Rotational cross sections and rate coefficients for e-CO and e-HCN collisions under interstellar conditions

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Rotational cross sections and rate coefficients for e-CO and e-HCN collisions have been calculated in the energy range relevant to dark interstellar clouds by using the close-coupling method. Gordon's technique has been used for solving the coupled Schrödinger equations. Initial rotational levels $j = 0$, 1, and 2 of CO and HCN have been considered. The rotational cross sections have been calculated in the energy range 0.0006 to 0.1 eV and the rate coefficients in the temperature range 5–100 K. The cross sections and rate coefficients thus obtained have been compared with Born and unitarized time-dependent perturbation calculations.

I. INTRODUCTION

The study of collision-induced rotational transitions of molecules has recently been drawing considerable attention due to the importance of this process in the interpretation of the spectral data obtained from interstellar sources. Until now most of the calculations of the cross sections and rate coefficients have been confined to the molecules CO, CS, OCS, HCN, etc., with H_2 as the collision partner[1-3] which is the most abundant molecular species in dense interstellar clouds. However, recently it has been shown[4,5] that for the interpretation of the spectral data for strongly polar molecules like HCN, CS, etc., it is absolutely necessary to consider electron-molecule collision in addition to H_2-molecule collision. Even for CO which has a comparatively small dipole moment, the electron-molecule collisions are important when the ratio of the densities of electron and H_2, $n(e)/n(H_2) \geq 10^{-3}$. Near the center of dense interstellar clouds such as Orion A, $n(e)/n(H_2)$ has been estimated to be ~10^{-6}. However, the ionization due to the cosmic ultraviolet radiation increases as the distance from the center of the cloud increases. Thus the ratio of electron density to that of hydrogen density is likely to be higher near the periphery of the cloud. Philips and Huggins[6] have also suggested that for dense interstellar clouds having infrared sources, the density of electrons may be quite high. The above discussions show conclusively the importance of the study of electron-molecule collisions existent in the interstellar clouds.

We have therefore taken up a program to calculate the rotational cross sections and rate coefficients for electron-molecule collisions under interstellar conditions. For molecules having sizable dipole moments, it is necessary to use close coupling method for the calculations. The usual technique used for such calculations is quite expensive. Gordon[7,8] has developed a technique for close-coupling calculations for which the time required is considerably less. Until now this technique has been mostly used for the study of atom-molecule[9,10] and molecule-molecule collisions.[11] However, it has also been used for the study of electron-CsF (Ref. 12) and proton-CN (Ref. 13) collisions.

We have reported in this paper the results of our calculations for e-CO and e-HCN systems. After H_2, CO is the most abundant species in dark interstellar clouds. For e-CO collisions, some calculations of rotational cross sections have been made by the following methods, viz., (1) Born approximation,[14,15] (2) unitarized time-dependent perturbation (UTDP) theory,[16] and (3) close-coupling (CC) method.[17,18] However, in these calculations the energy ranges are not sufficient for obtaining rate coefficients under interstellar conditions. Using the close-coupling theory, Allison and Dalgarno[19] have computed the rotational rate coefficients of e-CN collisions in the temperature range 5–1000 K. But their calculations at lower temperatures are somewhat uncertain. This is because they have extrapolated the calculated cross sections from 0.01 to 0.001 eV for the $0 \rightarrow 1$ and to 0.002 eV for the $0 \rightarrow 2$ transitions. For e-HCN collisions there are some calculations of rate coefficient at 100 K performed by Dickison et al.[4] using the time-dependent perturbation theory. We have calculated the cross sections for the rotational states 0, 1, and 2 of CO and HCN in the energy range 0.0006 to 0.1 eV and the rate coefficients in the temperature range 5–100 K. In e-CO collisions, for convergence of the CC calculations with basis sets initial rotational levels $j = 0-2$ were sufficient. The calculations converged very well. The CC basis here is the same as that used by Crawford and Dalgarno[17] but smaller than that used by Chandra.[18]

In e-HCN collisions, for sufficient convergence of the CC calculations with basis sets initial rotational levels $j = 0-3$ have been considered. In this case the calculations converged to within about $\pm 10\%$ for the range of partial waves and energies considered. Test calculations were performed to check this point. No other CC calculation for e-HCN was available to compare with our results.

II. METHOD OF CALCULATION

The close-coupling method of Arthurs and Dalgarno[20] has been used for calculation of rotational cross sections of CO and HCN by electron impact at temperatures existent in dark interstellar clouds. The expression of cross section for rotational transition $j \to j'$ is given by

$$\sigma_{jj'}(E_{\text{rel}}) = \sum_{J=0}^{\infty} \sigma_{jj'}^{J}(E_{\text{rel}}) = \frac{\pi}{(2j+1)k_{jj}^{2}} \sum_{J=0}^{\infty} \sum_{l=|J-j|}^{J+j} \sum_{l'=|J-j'|}^{J+j'} (2J+1) \left| T_{jl,j'l'}^{J}(E_{\text{rel}} + E_j) \right|^2 . \tag{1}$$

The transition matrix elements $T_{jl,j'l'}^{J}(E)$ were obtained by solving a set of coupled differential equations by Gordon's method[7,8] at each J and at total energy $E = E_{\text{rel}} + E_j$, E_{rel} being the relative kinetic energy of the system and E_j the rotational energy of the molecule. J is the total angular momentum quantum number which is conserved during a collision and $k_{jj} = (2\mu E_{\text{rel}})^{1/2}/\hbar$ is the wave number for the entrance channel, μ being the reduced mass of the system.

For electron-molecule collisions, since the interaction potential is of longer range, a large number of J value is required to get convergence of the total cross section $\sigma_{jj'}$. For example, for obtaining proper convergence at $E = 0.1$ eV the maximum value of J was about 150 where the partial cross section $\sigma_{jj'}^{J}$ decreased to less than one hundredth of its maximum value. To reduce the computation time, we computed the partial cross sections $\sigma_{jj'}^{J}$ at some J values (e.g., 20) from $J = 0$ to $J = 150$ and obtained the cross sections at other J values by a suitable interpolation method OPLSPA.[21] The density of J values was higher near J_{min} where the partial opacities showed a peak. It was then gradually reduced with higher J where $\sigma_{jj'}^{J}$ decreased smoothly.

The rate coefficient at temperature T is the product of the cross section averaged over Boltzmann distribution and the average velocity of the system. The expression of the rate coefficient for the transition $j \to j'$ at temperature T is given by

$$R_{jj'}(T) = \left(\frac{8kT}{\pi\mu} \right)^{1/2} \left(\frac{1}{kT} \right)^2 \int_0^{\infty} \sigma_{jj'}(E_{\text{rel}}) \exp(-E_{\text{rel}}/kT)$$
$$\times E_{\text{rel}} \, dE_{\text{rel}} , \tag{2}$$

where k is the Boltzmann constant. Integration in Eq. (2) was done by the spline integration me-thod.[22] All the calculations were performed on the Burroughs 6700 computer at the Regional Computer Center, Calcutta.

III. INTERACTION POTENTIAL

The interaction potential for e-CO or e-HCN system may be represented as the sum of terms representing the polarization interaction $V_p(\vec{r})$, the dipole interaction $V_d(\vec{r})$, and the quadrupole interaction $V_q(\vec{r})$. The form of the potential is thus[16]

$$V(\vec{r}) = V_p(\vec{r}) + V_d(\vec{r}) + V_q(\vec{r}) , \tag{3}$$

where

$$V_p(\vec{r}) = -\frac{\alpha e^2}{2r^4} - \frac{\alpha' e^2}{2r^4} P_2(\cos\theta) ,$$
$$V_d(\vec{r}) = \frac{eD}{r^2} P_1(\cos\theta) , \tag{4}$$
$$V_q(\vec{r}) = \frac{e\alpha}{r^3} P_2(\cos\theta) ,$$

$\vec{r}$ being the position vector of the electron relative to the center of mass of the molecule and θ the angle between $\vec{r}$ and the molecular axis. α and α' are, respectively, the spherical and anisotropic parts of the molecular polarizability. α' is given by $\alpha' = \frac{2}{3}(\alpha_{||} - \alpha_{\perp})$, $\alpha_{||}$ and $\alpha_{\perp}$ being, respectively, the parallel and perpendicular components of the polarizability. D and Q are, respectively, the dipole and quadrupole moments of the molecule. It may be pointed out here that higher multipole terms which might become very important for atom-molecule or molecule-molecule collisions are not so important for electron-molecule interaction even at the short range. In the latter case, the longer-range dipole and quadrupole and the shorter-range polarization terms are most important. For electron-mole-

TABLE I. Molecular parameters of CO and HCN used in the calculations.

Parameters \ Molecule	CO	HCN
Isotropic polarizability α (Å^3)	1.977 [a]	2.59 [b]
Anisotropic polarizability α' (Å^3)	0.355 [a]	1.33 [b]
Dipole moment D (D)	0.112 [c]	2.99 [c]
Quadrupole moment Q (D Å)	−2.5 [c]	4.40 [c]
Rotational constant B_e (cm^{-1})	1.9313 [d]	1.4878 [e]
Equilibrium distance r_e (cm^{-1})	1.128 [d]	2.22 [e]

[a] Reference 23.
[b] Reference 24.
[c] Reference 25.
[d] Reference 26.
[e] Reference 27.

cule interaction, also the short-range exchange forces are yet quite unknown. Hence we have not considered the higher multipole and the exchange terms. A number of previous workers[14,16-18] have also used almost similar type of potential as in Eqs. (3) and (4). The values of the molecular parameters used in the calculations are given in Table I.

As the interaction potential for electron-molecule collision is purely attractive at small r, some difficulties were faced in solving the coupled differential equations by Gordon's method. To overcome this difficulty, we have assumed the existence of a "flexible" repulsive potential wall for values of r less than the internuclear distance (r_e) of the molecule. Without a repulsive potential at the short range, Gordon's method does not work well. Arthurs and Dalgarno[20] and Rudge[28] also assumed an infinite potential wall at small r values for e-H$_2$ and e-alkali halides collisions, respectively. For e-CO the wall was assumed at $\sigma = r_e/2$ whereas for e-HCN the wall was assumed at $\sigma = r_e/3$. It may be noted here that by flexible potential wall it is meant that σ and the slope of the (potential) wall were varied in such a way that the effect of the wall, which was an artifact, vanished at $r \geq r_e$. The reason of taking a flexible (potential) wall was to see whether the

TABLE II. Rotational cross sections $\sigma_{jj'}$ (Å^2) for e-CO collision at total energy E (eV) and various rotational states j,j'.

$\sigma_{jj'}$	Method	0.0006	0.0008	0.001	0.002	0.003	0.004	0.005	0.006	0.008	0.01	0.03	0.05	0.075	0.1
σ_{01}	CC [a]	96.57	109.4	108.5	86.88	66.90	53.70	45.10	38.92	30.69	25.50	9.60	5.95	4.13	3.20
	Born [b]	100.1	115.9	113.1	83.24	64.85	53.45	45.69	40.05	32.35	27.30	11.41	7.48	5.32	4.17
	UTDP [b]	107.1	102.6	95.92	69.44	54.67	45.46	39.13	34.49	28.10	23.86	10.22	6.77	4.85	3.82
	CC [c]							45.06			26.87	11.20	7.34		4.09
	CC [d]							44.38			26.15	10.47	6.67		3.58
σ_{12}	CC				39.41	33.35	29.36	26.10	23.51	19.38	16.27	6.43	4.02	2.70	2.15
	Born				38.43	34.93	29.78	25.82	22.81	18.59	15.77	6.72	4.44	3.18	2.50
	UTDP				34.60	29.16	24.80	21.60	19.18	15.78	13.49	5.93	3.97	2.86	2.26
	CC														
	CC							24.98			15.01	6.10	3.90		2.11
σ_{02}	CC				0.62	0.84	0.93	0.97	1.00	1.03	1.05	1.12	1.16	1.23	1.30
	Born				0.56	0.76	0.84	0.88	0.91	0.94	0.95	0.96	0.94	0.92	0.90
	UTDP														
	CC							0.96			1.03	1.07	1.08		1.11
	CC							0.68			0.73	0.75	0.76		0.79

[a] This work.
[b] Calculated from Dickinson and Richards's formulas (Ref. 16).
[c] Crawford and Dalgarno's calculation (Ref. 17).
[d] Chandra's calculation (Ref. 18).

cross sections were sensitive to the position (σ) or slope of the wall. In the case of e-CO, it was found that the cross sections were quite insensitive to σ or to the slope of the wall at $r < r_e$. But in case of e-HCN, the cross sections were somewhat sensitive to σ or to the slope of the wall.

IV. RESULTS AND DISCUSSION

The values of the rotational excitation cross sections $\sigma_{jj'}$ for $j,j' = 0$, 1, and 2 obtained for e-CO and e-HCN systems have been given in Tables II and III. These are also shown as function of total energy E in Figs. 1(a) and 1(b) for $\Delta j = 1$ and 2, respectively. The deexcitation cross
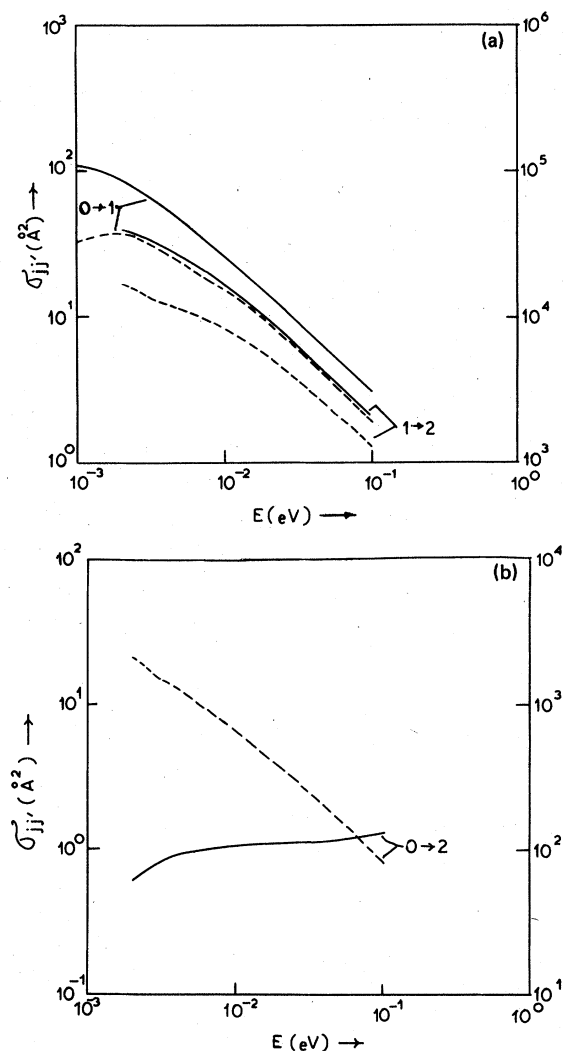

FIG. 1. Rotational cross sections $\sigma_{jj'}$ as a function of total energy E for (a) $\Delta j = 1$ and (b) $\Delta j = 2$, where $\Delta j = j' - j$. The solid curves with the left-hand scale are for e-CO and the dotted curves with the right-hand scale are for e-HCN collisions.

TABLE III. Rotational cross sections $\sigma_{jj'}$ (Å²) for e-HCN collision at total energy E (eV) and various rotational states j,j'.

$\sigma_{jj'}$	Method	0.0006	0.0008	0.001	0.002	0.003	0.004	0.005	0.006	0.007	0.01	0.03	0.05	0.075	0.1
σ_{01}	CC[a]	40 200	53 760	33 370	37 210	31 880	26 000	23 760	20 410	16 970	15 360	6037	3692	2481	1874
	Born[b]	107 100	103 800	95 910	65 890	50 430	41 190	35 010	30 570	24 560	20 660	8526	5570	3953	3093
	UTDP[b]	67 171	66 260	62 863	46 737	37 127	31 022	26 788	23 666	19 337	16 455	7102	4713	3381	2662
σ_{12}	CC				17 370	13 630	12 690	11 660	10 780	9400	8 291	3822	2447	1679	1274
	Born				34 400	28 040	23 320	20 000	17 550	14 200	12 000	5046	3322	2372	1862
	UTDP				22 013	18 997	16 377	14 387	12 855	10 658	9 157	4093	2750	1989	1576
σ_{02}	CC				2 126	1 508	1 292	1 121	983	792	666	263	164	110	81
	Born				2.34	2.82	3.05	3.20	3.30	3.44	3.53	3.99	4.24	4.49	4.69
	UTDP														

[a] This work.
[b] Calculated from Dickinson and Richards's formulas (Ref. 16).

TABLE IV. Rotational rate coefficients $R_{jj'}$ (cm^3/sec) for e–CO collision at temperature T(K) and various rotational states j, j'.

$R_{jj'}$	Method	5	10	15	20	30	40	50	60	70	80	90	100
R_{01}	CC[a]	0.98(−8)[c]	1.57(−8)	1.77(−8)	1.84(−8)	1.85(−8)	1.82(−8)	1.77(−8)	1.73(−8)	1.68(−8)	1.64(−8)	1.60(−8)	1.56(−8)
	Born[b]	1.01(−8)	1.58(−8)	1.77(−8)	1.83(−8)	1.85(−8)	1.83(−8)	1.79(−8)	1.75(−8)	1.70(−8)	1.66(−8)	1.62(−8)	1.59(−8)
	UTDP[b]	0.90(−8)	1.36(−8)	1.50(−8)	1.56(−8)	1.58(−8)	1.56(−8)	1.53(−8)	1.49(−8)	1.46(−8)	1.44(−8)	1.41(−8)	1.38(−8)
R_{12}	CC	0.15(−8)	0.47(−8)	0.64(−8)	0.73(−8)	0.83(−8)	0.88(−8)	0.89(−8)	0.90(−8)	0.90(−8)	0.89(−8)	0.89(−8)	0.88(−8)
	Born	0.15(−8)	0.47(−8)	0.64(−8)	0.73(−8)	0.83(−8)	0.86(−8)	0.88(−8)	0.88(−8)	0.87(−8)	0.86(−8)	0.85(−8)	0.84(−8)
	UTDP	0.17(−8)	0.43(−8)	0.56(−8)	0.64(−8)	0.71(−8)	0.73(−8)	0.74(−8)	0.74(−8)	0.74(−8)	0.73(−8)	0.73(−8)	0.72(−8)
R_{02}	CC	0.11(−10)	0.68(−10)	1.29(−10)	1.82(−10)	2.73(−10)	3.48(−10)	4.11(−10)	4.66(−10)	5.16(−10)	5.61(−10)	6.04(−10)	6.44(−10)
	Born	0.10(−10)	0.62(−10)	1.17(−10)	1.65(−10)	2.48(−10)	3.16(−10)	3.73(−10)	4.22(−10)	4.65(−10)	5.04(−10)	5.40(−10)	5.74(−10)
	UTDP												

[a] This work.
[b] Calculated from Dickinson and Richards's formulas (Ref. 16).
[c] The number in the parenthesis represents the power of ten by which the entry is to be multiplied.

TABLE V. Rotational rate coefficients $R_{jj'}$ (cm^3/sec) for e–HCN collision at temperature T(K) and various rotational status j, j'.

$R_{jj'}$	Method	5	10	15	20	30	40	50	60	70	80	90	100
R_{01}	CC[a]	3.18(−6)[c]	5.66(−6)	6.97(−6)	7.67(−6)	8.40(−6)	8.72(−6)	8.86(−6)	8.90(−6)	8.86(−6)	8.79(−6)	8.69(−6)	8.58(−6)
	Born[b]	9.76(−6)	13.83(−6)	14.87(−6)	15.08(−6)	14.87(−6)	14.47(−6)	14.04(−6)	13.61(−6)	13.20(−6)	12.83(−6)	12.49(−6)	12.19(−6)
	UTDP[b]	6.60(−6)	9.34(−6)	10.24(−6)	10.58(−6)	10.71(−6)	10.60(−6)	10.42(−6)	10.23(−6)	10.03(−6)	9.85(−6)	9.67(−6)	9.50(−6)
R_{12}	CC	0.56(−6)	1.87(−6)	2.67(−6)	3.14(−6)	3.70(−6)	4.01(−6)	4.20(−6)	4.31(−6)	4.37(−6)	4.41(−6)	4.42(−6)	4.42(−6)
	Born	1.11(−6)	3.70(−6)	5.14(−6)	5.90(−6)	6.60(−6)	6.85(−6)	6.91(−6)	6.88(−6)	6.80(−6)	6.71(−6)	6.61(−6)	6.51(−6)
	UTDP	1.44(−6)	3.11(−6)	3.95(−6)	4.40(−6)	4.83(−6)	4.99(−6)	5.04(−6)	5.05(−6)	5.05(−6)	5.00(−6)	4.96(−6)	4.91(−6)
R_{02}	CC	0.35(−7)	1.69(−7)	2.62(−7)	3.14(−7)	3.65(−7)	3.86(−7)	3.94(−7)	3.95(−7)	3.93(−7)	3.89(−7)	3.84(−7)	3.79(−7)
	Born	0.41(−10)	2.44(−10)	4.47(−10)	6.23(−10)	9.26(−10)	11.81(−10)	14.00(−10)	15.95(−10)	17.72(−10)	19.31(−10)	20.91(−10)	22.38(−10)
	UTDP												

[a] This work.
[b] Calculated from Dickinson and Richards's formulas (Ref. 16).
[c] The number in the parenthesis denotes the power of ten by which the entry is to be multiplied.
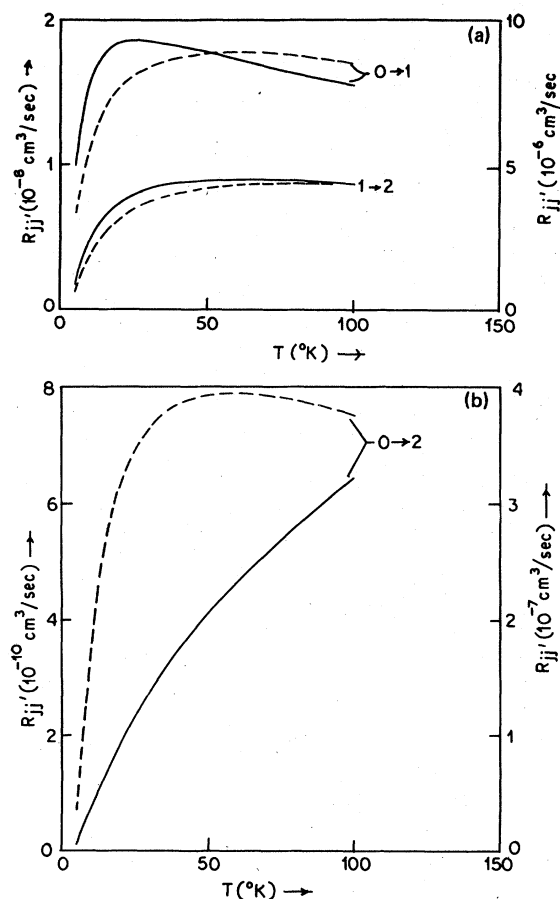
FIG. 2. Rotational rate coefficients $R_{jj'}$ as a function of temperature T for (a) $\Delta j = 1$ and (b) $\Delta j = 2$, where $\Delta j = j' - j$. The solid curves with the left-hand scale are for e-CO and the dotted curves with the right-hand scale are for e-HCN collisions.

sections are not reported since these can be obtained directly from the excitation cross sections using the detailed balance principle. As seen in Fig. 1(a), for both e-CO and e-HCN systems σ_{01} and σ_{12} decrease smoothly with energy in the range 0.002–0.1 eV. Figure 1(b) shows that σ_{02} for e-CO increases slightly with energy in the range 0.002–0.1 eV but that for e-HCN it decreases smoothly in the same range of energy.

The values of the excitation rate coefficients $R_{jj'}$ have been given in Tables IV and V for e-CO and e-HCN systems, respectively. These are

also plotted as a function of temperature T in Figs. 2(a) and 2(b) for $\Delta j = 1$ and 2, respectively. The deexcitation rate coefficients can be obtained with the help of the detailed balance principle and hence are not reported here. Figure 2(a) shows that for both e-CO and e-HCN, R_{01} at first rapidly increases and then slowly decreases with temperature, whereas R_{12} at first smoothly increases and then becomes almost constant with temperature. Figure 2(b) shows that R_{02}, for e-CO, steadily increases with temperature, but that, for e-HCN, at first sharply rises and then slowly falls as the temperature increases.

The cross sections and rate coefficients have also been compared with Born and unitarized time-dependent perturbation calculations[16] in Tables II–V. It is seen that Born results are quite good for e-CO but very bad for e-HCN collisions. The unitarized time-dependent results are quite bad for both the systems. In Table II we have also compared our results with those calculated by Crawford and Dalgarno[17] and Chandra[18] for e-CO cross sections using the close-coupling theory. The overestimation of their cross sections at higher energies is perhaps due to the fact that after a few J values, the close-coupling Born method was used to calculate the cross sections. It may again be mentioned that the potential used in this work is almost similar to that used by Crawford and Dalgarno[17] or Chandra.[18] The basis set used here is the same as that used by Crawford and Dalgarno[17] but smaller than that used by Chandra.[18]

For application to the interpretation of the spectral data obtained from interstellar sources it is interesting to compare the rate coefficients for e-CO and e-HCN collisions with those for H_2-CO collisions obtained by Green and Thaddeus.[2] It is seen that in the temperature range of interest to us, the rate coefficients for $\Delta j = 1$ transition in e-CO collisions are in general 10^2 to 10^3 times higher, and those for e-HCN collisions are 10^4 to 10^6 times higher than the corresponding values for the H_2-CO system.

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