Inelastic scattering of CN radical with para- and ortho-H_2

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The CN molecule is one of the most widely distributed in the interstellar medium (ISM). In diffuse molecular gas, CN plays a role as a tracer of high density gas. The CN thermal lines also probe dense regions in molecular clouds, circulstellar envelopes. The cyano radical is also of great interest in combustion chemistry and atmospheric physics.

Modelling of molecular emission spectra from ISM requires the knowledge of accurate rate coefficients for excitation by collisions with the most abundant species, like He and H_2. The extensive study of CN collisions with He atom was already done in ref. [1]. Thus, the present work is focused on the collisions with hydrogen molecule.

At low temperatures, molecular collisions induce only the rotational energy transfer in CN and H_2 molecules due to a large activation energy (~1100 cm-1) for HCN molecule formation. Thus, rotational (de-)excitation can be studied neglecting reaction pathways [2]. We present state-to-state and total rotational energy transfer rate coefficients and state-to-state cross sections between the first 16 rotational levels of CN($X^2\Sigma^+$), being in the ground vibrational state, in collisions with H_2, the most abundant collisional partners in cold molecular clouds. The Close Coupling (CC) calculations were carried out for a 4D potential energy surface (PES) calculated at highly correlated *ab initio* "coupled-cluster" method. The quality of the PES was checked by comparison with the experimental data. The zero-order corrected dissociation energies D_0 are 27.73 cm−1 and 38.75 cm−1 for the complex with para-, and ortho-H_2, respectively. These theoretical results obtained using our new PES are in excellent agreement with experimental value for CN-ortho-H_2: 38±1 cm−1 [3]. Rate coefficients were also compared with experimental results of Brunet et al. [4]. A good agreement between theoretical and experimental results was found. The fine-structure resolved cross sections were obtained by the recoupling of CC S-matrix. State-to-state cross sections were calculated for the first 25 fine levels of CN molecule in collisions with para-H_2 (j=0) and ortho-H_2 (j=1). Significant differences exist between para- and ortho-H2 results. The propensity rules between fine-structure levels are also studied, and it is shown that the cross sections for $\Delta j = \Delta N$ transitions are much larger than those for $\Delta j \neq \Delta N$ transitions, as expected from theoretical considerations.

We expect that the obtained results will serve as a valuable tool for the interpretation of the CN emission lines observed with current and future telescopes and also in determination of physical conditions in interstellar clouds.

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