

POTENTIAL ENERGY SURFACES AND VIBRATIONAL ENERGY LEVELS OF DCCI AND HCCI IN THEIR THREE LOW-LYING STATES^a

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We present *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 DCCI 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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