Radiative electron attachment to molecules of astrophysical interest: Direct and indirect mechanisms

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Résumé

A first-principle theoretical approach to study the process of radiative electron attachment is developed and applied to the negative molecular ions CN-, C4H-, and C2H-. Among these anions, the first two have already been observed in the interstellar space. Cross sections and rate coefficients for formation of these ions by radiative electron attachment to the corresponding neutral radicals are calculated. For completeness of the theoretical approach, two pathways for the process have been considered: (i) A direct pathway, in which the electron in collision with the molecule spontaneously emits a photon and forms a negative ion in one of the lowest vibrational levels, and (ii) an indirect, or two-step pathway, in which the electron is initially captured through non-Born-Oppenheimer coupling into a vibrationally resonant excited state of the anion, which then stabilizes by radiative decay. We have developed a general theoretical model to describe the two pathways. The contribution of the indirect pathway to the formation of cosmic anions was found to be negligible in comparison to the direct mechanism. The obtained total rate coefficients of radiative electronic attachment at 30K are 7x10-16 cm3/s for CN-, 7x10-17 cm3/s for C2H-, and 2x10-16 cm3/s for C4H-. These rates weakly depend on temperature between 10K and 100 K. The validity of our calculations is verified by comparing the present theoretical results with data from recent photodetachment experiments performed for the CN-, C4H-, and C2H- ions.

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