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EMPIRICAL POTENTIAL SURFACES FOR THE ELECTRONIC GROUND STATES OF BEOH, C3H+, AND C3H

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Introduction
To simulate molecular spectra we require an analytical, parameterized representation of the potential energy surface (PES) for the particular electronic state of the molecule under study. The PES parameter values can be obtained by least-squares fits of 1. ab initio energies or 2. experimentally derived rovibronic energy spacings.

The experimental data are mostly too limited for the determination of a PES, so we normally use Method (1) to determine initial parameter values and then refine these by Method (2). If the experimental information is too limited for the refinement, we simultaneously fit the experimental and the ab initio energies with an appropriate weighting of the two data types.

For BeOH/BeO, experimental data and ab initio energies are taken from Mascalitolo et al. (2013). For C3H+, the experimental data are compiled by Neele and the ab initio energies are newly calculated at the RCCSD(T)/aug-cc-pVQZ level of theory. Finally, for C3H and its isotopologues, the experimental data are compiled from diverse sources and the ab initio energies are newly calculated at the CCSD(T)/aug-cc-pVQZ level of theory.

Morbid Calculations
We are presently applying the extended Morbid program to obtain PES for the electronic ground states of BeOH (BeOH, HCO), and C3H. In this approach the following analytical expansion for the potential energy function is used:

\[ V(\Delta r_{ij}, \Delta r_{kl}) = \sum \alpha_{ijkl} \phi_{ijkl} \left( \Delta r_{ij} - \Delta r_{ij}^0 \right) \left( \Delta r_{kl} - \Delta r_{kl}^0 \right) \]

\[ (i - 1) \phi_{ijkl} = \text{the quantum of the distance } r_{ij} \text{ between the } i \text{th and } j \text{th nucleus; } (i + 1) \phi_{ijkl} = \text{the other quantum of the same distance.} \]

In order to optimise those in a fitting to a set of experimental data, we use Method (2) to determine initial parameter values and then refine these by Method (1). For the future we hope to further improve the potential energy parameters for HCO by adding the available experimental data of DCO\(^+\) to the input data of the fitting.

Conclusion and Outlook
The work is supported by the Deutsche Forschungsgemeinschaft (Project Ji 247/24-1) and the Japan Research–Wienoch-Bergero, S. Yurchenko, W. Theil, and P. Jensen, J. Mol. Spectrosc. 245, 120-140 (2007).