

Calculation of the predissociation spectra of the $^{35}\text{Cl}^-(\text{H}_2)$ complex and its isotopologue $^{35}\text{Cl}^-(\text{D}_2)$ recently measured in an ionic trap at low temperature

M. Lara-Moreno, P. Halvick and T. Stoecklin

UMR5255-CNRS, Université de Bordeaux, 351 cours de la libération, F-33405 Talence, France.

The predissociation spectra of the $^{35}\text{Cl}^-(\text{H}_2)$ and $^{35}\text{Cl}^-(\text{D}_2)$ complexes are determined within an accurate quantum approach and compared to those recently measured in an ionic trap at 8 K and 22 K. [1,2] The calculations are performed using an existing three-dimensional potential energy surface [3]. A variational approach is used for the accurate quantum calculations of the rovibrational bound states. Several methods are compared for the search and the characterization of the resonant states. A good agreement between the calculated and measured spectra is obtained, despite a slight shift to the red of the calculated spectra. The comparison shows that only the ortho or para contribution is observed in the measured $^{35}\text{Cl}^-(\text{H}_2)$ or $^{35}\text{Cl}^-(\text{D}_2)$ spectrum, respectively. This result is attributed to the rapid para \leftrightarrow ortho conversion of the complexes by collision with H_2 or D_2 molecules inside the trap at low temperature. Quantum numbers are assigned to the rovibrational resonant states. It demonstrates that the main features observed in the measured predissociation spectra correspond to a progression in the intermonomer vibrational stretching mode.

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