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Highly correlated ab initio calculations of various Monosubstituted Isotopologues of Acetone (CH_3-CO-CH_3)

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Abstract

Explicitly correlated coupled cluster calculations (CCSD(T)-F12) of structural and spectroscopic parameters have been performed for various monosubstituted isotopologues containing ^{18}O, ^{13}C and D of acetone, an astrophysically detected molecule. [1,2] We provide rotational and centrifugal distortion constants. The far infrared region is explored with second order perturbation theory and a variational procedure of reduced dimensionality that take into consideration the interconversion of the nine minima of the potential energy surface. The surface and the parameters of the torsional Hamiltonian were obtained at the CCSD(T)-F12/AVTZ level of theory. The methyl torsional barrier of the main isotopologue was computed to be 245.7 cm^{-1} and varies slightly due to isotopic substitution. In the monodeuterated species, the two inequivalent internal rotors are hindered by barriers of 244.0 cm^{-1} and 244.7 cm^{-1}. The torsional fundamentals of the main variety are localized at 78.636 cm^{-1} (ν_{12}) and 128.904 cm^{-1} (ν_{17}). The gaps between splitting components are lower than 0.02 cm^{-1} and 0.2 cm^{-1} in the main isotopologue and in the varieties containing ^{18}O and ^{13}C, respectively. In the monodeuterated species the subcomponents are separated~15cm^{-1}.

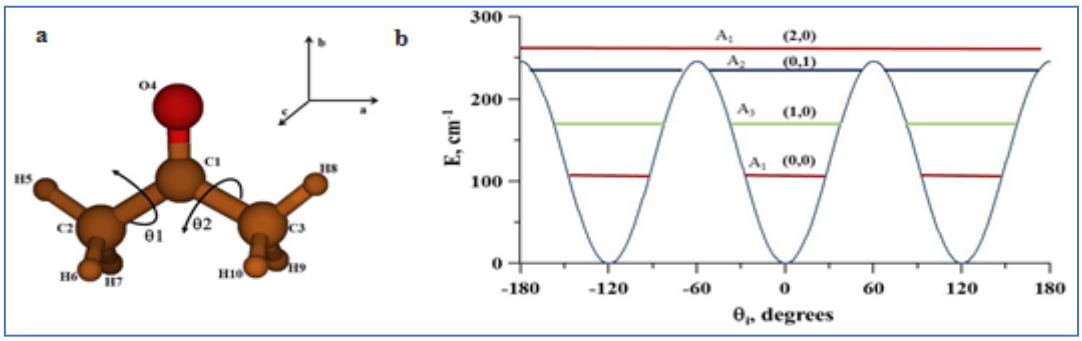

Fig.1: a) The C_{2V} equilibrium structure of acetone and the independent variables θ_1 and θ_2; **b**) non-degenerate torsional energy levels of the main isotopologue (in cm^{-1}).

References

[1] Combes, F.; Gerin, M.; Wootten, A.; Wlodarczak, G.; Clausset, F.; Encrenaz, P. J.; Acetone in interstellar space, Astron. Astrophys, 1987, 180, L13-L16.
[2] Snyder, L.E.; Lovas, F.J.; Mehringer, D.M.; Miao, N.Y., Kuan, Y.-J.; Hollis J.M.; Jewell, P.R.; Confirmation of interstellar acetone, Astrophys. J. 2002, 578, 245-255.