3D Potential energy surface and collisional excitation of $^{23}Na^{35}Cl$ by He

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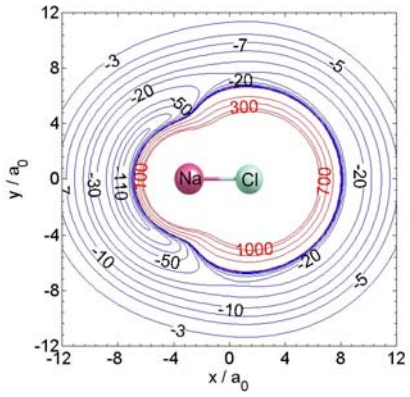
One of the most interesting astronomical objects is the circumstellar envelope of the carbon star IRC+10216. A half of all detected interstellar molecules is presented in this envelope. First observations of the metal halides like NaCl, KCl, AlCl and AlF were made by J. Cernicaro and M. Guélin in 1987 in IRC+10216 [1]. In 2012 radiative transfer modelling [2] of IRC+10216 have shown that a simple assumption of local thermodynamical equilibrium for such molecules as NaCl and KCl leads to a poor agreement with astronomical observations. This means that rotational excitation of these molecules is likely controlled by inelastic collisions with He and H_2. However, it is not possible to get reliable model without accurate collisional rate coefficients.

In the present work we have investigated the NaCl-He collisional system. A 3D potential energy surface (PES) was calculated at CCSD(T) level of theory with a large aug-cc-pWCVQZ basis set taking into account the Basis Set Superposition Error correction. The global minimum corresponds to a linear structure with He atom approaching Na atom. The molecular dynamics calculations were carried out for the ground vibrational state of $^{23}Na^{35}Cl$ using Close-Coupling (CC) method, Coupled States (CS) and Infinite Order Sudden (IOS) Approximations for the first 36 (j = 0 - 35) rotational levels of NaCl molecule for total energies up to 1000 cm^{-1}. A bad agreement is found between CC and CS/IOS results for collisional inelastic cross sections. The hyperfine structure of $^{23}Na^{35}Cl$ (I_{Na}=3/2, I_{Cl}=3/2) was taken into account by recoupling technique of CC scattering S-matrix.



We expect that present rate coefficients will help significantly in interpretation of NaCl emision spectra observed by current and future telescopes.

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[1] J. Cernicharo, M. Guélin, *A&A* **1987**, *183*, L10.
[2] M. Agundez, J. P. Fonfrıa, J. Cernicharo, C. Kahane, F. Daniel, and M. Guelin. *A&A* **2012**, *54*, A48.1-A48.26.