EQUILIBRIUM MOLECULAR STRUCTURE AND SPECTROSCOPIC PARAMETERS OF METHYL CARBAMATE

J. DEMAISON, *CNRS, Laboratoire PhLAM, Université de Lille 1, F-59655 Villeneuve d'Ascq, France*; A. G. CSÀSZÀR, *Department of Theoretical Chemistry, Eötvös University, P.O. Box 32, H-1518 Budapest 112, Hungary*; V. SZALAY, *Crystal Physics Laboratory, Research Institute for Solid State Physics and Optics, Hungarian Academy of Sciences, P.O.Box 49, H-1525 Budapest, Hungary*; I. KLEINER, *CNRS, Laboratoire Inter-Universitaire des Systèmes Atmosphériques, 61 av Général de Gaulle, 94010 Créteil, Cedex, France*; H. MØLLENDAL, *Department of Chemistry, The University of Oslo, P.O. Box 1033, Blindern, NO-0315 Oslo, Norway*.

A careful analysis of all related experimental and high-level first-principles results yield a reliable estimate of the equilibrium structure of methyl carbamate (MC), $H_2NC(O)OCH_3$, a molecule of biological interest (and for which there are pharmaceutical applications). One goal of this study is to check the predictive power of different quantum chemical methods in prevision of spectroscopic study of larger molecules of biological interest. MC is also of astrobiological interest as its interstellar detection appears plausible since it might be more abundant than glycine, its structural isomer, and its rotational spectrum is more intense. The experimental information used in the present study involves ground-state rotational constants, dipole moments, quadrupole coupling constants and the potential barrier hindering the internal rotation of the methyl group. The first-principles computational results include large basis set geometry optimizations up to the CCSD(T) level, equilibrium dipole moments, quartic force fields used in calculation of equilibrium, vibrationally averaged spectroscopic parameters and the barrier hindering the internal rotation of the methyl group. A special aspect of the geometrical structure of MW which is discussed concerns the planarity of the C(O)NH linkage.