CONSISTENT ASSIGNMENT OF THE VIBRATIONS OF MONOHALOSUBSTITUTED BENZENES

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When substituted benzenes become a focus of a spectroscopic study there are various well known vibrational labelling schemes present, however it was shown in recent works the description of monohalobenzene vibrations in terms of benzene modes (ie. Wilson notation) is questionable in some cases. A new scheme is presented which uses the motions of monofluorobenzene vibrations as a basis for labelling vibrational assignments of monosubstituted benzenes. The scheme has been successfully applied to the ground and excited states of toluene and its deuterated-methyl group isotopologue. Here we present the application of the scheme to fluorobenzene and its fully deuterated analogue. One-colour resonance-enhanced multiphoton ionization (REMPI) spectroscopy was employed in order to characterise the fluorobenzene and fluorobenzene-d$_5$ excited state.

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