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| A DESULFONYLATION PROCESS AS EASY ROUTE FOR SYNTHESIS OF 1,4-DINITRO-1,3-DIENES:  MECHANISTIC STUDY |
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**Supplemental Materials**

**Table S 1:** Optimized geometry for transition state for decomposition reaction of 2,5-dinitro-3,4-dimethyl-thiolene 1,1-dioxides 1a in gas phase according to B3LYP/6-31G(d) calculations.

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Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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1 6 0 1.388720 -0.867249 -0.145696

2 6 0 1.348121 0.025354 0.947484

3 6 0 2.654626 0.520708 1.527638

4 1 0 3.254147 -0.319617 1.895759

5 1 0 3.253448 1.046046 0.772767

6 1 0 2.485864 1.198915 2.366325

7 6 0 2.742430 -1.351165 -0.631254

8 1 0 3.236781 -1.936182 0.153270

9 1 0 2.645169 -1.999066 -1.504464

10 1 0 3.407226 -0.518150 -0.889017

11 6 0 0.324514 -1.029366 -1.055191

12 1 0 0.586037 -1.396717 -2.044228

13 6 0 0.200692 0.772344 1.280457

14 1 0 0.317860 1.710613 1.813207

15 7 0 -1.046858 -1.582006 -0.778973

16 8 0 -2.031717 -0.863021 -0.778071

17 8 0 -1.031339 -2.801588 -0.681643

18 7 0 -1.086753 0.179885 1.674181

19 8 0 -1.136748 -1.040878 1.826936

20 8 0 -1.998354 0.970783 1.894387

21 16 0 -0.213127 1.348574 -1.007552

22 8 0 1.058672 1.992821 -1.375389

23 8 0 -1.459995 1.995390 -1.417454

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**Table S 2:** Optimized geometry for transition state for decomposition reaction of 2,5-dinitro-3,4-dimethyl-thiolene 1,1-dioxides 1b in gas phase according to B3LYP/6-31G(d) calculations.

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Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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1 6 0 0.808532 1.186290 0.317531

2 6 0 -0.496583 1.597523 -0.018746

3 6 0 -0.697695 2.943819 -0.682807

4 1 0 -1.710281 3.043706 -1.079800

5 1 0 -0.554937 3.750260 0.048261

6 1 0 0.012807 3.114089 -1.498786

7 6 0 1.959300 2.143114 0.095492

8 1 0 1.691692 3.131940 0.479405

9 1 0 2.870747 1.814689 0.593372

10 1 0 2.189525 2.246137 -0.971319

11 6 0 1.019853 -0.168512 0.645267

12 6 0 -1.596158 0.699946 -0.096598

13 1 0 -2.433735 0.975546 -0.729040

14 7 0 -2.162232 -0.057129 1.045395

15 8 0 -1.487458 -0.227552 2.062072

16 8 0 -3.314812 -0.445718 0.888293

17 16 0 -0.476505 -1.055097 -1.067710

18 8 0 -0.090854 -0.595390 -2.405714

19 8 0 -1.105277 -2.366894 -0.892404

20 7 0 2.358494 -0.760181 0.574899

21 8 0 3.096830 -0.429669 -0.353420

22 8 0 2.625754 -1.583028 1.448890

23 1 0 0.407471 -0.700708 1.356637

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