



Abstract The Superrotor Model for the Rovibrational Motion

Hanno Schmiedt ¹, Stephan Schlemmer ¹ and Per Jensen ^{2,*}

¹ I. Physikalisches Institut, Universität zu Köln, Zülpicher Straße 77, D-50937 Köln, Germany; schmiedt@ph1.uni-koeln.de (H.S.); schlemmer@ph1.uni-koeln.de (S.S.)

of CH⁺₅, an Extremely Flexible Molecule ⁺

- ² Physikalische und Theoretische Chemie, Bergische Universitaet Wuppertal, Gauss-Strasse 20, D-42119 Wuppertal, Germany
- * Correspondence: jensen@uni-wuppertal.de
- Presented at Symmetry 2017—The First International Conference on Symmetry, Barcelona, Spain, 16–18 October 2017.

Published: 3 January 2018

We discuss here the low-energy rotation-vibration problem in CH_5^+ , an extremely flexible molecule lacking a well-defined structure. Using SO(5) symmetry we determine zeroth order energies, and complete nuclear permutation S_5 symmetries, using a five-dimensional model involving rotation and two vibrations (which one might imagine as internal rotations of a 2-protonmoiety relative to a 3-proton-moiety). These two vibrations are presumed to be unhindered by the molecular potential function and their analytical form is not determined. The other ten vibrational degrees of freedom are presumed to be "rigid" (or averaged over). The general energy expression for this "rigid superrotor" is relatively simple and contains one parameter only, the rotational constant B, together with two non-negative integers defining the irreducible representations of SO(5). The superrotor predictions agree favourably with the available experimental data.



© 2018 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (http://creativecommons.org/licenses/by/4.0/).