FOURFOLD CLUSTERS OF ROVIBRATIONAL ENERGIES IN $H_2Te$ AND $H_2Po$

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An interesting novel pattern in rotation-vibration spectra is the cluster effect (i. e., the formation of four-member groups of nearly degenerate rotation-vibration energy levels at higher $J$ and $K_a$ values[a]) in the molecules $H_2S$, $H_2Se$, $H_2Te$, and $H_2Po$. In the cluster states, local mode behaviour is induced by rotational excitation so that it occurs in the lowest vibrational states. We report here investigations of the cluster effect in the vibrational ground states of the $H_2Te$ and $H_2Po$ molecules. For $H_2Te$, we have obtained a new potential energy function by fitting to the available spectroscopic data, and for $H_2Po$, we have calculated the potential energy function *ab initio* by means of the CCSD(T) method, using an Averaged Relativistic Effective Potential for Po. With the new potential energy functions, the rotation-vibration energies of $H_2{}^{130}Te$ and $H_2{}^{209}Po$ have been calculated with the MORBID (Morse Oscillator Rigid Bender Internal Dynamics) Hamiltonian and computer program. In particular, we have calculated the rotational energy manifolds for $J \leq 40$ in the vibrational ground states.

An interesting aspect of the cluster effect is the change in vibrational ground state cluster formation taking place for the sequence of molecules $H_2O \rightarrow H_2S \rightarrow H_2Se \rightarrow H_2Te \rightarrow H_2Po$. The $H_2O$ molecule does not exhibit any discernible cluster formation at $J \leq 40$, but for all the other molecules the cluster size decreases rapidly with increasing $J$. For $H_2Te$ and $H_2Po$, in which the central mass is effectively infinite compared with the hydrogen mass, a limiting behaviour is reached which would not change further if the central mass were made heavier.

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