PREDICTED MICROWAVE SPECTRUM AS A SIMULTANEOUS PRODUCT OF BOTH LINEAR AND T-SHAPED CONFORMERS OF THE GROUND STATE He–Cl_2 SYSTEM

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Lowest energy rovibrational states are calculated for a high quality *ab initio* potential energy surface (PES) of the $HeCl_2$ Van Der Waals complex. The PES has wells of comparable depths for both linear (L) and T-shaped (T) conformers and thus produces two sets of rovibrational levels, the set associated with the L-well having higher energies due to difference between the two D_0 values.
Although the ground rovibrational levels of each conformer lie above the potential barrier separating the two wells, the associated wavefunctions reflect the presence of the other well only weakly, as indicated by the low local maxima in the probability densities at the other well positions. The presence of the L-well is found to affect the order of the rotational levels associated with the T-well.
The microwave spectra originating from each of the two conformers are simulated, and suggest a possibility for direct confirmation of the existence of the L-well. The positions of spectral lines associated with the T-shaped conformer are found to be quite sensitive to the binding energy for the linear conformer.