Electronic Supplementary Material (ESI) for CrystEngComm.

SUPPORTING INFORMATION

Thermal and Photochemical Control of Nitro-Nitrito Linkage Isomerism in Single-Crystals of [Ni(medpt)(NO_2)(η^2-ONO)]

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Table S1: Single-crystal X-ray data for the room temperature structure of **1**

Temperature	100(2) K
Radiation source	Mo K_α
Wavelength	0.71073 Å
Empirical formula	C7 H19 N5 Ni1 O4
Formula weight	443.97
Crystal size	0.50 x 0.40 x 0.10 mm^3
Crystal system	Monoclinic
Space group	$P2_1/m$
Unit cell dimensions	a = 7.235(5) Å b = 23.768(5) Å β = 103.920(5)° c = 11.072(5) Å
Volume	1848(2) $Å^3$
Z	6
Density (calculated)	1.596 M g m^{-3}
Absorption coeff. μ	1.588 mm^{-1}
F(000)	936
R(int)	0.0265
R1 (obs. data)	0.0305
wR2 (all data)	0.0724
Reflections (indep.)	5760

Hydrogen Bonding Tables

(i) Ground state nitro-(η^1-NO_2) isomer

Table S2: Intermolecular hydrogen bonding data for the slow cooled GS structure of **1** at 100 K

	(D-H) / Å	**(H...A) / Å**	**(D...A) / Å**	**<(DHA) / °**
N(5)-H(5D)...O(11) #1	0.92(2)	2.19(2)	3.06(1)	157(3)
N(5)-H(5C)...O(3) #2	0.92(2)	2.19(2)	3.01(1)	148(3)

Symmetry operations for equivalent atoms: **#1 =** x,-y+1/2,z ; **#2 =** -x,-y,-z+2

(ii) Metastable structure

TableS3: Intermolecular hydrogen bonding data for the metastable structure of **1** at 100 K

	(D-H) / Å	**(H...A) / Å**	**(D...A) / Å**	**<(DHA) / °**
N(23)-H(23D)...O(2A) #1	0.92(2)	2.56(2)	3.19(1)	126(3)
N(5)-H(5C)...O(22A) #2	0.92(2)	2.65(2)	3.29(1)	127(3)
N(23)-H(23C)...O(11)	0.92(2)	2.28(2)	3.15(1)	159(3)

N(5)-H(5D)...O(12)	0.92(2)	2.13(2)	3.00(1)	157(3)
N(23)-H(23C)...O(12A)	0.92(2)	2.08(2)	2.96(1)	159(3)
N(23)-H(23D)...O(4) #1	0.92(2)	2.22(2)	3.05(1)	150(3)
N(5)-H(5C)...O(23) #2	0.92(2)	2.17(2)	3.01(1)	151(3)

Symmetry operations for equivalent atoms: **#1 =** -x, y+1/2, -z; **#2 =** -x, y-1/2, -z

Solid State UV/vis Absorption Spectrum of 1

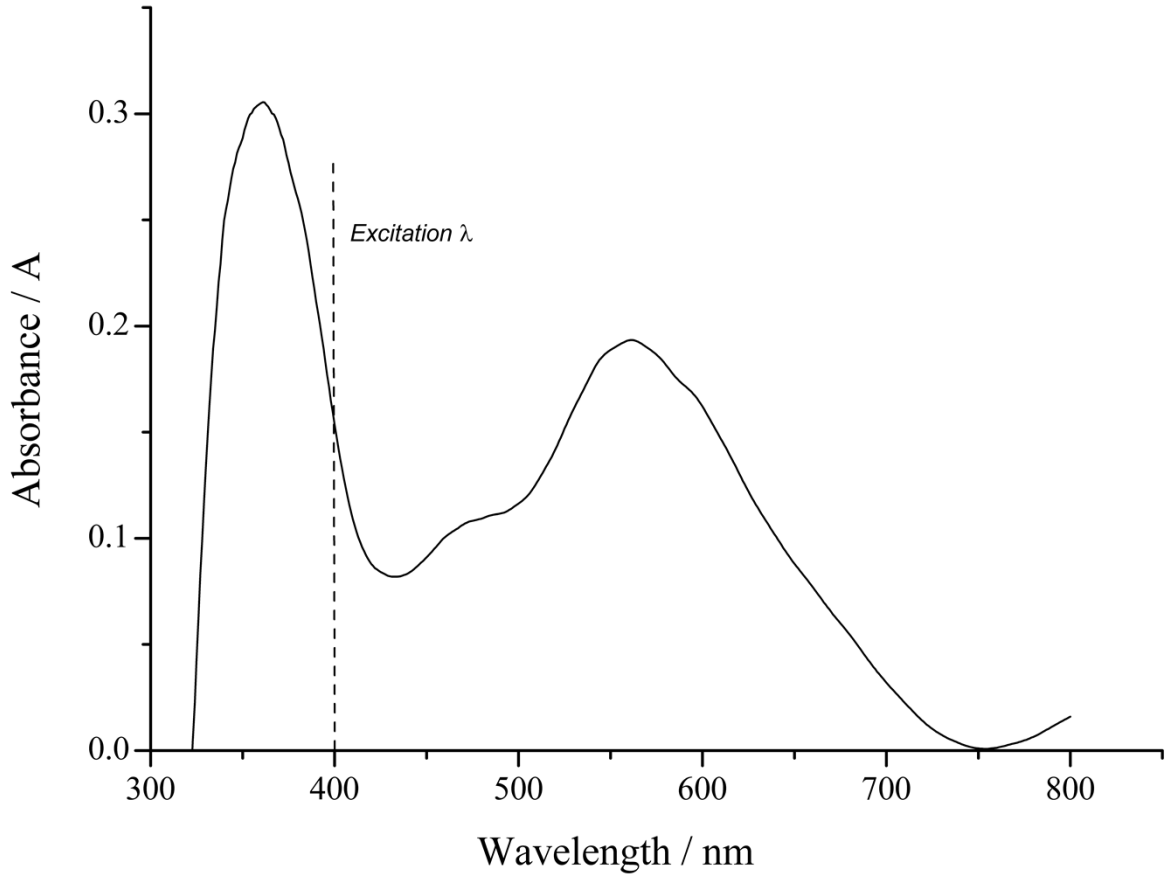
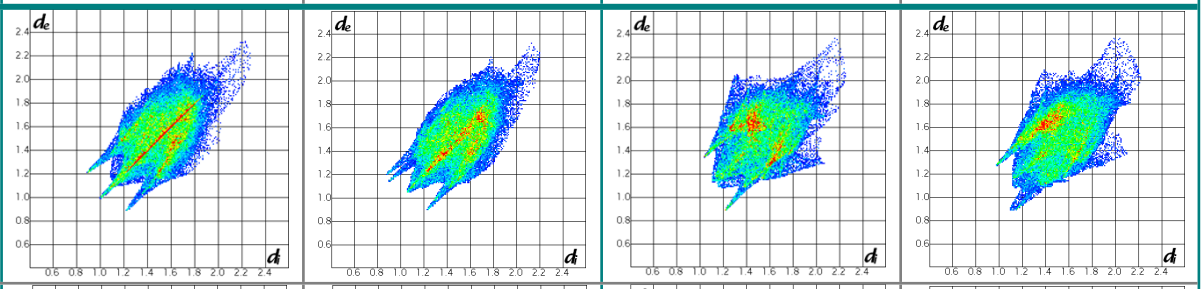
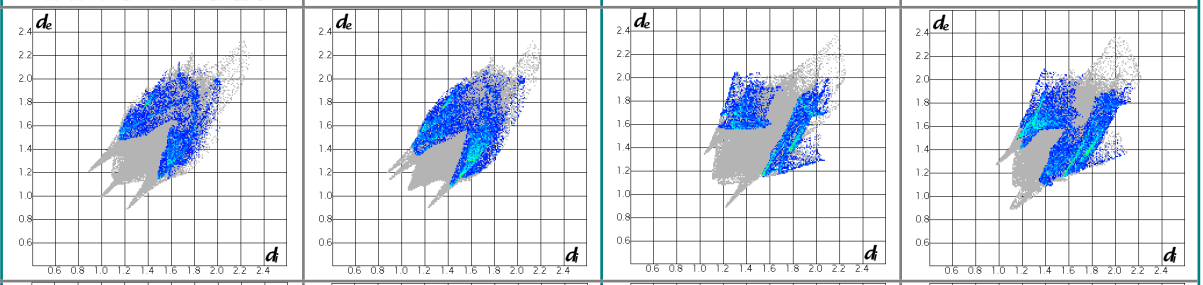
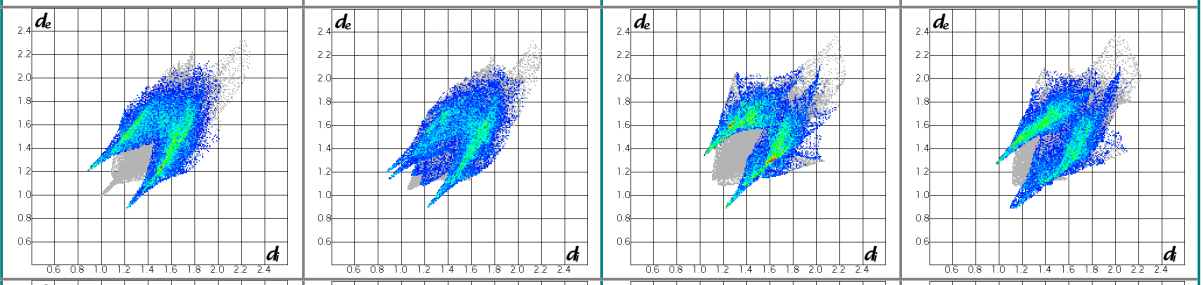


Figure S1: Solid state UV/vis spectrum for complex **1**, showing the choice of excitation wavelength

Table S4: Crystal Explorer fingerprint plots showing changes in intermolecular interactions on photoactivation of **1**

	Molecule A		Molecule B	
	GS	400 nm MS	GS	400 nm MS
All contacts				
N...H contacts				
O…H contacts				
H…H contacts