POTENTIAL ENERGY SURFACES AND VIBRATIONAL ENERGY LEVELS OF DCCl AND HCCI IN THEIR THREE LOW-LYING STATES

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We present \textit{ab initio} multi-reference configuration interaction (MRCI) calculations of potential energy surfaces of HCCI in its three low-lying electronic states ($\tilde{X}^1A'$, $\tilde{a}^3A''$ and $\tilde{A}^1A''$) and for the spin-orbit coupling between the $\tilde{X}$ and $\tilde{a}$ states. The two singlet states become a degenerate $^1\Delta$ state in collinear geometries. The potential energy surfaces are interpolated from 6075 MRCI energy points. The final surfaces are slightly adjusted using a coordinate and energy scaling approach. The $T_e$ values of the $\tilde{a}^3A''$ and $\tilde{A}^1A''$ states are computed to be 2122.0 and 12209.8 cm$^{-1}$, respectively. Vibrational energy levels of the three states of DCCl and HCCI taking into account the Renner-Teller effect and spin-orbit coupling are computed. The calculated vibronic energy levels are in good agreement with the available experimental values.

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