Synthesis and Kinetics of sterically altered Photochromic Dithizonatomercury Complexes

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Supporting Information

Table S1. Rates of the spontaneous back reaction of (4-OPh)DPM in various solvents at 10 °C.

Solvent	Rate (s^{-1})	Molar mass ($g.mol^{-1}$)	Dielectric constant (ε)	Dipole moment (D)	$\lambda_{blue\ isomer}$ (nm)
Acetone	0.069	58.08	20.7	2.88	610
THF	0.044	72.11	7.6	1.75	606
DCM	0.032	84.93	8.9	1.60	604
Diethylether	0.015	74.12	4.3	1.15	608
Chloroform	0.013	119.38	4.8	1.04	602
Toluene	0.009	92.14	2.4	0.36	615

Table S2. Crystal data and Refinement parameters of structures (2-OPh)NF and (4-OPh)NF. (NF - Nitroformazan)

Compound	**(2-OPh)NF**	**(4-OPh)NF**
Empirical formula	$C_{25}H_{19}N_5O_4$	$C_{25}H_{19}N_5O_4$
Formula weight	453.45	453.45
Temperature	100 (2) K	100 (2) K
Wavelength	0.71073 Å	0.71073 Å
Crystal system	Monoclinic	Monoclinic
Space group	$P2_1/c$	$P2_1/c$
Unit cell dimensions	a = 13.701(3) Å, b = 6.4469(13)Å, c = 25.367(5) Å α = 90, β = 102.51(3), γ = 90.0°	a = 16.689 (3) Å, b = 10.481 (2) Å, c = 26.364 (5) Å α = 90, β = 102.917(7), γ= 90.0°
Volume	2187.4(8) $Å^3$	4494.9 (16) $Å^3$
Z	4	8
Density (calculated)	1.374 Mg m^{-3}	1.340 Mg m^{-3}
Absorption coefficient	0.094 mm^{-1}	0.094 mm^{-1}
F(000)	944	1888.0
Crystal colour	Orange red	Orange red
Crystal size	0.465 × 0.304 × 0.212 mm	0.756 x 0.540 x 0.464 mm
Theta range for data	3.133 to 26.999 º	1.252 to 26.998 º
Theta range for data collection	h = −17→17, k = −8→8, l = −32→32	h = −21→21, k = −13→13, l = −33→33
Index ranges		
Reflections collected	52922	105962
Independent reflections	4753 [R(int) = 0.1541]	9819 [R(int) = 0.1142]
Absorption correction	multi-scan	multi-scan
Max. and min. Transition	0.964 and 0.960	0.957 and 0.941
Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Data/restraints/parameters	4753 / 12 / 318	9819 / 0 / 613
Goodness of fit on F^2	1.126	1.030
Final R indices[I > 2sigma(I)]	R_1 = 0.1140, wR_2 = 0.3000	R_1 = 0.0672, wR_2 = 0.1710
R indices (all data)	R_1 = 0.1896, wR_2 = 0.3671	R_1 = 0.0852, wR_2 = 0.1846
Extinction coefficient	0.001(2)	n/a
Largest diff. peak and hole	1.000 e.$Å^{-3}$ and −0.676 e.$Å^{-3}$	0.373 e.$Å^{-3}$ and −0.288 e.$Å^{-3}$

Table S3. Selected bond lengths (Å)

Parameters	(2-OPh)NF	(4-OPh)NF	(4-OMe)NF[1]
N1-N2	1.296(5)	1.297(2)	1.300(2)
N3-N4	1.279(5)	1.297(3)	1.290(2)
C1-N2	1.316(5)	1.332(2)	1.325(1)
C1-N3	1.359(6)	1.348(3)	1.356(2)
C1-N5	1.461(6)	1.472(3)	1.468(2)
O1-N5	1.238(6)	1.219(3)	1.234(1)
O2-N5	1.198(5)	1.216(3)	1.229(2)

Table S4. Selected bond angles (°)

Parameters	(2-OPh) NF	(4-OPh) NF	(4-OMe)NF
N1-N2-C1	118.0(4)	115.4(2)	117.7(1)
N4-N3-C1	114.4(3)	114.0(2)	114.2(1)
N2-N1-C2	115.4(3)	120.6(2)	117.1(1)
N3-N4-C14	117.1(3)	117.8(2)	115.3(1)
N2-C1-N3	133.8(3)	134.0(1)	134.1(1)
O1-N5-C1	117.5(4)	118.2(2)	118.2(1)
O1-N5-O2	122.5(4)	123.9(2)	123.5(1)
O2-N5-C1	119.9(4)	117.9(2)	118.3(1)
C5-O3-C8	118.7(3)	121.7(2)	117.4(1)
C17-O4-C20	116.3(3)	116.3(2)	116.8(1)

Table S5. Selected torsion angles (°)

Parameters	(2-OPh)NF	(4-OPh)NF	(4-OMe)NF
O1-N5-C1-N2	-14.8(6)	-18.8(3)	14.1(2)
N5-C1-N2-N1	-176.9(3)	-178.8(2)	178.1(1)
C1-N2-N1-C2	-177.0(4)	-173.6(2)	171.5(1)
N2-N1-C2-C3	32.3(4)	2.6(2)	17.6(1)
C13-O3-C20-C21	113.1(3)	50.6(2)	-
N3-N4-C8-C9	7.7(6)	166.8(3)	6.3(2)
C7-O4-C14-C15	64.3(5)	-93.0(3)	-

[1] K. G. von Eschwege, F. Muller and T. N. Hill, *Acta Cryst.* (2012) **E68**, o609.

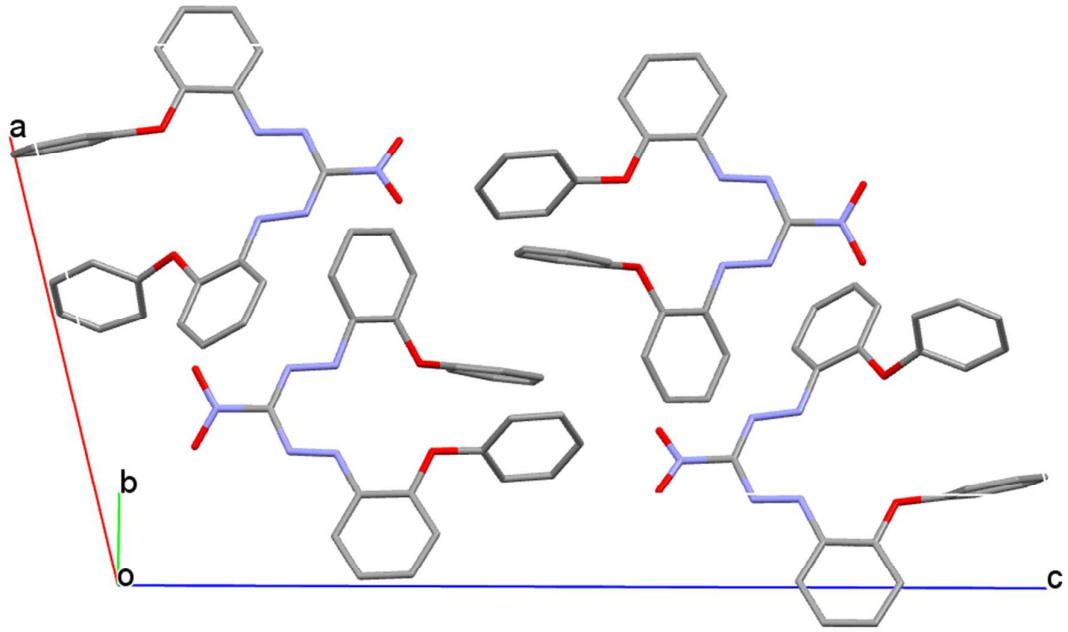

Figure S1. Crystal packing diagram of 2-phenoxynitroformazan. Grey = C, Blue = N, Red = O.

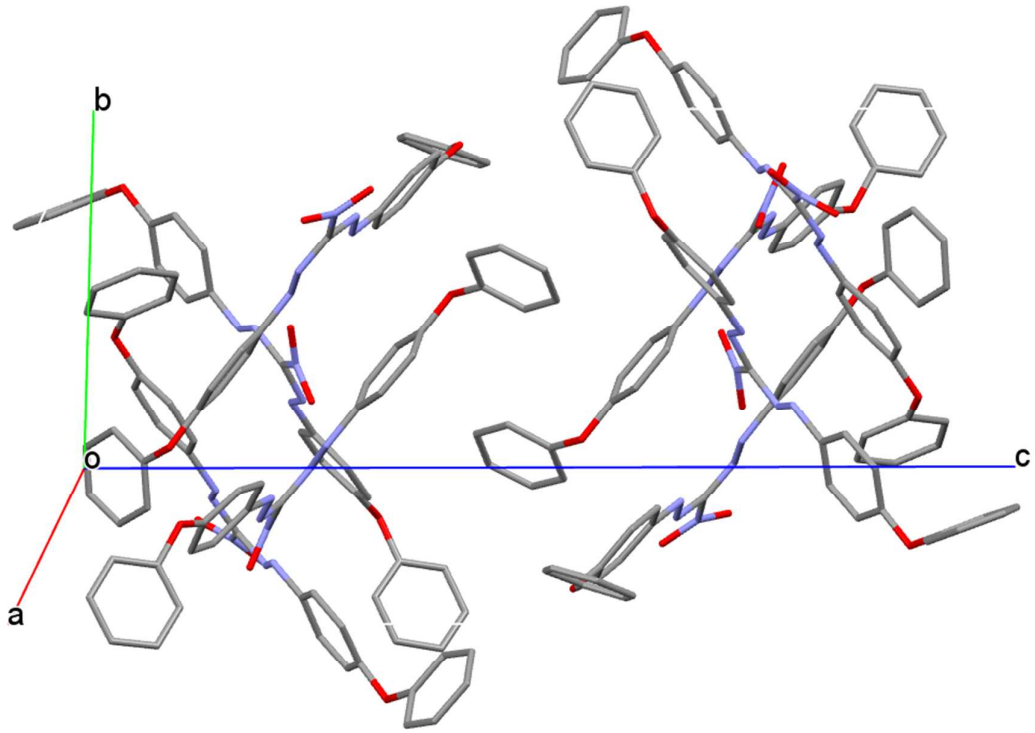

Figure S2. Crystal packing diagram of 4-phenoxynitroformazan. Grey = C, Blue = N, Red = O.