Geophysical Research Abstracts
Vol. 13, EGU2011-2378, 2011
EGU General Assembly 2011

Toward a Line List for Methane

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The importance of specific parts of high-resolution, rotational-vibrational spectra of stable small molecules in astronomy, astrochemistry, and astrophysics, as well as in atmospheric studies created a great deal of interest in complete line lists of these molecules (e.g., H2O, NH3, and CH4). Only extremely small parts of line lists can be determined experimentally. Thus, line lists need to be generated synthetically, via complex and sophisticated quantum mechanical procedures. Newly developed quantum chemical techniques are described which allow the ab initio computation and the full assignment of rotational-vibrational states of methane isotopologues. Computed results up to J = 50 are presented for the parent isotopologue via our nearly variational DEWE protocol (DEWE denotes Discrete variable representation of the Eckart-Watson Hamiltonian with an Exact inclusion of a potential energy surface expressed in arbitrary coordinates). Since accuracy of computed data does not match that of the best experiments, line lists should include as much high-quality experimental information as possible. Computed line lists can be improved via our Hamiltonian-free inversion protocol MARVEL (MARVEL stands for Measured Active Rotational-Vibrational Energy Levels). MARVEL results obtained for several water isotopologues highlight the utility of this approach for arbitrary species.