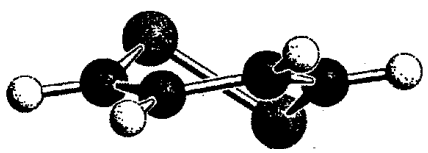
Application of TD-DFT in Calculating UV/Vis Spectral Absorption Data of Sulfur Organic Compounds

Maxime Petiau, Jürgen Fabian*

Institut für Organische Chemie der Technischen Universität Dresden, D-01062 Dresden

Parametrized quantum chemical methods provide useful information about electronic transitions but may seriously fail in some cases. The puckered 1,2-dithiin ($C_4H_4S_2$) (cf. formula below), for example, is predicted as an UV absorber by the semiempirical CNDO/S and ZINDO/S methods and as an infrared absorber by PM3/PECI while this compound is actually red in color.



The position of the "color band" is well reproduced at the CASSCF/CASPT2 level of theory. A similar good result was achieved by the computationally less demanding time-dependent functional theory (TD-DFT). Scope and limitation of TD-DFT (B3LYP/6-31+G*) is demonstrated with a series of organic thiocarbonyls, sulfides and disulfides.