

Electric dipole transition moments between the $^2\Sigma_u^+$ and $^2\Sigma_g^+$ states of the He_2^+ ion

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The electric dipole transition moments of the He_2^+ molecular ion between its two lowest $^2\Sigma_u^+$ states and its first six excited $^2\Sigma_g^+$ states are computed at various internuclear distances between 0.8 and 4.0 a_0 . The results are obtained with two different AO basis sets at the multireference CI level of treatment and show strong variations in the regions of various avoided crossings of the $^2\Sigma_g^+$ states. Predictions of the radiative transition probabilities between various He_2^+ vibrational levels in several $^2\Sigma_g^+ \rightarrow ^2\Sigma_u^+$ band systems are made on this basis.

1. Introduction

The He_2^+ ion continues to draw considerable attention because of its importance in the interpretation of excitation and electron transfer cross sections, as well as because of its presence in helium discharges and plasmas (see refs. [1–5], and references therein). Some of our previous work has examined various aspects of the diabaticity of the $^2\Sigma_u^+$ and $^2\Sigma_g^+$ states of this ion [1–4]. Recently, Ackermann and Hogreve [5] calculated accurate vibrational and rotational levels based on ab initio $^2\Sigma_{u,g}^+$ and $^2\Pi_{u,g}$ potential energy curves, and Nicolaides et al. [6] used the $^2\Sigma_g^+$ states of He_2^+ as an example for the direct construction of diabatic states. In spite of these extensive studies, however, there is still a lack of computations of transition probabilities between the various electronic states of this ion. Consequently, in the present paper we report calculated transition moments between the two lowest

$^2\Sigma_u^+$ states and the first six excited $^2\Sigma_g^+$ states of the He_2^+ ion and employ these data to compute transition probabilities between various vibrational levels of the He_2^+ system.

2. Computational details

The calculations of the potential energy curves of the present study were done with the MRD-CI programs of Buenker and Peyerimhoff [7–9], using the AO basis set of Sunil et al. [10]. The first two $^2\Sigma_u^+$ and the first six $^2\Sigma_g^+$ states were treated by employing the set of molecular orbitals which was generated in the corresponding SCF calculation of the lowest $1^2\Sigma_u^+$ state. All single and double excitations with respect to a series of reference configurations have been included in the CI calculations undertaken. This procedure results in about 6000 configurations for the $^2\Sigma_u^+$ states and about 8000 configurations for the $^2\Sigma_g^+$ states.

The calculations were done in formal D_{2h} symmetry, and as a result, the first $^2\Delta_g$ state appeared among the six excited $^2\Sigma_g^+$ states obtained, since both

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types correlate with the A_g irreducible representation of D_{2h} . A corresponding ${}^2\Delta_g$ state was not found in earlier calculations [4] because of the absence of the necessary Rydberg d orbital in the AO basis set employed.

From the computed wavefunctions of the above states, the electric dipole transition moment components along the internuclear axis were calculated between the various ${}^2\Sigma_u^+$ and the ${}^2\Sigma_g^+$ states. The corresponding moments between ${}^2\Sigma_u^+$ and the ${}^2\Delta_g$ state are zero by symmetry.

As a check on the accuracy of these results, a second calculation was carried out using a larger basis set, as shown in table 1. In this case only the $1^2\Sigma_u^+$ and the $1^2\Sigma_g^+$ states were calculated, as well as the transition moment between them (calculation B). The energies of both of these states were somewhat lower than the corresponding energies of calculation A within the smaller basis, and of about the same quality as the corresponding energies given by Ackermann and Hogreve [5]. The $1^2\Sigma_u^+ - 1^2\Sigma_g^+$ transition moments for the two calculations agree to within several thousandths of an atomic unit. These results give increased confidence regarding the ac-

curacy for the additional transition moment data of calculation A.

3. Results of the calculations

3.1. Potential curves and transition moments

The total energies computed for the He_2^+ ion are given in table 2 for the first two ${}^2\Sigma_u^+$ electronic states, and in table 3 for the lowest six ${}^2\Sigma_g^+$ states. The data for the lowest ${}^2\Sigma_u^+$ and ${}^2\Sigma_g^+$ states are taken from the theoretical treatment employing the larger AO basis (calculation B); all other results in the tables stem from calculation A. The potential curves originating from treatment A are plotted in fig. 1. The He_2^+ ground state possesses a $1\sigma_g^2 1\sigma_u$ configuration and has an equilibrium bond length of $2.05 a_0$. The $2^2\Sigma_u^+$ corresponds to a $1\sigma_u \rightarrow 2p\sigma$ Rydberg excita-

Table 1
The AO basis set for calculation B ^{a)}

Type	Origin	Exponent α (a_0^{-2})	Contraction coefficients
s	He	833.052200	0.000530
s	He	124.505150	0.004150
s	He	28.099350	0.021340
s	He	7.921657	1.000000
s	He	2.580737	1.000000
s	He	0.918171	1.000000
s	He	0.347207	1.000000
s	He	0.137777	1.000000
s	bond center	0.055000	1.000000
s	bond center	0.027000	1.000000
p	He	7.320000	1.000000
p	He	2.530000	1.000000
p	He	0.870000	1.000000
p	He	0.300000	1.000000
d	He	4.140000	1.000000
d	He	1.380000	1.000000
d	He	0.460000	1.000000
f	He	2.340000	1.000000
f	He	0.780000	1.000000

^{a)} Calculation A was done with the Sunil et al. basis set [10].

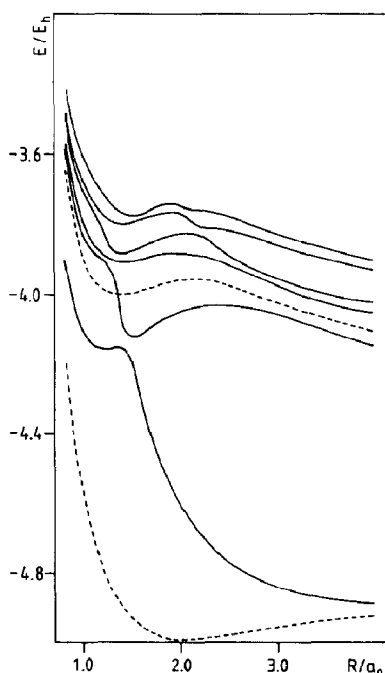
Table 2
Total energies for the two lowest $n^2\Sigma_u^+$ states of He_2^+ (for $n=1$ from calculation B, for $n=2$ from A) as a function of bond distance R

$R (a_0)$	$E (E_h)$	
	$1^2\Sigma_u^+$	$2^2\Sigma_u^+$
0.80	-4.1720	-3.6419
0.90	-4.4025	-3.8044
1.00	-4.5693	-3.9018
1.10	-4.6921	-3.9578
1.20	-4.7828	-3.9871
1.30	-4.8497	-3.9994
1.40	-4.8985	-4.0010
1.50	-4.9336	-3.9965
1.60	-4.9581	-3.9886
1.70	-4.9747	-3.9798
1.80	-4.9851	-3.9712
1.90	-4.9910	-3.9640
2.00	-4.9934	-3.9589
2.10	-4.9932	-3.9563
2.20	-4.9913	-3.9568
2.40	-4.9840	-3.9681
2.60	-4.9745	-3.9881
2.80	-4.9645	-4.0082
3.00	-4.9549	-4.0262
3.20	-4.9462	-4.0426
3.40	-4.9385	-4.0582
3.60	-4.9320	-4.0737
3.80	-4.9264	-4.0890
4.00	-4.9219	-4.1040

Table 3

Total energies E for the first six excited $m\ ^2\Sigma_g^+$ and the first $^2\Delta_g$ states of He_2^+ (for $m=1$ from calculation B, otherwise from A) as a function of bond distance R

$R\ (a_0)$	$E\ (E_h)$						
	$1\ ^2\Sigma_g^+$	$2\ ^2\Sigma_g^+$	$3\ ^2\Sigma_g^+$	$4\ ^2\Sigma_g^+$	$5\ ^2\Sigma_g^+$	$6\ ^2\Sigma_g^+$	$^2\Delta_g$
0.80	-3.8922	-3.5825	-3.5763	-3.4803	-3.4703	-3.3986	-3.5419
0.90	-4.0316	-3.7329	-3.7313	-3.6326	-3.6249	-3.5493	-3.6950
1.00	-4.1088	-3.8226	-3.8186	-3.7206	-3.7154	-3.6357	-3.7844
1.10	-4.1471	-3.8741	-3.8650	-3.7688	-3.7664	-3.6824	-3.8339
1.20	-4.1612	-3.9014	-3.8864	-3.7944	-3.7919	-3.7176	-3.8580
1.30	-4.1607	-3.9323	-3.8964	-3.8846	-3.7995	-3.7972	-3.8663
1.40	-4.1549	-4.0698	-3.9077	-3.8871	-3.7997	-3.7963	-3.8649
1.50	-4.2180	-4.1236	-3.9045	-3.8779	-3.7947	-3.7886	-3.8580
1.60	-4.3246	-4.1099	-3.8982	-3.8662	-3.7872	-3.7782	-3.8485
1.70	-4.4155	-4.0932	-3.8915	-3.8540	-3.7791	-3.7672	-3.8384
1.80	-4.4915	-4.0772	-3.8857	-3.8426	-3.7719	-3.7571	-3.8290
1.90	-4.5551	-4.0629	-3.8819	-3.8331	-3.7667	-3.7491	-3.8212
2.00	-4.6083	-4.0512	-3.8807	-3.8262	-3.7667	-3.7563	-3.8157
2.10	-4.6527	-4.0422	-3.8823	-3.8227	-3.7923	-3.7616	-3.8125
2.20	-4.6901	-4.0360	-3.8869	-3.8294	-3.8116	-3.7639	-3.8118
2.40	-4.7478	-4.0315	-3.9036	-3.8698	-3.8169	-3.7746	-3.8185
2.60	-4.7890	-4.0355	-3.9271	-3.9036	-3.8281	-3.7913	-3.8283
2.80	-4.8185	-4.0456	-3.9528	-3.9310	-3.8416	-3.8105	-3.8433
3.00	-4.8400	-4.0598	-3.9773	-3.9535	-3.8570	-3.8298	-3.8596
3.20	-4.8556	-4.0767	-3.9990	-3.9721	-3.8730	-3.8479	-3.8757
3.40	-4.8672	-4.0949	-4.0171	-3.9878	-3.8885	-3.8642	-3.8911
3.60	-4.8758	-4.1130	-4.0317	-4.0011	-3.9033	-3.8788	-3.9052
3.80	-4.8823	-4.1300	-4.0438	-4.0128	-3.9170	-3.8917	-3.9181
4.00	-4.8872	-4.1453	-4.0537	-4.0229	-3.9295	-3.9032	-3.9298



tion, resulting in a decrease in bond length of $0.7\ a_0$, close to the corresponding value for the $1\Sigma_g^+$ ground state of H_2 . Since the upper orbitals of the two $^2\Sigma_u^+$ states correlate with the $2p\sigma$ and $3p\sigma$ AOs of the united atom (Be^+), respectively, it is not surprising that an avoided crossing between their potential curves is not observed.

The situation for the $^2\Sigma_g^+$ states is quite different, however, since in this case one can speak of a valence-type diabatic state of $1\sigma_g1\sigma_u^2$ configuration, with a purely repulsive potential curve expected on the basis of its negative bond order. The other states of this symmetry also result from Rydberg excitations with a $1\sigma_g^2$ core, and so their corresponding diabatic potential curves run nearly parallel to that of the computed $2^2\Sigma_u^+$ state already mentioned. As a result the adiabatic CI potential curves for the var-

◀ Fig. 1. Potential energy curves for the $n\ ^2\Sigma_u^+$ states ($n=1$ and 2 ; dashed lines) and the $m\ ^2\Sigma_g^+$ states ($m=1$ to 6 ; solid lines) of the He_2^+ ion.

ious $^2\Sigma_g^+$ states undergo a complicated series of avoided crossings within a narrow range of internuclear distance, as seen from fig. 1. The five Rydberg upper orbitals involved are the $2s\sigma$, $3s\sigma$, $3d\sigma$, $4s\sigma$ and $5s\sigma$ respectively. The potential energy data for the lowest state of $^2\Delta_g$ symmetry is also included in table 3. This state corresponds to a $3d\delta$ (Rydberg) orbital and its potential curve has a minimum at nearly the same bond distance as does the $2^2\Sigma_u^+(1\sigma_u \rightarrow 2p\sigma)$ state. In this case there are no lower states of the same symmetry with which to interact and produce further avoided crossings.

The corresponding computed electric dipole transition moments are given in tables 4 and 5. In table 4, transitions from the $^2\Sigma_u^+$ ground state to each of the six $^2\Sigma_g^+$ states discussed above are considered, and in table 5, the analogous data for $2^2\Sigma_u^+ \rightarrow m^2\Sigma_g^+$ transitions are given. For a more detailed discussion the transition moments μ_{nm} between the

two $n^2\Sigma_u^+$ states ($n=1$ and 2) and the first three $m^2\Sigma_g^+$ species ($m=1, 2$ and 3) are shown in figs. 2 and 3. In regions of bond distances without avoided crossings between the states considered, the calculated data can be represented by smooth curves. For increasing R , μ_{11} increases nearly linearly, consistent with the ionic character of the system and the fact that both states lead to the same dissociation limit: $\text{He } ^1S_g(1s^2) + \text{He}^+ ^2S_g(1s)$. With the center of mass of the molecular ion located in the origin of the coordinate system, a relation $\mu(R) = eR/2$ as $R \rightarrow \infty$ is expected, and this behavior is reflected by the results for μ_{11} given in table 4. The μ_{12} and μ_{13} transition moments to states with Rydberg character remain small in the limit of dissociation, with the upper states leading to $\text{He } ^3,^1S_g(1s2s) + \text{He}^+ ^2S_g(1s)$, respectively.

The series of avoided crossings around $R = 1.4 a_0$ leads to strong mixing of the character of the excited $^2\Sigma_g^+$ states, and thus the well-separated transition

Table 4

Electric dipole transition moments μ_{1m} between the $1^2\Sigma_u^+$ ground state and the first excited $m^2\Sigma_g^+$ states of He_2^+ as a function of bond distance R

$R (a_0)$	$\mu_{1m} (e a_0)$					
	$m=1$	$m=2$	$m=3$	$m=4$	$m=5$	$m=6$
0.80	0.824	0.173	0.475	0.061	0.296	0.156
0.90	0.717	0.291	0.337	0.073	0.266	0.170
1.00	0.628	0.384	0.109	0.086	0.234	0.186
1.10	0.558	0.336	0.137	0.094	0.200	0.187
1.20	0.508	0.274	0.164	0.085	-0.124	0.412
1.30	0.483	0.195	0.481	0.345	-0.213	0.223
1.40	0.556	0.470	0.395	0.070	-0.261	-0.013
1.50	0.754	-0.161	0.366	0.087	-0.247	-0.039
1.60	0.769	-0.239	0.361	0.089	-0.242	-0.047
1.70	0.805	-0.237	0.365	0.086	-0.243	-0.050
1.80	0.846	-0.221	0.375	0.081	-0.246	-0.050
1.90	0.888	-0.202	0.388	0.074	-0.253	-0.048
2.00	0.930	-0.180	0.404	0.061	-0.253	0.082
2.10	0.974	-0.156	0.422	0.037	-0.142	0.233
2.20	1.018	-0.131	0.441	-0.042	-0.117	0.243
2.40	1.109	-0.074	0.478	-0.053	-0.066	0.243
2.60	1.203	0.009	0.502	0.025	-0.043	0.234
2.80	1.300	0.064	0.506	0.049	-0.024	0.218
3.00	1.400	0.140	0.486	0.102	0.006	0.198
3.20	1.501	0.210	0.445	0.148	0.008	0.175
3.40	1.604	0.263	0.396	0.180	0.016	0.154
3.60	1.708	0.298	0.349	0.201	0.019	0.136
3.80	1.813	0.317	0.309	0.217	0.018	0.121
4.00	1.918	0.324	0.275	0.228	0.015	0.108

Table 5

Electric dipole transition moments μ_{2m} between the $2^2\Sigma_u^+$ state and the first excited $m^2\Sigma_g^+$ states of He_2^+ as a function of bond distance R

$R (a_0)$	$\mu_{2m} (e a_0)$					
	$m=1$	$m=2$	$m=3$	$m=4$	$m=5$	$m=6$
0.80	1.519	2.194	-2.779	-0.249	-0.555	0.244
0.90	1.618	1.244	-3.124	-0.299	-0.478	0.313
1.00	1.725	2.110	-2.408	-0.360	-0.397	0.368
1.10	1.809	2.203	-2.136	-0.393	-0.352	0.410
1.20	1.876	2.270	-1.883	-0.338	-0.454	0.330
1.30	1.919	1.846	0.067	-2.222	-0.495	-0.044
1.40	1.842	0.944	2.016	-1.853	-0.376	-0.367
1.50	0.340	2.054	2.096	-1.691	-0.375	-0.397
1.60	0.072	2.116	2.117	-1.576	-0.405	-0.407
1.70	0.020	2.149	2.126	-1.471	-0.448	-0.408
1.80	0.001	2.182	2.133	-1.367	-0.506	-0.401
1.90	-0.009	2.210	2.134	-1.254	-0.583	-0.368
2.00	-0.017	2.232	2.120	-1.117	-0.764	0.078
2.10	-0.028	2.236	2.085	-0.837	-0.910	0.571
2.20	-0.044	2.203	1.985	0.186	-1.270	0.637
2.40	-0.087	1.895	1.391	1.614	-0.804	0.559
2.60	-0.087	1.508	0.741	2.126	-0.476	0.413
2.80	-0.045	1.309	-0.647	2.214	-0.306	0.360
3.00	0.018	1.167	-0.855	2.152	-0.189	0.356
3.20	0.095	1.015	-1.089	1.997	-0.094	0.371
3.40	0.183	0.847	-1.236	1.776	0.003	0.370
3.60	0.273	0.685	-1.272	1.509	0.074	0.352
3.80	0.353	0.552	-1.219	1.237	0.132	0.318
4.00	0.413	0.456	-1.122	1.000	0.160	0.281

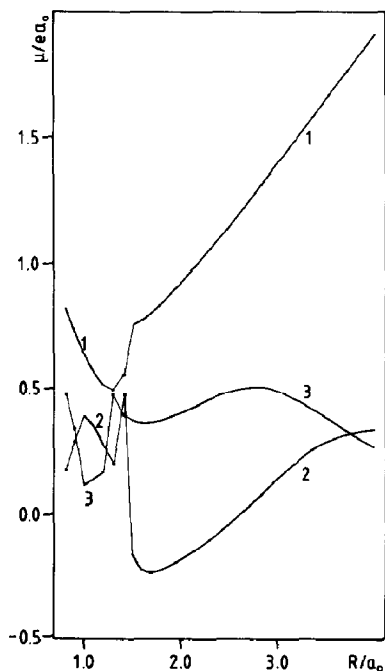


Fig. 2. Electric dipole transition moments μ_{1m} between the $1^2\Sigma_u^+$ and $m^2\Sigma_g^+$ states ($m=1$ to 3) of the He_2^+ ion as a function of bond distance R .

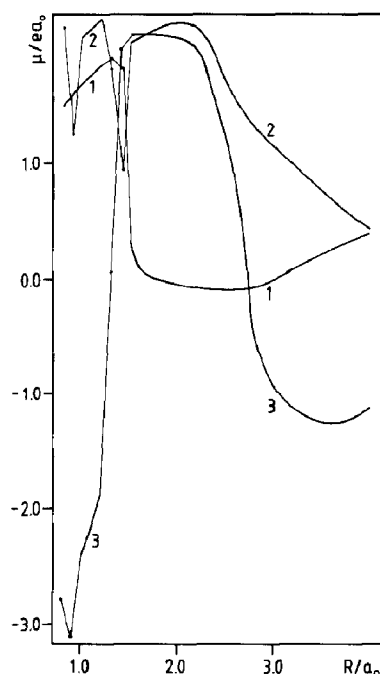


Fig. 3. Electric dipole transition moments μ_{2m} between the $2^2\Sigma_u^+$ and $m^2\Sigma_g^+$ states ($m=1$ to 3) of the He_2^+ ion as a function of bond distance R .

moments at somewhat longer bond distances (e.g. 0.81, -0.24 and 0.37 $e a_0$ at $R=1.7 a_0$) suddenly come close to each other, with values of 0.56, 0.47 and 0.40 $e a_0$, at $R=1.4 a_0$. Therefore, in this region of bond distances the calculated moments are given only by dots connected by thin straight lines indicating to which transition they belong. For smaller bond distances, the $1^2\Sigma_g^+$ state is unaffected by any perturbation from other states, as can be seen from fig. 1, and thus the μ_{11} data can again be represented by a smooth curve. The situation is different for μ_{12} and μ_{13} , reflecting additional mixing effects at smaller R values. Therefore, these results are also plotted pointwise with thin connecting lines.

The corresponding μ_{2m} data for transitions starting from the Rydberg $2^2\Sigma_u^+$ state (table 5 and fig. 3) are noticeably different from those first discussed. Quite large values are computed for each of the transitions to the lowest three $2^2\Sigma_g^+$ states at relatively small R values. Especially large results are computed for the $2^2\Sigma_g^+ - 2^2\Sigma_u^+$ transition. These data show that the intensities of Rydberg-Rydberg transitions can be quite high, even though those involving one Rydberg and one valence state are invariably found to be relatively small. The effect of the various avoided crossings is again evident in this series of results, and

the same way of plotting is used in fig. 3 as before in fig. 2.

3.2. Vibrational transition probabilities

The potential curves in fig. 1 show that the $2^2\Sigma_g^+$ state possesses an energy minimum in the neighborhood of $R=2.0 a_0$ by virtue of a rather strongly avoided crossing with the lowest state of this symmetry. A vibrational treatment employing the Numerov-Cooley method [11] has been carried out for this adiabatic state, as well as for the two $2^2\Sigma_u^+$ states also treated, in order to compute the radiative transition probabilities of the associated vibrational levels. The corresponding electric-dipole transition moments for the $2^2\Sigma_g^+ - X^2\Sigma_u^+$ and $2^2\Sigma_u^+ - 2^2\Sigma_g^+$ pairs of states (tables 4 and 5) have then been averaged over the various vibrational wavefunctions. The vibrational transition moments $R_{v'v''}$ are then employed to compute the corresponding optical $f_{v'v''}$ values:

$$f_{v'v''} = \frac{2}{3} |R_{v'v''}|^2 \Delta E_{v'v''},$$

where $\Delta E_{v'v''}$ is the transition energy in E_h . These results are shown in table 6.

The $X^2\Sigma_u^+$ state of He_2^+ has a large series of bound

Table 6

f values (multiplied by 10^4) between several vibrational levels v_g (with relative energies E_g in cm^{-1}) of the $2^2\Sigma_g^+$ state and v_u (with relative energies E_u in cm^{-1}) of the $n^2\Sigma_u^+$ states of He_2^+

n	v_u	E_u	$v_g=0$ $E_g=0^a$	$v_g=1$ $E_g=6024$	$v_g=2$ $E_g=10573$	$v_g=3$ $E_g=14060$
1	0	0	0.95	15.15	57.42	78.03
1	1	1751	4.05	37.05	51.11	0.73
1	2	3418	9.37	48.82	16.35	14.59
1	3	5002	15.60	45.22	0.23	20.84
1	4	6503	20.91	32.09	5.58	9.46
1	5	7923	23.89	17.80	16.57	0.55
1	6	9259	24.05	7.42	22.33	2.03
1	7	10515	21.85	1.97	21.34	8.78
1	8	11688	18.09	0.13	16.49	14.28
1	9	12777	13.76	0.14	10.95	16.02
1	10	13792	9.91	0.68	6.60	15.06
2	0	0	1087.03	47.36	23.93	9.73
2	1	3063	1856.01	290.59	6.35	9.50
2	2	5782	27.75	2030.11	124.20	6.74
2	3	7997	189.82	70.71	1845.67	270.04

^a) The energy difference between the $v_g=0$ and $nv_u=0$ levels is 194100 cm^{-1} for $n=1$ and 24390 cm^{-1} for $n=2$ (with $2^2\Sigma_u^+$ lying higher).

levels and results are given from $v''=0$ to 10 (v_u , $n=1$). By contrast only four quasi-bound vibrational levels v' (v_g) are found for the $2^2\Sigma_g^+$ state, each of which is subject to predissociation [2], as well as to spontaneous emission into the electronic ground state. The optical f values for the $2^2\Sigma_g^+(v')-X^2\Sigma_u^+$ transition show a maximum at $v''=5-6$ for $v'=0$. The f values tend to be larger for the $v'=1$ and 2 levels and reach a maximum for lower v'' (2-3 for $v'=1$ and 0-1 for $v'=2$). There is a v' progression with increasing intensity relative to $v''=0$, whereas for higher v'' levels a maximum is reached at $v'=2$ or lower. The T_0 value for the $2^2\Sigma_g^+-X^2\Sigma_u^+$ transition is computed to be 194100 cm^{-1} , and the absorption lines are expected to be somewhat broadened by predissociation.

Similar calculations have been carried out for the $2^2\Sigma_u^+-2^2\Sigma_g^+$ transition, whereby in this case the ungerade state is only found to possess four bound vibrational levels v' (v_u , $n=2$). Results are given in table 6 for transitions involving the above four levels v'' (v_g) of the $2^2\Sigma_g^+$ state. As mentioned above, the transition moment is relatively large between these two Rydberg states. Thus the computed f values for this transition are found to be notably larger than for the $2^2\Sigma_g^+-X^2\Sigma_u^+$ band system, whereas the corresponding transition energies are much smaller. It is hoped that these results will aid in the search for these and other transitions in the He_2^+ spectrum.

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