

Theoretical Investigation of Stilbene as Photochromic Spin Coupler

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Abstract

Density functional theory based calculations are used here to investigate the magnetic behavior, spectroscopic transitions and possible photomagnetic properties of stilbene derivatives using photochromicity of *cis*- and *trans*- forms of the parent molecule. Nitronyl nitroxide (NN), iminonitroxide (IN), tetrathiafulvalene cation (TTF) and verdazyl (VER) are used as monoradical centers at p, p' positions. The B3LYP functional with the usual broken symmetry approach and a sufficiently large basis set is chosen to obtain reliable estimates of the *intra*-molecular exchange coupling constants (J). It is found that with stilbene as spacer, the coupling of TTF with NN, IN and VER is always antiferromagnetic with J generally large and negative. Although J values obtained for *cis*- and *trans*- forms are both negative, the difference in J values is quite large. Spectroscopic transition energies and corresponding oscillator strengths of *cis*- and *trans*- stilbene diradicals are estimated by TDDFT calculations using the same functional. Interestingly, the spectral features of the diradicals are similar to those of *cis*- and *trans*- stilbene, which suggests that stilbene diradicals would have good photoswitching properties. Finally, we show that when these diradicals are placed in a matrix, photochromicity would be accompanied by a significant change in paramagnetic susceptibility.

