Rotational Relaxation of AlNC and AlCN by para-H_2(j = 0) at Low Temperatures

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Abstract
An accurate determination of the abundances of metal-containing molecules in the interstellar medium or circumstellar gas requires knowledge of molecular data, including the collisional rate coefficients. This work is focused on the study of the collision of the aluminum isocyanide (AlNC) molecule, as well as its isomer AlCN, with para-H2 (j = 0). For the AlNC + H2 and AlCN + H2 complexes, averaged potential energy surfaces are developed from ab initio energies computed at the coupled cluster with the single, double, and perturbative triple excitation level of theory. Such surfaces are used in close-coupling calculations. The rate coefficients at low temperature are compared with those for the collisions with He. The use of the mass scaling procedure is a good approximation in the case of AlCN. However, for the collision with AlNC, a different propensity rule is found between the rates with He and para-H2 (j = 0). Finally, rotational rate coefficients for the lowest 26 rotational levels of both molecules, AlCN and AlNC, by collision with para-H2 (j = 0) are reported.

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