METHANE HIGH-T PARTITION FUNCTION FROM CONTACT TRANSFORMATIONS AND VARIATIONAL CALCULATIONS

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Precise knowledge of methane absorption is often crucial in the study of planetary systems because its spectral features are used to determine the physical properties of these atmospheres. The Total Internal Partition Sum. [1] [2] [3] of methane enables one to calculate a wide range of spectroscopic and thermodynamic characteristics. In our approach, we obtain the partition function from 10-3000K by modelling rovibrational energy levels, by consistently combining, for lower polyads individual levels obtained from exact rovibrational calculations and for higher polyads energy levels from statistical estimations based on extrapolations with appropriate physical approximations. In both cases high order contact transformation Hamiltonian was applied [4] to obtain effective Hamiltonian from potential energy surface [5] [6] To estimate contributions from higher polyads, we fit the average contributions of the polyads to the partition function obtained from exact calculations at a particular temperature at each polyad with a second order polynomial. The values from the polynomial fit are used to make an estimation formula for higher polyad contributions with the power function to good accuracy. The value of Total internal partition sum is compared with previous reports. This work is supported by French-Russian LIA SAMIA and partly the Tomsk State University Academic D.I. Mendeleev Fund Program.

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p-number: p187 **Submitted on Sun Jun 14 19:36:25 CEST 2015**