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C5N– in collision with He: rotational transitions in the ISM

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In the last years, several C-bearing and (C,N)-bearing chains of molecular anions have been detected in the interestellar medium (ISM). Since experimental treatments are still challenging, computational methods have to be used to understand their chemistry. The C_5N^- anion is one of the largest (C,N)-bearing chains and, although there are several theoretical studies [1-3] that describe the dynamics of the smaller (CN^-,C_3N^-) + He/H_2 systems, for the moment there has been no study reported for the collision between this molecular anion with He or H_2.

We have performed quantum scattering calculations using a new ab initio potential energy surface (PES) where the interaction potential between C_5N^- and He was obtained using CCSD(T) approach and the complete basis set (CBS) limit (see Figure 1). Given the ISM conditions of this system, we calculate the state-to-state (de-)excitation cross sections and the respective rate coefficients as a function of temperature. These results have been also compared by those obtained for the C_3N^-/C_5N^- + H_2 system.

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