

Photoelectron spectroscopy, a new technique for studying molecular conformations

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The use of carbon 1s photoelectron spectroscopy as a method for determining the conformational distribution of a chemical compound is discussed with application to a series of substituted propenes. The method relies on quantum chemical calculations for predicting shifts in ionisation energies between conformers and vibrational Franck-Condon profiles for the lineshape of photoelectron spectra.