Rotational relaxation of AIO+(1?+) in collision with He

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The rate coefficients for the rotational de-excitation of AIO+ by collisions with He are determined. The possible production mechanisms of the AIO+ ion in both diffuse and dense molecular clouds are first discussed. A set of ab initio interaction energies is computed at the CCSD(T)-F12 level of theory, and a three-dimensional analytical model of the potential energy surface is obtained using a linear combination of reproducing kernel Hilbert space polynomials together with an analytical long range potential. The nuclear spin free closecoupling equations are solved and the de-excitation rotational rate coefficients for the lower 15 rotational states of AIO+ are reported. A propensity rule to favour ?j = -1 transitions is obtained while the hyperfine resolved state-to-state rate coefficients are also discussed. © 2017 The Author(s).

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