THE ANALYSIS OF HIGH RESOLUTION SPECTRA OF ASYMMETRICALLY DEUTERATED METHOXY RADICALS CH_2DO AND CHD_2O

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Asymmetric deuteration of methoxy radical reduces the symmetry of normal vibrations, while the electronic wavefunction essentially retains its threefold symmetry. Although the vibrational modes are no longer degenerate, the asymmetry induced by deuteration can be treated as a perturbation and the molecule can still be analyzed using theory similar to that which has been employed for the isotopically symmetric CH_3O and CD_3O. The treatment of the rotationally-resolved spectra of these molecules is especially interesting since the angular momentum is no longer directed along one of the principal inertial axes. We have recently proposed the methods[b] for handling this kind of a problem. This presentation describes the application of these methods to the global analysis of the high resolution data on CH_2DO and CHD_2O radicals, including microwave spectra[c], laser induced fluorescence (LIF) and stimulated emission pumping (SEP) spectra.[d] The analysis of these data along with those existing for the symmetric species[e] provides quantitative insight into the mechanism of Jahn-Teller interaction, spin-orbit interaction, and the effects of deuteration and symmetry reduction on these phenomena.

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[b] D.Melnik, J.Liu, R.F.Curl, and T.A.Miller, *Mol.Physics*, **105**, 529 (2007)

[c] D. Melnik *et al.* 59^{th} International Symposium on Molecular Spectroscopy, **WJ09**, (2004)

[d] J.Liu *et al.* 62^{nd} International Symposium on Molecular Spectroscopy, **RF02**, (2007)

[e] *see preceding talk.*