THE INTERMOLECULAR POTENTIAL SURFACE OF INERT GAS HALOGEN COMPLEXES AS PROBED BY HeClF

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We report the intermolecular potential of HeClF as studied by *ab initio* theory and microwave spectroscopy. The potential surface was calculated at the MP4 level and is characterized by three minima, the deepest of which is -58.1 cm at 0° and 3.57 Å , the next is -35.2 cm^{-1} at 110° and 3.30 Å , and the shallowest is -32.3 cm^{-1} at 180° and 3.95 Å . The rotation-vibration levels calculated from the *ab initio* potential fall into three catagories with the He atom localized in each of the three minima. These configurations can be viewed as different isomeric forms or as vibrational states of HeClF. Pure rotational transitions have been observed for the two lowest energy vibrational states (linear and T-shaped) and these are in good agreement with predictions from the *ab initio* surface. Two linear $\rightarrow$ T-shaped transitions have been observed for the complex. The observed vibrational interval between the linear and the T-shaped forms differ from predictions by 0.9 cm^{-1}. The nuclear hyperfine structure and electric dipole moments measured are also in good agreement with those calculated from the *ab initio* surface. The potential surface with multiple minima observed here appears to be a general phenomena for inert gas halogen complexes. This is the first experimental observation of both a linear and a T-shaped form for this kind of complex.

Spectroscopic constants for the linear form of $He^{35}ClF$ are $B = 5586.389(7)$ MHz, $D = 1.367(1)$ MHz, $eqQ_{J=1} = -133.70(6)$ MHz, $eqQ_{J=2} = -133.79(6)$ MHz and $\mu = 0.880(1)$ D. Constants for the T-shaped form are $B = 7042.256(12)$ MHz, $eqQ_{J=1} = -40.02$ MHz, $eqQ_{J=2} = -50.33$ MHz and $\mu = 0.614(7)$ D.