SYMMETRY IN THE GENERALIZED ROTOR MODEL FOR EXTREMELY FLOPPY MOLECULES

Conference Paper · June 2016

DOI: 10.15278/isms.2016.MF02

3 authors:

Hanno Schmiedt
University of Cologne
10 PUBLICATIONS **17** CITATIONS
SEE PROFILE

Stephan Schlemmer
I. Physikalisches Institut, Universität zu Köln
281 PUBLICATIONS **3,548** CITATIONS
SEE PROFILE

Per Jensen
Bergische Universität Wuppertal
337 PUBLICATIONS **6,814** CITATIONS
SEE PROFILE

SYMMETRY IN THE GENERALIZED ROTOR MODEL FOR EXTREMELY FLOPPY MOLECULES

HANNO SCHMIEDT, *I. Physikalisches Institut, University of Cologne, Cologne, Germany*; PER JENSEN, *Faculty of Mathematics and Natural Sciences, University of Wuppertal, Wuppertal, Germany*; STEPHAN SCHLEMMER, *I. Physikalisches Institut, University of Cologne, Cologne, Germany*.

Protonated methane CH_5^+ is unique: It is an extremely fluxional molecule. All attempts to assign quantum numbers to the high-resolution transitions obtained over the last 20 years have failed because molecular rotation and vibration cannot be separated in the conventional way[ab]. The first step towards a theoretical description is to include internal rotational degrees of freedom into the overall ones, which can be used to formulate a fundamentally new zero order approximation for the (now) generalized rotational states and energies. Predictions from this simple five-dimensional rotor model compare very favorably with the combination differences of protonated methane found in recent low temperature experiments[c]. This talk will focus on symmetry aspects and implications of permutation symmetry for the generalized rotational states. Furthermore, refinements of the theory will be discussed, ranging from the generalization to even higher-dimensional rotors to explicit symmetry breaking and corresponding energy splittings. The latter includes the link to well-known theories of internal rotation dynamics and will show the general validity of the presented theory.

[a] Schmiedt, H., et al.; *J. Chem. Phys.* **143** (15), 154302 (2015)
[b] Wodraszka, R. et al.; *J. Phys. Chem. Lett.* **6**, 4229-4232 (2015)
[c] Asvany, O. et al.; *Science*, **347**, (6228), 1346-1349 (2015)