THE MICROWAVE SPECTRUM OF PARTIALLY DEUTERATED SPECIES OF DIMETHYL ETHER

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Dimethyl ether is a molecule of astrophysical interest spectroscopically well characterized. It is one of the simplest molecules with two methyl groups undergoing large amplitude internal rotations. Due to deuterium enrichment in the interstellar medium, 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.

It is hoped that the present results will allow us to understand the microwave spectrum of the mono deuterated species CH$_2$DOCH$_3$ 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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