Microwave spectroscopy of trimethylgermanium iodide: Internal dynamics of a highly flexible molecule

David Schmitz[a], Alvin Shubert[a], Thomas Betz[a], Wolfgang Jäger[b], Melanie Schnell[a]

[a] Center for Free-Electron Laser Science, Hamburg, and Max-Planck-Institut für Kernphysik, Heidelberg
[b] Department of Chemistry, University of Alberta, Edmonton, Alberta T6G 2G2, Canada

The internal rotations of the three methyl groups of trimethylgermanium iodide ((CH3)3GeI) give rise to a complex splitting pattern in its microwave rotational spectrum. The understanding and correct interpretation of this pattern provides information not only about the internal motion, but also about the molecular structure, tunneling pathways, and the electron distribution within the molecule.
This contribution will present the interpretation of our measurements performed with three different microwave spectrometers with different spectral resolutions and covering different frequency regions.
A group-theoretical approach was used to make assignments to the spectra and understand the splitting pattern. Furthermore, ab-initio calculations were performed in order to model the potential energy surface and investigate tunneling pathways. Finally, the results were compared with prior studies on trimethylgermanium chloride ((CH3)3GeCl) [1] and trimethylgermanium bromide ((CH3)3GeBr) [2].

[1] Schnell et al., *Phys. Chem. Chem. Phys.* **2006**, *8*, 2225-31.
[2] Schnell et al., *Chem. Phys.* **2008**, *343*, 121-128.