Molecular anions: Rotational (de)-excitation and dipole bound states.

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Résumé

Since their recent detection in the interstellar medium, anions have raised the question of their possible mechanisms of formation, destruction and excitation. Radiative electron attachment is thought to be the most probable most probable mechanism of formation. A key point for this hypothesis is the abundance ratio [A-]/[A] for this anions is estimated to be approximately 1 % . There are however at the moment a lack of experimental and theoretical data allowing to asses this hypothesis. Among the observed anions, we will focus our attention C3N- and C4H-.
To improve the measurement of the abundance ratio of C3N- a quantum mechanical treatment of the rotational (de-)excitation by collisions with He and H2 is reported. Full close-coupling calculations are performed within the rigid rotor approximation and rate coefficients for the rotational transitions among the first 31 levels of C3N- are obtained for temperatures between 1 and 300 K. Calculations of the ro-vibrational bound states are carried out by using a discrete variable representation method based on Sturmians functions. The first theoretical predictions of the absorption spectra for the van der Waals complexes in the microwave region is also provided.
$C4H^-$/[C4H] ratio is most elegantly explained by the dipole-bound formation hypothesis. No dipole-bound state was found for C4H 2Σ ground state conversely to its low-lying 2Π excited state which own a large dipole moment enough to capture the additional electron. The calculated C4H- dipole-bound state energy have been found to be in good agreement with the experimental observations.

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