

## A VARIATIONAL TREATMENT OF THE RENNER-TELLER EFFECT

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For a triatomic molecule we have developed a rovibronic Hamiltonian that allows for the Renner-Teller effect (i.e., for the effect of electronic angular momentum)<sup>a,b</sup>. The Hamiltonian is based on the MORBID Hamiltonian developed by Jensen<sup>c</sup>, which itself is based on the Hougen-Bunker-Johns Hamiltonian<sup>d</sup>. We determine the eigenfunctions and eigenvalues of this Hamiltonian in a variational manner, and the computer program we have developed is called RENNER; we have used RENNER to calculate the rovibronic energies of CH<sub>2</sub>, CH<sub>2</sub><sup>+</sup>, HO<sub>2</sub> and other molecules. As well as calculating rovibronic energies from potential energy surfaces we are able to calculate intensities from dipole moment surfaces, and we can simulate spectra that involve electronic states subject to the Renner-Teller effect. Although there is a breakdown of the Born-Oppenheimer approximation one can still understand the situation using potential energy curves and dipole moment surfaces, but the shapes of the potential energy curves and dipole moment surfaces depend on the value of the rotational quantum number  $K$ . This will be explained using our results for the CH<sub>2</sub><sup>+</sup> molecule as an example<sup>e</sup>.

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<sup>a</sup>G. Osmann, P. R. Bunker, P. Jensen, R. J. Buenker, J.-P. Gu and G. Hirsch, *J. Mol. Spectrosc.* **197**, 262 (1999), and references therein.

<sup>b</sup>Section 13.4.1 of the book *Molecular Symmetry and Spectroscopy*, 2nd Edition, by P. R. Bunker and P. Jensen, NRC Research Press, Ottawa 1998. See <http://www.nrc.ca/cisti/journals/41653> for the table of contents and ordering information.

<sup>c</sup>P. Jensen, *J. Mol. Spectrosc.* **128**, 478 (1988); **132**, 429 (1988).

<sup>d</sup>J. T. Hougen, P. R. Bunker and J. W. C. Johns, *J. Mol. Spectrosc.* **34**, 136 (1970).

<sup>e</sup>G. Osmann, P. R. Bunker, P. Jensen, and W. P. Kraemer, *Chem. Phys.* **225**, 33 (1997).