.341476230E+04	7.695202160E+04	-5.681458730E+04	1.663383310E+04
Residuals: min=3.963E - 09, max=1.760E - 03, mean=2.548E - 05.							

Table 234: Fitting coefficients for C_p/R of C^{2+} ΔE=250 cm^{-1}

T interval (K)	a_1	a_2	a_3	a_4	a_5	a_6	a_7
50 - 2000	3.443568470E - 15	-9.282134860E - 12	2.500000010E+00	-9.180462680E - 07	3.533197530E - 05	1.776985210E - 03	-9.660159490E - 02
2000 - 10000	-2.390508460E - 04	3.665297390E - 02	2.925179400E - 01	6.606425289E+01	-1.013377941E+03	7.153605968E+03	-1.491380760E+04
10000 - 15000	6.390405140E - 02	-3.860575410E+00	9.868694331E+01	-1.246227287E+03	8.637214459E+03	-2.933518910E+04	3.883388640E+04
15000 - 25000	1.098715300E - 01	-1.261572620E+00	-7.475184980E+00	1.751998786E+02	-5.331695702E+02	-6.312712024E+01	1.537919357E+03
25000 - 35000	-9.331007265E+01	1.928273467E+03	-1.646726500E+04	7.419789060E+04	-1.848712620E+05	2.394206080E+05	-1.239294310E+05
35000 - 50000	-3.006342552E+02	-4.628487321E+03	8.545497180E+04	-4.666993570E+05	1.193904170E+06	-1.480252920E+06	7.189728500E+05
Residuals: min=1.372E - 12, max=5.275E - 03, mean=2.324E - 04.							

Table 235: Fitting coefficients for C_p/R of C^{2+} ΔE=500 cm^{-1}

T interval (K)	a_1	a_2	a_3	a_4	a_5	a_6	a_7
50 - 2000	2.666855500E - 15	-7.407561070E - 12	2.500000000E+00	-8.521384420E - 07	3.731795820E - 05	1.480684950E - 03	-9.109917070E - 02
2000 - 10000	-2.390505090E - 04	3.665292610E - 02	2.925206100E - 01	6.606417825E+01	-1.013376832E+03	7.153597633E+03	-1.491378430E+04
10000 - 15000	6.390524500E - 02	-3.860637470E+00	9.868827905E+01	-1.246242518E+03	8.637311522E+03	-2.933551700E+04	3.883434500E+04
15000 - 25000	-2.024427000E - 01	9.080950260E+00	-1.498893748E+02	1.219174879E+03	-4.831384496E+03	9.363837092E+03	-7.070081188E+03
25000 - 35000	-1.414620992E+01	2.781308844E+02	-2.229156354E+03	9.245658166E+03	-2.019176130E+04	2.055324950E+04	-5.857753750E+03
35000 - 50000	3.806607420E+03	-5.640179430E+04	3.461086020E+05	-1.124547370E+06	2.037688910E+06	-1.949670010E+06	7.688574680E+05
Residuals: min=3.581E - 12, max=1.438E - 03, mean=6.481E - 05.							

Table 236: Fitting coefficients for C_p/R of C^{2+} ΔE=1000 cm^{-1}

T interval (K)	a_1	a_2	a_3	a_4	a_5	a_6	a_7
50 - 2000	2.287505310E - 15	-6.386582860E - 12	2.500000000E+00	-7.695180960E - 07	3.489057610E - 05	1.324325670E - 03	-8.430333740E - 02
2000 - 10000	-2.390510200E - 04	3.665299870E - 02	2.925165500E - 01	6.606429187E+01	-1.013378522E+03	7.153610347E+03	-1.491382220E+04
10000 - 15000	6.380224840E - 02	-3.855585530E+00	9.858541456E+01	-1.245129625E+03	8.630563907E+03	-2.931377790E+04	3.880526940E+04
15000 - 25000	-3.162755700E - 01	1.285330052E+01	-2.018726207E+02	1.600537523E+03	-6.402779586E+03	1.281310900E+04	-1.022234890E+04
25000 - 35000	-1.812985650E+00	2.866151644E+01	-1.625017951E+02	3.426879948E+02	5.427003702E+02	-3.492151611E+03	4.237373371E+03
35000 - 50000	3.331004151E+02	-4.551033151E+03	2.521978330E+04	-7.168083780E+04	1.081332400E+05	-7.914285820E+04	2.026329300E+04
Residuals: min=1.260E - 12, max=3.779E - 04, mean=3.548E - 05.							

Table 237: Fitting coefficients for C_p/R of C^{3+} ΔE=250 cm^{-1}

T interval (K)	a_1	a_2	a_3	a_4	a_5	a_6	a_7
50 - 2000	2.351299960E - 15	-6.436212770E - 12	2.500000000E+00	-7.231578820E - 07	3.233447340E - 05	1.153793580E - 03	-7.365771000E - 02
2000 - 10000	-2.181030840E - 06	1.128249560E - 04	2.511609490E+00	-1.152298240E+00	3.759937098E+01	-5.403342081E+02	2.910699008E+03
10000 - 15000	1.715619020E - 02	-8.944858800E - 01	2.149344186E+01	-2.061977566E+02	1.167726237E+03	-3.116546127E+03	3.187968451E+03
15000 - 25000	-6.129980490E - 02	1.801773190E+00	-1.707909961E+01	8.778873897E+01	-9.101539538E+01	-2.468181597E+02	4.675486979E+02
25000 - 35000	4.074617370E+00	-8.794978169E+01	7.933960554E+02	-3.808979899E+03	1.042428390E+04	-1.533493000E+04	9.451635651E+03
35000 - 50000	-5.948929806E+02	8.795848379E+03	-5.389985700E+04	1.749768900E+05	-3.165683420E+05	3.015513800E+05	-1.174592650E+05
Residuals: min=4.315E - 13, max=5.489E - 04, mean=3.399E - 05.							

Table 238: Fitting coefficients for C_p/R of C^{3+} ΔE=500 cm^{-1}

T interval (K)	a_1	a_2	a_3	a_4	a_5	a_6	a_7
50 - 2000	1.851103500E - 15	-5.349672510E - 12	2.500000000E+00	-6.586511700E - 07	2.983072590E - 05	9.940985350E - 04	-6.452101630E - 02
2000 - 10000	-2.180801750E - 06	1.127926730E - 04	2.511611270E+00	-1.152347700E+00	3.760009927E+01	-5.403396299E+02	2.910715035E+03
10000 - 15000	1.713905570E - 02	-8.936432300E - 01	2.147623936E+01	-2.060111532E+02	1.166591869E+03	-3.112881954E+03	3.183055014E+03
15000 - 25000	-6.194308400E - 02	1.823157340E+00	-1.737408936E+01	8.995010649E+01	-9.988613927E+01	-2.274823826E+02	4.500617842E+02
25000 - 35000	2.544247060E+00	-5.285110574E+01	4.586762584E+02	-2.109104542E+03	5.572949476E+03	-7.953579421E+03	4.771192854E+03
35000 - 50000	-8.281681319E+01	1.191043278E+03	-7.034341369E+03	2.172873500E+04	-3.655615720E+04	3.111237530E+04	-9.990844271E+03
Residuals: min=6.537E - 12, max=7.869E - 05, mean=8.443E - 06.							

Table 239: Fitting coefficients for C_p/R of C^{3+} ΔE=1000 cm^{-1}

T interval (K)	a_1	a_2	a_3	a_4	a_5	a_6	a_7
50 - 2000	1.700179030E - 15	-4.712664500E - 12	2.500000000E+00	-6.001069550E - 07	2.811751750E - 05	1.024780030E - 03	-6.715116480E - 02
2000 - 10000	-2.180562250E - 06	1.127595160E - 04	2.511613070E+00	-1.152396830E+00	3.760081223E+01	-5.403448702E+02	2.910730354E+03
10000 - 15000	1.708892880E - 02	-8.911830000E - 01	2.142611467E+01	-2.054685168E+02	1.163299756E+03	-3.102269075E+03	3.168851826E+03
15000 - 25000	-6.171294310E - 02	1.816202850E+00	-1.728762570E+01	8.938493751E+01	-9.784225522E+01	-2.313479382E+02	4.530356179E+02
25000 - 35000	6.217137600E - 01	-1.224407363E+01	1.010224755E+02	-4.270834039E+02	1.116211092E+03	-1.642434354E+03	1.037522470E+03
35000 - 50000	-9.908538320E+00	1.293648590E+02	-6.605729635E+02	1.615507133E+03	-1.593901375E+03	-2.800386577E+02	1.146079982E+03
Residuals: min=4.690E - 12, max=3.535E - 05, mean=2.865E - 06.							

Table 240: Fitting coefficients for C_p/R of C^{4+} ΔE=250 cm^{-1}

T interval (K)	a_1	a_2	a_3	a_4	a_5	a_6	a_7
50 - 50000	0.000000000E+00	0.000000000E+00	2.500000000E+00	0.000000000E+00	0.000000000E+00	0.000000000E+00	0.000000000E+00

Table 241: Fitting coefficients for C_p/R of C^{4+} ΔE=500 cm^{-1}

T interval (K)	a_1	a_2	a_3	a_4	a_5	a_6	a_7
50 - 50000	0.000000000E+00	0.000000000E+00	2.500000000E+00	0.000000000E+00	0.000000000E+00	0.000000000E+00	0.000000000E+00

Table 242: Fitting coefficients for C_p/R of C^{4+} ΔE=1000 cm^{-1}

T interval (K)	a_1	a_2	a_3	a_4	a_5	a_6	a_7
50 - 50000	0.000000000E+00	0.000000000E+00	2.500000000E+00	0.000000000E+00	0.000000000E+00	0.000000000E+00	0.000000000E+00

Table 243: Fitting coefficients for C_p/R of C^-

T interval (K)	a_1	a_2	a_3	a_4	a_5	a_6	a_7
50 - 2000	-3.289364480E - 09	1.062992130E - 05	2.490536860E+00	2.722975300E+00	-1.862720509E+02	-1.705997880E+04	1.671681010E+06
2000 - 10000	3.092919310E - 04	3.016641580E - 02	-4.932946130E+00	3.813116258E+02	-6.944753419E+03	5.547822200E+04	-1.658941890E+05
10000 - 15000	-7.308849050E - 03	3.079724900E - 01	-2.115618900E - 01	6.351183750E+00	4.772357730E+01	-3.325106497E+02	6.030330877E+02
15000 - 25000	-3.388873340E - 03	2.141828600E - 01	2.483223800E - 01	1.276847953E+01	-4.150416339E+01	7.311353479E+01	-5.433384284E+01
25000 - 35000	8.815689130E - 04	8.925666950E - 02	1.745529660E+00	3.307322520E+00	-8.136567450E+00	1.068953522E+01	-5.857276350E+00
35000 - 50000	1.027708400E - 01	-1.415827010E+00	1.102992353E+01	-2.736455885E+01	4.923420895E+01	-4.708710929E+01	1.869975062E+01
Residuals: min=1.717E - 09, max=2.814E - 03, mean=1.016E - 04.							

see errata

Table 244: Fitting coefficients for C_p/R of C_2

T interval (K)	a_1	a_2	a_3	a_4	a_5	a_6	a_7
50 - 1000	1.860885460E - 06	-5.132983540E - 03	5.597999660E+00	1.806571612E+03	-7.339718720E+05	9.278964750E+07	-3.830369230E+09
1000 - 3000	-6.213344240E - 07	3.419404650E - 04	4.147727190E+00	-1.140061172E+01	3.706522991E+03	-1.183321090E+05	1.196429250E+06
3000 - 6000	6.118942080E - 04	-9.151837980E - 02	8.969679950E+00	-7.676711417E+01	7.237235589E+02	5.860434460E+00	-2.600236670E+04
6000 - 10000	-1.447566740E - 02	1.085999410E+00	-2.778013816E+01	4.926012502E+02	-3.554693260E+03	1.081816230E+04	-9.009146497E+03
10000 - 35000	-1.380212640E - 02	-1.390283900E - 01	1.614826656E+01	-1.203652104E+02	4.761592477E+02	-9.126214128E+02	6.890235744E+02
35000 - 50000	-7.436879590E - 03	6.776237100E - 01	-4.880836800E - 01	8.072924830E+00	-1.297490734E+01	1.143642607E+01	-4.269570470E+00
Residuals: min=1.231E - 09, max=5.327E - 02, mean=3.816E - 04.							

Table 245: Fitting coefficients for C_p/R of C_2^+

T interval (K)	a_1	a_2	a_3	a_4	a_5	a_6	a_7
50 - 1000	4.622162160E - 08	-2.513797490E - 04	3.983593550E+00	-3.928371751E+02	1.311819460E+05	-1.395501880E+07	5.050593600E+08
1000 - 3000	7.370176550E - 06	-8.110849390E - 03	5.301805440E+00	-4.467462573E+01	1.464801658E+03	-2.568022620E+04	1.891525620E+05
3000 - 6000	3.035282160E - 04	-4.994164390E - 02	7.559677450E+00	-9.716434302E+01	1.674756749E+03	-1.408914750E+04	4.124751390E+04
6000 - 10000	-7.642351290E - 03	6.709568500E - 01	-1.953796925E+01	4.410207047E+02	-4.249299864E+03	1.988432530E+04	-3.690923250E+04
10000 - 35000	-2.060280560E - 02	4.669515300E - 01	2.861713340E+00	-2.137979651E+01	1.087515001E+02	-2.302392540E+02	1.830211408E+02
35000 - 50000	2.667907660E - 03	3.213244900E - 01	9.242689300E - 01	4.131726720E+00	-6.191292320E+00	5.021560290E+00	-1.717473640E+00
Residuals: min=4.534E - 09, max=1.147E - 03, mean=3.961E - 05.							

Table 246: Fitting coefficients for C_p/R of C_2^-

T interval (K)	a_1	a_2	a_3	a_4	a_5	a_6	a_7
50 - 1000	1.435274350E - 07	-5.784888480E - 04	4.280274100E+00	-4.462677097E+02	1.094131370E+05	-9.488112560E+06	2.906476440E+08
1000 - 3000	-1.427095230E - 06	-4.427878700E - 03	4.281160380E+00	4.796027325E+01	-2.186713938E+03	3.531489250E+04	2.767677140E+04
3000 - 6000	3.262245270E - 03	-6.616438500E - 01	5.697896661E+01	-2.101529258E+03	4.423390830E+04	-4.505189300E+05	1.764162850E+06
6000 - 10000	6.111457460E - 02	-4.184533690E+00	1.113604399E+02	-1.248784366E+03	7.087421608E+03	-1.718115320E+04	6.829858336E+03
10000 - 35000	-3.194983270E - 02	1.024516270E+00	-3.941341850E+00	2.620712271E+01	-7.107629087E+01	1.142197261E+02	-8.012429278E+01
35000 - 50000	2.469328510E - 03	4.292547800E - 01	8.159715000E - 01	3.460795500E+00	-3.853238630E+00	2.082804160E+00	-3.616175800E - 01
Residuals: min=1.421E - 09, max=1.052E - 03, mean=1.885E - 05.							

Table 247: Fitting coefficients for C_p/R of C_3

T interval (K)	a_1	a_2	a_3	a_4	a_5	a_6	a_7
50 - 1000	-6.079368780E - 08	-2.609232070E - 04	5.810964320E+00	-6.276057517E+02	1.834545000E+05	-1.781370840E+07	6.028427140E+08
1000 - 3000	-2.198880410E - 05	4.918901190E - 03	3.700437600E+00	3.662333992E+02	-2.055120280E+04	5.317198830E+05	-4.658918990E+06
3000 - 6000	1.823893630E - 03	-4.888694000E - 01	5.370914272E+01	-2.218936626E+03	5.318618670E+04	-5.836611170E+05	2.386181250E+06
6000 - 10000	1.256694500E - 01	-8.901642450E+00	2.452940255E+02	-3.009782469E+03	1.956499310E+04	-6.162419600E+04	6.778303800E+04
10000 - 35000	-2.929395110E - 02	1.196522090E+00	-4.989293340E+00	7.485395840E+01	-3.560221050E+02	7.647749546E+02	-6.196212840E+02
35000 - 50000	-1.493243200E - 01	2.467970140E+00	-4.246045270E+00	1.022294713E+01	-8.295373590E+00	2.832899570E+00	-9.771477870E - 03
Residuals: min=6.818E - 10, max=8.450E - 04, mean=5.593E - 05.							

see errata

Table 248: Fitting coefficients for C_p/R of CN

T interval (K)	a_1	a_2	a_3	a_4	a_5	a_6	a_7
50 - 1000	1.485364830E - 07	-6.316412640E - 04	4.424462010E+00	-5.867163249E+02	1.613194670E+05	-1.564754980E+07	5.306351710E+08
1000 - 3000	5.261222290E - 06	-1.005519890E - 02	5.825838430E+00	-9.414443503E+01	4.383393883E+03	-9.383955500E+04	7.866005240E+05
3000 - 6000	8.719472930E - 04	-1.383986500E - 01	1.306723398E+01	-2.668225996E+02	4.848415199E+03	-4.369685880E+04	1.467170050E+05
6000 - 15000	-8.657132210E - 03	8.500818200E - 01	-2.917209079E+01	6.863062658E+02	-7.137598196E+03	3.594106500E+04	-7.151210020E+04
15000 - 35000	-4.026934260E - 02	1.131287650E+00	-4.677546780E+00	2.155918567E+01	-2.498267511E+01	-1.189297934E+01	3.645902311E+01
35000 - 50000	-5.665630430E - 02	1.225672610E+00	-4.638124050E+00	2.214538932E+01	-3.871070265E+01	3.612674126E+01	-1.405038828E+01
Residuals: min=3.433E - 09, max=1.239E - 03, mean=2.285E - 05.							

Table 249: Fitting coefficients for C_p/R of CN^+

T interval (K)	a_1	a_2	a_3	a_4	a_5	a_6	a_7
50 - 1000	1.485364830E - 07	-6.316412640E - 04	4.424462010E+00	-5.867163249E+02	1.613194670E+05	-1.564754980E+07	5.306351710E+08
1000 - 3000	5.261222290E - 06	-1.005519990E - 02	5.825838430E+00	-9.414443503E+01	4.383393883E+03	-9.383955500E+04	7.866005240E+05
3000 - 6000	8.719472930E - 04	-1.383986500E - 01	1.306723529E+01	-2.668225996E+02	4.848415199E+03	-4.369685880E+04	1.467170050E+05
6000 - 10000	-8.657132210E - 03	8.500818200E - 01	-2.917209079E+01	6.863062658E+02	-7.137598196E+03	3.594106500E+04	-7.151210020E+04
10000 - 35000	-4.026934260E - 02	1.131287650E+00	-4.677546780E+00	2.155918567E+01	-2.498267511E+01	-1.189297934E+01	3.645902311E+01
35000 - 50000	-5.665630430E - 02	1.225672610E+00	-4.638124050E+00	2.214538932E+01	-3.871070265E+01	3.612674126E+01	-1.405038828E+01
Residuals: min=1.082E - 09, max=7.562E - 04, mean=2.754E - 05.							

Table 250: Fitting coefficients for C_p/R of CN^-

T interval (K)	a_1	a_2	a_3	a_4	a_5	a_6	a_7
50 - 1000	9.295510650E - 08	-3.563055720E - 04	3.940361060E+00	-2.192745830E+02	4.312855210E+04	-2.270925400E+06	2.337774620E+07
1000 - 3000	5.639105840E - 05	-2.288883040E - 02	6.381056750E+00	-8.873654568E+01	2.600881793E+03	-4.107503530E+04	2.774473660E+05
3000 - 6000	-3.057679980E - 06	-8.253264820E - 03	4.901969220E+00	-9.105660290E+00	1.767922217E+02	-1.430185175E+03	5.392227485E+03
6000 - 10000	1.658195440E - 03	-1.309462600E - 01	8.473161360E+00	-5.891620618E+01	4.744311080E+02	-1.456985166E+03	3.888937100E+02
10000 - 35000	3.904297050E - 02	-9.966159800E - 01	1.151041890E+01	1.187080418E+01	-2.538464038E+02	7.400868707E+02	-6.868213084E+02
35000 - 50000	-3.589237300E - 01	5.010015730E+00	-2.012716476E+01	5.688312607E+01	-8.373417940E+01	6.790235416E+01	-2.352980947E+01
Residuals: min=1.138E - 10, max=1.148E - 03, mean=9.355E - 05.							

Table 251: Fitting coefficients for C_p/R of CO

T interval (K)	a_1	a_2	a_3	a_4	a_5	a_6	a_7
50 - 1000	9.295511200E - 08	-3.563055960E - 04	3.940361100E+00	-2.192746030E+02	4.312855720E+04	-2.270925970E+06	2.337776920E+07
1000 - 3000	5.653187800E - 05	-2.293843550E - 02	6.388123240E+00	-8.925695630E+01	2.621761228E+03	-4.150768530E+04	2.810679130E+05
3000 - 6000	2.798419720E - 04	-5.560352620E - 02	8.219040420E+00	-1.337573632E+02	2.830851848E+03	-3.183793920E+04	1.521183080E+05
6000 - 15000	3.238063300E - 01	-2.204836363E+01	6.127529289E+02	-8.624761949E+03	6.543231930E+04	-2.470086550E+05	3.624162220E+05
15000 - 35000	1.096573440E+00	-4.776902525E+01	6.902925837E+02	-4.505267898E+03	1.520898810E+04	-2.591996640E+04	1.772646140E+04
35000 - 50000	6.252322600E - 01	-3.276049780E+00	8.121293300E+00	8.165989460E+00	-3.926469228E+01	4.925998929E+01	-2.167926527E+01
Residuals: min=7.296E - 10, max=2.093E - 03, mean=2.435E - 04.							

Table 252: Fitting coefficients for C_p/R of CO^+

T interval (K)	a_1	a_2	a_3	a_4	a_5	a_6	a_7
50 - 1000	8.567001370E - 08	-3.266533550E - 04	3.899686140E+00	-1.953073194E+02	3.692033370E+04	-1.649321270E+06	1.886693000E+06
1000 - 3000	5.272301600E - 05	-2.140387020E - 02	6.141682520E+00	-7.400828767E+01	2.317819423E+03	-4.701680250E+04	5.065153240E+05
3000 - 6000	1.797544980E - 03	-3.048771600E - 01	2.465430355E+01	-6.760362909E+02	1.177293120E+04	-9.411506110E+04	2.851346660E+05
6000 - 10000	-8.951770640E - 03	7.095139000E - 01	-1.621400096E+01	2.238669790E+02	3.643800673E+02	-1.534432660E+04	5.441010590E+04
10000 - 35000	2.538643040E - 02	-2.432955320E+00	5.784867473E+01	-4.376116726E+02	1.672236096E+03	-3.151172738E+03	2.354493845E+03
35000 - 50000	3.425542900E - 02	6.779293800E - 01	-1.860660400E+00	1.311321027E+01	-2.150522085E+01	1.867661935E+01	-6.763084600E+00
Residuals: min=1.127E - 09, max=1.534E - 03, mean=1.947E - 04.							

Table 253: Fitting coefficients for C_p/R of CO_2

T interval (K)	a_1	a_2	a_3	a_4	a_5	a_6	a_7
50 - 1000	-6.541202270E - 07	2.740758940E - 03	-2.764186200E - 01	1.956385613E+03	-2.769687920E+05	2.128976190E+07	-6.656340990E+08
1000 - 3000	6.860267870E - 05	-3.582886450E - 02	1.051426355E+01	-1.502815747E+02	4.518558018E+03	-7.616338400E+04	5.557995820E+05
3000 - 6000	-9.731215180E - 04	1.574367700E - 01	-4.492492180E+00	4.750328343E+02	-1.025662150E+04	1.119194530E+05	-4.540342030E+05
6000 - 15000	-1.559598400E - 01	1.019080933E+01	-2.554586119E+02	3.343667541E+03	-2.145696180E+04	6.613975880E+04	-7.734196380E+04
15000 - 35000	-5.972665800E - 01	1.295464900E+01	-9.268692023E+01	3.811120848E+02	-8.429049684E+02	9.708735088E+02	-4.518054217E+02
35000 - 50000	7.123245240E - 02	7.429147400E - 01	-4.061372200E - 01	1.307421936E+01	-2.942146424E+01	3.176545726E+01	-1.343181163E+01
Residuals: min=3.596E - 09, max=1.251E - 03, mean=3.327E - 05.							

Table 254: Fitting coefficients for C_p/R of CO_2^+

T interval (K)	a_1	a_2	a_3	a_4	a_5	a_6	a_7
50 - 1000	-2.620914720E - 07	9.054036550E - 04	2.482830670E+00	9.648328971E+02	-7.376667470E+04	2.011279550E+06	4.296632790E+06
1000 - 3000	1.121763120E - 05	-1.718781290E - 02	9.193155910E+00	-9.472350385E+01	3.080933148E+03	-5.438724950E+04	4.036339740E+05
3000 - 6000	4.272962000E - 04	-7.225268320E - 02	1.176599085E+01	-1.289680868E+02	2.048074217E+03	-1.532008110E+04	3.629151600E+04
6000 - 10000	-1.080283250E - 02	9.185363800E - 01	-2.427469207E+01	5.582051779E+02	-5.113612878E+03	2.257715450E+04	-3.987408900E+04
10000 - 35000	1.955767290E - 03	-4.513481600E - 01	1.989171600E+01	-1.172303208E+02	3.854712634E+02	-6.463690782E+02	4.419848440E+02
35000 - 50000	-9.076771950E - 02	1.834815280E+00	-3.690871430E+00	1.262683892E+01	-1.573582228E+01	1.108674480E+01	-3.396605180E+00
Residuals: min=7.890E - 10, max=2.291E - 03, mean=2.683E - 05.							

Table 255: Fitting coefficients for C_p/R of e$^-$

T interval (K)	a_1	a_2	a_3	a_4	a_5	a_6	a_7
50 - 50000	0.000000000E+00	0.000000000E+00	2.500000000E+00	0.000000000E+00	0.000000000E+00	0.000000000E+00	0.000000000E+00

Table 256: Fitting coefficients for C_p/R of N ΔE=250 cm^{-1}

T interval (K)	a_1	a_2	a_3	a_4	a_5	a_6	a_7
50 - 2000	1.359215170E - 10	-4.651413160E - 07	2.500472580E+00	-1.839834300E - 01	3.062985027E+01	-2.209625564E+03	5.686369710E+04
2000 - 10000	1.339206600E - 03	-2.333933500E - 01	1.882097603E+01	-5.765070190E+02	1.049369770E+04	-8.832768070E+04	2.823323920E+05
10000 - 15000	-1.755376876E+01	9.652843180E+02	-2.209689160E+04	2.693283230E+05	-1.839003060E+06	6.649975970E+06	-9.895361200E+06
15000 - 25000	4.208357626E+02	-1.216238420E+04	1.435306990E+05	-8.859125740E+05	3.022284600E+06	-5.412571600E+06	3.980439130E+06
25000 - 35000	1.721579110E+00	9.279811505E+01	-1.473451474E+03	8.686224458E+03	-2.536670830E+04	3.714096980E+04	-2.185684270E+04
35000 - 50000	7.130195350E+00	-8.168517310E+01	4.012953097E+02	-1.052000227E+03	1.573186395E+03	-1.260025856E+03	4.211568942E+02
Residuals: min=7.922E - 09, max=7.048E - 03, mean=3.047E - 04.							

Table 257: Fitting coefficients for C_p/R of N ΔE=500 cm^{-1}

T interval (K)	a_1	a_2	a_3	a_4	a_5	a_6	a_7
50 - 2000	1.359421140E - 10	-4.652062360E - 07	2.500472640E+00	-1.840010200E - 01	3.063215707E+01	-2.209756183E+03	5.686633980E+04
2000 - 10000	7.743034400E - 04	-1.457740500E - 01	1.341597941E+01	-4.068612352E+02	7.633045359E+03	-6.369069980E+04	1.973536090E+05
10000 - 15000	-5.748799070E+00	3.070288707E+02	-6.828336821E+03	8.090447610E+04	-5.360765060E+05	1.875083850E+06	-2.681140140E+06
15000 - 25000	-2.453085363E+02	8.022795351E+03	-1.077183790E+05	7.588824590E+05	-2.956078810E+06	6.041102550E+06	-5.067824430E+06
25000 - 35000	-1.155644660E+02	2.260599044E+03	-1.807353300E+04	7.635263670E+04	-1.804656060E+05	2.268043660E+05	-1.185510560E+05
35000 - 50000	1.364148434E+01	-1.562554800E+02	7.745009671E+02	-2.081186931E+03	3.208582767E+03	-2.671524964E+03	9.359065044E+02
Residuals: min=4.305E - 09, max=2.561E - 03, mean=9.066E - 05.							

Table 258: Fitting coefficients for C_p/R of N ΔE=1000 cm^{-1}

T interval (K)	a_1	a_2	a_3	a_4	a_5	a_6	a_7
50 - 2000	1.359428160E - 10	-4.652086330E - 07	2.500472640E+00	-1.840017200E - 01	3.063224631E+01	-2.209761032E+03	5.686643360E+04
2000 - 10000	5.729895450E - 04	-1.145450700E - 01	1.148923136E+01	-3.463746508E+02	6.612846903E+03	-5.490190110E+04	1.670289550E+05
10000 - 15000	-1.412822390E+00	7.587508544E+01	-1.698072545E+03	2.029569030E+04	-1.348963630E+05	4.695258230E+05	-6.583571990E+05
15000 - 25000	-6.031810034E+01	1.783330825E+03	-2.132744380E+04	1.312691160E+05	-4.354161170E+05	7.344496820E+05	-4.886929840E+05
25000 - 35000	-4.250515959E+01	5.976267506E+02	-3.032269654E+03	6.144003114E+03	-2.869175366E+02	-1.581789330E+04	1.594850860E+04
35000 - 50000	-1.073143800E - 03	4.017583524E+01	-3.625830438E+02	1.376534903E+03	-2.660980526E+03	2.620164702E+03	-1.046887408E+03
Residuals: min=9.423E - 09, max=2.259E - 03, mean=8.710E - 05.							

Table 259: Fitting coefficients for C_p/R of N^+ ΔE=250 cm^{-1}

T interval (K)	a_1	a_2	a_3	a_4	a_5	a_6	a_7
50 - 2000	-1.260456990E - 07	1.000811230E - 03	1.987862890E+00	1.136306439E+02	-1.192066780E+04	5.801985260E+05	-1.053042190E+07
2000 - 10000	-3.265922670E - 04	4.752341590E - 02	-3.089116870E - 02	5.823472502E+01	-5.209808049E+02	1.964607618E+03	-1.777827422E+03
10000 - 15000	4.306802400E - 02	-2.273770830E+00	5.200906515E+01	-5.655727223E+02	3.661471544E+03	-1.265607370E+04	1.832232770E+04
15000 - 25000	-1.576274519E+01	4.954058332E+02	-6.388035149E+03	4.309365770E+04	-1.588305940E+05	2.987151530E+05	-2.168068010E+05
25000 - 35000	-1.675742612E+03	2.918014520E+04	-2.007110810E+05	6.776664200E+05	-1.105820550E+06	6.439986330E+05	1.140354840E+05
35000 - 50000	-2.931853127E+03	3.888180580E+04	-2.133648990E+05	6.218168010E+05	-1.016558580E+06	8.847218340E+05	-3.204176610E+05
Residuals: min=1.607E - 08, max=4.303E - 03, mean=1.975E - 04.							

Table 260: Fitting coefficients for C_p/R of N^+ ΔE=500 cm^{-1}

T interval (K)	a_1	a_2	a_3	a_4	a_5	a_6	a_7
50 - 2000	-1.260457000E - 07	1.000811230E - 03	1.987862890E+00	1.136306443E+02	-1.192066790E+04	5.801985270E+05	-1.053042190E+07
2000 - 10000	-3.265860360E - 04	4.752253300E - 02	-3.084208540E - 02	5.823335456E+01	-5.209604884E+02	1.964455363E+03	-1.777374532E+03
10000 - 15000	1.835595120E - 02	-9.795295600E - 01	2.377879421E+01	-2.372552212E+02	1.513826494E+03	-5.162377430E+03	7.423006245E+03
15000 - 25000	-2.025201470E+00	5.926872190E+01	-6.850161305E+02	3.905452468E+03	-1.035321900E+04	7.161308808E+03	1.132217430E+04
25000 - 35000	1.492703988E+03	-3.146632350E+04	2.748405230E+05	-1.271570300E+06	3.281930870E+06	-4.473619080E+06	2.513605470E+06
35000 - 50000	3.706396409E+03	-5.429619820E+04	3.271596840E+05	-1.038971820E+06	1.837340120E+06	-1.718314230E+06	6.648614920E+05
Residuals: min=3.017E - 08, max=4.303E - 03, mean=1.320E - 04.							

Table 261: Fitting coefficients for C_p/R of N^+ ΔE=1000 cm^{-1}

T interval (K)	a_1	a_2	a_3	a_4	a_5	a_6	a_7
50 - 2000	-1.260457070E - 07	1.000811250E - 03	1.987862880E+00	1.136306498E+02	-1.192066860E+04	5.801985680E+05	-1.053042270E+07
2000 - 10000	-3.265922280E - 04	4.752341030E - 02	-3.089085200E - 02	5.823471597E+01	-5.209806677E+02	1.964606568E+03	-1.777824238E+03
10000 - 15000	3.560949240E - 03	-2.225017100E - 01	7.659352790E+00	-5.438159349E+01	3.476332180E+02	-1.197427787E+03	1.805823340E+03
15000 - 25000	-2.790198800E - 01	6.647343380E+00	-4.579168083E+01	-2.739469917E+01	2.066273292E+03	-9.888252761E+03	1.528764280E+04
25000 - 35000	3.689027953E+02	-7.404623574E+03	6.133247880E+04	-2.676682930E+05	6.473296960E+05	-8.198511020E+05	4.240786420E+05
35000 - 50000	4.962925269E+02	-4.759863403E+03	1.400560420E+04	3.377180354E+02	-7.555718840E+04	1.361514970E+05	-7.615031510E+04
Residuals: min=6.584E - 10, max=4.303E - 03, mean=1.203E - 04.							

Table 262: Fitting coefficients for C_p/R of N^{2+} ΔE=250 cm^{-1}

T interval (K)	a_1	a_2	a_3	a_4	a_5	a_6	a_7
50 - 2000	-9.409084680E - 07	2.441579530E - 03	1.635404590E+00	1.434831285E+02	-1.202077580E+04	4.909278450E+05	-7.755825460E+06
2000 - 10000	-2.173658320E - 05	3.412037490E - 03	2.306557820E+00	5.264111470E+00	-6.803383672E+01	3.104186673E+02	4.167935188E+02
10000 - 15000	4.914814540E - 03	-3.209474700E - 01	1.075565395E+01	-1.054998947E+02	6.821315638E+02	-1.997887939E+03	2.254466063E+03
15000 - 25000	1.132425300E - 01	-3.761732000E+00	5.572800446E+01	-4.139956925E+02	1.846824643E+03	-4.270447608E+03	4.013155153E+03
25000 - 35000	-6.993948090E+00	1.218512462E+02	-7.908004229E+02	2.098547730E+03	-1.434436631E+02	-9.358132171E+03	1.260004250E+04
35000 - 50000	4.978903285E+03	-7.299738630E+04	4.430231190E+05	-1.422976600E+06	2.547925570E+06	-2.408141300E+06	9.377265140E+05
Residuals: min=8.276E - 09, max=6.740E - 03, mean=1.253E - 04.							

Table 263: Fitting coefficients for C_p/R of N^{2+} ΔE=500 cm^{-1}

T interval (K)	a_1	a_2	a_3	a_4	a_5	a_6	a_7
50 - 2000	-9.409084510E - 07	2.441579480E - 03	1.635404640E+00	1.434831120E+02	-1.202077350E+04	4.909277110E+05	-7.755822660E+06
2000 - 10000	-2.173633750E - 05	3.412002020E - 03	2.306559830E+00	5.264054190E+00	-6.803297142E+01	3.104120680E+02	4.168134647E+02
10000 - 15000	4.839634600E - 03	-3.172586400E - 01	1.068051877E+01	-1.046867331E+02	6.771996325E+02	-1.981993393E+03	2.233200731E+03
15000 - 25000	5.424181580E - 03	-2.046895100E - 01	6.946539720E+00	-5.795603090E+01	3.878078023E+02	-1.086589691E+03	1.121628925E+03
25000 - 35000	1.964678600E+00	-4.677571664E+01	4.730721333E+02	-2.570989180E+03	8.079407440E+03	-1.374858740E+04	9.873628589E+03
35000 - 50000	-6.473866653E+01	1.352703895E+03	-1.109697520E+04	4.667457310E+04	-1.070350410E+05	1.273603030E+05	-6.132453130E+04
Residuals: min=1.207E - 08, max=6.740E - 03, mean=4.314E - 05.							

Table 264: Fitting coefficients for C_p/R of N^{2+} ΔE=1000 cm^{-1}

T interval (K)	a_1	a_2	a_3	a_4	a_5	a_6	a_7
50 - 2000	-9.409084490E - 07	2.441579470E - 03	1.635404650E+00	1.434831093E+02	-1.202077190E+04	4.909276880E+05	-7.755822180E+06
2000 - 10000	-2.173674820E - 05	3.412060780E - 03	2.306556530E+00	5.264147400E+00	-6.803436854E+01	3.104226496E+02	4.167816754E+02
10000 - 15000	4.986258440E - 03	-3.244505500E - 01	1.082695665E+01	-1.062710536E+02	6.868056029E+02	-2.012941402E+03	2.274593042E+03
15000 - 25000	-2.211006140E - 02	7.029216200E - 01	-5.491481570E+00	3.277158076E+01	1.618087519E+01	-2.758749392E+02	3.854730676E+02
25000 - 35000	1.420378570E - 02	-2.091924020E+00	3.995258882E+01	-2.953052716E+02	1.239362429E+03	-2.593099664E+03	2.159882139E+03
35000 - 50000	-5.978771099E+01	9.548765080E+02	-6.359511006E+03	2.260189880E+04	-4.500464370E+04	4.740478030E+04	-2.045355190E+04
Residuals: min=7.728E - 10, max=6.740E - 03, mean=3.247E - 05.							

Table 265: Fitting coefficients for C_p/R of N^{3+} ΔE=250 cm^{-1}

T interval (K)	a_1	a_2	a_3	a_4	a_5	a_6	a_7
50 - 2000	-1.466381650E - 14	4.518775510E - 11	2.500000210E+00	1.165186340E - 05	-1.507328630E - 03	8.459855840E - 02	-1.701484600E+00
2000 - 10000	1.023489970E - 05	-2.130738460E - 03	2.675498320E+00	-7.344390070E+00	1.653107369E+02	-1.906354289E+03	8.849206743E+03
10000 - 15000	4.165218280E - 02	-2.126364660E+00	4.620580265E+01	-4.509832595E+02	2.342359563E+03	-5.240507099E+03	3.601504049E+03
15000 - 25000	-3.198968500E - 01	9.368556630E+00	-1.021508921E+02	5.297684154E+02	-1.062286982E+03	2.533236016E+02	1.118150850E+03
25000 - 35000	2.131932360E+00	-4.015692166E+01	3.011276896E+02	-1.129376713E+03	2.413164227E+03	-2.821719352E+03	1.428466208E+03
35000 - 50000	4.061151234E+01	-6.646606637E+02	4.550416050E+03	-1.664830600E+04	3.450139330E+04	-3.843944200E+04	1.800930510E+04
Residuals: min=1.358E - 12, max=6.628E - 05, mean=5.587E - 06.							

Table 266: Fitting coefficients for C_p/R of N^{3+} ΔE=500 cm^{-1}

T interval (K)	a_1	a_2	a_3	a_4	a_5	a_6	a_7
50 - 2000	-8.754623320E - 15	2.804864670E - 11	2.499999970E+00	8.188410740E - 06	-1.107233240E - 03	6.412161760E - 02	-1.318724760E+00
2000 - 10000	1.023524500E - 05	-2.130787420E - 03	2.675501040E+00	-7.344466220E+00	1.653118671E+02	-1.906362770E+03	8.849232002E+03
10000 - 15000	4.174624780E - 02	-2.130986860E+00	4.630008689E+01	-4.520051548E+02	2.348566503E+03	-5.260539599E+03	3.628343874E+03
15000 - 25000	-3.199054800E - 01	9.368824750E+00	-1.021543456E+02	5.297919998E+02	-1.062377047E+03	2.535059656E+02	1.117997880E+03
25000 - 35000	9.678625500E - 01	-1.605011747E+01	9.332928805E+01	-1.748876116E+02	-5.137714832E+01	5.707335151E+02	-5.169366581E+02
35000 - 50000	1.669335202E+01	-2.760614134E+02	1.899180128E+03	-6.921201246E+03	1.425083590E+04	-1.574636490E+04	7.309905323E+03
Residuals: min=1.162E - 11, max=6.628E - 05, mean=3.122E - 06.							

Table 267: Fitting coefficients for C_p/R of N^{3+} ΔE=1000 cm^{-1}

T interval (K)	a_1	a_2	a_3	a_4	a_5	a_6	a_7
50 - 2000	-6.628534020E - 15	2.162363770E - 11	2.499999980E+00	6.326573280E - 06	-8.510532150E - 04	4.915222770E - 02	-1.009410840E+00
2000 - 10000	1.023502900E - 05	-2.130757070E - 03	2.675499370E+00	-7.344419970E+00	1.653111873E+02	-1.906357715E+03	8.849217072E+03
10000 - 15000	4.162661570E - 02	-2.125110920E+00	4.618028070E+01	-4.507071949E+02	2.340686062E+03	-5.235116402E+03	3.594295141E+03
15000 - 25000	-3.198387900E - 01	9.366747550E+00	-1.021275448E+02	5.296086659E+02	-1.061675766E+03	2.520836676E+02	1.119192853E+03
25000 - 35000	1.359289310E+00	-2.387433012E+01	1.581616126E+02	-4.597908039E+02	6.484811842E+02	-3.397215858E+02	-2.740824181E+01
35000 - 50000	1.245594090E+01	-1.957459215E+02	1.278661094E+03	-4.401753717E+03	8.552464441E+03	-8.913557659E+03	3.906265615E+03
Residuals: min=5.936E - 12, max=6.628E - 05, mean=4.075E - 06.							

Table 268: Fitting coefficients for C_p/R of N^{4+} ΔE=250 cm^{-1}

T interval (K)	a_1	a_2	a_3	a_4	a_5	a_6	a_7
50 - 2000	-6.222977480E - 15	1.989486030E - 11	2.500000230E+00	5.467265530E - 06	-7.175921370E - 04	4.054302190E - 02	-8.170279800E - 01
2000 - 10000	6.945030800E - 06	-1.118822960E - 03	2.572262930E+00	-2.397183380E+00	4.318017420E+01	-4.019614539E+02	1.517923351E+03
10000 - 15000	6.760096990E - 03	-2.975401700E - 01	7.531721260E+00	-3.862735672E+01	1.065561079E+02	1.307673790E+02	-6.222236035E+02
15000 - 25000	2.186009980E - 02	-9.643120500E - 01	1.953070743E+01	-1.518370056E+02	6.990095615E+02	-1.502693028E+03	1.233020792E+03
25000 - 35000	-1.894478300E - 01	4.544202040E+00	-4.014085748E+01	1.925669341E+02	-4.194552941E+02	4.369627638E+02	-1.712980630E+02
35000 - 50000	1.495493390E+00	-2.111371194E+01	1.220755665E+02	-3.516640892E+02	6.003282953E+02	-5.719087219E+02	2.385321791E+02
Residuals: min=2.877E - 12, max=8.597E - 06, mean=9.602E - 07.							

Table 269: Fitting coefficients for C_p/R of N^{4+} ΔE=500 cm^{-1}

T interval (K)	a_1	a_2	a_3	a_4	a_5	a_6	a_7
50 - 2000	-5.404962970E - 15	1.727295240E - 11	2.499999980E+00	4.871867700E - 06	-6.456584380E - 04	3.678708740E - 02	-7.469233000E - 01
2000 - 10000	6.944970580E - 06	-1.118814670E - 03	2.572262480E+00	-2.397171250E+00	4.317999947E+01	-4.019601797E+02	1.517919655E+03
10000 - 15000	6.585815210E - 03	-2.889791600E - 01	7.357150400E+00	-3.673588001E+01	9.507088464E+01	1.678243715E+02	-6.718592756E+02
15000 - 25000	2.186270710E - 02	-9.643928800E - 01	1.953174527E+01	-1.518440707E+02	6.990364562E+02	-1.502747313E+03	1.233066184E+03
25000 - 35000	-2.515244500E - 01	5.806284580E+00	-5.080485202E+01	2.404998708E+02	-5.403355605E+02	5.991301841E+02	-2.617158554E+02
35000 - 50000	7.301077900E - 01	-9.545483390E+00	4.919213271E+01	-1.065942124E+02	1.363447256E+02	-1.027838402E+02	4.056111573E+01
Residuals: min=3.446E - 12, max=8.597E - 06, mean=9.643E - 07.							

Table 270: Fitting coefficients for C_p/R of N^{4+} ΔE=1000 cm^{-1}

T interval (K)	a_1	a_2	a_3	a_4	a_5	a_6	a_7
50 - 2000	-4.762243630E - 15	1.543334390E - 11	2.499999990E+00	4.503150220E - 06	-6.036683580E - 04	3.470220710E - 02	-7.100872200E - 01
2000 - 10000	6.945013990E - 06	-1.118820660E - 03	2.572262810E+00	-2.397180060E+00	4.318012673E+01	-4.019611100E+02	1.517922359E+03
10000 - 15000	6.657486470E - 03	-2.924992900E - 01	7.428920880E+00	-3.751340380E+01	9.979140050E+01	1.525958984E+02	-6.514646752E+02
15000 - 25000	2.186755620E - 02	-9.645439400E - 01	1.953369434E+01	-1.518573888E+02	6.990874599E+02	-1.502850759E+03	1.233153099E+03
25000 - 35000	-2.630828400E - 01	6.042339270E+00	-5.280788807E+01	2.495388818E+02	-5.632136705E+02	6.299232305E+02	-2.789346119E+02
35000 - 50000	4.746969100E - 01	-5.689727680E+00	2.493234541E+01	-2.513981324E+01	-1.763508673E+01	5.266028073E+01	-2.493515795E+01
Residuals: min=2.270E - 12, max=8.597E - 06, mean=9.608E - 07.							

Table 271: Fitting coefficients for C_p/R of N^-

T interval (K)	a_1	a_2	a_3	a_4	a_5	a_6	a_7
50 - 2000	-6.263710240E - 08	3.740473190E - 04	2.327115410E+00	3.653919526E+01	-3.694327379E+03	1.713915440E+05	-2.848723270E+06
2000 - 10000	-2.046846510E - 04	4.162023080E - 02	-6.231933300E - 01	1.039566030E+02	-1.458549904E+03	9.736083376E+03	-2.556638750E+04
10000 - 15000	-9.973189220E - 04	1.803361130E - 03	3.427788360E+00	-9.240681810E+00	4.355254151E+01	-1.057058482E+02	1.074235444E+02
15000 - 25000	-1.210119490E - 03	1.948643230E - 02	3.032321780E+00	-5.174527550E+00	2.165072086E+01	-4.489729209E+01	3.765166885E+01
25000 - 35000	-5.505766280E - 02	1.152034440E+00	-6.954214960E+00	4.223973113E+01	-1.067159576E+02	1.438863640E+02	-8.074442797E+01
35000 - 50000	4.982482240E - 02	-6.634201500E - 01	6.548620210E+00	-1.283033894E+01	2.260316067E+01	-2.108135490E+01	8.146558890E+00
Residuals: min=1.213E - 10, max=1.243E - 03, mean=1.979E - 05.							

Table 272: Fitting coefficients for C_p/R of N_2

T interval (K)	a_1	a_2	a_3	a_4	a_5	a_6	a_7
50 - 1000	6.026782720E - 08	-2.246595750E - 04	3.762803150E+00	-1.170457022E+02	1.733674690E+04	2.380174270E+05	-6.115721610E+07
1000 - 3000	6.525819040E - 05	-2.444075800E - 02	6.324131400E+00	-7.785287656E+01	2.060274113E+03	-2.927364000E+04	1.776979730E+05
3000 - 6000	2.378286940E - 04	-4.919400430E - 02	7.691775090E+00	-1.117484848E+02	2.309560646E+03	-2.532306080E+04	1.179106810E+05
6000 - 15000	1.801282700E - 01	-1.208300191E+01	3.309729225E+02	-4.491580740E+03	3.254254260E+04	-1.139056770E+05	1.490788260E+05
15000 - 35000	3.478740340E+00	-1.043903124E+02	1.222548664E+03	-7.065203074E+03	2.193370830E+04	-3.514797090E+04	2.291752250E+04
35000 - 50000	4.092196300E - 02	4.700772190E+00	-3.348084150E+01	1.209076047E+02	-2.143196082E+02	1.969677000E+02	-7.435172218E+01
Residuals: min=9.482E - 09, max=1.842E - 03, mean=1.840E - 04.							

Table 273: Fitting coefficients for C_p/R of N_2^+

T interval (K)	a_1	a_2	a_3	a_4	a_5	a_6	a_7
50 - 1000	8.778922150E - 08	-3.351825460E - 04	3.911201190E+00	-2.019940564E+02	3.865458690E+04	-1.830639230E+06	8.708991130E+06
1000 - 3000	2.511168040E - 04	-9.943534210E - 02	1.844641328E+01	-1.048422726E+03	4.170947850E+04	-7.722152240E+05	5.453626990E+06
3000 - 6000	1.187635750E - 03	-6.178089450E - 02	-1.022755040E+00	4.634960077E+02	-1.085267290E+04	1.129914540E+05	-4.459144230E+05
6000 - 15000	-3.533846130E - 02	2.165693470E+00	-4.689127612E+01	6.307182057E+02	-3.805347479E+03	1.035690840E+04	-9.616725755E+03
15000 - 35000	-1.011921600E - 01	1.537971620E+00	3.992064490E+00	-6.385835852E+01	2.912700846E+02	-5.560187141E+02	4.003651129E+02
35000 - 50000	-1.254089100E - 01	2.747714980E+00	-1.302198287E+01	4.605455968E+01	-7.704239517E+01	6.907418239E+01	-2.592065555E+01
Residuals: min=2.993E - 09, max=1.117E - 03, mean=2.114E - 05.							

Table 274: Fitting coefficients for C_p/R of N_2^-

T interval (K)	a_1	a_2	a_3	a_4	a_5	a_6	a_7
50 - 1000	1.252514670E - 07	-4.915972910E - 04	4.134148250E+00	-3.396725953E+02	7.604694290E+04	-5.712668110E+06	1.469747350E+08
1000 - 3000	4.392250980E - 05	-1.985157460E - 02	6.244111520E+00	-8.740158393E+01	2.699228106E+03	-4.472388830E+04	3.151574060E+05
3000 - 6000	-7.262906620E - 05	3.355539190E - 03	4.206303430E+00	1.340036150E+01	-2.407805143E+02	2.704916922E+03	-1.187541300E+04
6000 - 15000	-8.029180040E - 03	5.077310600E - 01	-8.142307870E+00	1.530312032E+02	-8.370072170E+02	1.638007838E+03	-2.055351664E+02
15000 - 35000	1.559354780E - 02	-1.080195580E+00	2.399747466E+01	-1.406797506E+02	4.578907693E+02	-7.409730896E+02	4.792431938E+02
35000 - 50000	-2.977056920E - 02	1.075657230E+00	-3.216252330E+00	1.795344690E+01	-2.746946706E+01	2.021226248E+01	-5.652007200E+00
Residuals: min=6.999E - 10, max=1.258E - 03, mean=1.364E - 05.							

Table 275: Fitting coefficients for C_p/R of N_3

T interval (K)	a_1	a_2	a_3	a_4	a_5	a_6	a_7
50 - 1000	-8.181858500E - 07	3.406619080E - 03	-4.487466900E - 01	1.770372856E+03	-2.097548520E+05	1.371153120E+07	-3.802581690E+08
1000 - 3000	5.607380430E - 05	-3.375083140E - 02	1.046010829E+01	-1.506477097E+02	4.521062218E+03	-7.426306440E+04	5.146680830E+05
3000 - 6000	5.348758940E - 04	-1.090875100E - 01	1.504018504E+01	-2.760774678E+02	5.553984921E+03	-5.670838250E+04	2.164205940E+05
6000 - 15000	1.582157330E - 02	-1.010875980E+00	3.139690720E+01	-2.485088549E+02	1.034999544E+03	-1.915515455E+03	8.387737125E+02
15000 - 35000	-4.822620640E - 02	1.317343120E+00	-3.293413430E+00	1.766159945E+01	-3.502047075E+01	4.007918384E+01	-1.996791946E+01
35000 - 50000	1.291314890E - 02	3.736365900E - 01	2.894278040E+00	-4.457574680E+00	1.052440331E+01	-1.116322233E+01	4.621890670E+00
Residuals: min=5.259E - 10, max=1.429E - 03, mean=9.199E - 06.							

Table 276: Fitting coefficients for C_p/R of NO

T interval (K)	a_1	a_2	a_3	a_4	a_5	a_6	a_7
50 - 1000	1.346640380E - 07	-5.333773380E - 04	4.198885080E+00	-3.838810262E+02	8.892485660E+04	-7.118696140E+06	1.992922550E+08
1000 - 3000	3.987553700E - 05	-1.878000310E - 02	6.186088850E+00	-8.603653213E+01	2.716156638E+03	-4.573828610E+04	3.284501640E+05
3000 - 6000	-8.205872510E - 04	1.205117600E - 01	-3.317181910E+00	2.669647051E+02	-4.910380278E+03	4.653358710E+04	-1.668984420E+05
6000 - 15000	-3.742503470E - 02	2.255826190E+00	-4.684414345E+01	5.247635557E+02	-2.033594737E+03	1.526351150E+02	1.046998090E+04
15000 - 35000	-5.313270880E - 02	-6.567835000E - 01	3.388158542E+01	-2.449877019E+02	8.608507866E+02	-1.470339063E+03	9.953195904E+02
35000 - 50000	-9.327069780E - 02	2.391062770E+00	-1.016994208E+01	3.480056503E+01	-5.368883565E+01	4.433883200E+01	-1.532036817E+01
Residuals: min=9.260E - 10, max=1.230E - 03, mean=2.741E - 05.							

Table 277: Fitting coefficients for C_p/R of NO^+

T interval (K)	a_1	a_2	a_3	a_4	a_5	a_6	a_7
50 - 1000	5.792277660E - 08	-2.153683800E - 04	3.750569680E+00	-1.102104795E+02	1.566614530E+04	3.954638350E+05	-6.625645550E+07
1000 - 3000	6.570421560E - 05	-2.445858420E - 02	6.303542240E+00	-7.574575156E+01	1.976625579E+03	-2.751289010E+04	1.630914510E+05
3000 - 6000	2.288387600E - 04	-4.856673390E - 02	7.685519870E+00	-1.123918127E+02	2.337963884E+03	-2.565607830E+04	1.191468310E+05
6000 - 15000	2.190458300E - 01	-1.486104775E+01	4.120460190E+02	-5.724870342E+03	4.280722400E+04	-1.578948480E+05	2.241934780E+05
15000 - 35000	2.318981990E+00	-7.462539219E+01	9.188537727E+02	-5.480164214E+03	1.740551260E+04	-2.837884320E+04	1.876084940E+04
35000 - 50000	3.192252500E - 01	3.996686500E - 01	-8.563833990E+00	4.458223298E+01	-8.315079703E+01	7.680272777E+01	-2.847420293E+01
Residuals: min=2.237E - 09, max=1.822E - 03, mean=1.910E - 04.							

Table 278: Fitting coefficients for C_p/R of NO_2

T interval (K)	a_1	a_2	a_3	a_4	a_5	a_6	a_7
50 - 1000	-2.697204500E - 07	9.836504190E - 04	2.962700280E+00	2.593169294E+02	8.211180320E+04	-1.269235490E+07	5.138750590E+08
1000 - 3000	2.468689610E - 05	-2.090014930E - 02	8.630275410E+00	-4.349794074E+01	-1.269449273E+03	9.057468780E+04	-1.116358690E+06
3000 - 6000	-1.910039490E - 03	2.735113900E - 01	-8.712327730E+00	4.160336177E+02	-4.811949894E+03	2.445859970E+04	-4.720137420E+04
6000 - 15000	1.039942500E - 02	-6.011238200E - 01	1.715398198E+01	7.117724470E+00	-1.162544447E+03	7.112766526E+03	-1.357302830E+04
15000 - 35000	-9.986069590E - 02	2.586272280E+00	-1.398567509E+01	6.248997702E+01	-1.347617616E+02	1.582447230E+02	-7.863681672E+01
35000 - 50000	-6.664419850E - 03	9.024785900E - 01	-1.238973370E+00	1.077328057E+01	-1.626908523E+01	1.305140938E+01	-4.401098860E+00
Residuals: min=2.745E - 09, max=1.861E - 03, mean=1.548E - 05.							

Table 279: Fitting coefficients for C_p/R of N_2O

T interval (K)	a_1	a_2	a_3	a_4	a_5	a_6	a_7
50 - 1000	-4.526850610E - 07	2.120293790E - 03	1.531157600E - 01	1.977996709E+03	-2.978767240E+05	2.401839040E+07	-7.778917320E+08
1000 - 3000	-1.084954550E - 06	-1.635835990E - 02	9.164057840E+00	-1.841781481E+02	1.312988230E+04	-4.373227360E+05	4.671740230E+06
3000 - 6000	1.855159360E - 03	-3.153777200E - 01	2.569717629E+01	-4.081966004E+02	1.442211901E+03	2.721012030E+04	-1.818655820E+05
6000 - 15000	-1.345955500E - 01	8.534034810E+00	-1.990972365E+02	2.316624384E+03	-1.277772300E+04	3.107676700E+04	-2.214900680E+04
15000 - 35000	-4.467485800E - 01	9.116539440E+00	-6.050466674E+01	2.181281613E+02	-3.827398356E+02	2.871978760E+02	-3.236338211E+01
35000 - 50000	1.749342700E - 01	-1.091286800E+00	7.549205510E+00	-1.268346743E+01	1.971473201E+01	-1.762122811E+01	6.860942020E+00
Residuals: min=2.861E - 09, max=3.402E - 03, mean=5.611E - 05.							

Table 280: Fitting coefficients for C_p/R of N_2 O^+

T interval (K)	a_1	a_2	a_3	a_4	a_5	a_6	a_7
50 - 1000	-2.138420250E-07	9.444413210E-04	2.194231940E+00	1.234962899E+03	-1.510199160E+05	1.046401830E+07	-3.148470090E+08
1000 - 3000	-1.918150820E-05	-1.133396020E-02	9.378389980E+00	-2.342226822E+02	1.593549280E+04	-5.043873910E+05	5.256369080E+06
3000 - 6000	3.890807900E-03	-6.409953000E-01	4.744182904E+01	-1.165855790E+03	1.591064060E+04	-1.143406180E+05	3.437310550E+05
6000 - 15000	-9.955444240E-03	7.082549500E-01	-8.564872200E+00	1.008113189E+02	-5.277093637E+02	1.499834124E+03	-1.805339141E+03
15000 - 35000	7.015703730E-03	4.733631300E-02	2.439452550E+00	6.579443000E-01	-3.363324470E+00	6.926506060E+00	-5.213707420E+00
35000 - 50000	1.326079000E-01	-1.764769250E+00	1.336214230E+01	-3.468089384E+01	6.173249966E+01	-5.832618369E+01	2.287995855E+01
Residuals: min=5.608E-10, max=3.759E-03, mean=1.821E-05.							

Table 281: Fitting coefficients for C_p/R of NCO

T interval (K)	a_1	a_2	a_3	a_4	a_5	a_6	a_7
50 - 1000	-4.110511480E-07	2.018119220E-03	7.180589400E-01	1.759079029E+03	-2.544850530E+05	2.028397920E+07	-6.630255350E+08
1000 - 3000	3.772206030E-05	-2.612533710E-02	9.871941250E+00	-1.236749209E+02	3.773742187E+03	-6.273792720E+04	4.398820800E+05
3000 - 6000	2.275857030E-04	-6.465528340E-02	1.274474514E+01	-2.193733102E+02	4.919737252E+03	-5.477280980E+04	2.238898880E+05
6000 - 10000	4.949228290E-03	-2.814742200E-01	1.123555077E+01	5.245775154E+01	-1.586109283E+03	1.073598500E+04	-2.514127160E+04
10000 - 35000	-1.425799500E-02	3.325396000E-01	7.614224090E+00	-4.163473361E+01	1.381728165E+02	-2.248339281E+02	1.476300680E+02
35000 - 50000	-7.748116520E-02	1.641067150E+00	-4.073733120E+00	1.554612209E+01	-2.211609502E+01	1.756282387E+01	-5.997704380E+00
Residuals: min=2.397E-09, max=5.419E-03, mean=3.149E-05.							

Table 282: Fitting coefficients for C_p/R of O ΔE=250 cm^{-1}

T interval (K)	a_1	a_2	a_3	a_4	a_5	a_6	a_7
50 - 2000	-3.110024390E - 07	6.948659320E - 04	2.511950330E+00	-3.817118589E+01	5.957608985E+03	-3.469300540E+05	6.988382380E+06
2000 - 10000	2.336680340E - 04	-4.042040830E - 02	5.459962580E+00	-1.151203867E+02	2.388915630E+03	-2.285629570E+04	8.273620880E+04
10000 - 15000	-8.802068260E+00	4.703636449E+02	-1.046327610E+04	1.239687220E+05	-8.225999420E+05	2.887698630E+06	-4.158492880E+06
15000 - 25000	-1.897141601E+02	6.601629878E+03	-9.364823560E+04	6.926907140E+05	-2.817307380E+06	5.983534050E+06	-5.196297510E+06
25000 - 35000	-8.788983228E+01	1.793349740E+03	-1.483746220E+04	6.455695340E+04	-1.566302250E+05	2.015819730E+05	-1.077017500E+05
35000 - 50000	1.401316243E+01	-1.674676200E+02	8.613338123E+02	-2.395246169E+03	3.810612036E+03	-3.267244538E+03	1.176604861E+03
Residuals: min=1.087E - 10, max=6.196E - 03, mean=2.844E - 04.							

Table 283: Fitting coefficients for C_p/R of O ΔE=500 cm^{-1}

T interval (K)	a_1	a_2	a_3	a_4	a_5	a_6	a_7
50 - 2000	-3.110024260E - 07	6.948658890E - 04	2.511950370E+00	-3.817119824E+01	5.957610631E+03	-3.469301480E+05	6.988384290E+06
2000 - 10000	-7.443769920E - 05	7.486293960E - 03	2.495795660E+00	-2.174202182E+01	8.073211452E+02	-9.162555715E+03	3.520504080E+04
10000 - 15000	-2.037605470E+00	1.082943512E+02	-2.392046258E+03	2.813947100E+04	-1.845426220E+05	6.357626320E+05	-8.859955340E+05
15000 - 25000	-1.059987860E+02	3.217246825E+03	-3.982105980E+04	2.564854880E+05	-9.044023260E+05	1.655888070E+06	-1.231372010E+06
25000 - 35000	-9.784839883E+01	1.696097876E+03	-1.199497210E+04	4.475568170E+04	-9.318620810E+04	1.027811680E+05	-4.690356510E+04
35000 - 50000	6.747289530E+00	-5.056908747E+01	1.398191924E+02	-1.032023596E+02	-2.089262838E+02	4.507190543E+02	-2.460980823E+02
Residuals: min=2.823E - 09, max=6.196E - 03, mean=1.379E - 04.							

Table 284: Fitting coefficients for C_p/R of O ΔE=1000 cm^{-1}

T interval (K)	a_1	a_2	a_3	a_4	a_5	a_6	a_7
50 - 2000	-3.110023960E - 07	6.948657950E - 04	2.511950450E+00	-3.817122620E+01	5.957614438E+03	-3.469303700E+05	6.988388890E+06
2000 - 10000	-1.826466740E - 04	2.431458850E - 02	1.454326770E+00	1.107608359E+01	2.512708445E+02	-4.346133405E+03	1.847880440E+04
10000 - 15000	-5.110651000E - 01	2.733963507E+01	-6.060352386E+02	7.192388230E+03	-4.721691830E+04	1.613386240E+05	-2.186164420E+05
15000 - 25000	1.016890976E+01	-3.947926757E+02	6.230052915E+03	-5.100772300E+04	2.279456980E+05	-5.242159580E+05	4.847191710E+05
25000 - 35000	1.112201170E+02	-2.328524211E+03	1.983976990E+04	-8.819904250E+04	2.170424530E+05	-2.815507980E+05	1.509018230E+05
35000 - 50000	-2.812137896E+01	4.065081766E+02	-2.332872820E+03	7.023709995E+03	-1.178082770E+04	1.049421210E+04	-3.886704312E+03
Residuals: min=2.287E - 09, max=6.196E - 03, mean=7.147E - 05.							

Table 285: Fitting coefficients for C_p/R of O^+ ΔE=250 cm^{-1}

T interval (K)	a_1	a_2	a_3	a_4	a_5	a_6	a_7
50 - 2000	-9.018569000E - 15	2.927466950E - 11	2.499999970E+00	8.781501850E - 06	-1.194882820E - 03	6.954367360E - 02	-1.436894610E+00
2000 - 10000	6.315837630E - 04	-9.682227270E - 02	8.231141960E+00	-1.625272610E+02	2.185117876E+03	-1.146722760E+04	1.879835230E+04
10000 - 15000	-2.795762460E - 02	1.868083050E+00	-4.650597489E+01	6.247753070E+02	-3.912022041E+03	1.209183460E+04	-1.489969710E+04
15000 - 25000	1.572980340E+00	-5.540554130E+01	8.118308862E+02	-6.279126194E+03	2.755083480E+04	-6.500693020E+04	6.453508870E+04
25000 - 35000	-3.457471673E+01	1.316293036E+03	-1.723623900E+04	1.097778770E+05	-3.714611000E+05	6.429920470E+05	-4.471700640E+05
35000 - 50000	2.465623990E+03	-2.889711930E+04	1.326153250E+05	-2.951790620E+05	3.095082840E+05	-1.003837680E+05	-3.059988930E+04
Residuals: min=1.342E - 11, max=2.047E - 03, mean=1.556E - 04.							

Table 286: Fitting coefficients for C_p/R of O^+ ΔE=500 cm^{-1}

T interval (K)	a_1	a_2	a_3	a_4	a_5	a_6	a_7
50 - 2000	-6.033566300E - 15	1.950078080E - 11	2.499999980E+00	6.027162580E - 06	-8.341378660E - 04	4.914643160E - 02	-1.024467810E+00
2000 - 10000	6.315839200E - 04	-9.682229540E - 02	8.231143250E+00	-1.625272815E+02	2.185118433E+03	-1.146723180E+04	1.879836520E+04
10000 - 15000	-2.764501690E - 02	1.853558680E+00	-4.622729019E+01	6.219509176E+02	-3.896091964E+03	1.204449050E+04	-1.484189000E+04
15000 - 25000	1.341622970E+00	-4.719902035E+01	6.902072694E+02	-5.314491315E+03	2.322921360E+04	-5.462898340E+04	5.408903650E+04
25000 - 35000	-1.165071464E+02	2.888325498E+03	-2.950526550E+04	1.591790420E+05	-4.780634330E+05	7.566627870E+05	-4.912091200E+05
35000 - 50000	-7.991187063E+02	1.750616330E+04	-1.400568640E+05	5.528517510E+05	-1.163365520E+06	1.254877600E+06	-5.470646380E+05
Residuals: min=9.524E - 12, max=2.003E - 03, mean=1.428E - 04.							

Table 287: Fitting coefficients for C_p/R of O^+ ΔE=1000 cm^{-1}

T interval (K)	a_1	a_2	a_3	a_4	a_5	a_6	a_7
50 - 2000	-5.370796960E - 15	1.688429130E - 11	2.499999990E+00	4.789687600E - 06	-6.448581720E - 04	3.729984770E - 02	-7.680352600E - 01
2000 - 10000	6.315839730E - 04	-9.682230310E - 02	8.231143690E+00	-1.625273106E+02	2.185118629E+03	-1.146723330E+04	1.879836980E+04
10000 - 15000	-3.024745190E - 02	1.986048400E+00	-4.903119813E+01	6.535261968E+02	-4.095652371E+03	1.271568140E+04	-1.578049880E+04
15000 - 25000	6.017060300E - 01	-2.116883251E+01	3.075078627E+02	-2.302559624E+03	9.835232542E+03	-2.269067750E+04	2.215420560E+04
25000 - 35000	-8.336190171E+01	1.843100094E+03	-1.697695170E+04	8.337228000E+04	-2.296825270E+05	3.354873360E+05	-2.017382560E+05
35000 - 50000	-3.099104135E+03	4.432602140E+04	-2.612744750E+05	8.115840190E+05	-1.400419850E+06	1.273283730E+06	-4.770061420E+05
Residuals: min=6.789E - 12, max=8.333E - 04, mean=5.711E - 05.							

Table 288: Fitting coefficients for C_p/R of O^{2+} ΔE=250 cm^{-1}

T interval (K)	a_1	a_2	a_3	a_4	a_5	a_6	a_7
50 - 2000	-8.314352060E-07	2.391005430E-03	2.066910750E+00	7.385691470E+00	4.421157370E+03	-3.702919910E+05	8.592895070E+06
2000 - 10000	3.682481690E-05	-9.915340600E-03	3.457871750E+00	-4.152530504E+01	8.361435155E+02	-6.863192948E+03	2.050633510E+04
10000 - 15000	7.418506970E-03	-3.674309000E-01	9.406868780E+00	-6.242259632E+01	3.403498232E+02	-1.004676235E+03	1.273028456E+03
15000 - 25000	2.191768170E-02	-7.438363300E-01	1.269042698E+01	-6.780482160E+01	2.583974795E+02	-5.138560723E+02	4.357950992E+02
25000 - 35000	1.259921769E+01	-2.807726895E+02	2.619612044E+03	-1.306272100E+04	3.685770440E+04	-5.576202590E+04	3.537519830E+04
35000 - 50000	-1.311180429E+03	2.097702150E+04	-1.395361480E+05	4.936984240E+05	-9.789171610E+05	1.029817730E+06	-4.479327850E+05
Residuals: min=7.833E-11, max=1.148E-02, mean=1.215E-04.							

Table 289: Fitting coefficients for C_p/R of O^{2+} ΔE=500 cm^{-1}

T interval (K)	a_1	a_2	a_3	a_4	a_5	a_6	a_7
50 - 2000	-8.314354320E-07	2.391005910E-03	2.066910120E+00	7.385894090E+00	4.421130481E+03	-3.702904560E+05	8.592863840E+06
2000 - 10000	3.682491580E-05	-9.915354310E-03	3.457872500E+00	-4.152532546E+01	8.361438124E+02	-6.863195133E+03	2.050634360E+04
10000 - 15000	7.281444730E-03	-3.607015600E-01	9.269718220E+00	-6.093733183E+01	3.313358163E+02	-9.756076826E+02	1.234113050E+03
15000 - 25000	8.585347070E-03	-3.077665800E-01	6.766018530E+00	-2.500502017E+01	8.496088535E+01	-1.400024740E+02	1.008213679E+02
25000 - 35000	4.817597030E+00	-1.066331839E+02	9.900116363E+02	-4.895483873E+03	1.372236960E+04	-2.061705400E+04	1.298977650E+04
35000 - 50000	-5.496013966E+02	8.369563621E+03	-5.299745610E+04	1.784877150E+05	-3.366732000E+05	3.364890920E+05	-1.386775570E+05
Residuals: min=5.810E-09, max=1.148E-02, mean=1.068E-04.							

Table 290: Fitting coefficients for C_p/R of O^{2+} ΔE=1000 cm^{-1}

T interval (K)	a_1	a_2	a_3	a_4	a_5	a_6	a_7
50 - 2000	-8.314354930E-07	2.391006110E-03	2.066909940E+00	7.385949270E+00	4.421123159E+03	-3.702900380E+05	8.592855340E+06
2000 - 10000	3.682460240E-05	-9.915310510E-03	3.457870100E+00	-4.152525931E+01	8.361428442E+02	-6.863187962E+03	2.050632040E+04
10000 - 15000	7.338710680E-03	-3.635119100E-01	9.326970920E+00	-6.155707725E+01	3.350954018E+02	-9.877264928E+02	1.250330218E+03
15000 - 25000	5.457931040E-03	-2.031393000E-01	5.312297400E+00	-1.426723383E+01	4.048851197E+01	-4.207235553E+01	1.123772668E+01
25000 - 35000	1.572108910E+00	-3.531992714E+01	3.345765374E+02	-1.668126240E+03	4.736572806E+03	-7.193159623E+03	4.576158322E+03
35000 - 50000	-1.184184652E+02	1.788867959E+03	-1.121249820E+04	3.728529690E+04	-6.911822530E+04	6.741558810E+04	-2.679146010E+04
Residuals: min=3.074E-09, max=1.148E-02, mean=9.622E-05.							

Table 291: Fitting coefficients for C_p/R of O^{3+} ΔE=250 cm^{-1}

T interval (K)	a_1	a_2	a_3	a_4	a_5	a_6	a_7
50 - 1000	1.744536700E - 06	-6.306394270E - 03	9.135635730E+00	-2.151250712E+03	3.268753770E+05	-2.391542110E+07	6.794464760E+08
1000 - 10000	9.151799570E - 06	-2.994641150E - 04	2.523873600E+00	-1.053118460E+00	2.494327478E+01	-2.963523554E+02	1.386542288E+03
10000 - 15000	2.422149070E - 03	-1.221664200E - 01	4.805401330E+00	-1.834109098E+01	3.076970310E+01	2.925532044E+02	-8.385581590E+02
15000 - 25000	-1.167739710E - 02	2.439679100E - 01	1.835491460E+00	-1.895511435E+01	1.678087002E+02	-4.350735153E+02	3.863767497E+02
25000 - 35000	3.740688700E+00	-7.566947186E+01	6.390905120E+02	-2.858460539E+03	7.245210841E+03	-9.780054927E+03	5.484633535E+03
35000 - 50000	8.051678300E - 01	-2.061572448E+01	1.878445134E+02	-8.246690046E+02	2.004754289E+03	-2.533099014E+03	1.308270244E+03
Residuals: min=5.625E - 09, max=8.038E - 03, mean=3.745E - 05.							

Table 292: Fitting coefficients for C_p/R of O^{3+} ΔE=500 cm^{-1}

T interval (K)	a_1	a_2	a_3	a_4	a_5	a_6	a_7
50 - 1000	1.744536710E - 06	-6.306394320E - 03	9.135635800E+00	-2.151250746E+03	3.268753850E+05	-2.391542200E+07	6.794465110E+08
1000 - 10000	9.151788990E - 06	-2.994618620E - 04	2.523873430E+00	-1.053111980E+00	2.494315546E+01	-2.963512934E+02	1.386538666E+03
10000 - 15000	2.766260340E - 03	-1.390617600E - 01	5.149755460E+00	-2.207035758E+01	5.340303061E+01	2.195631597E+02	-7.408410313E+02
15000 - 25000	-1.166623540E - 02	2.436211600E - 01	1.839953410E+00	-1.898555454E+01	1.679248256E+02	-4.353084055E+02	3.865735757E+02
25000 - 35000	4.126058400E - 01	-8.025265240E+00	6.767635902E+01	-2.906266701E+02	7.707132319E+02	-1.095441199E+03	6.429259643E+02
35000 - 50000	4.250347860E+00	-6.743841498E+01	4.483423071E+02	-1.579282553E+03	3.192548709E+03	-3.477604727E+03	1.592355234E+03
Residuals: min=3.396E - 09, max=8.038E - 03, mean=3.546E - 05.							

Table 293: Fitting coefficients for C_p/R of O^{3+} ΔE=1000 cm^{-1}

T interval (K)	a_1	a_2	a_3	a_4	a_5	a_6	a_7
50 - 1000	1.744536710E - 06	-6.306394320E - 03	9.135635790E+00	-2.151250742E+03	3.268753840E+05	-2.391542190E+07	6.794465080E+08
1000 - 10000	9.151790540E - 06	-2.994621910E - 04	2.523873450E+00	-1.053112920E+00	2.494317256E+01	-2.963514445E+02	1.386539178E+03
10000 - 15000	2.690325930E - 03	-1.353320300E - 01	5.073709250E+00	-2.124650618E+01	4.840132873E+01	2.356980835E+02	-7.624482633E+02
15000 - 25000	-1.166616430E - 02	2.436184200E - 01	1.839995440E+00	-1.898588780E+01	1.679262740E+02	-4.353116908E+02	3.865766236E+02
25000 - 35000	1.552925800E - 01	-2.756132850E+00	2.281835873E+01	-8.739616197E+01	2.539045972E+02	-3.959776809E+02	2.492680398E+02
35000 - 50000	1.689180080E+00	-2.628108999E+01	1.717775775E+02	-5.839977033E+02	1.168114322E+03	-1.269316901E+03	5.823078464E+02
Residuals: min=3.811E - 09, max=8.038E - 03, mean=3.543E - 05.							

Table 294: Fitting coefficients for C_p/R of O^{4+} ΔE=250 cm^{-1}

T interval (K)	a_1	a_2	a_3	a_4	a_5	a_6	a_7
50 - 2000	9.824704850E - 15	-3.184131710E - 11	2.500000030E+00	-9.309184570E - 06	1.248389730E - 03	-7.174629560E - 02	1.467002090E+00
2000 - 10000	1.906379500E - 05	-3.055721230E - 03	2.696177600E+00	-6.461328350E+00	1.154121788E+02	-1.063979354E+03	3.973896925E+03
10000 - 15000	-2.431608050E - 03	2.373084600E - 01	-5.694778340E+00	1.380906770E+02	-1.221296097E+03	5.318988838E+03	-8.412701375E+03
15000 - 25000	1.332963800E - 01	-5.280852230E+00	8.820928419E+01	-7.186591376E+02	3.201188115E+03	-6.931863718E+03	5.818455327E+03
25000 - 35000	-1.340518680E+00	3.178705457E+01	-3.014634890E+02	1.473211508E+03	-3.757091181E+03	4.889066944E+03	-2.577081914E+03
35000 - 50000	4.338511990E+00	-6.495345841E+01	3.892188650E+02	-1.172001989E+03	1.973777084E+03	-1.769055759E+03	6.629049434E+02
Residuals: min=9.964E - 13, max=2.451E - 05, mean=1.548E - 06.							

Table 295: Fitting coefficients for C_p/R of O^{4+} ΔE=500 cm^{-1}

T interval (K)	a_1	a_2	a_3	a_4	a_5	a_6	a_7
50 - 2000	6.877672870E - 15	-2.199951440E - 11	2.500000020E+00	-6.525395900E - 06	8.938137720E - 04	-5.239195470E - 02	1.089564440E+00
2000 - 10000	1.906375010E - 05	-3.055714970E - 03	2.696177260E+00	-6.461318920E+00	1.154120411E+02	-1.063978337E+03	3.973893939E+03
10000 - 15000	-2.136683930E - 03	2.228354000E - 01	-5.399941180E+00	1.348992408E+02	-1.201936338E+03	5.256585514E+03	-8.329196601E+03
15000 - 25000	1.332949700E - 01	-5.280807920E+00	8.820870877E+01	-7.186551769E+02	3.201173191E+03	-6.931832616E+03	5.818428461E+03
25000 - 35000	-1.344253130E+00	3.186297422E+01	-3.021049290E+02	1.476094487E+03	-3.764361195E+03	4.898819474E+03	-2.582519204E+03
35000 - 50000	3.637885280E+00	-5.440419256E+01	3.230688584E+02	-9.508518168E+02	1.557967096E+03	-1.352075258E+03	4.886289158E+02
Residuals: min=1.516E - 11, max=2.451E - 05, mean=1.547E - 06.							

Table 296: Fitting coefficients for C_p/R of O^{4+} ΔE=1000 cm^{-1}

T interval (K)	a_1	a_2	a_3	a_4	a_5	a_6	a_7
50 - 2000	6.465945040E - 15	-2.058892160E - 11	2.500000020E+00	-5.879376310E - 06	7.916256390E - 04	-4.582112930E - 02	9.442160000E - 01
2000 - 10000	1.906366110E - 05	-3.055702220E - 03	2.696176540E+00	-6.461298740E+00	1.154117390E+02	-1.063976053E+03	3.973887091E+03
10000 - 15000	-2.409426590E - 03	2.362166300E - 01	-5.672468010E+00	1.378484485E+02	-1.219822195E+03	5.314223350E+03	-8.406304904E+03
15000 - 25000	1.332905500E - 01	-5.280670530E+00	8.820693929E+01	-7.186430938E+02	3.201126732E+03	-6.931739201E+03	5.818350111E+03
25000 - 35000	-1.342939630E+00	3.183629105E+01	-3.018796513E+02	1.475082719E+03	-3.761811718E+03	4.895401967E+03	-2.580615273E+03
35000 - 50000	3.371031370E+00	-5.041941553E+01	2.982793585E+02	-8.685949509E+02	1.404382818E+03	-1.199043346E+03	4.250386277E+02
Residuals: min=3.626E - 12, max=2.451E - 05, mean=1.542E - 06.							

Table 297: Fitting coefficients for C_p/R of O^-

T interval (K)	a_1	a_2	a_3	a_4	a_5	a_6	a_7
50 - 5000	-2.596126790E - 07	6.006711370E - 04	2.408996970E+00	8.704633880E+00	-5.393932849E+02	1.573968710E+04	-1.227026950E+05
5000 - 10000	-1.272340250E - 03	1.735964000E - 01	-6.200039350E+00	1.995455748E+02	-2.094042516E+03	1.070157390E+04	-2.185860000E+04
10000 - 15000	9.074529720E - 03	-5.244110400E - 01	1.359774259E+01	-1.023212757E+02	5.126021669E+02	-1.370727300E+03	1.542882725E+03
15000 - 25000	-5.892574320E - 03	7.285336570E - 02	3.597325130E+00	-1.234324197E+01	5.363911828E+01	-1.122445297E+02	9.388183057E+01
25000 - 35000	2.951500700E - 01	-5.982299820E+00	5.396417934E+01	-2.335531144E+02	5.925558654E+02	-7.983691161E+02	4.466373570E+02
35000 - 50000	1.237819000E - 01	-1.698783440E+00	1.295617493E+01	-3.377301032E+01	6.081249387E+01	-5.804453445E+01	2.297501613E+01
Residuals: min=6.331E - 09, max=8.415E - 03, mean=8.011E - 05.							

Table 298: Fitting coefficients for C_p/R of O_2

T interval (K)	a_1	a_2	a_3	a_4	a_5	a_6	a_7
50 - 1000	1.286643900E - 07	-5.447623260E - 04	4.292237430E+00	-4.987804747E+02	1.359060290E+05	-1.302795170E+07	4.382832040E+08
1000 - 3000	4.935635510E - 05	-2.644043510E - 02	8.281896790E+00	-3.004655985E+02	1.308263260E+04	-2.602687870E+05	2.005170950E+06
3000 - 6000	1.785970300E - 03	-2.290593300E - 01	1.509597479E+01	-2.167750454E+02	2.235883547E+03	-3.406044142E+03	-6.094112890E+04
6000 - 15000	2.848213050E - 02	-1.465439240E+00	2.912253079E+01	-8.319486880E+01	-1.143978609E+03	9.557724208E+03	-2.094567130E+04
15000 - 35000	-8.117072020E - 02	2.436807180E+00	-1.946878746E+01	1.083761927E+02	-2.978689514E+02	4.336679723E+02	-2.619788384E+02
35000 - 50000	-5.893687460E - 02	1.254275230E+00	-4.576388740E+00	2.309555490E+01	-4.227443670E+01	4.077379350E+01	-1.621174994E+01
Residuals: min=2.307E - 10, max=6.239E - 04, mean=1.760E - 05.							

Table 299: Fitting coefficients for C_p/R of O_2^+

T interval (K)	a_1	a_2	a_3	a_4	a_5	a_6	a_7
50 - 1000	1.352381120E - 07	-5.358964260E - 04	4.202739110E+00	-3.859765498E+02	8.966212960E+04	-7.194857110E+06	2.020766760E+08
1000 - 3000	4.062383760E - 05	-1.907963730E - 02	6.235487100E+00	-8.951174036E+01	2.917667970E+03	-5.049349280E+04	3.769164750E+05
3000 - 6000	-1.405383600E - 03	2.253872400E - 01	-1.108315259E+01	5.703726498E+02	-1.140039440E+04	1.181227050E+05	-4.706276780E+05
6000 - 15000	-1.315709900E - 01	9.048972990E+00	-2.437955347E+02	3.424192749E+03	-2.457491630E+04	8.824160100E+04	-1.264163460E+05
15000 - 35000	-3.441008800E - 01	7.876333110E+00	-6.001427647E+01	2.653550977E+02	-6.387884071E+02	8.261398061E+02	-4.475832829E+02
35000 - 50000	5.805008510E - 02	2.660863300E - 01	5.952212000E - 01	5.750515210E+00	-9.125802390E+00	7.485180970E+00	-2.506142850E+00
Residuals: min=2.722E - 09, max=1.227E - 03, mean=1.682E - 05.							

Table 300: Fitting coefficients for C_p/R of O_2^-

T interval (K)	a_1	a_2	a_3	a_4	a_5	a_6	a_7
50 - 1000	-1.875638610E-07	6.413030510E-04	2.900530310E+00	1.136899366E+02	4.535688420E+04	-7.541177380E+06	3.274593130E+08
1000 - 3000	-2.297649740E-06	-3.889104340E-03	4.901240140E+00	-2.025968078E+01	9.500008819E+02	-1.991335670E+04	2.095996200E+05
3000 - 6000	2.313139050E-03	-4.007361500E-01	3.266494406E+01	-1.024193496E+03	2.033460180E+04	-2.009514860E+05	7.672521180E+05
6000 - 15000	4.473808080E-02	-3.059184730E+00	8.515511337E+01	-1.019299271E+03	6.647686621E+03	-2.247219040E+04	3.118356490E+04
15000 - 35000	-2.513364230E-02	1.027790840E+00	-7.019804140E+00	4.616782501E+01	-1.259065958E+02	1.833978374E+02	-1.113459484E+02
35000 - 50000	3.015243790E-02	-1.101852200E-01	2.950712500E+00	-1.157714990E+00	1.781807990E+00	-1.486039430E+00	5.113758500E-01
Residuals: min=5.271E-10, max=3.293E-03, mean=2.479E-05.							

Table 301: Fitting coefficients for C_p/R of O_3

T interval (K)	a_1	a_2	a_3	a_4	a_5	a_6	a_7
50 - 1000	-8.182867830E-07	3.101791730E-03	3.458955800E-01	1.508400566E+03	-1.260443920E+05	2.371173690E+06	1.118559040E+08
1000 - 3000	1.427394180E-03	-4.597364500E-01	5.939707430E+01	-2.352888625E+03	3.948257166E+03	2.517553430E+06	-4.548923470E+07
3000 - 6000	3.109355200E-01	-4.332002065E+01	2.413898983E+03	-6.825888780E+04	1.054835170E+06	-8.523588390E+06	2.831143830E+07
6000 - 15000	9.547897790E-03	5.005139900E-01	-1.688676851E+01	3.167788762E+02	-2.534615183E+03	1.011838220E+04	-1.618806770E+04
15000 - 35000	1.142779610E-02	-8.942893620E-02	4.393588850E+00	-9.759771570E+00	2.623762387E+01	-3.731864019E+01	2.218643553E+01
35000 - 50000	-9.808983860E-02	1.560406540E+00	-6.129441410E+00	2.686135886E+01	-4.765279880E+01	4.520882600E+01	-1.786052480E+01
Residuals: min=1.726E-09, max=5.989E-03, mean=4.620E-05.							

Table 302: Fitting coefficients for C_p/R of O_3^-

T interval (K)	a_1	a_2	a_3	a_4	a_5	a_6	a_7
50 - 1000	-8.462283090E-07	3.441297740E-03	-2.072775800E+00	2.303418984E+03	-3.180303710E+05	2.122227580E+07	-5.538223200E+08
1000 - 3000	-5.839175650E-05	9.397650450E-03	4.408756780E+00	3.540222302E+01	1.631095959E+03	-1.231938600E+05	1.778128810E+06
3000 - 6000	6.036791400E-03	-1.017108890E+00	7.430437570E+01	-2.359408048E+03	4.235289840E+04	-3.783236520E+05	1.323739820E+06
6000 - 15000	7.882741980E-02	-4.908222660E+00	1.224505764E+02	-1.353484491E+03	8.041228250E+03	-2.454889930E+04	3.043651290E+04
15000 - 35000	-4.901475970E-02	1.756309500E+00	-1.389624106E+01	8.012753939E+01	-2.197961436E+02	3.215300899E+02	-1.958203595E+02
35000 - 50000	6.605317210E-02	-5.088360800E-01	5.273755360E+00	-8.562093450E+00	1.518476344E+01	-1.447598484E+01	5.764540280E+00
Residuals: min=3.055E-09, max=4.915E-03, mean=2.669E-05.							

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