

Supporting information

Nitric oxide release and related light-induced cytotoxicity of ruthenium nitrosyls with coordinated nicotinate derivatives

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Table S1. Crystal data and refinement details.

Identification code	[RuNO(Et-nic) ₂ (NO ₂) ₂ OH] (I)	[RuNO(Me-nic) ₂ (NO ₂) ₂ OH] (II)	[RuNO(Et-nic) ₂ (NO ₂) ₂ OH] (III)
Empirical formula	C ₁₆ H ₁₉ N ₅ O ₁₀ Ru	C ₁₄ H ₁₅ N ₅ O ₁₀ Ru	C ₂₀ H ₁₀ N ₅ O ₁₀ Ru
Formula weight	542.43	514.38	581.4
Temperature/K	150	150	150
Crystal system	orthorhombic	monoclinic	monoclinic
Space group	Pbca	P2 ₁ /c	Cc
a/Å	12.8083(5)	10.3004(9)	10.5495(12)
b/Å	15.1963(6)	16.2916(12)	17.8137(18)
c/Å	21.7231(9)	11.4935(9)	11.4884(19)
α/°	90	90	90
β/°	90	94.844(3)	96.879(3)
γ/°	90	90	90
Volume/Å ³	4228.2(3)	1921.8(3)	2143.4(5)
Z	8	4	4
ρ _{calc} /cm ³	1.704	1.778	1.802
μ/mm ⁻¹	0.806	0.881	0.802
F(000)	2192	1032	1156
Crystal size/mm ³	0.04 × 0.05 × 0.24	0.04 × 0.04 × 0.08	0.01 × 0.02 × 0.10
Radiation	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)

2 θ range for data collection/ $^{\circ}$	3.75 to 72.652	3.968 to 64.244	4.512 to 52.754
Index ranges	$-20 \leq h \leq 21, -24 \leq k \leq 24, -35 \leq l \leq 36$	$-15 \leq h \leq 13, -24 \leq k \leq 24, -16 \leq l \leq 15$	$-13 \leq h \leq 12, -22 \leq k \leq 21, -14 \leq l \leq 14$
Reflections collected	158947	24070	13119
Independent reflections	9852 [$R_{\text{int}} = 0.0760, R_{\text{sigma}} = 0.0364$]	6065 [$R_{\text{int}} = 0.0487, R_{\text{sigma}} = 0.0505$]	3874 [$R_{\text{int}} = 0.0789, R_{\text{sigma}} = 0.0847$]
Data/restraints/parameters	9852/0/292	6065/0/274	3874/2/292
Goodness-of-fit on F^2	1.078	1.053	1.051
Final R indexes [$I \geq 2\sigma(I)$]	$R_1 = 0.0424, wR_2 = 0.1035$	$R_1 = 0.0350, wR_2 = 0.0753$	$R_1 = 0.0432, wR_2 = 0.0841$
Final R indexes [all data]	$R_1 = 0.0696, wR_2 = 0.1158$	$R_1 = 0.0490, wR_2 = 0.0834$	$R_1 = 0.0675, wR_2 = 0.1041$
Largest diff. peak/hole / $e \text{ \AA}^{-3}$	0.63/-1.41	0.47/-0.64	0.84/-0.56
Flack parameter	-	-	0.43(4)

Table S2. Selected bond lengths and angles of **(I)**, **(II)** and $[\text{RuNO}(\text{Et-nic})_2(\text{NO}_2)_2\text{OH}]$ crystallized in Cc (**(I)'**).

Bond/angle	(I)	(II)	(I)'
Ru-NO	1.767(2)	1.762(2)	1.750(8)
N-O	1.150(2)	1.150(3)	1.15(1)
Ru-OH	1.910(2)	1.933(2)	1.930(6)
Ru-NO ₂	2.069(2); 2.072(2)	2.061(2); 2.080(2)	2.071(9); 2.075(9)
Ru-N _{nic}	2.122(2); 2.123(2)	2.113(2); 2.131(2)	2.12(1); 2.12(1)
Ru-N-O	173.4(2)	171.0(2)	170.4(8)
HO-Ru-NO ₂	89.1(1); 89.5(1)	88.1(1); 86.7(1)	87.6(3); 88.3(3)
HO-Ru-N _{nic}	86.6(1); 86.8(1)	87.2(7); 85.7(1)	85.9(3); 87.2(3)

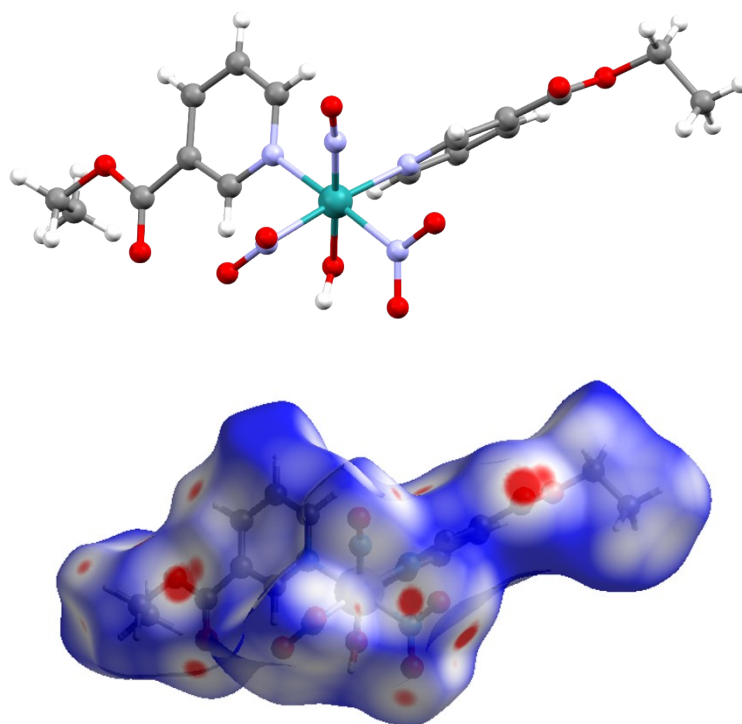


Fig. S1. Three-dimensional Hirshfeld surface map of **(I)**, generated for the whole intermolecular interactions. The red areas show the most pronounced interactions, where the strongest are formed by the oxygen atoms of nitrites and ether groups.

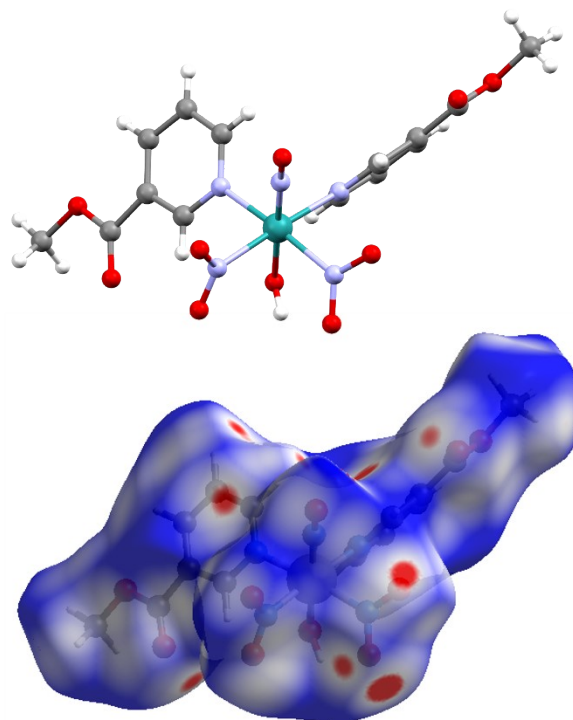


Fig. S2. Three-dimensional Hirshfeld surface map of **(II)**, generated for the whole intermolecular interactions. The red areas show the most pronounced interactions, where the strongest are formed by the oxygen atoms of nitrites and ether groups.

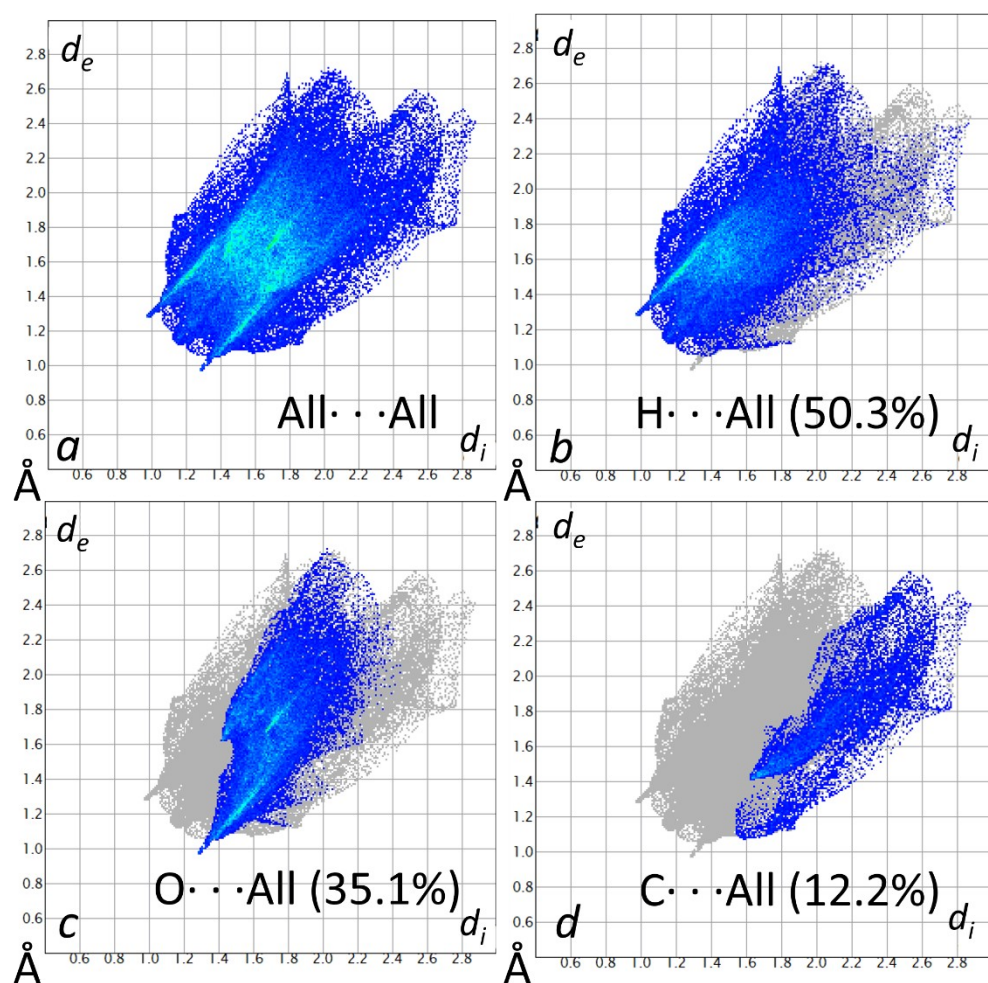


Fig. S3. Selected two-dimensional fingerprint plots based on the Hirshfeld surfaces of the (II) for the all (a), hydrogen (b), oxygen (c) and carbon (d) intermolecular interactions.

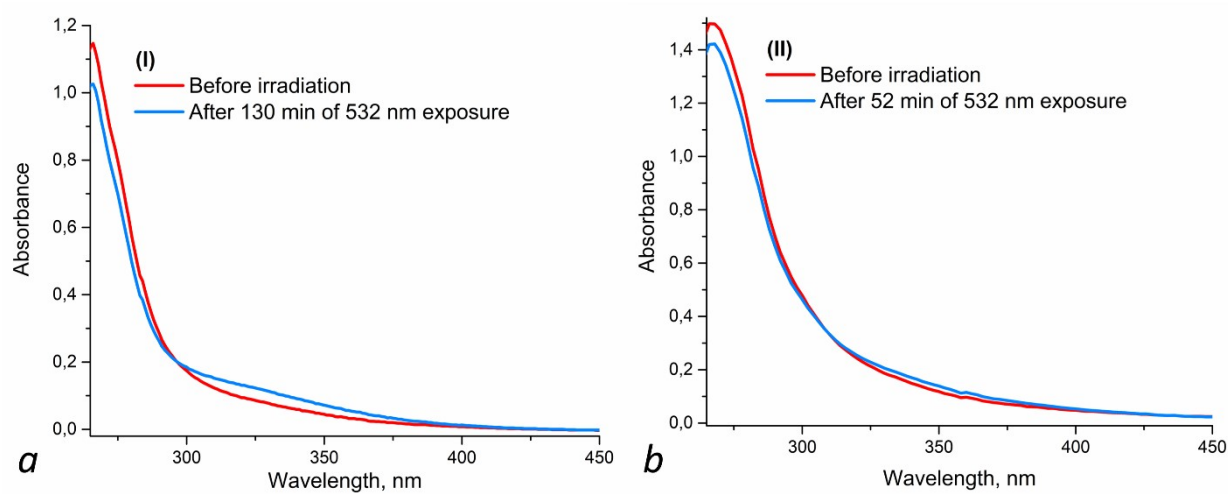


Fig. S4. The evolution of UV-vis spectra of (I) (a) and (II) (b) after irradiation at 532 nm.

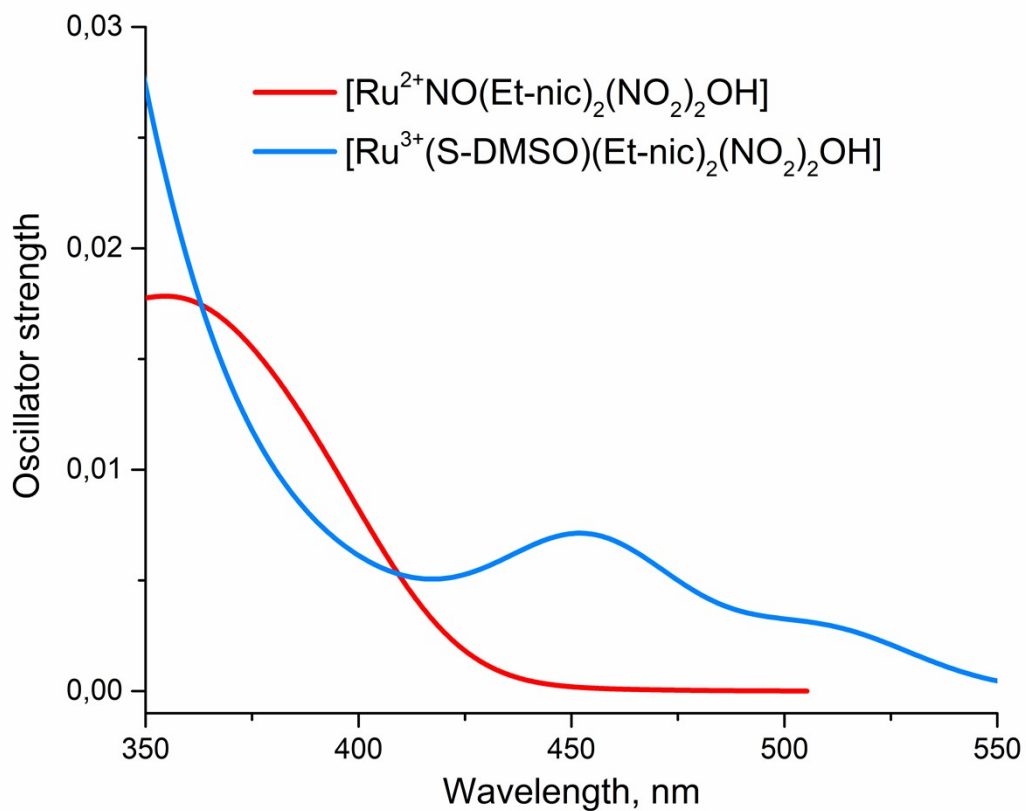


Fig. S5. Calculated (DFT, B3LYP, TZP) UV-vis spectra of **(I)** and its corresponding product of the photolysis.

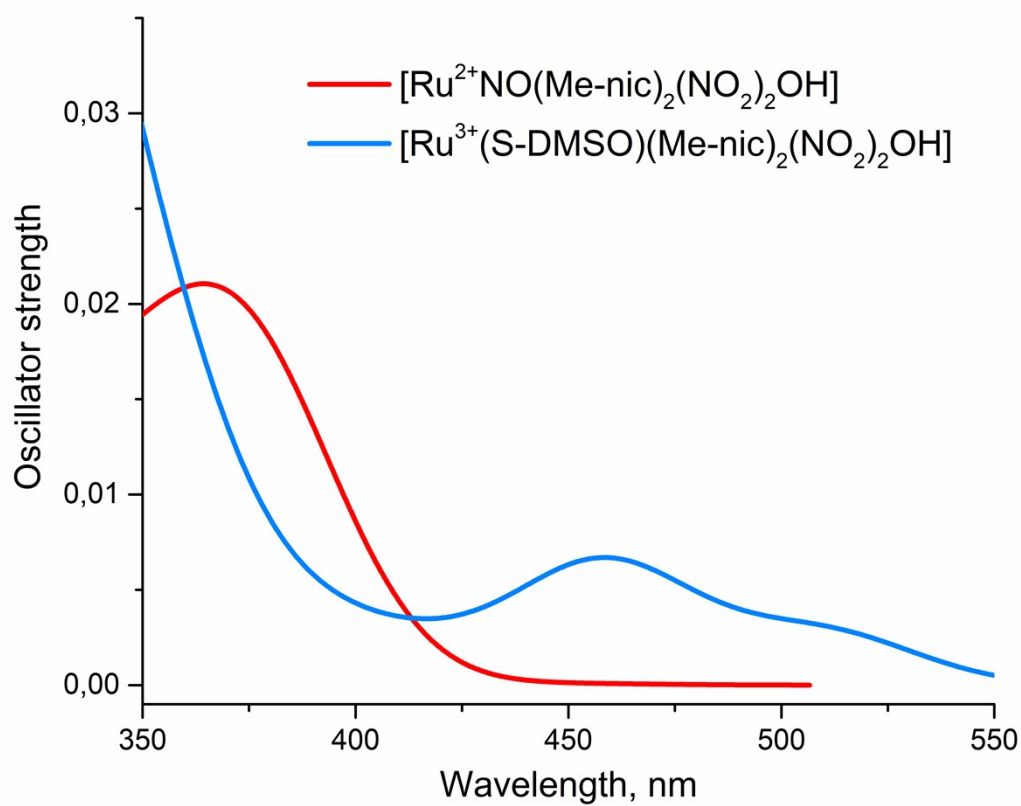


Fig. S6. Calculated (DFT, B3LYP, TZP) UV-vis spectra of **(II)** and its corresponding product of the photolysis.

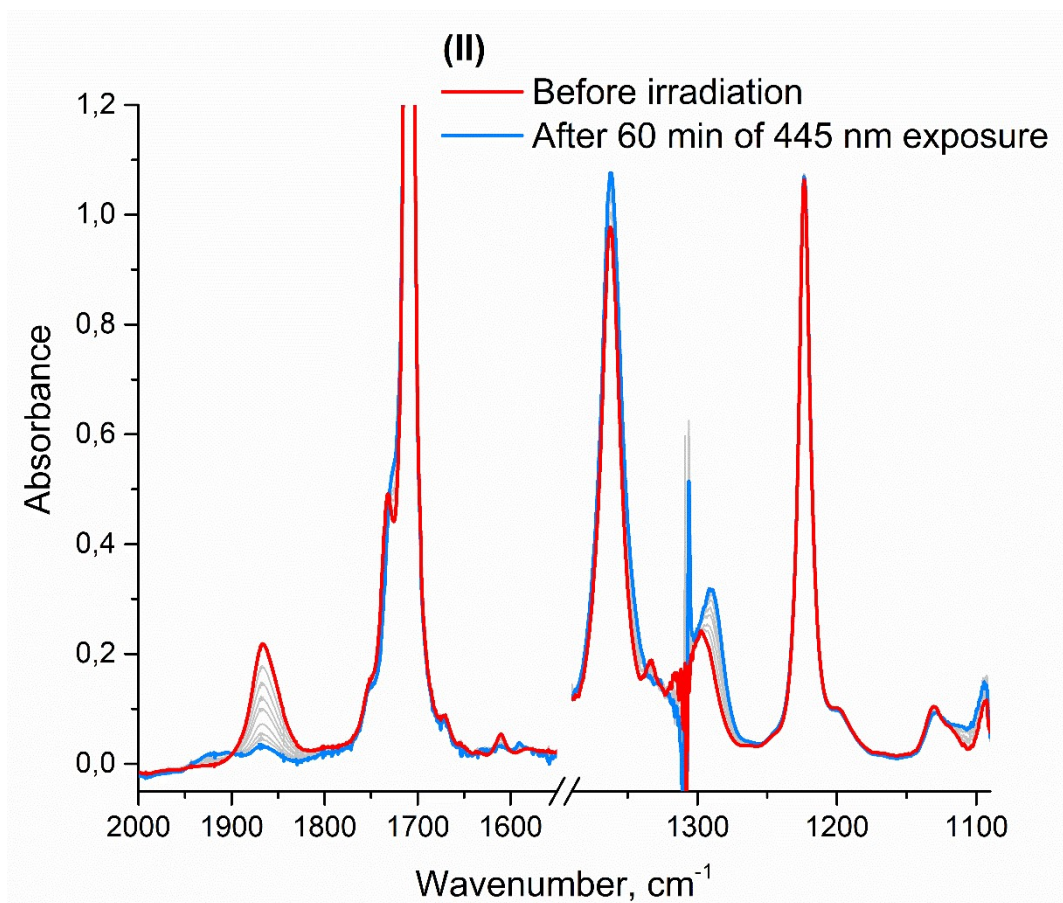


Fig. S7. The evolution of IR spectra of (II) in after 445 nm exposure.