POTENTIAL ENERGY SURFACES AND VIBRATIONAL ENERGY LEVELS OF DCCl AND HCCl IN THEIR THREE LOW-LYING STATES[a]

HUA-GEN YU, TREVOR J. SEARS and JAMES T. MUCKERMAN, *Chemistry Department, Brookhaven National Laboratory, Upton, NY 11973-5000 USA*.

We present *ab initio* multi-reference configuration interaction (MRCI) calculations of potential energy surfaces of HCCl 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 HCCl 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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