THE DOUBLE RENNER EFFECT IN A TRIATOMIC MOLECULE

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The electronic energy of a triatomic molecule can be doubly degenerate at linear configurations but split into two non-degenerate components at bent geometries. This is termed the Renner effect. If two different linear geometries are accessible to the molecule and the electronic energy is doubly degenerate at these geometries, we speak about the 'double Renner effect.'

For example, a double Renner effect will occur if the triatomic molecule ABC isomerizes between two linear minima ABC and BCA, say, and the electronic energy is doubly degenerate at these minima. An example of this is afforded by the two isomers MgNC and MgCN in the $\tilde{A}\ ^2\Pi$ electronic state.

Also ABB molecules can exhibit the double Renner effect. In the $\widetilde{X}\ ^2A''$ and $\widetilde{A}\ ^2A'$ electronic states of HOO, the proton orbits the OO moiety with two equivalent minima on each potential surface at bent geometries. At the two linear geometries HOO and OOH (which correspond to maxima on the potential energy surface) the two electronic states are degenerate as a Π state. The two equivalent minima on each surface are separated by a maximum corresponding to a T-shaped geometry.

We have developed a program for calculating the rovibronic energies for a triatomic molecule in 'double-Renner'-degenerate electronic states. Our program can treat both ABC- and ABB-type molecules.

The new program has been applied to $\tilde{A}\ ^2\Pi$ MgNC/MgCN, and to HOO in the $\widetilde{X}\ ^2A''$ and $\widetilde{A}\ ^2A'$ states.

We present detailed analyses of rotation-bending-electronic wavefunctions aimed at providing further insight into the nature of the double-Renner interaction.