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Spectroscopic data of methane for astrophysics ROBERT WARMBIER, RALF SCHNEIDER, Max-Planck-Institute for plasmaphysics, AMIT R. SHARMA, BASTIAAN J. BRAAMS, JOEL M. BOWMAN, Emory University, STUART CARTER, University of Reading, PETER H. HAUSCHILDT, Hamburger Sternwarte — Adequate spectroscopic information of small to medium size molecules is a vital part for the understanding of processes in plasma physics and astrophysics. The demands for this information vary in terms of resolution/accuracy, completeness and consistence, depending on the task. While for many molecules experimental and/or theoretical data is available, these do not always fit the prerequisites. We showed for the example of methane (Warmbieret al. A&A 495, 655-661 (2009)) that we can calculate complete and consistent datasets of rovibrational transitions for a large temperature range with a sufficient accuracy for applications like atmospheric radiation transport. We are going to present an improved potential energy surface. The higher accuracy of the rovibrational energies levels allows line-by-line comparisons with experimental data. We will use an improved version of the quantum chemistry code MULTIMODE (publication pending;S. Carter, A. R. Sharma, P. Rosmus, and J.M. Bowman) to test the adiabatic dipole transition moments used before against the full rotational ones. This will offer a generic approach to calculate spectroscopic information of polyatomic molecules fitting a wide range of requirements.

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