

AB initio calculations applied to the study of organic non-rigid molecules with (at least) three interacting torsional modes.

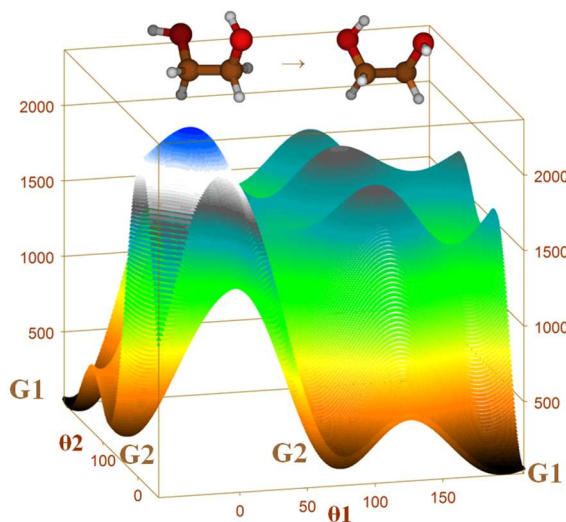
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Methods applicable to the spectroscopic study of non-rigid organic molecular species with various large amplitude motions (torsional or inversion modes), are presented. Recent studies of species containing C, H, O, and N are presented as examples^{a,b,c}.

Many organic molecules display non-rigidity. Vibrational modes of inversion and torsion interconvert different conformers separated by relatively low barriers. Some conformers can be stabilized by the presence of hydrogen intermolecular bonds that can determine their geometry, symmetry and internal dynamics. When a species displays three or more large amplitude motions, which cannot be separated because they interact strongly, the variational calculation of vibrational levels is complex and requires to search how to reduce the computational consuming. Especially tricky is the classification of the vibrational levels and their splittings.



Paths connecting the G1 and G2 conformers of ethylene glycol

References:

^a Weak intramolecular interaction effects on the low temperature spectra of ethylene glycol, an astrophysical species, Boussasi, R.; Senent, M.L.; Jaïdane, N.; J.Chem.Phys., 2016, 144, 164110. <http://dx.doi.org/10.1063/1.4947088>

^b Ab initio study of the large amplitude motions of methoxy-methanol (CH₃-O-CH₂OH), Missaoui, D.; Brahem, S.; Najar, F.; Yazidi, O.; Senent, M.L.; ACS Earth and Space Chemistry, 2024, 8, 1236. <https://doi.org/10.1021/acsearthspacechem.4c00053>

^c Theoretical spectroscopic study of isopropyl alcohol (CH₃-CHOH-CH₃), Salah, M.; Marachi, K.; Komiha, N.; Senent, M.L. Astrophys. J., 2024, 963, 143 -154. <https://doi.org/10.3847/1538-4357/ad1fef>