Electronic Supplementary Material (ESI) for RSC Advances.

Supporting information

Site-specific orthometallation *via* C–H bond activation and syntheses of ruthenium (III) organometallics: Studies on nitric oxide (NO) reactivity and photorelease of coordinated NO

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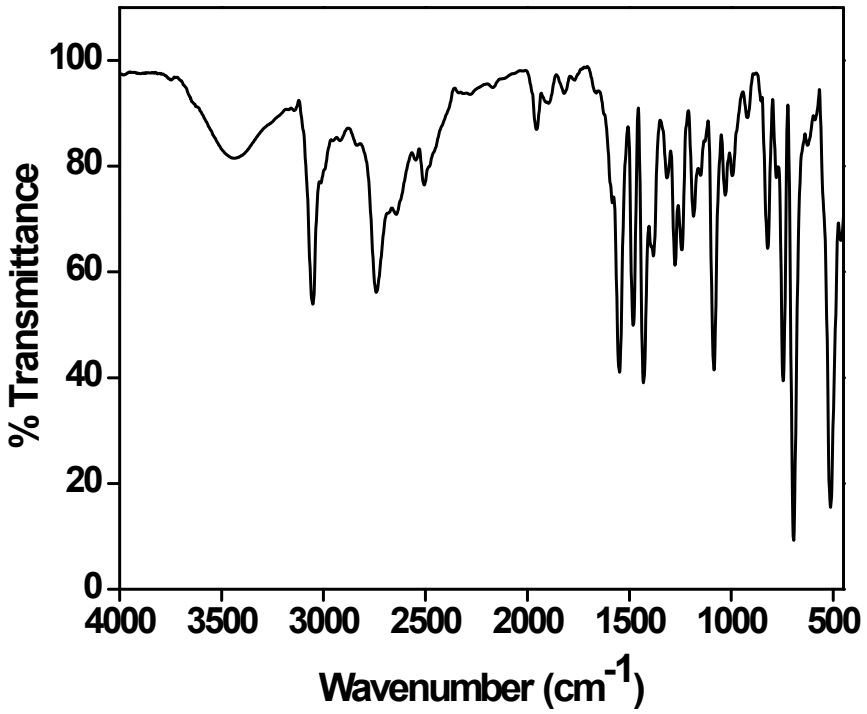

Figure S1. Infrared spectrum of complex **1**. IR (KBr disk, cm^{-1}): 1558 (ν_{CONH}), 746, 692, 520 (ν_{PPh3}) cm^{-1}.

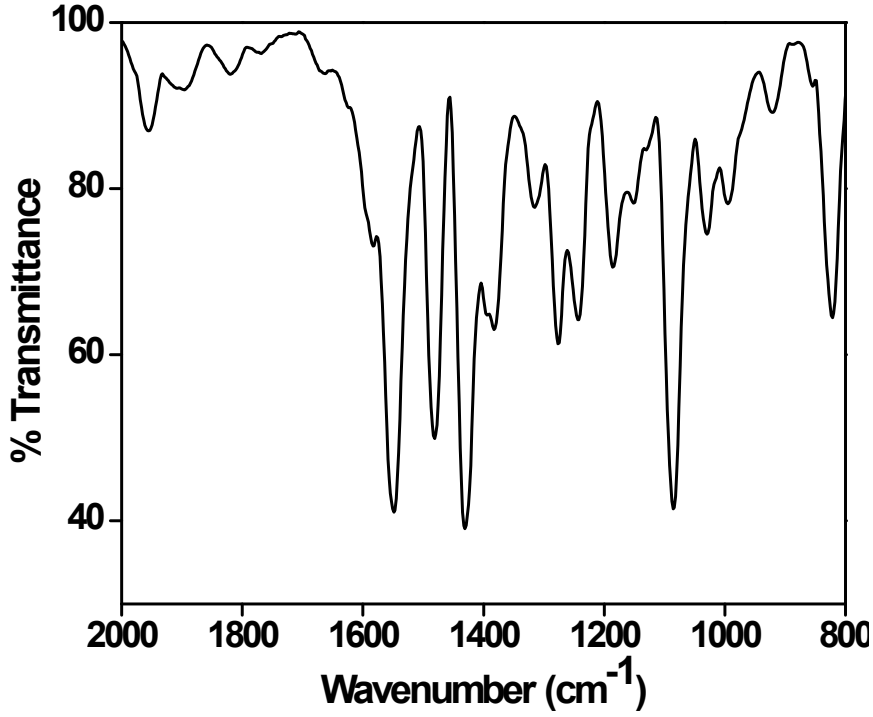

Figure S2. Magnified infrared spectrum of complex **1** in the CO stretching region. IR (KBr disk, cm^{-1}): 1558 (ν_{CONH}) cm^{-1}.

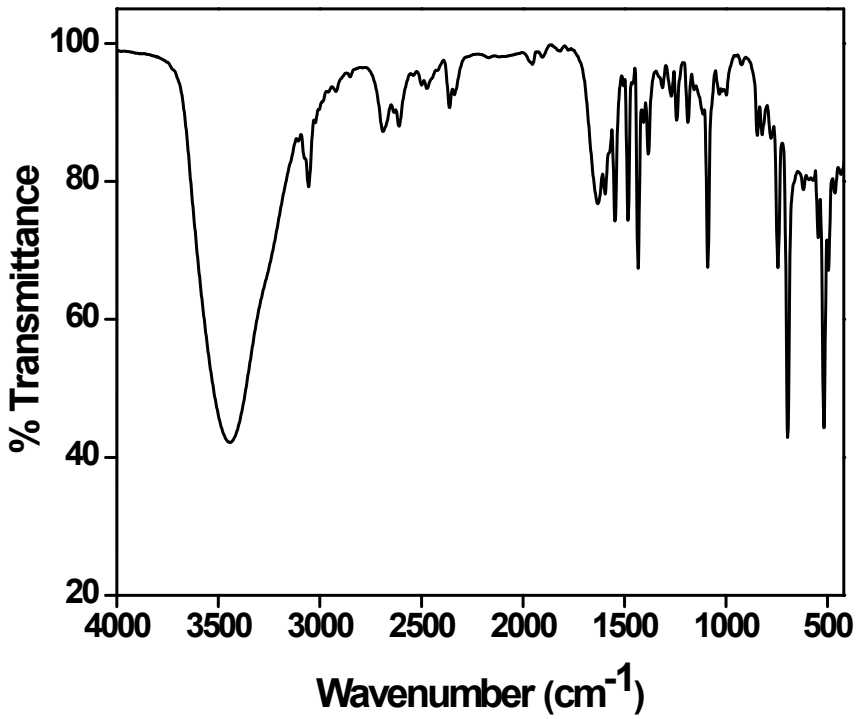

Figure S3. Infrared spectrum of complex **2**. IR (KBr disk, cm^{-1}): 1635 (ν_{CONH}), 746, 694, 522 (ν_{PPh3}) cm^{-1}.

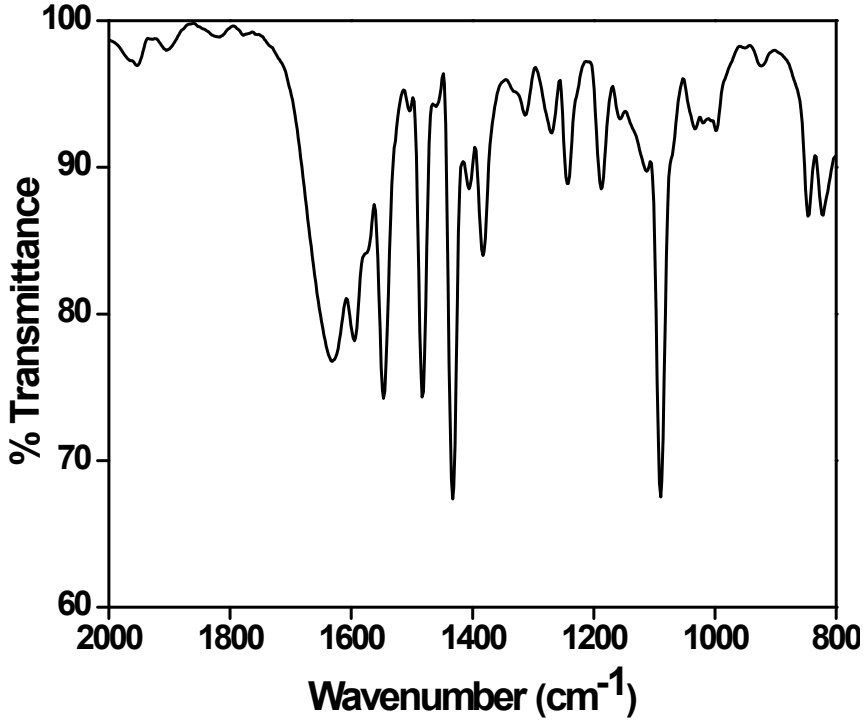

Figure S4. Magnified infrared spectrum of complex **2** in the CO stretching region. IR (KBr disk, cm^{-1}): 1635 (ν_{CONH}) cm^{-1}.

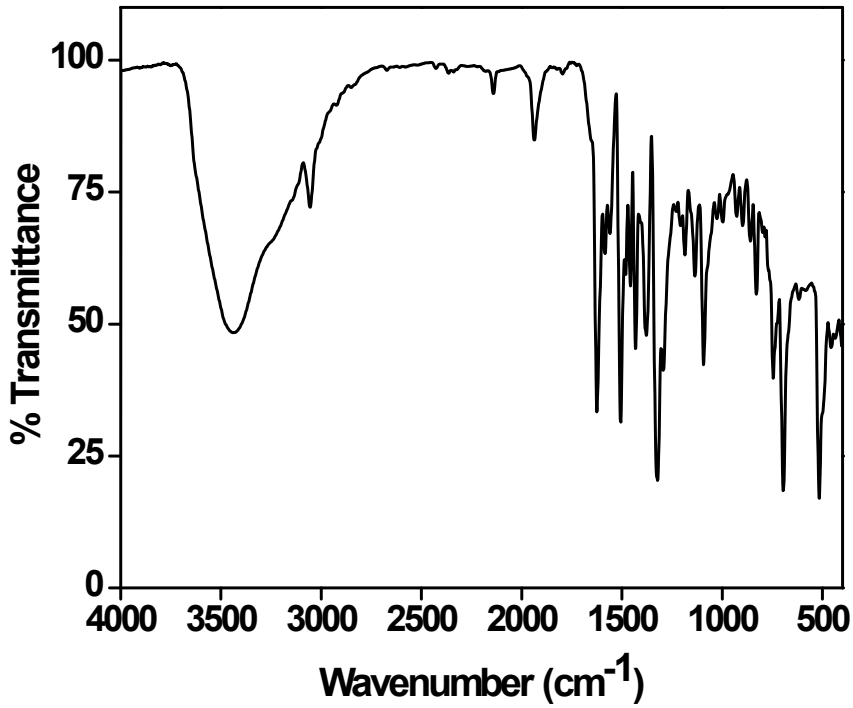

Figure S5. Infrared spectrum of complex **3**. IR (KBr disk, cm^{-1}): 1632 (ν_{CONH}), 744, 694, 515 (ν_{PPh3}) cm^{-1}.

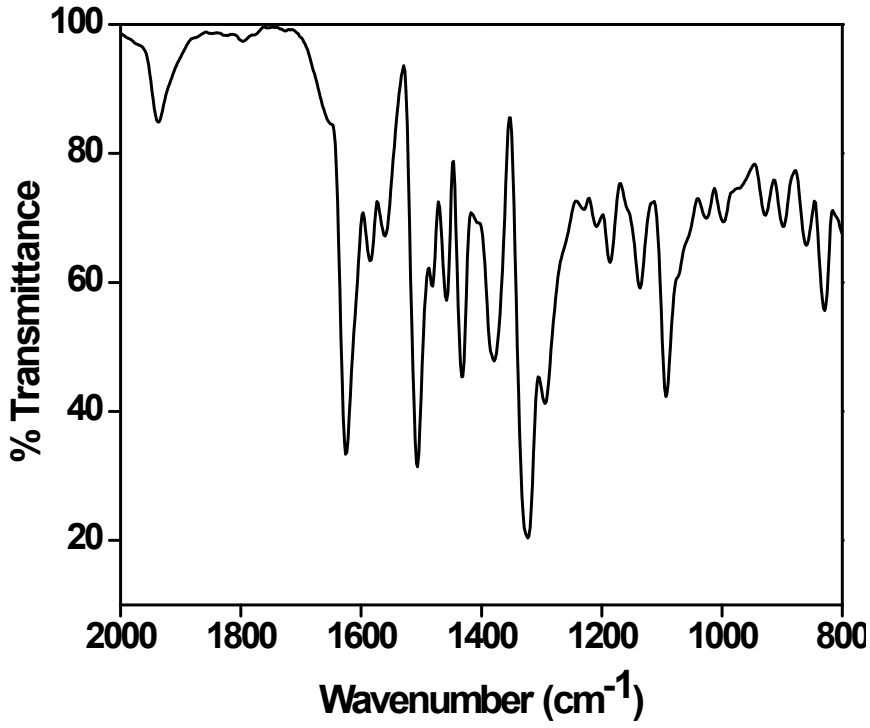

Figure S6. Magnified infrared spectrum of complex **3** in the CO stretching region. IR (KBr disk, cm^{-1}): 1632 (ν_{CONH}) cm^{-1}.

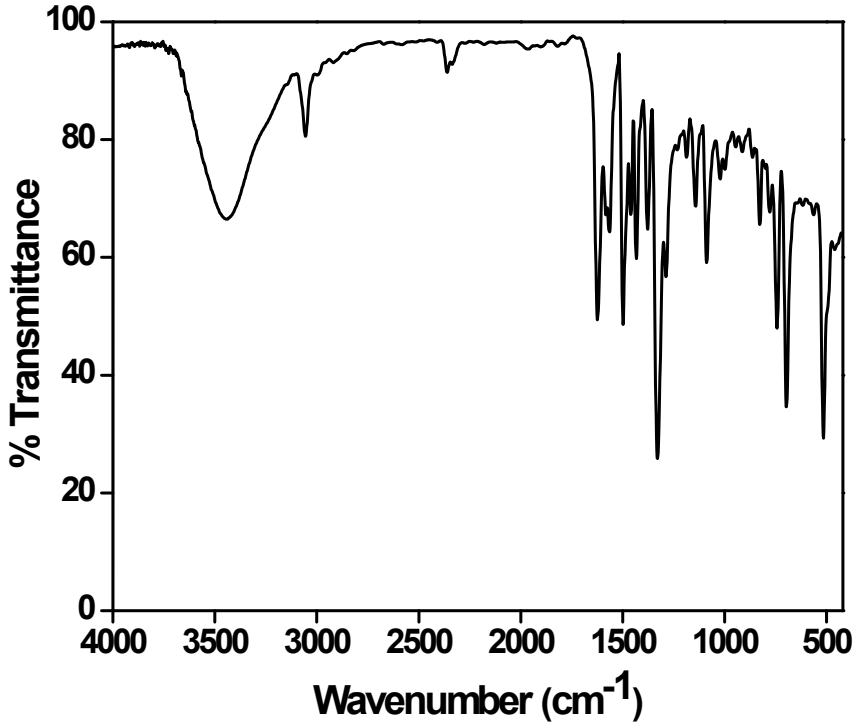

Figure S7. Infrared spectrum of complex **4**. IR (KBr disk, cm^{-1}): 1625 (ν_{CONH}), 742, 692, 514 (ν_{PPh3}) cm^{-1}.

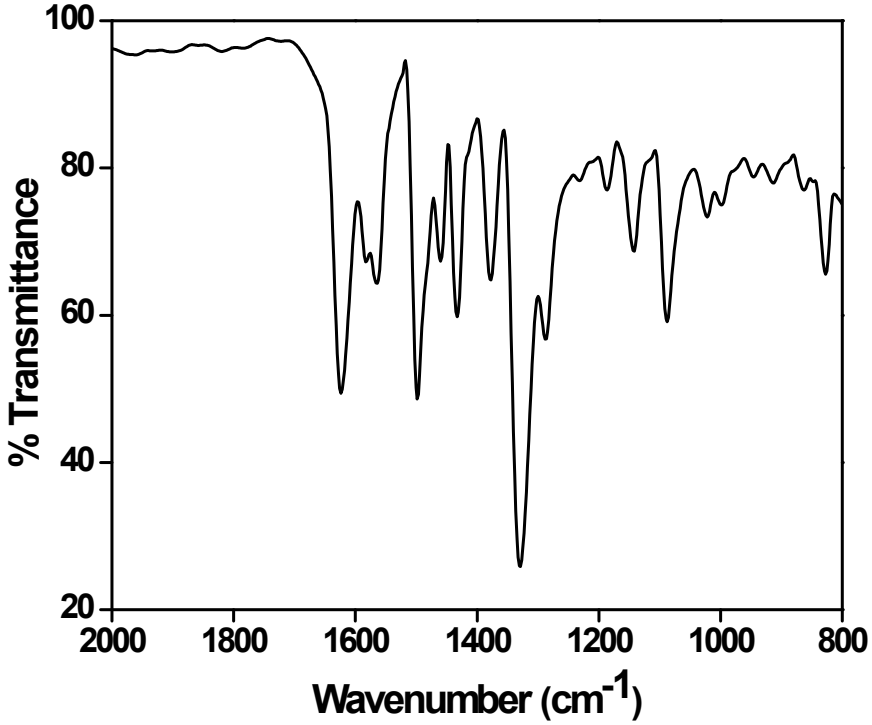

Figure S8. Magnified infrared spectrum of complex **4** in the CO stretching region. IR (KBr disk, cm^{-1}): 1625 (ν_{CONH}) cm^{-1}.

Table S1. Data for IR spectral studies.

Complex	IR data (cm^{-1}, KBr pellets)			
	ν_{CONH}	ν_{NO}	ν_{ClO4}	ν_{PPh3}
1	1558	–	–	746, 692, 520
2	1635	–	–	746, 694, 522
3	1632	–	–	744, 694, 515
4	1625	–	–	742, 692, 514
1a	1635	1880	1092, 620	730, 692, 530
2a	1585	1870	1092, 612	746, 692, 522
3a	1645	1830	1092, 612	746, 694, 520
4a	1655	1845	1090, 614	742, 692, 514

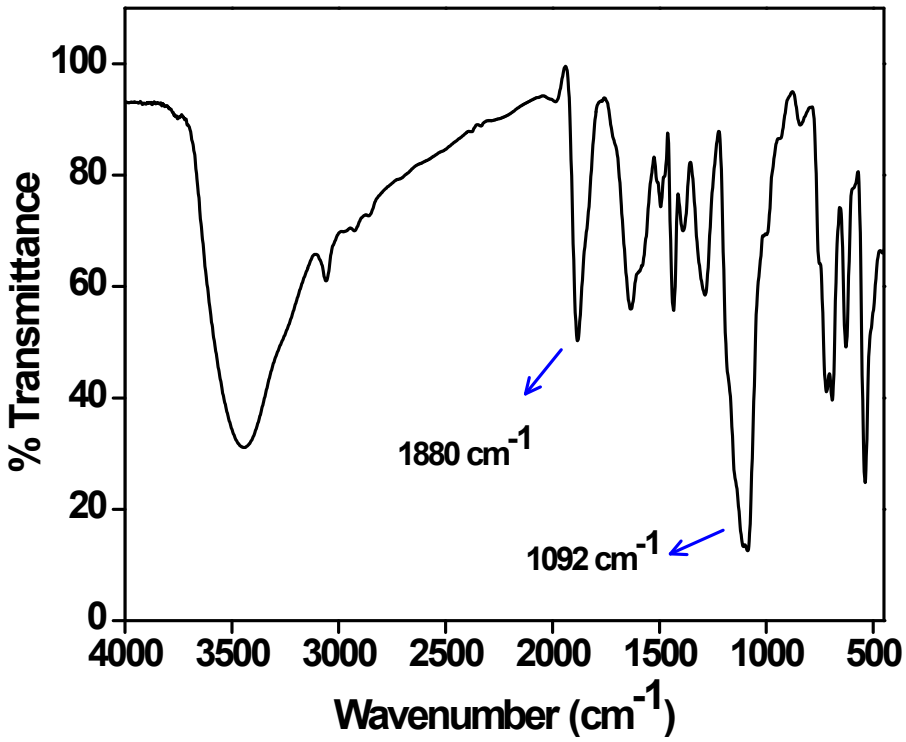

Figure S9. Infrared spectrum of complex **1a**. IR (KBr disk, cm^{-1}): 1880 (ν_{NO}), 1635 (ν_{CONH}), 1092, 620 (ν_{ClO4}), 730, 692, 530 (ν_{PPh3}) cm^{-1}.

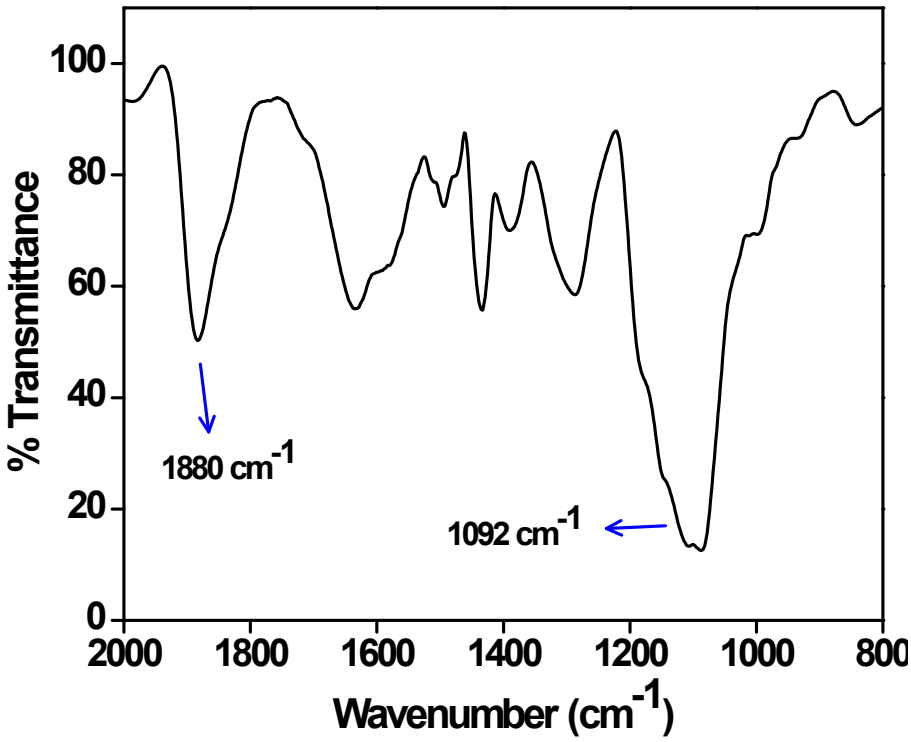

Figure S10. Magnified infrared spectrum of complex **1a** in the CO stretching region. IR (KBr disk, cm^{-1}): 1880 (ν_{NO}), 1635 (ν_{CONH}), 1092, 620 (ν_{ClO4}) cm^{-1}.

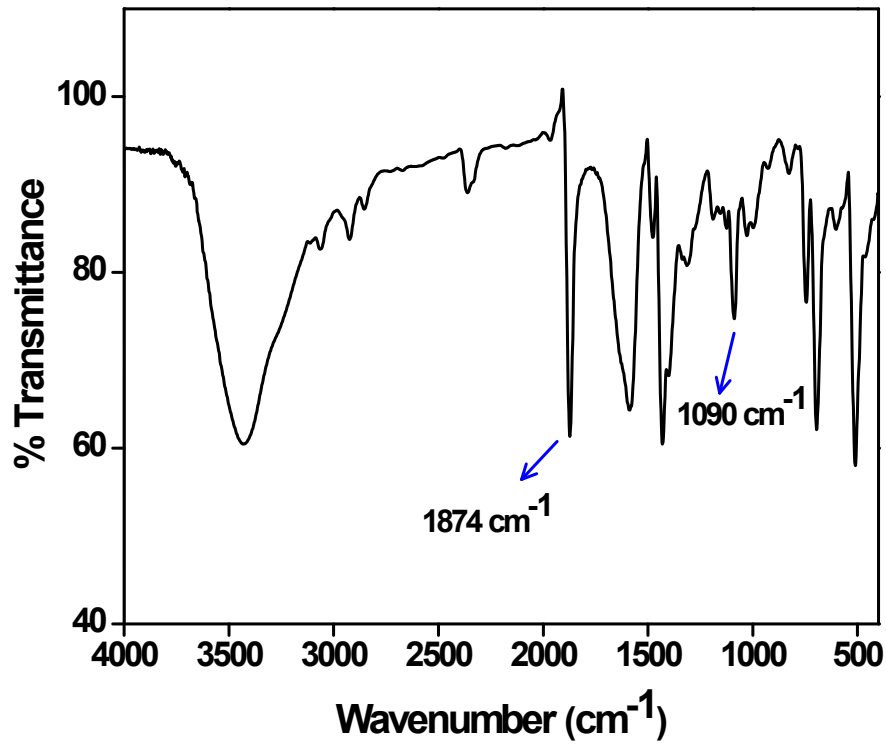

Figure S11. Infrared spectrum of complex **2a**. IR (KBr disk, cm^{-1}): 1874 (ν_{NO}), 1590 (ν_{CONH}), 1090, 608 (ν_{ClO4}), 748, 698, 512 (ν_{PPh3}) cm^{-1}.

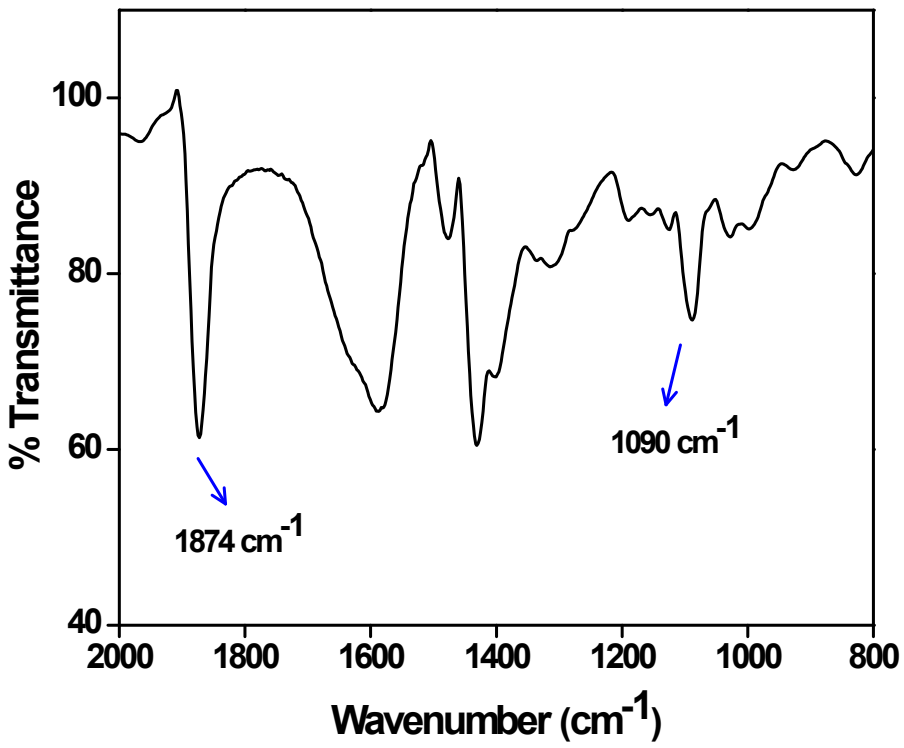

Figure S12. Magnified infrared spectrum of complex **2a** in the CO stretching region. IR (KBr disk, cm^{-1}): 1874 (ν_{NO}), 1590 (ν_{CONH}), 1090, 608 (ν_{ClO4}) cm^{-1}.

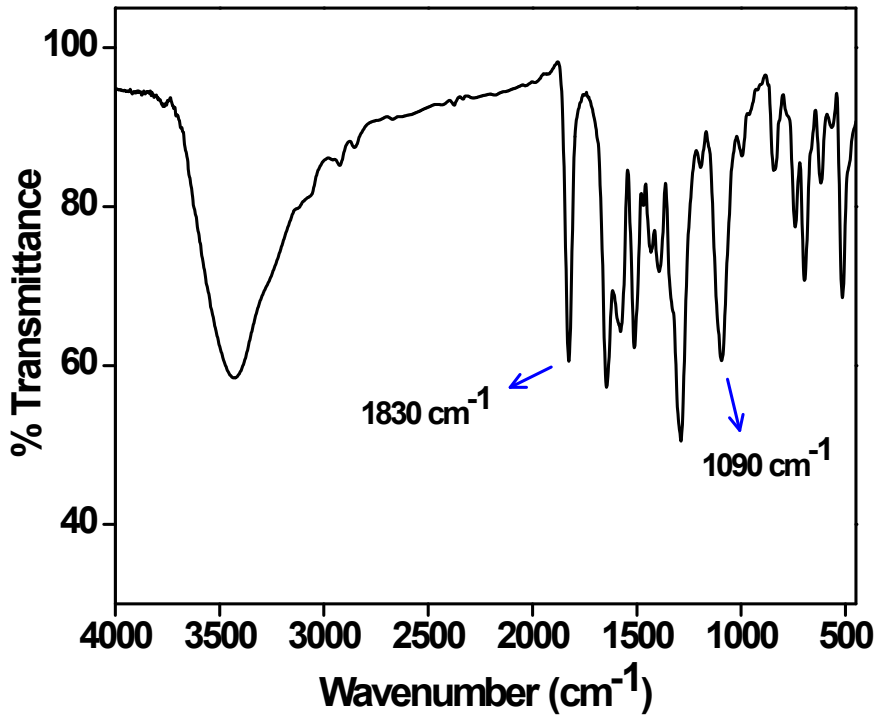

Figure S13. Infrared spectrum of complex **3a**. IR (KBr disk, cm^{-1}): 1830 (ν_{NO}), 1645 (ν_{CONH}), 1090, 620 (ν_{ClO4}), 746, 692, 520 (ν_{PPh3}) cm^{-1}.

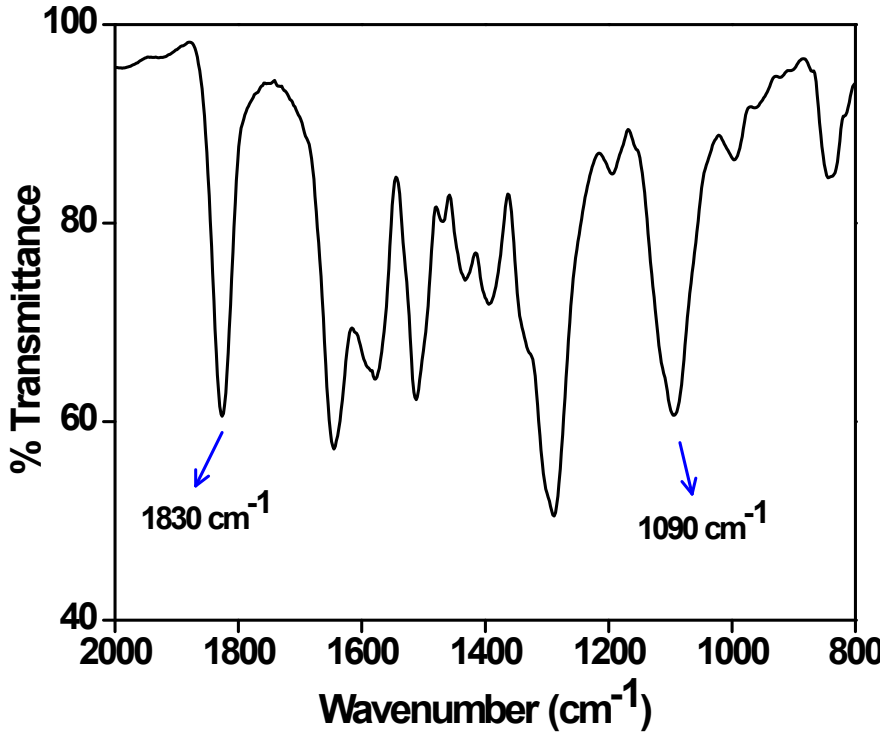

Figure S14. Magnified infrared spectrum of complex **3a** in the CO stretching region. IR (KBr disk, cm^{-1}): 1830 (ν_{NO}), 1645 (ν_{CONH}), 1090, 620 (ν_{ClO4}) cm^{-1}.

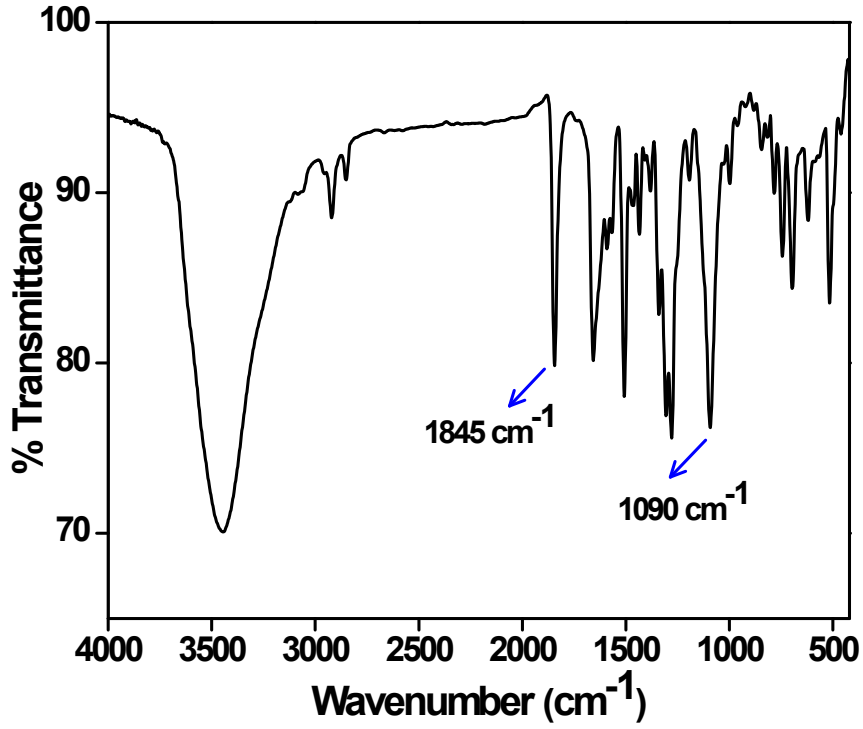

Figure S15. Infrared spectrum of complex **4a**. IR (KBr disk, cm^{-1}): 1845 (ν_{NO}), 1655 (ν_{CONH}), 1090, 614 (ν_{ClO4}), 742, 692, 514 (ν_{PPh3}) cm^{-1}.

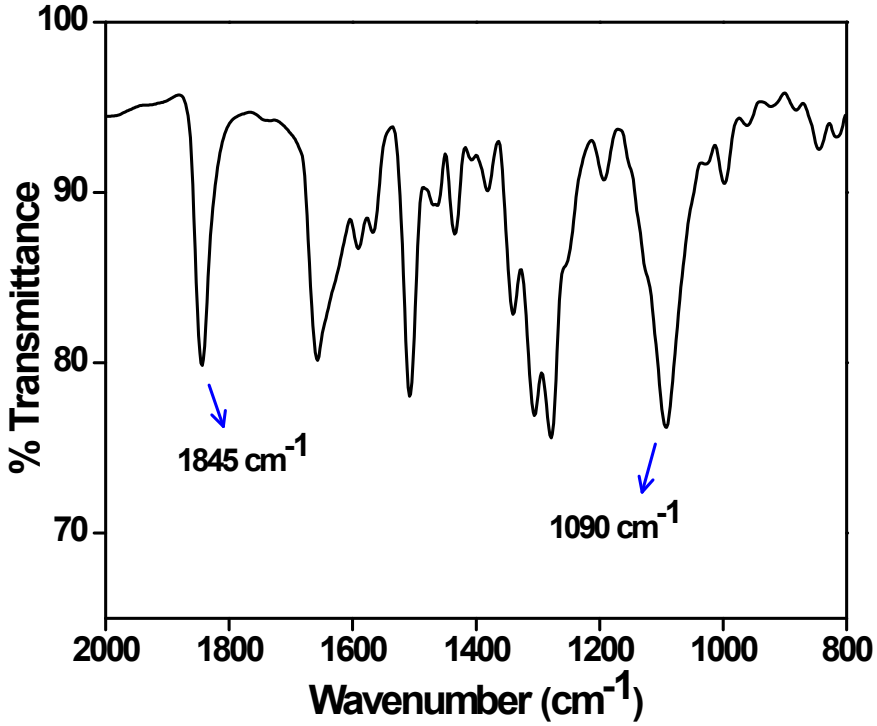

Figure S16. Magnified infrared spectrum of complex **4a** in the CO stretching region. IR (KBr disk, cm^{-1}): 1845 (ν_{NO}), 1655 (ν_{CONH}), 1090, 614 (ν_{ClO4}) cm^{-1}.

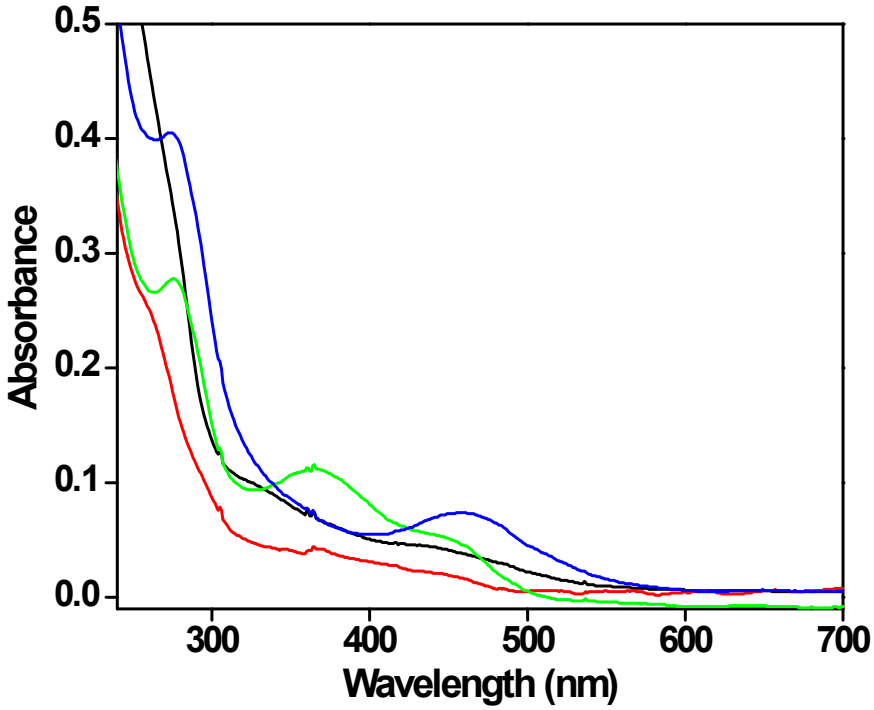

Figure S17. Electronic absorption spectra of complexes **1** (—), **2** (—), **3** (—) and **4** (—) in dichloromethane solutions.

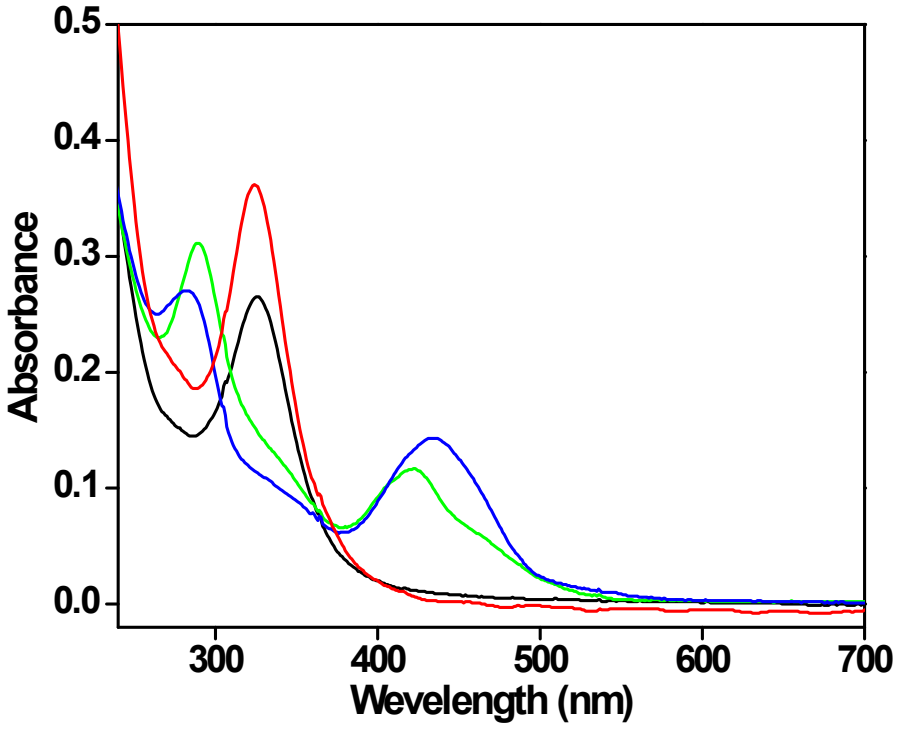

Figure S18. Electronic absorption spectra of ruthenium nitrosyl complexes **1a** (—), **2a** (—), **3a** (—) and **4a** (—) in dichloromethane solutions.

Table S2. Electronic spectral data for ruthenium complexes in dichloromethane solutions.

Complex	λ_{max}/nm (ε / $M^{-1}cm^{-1}$)
1	270 (17280), 335 (4041), 445 (1942)
2	262 (17596), 365 (2804)
3	274 (28626), 460 (5042)
4	274 (25615), 365 (10570), 460 (4966)
1a	326 (21370)
2a	324 (29668)
3a	282 (27107), 434 (20867)
4a	288 (30266), 424 (14372)

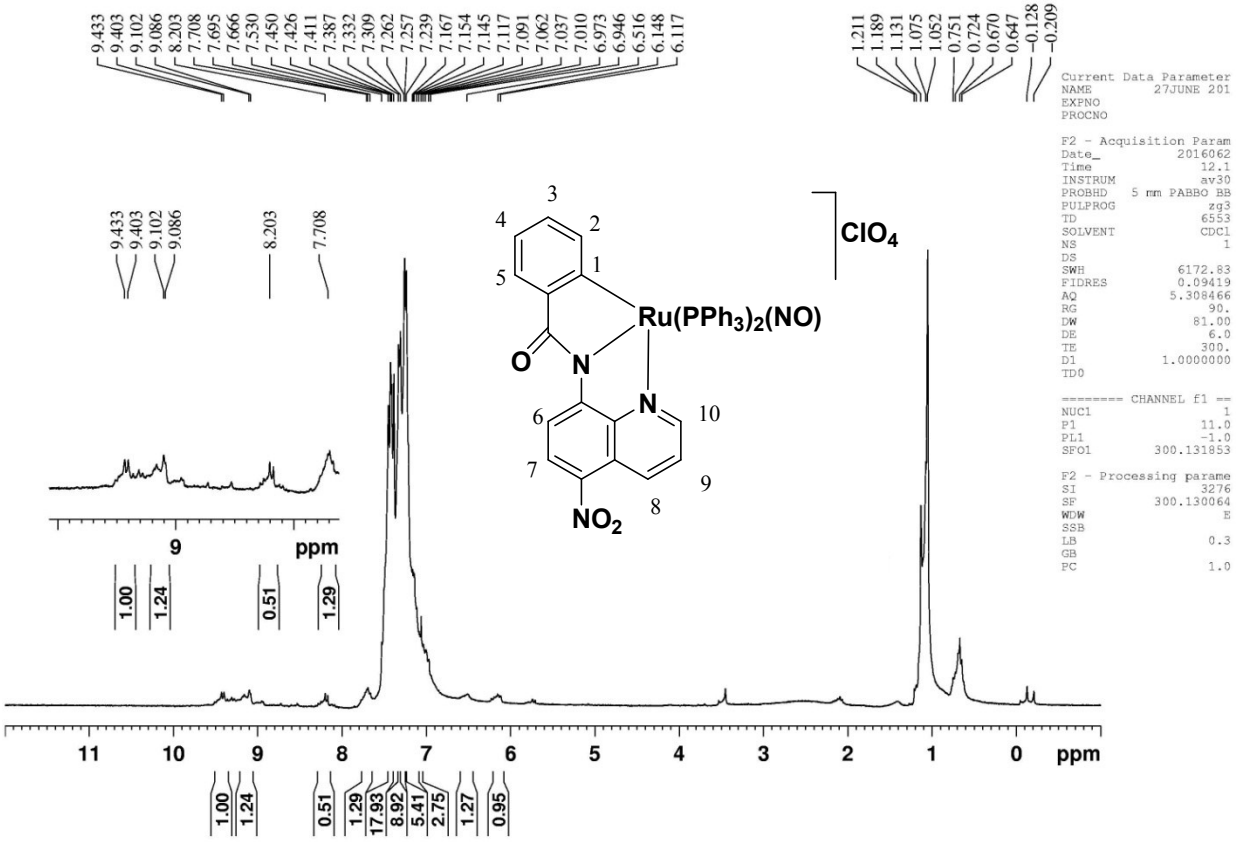

Figure S19. ^{1}H NMR spectrum of complex **1a** in $CDCl_3$ at room temperature.

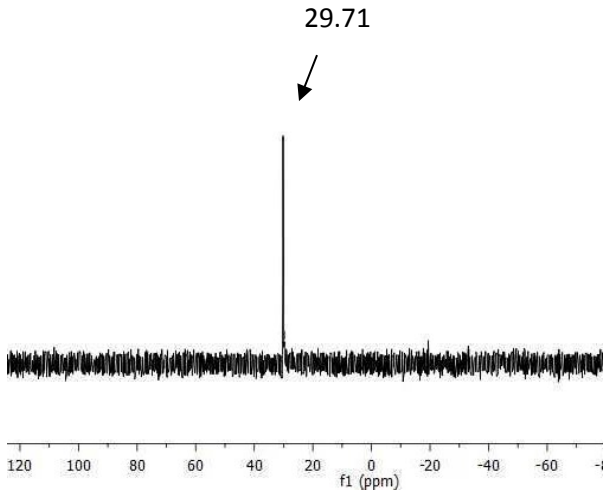

Figure S20. ^{31}P NMR spectrum of complex **1a** in $CDCl_3$ at room temperature.

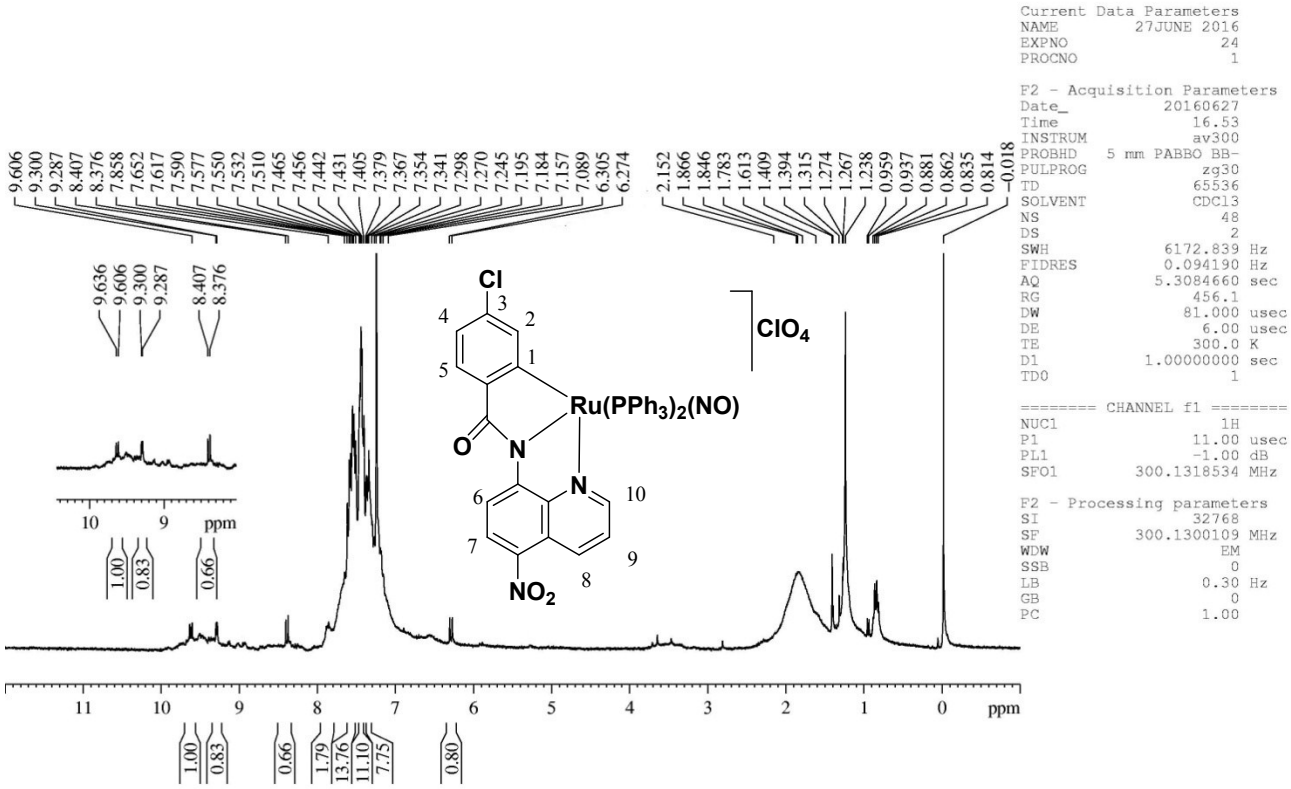

Figure S21. ^{1}H NMR spectrum of complex **2a** in $CDCl_3$ at room temperature.

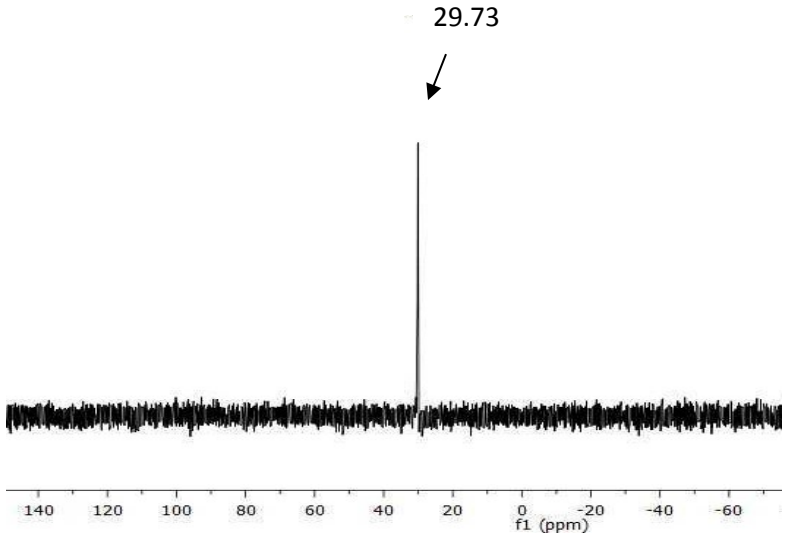

Figure S22. ^{31}P NMR spectrum of complex **2a** in $CDCl_3$ at room temperature.

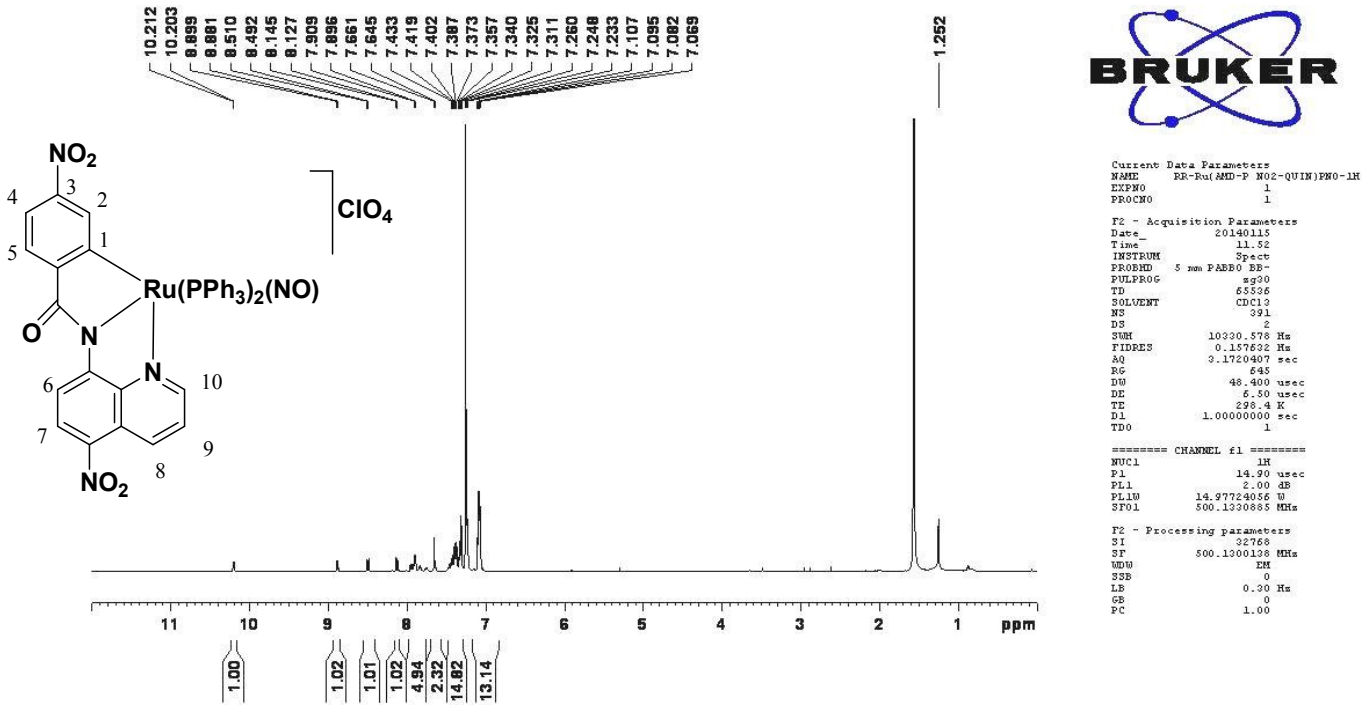

Figure S23. ^{1}H NMR spectrum of complex **3a** in $CDCl_3$ at room temperature.

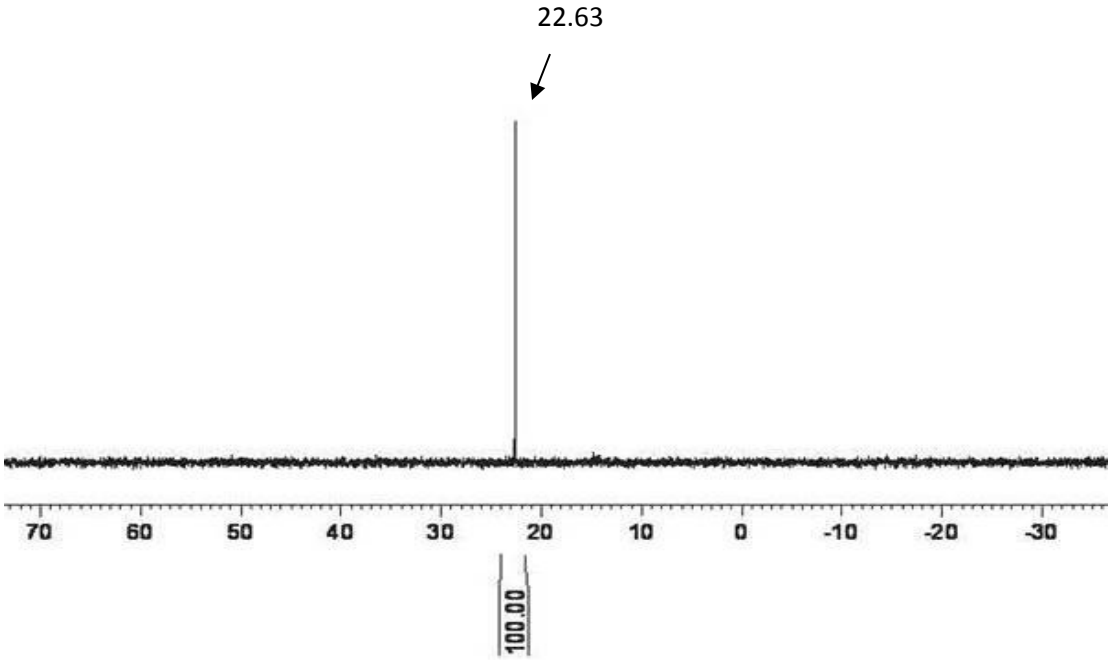

Figure S24. ^{31}P NMR spectrum of complex **3a** in $CDCl_3$ at room temperature.

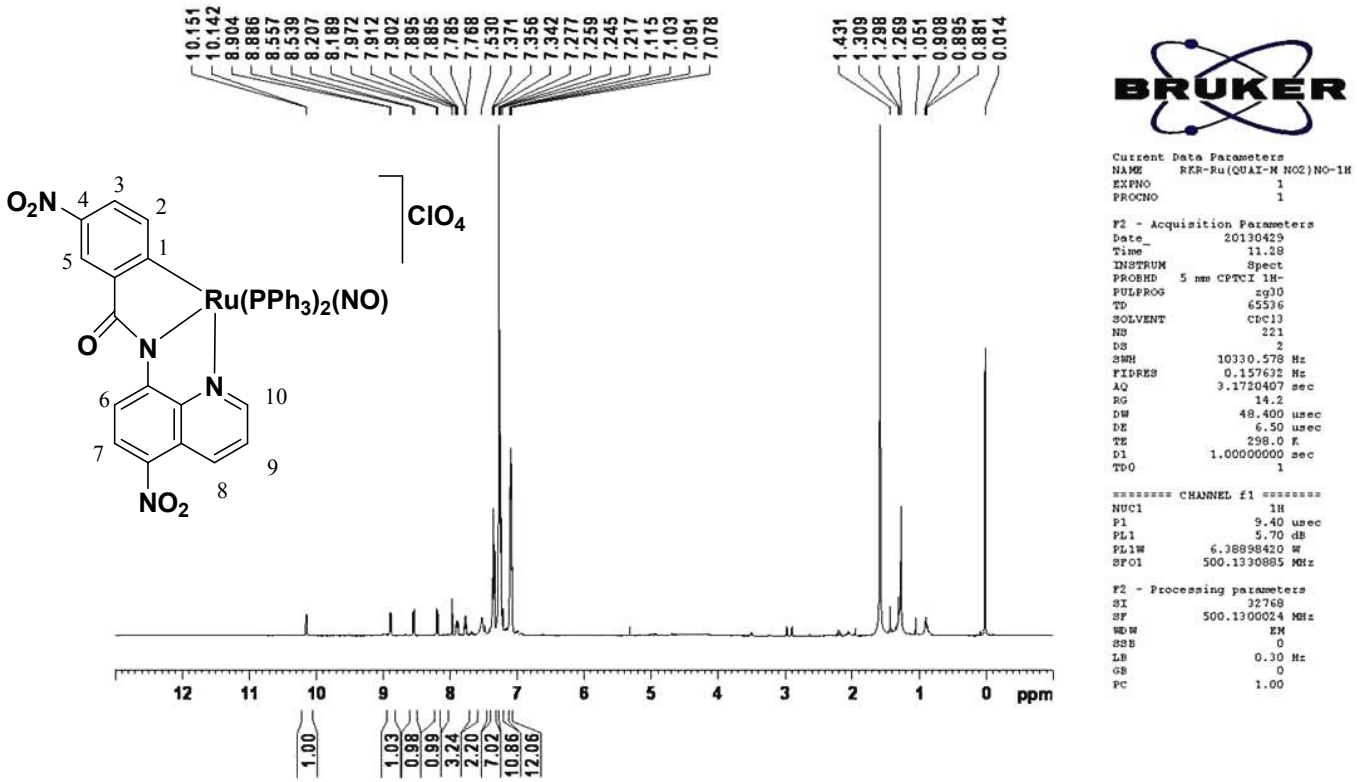

Figure S25. ^{1}H NMR spectrum of complex **4a** in $CDCl_3$ at room temperature.

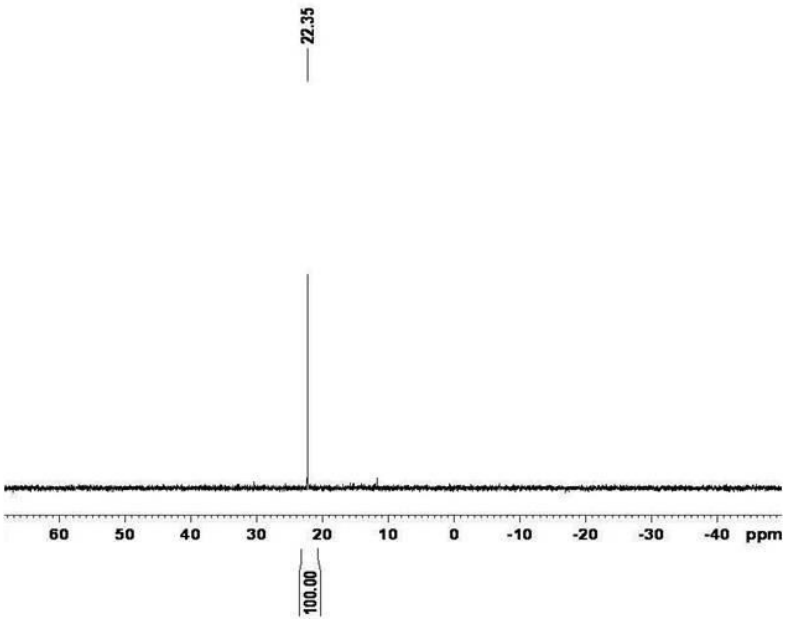

Figure S26. ^{31}P NMR spectrum of complex **4a** in $CDCl_3$ at room temperature.

Table S3 ^{1}H NMR Spectral Data (δ, ppm) of nitrosyl complexs **1a**, **2a**, **3a** and **4a**.

Comp.	10–H	5–H	8–H	3–H	7–H	Other protons
1a	9.42	9.09	8.20	–	–	7.71–6.13 (PPh_3, 30H and ligand–H)
2a	9.62	9.29	8.39	–	–	7.86–6.29 (PPh_3, 30H and ligand–H)
3a	10.21	8.89	8.50	8.13	7.90	7.90 –7.06 (PPh_3, 30H and ligand–H)
4a	10.15	8.89	8.54	8.19	7.45	7.97–7.07 (PPh_3, 30H and ligand–H)

Table S4 Comparison table of nitrosyl complexs **1a**, **2a**, **3a** and **4a** for ν_{NO} and ^{31}P NMR data and substituents in ligand frame

Complexes	**ν_{NO}(cm^{-1})**	**^{31}P (ppm)**	**Substituents in the ligand frame**
1a	1880	29.71	-H
2a	1870	29.73	-Cl
3a	1830	22.63	$-NO_2$
4a	1845	22.35	$-NO_2$

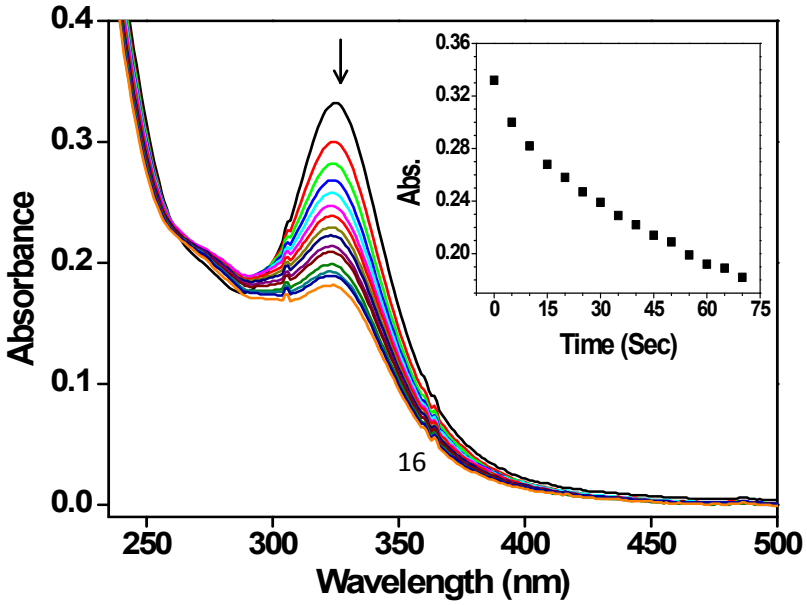

Figure S27. Photodissociation of NO from complex **2a** (~ 1.5 x 10^{-5} M) in dichloromethane solutions under illumination with a UV light (λ_{irr} = 365 nm). Repetitive scans were taken in 5 seconds intervals. Inset: Changes in absorbance with time at λ = 324 nm at room temperature.

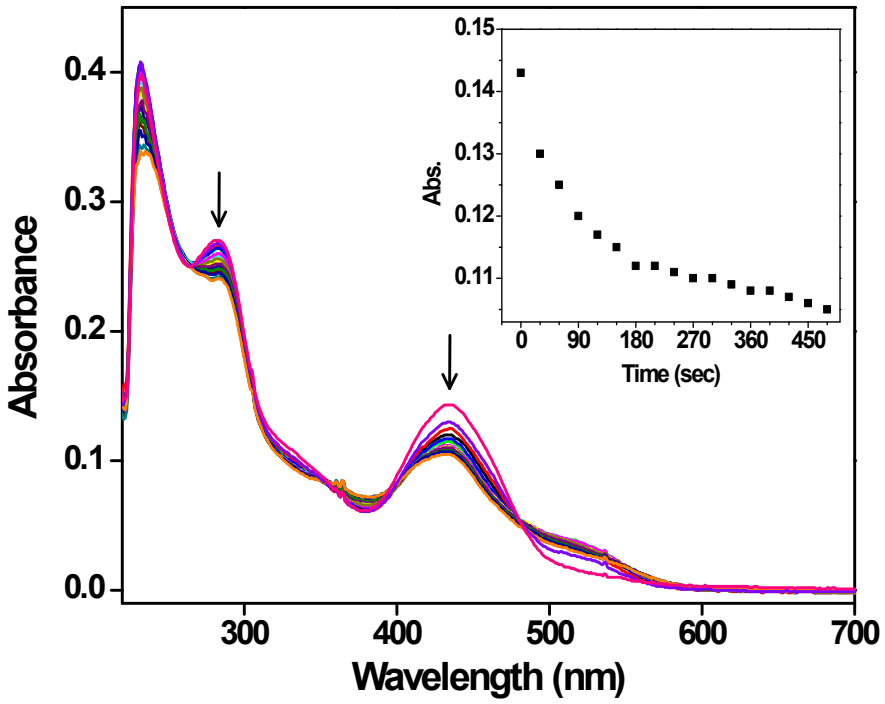

Figure S28. Photodissociation of NO from complex **3a** (~ 1.5 x 10^{-5} M) in dichloromethane solutions under illumination with a UV light (λ_{irr} = 365 nm). Repetitive scans were taken in 30 seconds intervals. Inset: Changes in absorbance with time at λ = 434 nm at room temperature.

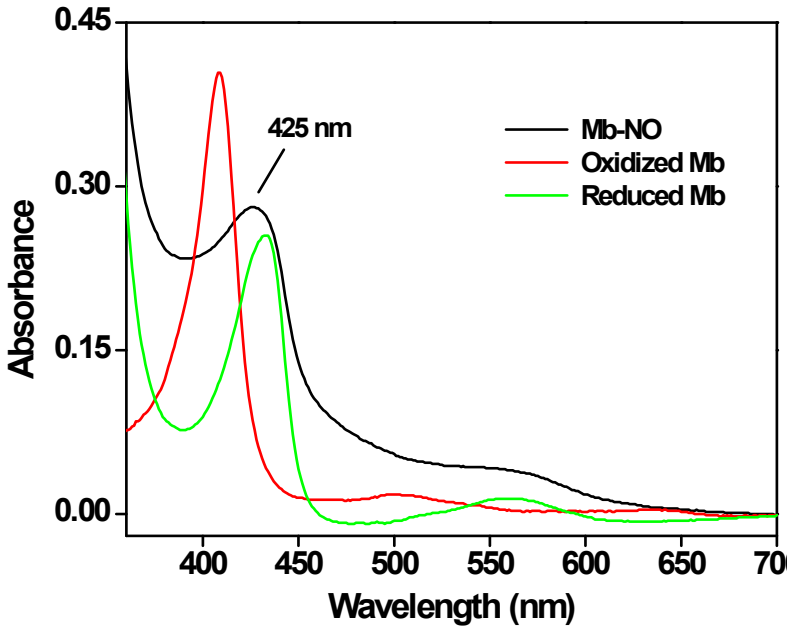

Figure S29. Electronic spectra for conversion of reduced Mb to Mb−NO adducts upon reaction with **2a** in buffer solutions (50 mM phosphate buffer, pH 6.8) under exposure of UV light. Red line, oxidized Mb (intense band at ~ 409 nm); blue line, reduced Mb (at ~ 433 nm, with excess of sodium dithionite); Black line, Mb–NO adduct (at ~ 425 nm), obtained by Mb and solution of **2a** (~ 10^{-5} M) exposed to UV light (λ_{irr} = 365 nm) for 2-3 minutes at room temperature.

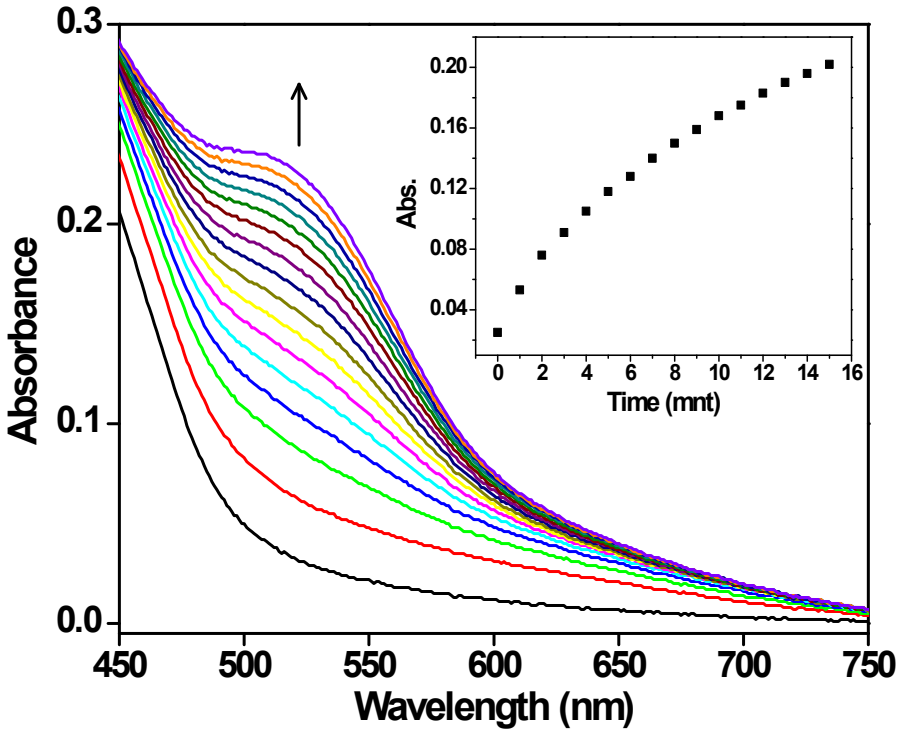

Figure S30. Electronic spectra of dye formation when Griess reagent (100 μL) was treated with complex **2a** (50 μM) in the presence of UV light (λ_{irr} = 365 nm). Repetitive scans were taken in 1 minute intervals. Inset: Time dependent changes in absorbance at λ = 538 nm at room temperature.

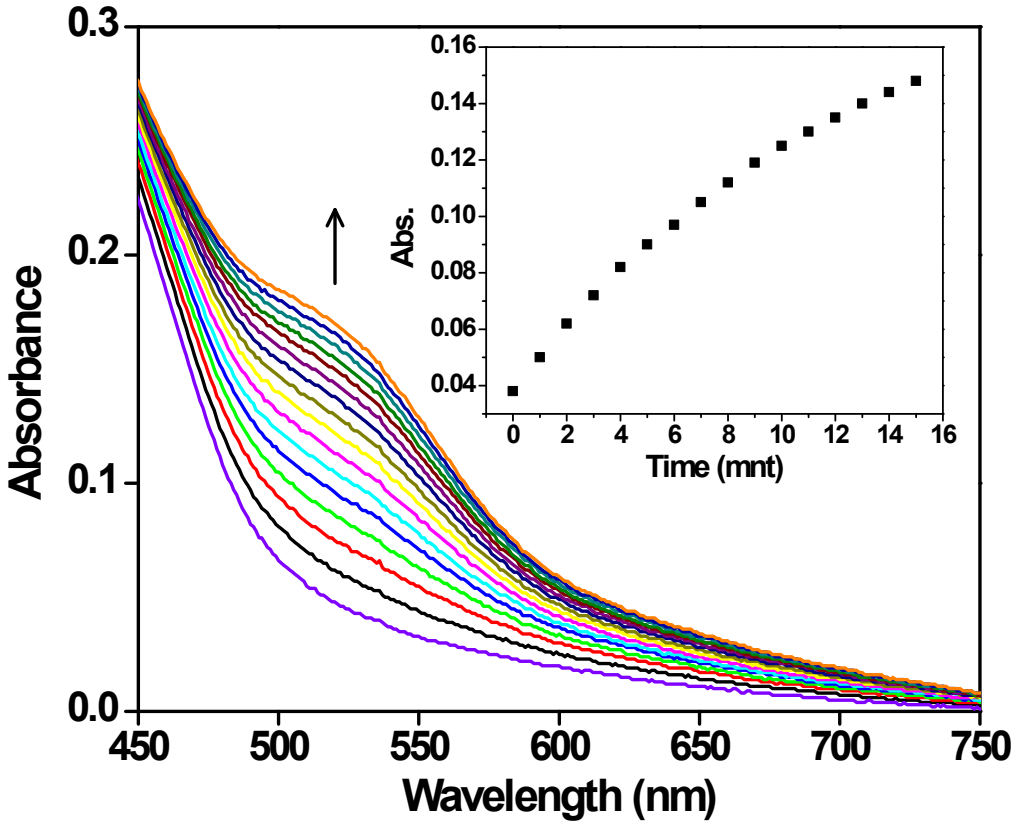

Figure S31. Electronic spectra of dye formation when Griess reagent (100 μL) was treated with complex **2a** (50 μM) in the presence of visible light (100 Watt tungsten lamp). Repetitive scans were taken in 1 minute intervals. Inset: Time dependent changes in absorbance at λ = 538 nm at room temperature.

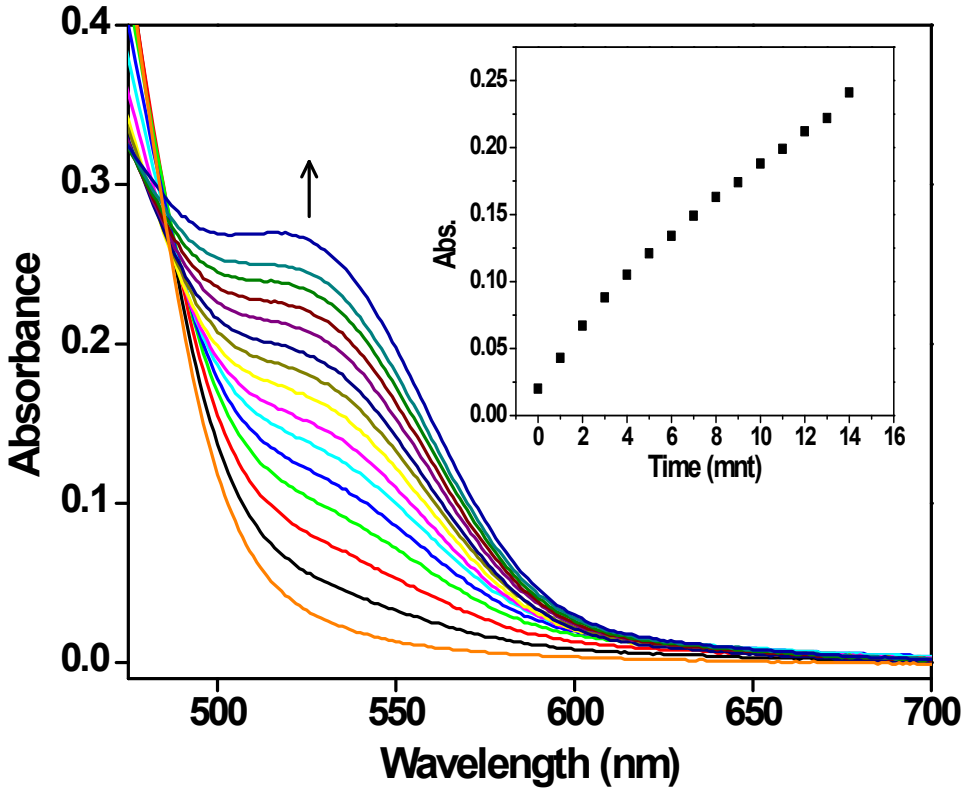

Figure S32. Electronic spectra of dye formation when Griess reagent (100 μL) was treated with complex **4a** (50 μM) in the presence of visible light (100 Watt tungsten lamp). Repetitive scans were taken in 1 minute intervals. Inset: Time dependent changes in absorbance at λ = 538 nm at room temperature.

CIF_4a

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_exptl_absorpt_correction_T_max  0.906
_exptl_absorpt_process_details   '(SADABS; Bruker, 2000)'

_exptl_special_details
;
 ?
;

_diffrn_ambient_temperature      296(2)
_diffrn_radiation_wavelength     0.71073
_diffrn_radiation_type           MoK\a
_diffrn_radiation_source         'fine-focus sealed tube'
_diffrn_radiation_monochromator  graphite
_diffrn_measurement_device_type  'CCD area detector'
_diffrn_measurement_method       'phi omega scans'
_diffrn_detector_area_resol_mean  ?
_diffrn_standards_number         ?
_diffrn_standards_interval_count  ?
_diffrn_standards_interval_time  ?
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_diffrn_reflns_av_R_equivalents  0.0258
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_diffrn_reflns_av_sigmaI/netI     0.0183
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_diffrn_reflns_limit_k_max       16
_diffrn_reflns_limit_l_min       -25
_diffrn_reflns_limit_l_max       25
_diffrn_reflns_theta_min         1.07
_diffrn_reflns_theta_max         28.34
_reflns_number_total             13031
_reflns_number_gt                11073
_reflns_threshold_expression     >2sigma(I)

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_computing_cell_refinement       'Bruker Kappa Apex'
_computing_data_reduction        'Bruker SAINT'
_computing_structure_solution    'SHELXL-97 (Sheldrick, 1997)'
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_computing_molecular_graphics    'Bruker SHELXTL'
_computing_publication_material  'Bruker SHELXTL'

_refine_special_details
;
 Refinement of F^2^ against ALL reflections.  The weighted R-factor wR and
 goodness of fit S are based on F^2^, conventional R-factors R are based
 on F, with F set to zero for negative F^2^. The threshold expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
 not relevant to the choice of reflections for refinement.  R-factors based
 on F^2^ are statistically about twice as large as those based on F, and R-
 factors based on ALL data will be even larger.
;

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_refine_ls_weighting_details
'calc w=1/[\s^2^(Fo^2^)+(0.1000P)^2^+0.8858P] where P=(Fo^2^+2Fc^2^)/3'
_atom_sites_solution_primary     direct
_atom_sites_solution_secondary   difmap
_atom_sites_solution_hydrogens   geom
_refine_ls_hydrogen_treatment    mixed
_refine_ls_extinction_method     none
_refine_ls_extinction_coef       ?
_refine_ls_number_reflns         13031
_refine_ls_number_parameters     668
_refine_ls_number_restraints     0
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Ru1 Ru 0.889815(16) 0.601451(16) 0.710306(9) 0.02807(8) Uani 1 1 d . . .
P2 P 0.80565(6) 0.45688(6) 0.75407(3) 0.03112(14) Uani 1 1 d . . .
P1 P 0.97895(6) 0.74544(6) 0.67598(4) 0.03176(14) Uani 1 1 d . . .
N2 N 0.8801(2) 0.64052(19) 0.81023(11) 0.0320(4) Uani 1 1 d . . .
N3 N 0.9123(2) 0.5581(2) 0.62590(12) 0.0343(4) Uani 1 1 d . . .
N1 N 0.7060(2) 0.74287(19) 0.71535(12) 0.0336(4) Uani 1 1 d . . .
C53 C 1.0600(2) 0.4780(2) 0.74841(14) 0.0327(5) Uani 1 1 d . . .
C1 C 0.8576(3) 0.8934(2) 0.66073(16) 0.0398(6) Uani 1 1 d . . .
C45 C 0.6752(2) 0.7783(2) 0.78039(14) 0.0346(5) Uani 1 1 d . . .
C19 C 0.6749(2) 0.4688(2) 0.70564(15) 0.0362(5) Uani 1 1 d . . .
O1 O 0.9334(2) 0.5231(2) 0.57315(11) 0.0564(6) Uani 1 1 d . . .
C46 C 1.0815(2) 0.4881(2) 0.81727(14) 0.0366(5) Uani 1 1 d . . .
C37 C 0.7692(2) 0.7244(2) 0.83327(14) 0.0345(5) Uani 1 1 d . . .
C7 C 1.0886(3) 0.7453(3) 0.73725(17) 0.0430(6) Uani 1 1 d . . .
C31 C 0.7516(3) 0.4721(3) 0.84422(14) 0.0395(6) Uani 1 1 d . . .
Cl1 Cl 0.68202(11) 0.76755(9) 0.45307(5) 0.0701(3) Uani 1 1 d . . .
C14 C 1.0639(3) 0.7293(3) 0.59320(16) 0.0414(6) Uani 1 1 d . . .
C15 C 1.1332(3) 0.6191(3) 0.57304(16) 0.0423(6) Uani 1 1 d . . .
H15 H 1.1321 0.5522 0.6002 0.051 Uiso 1 1 calc R . .
C9 C 1.0539(3) 0.7765(3) 0.80466(18) 0.0507(7) Uani 1 1 d . . .
H9 H 0.9728 0.7981 0.8194 0.061 Uiso 1 1 calc R . .
C6 C 0.7822(3) 0.9198(3) 0.6027(2) 0.0553(8) Uani 1 1 d . . .
H6 H 0.7998 0.8638 0.5725 0.066 Uiso 1 1 calc R . .

C17 C 1.2046(3) 0.6078(3) 0.51242(18) 0.0526(8) Uani 1 1 d . . .
H17 H 1.2510 0.5334 0.4993 0.063 Uiso 1 1 calc R . .
C8 C 1.1407(4) 0.7752(4) 0.8497(2) 0.0682(11) Uani 1 1 d . . .
H8 H 1.1173 0.7963 0.8944 0.082 Uiso 1 1 calc R . .
C4 C 0.6556(4) 1.1100(4) 0.6327(3) 0.0790(13) Uani 1 1 d . . .
H4 H 0.5881 1.1826 0.6238 0.095 Uiso 1 1 calc R . .
C12 C 1.2127(3) 0.7107(4) 0.7171(2) 0.0661(10) Uani 1 1 d . . .
H12 H 1.2378 0.6878 0.6729 0.079 Uiso 1 1 calc R . .
C5 C 0.6816(4) 1.0275(3) 0.5893(3) 0.0699(11) Uani 1 1 d . . .
H5 H 0.6318 1.0433 0.5505 0.084 Uiso 1 1 calc R . .
C13 C 1.0651(4) 0.8281(3) 0.5510(2) 0.0764(13) Uani 1 1 d . . .
H13 H 1.0174 0.9033 0.5627 0.092 Uiso 1 1 calc R . .
C2 C 0.8312(4) 0.9794(3) 0.7042(2) 0.0621(9) Uani 1 1 d . . .
H2 H 0.8814 0.9655 0.7425 0.074 Uiso 1 1 calc R . .
C10 C 1.2616(5) 0.7426(5) 0.8282(3) 0.0897(16) Uani 1 1 d . . .
H10 H 1.3192 0.7424 0.8583 0.108 Uiso 1 1 calc R . .
C16 C 1.2070(4) 0.7040(4) 0.4726(2) 0.0732(12) Uani 1 1 d . . .
H16 H 1.2555 0.6956 0.4323 0.088 Uiso 1 1 calc R . .
C11 C 1.2970(4) 0.7103(5) 0.7622(3) 0.0928(16) Uani 1 1 d . . .
H11 H 1.3785 0.6882 0.7480 0.111 Uiso 1 1 calc R . .
C3 C 0.7290(5) 1.0863(4) 0.6897(3) 0.0868(15) Uani 1 1 d . . .
H3 H 0.7099 1.1432 0.7195 0.104 Uiso 1 1 calc R . .
C18 C 1.1387(5) 0.8134(4) 0.4910(3) 0.0945(18) Uani 1 1 d . . .
H18 H 1.1411 0.8792 0.4631 0.113 Uiso 1 1 calc R . .
C25 C 0.9145(3) 0.3037(2) 0.74997(17) 0.0407(6) Uani 1 1 d . . .
C24 C 0.6130(3) 0.3988(3) 0.73181(18) 0.0485(7) Uani 1 1 d . . .
H24 H 0.6366 0.3501 0.7746 0.058 Uiso 1 1 calc R . .
C36 C 0.6275(3) 0.5346(3) 0.85809(17) 0.0496(7) Uani 1 1 d . . .
H36 H 0.5706 0.5624 0.8216 0.060 Uiso 1 1 calc R . .
C20 C 0.6374(3) 0.5395(3) 0.64161(16) 0.0435(6) Uani 1 1 d . . .
H20 H 0.6781 0.5856 0.6230 0.052 Uiso 1 1 calc R . .
C23 C 0.5171(3) 0.4022(4) 0.6942(2) 0.0600(9) Uani 1 1 d . . .
H23 H 0.4771 0.3548 0.7116 0.072 Uiso 1 1 calc R . .
C32 C 0.8351(3) 0.4326(3) 0.89963(16) 0.0458(7) Uani 1 1 d . . .
H32 H 0.9189 0.3919 0.8912 0.055 Uiso 1 1 calc R . .
C21 C 0.5404(3) 0.5427(3) 0.60484(19) 0.0565(8) Uani 1 1 d . . .
H21 H 0.5158 0.5910 0.5620 0.068 Uiso 1 1 calc R . .
C22 C 0.4806(3) 0.4740(4) 0.6319(2) 0.0619(10) Uani 1 1 d . . .
H22 H 0.4148 0.4767 0.6076 0.074 Uiso 1 1 calc R . .
C33 C 0.7937(4) 0.4539(4) 0.96723(17) 0.0610(9) Uani 1 1 d . . .
H33 H 0.8499 0.4268 1.0040 0.073 Uiso 1 1 calc R . .
C35 C 0.5875(4) 0.5559(4) 0.9264(2) 0.0648(10) Uani 1 1 d . . .
H35 H 0.5042 0.5984 0.9353 0.078 Uiso 1 1 calc R . .
C34 C 0.6710(4) 0.5143(4) 0.98048(19) 0.0661(10) Uani 1 1 d . . .
H34 H 0.6440 0.5271 1.0262 0.079 Uiso 1 1 calc R . .
C28 C 1.0807(4) 0.0751(4) 0.7355(3) 0.0842(15) Uani 1 1 d . . .

H28 H 1.1369 -0.0016 0.7308 0.101 Uiso 1 1 calc R . .
C30 C 0.9519(4) 0.2163(3) 0.8075(2) 0.0707(11) Uani 1 1 d . . .
H30 H 0.9209 0.2340 0.8519 0.085 Uiso 1 1 calc R . .
C26 C 0.9613(4) 0.2734(3) 0.6849(2) 0.0605(9) Uani 1 1 d . . .
H26 H 0.9366 0.3302 0.6454 0.073 Uiso 1 1 calc R . .
C27 C 1.0448(4) 0.1591(4) 0.6780(3) 0.0753(12) Uani 1 1 d . . .
H27 H 1.0765 0.1396 0.6340 0.090 Uiso 1 1 calc R . .
C29 C 1.0350(5) 0.1033(4) 0.7990(3) 0.0916(16) Uani 1 1 d . . .
H29 H 1.0599 0.0455 0.8380 0.110 Uiso 1 1 calc R . .
C43 C 0.5088(3) 0.8854(3) 0.67311(19) 0.0534(8) Uani 1 1 d . . .
H43 H 0.4554 0.9220 0.6351 0.064 Uiso 1 1 calc R . .
C38 C 0.7423(3) 0.7576(3) 0.89985(17) 0.0481(7) Uani 1 1 d . . .
H38 H 0.8022 0.7244 0.9348 0.058 Uiso 1 1 calc R . .
C44 C 0.6254(3) 0.7955(3) 0.66382(16) 0.0431(6) Uani 1 1 d . . .
H44 H 0.6469 0.7719 0.6195 0.052 Uiso 1 1 calc R . .
C39 C 0.6251(3) 0.8410(3) 0.91432(18) 0.0537(8) Uani 1 1 d . . .
H39 H 0.6078 0.8624 0.9593 0.064 Uiso 1 1 calc R . .
C40 C 0.5363(3) 0.8914(3) 0.86519(19) 0.0501(7) Uani 1 1 d . . .
C42 C 0.4739(3) 0.9189(3) 0.7373(2) 0.0542(8) Uani 1 1 d . . .
H42 H 0.3956 0.9772 0.7439 0.065 Uiso 1 1 calc R . .
C41 C 0.5563(3) 0.8654(3) 0.79449(17) 0.0424(6) Uani 1 1 d . . .
N4 N 0.4156(3) 0.9751(3) 0.8866(2) 0.0668(9) Uani 1 1 d . . .
O2 O 0.4103(3) 1.0220(3) 0.9380(2) 0.0949(11) Uani 1 1 d . . .
O3 O 0.3251(3) 0.9884(5) 0.8553(2) 0.1232(17) Uani 1 1 d . . .
C47 C 1.1906(3) 0.4147(3) 0.85188(16) 0.0442(6) Uani 1 1 d . . .
H47 H 1.2038 0.4223 0.8976 0.053 Uiso 1 1 calc R . .
C49 C 1.2614(3) 0.3135(3) 0.74951(17) 0.0442(6) Uani 1 1 d . . .
H49 H 1.3217 0.2533 0.7278 0.053 Uiso 1 1 calc R . .
C48 C 1.2788(3) 0.3305(3) 0.81663(18) 0.0478(7) Uani 1 1 d . . .
C50 C 1.1512(2) 0.3887(2) 0.71536(15) 0.0378(5) Uani 1 1 d . . .
H50 H 1.1382 0.3794 0.6700 0.045 Uiso 1 1 calc R . .
C51 C 0.9818(2) 0.5790(2) 0.85400(14) 0.0358(5) Uani 1 1 d . . .
O4 O 0.9901(2) 0.5941(2) 0.91409(11) 0.0488(5) Uani 1 1 d . . .
O7 O 0.6517(8) 0.6932(8) 0.4211(5) 0.224(4) Uani 1 1 d . . .
O6 O 0.6663(7) 0.8447(6) 0.3964(4) 0.220(4) Uani 1 1 d . . .
O8 O 0.7977(8) 0.7163(7) 0.4771(6) 0.271(5) Uani 1 1 d . . .
O5 O 0.5945(9) 0.8223(11) 0.4989(3) 0.290(6) Uani 1 1 d . . .
N6 N 1.3983(3) 0.2545(3) 0.85178(19) 0.0671(9) Uani 1 1 d . . .
O10 O 1.4781(3) 0.1812(3) 0.81900(17) 0.0859(10) Uani 1 1 d . . .
O9 O 1.4125(3) 0.2685(4) 0.9108(2) 0.1083(14) Uani 1 1 d . . .
Cl2 Cl 0.7107(3) 0.2102(3) 0.9670(2) 0.1987(13) Uani 1 1 d . . .
Cl3 Cl 0.8448(6) -0.0081(7) 0.9243(6) 0.563(9) Uani 1 1 d . . .
C54 C 0.7171(8) 0.0918(8) 0.9379(5) 0.147(3) Uani 1 1 d . . .
H54A H 0.6738 0.0574 0.9714 0.177 Uiso 1 1 calc R . .
H54B H 0.6712 0.1176 0.8942 0.177 Uiso 1 1 calc R . .

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P2 0.0312(3) 0.0325(3) 0.0315(3) -0.0030(2) -0.0023(2) -0.0154(3)
P1 0.0314(3) 0.0305(3) 0.0355(3) -0.0069(2) 0.0011(3) -0.0145(3)
N2 0.0332(10) 0.0352(11) 0.0289(10) -0.0079(8) -0.0002(8) -0.0145(9)
N3 0.0352(11) 0.0355(11) 0.0340(11) -0.0048(9) -0.0028(9) -0.0162(9)
N1 0.0319(10) 0.0346(11) 0.0335(10) -0.0036(8) -0.0021(8) -0.0132(9)
C53 0.0313(11) 0.0332(12) 0.0347(12) -0.0027(10) -0.0034(10) -0.0148(10)
C1 0.0366(13) 0.0317(13) 0.0503(16) -0.0024(11) 0.0021(12) -0.0150(11)
C45 0.0350(12) 0.0327(12) 0.0378(13) -0.0067(10) 0.0024(10) -0.0157(10)
C19 0.0319(12) 0.0379(13) 0.0427(14) -0.0114(11) -0.0018(10) -0.0164(10)
O1 0.0728(16) 0.0710(16) 0.0347(11) -0.0233(10) 0.0057(10) -0.0348(13)
C46 0.0360(13) 0.0378(13) 0.0366(13) -0.0042(10) -0.0036(10) -0.0159(11)
C37 0.0358(12) 0.0348(13) 0.0352(12) -0.0089(10) 0.0030(10) -0.0162(10)
C7 0.0416(14) 0.0362(14) 0.0549(17) -0.0060(12) -0.0107(13) -0.0185(11)
C31 0.0474(15) 0.0442(15) 0.0325(13) -0.0035(11) 0.0019(11) -0.0255(12)
Cl1 0.0856(7) 0.0601(5) 0.0513(5) -0.0034(4) -0.0197(5) -0.0168(5)
C14 0.0428(14) 0.0421(15) 0.0412(14) -0.0055(11) 0.0092(12) -0.0210(12)
C15 0.0425(14) 0.0454(15) 0.0411(14) -0.0084(12) 0.0049(12) -0.0205(12)
C9 0.0606(19) 0.0466(17) 0.0537(18) -0.0085(14) -0.0068(15) -0.0295(15)
C6 0.0524(18) 0.0434(17) 0.069(2) 0.0021(15) -0.0132(16) -0.0203(14)
C17 0.0495(17) 0.062(2) 0.0482(17) -0.0163(15) 0.0106(14) -0.0234(15)
C8 0.090(3) 0.062(2) 0.060(2) -0.0069(18) -0.026(2) -0.036(2)
C4 0.052(2) 0.044(2) 0.122(4) 0.008(2) -0.004(2) -0.0074(16)
C12 0.0412(17) 0.071(2) 0.088(3) -0.030(2) -0.0055(17) -0.0186(16)
C5 0.055(2) 0.052(2) 0.096(3) 0.017(2) -0.022(2) -0.0223(17)
C13 0.085(3) 0.047(2) 0.090(3) -0.0077(19) 0.041(2) -0.0272(19)
C2 0.061(2) 0.0422(17) 0.074(2) -0.0168(16) -0.0005(18) -0.0104(15)
C10 0.074(3) 0.089(3) 0.109(4) -0.017(3) -0.046(3) -0.030(2)
C16 0.074(3) 0.074(3) 0.059(2) -0.0017(19) 0.026(2) -0.027(2)
C11 0.047(2) 0.101(4) 0.131(5) -0.028(3) -0.024(3) -0.024(2)
C3 0.076(3) 0.047(2) 0.117(4) -0.025(2) 0.005(3) -0.003(2)
C18 0.108(4) 0.064(3) 0.093(3) 0.009(2) 0.052(3) -0.033(3)
C25 0.0353(13) 0.0340(13) 0.0547(17) -0.0065(12) -0.0016(12) -0.0161(11)
C24 0.0441(15) 0.0525(17) 0.0571(18) -0.0069(14) -0.0024(14) -0.0279(14)
C36 0.0484(16) 0.0584(19) 0.0426(16) -0.0104(14) 0.0037(13) -0.0224(15)
C20 0.0407(14) 0.0469(16) 0.0437(15) -0.0069(12) -0.0060(12) -0.0182(12)
C23 0.0438(17) 0.068(2) 0.082(3) -0.0183(19) -0.0001(17) -0.0348(16)
C32 0.0496(16) 0.0552(18) 0.0392(14) 0.0009(13) -0.0065(12) -0.0301(14)

C21 0.0474(17) 0.066(2) 0.0519(18) -0.0123(16) -0.0147(15) -0.0166(16)
C22 0.0363(15) 0.079(3) 0.078(3) -0.031(2) -0.0094(16) -0.0240(16)
C33 0.081(3) 0.083(3) 0.0349(15) -0.0010(16) -0.0081(16) -0.050(2)
C35 0.061(2) 0.083(3) 0.058(2) -0.027(2) 0.0214(18) -0.035(2)
C34 0.087(3) 0.091(3) 0.0404(17) -0.0197(18) 0.0115(18) -0.054(2)
C28 0.059(2) 0.042(2) 0.139(5) -0.017(3) -0.009(3) -0.0067(17)
C30 0.085(3) 0.0445(19) 0.065(2) 0.0009(17) -0.010(2) -0.0116(18)
C26 0.072(2) 0.0433(17) 0.066(2) -0.0140(16) 0.0155(18) -0.0240(16)
C27 0.074(3) 0.058(2) 0.099(3) -0.036(2) 0.027(2) -0.029(2)
C29 0.110(4) 0.044(2) 0.088(3) -0.002(2) -0.028(3) -0.001(2)
C43 0.0393(15) 0.0526(18) 0.0562(19) -0.0010(15) -0.0113(14) -0.0084(13)
C38 0.0498(17) 0.0523(17) 0.0425(15) -0.0162(13) 0.0018(13) -0.0190(14)
C44 0.0418(14) 0.0458(16) 0.0382(14) -0.0041(12) -0.0053(12) -0.0150(12)
C39 0.0590(19) 0.0577(19) 0.0457(16) -0.0250(15) 0.0145(15) -0.0221(16)
C40 0.0422(15) 0.0479(17) 0.0594(19) -0.0236(15) 0.0158(14) -0.0151(13)
C42 0.0375(15) 0.0448(17) 0.068(2) -0.0094(15) 0.0007(14) -0.0056(12)
C41 0.0383(14) 0.0367(14) 0.0518(16) -0.0109(12) 0.0072(12) -0.0148(11)
N4 0.0512(17) 0.067(2) 0.072(2) -0.0256(17) 0.0179(16) -0.0122(15)
O2 0.080(2) 0.093(2) 0.095(2) -0.056(2) 0.0230(18) -0.0085(17)
O3 0.0475(17) 0.182(4) 0.119(3) -0.080(3) 0.0149(19) -0.011(2)
C47 0.0403(14) 0.0477(16) 0.0403(14) -0.0021(12) -0.0113(12) -0.0140(12)
C49 0.0376(14) 0.0391(15) 0.0498(16) -0.0055(12) 0.0008(12) -0.0107(11)
C48 0.0380(14) 0.0437(16) 0.0535(17) 0.0005(13) -0.0108(13) -0.0103(12)
C50 0.0343(12) 0.0392(14) 0.0389(13) -0.0074(11) 0.0016(11) -0.0144(11)
C51 0.0373(13) 0.0404(14) 0.0311(12) -0.0050(10) -0.0026(10) -0.0172(11)
O4 0.0484(12) 0.0600(13) 0.0357(10) -0.0132(9) -0.0091(9) -0.0175(10)
O7 0.215(8) 0.230(8) 0.275(9) -0.149(8) -0.016(7) -0.101(7)
O6 0.154(6) 0.166(6) 0.240(8) 0.107(6) 0.015(5) -0.018(4)
O8 0.214(8) 0.173(6) 0.376(12) 0.039(7) -0.222(9) -0.028(5)
O5 0.223(8) 0.488(16) 0.095(4) -0.135(7) 0.016(5) -0.060(10)
N6 0.0479(16) 0.065(2) 0.069(2) -0.0026(16) -0.0174(15) -0.0044(14)
O10 0.0471(14) 0.090(2) 0.079(2) -0.0075(17) -0.0071(14) 0.0103(14)
O9 0.076(2) 0.109(3) 0.098(3) -0.029(2) -0.050(2) 0.0134(19)
Cl2 0.212(3) 0.176(2) 0.259(3) -0.102(2) 0.050(3) -0.114(2)
Cl3 0.358(8) 0.560(12) 1.03(2) -0.627(14) 0.454(11) -0.336(9)
C54 0.112(6) 0.157(7) 0.171(8) -0.056(6) -0.018(5) -0.042(5)

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;
All esds (except the esd in the dihedral angle between two l.s. planes)
are estimated using the full covariance matrix. The cell esds are taken
into account individually in the estimation of esds in distances, angles
and torsion angles; correlations between esds in cell parameters are only
used when they are defined by crystal symmetry. An approximate (isotropic)
treatment of cell esds is used for estimating esds involving l.s. planes.
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P2 C31 1.821(3) . ?
P2 C25 1.827(3) . ?
P1 C1 1.809(3) . ?
P1 C7 1.822(3) . ?
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N2 C37 1.398(3) . ?
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C45 C37 1.434(4) . ?
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C7 C12 1.409(5) . ?
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C31 C32 1.393(4) . ?
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Cl1 O7 1.375(6) . ?
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C14 C13 1.389(5) . ?
C15 C17 1.390(4) . ?
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C8 H8 0.9300 . ?
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Ru1 N1 C45 C37 4.3(3) . . . . ?
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Ru1 C53 C46 C51 2.4(3) . . . . ?
C51 N2 C37 C38 -1.0(4) . . . . ?
Ru1 N2 C37 C38 175.9(2) . . . . ?
C51 N2 C37 C45 -180.0(2) . . . . ?
Ru1 N2 C37 C45 -3.1(3) . . . . ?
N1 C45 C37 C38 179.9(3) . . . . ?
C41 C45 C37 C38 0.7(4) . . . . ?
N1 C45 C37 N2 -1.0(3) . . . . ?
C41 C45 C37 N2 179.8(2) . . . . ?
C1 P1 C7 C9 59.5(3) . . . . ?
C14 P1 C7 C9 168.6(3) . . . . ?
Ru1 P1 C7 C9 -64.8(3) . . . . ?
C1 P1 C7 C12 -121.7(3) . . . . ?
C14 P1 C7 C12 -12.7(3) . . . . ?
Ru1 P1 C7 C12 113.9(3) . . . . ?
C19 P2 C31 C36 -26.6(3) . . . . ?
C25 P2 C31 C36 -135.3(3) . . . . ?
Ru1 P2 C31 C36 98.9(2) . . . . ?

C19 P2 C31 C32 160.4(2) . . . . ?
C25 P2 C31 C32 51.7(3) . . . . ?
Ru1 P2 C31 C32 -74.1(3) . . . . ?
C1 P1 C14 C15 -155.8(3) . . . . ?
C7 P1 C14 C15 91.8(3) . . . . ?
Ru1 P1 C14 C15 -35.7(3) . . . . ?
C1 P1 C14 C13 27.8(4) . . . . ?
C7 P1 C14 C13 -84.6(3) . . . . ?
Ru1 P1 C14 C13 147.9(3) . . . . ?
C13 C14 C15 C17 1.3(5) . . . . ?
P1 C14 C15 C17 -175.2(3) . . . . ?
C12 C7 C9 C8 1.3(5) . . . . ?
P1 C7 C9 C8 -179.9(3) . . . . ?
C2 C1 C6 C5 -1.5(5) . . . . ?
P1 C1 C6 C5 175.4(3) . . . . ?
C14 C15 C17 C16 -0.1(6) . . . . ?
C7 C9 C8 C10 -0.3(6) . . . . ?
C9 C7 C12 C11 -1.5(6) . . . . ?
P1 C7 C12 C11 179.7(4) . . . . ?
C3 C4 C5 C6 -0.1(7) . . . . ?
C1 C6 C5 C4 0.5(6) . . . . ?
C15 C14 C13 C18 -1.9(7) . . . . ?
P1 C14 C13 C18 174.6(4) . . . . ?
C6 C1 C2 C3 2.1(6) . . . . ?
P1 C1 C2 C3 -174.6(4) . . . . ?
C9 C8 C10 C11 -0.4(7) . . . . ?
C15 C17 C16 C18 -0.5(7) . . . . ?
C7 C12 C11 C10 0.8(8) . . . . ?
C8 C10 C11 C12 0.2(9) . . . . ?
C5 C4 C3 C2 0.7(8) . . . . ?
C1 C2 C3 C4 -1.7(8) . . . . ?
C17 C16 C18 C13 -0.1(9) . . . . ?
C14 C13 C18 C16 1.3(9) . . . . ?
C19 P2 C25 C26 66.2(3) . . . . ?
C31 P2 C25 C26 177.0(3) . . . . ?
Ru1 P2 C25 C26 -59.0(3) . . . . ?
C19 P2 C25 C30 -113.1(3) . . . . ?
C31 P2 C25 C30 -2.4(4) . . . . ?
Ru1 P2 C25 C30 121.6(3) . . . . ?
C20 C19 C24 C23 -0.4(5) . . . . ?
P2 C19 C24 C23 -176.9(3) . . . . ?
C32 C31 C36 C35 -0.7(5) . . . . ?
P2 C31 C36 C35 -173.9(3) . . . . ?
C24 C19 C20 C21 1.0(5) . . . . ?
P2 C19 C20 C21 177.4(3) . . . . ?
C19 C24 C23 C22 -0.7(6) . . . . ?

C36 C31 C32 C33 1.2(5) . . . . ?
P2 C31 C32 C33 174.3(3) . . . . ?
C19 C20 C21 C22 -0.5(5) . . . . ?
C24 C23 C22 C21 1.3(6) . . . . ?
C20 C21 C22 C23 -0.7(6) . . . . ?
C31 C32 C33 C34 -0.4(5) . . . . ?
C31 C36 C35 C34 -0.5(6) . . . . ?
C32 C33 C34 C35 -0.8(6) . . . . ?
C36 C35 C34 C33 1.3(6) . . . . ?
C26 C25 C30 C29 0.9(7) . . . . ?
P2 C25 C30 C29 -179.7(4) . . . . ?
C30 C25 C26 C27 -1.0(6) . . . . ?
P2 C25 C26 C27 179.6(3) . . . . ?
C29 C28 C27 C26 0.0(8) . . . . ?
C25 C26 C27 C28 0.6(7) . . . . ?
C27 C28 C29 C30 -0.1(9) . . . . ?
C25 C30 C29 C28 -0.4(9) . . . . ?
N2 C37 C38 C39 -178.3(3) . . . . ?
C45 C37 C38 C39 0.7(4) . . . . ?
C45 N1 C44 C43 -0.7(4) . . . . ?
Ru1 N1 C44 C43 179.5(2) . . . . ?
C42 C43 C44 N1 -1.9(5) . . . . ?
C37 C38 C39 C40 -0.3(5) . . . . ?
C38 C39 C40 C41 -1.5(6) . . . . ?
C38 C39 C40 N4 178.2(3) . . . . ?
C44 C43 C42 C41 1.7(5) . . . . ?
C43 C42 C41 C45 1.0(5) . . . . ?
C43 C42 C41 C40 178.4(3) . . . . ?
N1 C45 C41 C42 -3.7(4) . . . . ?
C37 C45 C41 C42 175.4(3) . . . . ?
N1 C45 C41 C40 178.6(3) . . . . ?
C37 C45 C41 C40 -2.3(4) . . . . ?
C39 C40 C41 C42 -174.7(3) . . . . ?
N4 C40 C41 C42 5.7(5) . . . . ?
C39 C40 C41 C45 2.7(5) . . . . ?
N4 C40 C41 C45 -176.9(3) . . . . ?
C39 C40 N4 O2 22.2(6) . . . . ?
C41 C40 N4 O2 -158.1(4) . . . . ?
C39 C40 N4 O3 -152.8(5) . . . . ?
C41 C40 N4 O3 26.8(6) . . . . ?
C53 C46 C47 C48 0.0(4) . . . . ?
C51 C46 C47 C48 178.5(3) . . . . ?
C46 C47 C48 C49 -2.4(5) . . . . ?
C46 C47 C48 N6 177.4(3) . . . . ?
C50 C49 C48 C47 2.8(5) . . . . ?
C50 C49 C48 N6 -177.0(3) . . . . ?

C48 C49 C50 C53 -0.9(4) . . . . ?
C46 C53 C50 C49 -1.3(4) . . . . ?
Ru1 C53 C50 C49 179.7(2) . . . . ?
C37 N2 C51 O4 -4.4(4) . . . . ?
Ru1 N2 C51 O4 178.7(2) . . . . ?
C37 N2 C51 C46 174.5(2) . . . . ?
Ru1 N2 C51 C46 -2.4(3) . . . . ?
C47 C46 C51 O4 0.4(4) . . . . ?
C53 C46 C51 O4 178.9(3) . . . . ?
C47 C46 C51 N2 -178.6(3) . . . . ?
C53 C46 C51 N2 -0.1(3) . . . . ?
C47 C48 N6 O9 1.3(6) . . . . ?
C49 C48 N6 O9 -178.9(4) . . . . ?
C47 C48 N6 O10 -178.1(4) . . . . ?
C49 C48 N6 O10 1.7(5) . . . . ?

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_refine_diff_density_rms 0.115

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