

Vibrational Assignment of 1,4-(*E,E*)-Distyrylbenzene Supported by Isotopic Shifts and DFT Calculations

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Isotopic substitution is taking for decades a crucial role in assigning vibrational spectra. Among various possible isotopic substitutions, by far the most important one for vibrational analysis is the substitution of hydrogen (H) by deuterium (D). Theoretical values of vibrational frequencies depend upon force constants determined at the minimum of the adiabatic potential energy surface but this leads to a theoretical ratio of frequencies of XH and XD normal modes that always exceed experimental values, anharmonicity being responsible for a lower value of this ratio.

A model molecule of 1,4-(*E,E*)-distyrylbenzene (DSB, Figure 1.) was chosen to make a rather complex but reliable vibrational analysis. In order to make a thorough assignment of its infrared and Raman spectra, isotopic shifts in vibrational spectra of its isotopologues were investigated.

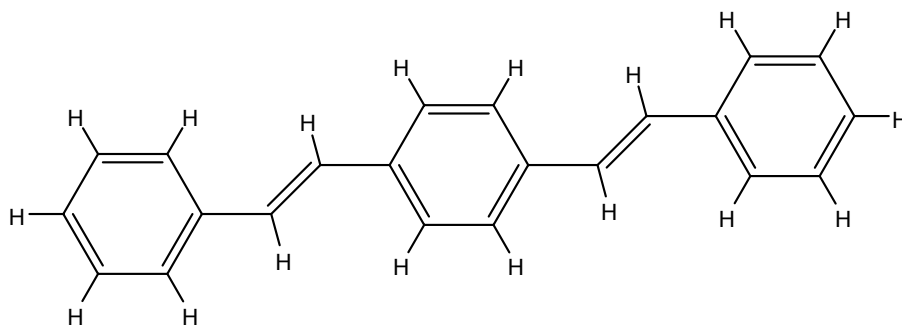


Figure 1: 1,4-(*E,E*)-distyrylbenzene (DSB)

Experimental trends were endorsed by DFT calculations coupled with the Pulay's scaling scheme and using vibrational perturbation theory. Further investigation of potential energy distribution among the normal modes is presented and comparison is made with the spectra of *trans*-stilbene, the precursor of the *para*-phenylenevinylene (PPV) series [1].

[1] T. Hrenar, R. Mitrić, Z. Meić, H. Meier, and U. Stalmach, *J. Mol. Struct.* 661-662 (2003) 33-40.