

Supporting Information

Redox and Photoisomerization Switching of the Second-Order Optical Nonlinearity of a Tetrathiafulvalene Derivative of Spiropyran Across Five States: A DFT Study

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Table S1. Annihilation of the Spin Contaminant for All Open-shell Systems

Compounds	Before	After
² 1-c ^{1e} oxidized	0.7538	0.7500
² 1-o ^{1e} oxidized	0.7577	0.7502
³ 1-c ^{2e} oxidized	2.0176	2.0002
³ 1-o ^{2e} oxidized	2.0480	2.0013

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