THE MICROWAVE SPECTRUM OF PARTIALLY DEUTERATED SPECIES OF DIMETHYL ETHER[a]

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Dimethyl ether is a molecule of astrophysical interest[b] spectroscopically well characterized.[c] It is one of the simplest molecules with two methyl groups undergoing large amplitude internal rotations. Due to deuterium enrichment in the interstellar medium,[d] one can reasonably expect that partially deuterated species of dimethyl ether might be detected. However, there are no spectroscopic results about the microwave spectrum of such species.

A theoretical calculation of the rotation-torsion energy levels of the partially deuterated species of dimethyl ether has been undertaken aided by *ab initio* calculations. The approach accounts for the complicated torsion-rotation interactions displayed by this molecule and for the fact that deuteration leads to changes of the bidimensional internal rotation effective potential energy surface. Due to zero-point energy contributions from the 19 small amplitude vibrational modes, this surface no longer displays G_{36} symmetry. Rotation-torsion energy levels are computed treating the two angles of internal rotation as active coordinates and evaluating Hamiltonian matrix elements with the help of Gaussian quadrature.[e]

It is hoped that the present results will allow us to understand the microwave spectrum of the mono deuterated species CH_2DOCH_3 which has been recorded in Lille with the new sub millimeter wave spectrometer (150–950 GHz) based on harmonic generation of solid-state sources.

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[b] Snyder, Buhl, and Schwartz, *Astrophys. J. Letters* **191** (1974) L79.

[c] Endres, Drouin, Pearson, Müller, Lewen, Schlemmer, and Giesen, *A&A* **504** (2009) 635.

[d] Solomon and Woolf, *Astrophys. J. Letters* **180** (1973) L89.

[e] Lauvergnat and Nauts, *J. Chem. Phys.* **116** (2002) 8560; and Light and Bačić, *J. Chem. Phys.* **87** (1987) 4008.