Rotational excitation of heteronuclear molecular ions by electron impact

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The Glauber approximation with allowance for Coulomb effects is used in the study of the rotational excitation of the CO^+, HCO^+, and N_2H^+ heteronuclear molecular ions from the $J = 0 \rightarrow 1$ state by electron impact.

The rotational excitation of molecular ions plays an important role in ionospheric studies and in the understanding of the constituents of interstellar matter.[1-7] Several new spectral lines have been detected which have led to the discovery of new molecular ions.[1,2] The existence of HCO^+ and N_2H^+ in interstellar matter has already been established.[4-7] The $J = 0 \rightarrow 1$ transition in N_2H^+ has been observed in interstellar clouds in IC 2162, NGC 6334, W31, W33, W49, W75, etc., and the $J = 0 \rightarrow 1$ transition in HCO^+ is observed in M17, NGC 1999, NGC 2023, IC 2162, etc.

On the theoretical side not much work has been done in the study of pure rotational excitation of molecular ions. Stabler[8] and Sampson[9] considered the rotational excitation of homonuclear molecular ions using the first-order time-dependent perturbation theory and an approximate form of the Coulomb wave function. Chu and Dalgarno[10] studied the rotational excitation of the heteronuclear CH^+ molecular ion in the Coulomb-Born approximation. Ray and Barua[11] used a semiclassical first-order time-dependent theory for the rotational excitation in HD^+. Dickinson and Muñoz[12] used an impact parameter method using hyperbolic paths and perturbation theory to study rotational excitation of HD^+, CH^+, and H_3O^+ ions.

In a recent paper Mathur[13] studied the rotational excitation of CH^+ by including Coulomb effects in the framework of the Glauber eikonal approximation. Here we extend this study to the calculation of rotational excitation cross sections and reaction rates for the $J = 0 \rightarrow 1$ transition in CO^+, HCO^+, and N_2H^+ molecular ions which are of great current astrophysical interest.

If we consider the target molecular ion to be a rigid rotator having a permanent dipole moment (D), the total cross sections (σ) and the rate coefficients (K_r) are evaluated using Eqs. (20) and (22) of Mathur.[13]

Figure 1 shows our results of the total cross sections for the $J = 0 \rightarrow 1$ rotational excitation of CO^+, HCO^+, and N_2H^+ at several incident electron energies. From the figure, it is noted that in all cases studied the cross section falls steeply near threshold. However, in the Coulomb-Born approximation, the cross section has a finite large value in the threshold region.[10] This drawback of the present theory is not surprising as the Glauber approximation is not expected to be good in the region close to the threshold. From the comparative study of the various molecular ions, it is observed

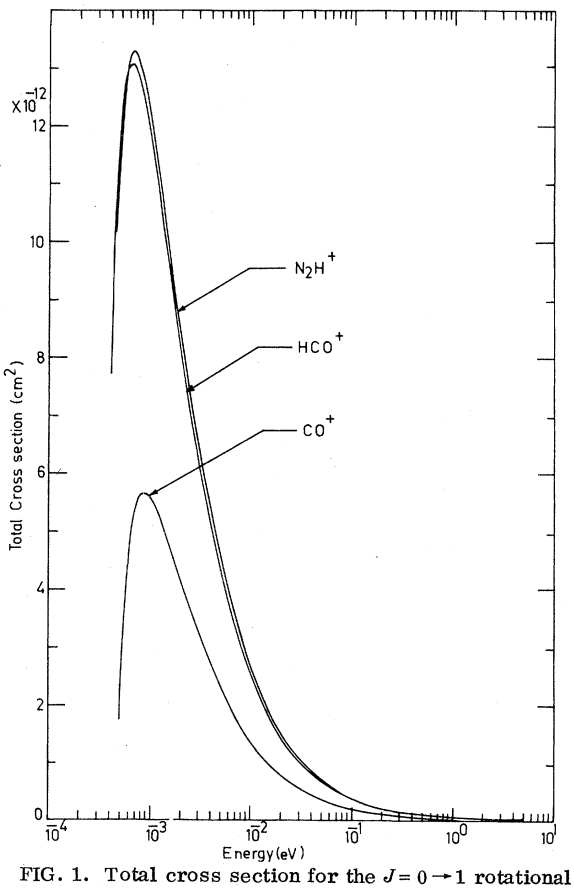

FIG. 1. Total cross section for the $J = 0 \rightarrow 1$ rotational excitation of CO^+, HCO^+, and N_2H^+ molecular ions at several incident electron energies. The solid curves give present results for these molecular ions which are labeled accordingly.

that the cross sections depend greatly upon the dipole moment. The HCO^+ and N_2H^+ molecular ions have nearly equal dipole moments of 3.3 and 3.4 D, respectively. The cross sections for these two ions are nearly the same except for some difference in the near threshold region. In the case of CO^+ the dipole moment is smaller (2.5 D) and therefore the cross sections are lower.

The dependence of the cross section on the dipole moment D, can be approximately given by the scaling law

$$\sigma = AD^n, \tag{1a}$$

where A and n are energy-dependent parameters. For higher energies (about $E > 0.5$ eV) these parameters can be expressed in the form

$$A = a(\ln E)/E + b/E \tag{1b}$$

and

$$n = 1/(c + dE), \tag{1c}$$

where a, b, c, and d are constants. The values of these constants are $a = 36.62$, $b = 103.91$, $c = 4.11 \times 10^{-1}$, and $d = 4.77 \times 10^{-3}$. In the above expressions D is to be taken in D, the energy E in eV, and σ is obtained in a_0^2, where a_0 is Bohr's radius.

The cross sections obtained by using Eq. (1) are found to be within 10% of the exact results [obtained from Eq. (20) of Mathur[13]] for energies above 0.5 eV, for all the molecular ions studied here. Therefore the above scaling law can be used to obtain a rough estimate of the cross sections for other ions in the high-energy region (far from the threshold).

The rate coefficients for a temperature range from 10 to 1000 °K are presented in Table I. As is evident from the table, the rate coefficients show an increase with the increase in dipole moment of the ion at all temperatures. However, we do not find any systematic fit to the calculated rates with dipole moment at various temperatures.

There is no experimental data available at present to compare our results for these molecular ions. However, it may be noted that the magnitude of these rotational cross sections and reaction rates are quite large, especially for HCO^+ and N_2H^+, and can easily be measured experimentally.

TABLE I. Rate coefficients in units of 10^{-8} $cm^3 sec^{-1}$ for ($J = 0$ to $J = 1$) rotational excitation of CO^+, HCO^+, and N_2H^+ at various temperatures.

T (°K)	CO^+	HCO^+	N_2H^+
10	740	1641	1686
20	893	1827	1911
30	915	1818	1913
40	905	1768	1865
50	887	1716	1812
60	869	1669	1760
70	848	1620	1712
80	830	1578	1667
100	796	1504	1588
150	729	1364	1440
200	679	1264	1333
300	609	1126	1188
400	560	1033	1089
600	495	909	959
800	452	828	873
1000	421	768	810

In conclusion, we note that the present approach provides a simple way for estimating the cross sections and reaction rates of some atmospherically interesting molecular ions.

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