INTERNAL AXIS MOLECULAR PARAMETERS OF METHYL MERCAPTAN-D1

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In this paper an internal axis method Hamiltonian model [1] has been applied to evaluate the torsional-rotational molecular parameters of asymmetrically substituted methyl mercaptan (CH2DSH) using previously observed microwave transitions. The torsional barrier potential functions V1, V2 and V3 have been determined. The observed microwave transition frequencies have also been fitted to an energy expansion model, which allowed accurate predictions of yet unobserved transition frequencies with microwave accuracies. These values are independent of the Hamiltonian model and will prove valuable for astrophysical detection. The results will be discussed in terms of matrix elements between various torsional sub-levels in the ground vibrational state.

[1] M. Liu and C.R. Quade, J. Mol. Spectrosc. 146, 238-251 (1991).