Supporting Information

Mechanistic Insights and Origin of Chemoselectivity for S–O bond Cleavage in Dinitrobenzenesulfonic Carbamates

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### Table S1.
The ZPE, $\delta$G, E+ZPE, and G of SP (stationary points) at the M06-2X/6-31G (d,p) level in solvent THF using IEFPCM model, E at B2, i.e. M06-2X/6-311+G (d,p) level in solvent THF using IEFPCM model (unit:a.u.) and sole imaginary frequency (unit:icm-1)

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<th>E+ZPE</th>
<th>G</th>
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### Table S2.
NBO charge analyses on TS2R/TS2S, M2 and TS2C

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Cartesian Coordinate for all stationary points

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