Supporting Information

Spectroscopic and Electronic Structure Studies of a DMSO Reductase Caltalytic Intermediate: Implications for Electron and Atom Transfer Reactivity

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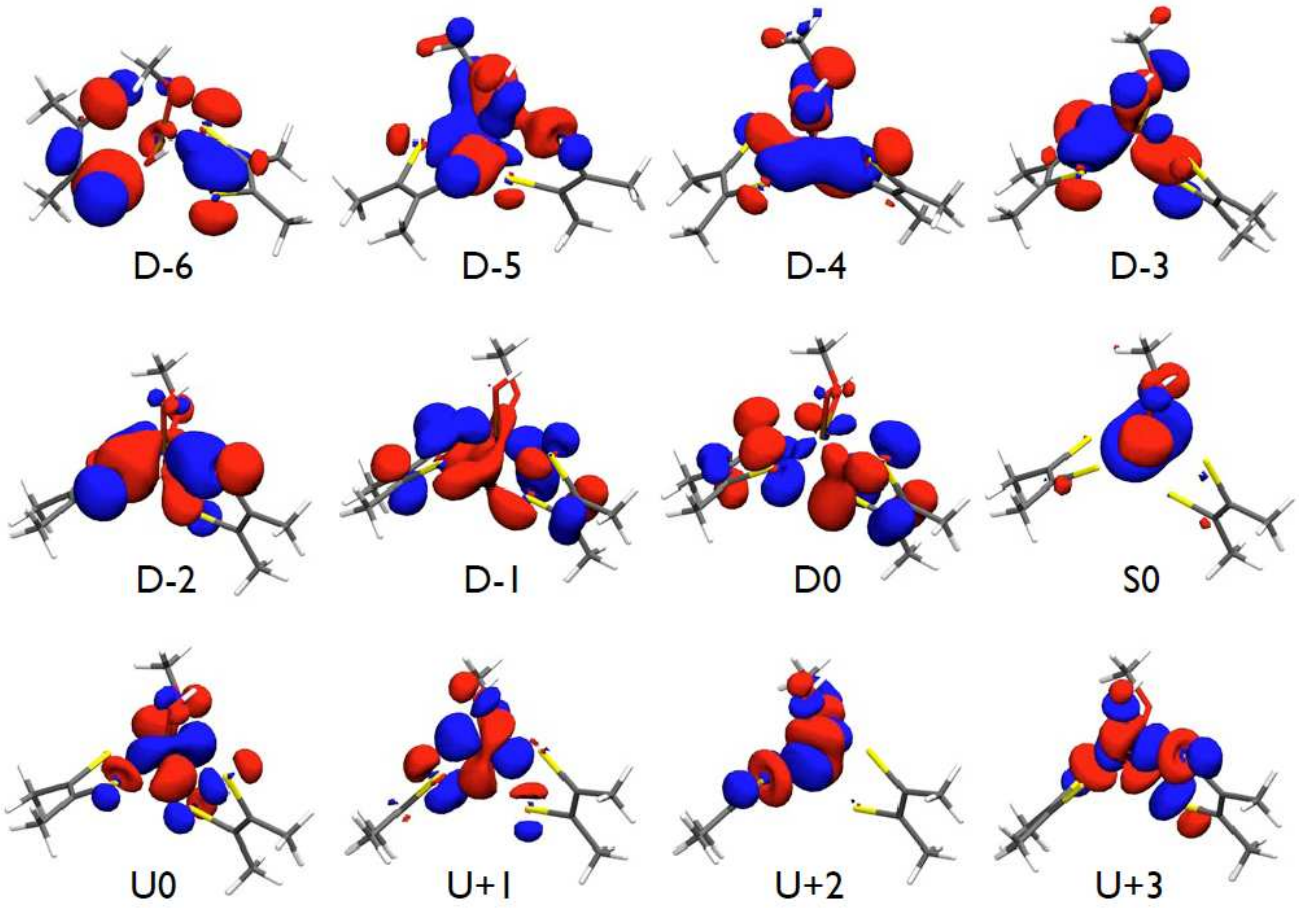
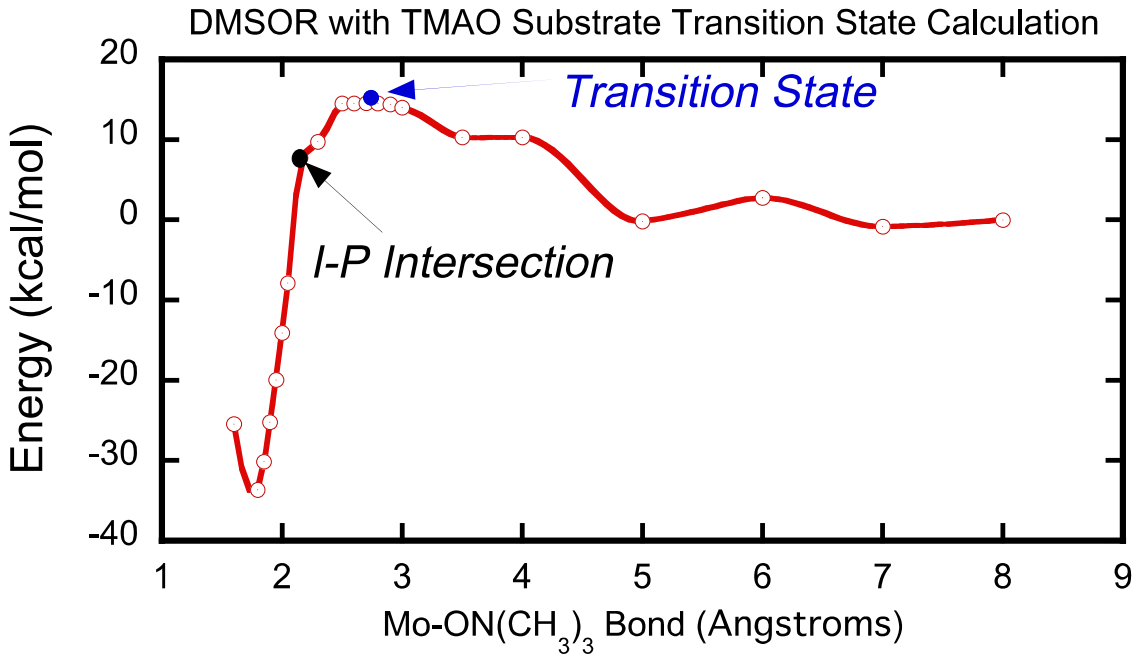
Contents:

S1. Active space orbitals used in SORCI calculations of the electronic absorption and MCD spectra for **1** (D = doubly occupied; S = singly occupied; U = unoccupied). Perspective view is looking down the pseudo 3-fold molecular "z" axis.



S2. Calculated reaction coordinate for DMSOR with TMAO as substrate showing the **TS** and the **I-P** intersection.



S3. C-term intensity for DMSOR intermediate at 5K and 7T.