## Electronic Supplementary Information

# Unexpected rearrangement of phenoxypicramide to 1,3-dinitro-10*H*-phenoxazine

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**Figure S1a.** [1]H-NMR spectrum of 1,3-dinitro-10*H*-phenoxazine.

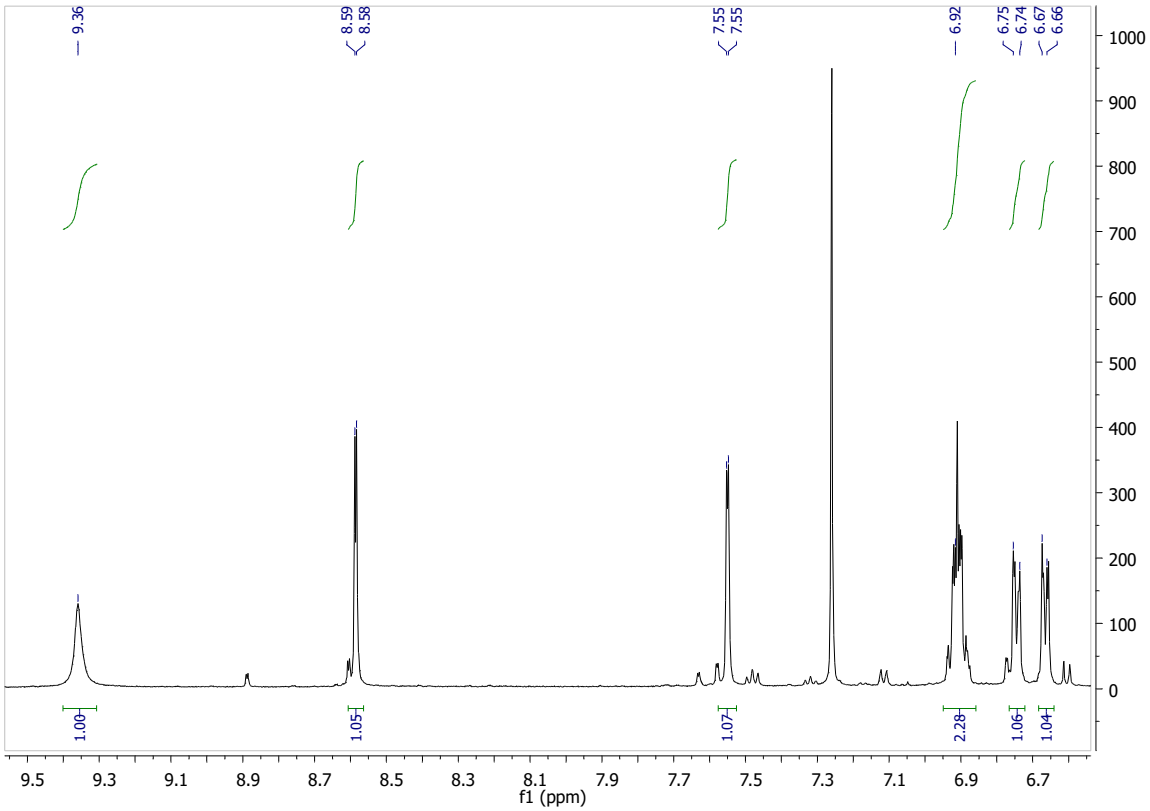


**Figure S1b.** [13]C-NMR spectrum of 1,3-dinitro-10*H*-phenoxazine.

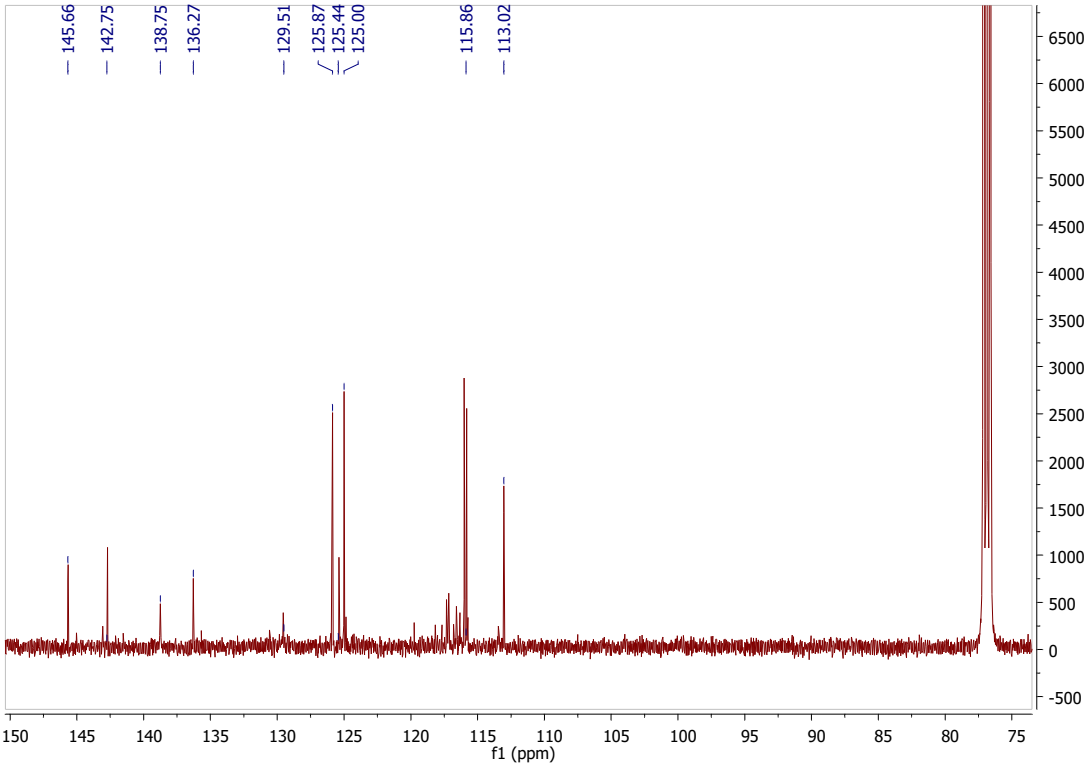


**Figure S1c.** IR spectrum of 1,3-dinitro-10*H*-phenoxazine

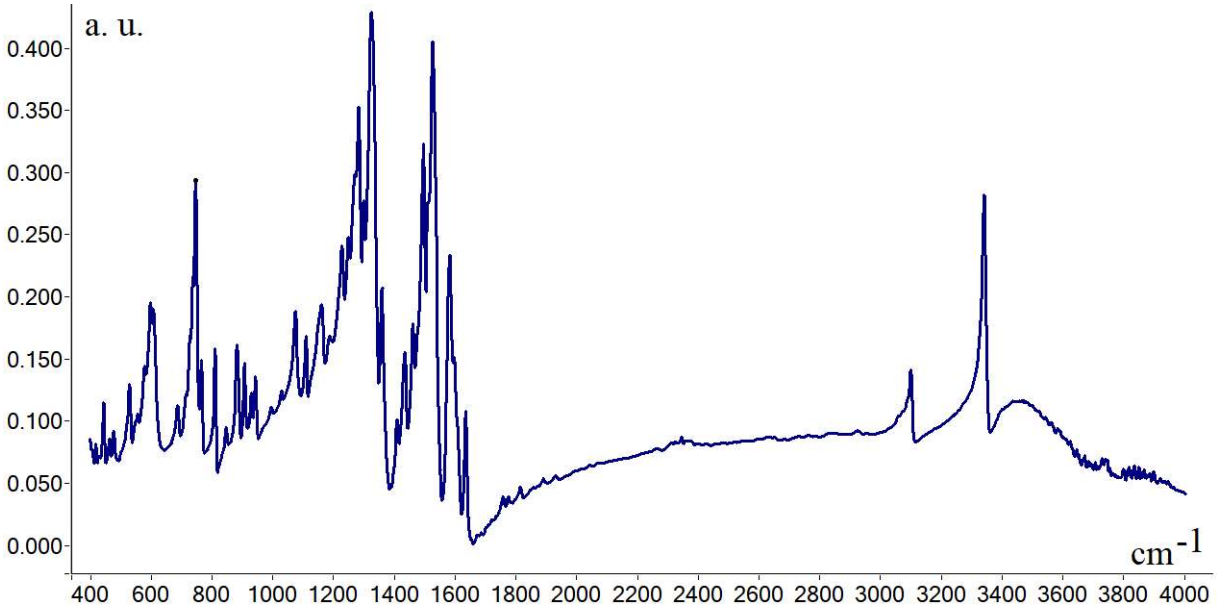


**Figure S1d.** ESI-MS spectrum of 1,3-dinitro-10*H*-phenoxazine.

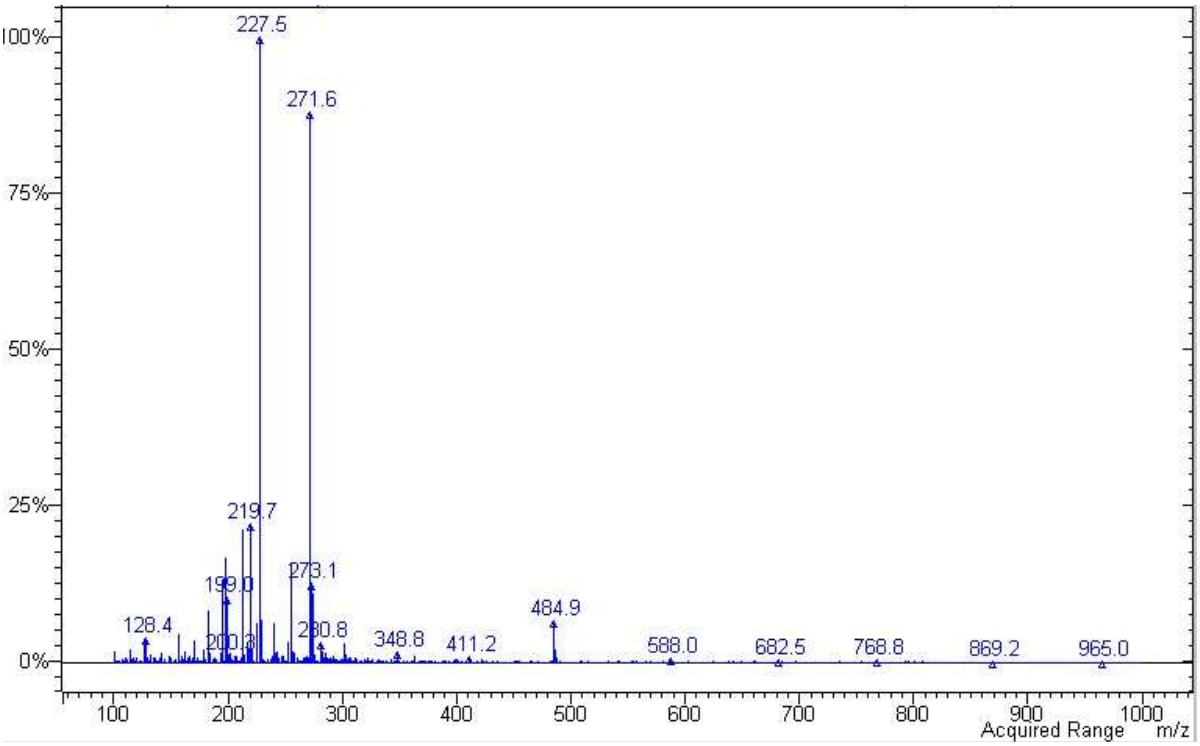


**Figure S2.** UV-Vis spectrum of 1,3-dinitro-10*H*-phenoxazine.

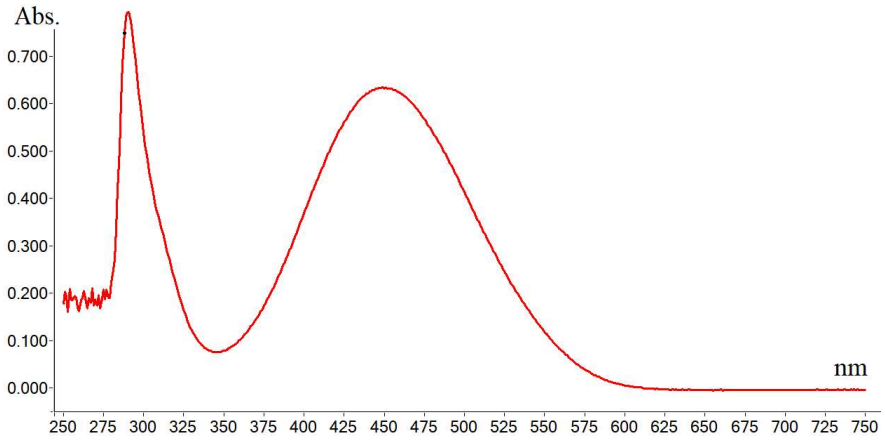


**Figure S3a.** Crystal packing for 1,3-dinitro-10*H*-phenoxazine along *a*, *b* and *c* axes.

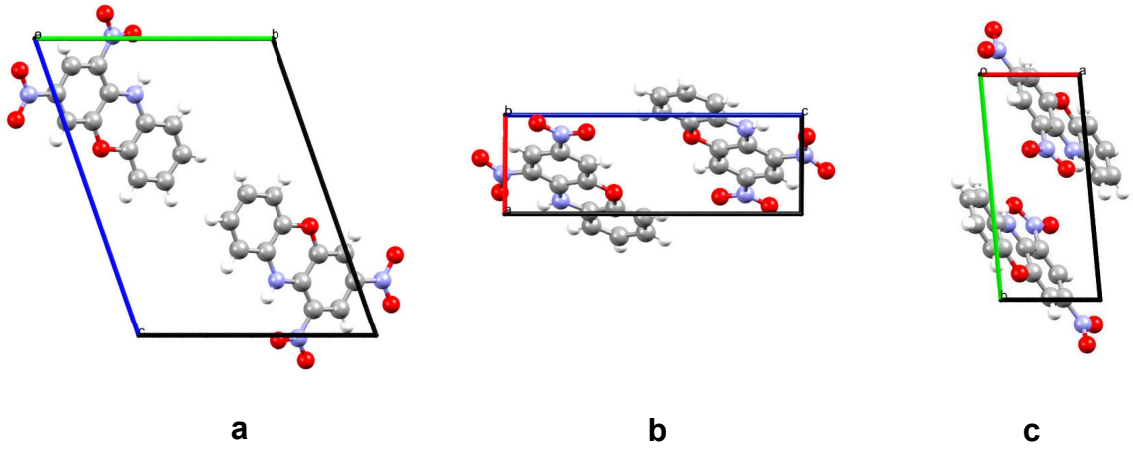


**Figure S3b.** Molecular structure details**.**

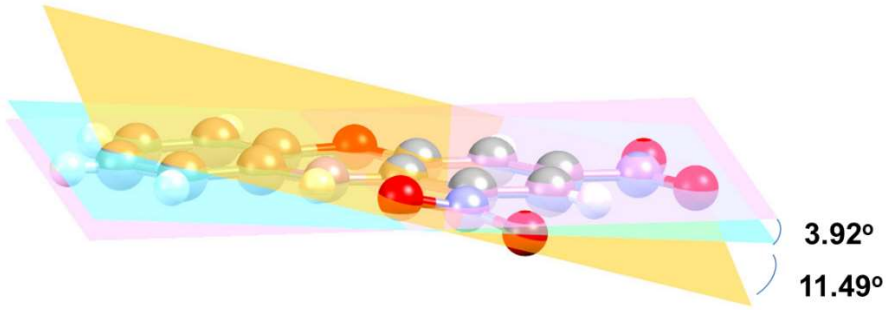

**Figure S4.** Simulation (in red) of the experimental ESR spectrum of 1,3-dinitro-10*H*-phenoxazinyl free radical (in blue).

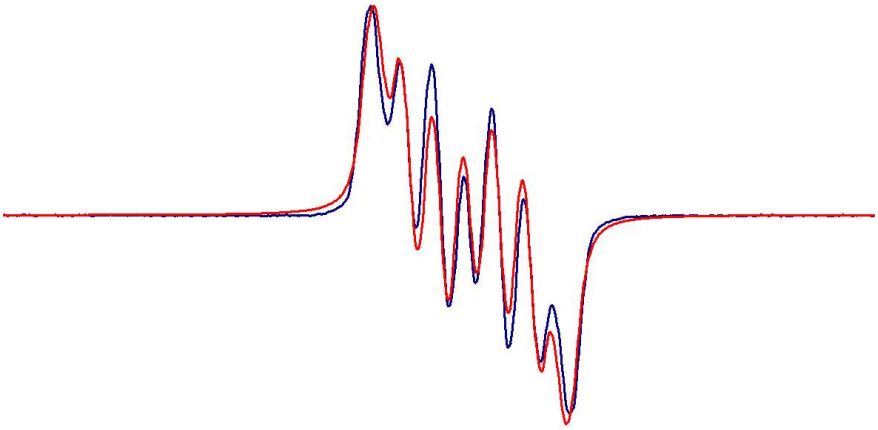

**Table S1.** Selected bond lengths (Å) and angles (°)**.**

| Bond lengths, (Å) | | Bond angles, (°) | |
|---|---|---|---|
| O1-C5 | 1.389(2) | C5-O1-C8 | 119.36(12) |
| O1-C8 | 1.369(2) | C6-N1-C7 | 121.77(12) |
| O2-N2 | 1.2218(18) | O2-N2-O3 | 123.61(17) |
| O3-N2 | 1.219(2) | O2-N2-C10 | 117.78(17) |
| O4-N3 | 1.218(2) | O3-N2-C10 | 118.60(13) |
| O5-N3 | 1.242(2) | O4-N3-O5 | 122.48(12) |
| N1-C6 | 1.403(2) | O4-N3-C12 | 119.32(15) |
| N1-C7 | 1.352(2) | O5-N3-C12 | 118.19(14) |
| N-C10 | 1.456(2) | C2-C1-C6 | 119.78(15) |
| N3-C12 | 1.4496(18) | C1-C2-C3 | 120.6(2) |
| C1-C2 | 1.385(3) | C2-C3-C4 | 119.7(2) |
| C1-C6 | 1.378(3) | C3-C4-C5 | 119.61(16) |
| C2-C3 | 1.382(2) | O1-C5-C4 | 118.15(14) |
| C3-C4 | 1.379(3) | O1-C5-C6 | 120.43(16) |
| C4-C5 | 1.366(3) | C4-C5 C6 | 121.42(18) |
| C5-C6 | 1.391(2) | N1-C6-C1 | 122.20(13) |
| C7-C8 | 1.4298(19) | N1-C6-C5 | 118.90(17) |
| C7-C12 | 1.412(2) | C1-C6-C5 | 118.90(17) |
| C8-C9 | 1.358(3) | N1-C7-C8 | 118.15(15) |
| C9-C10 | 1.396(3) | N1-C7-C12 | 126.34(13) |
| C10-C11 | 1.368(2) | C8-C7-C12 | 115.51(15) |

| | | | |
|---|---|---|---|
| C11-C12 | 1.393(2) | O1-C8-C7 | 120.97(16) |
| | | O1-C8-C9 | 116.89(13) |
| | | C7-C8-C9 | 122.12(16) |
| | | C8-C9-C10 | 119.53(14) |
| | | N2-C10-C9 | 118.78(13) |
| | | N2-C10-C11 | 119.49(17) |
| | | C9-C10-C11 | 121.72(17) |
| | | C10-C11-C12 | 118.31(17) |
| | | N3-C12-C7 | 120.80(15) |
| | | N3-C12-C11 | 116.40(15) |
| | | C7-C12-C11 | 122.81(13) |

**References**

1. Sheldrick, G. M. *Acta Cryst*., 2008, *A64*, 112-122.

2. Crystal Structure Analysis Package, CrystalStructure 4.2. Rigaku Corporation (2000-2015), Tokyo 196-8666, Japan.