RESONANCE RAMAN STUDIES OF BENZENE DERIVATIVES WITH METHOXY SUBSTITUTION: CONFORMATIONAL SYMMETRY BREAKING EFFECTS

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Resonance Raman intensities show that methoxy substitution induces considerable allowed character to the L_a transition of benzene. In symmetric 1,3,5-trisubstituted benzene derivatives the induced allowed character should cancel by symmetry. However, in 1,3,5-trimethoxybenzene the resonance Raman spectra show a strong fundamental transition of ν_8, the clear signature of an allowed transition. It is shown that this is due the presence of a C_s conformer of 1,3,5-trimethoxybenzene in which one of the three methoxy groups is rotated relative to the other two. This conclusion is supported by ab initio calculations of conformational energies, induced transition moment and the splitting of the ν_8 vibrational band. These results will be compared with those obtained from jet spectroscopy.