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

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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 $\text{H}_2$ or $\text{D}_2$ 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.