Electronic Supplementary Material (ESI) for Inorganic Chemistry Frontiers.

Supporting Information

Heterometallic ruthenium-osmium complexes: dual photodynamic and photothermal therapy for melanoma and drug-resistant lung tumor in vivo

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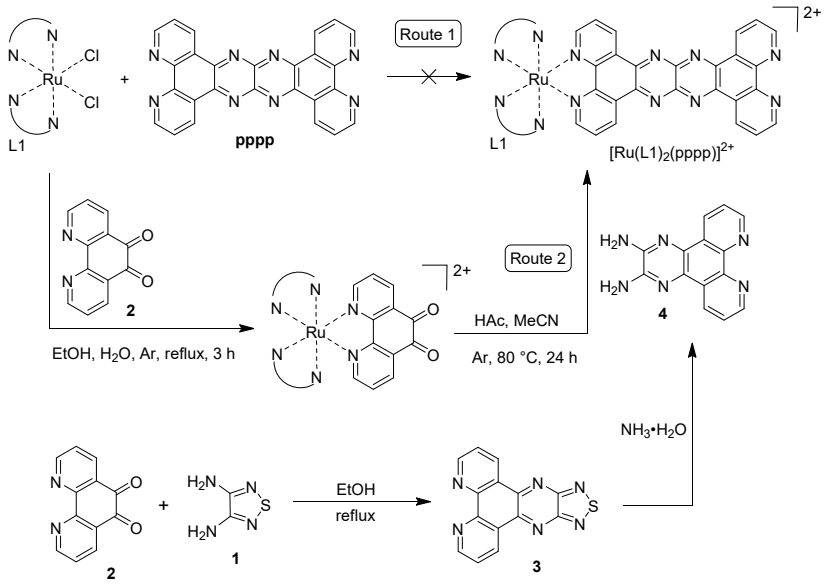
1. General

Instruments. ^{1}H and ^{13}C NMR spectra were recorded on a Bruker AVANCE NEO 400 MHz spectrometer. All chemical shifts are given relative to tetramethylsilane (TMS). Electron Spray ionization mass spectra (ESI-MS) were recorded on AB QSTAR Pulsar mass spectrometer. Microanalysis (C, H, and N) was carried out with a Perkin-Elmer 240Q elemental analyzer. High-performance liquid chromatography (HPLC) was record on an Agilent 1260 Infinity II system fitted with a RP-C18 column (Gemini-NX C18, 4.6 mm×250 mm, 25 °C) and a diode array detector. Solvent A (H_2O−0.1% HCOOH) and solvent B (CH_3CN) were used as the mobile phases which was eluted at a flow rate of 1 mL/min with the following gradient: 10%−100% B (0−30 min). UV−Vis spectra were recorded on a Perkin-Elmer Lambda 365 spectrophotometer equipped with a temperature controller accessory and circulating water system. Fluorescence spectra were recorded on a Hitachi F-4700 fluorescence spectrophotometer. Time-resolved photoluminescence spectra was tested on an Edinburgh FLS1000 Photoluminescence Spectrometer. FT-IR spectra were recorded on a Nicolet iS 10 FTIR spectrometer. Two-photon photoluminescence spectra were recorded on a SpectroPro300i instrument, and the pump laser beam came from a Ti:sapphire laser system (pulse duration, 200 fs; repetition rate, 76 MHz; Coherent Mira900-D). TPA cross-sections were measured by using the two-photon-induced fluorescence.

Materials. Potassium phthalimide, 3,4-dichloro-1,2,5-thiadiazole, acetonitrile (MeCN) and methylamine hydrochloride were purchased from Adamas-beta were synthesized according to the literature methods. CD_3CN and DMSO-d_6 were purchased from Energy Chemical. Aluminium oxide (200−300 mesh), ammonium hydroxide, ethylene glycol (ethylene glycol), ethanol (EtOH), N,N-dimethylformamide (DMF), trichloromethane ($CHCl_3$), acetone and toluene were purchased from Greagent. The compounds 3,4-diamino-1,2,5-thiadiazole (**1**), 1,10-phenanthroline-5,6-dione (**2**), [1,2,5]thiadiazolo[3',4':5,6]pyrazino[2,3-*f*][1,10]phenanthroline (**3**), pyrazino[2,3-*f*][1,10]phenanthroline-2,3-diamine (**4**), *cis*-$[Ru(L1)_2Cl_2]\cdot 2H_2O$ (L1 = bpy, phen, dip, or tbubpy, where bpy = 2,2'-bipyridine, phen = 1,10-phenanthroline, dip = 4,7-diphenyl-1,10-phenanthroline, and tbubpy = 4,4'-di-*tert*-butyl-2,2'-bipyridine), *cis*-$[Os(L2)_2Cl_2]\cdot 2H_2O$ (L2 = bpy, phen, dip, or tbubpy, where bpy = 2,2'-bipyridine, phen = 1,10-phenanthroline, dip = 4,7-diphenyl-1,10-phenanthroline, and tbubpy = 4,4'-di-*tert*-butyl-2,2'-bipyridine) were synthesized according to the literature.[1-4]

2. Synthesis and Characterization

2.1. Preparation of mononuclear precursors $[Ru(L1)_2(pppp)]^{2+}$:



Scheme S1. Synthetic route to the mononuclear $[Ru(L1)_2(pppp)]^{2+}$ precursors.

1,10-Phenanthroline-5,6-dione (**2**, 252 mg, 1.2 mmol) was refluxed with *cis*-$[Ru(L1)_2Cl_2]$ (1 mmol) in 30 mL of water/EtOH (1:1, v/v) for 3 h under Ar. The dark red solution was cooled to 20 °C. After removal of EtOH, NH_4PF_6 (1 g, 6.2 mmol) was added and stirred for 0.5 h. $[Ru(L1)_2(phendione)](PF_6)_2$ precipitated as brown solid, which was isolated by suction filtration, washed by small amount of water, EtOH and diethyl ether (3 × 10 mL), and dried in vacuo. The ligand pyrazino[2,3-*f*][1,10]phenanthroline-2,3-diamine (**4**, 157 mg, 0.6 mmol) was stirred with $[Ru(L1)_2(phendione)]$ (0.6 mmol) in 50 mL of MeCN/HAc (1:1, v/v) at 80 °C for 24 h under Ar. After removal of MeCN, the dark red solution was poured into 80 mL of water and neutralized with ammonia (1 M). The mononuclear $[Ru(L1)_2(pppp)](PF_6)_2$ precursors precipitated as red solid, which was isolated by suction filtration, washed by small amount of water, EtOH and diethyl ether (3 × 10 mL), and dried in vacuo. The crude product was purified by flash column chromatography on alumina (200–300 mesh) with MeCN/Tol (1:1−2:1) as eluent.

$[Ru(bpy)_2(pppp)](PF_6)_2$: Yield 536 mg, 76%. ^{1}H NMR (400 MHz, DMSO-d_6): 9.67 (s, 4H), 9.21 (s, 2H),8.92 (t, J = 9.6 Hz, 4H), 8.35 (s, 2H), 8.26 (td, J = 7.9, 1.5 Hz, 2H), 8.17 (td, J = 7.9, 1.5 Hz, 2H), 8.10 (s, 2H), 8.04 (s, 2H), 7.90 (d, J = 5.7 Hz, 2H), 7.85 (d, J = 5.2 Hz, 2H), 7.63 (t, J = 6.3 Hz, 2H), 7.45 (t, J = 6.3 Hz, 2H). MS (ESI) calcd for $C_{46}H_{28}N_{12}Ru$ $[M-2PF_6]^{2+}$: 425.08; Found: 425.04.

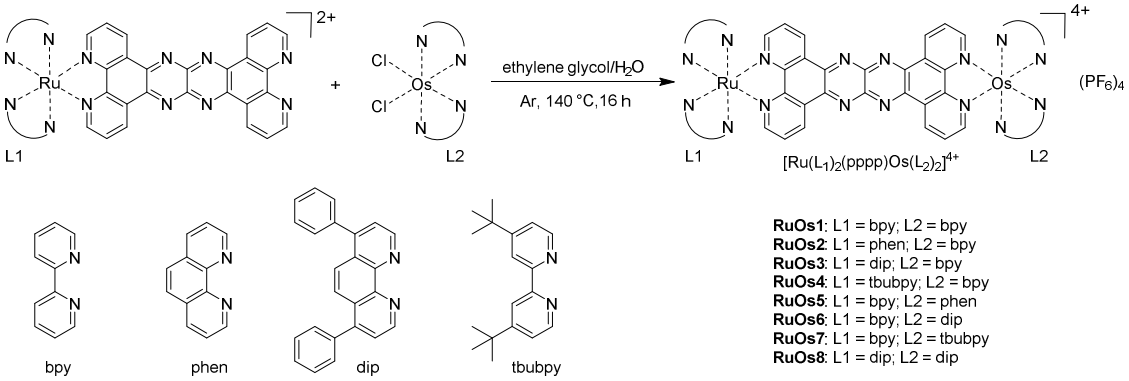
$[Ru(phen)_2(pppp)](PF_6)_2$: Yield 603 mg, 82%. ^{1}H NMR (400 MHz, DMSO-d_6): 9.55 (d, J = 39.7 Hz, 4H),

8.84 (t, J = 7.5 Hz, 4H), 8.78 (d, J = 7.5 Hz,2H), 8.54 (s, 2H), 8.44 (s, 4H), 8.39 (s, 2H), 8.11 (d, J = 5.4 Hz, 2H), 7.96 (s, 2H), 7.89 (t, J = 13.6 Hz, 2H), 7.82 (dd, J = 8.3, 5.3 Hz, 2H), 7.77 (dd, J = 8.3, 5.0 Hz, 2H). MS (ESI) calcd for $C_{50}H_{28}N_{12}Ru$ $[M-2PF_6]^{2+}$: 450.08; Found: 450.19.

$[Ru(dip)_2(pppp)](PF_6)_2$: Yield 660 mg, 72%. ^1H NMR (400 MHz, DMSO-d_6): 9.64 (d, J = 8.1 Hz, 4H), 9.11 (s, 2H), 8.58 (d, J = 5.5 Hz, 2H), 8.45 (s, 2H), 8.37 (d, J = 5.5 Hz, 2H), 8.31 (s, 4H), 8.07 (t, J = 6.9 Hz, 2H), 8.02 (s, 2H), 7.87 (d, J = 5.5 Hz, 4H), 7.76–7.63 (m, 20H). MS (ESI) calcd for $C_{50}H_{28}N_{12}Ru$ $[M-2PF_6]^{2+}$: 601.14; Found: 600.33.

$[Ru(tbubpy)_2(pppp)](PF_6)_2$: Yield 622 mg, 74%. ^1H NMR (400 MHz, DMSO-d_6): 9.54 (d, J = 33.4 Hz, 4H), 8.91 (d, J = 6.9 Hz, 6H), 8.29 (s, 2H), 8.08 (s, 2H), 7.98 (s, 2H), 7.88 (s, 2H), 7.76–7.61 (m, 4H), 7.45 (dd, J = 6.4, 1.8 Hz, 2H). MS (ESI) calcd for $C_{62}H_{60}N_{12}Ru$ $[M-2PF_6]^{2+}$: 537.20; Found: 537.20.

2.2. Preparation of hetero-dinuclear complexes $[Ru(L1)_2(pppp)Os(L2)_2]^{2+}$ (RuOs1−8):



Scheme S2. Synthetic route to the heteronuclear $[Ru(L1)_2(pppp)Os(L2)_2]^{2+}$.

$[Ru(L1)_2(pppp)](PF_6)_2$ (0.2 mmol) was stirred with *cis*-$[Os(L2)_2Cl_2]$ (0.22 mmol, 1.1 eq.), 1 mL water and 6 mL EG under Ar at 140 °C for 16 h. The black solution was cooled to 20 °C and poured into water (20 mL). Upon addition of NH_4PF_6 (1 g, 6.2 mmol) in water (5 mL), the heteronuclear Ru(II)-Os(II) complexes $[Ru(L1)_2(pppp)Os(L2)_2](PF_6)_4$ precipitated as black solid, which was isolated by suction filtration, washed by small amount of water, EtOH and diethyl ether (3 × 10 mL), and dried in vacuo. The crude product was purified by flash column chromatography on alumina (200–300 mesh) with MeCN/Tol (1:1−4:1) as eluent.

RuOs1 (L1 = bpy, L2 = bpy): dark brown solid. Yield 319 mg, 81%. Anal. Calcd for $C_{66}H_{44}F_{24}N_{16}P_4OsRu\cdot 2H_2O$: C, 40.27; H, 2.46; N, 11.39. Found: C, 39.99; H: 2.71; N: 11.12. ^1H NMR (400 MHz, DMSO-d_6) δ 9.78 (d, J = 8.1 Hz, 2H), 9.55 (d, J = 8.2 Hz, 2H), 8.90 (d, J = 17.2 Hz, 2H), 8.36 (d, J = 5.4 Hz, 2H), 8.30 (d, J = 5.2 Hz, 2H), 8.26 (t, J = 8.2 Hz, 2H), 8.17 (t, J = 7.7 Hz, 2H), 8.11 (t, J = 6.8 Hz, 2H), 8.06

(t, J = 7.6 Hz, 2H), 7.99 (q, J = 7.2 Hz, 4H), 7.85 (d, J = 5.6 Hz, 2H), 7.81 (d, J = 5.6 Hz, 1H), 7.76 (d, J = 5.6 Hz, 2H), 7.70 (d, J = 5.6 Hz, 2H), 7.63 (t, J = 6.7 Hz, 2H), 7.54 (t, J = 6.7 Hz, 2H), 7.43 (t, J = 6.8 Hz, 2H), 7.33 (t, J = 6.8 Hz, 2H). ^{13}C NMR (100 MHz, DMSO-d_6): δ 158.85, 158.47, 158.32, 156.71, 156.48, 152.04, 151.34, 138.19, 138.08, 137.61, 128.42, 127.99, 124.81, 124.65. MS (ESI) calcd for $C_{66}H_{44}N_{16}OsRu$ $[M-4PF_6]^{4+}$: 338.5643; Found: 338.5649. FTIR (KBr) ν_{max} (cm^{-1}): 3067 (CH, aryl), 2924 (CH, aryl), 2853 (CH, aryl), 1659 (C=C, aryl), 1603 (C=C, aryl), 1463 (C=C, aryl), 1445 (C=C, aryl), 1424 (CH, aryl), 1359 (CN, pyridyl), 1312 (CN, pyridyl), 1267 (CN, pyridyl), 1161 (CN, pyrazine), 1074 (CN, pyrazine), 1024 (CH, aryl), 841 (PF), 764 (C=C, aryl), 727 (C=C, aryl), 661 (CH, aryl), 558 (PF).

RuOs2 (L1 = phen, L2 = bpy): dark brown solid. Yield 295 mg, 73%. Anal. Calcd for $C_{70}H_{44}F_{24}N_{16}P_4OsRu\cdot 2H_2O$: C, 41.70; H, 2.40; N, 11.11. Found: C, 41.46; H, 2.67; N, 10.83. ^{1}H NMR (400 MHz, DMSO-d_6): 9.76 (d, J = 8.2 Hz, 2H), 9.55 (d, J = 8.1 Hz, 2H), 8.89 (dd, J = 12.0, 5.3 Hz, 4H), 8.82 (dd, J = 10.0, 5.6 Hz, 4H), 8.43 (s, 4H), 8.32 (s, 2H), 8.31 (d, J = 3.7 Hz, 2H), 8.08(d, J=3.4 Hz, 2H), 8.05 (t, J = 5.3 Hz, 2H), 8.00 (dd, J = 8.2, 4.7 Hz, 6H), 7.86 (dd, J = 8.3, 5.3 Hz, 2H), 7.80 (dd, J = 8.3, 5.3 Hz, 2H), 7.77 (d, J = 5.7 Hz, 2H), 7.72 (s, 2H), 7.54 (t, J = 4.4 Hz, 2H), 7.33 (t, J = 4.4 Hz, 2H). ^{13}C NMR (100 MHz, DMSO-d_6): δ 158.51, 158.38, 155.18, 154.20, 153.63, 153.28, 152.71, 151.98, 151.18, 150.55, 147.14, 147.09, 145.63, 143.48, 137.62, 137.52, 137.08, 134.24, 133.45, 130.53, 130.50, 130.16, 129.72, 128.70, 128.42, 128.15, 128.08, 126.39, 126.21, 124.72, 124.65. MS (ESI) calcd for $C_{70}H_{44}N_{16}OsRu$ $[M-4PF_6]^{4+}$: 350.5643; Found: 350.5637. FTIR (KBr) ν_{max} (cm^{-1}): 3066 (CH, aryl), 2923 (CH, aryl), 2852 (CH, aryl), 1667 (C=C, aryl), 1428 (CH, aryl), 1358 (CN, pyridyl), 1312 (CN, pyridyl), 1118 (CN, pyrazine), 1073 (CN, pyrazine), 839 (PF), 720 (C=C, aryl), 557 (PF).

RuOs3 (L1 = dip, L2 = bpy): dark brown solid. Yield 330 mg, 71%. Anal. Calcd for $C_{94}H_{60}F_{24}N_{16}P_4OsRu\cdot 2H_2O$: C, 48.65; H, 2.78; N, 9.66. Found: C, 48.39; H, 2.97; N, 9.42. ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.82 (d, J = 8.2 Hz, 2H), 9.55 (d, J = 8.1 Hz, 2H), 8.89 (dd, J = 13.0, 8.1 Hz, 4H), 8.45 (dd, J = 10.4, 5.4 Hz, 4H), 8.36 (d, J = 5.4 Hz, 2H), 8.33–8.27 (m, 6H), 8.08 (dt, J = 16.1, 7.3 Hz, 4H), 8.00 (q, J = 8.4, 7.6 Hz, 4H), 7.86 (d, J = 5.5 Hz, 4H), 7.76 (d, J = 5.6 Hz, 2H), 7.72–7.63 (m, 22H), 7.54 (t, J = 6.8 Hz, 2H), 7.33 (t, J = 6.8 Hz, 2H). ^{13}C NMR (100 MHz, DMSO-d_6): δ 158.57, 158.49, 158.43, 152.89, 152.60, 151.27, 150.58, 150.34, 148.23, 148.02, 137.71, 137.31, 135.50, 135.43, 130.02, 129.94, 129.76, 129.23, 128.50. 128.42, 128.32, 128.21, 126.65, 126.41, 126.10, 124.88, 124.77. MS (ESI) calcd for $C_{94}H_{60}N_{16}OsRu$ $[M-4PF_6]^{4+}$: 426.5956; Found: 426.5957. FTIR (KBr) ν_{max} (cm^{-1}): 3067 (CH, aryl), 2924 (CH, aryl), 2852 (CH, aryl), 1666 (C=C, aryl), 1606 (C=C, aryl), 1465 (C=C, aryl), 1447 (C=C, aryl), 1420 (CH, aryl), 1360

(CN, pyridyl), 1313 (CN, pyridyl), 1265 (CN, pyridyl), 1162 (CN, pyrazine), 1120 (CN, pyrazine), 839 (PF), 765 (C=C, aryl), 726 (C=C, aryl), 705 (C=C, aryl), 662 (CH, aryl), 558 (PF).

RuOs4 (L1 = tbubpy, L2 = bpy): dark brown solid. Yield 334 mg, 76%. Anal. Calcd for $C_{82}H_{76}F_{24}N_{16}P_4OsRu\cdot 2H_2O$: C, 44.92; H, 3.68; N, 10.22. Found: C, 44.71; H, 3.91; N, 9.96. ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.77 (d, J = 8.2 Hz, 2H), 9.54 (d, J = 8.1 Hz, 2H), 8.19–8.10 (m, 8H), 8.29 (s, 4H), 8.13 (t, J = 6.8 Hz, 2H), 8.07 (t, J = 7.8 Hz, 2H), 8.00 (q, J = 7.8, 7.2 Hz, 4H), 7.76 (d, J = 5.6 Hz, 2H), 7.72–7.62 (m, 8H), 7.54 (t, J = 6.8 Hz, 2H), 7.41 (d, J = 6.2 Hz, 2H), 7.33 (t, J = 6.8 Hz, 2H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 162.05, 161.95, 158.48, 158.40, 158.35, 156.44, 156.32, 151.33, 151.16, 150.66, 150.47, 150.27, 137.60, 137.48, 137.20, 128.41, 128.32, 128.20, 124.89, 124.76, 124.66, 124.36, 122.02, 121.91, 118.05, 35.54, 35.44, 30.06, 29.97. MS (ESI) calcd for $C_{82}H_{76}N_{16}OsRu$ $[M-4PF_6]^{4+}$: 394.6269; Found: 394.6271. FTIR (KBr) ν_{max} (cm^{-1}): 2961 (CH, aryl), 2924 (CH, aryl), 2852 (CH, aryl), 1671 (C=C, aryl), 1614 (C=C, aryl), 1465 (C=C, aryl), 1415 (CH, aryl), 1361 (CN, pyridyl), 1254 (CN, pyridyl), 1161 (CN, pyrazine), 1120 (CN, pyrazine), 1074 (CN, pyrazine), 1025 (CH, aryl), 840 (PF), 765 (C=C, aryl), 726 (C=C, aryl), 705 (C=C, aryl), 558 (PF).

RuOs5 (L1 = bpy, L2 = phen): dark brown solid. Yield 314 mg, 78%. Anal. Calcd for $C_{70}H_{44}F_{24}N_{16}P_4OsRu\cdot 2H_2O$: C, 41.70; H, 2.40; N, 11.11. Found: C, 41.39; H, 2.64; N, 10.91. ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.78 (d, J = 8.1 Hz, 2H), 9.51 (d, J = 8.1 Hz, 2H), 8.91 (t, J = 9.4 Hz, 4H), 8.62 (dd, J = 12.3, 8.2 Hz, 4H), 8.43 (s, 4H), 8.35 (d, J = 5.3 Hz, 2H), 8.27 (d, J = 7.9 Hz, 2H), 8.23 (d, J = 5.8 Hz, 4H), 8.17 (t, J = 7.9 Hz, 2H), 8.11 (dd, J = 8.2, 5.7 Hz, 2H), 7.99 (d, J = 5.3 Hz, 2H), 7.91–7.83 (m, 4H), 7.83–7.76 (m, 4H), 7.74 (dd, J = 8.3, 5.4 Hz, 2H), 7.63 (t, J = 6.7 Hz, 2H), 7.43 (t, J = 6.7 Hz, 2H). ^{13}C NMR (100 MHz, DMSO-d_6): δ 156.75, 156.52, 154.63, 152.06, 151.96, 151.57, 151.39, 149.18, 149.04, 145.61, 138.21, 138.12, 136.93, 130.76, 128.28, 128.00, 127.75, 126.54, 126.39, 124.69, 124.58. MS (ESI) calcd for $C_{70}H_{44}N_{16}OsRu$ $[M-4PF_6]^{4+}$: 350.5643; Found: 350.5647. FTIR (KBr) ν_{max} (cm^{-1}): 3087 (CH, aryl), 2924 (CH, aryl), 2852 (CH, aryl), 1670 (C=C, aryl), 1603 (C=C, aryl), 1469 (C=C, aryl), 1447 (C=C, aryl), 1428 (CH, aryl), 1360 (CN, pyridyl), 1313 (CN, pyridyl), 1161 (CN, pyrazine), 1120 (CN, pyrazine), 1074 (CN, pyrazine), 1024 (CH, aryl), 841 (PF), 765 (C=C, aryl), 720 (C=C, aryl), 558 (PF).

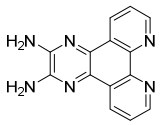
RuOs6 (L1 = bpy, L2 = dip): dark brown solid. Yield 367 mg, 79%. Anal. Calcd for $C_{94}H_{60}F_{24}N_{16}P_4OsRu\cdot 2H_2O$: C, 48.65; H, 2.78; N, 9.66. Found: C, 48.41; H, 3.04; N, 9.47. ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.78 (d, J = 8.2 Hz, 2H), 9.59 (d, J = 8.2 Hz, 2H), 8.90 (t, J = 9.4 Hz, 4H), 8.40 (d, J = 5.5 Hz, 2H), 8.35 (s, 4H), 8.31 (s, 4H), 7.83–7.76 (m, 6H), 8.14 (dt, J = 20.9, 7.3 Hz, 4H), 7.99 (t, J = 6.9 Hz, 2H), 7.85 (d, J = 5.7 Hz, 2H), 7.83–7.76 (m, 6H), 7.74–7.55 (m, 22H), 7.43 (t, J = 6.7 Hz, 2H). ^{13}C NMR (100 MHz, DMSO-

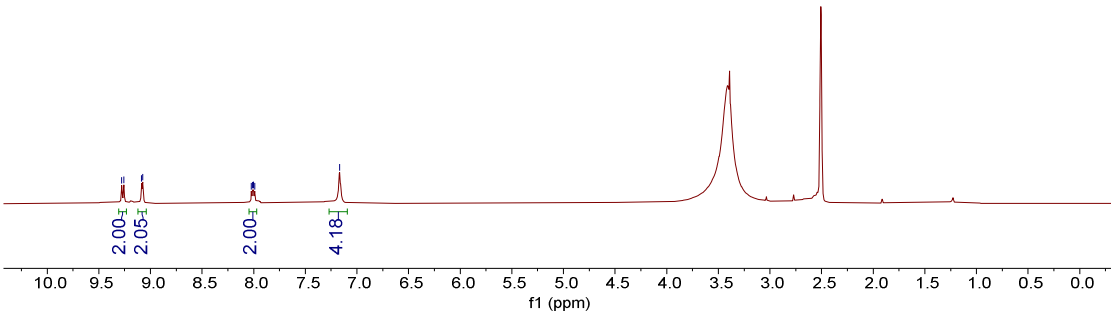
d_6): δ 156.74, 156.52, 152.31, 151.97, 151.38, 149.94, 147.95, 138.20, 138.10, 135.15, 135.11, 130.21, 130.12, 129.71, 129.14, 128.76, 128.46, 128.00, 127.81, 126.73, 126.37, 126.22, 124.68. MS (ESI) calcd for $C_{94}H_{60}N_{16}OsRu$ $[M-4PF_6]^{4+}$: 426.5956; Found: 426.5968. FTIR (KBr) ν_{max} (cm^{-1}): 3083 (CH, aryl), 2927 (CH, aryl), 2853 (CH, aryl), 1670 (C=C, styryl), 1603 (C=C, aryl), 1467 (C=C, aryl), 1446 (C=C, aryl), 1426 (CH, aryl), 1340 (CN, pyridyl), 1313 (CN, pyridyl), 1259 (CN, pyridyl), 1161 (CN, pyrazine), 1119 (CN, pyrazine), 1094 (CN, pyrazine), 1074 (CN, pyrazine), 1028 (CH, aryl), 837 (PF), 765 (C=C, aryl), 729 (C=C, aryl), 704 (C=C, aryl), 661 (CH, aryl), 558 (PF).

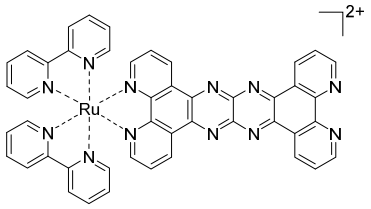
RuOs7 (L1 = bpy, L2 = tbubpy): dark brown solid. Yield 303 mg, 69%. Anal. Calcd for $C_{82}H_{76}F_{24}N_{16}P_4OsRu\cdot 2H_2O$: C, 44.92; H, 3.68; N, 10.22. Found: C, 44.68; H, 3.95; N, 10.01. ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.78 (d, J = 8.1 Hz, 2H), 9.52 (d, J = 8.1 Hz, 2H), 8.92 (t, J = 9.9 Hz, 8H), 8.37 (d, J = 5.5 Hz, 2H), 8.27 (t, J = 7.4 Hz, 4H), 8.18 (t, J = 7.9 Hz, 4H), 8.12 (dd, J = 8.2, 5.4 Hz, 2H), 8.01 (dd, J = 7.9, 5.5 Hz, 2H), 7.86 (d, J = 5.5 Hz, 2H), 7.81 (d, J = 5.3 Hz, 2H), 7.64 (t, J = 6.7 Hz, 2H), 7.61–7.55 (m, 6H), 7.44 (t, J = 6.6 Hz, 2H), 7.33 (d, J = 6.2 Hz, 2H). ^{13}C NMR (100 MHz, DMSO-d_6): δ 161.47, 158.04, 156.83, 156.71, 156.49 156.35, 151.96, 151.34, 150.58, 138.18, 138.01, 127.98, 125.30, 124.65, 124.47, 122.22, 35.39, 35.33, 30.23, 30.17, 30.11. MS (ESI) calcd for $C_{82}H_{76}N_{16}OsRu$ $[M-4PF_6]^{4+}$: 394.6269; Found: 394.6262. FTIR (KBr) ν_{max} (cm^{-1}): 3087 (CH, aryl), 2961 (CH, aryl), 2924 (CH, aryl), 2852 (CH, aryl), 1668 (C=C, aryl), 1615 (C=C, aryl), 1465 (C=C, aryl), 1445 (C=C, aryl), 1423 (CH, aryl), 1360 (CN, pyridyl), 1312 (CN, pyridyl), 1273 (CN, pyridyl), 1161 (CN, pyrazine), 1117 (CN, pyrazine), 1073 (CN, pyrazine), 1028 (CH, aryl), 842 (PF), 767 (C=C, aryl), 728 (C=C, aryl), 705 (C=C, aryl), 661 (CH, aryl), 558 (PF).

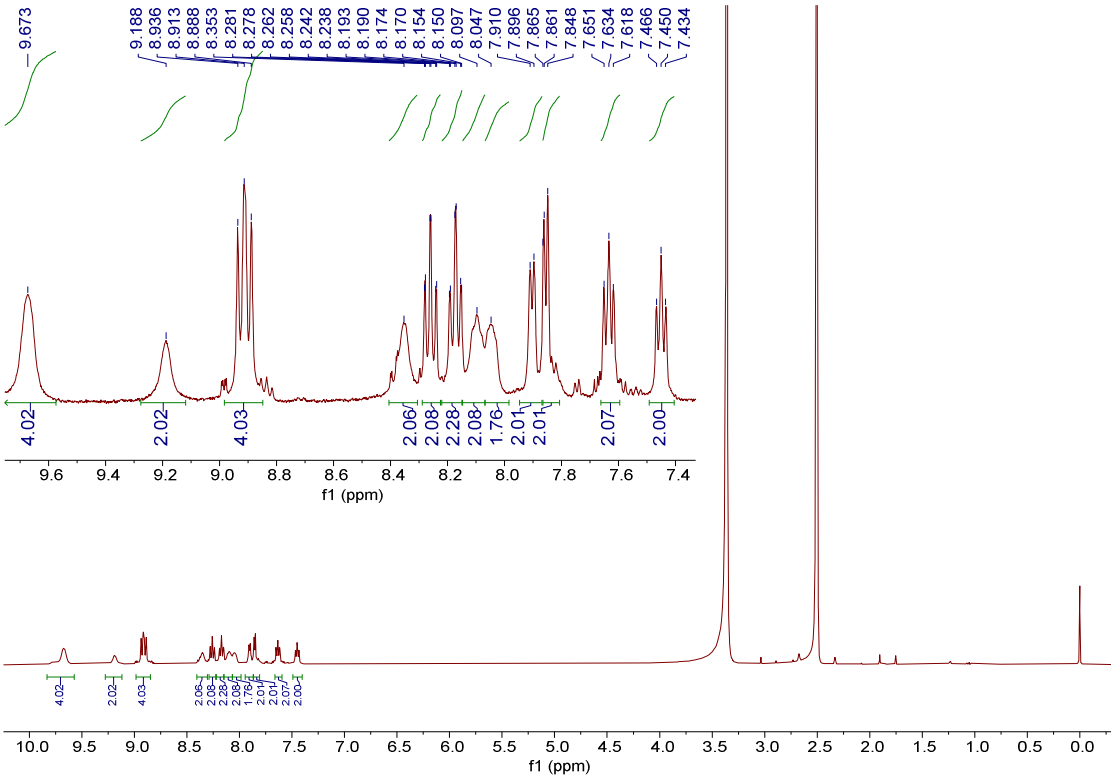
RuOs8 (L1 = dip, L2 = dip): dark brown solid. Yield 401 mg, 75%. Anal. Calcd for $C_{122}H_{76}F_{24}N_{16}P_4OsRu\cdot 2H_2O$: C, 54.82; H, 3.02; N, 8.38. Found: C, 54.56; H, 3.28; N, 8.14. ^{1}H NMR (400 MHz, DMSO-d_6): 9.83 (d, J = 8.2 Hz, 2H), 9.60 (d, J = 7.4 Hz, 2H), 8.45 (t, J = 12.6 Hz, 8H), 8.36 (s, 4H), 8.32 (s, 8H), 8.11 (s, 2H), 8.00 (s, 2H), 7.87 (s, 4H), 7.80 (s, 4H), 7.68 (d, J = 15.9 Hz, 40H). ^{13}C NMR (100 MHz, DMSO-d_6): δ 155.02, 154.41, 152.56, 152.33, 152.05, 151.77, 149.77, 149.73, 148.00, 147.78, 145.47, 143.38, 135.20, 135.14, 134.92, 134.88, 130.00, 129.90, 129.75, 129.66, 129.53, 128.98, 128.27, 128.06, 127.96, 126.50, 126.35, 126.23, 126.06, 125.85. MS (ESI) calcd for $C_{122}H_{76}N_{16}OsRu$ $[M-4PF_6]^{4+}$: 514.6269; Found: 514.6276. FTIR (KBr) ν_{max} (cm^{-1}): 3060 (CH, aryl), 2925 (CH, aryl), 2852 (CH, aryl), 1669 (C=C, aryl), 1669 (C=C, aryl), 1595 (C=C, styryl), 1556 (C=C, aryl), 1445 (C=C, aryl), 1417 (CH, aryl), 1401 (CH, aryl), 1359 (CN, pyridyl), 1161 (CN, pyrazine), 1120 (CN, pyrazine), 1095 (CN, pyrazine), 1021 (CH, aryl), 837 (PF), 766 (C=C, aryl), 737 (C=C, aryl), 703 (C=C, aryl), 557 (PF).

3. ^{1}H NMR, ^{13}C NMR, Mass, and FT-IR Spectra of Important Intermediates and RuOs1−8






2+
Ru
N


9.673
9.188
8.936
8.913
8.888
8.353
8.281
8.278
8.262
8.258
8.242
8.238
8.193
8.190
8.174
8.170
8.154
8.150
8.097
8.047
7.910
7.896
7.865
7.861
7.848
7.651
7.634
7.618
7.466
7.450
7.434
4.02
2.02
4.03
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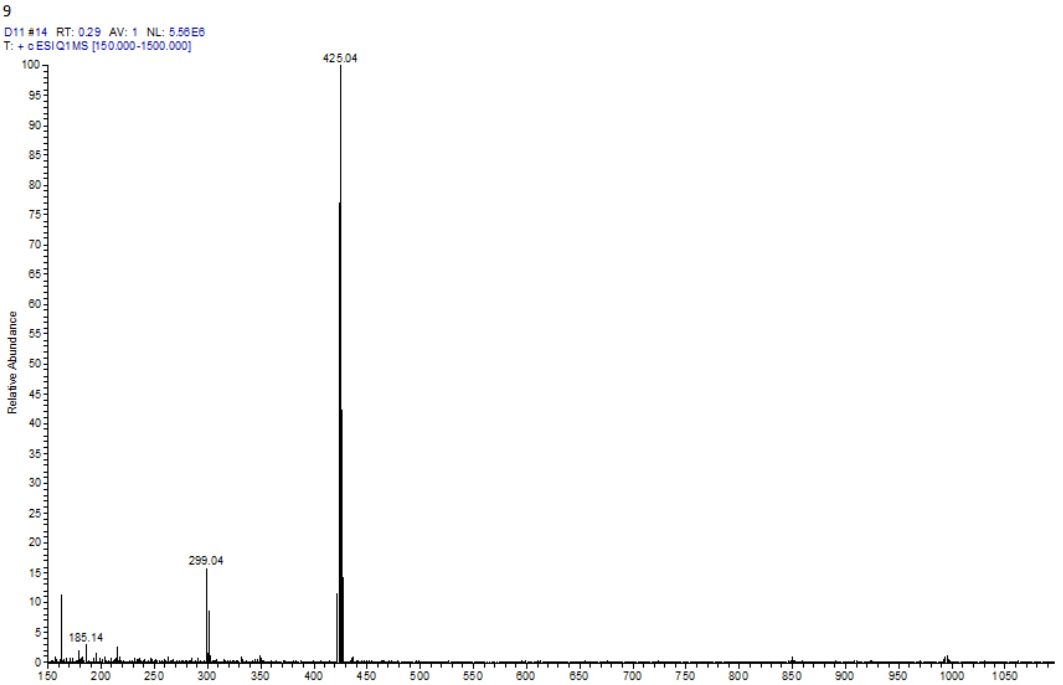
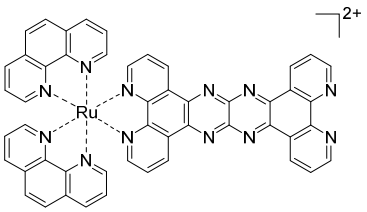
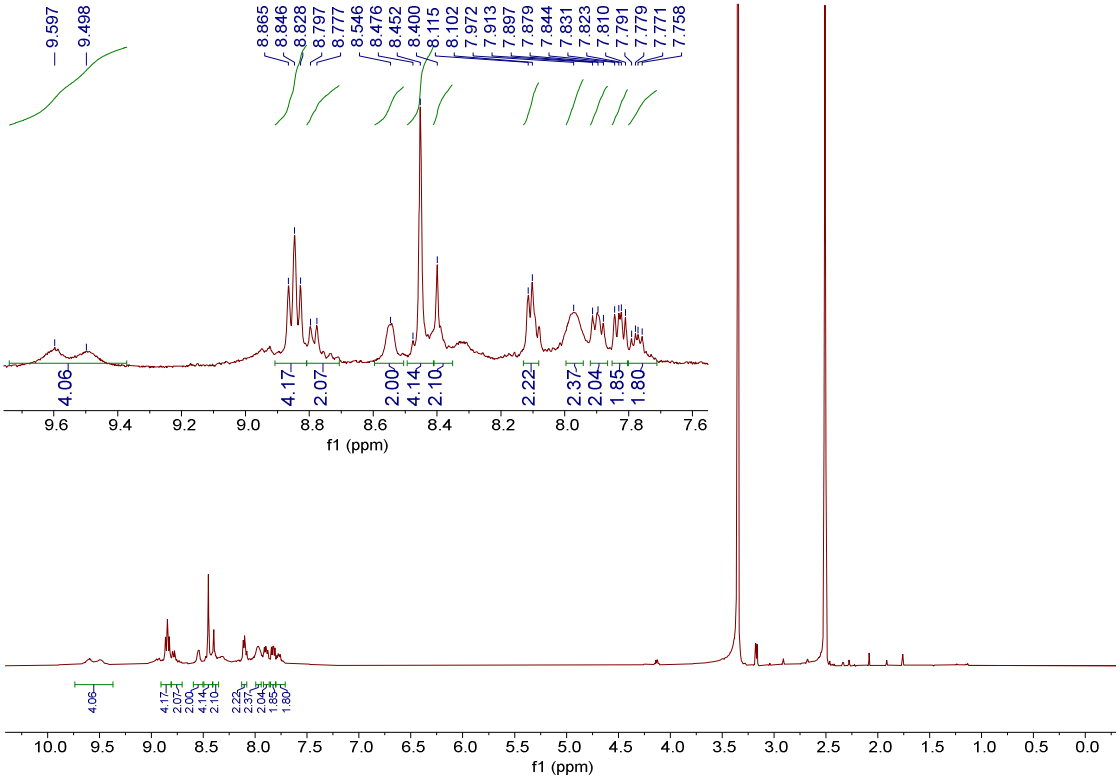
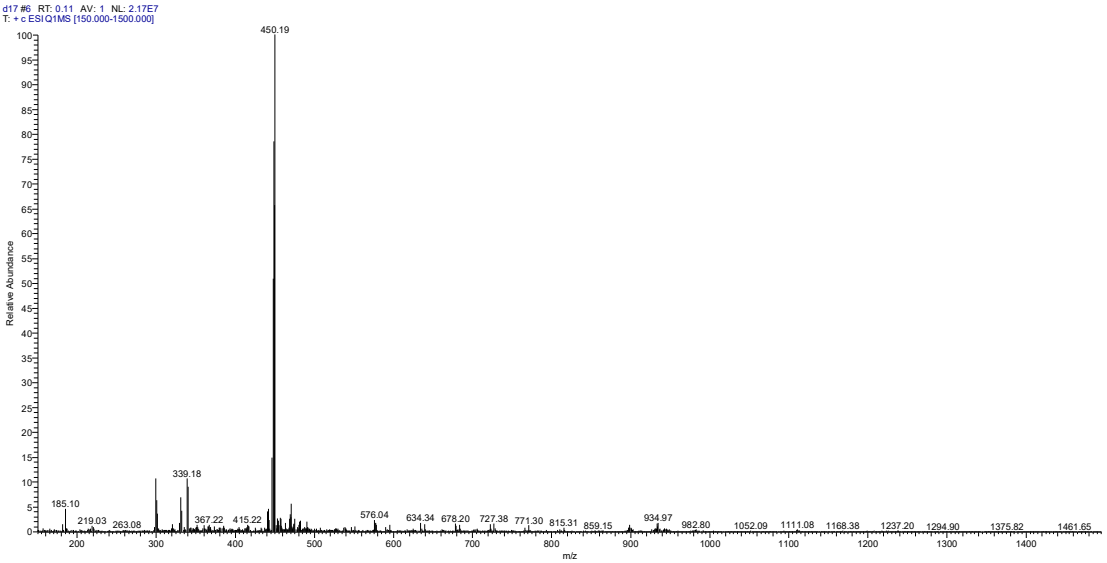
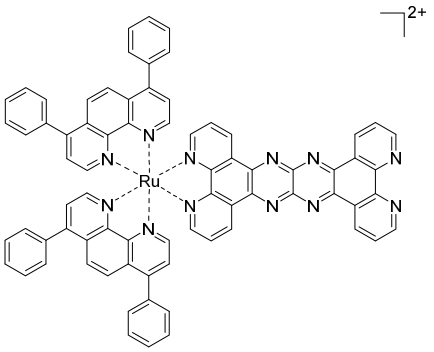
2.08
2.28
2.08
1.76
2.01
2.01
2.07
2.00
f1 (ppm)

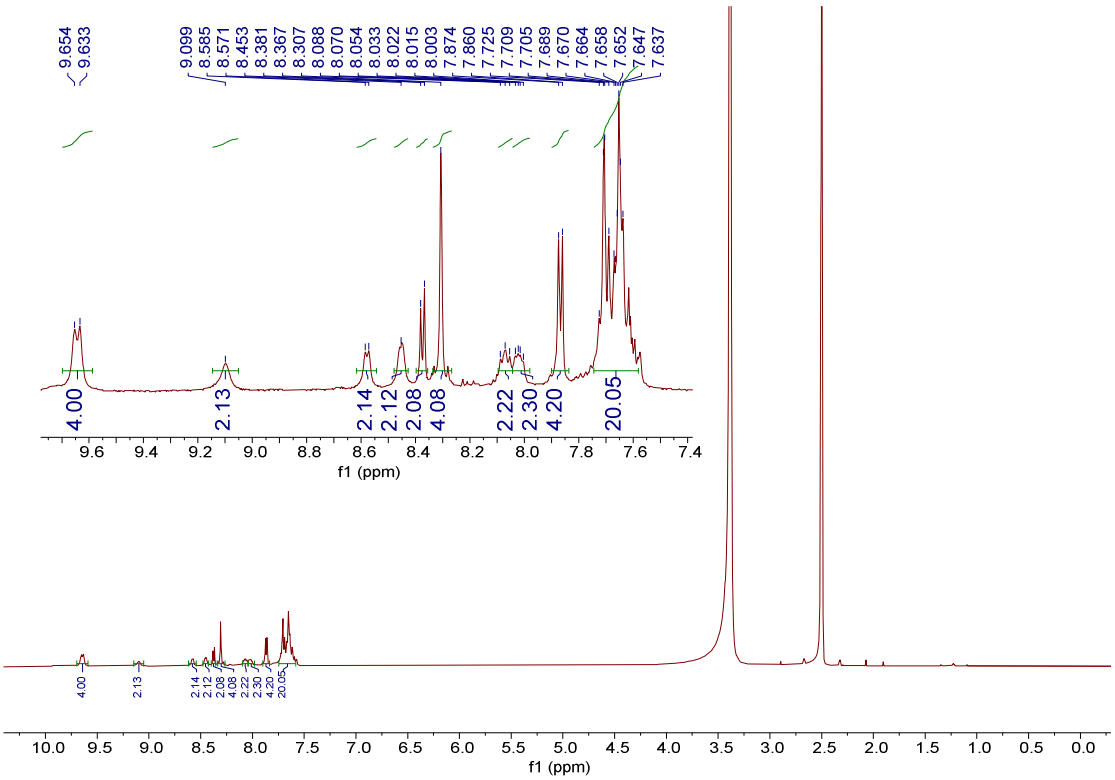

9
D11 #14 RT: 0.29 AV: 1 NL: 5.56E6
T: + c ESI Q1MS [150.000-1500.000]
425.04
299.04
185.14
Relative Abundance

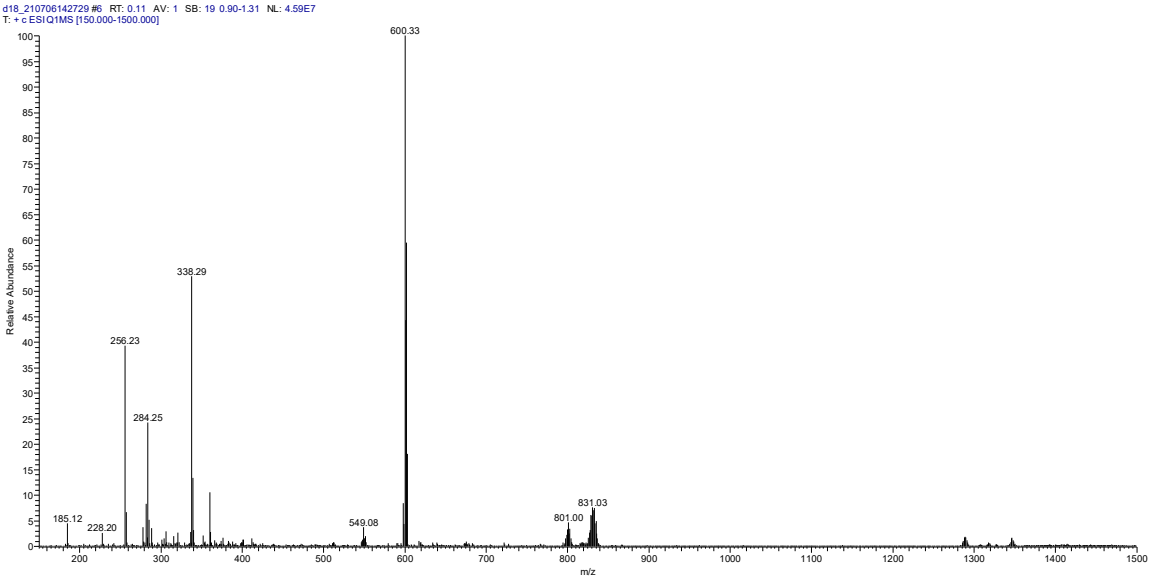

2+
Ru
N

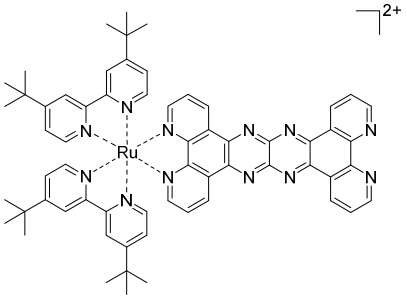

9.597
9.498
8.865
8.846
8.828
8.797
8.777
8.546
8.476
8.452
8.400
8.115
8.102
7.972
7.913
7.897
7.879
7.844
7.831
7.823
7.810
7.791
7.779
7.771
7.758
4.06
4.17
2.07
2.00
4.14
2.10
2.22
2.37
2.04
1.85
1.80
f1 (ppm)
f1 (ppm)

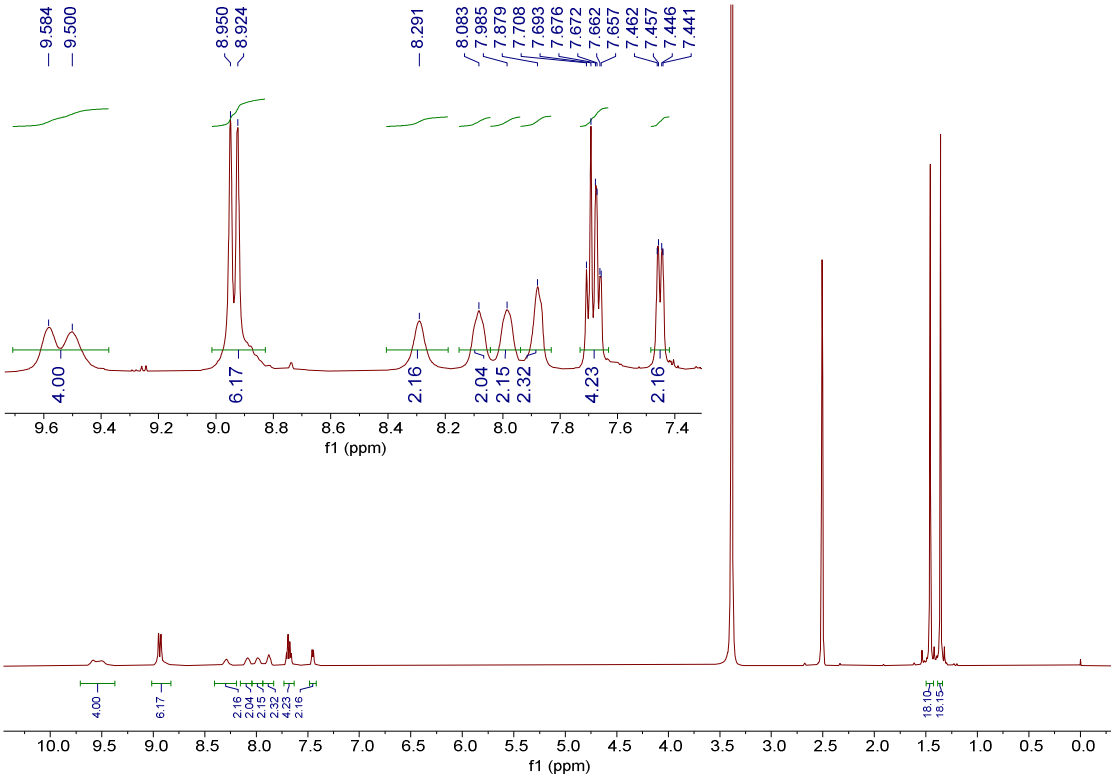

d17 #6 RT: 0.11 AV: 1 NL: 2.17E7
T: + c ESI Q1MS [150.000-1500.000]
450.19
339.18
185.10
219.03
263.08
367.22
415.22
576.04
634.34
678.20
727.38
771.30
815.31
859.15
934.97
982.80
1052.09
1111.08
1168.38
1237.20
1294.90
1375.82
1461.65
Relative Abundance
m/z

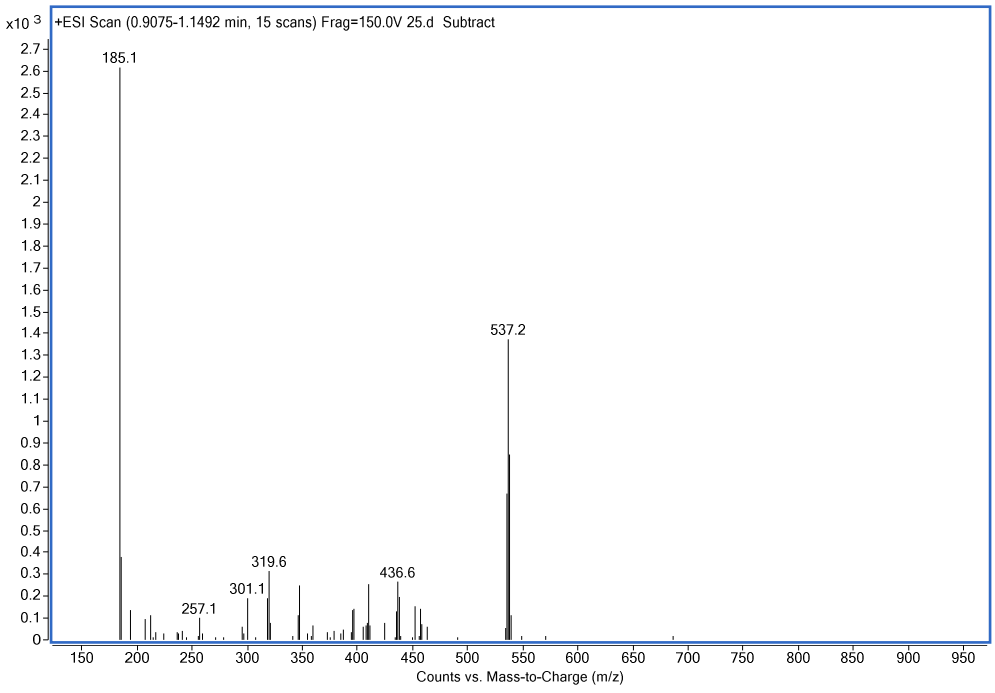

2+
Ru
N


9.654
9.633
9.099
8.585
8.571
8.453
8.381
8.367
8.307
8.088
8.070
8.054
8.033
8.022
8.015
8.003
7.874
7.860
7.725
7.709
7.705
7.689
7.670
7.664
7.658
7.652
7.647
7.637
4.00
2.13
2.14
2.12
2.08
4.08
2.22
2.30
4.20
20.05
f1 (ppm)
f1 (ppm)

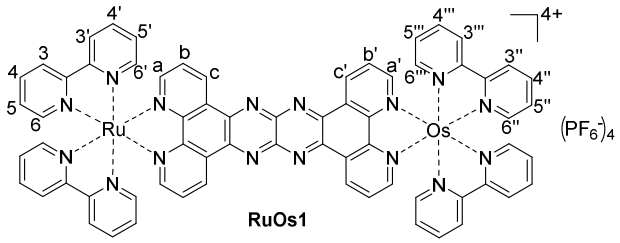

d18_210706142729 #6 RT: 0.11 AV: 1 SB: 19 0.90-1.31 NL: 4.59E7
T: + c ESI Q1MS [150.000-1500.000]
600.33
338.29
256.23
284.25
185.12
228.20
549.08
801.00
831.03
Relative Abundance
m/z

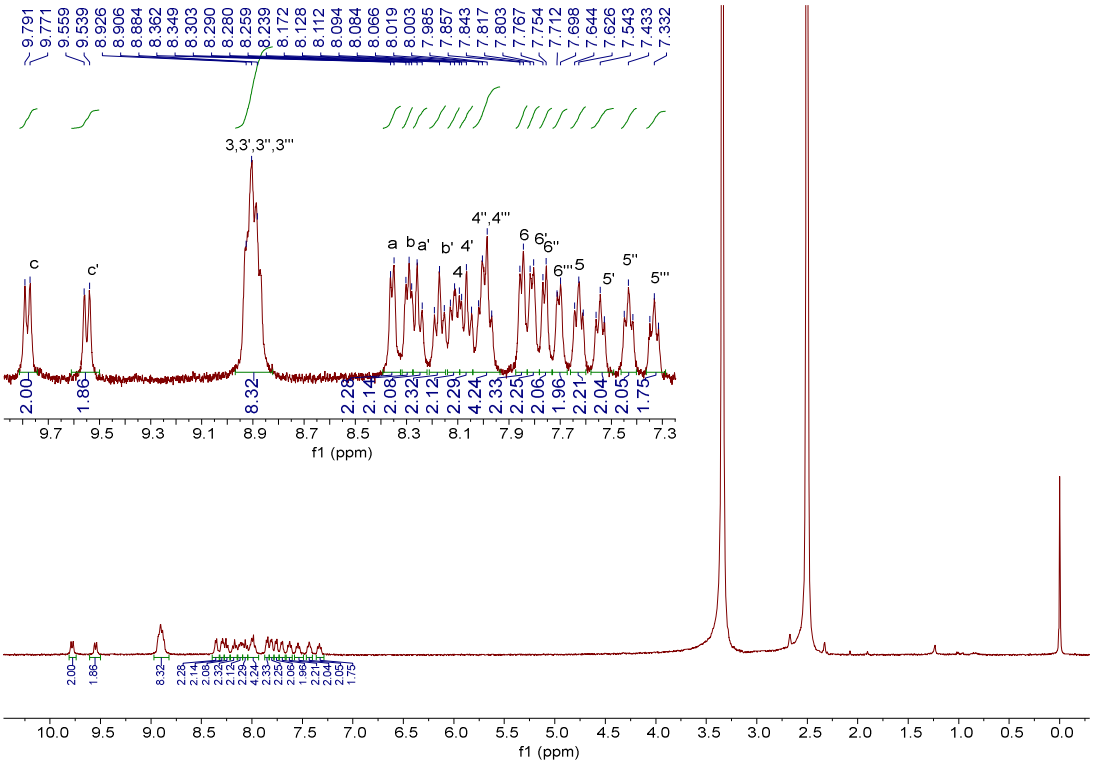

2+
Ru
N

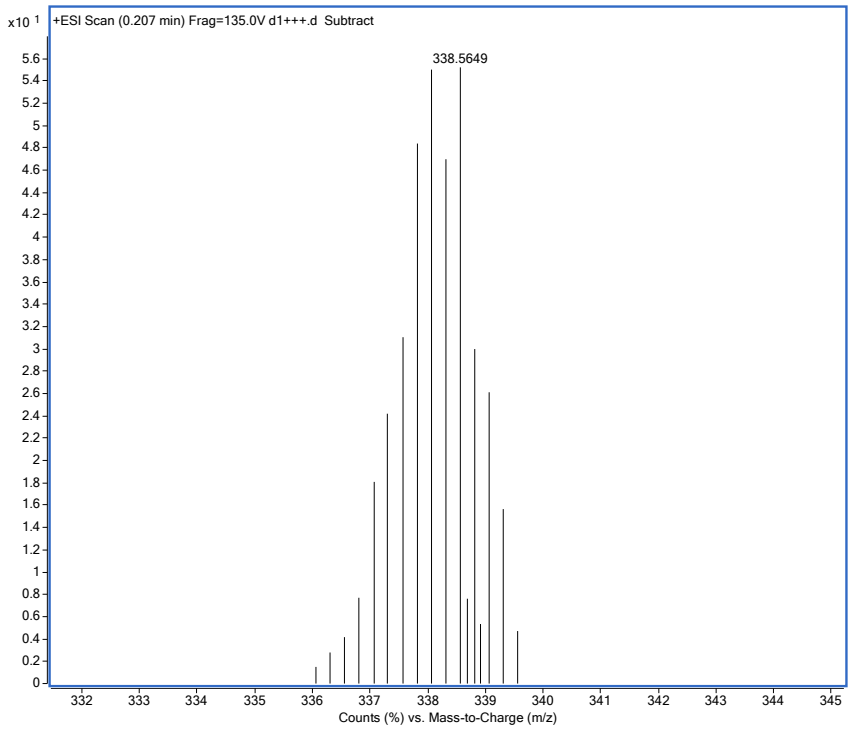

9.584
9.500
8.950
8.924
8.291
8.083
7.985
7.879
7.708
7.693
7.676
7.672
7.662
7.657
7.462
7.457
7.446
7.441
4.00
6.17
2.16
2.04
2.15
2.32
4.23
2.16
18.10
18.15
f1 (ppm)

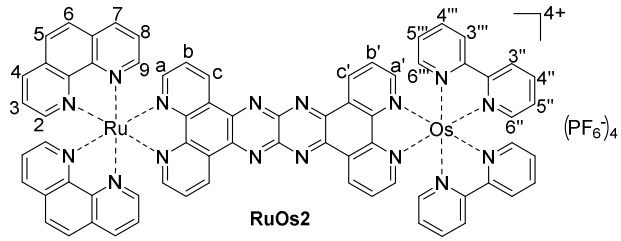

x10 3
+ESI Scan (0.9075-1.1492 min, 15 scans) Frag=150.0V 25.d Subtract
185.1
537.2
319.6
436.6
301.1
257.1
Counts vs. Mass-to-Charge (m/z)

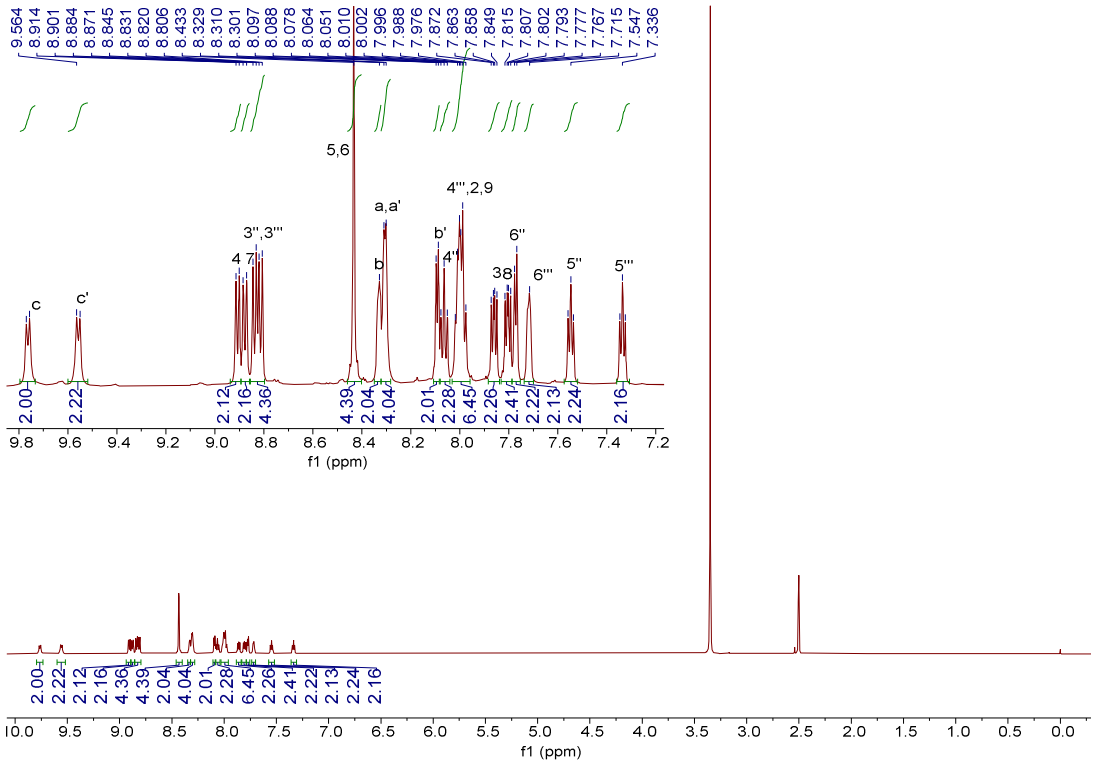
^{1}H NMR spectra and HRMS of RuOs1–8

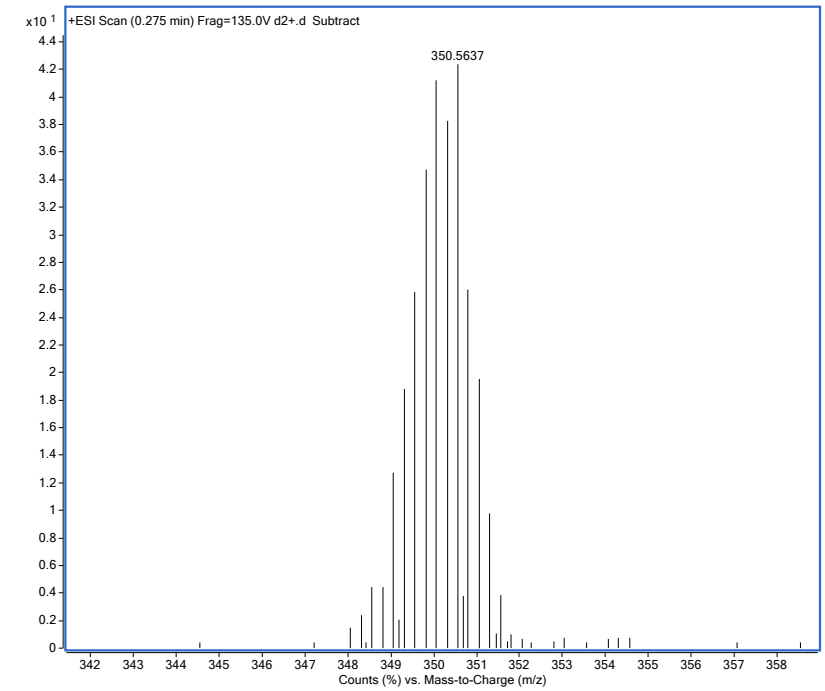


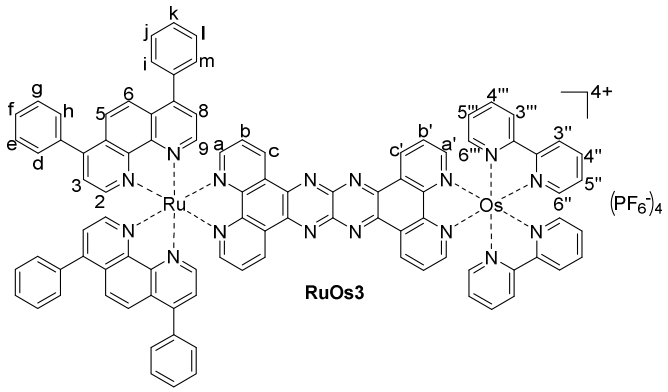


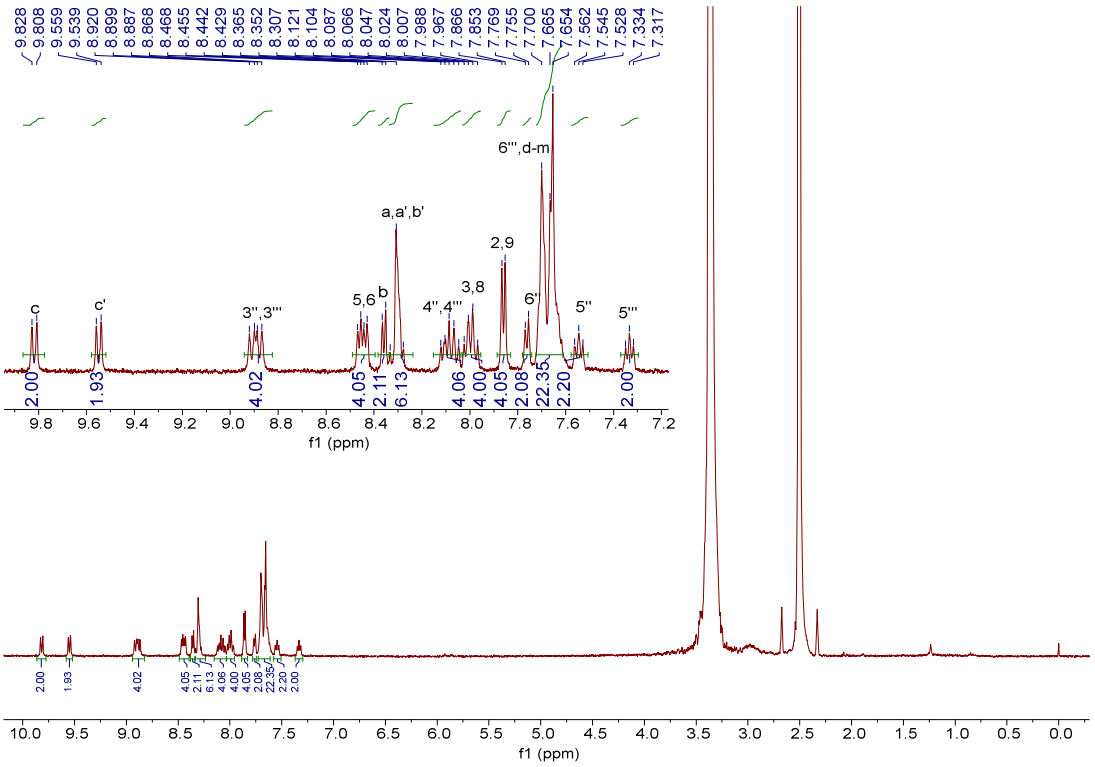


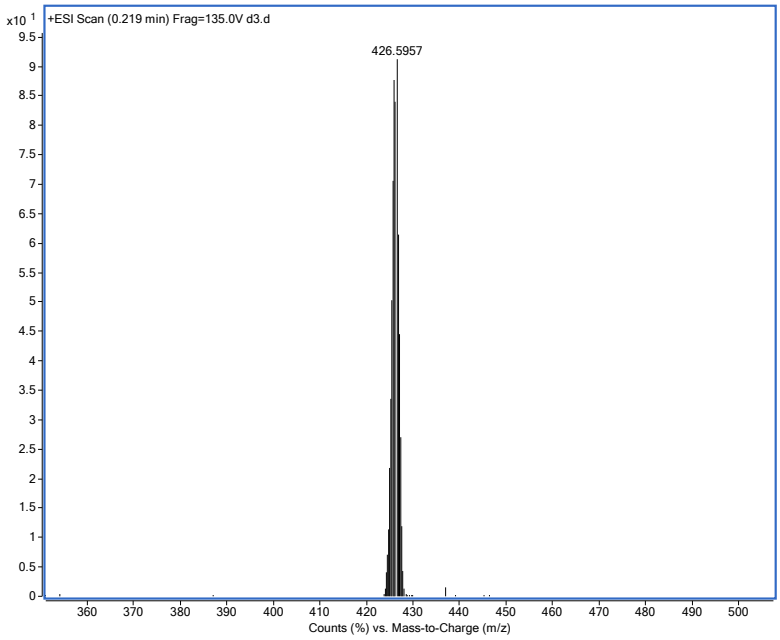

RuOs2
Ru
Os
4+
(PF6-)4

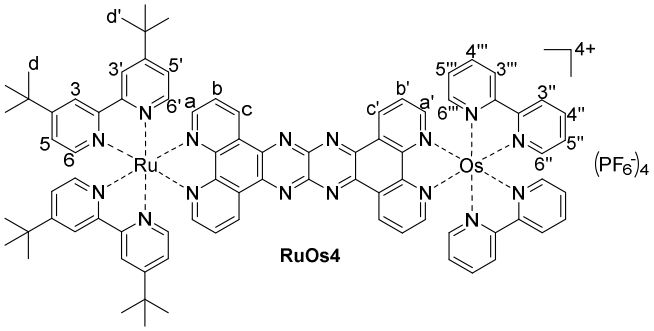

f1 (ppm)
5,6
a,a'
4''',2,9
3'',3'''
b'
6''
b
4'
38'
6'''
5''
5'''
c
c'
4 7
2.00
2.22
2.12
2.16
4.36
4.39
2.04
4.04
2.01
2.28
6.45
2.26
2.41
2.22
2.13
2.24
2.16

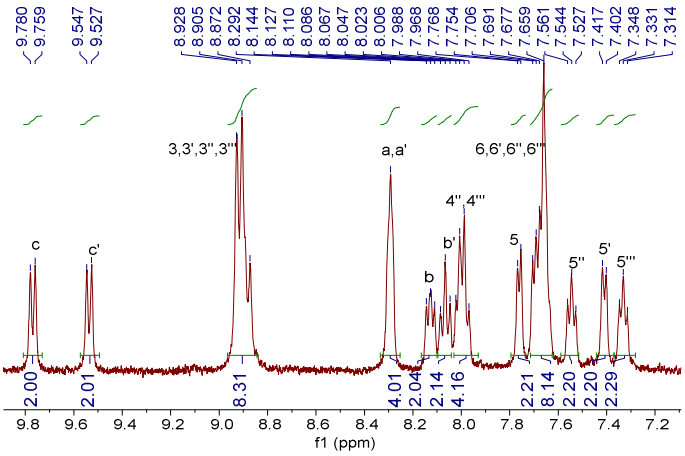

+ESI Scan (0.275 min) Frag=135.0V d2+.d Subtract
x10 1
350.5637
Counts (%) vs. Mass-to-Charge (m/z)


RuOs3
Ru
Os
4+
(PF6-)4

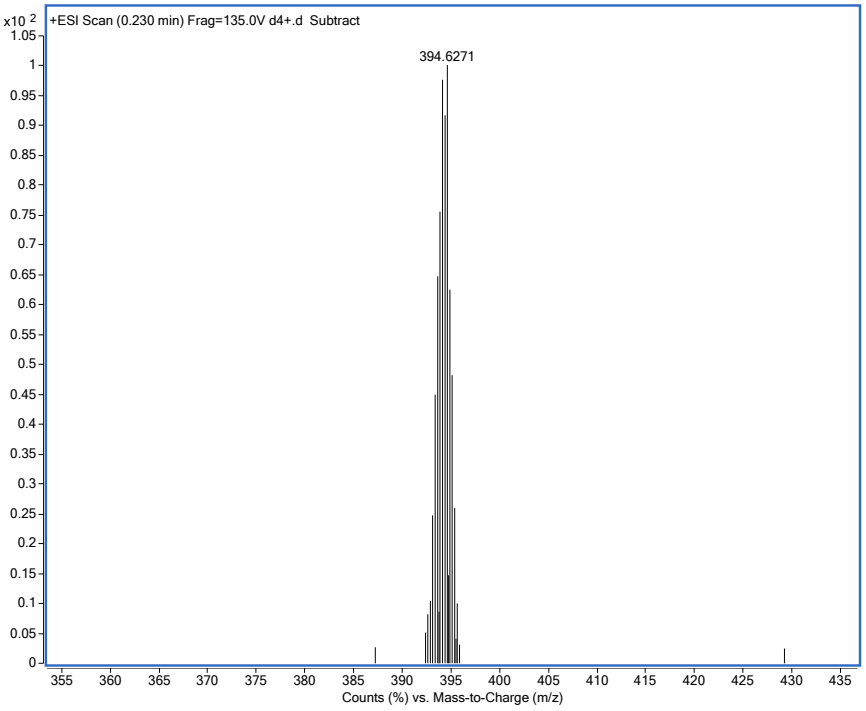

6''',d-m
a,a',b'
2,9
3,8
6'
5,6
b
4'',4'''
3'',3'''
c
c'
5''
5'''
f1 (ppm)

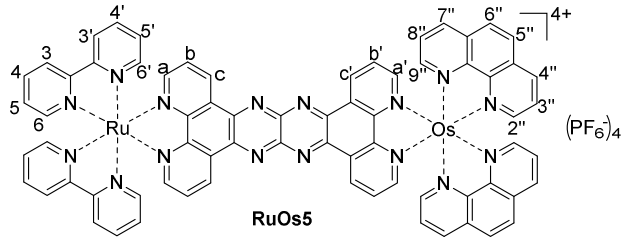

+ESI Scan (0.219 min) Frag=135.0V d3.d
426.5957
Counts (%) vs. Mass-to-Charge (m/z)

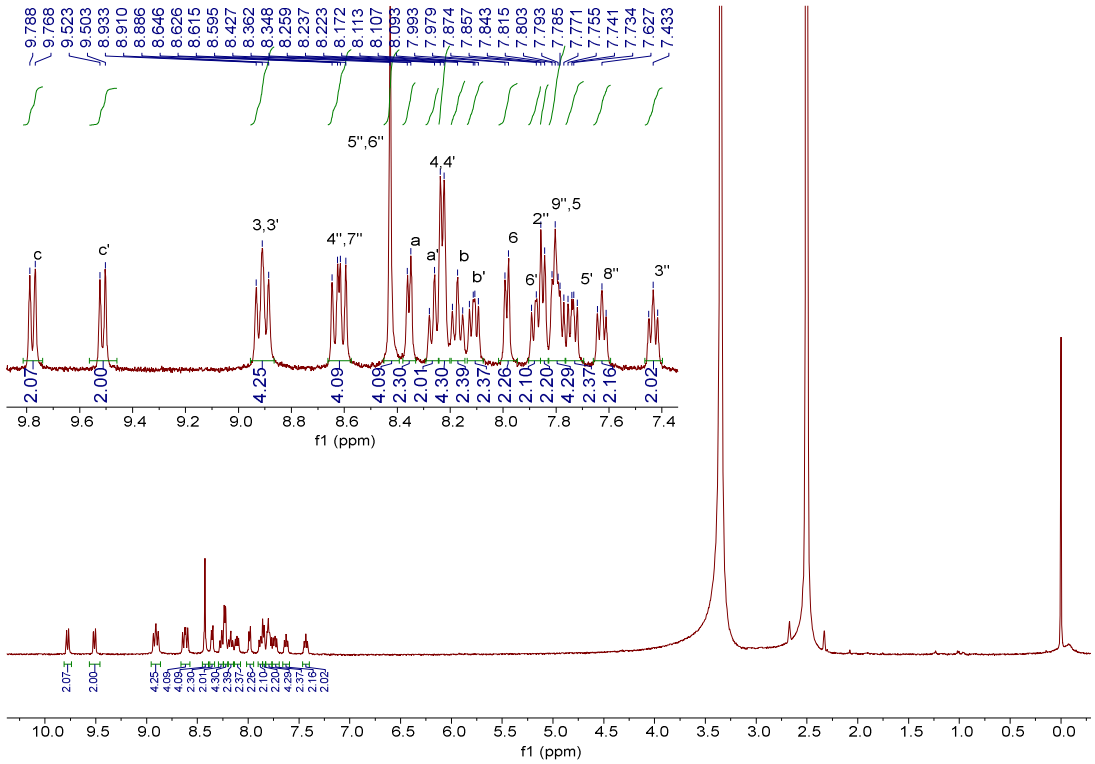

RuOs4
Ru
Os
4+
(PF6-)4

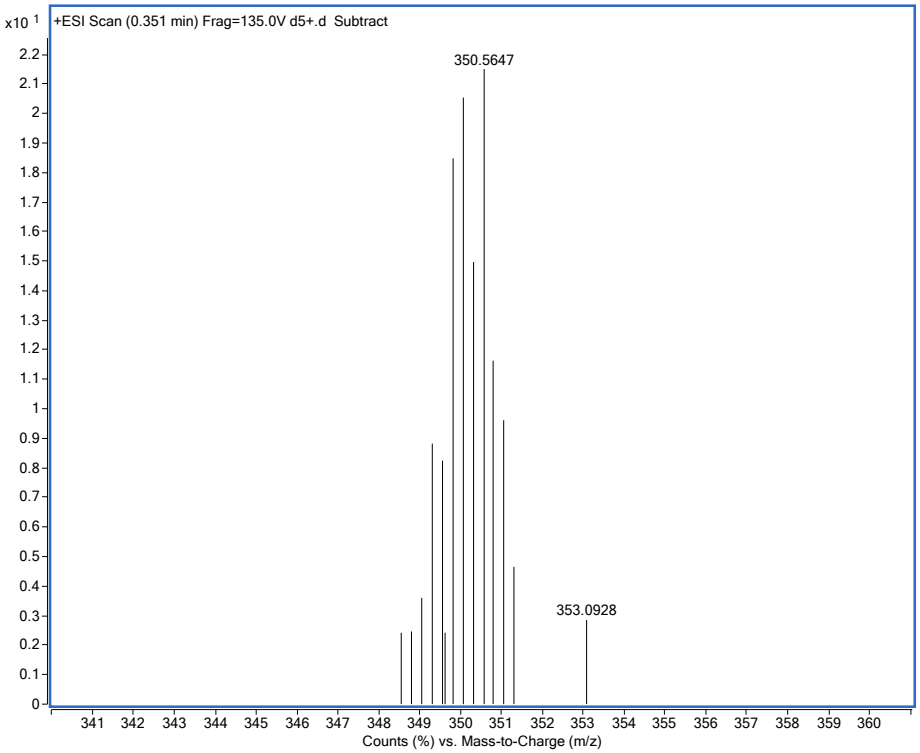

3,3',3'',3'''
a,a'
6,6',6'',6'''
4'', 4'''
f1 (ppm)

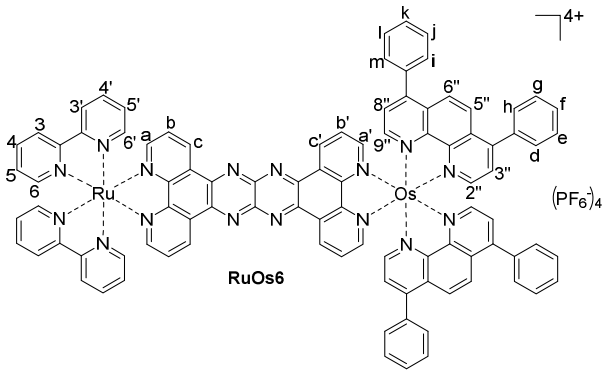
d d'
f1 (ppm)

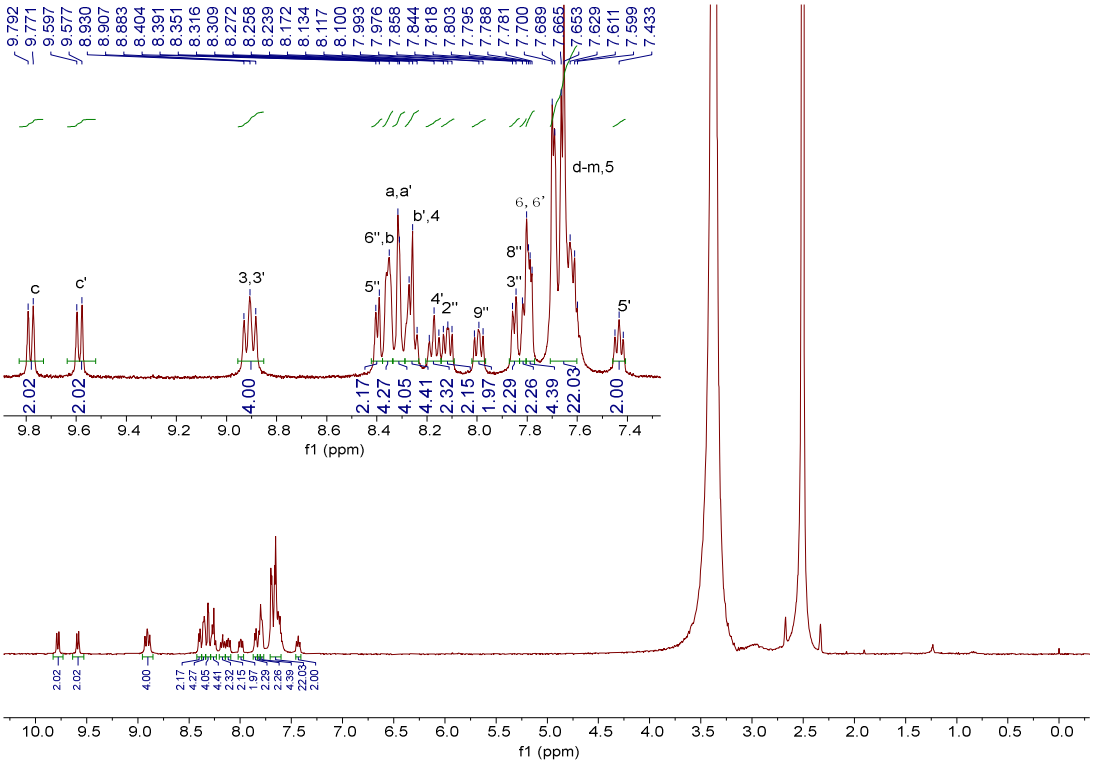

+ESI Scan (0.230 min) Frag=135.0V d4+.d Subtract
394.6271
Counts (%) vs. Mass-to-Charge (m/z)

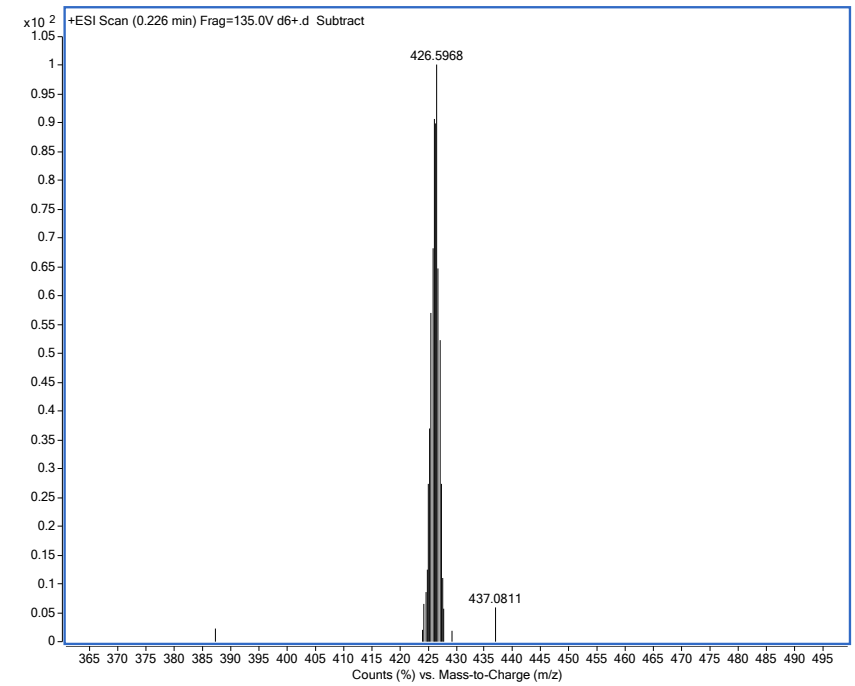

RuOs5

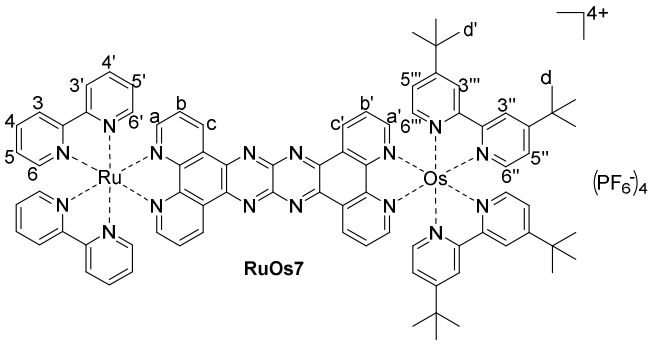

f1 (ppm)
f1 (ppm)

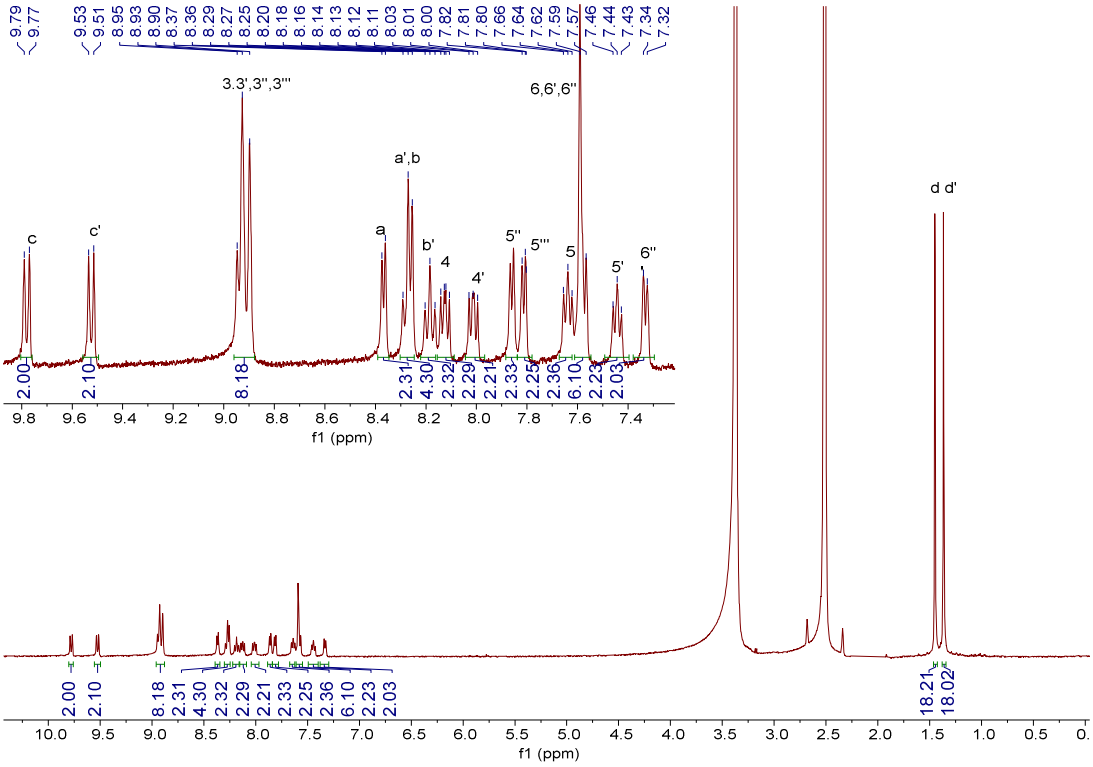

+ESI Scan (0.351 min) Frag=135.0V d5+.d Subtract
350.5647
353.0928
Counts (%) vs. Mass-to-Charge (m/z)

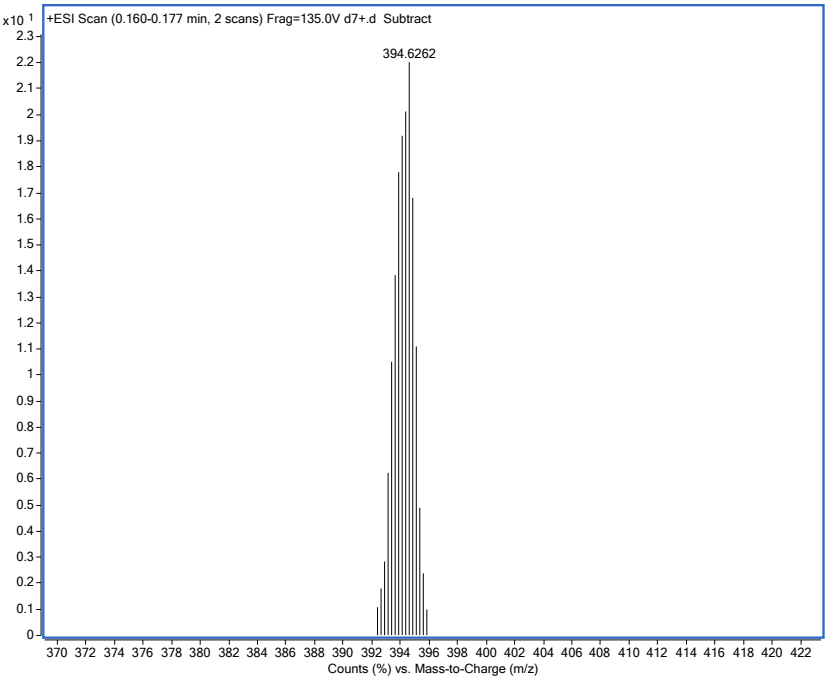

RuOs6
4+
(PF6-)4

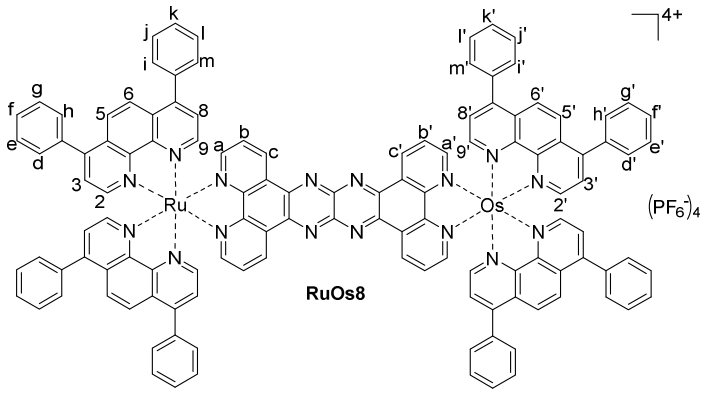

f1 (ppm)
d-m,5
a,a'
b',4
6,6'
6'',b
8''
5''
3''
3,3'
c
c'
4'
2''
9''
5'
2.02
2.02
4.00
2.17
4.27
4.05
4.41
2.32
2.15
1.97
2.29
2.26
4.39
22.03
2.00

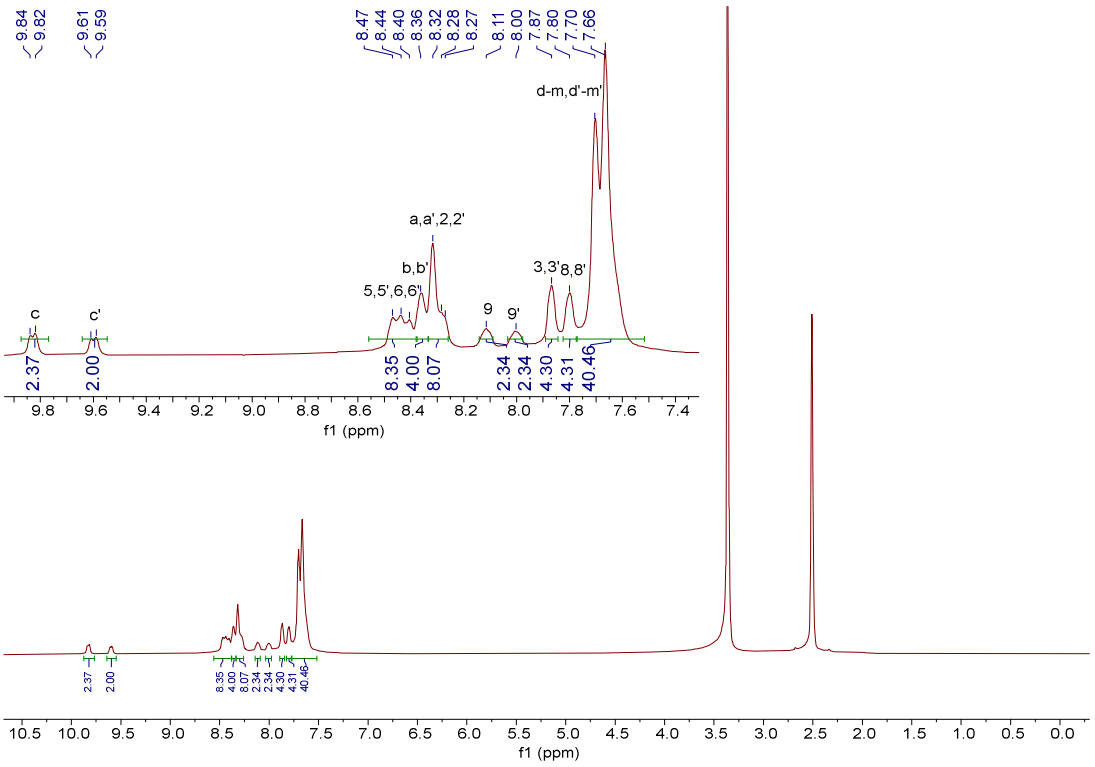

+ESI Scan (0.226 min) Frag=135.0V d6+.d Subtract
426.5968
437.0811
Counts (%) vs. Mass-to-Charge (m/z)

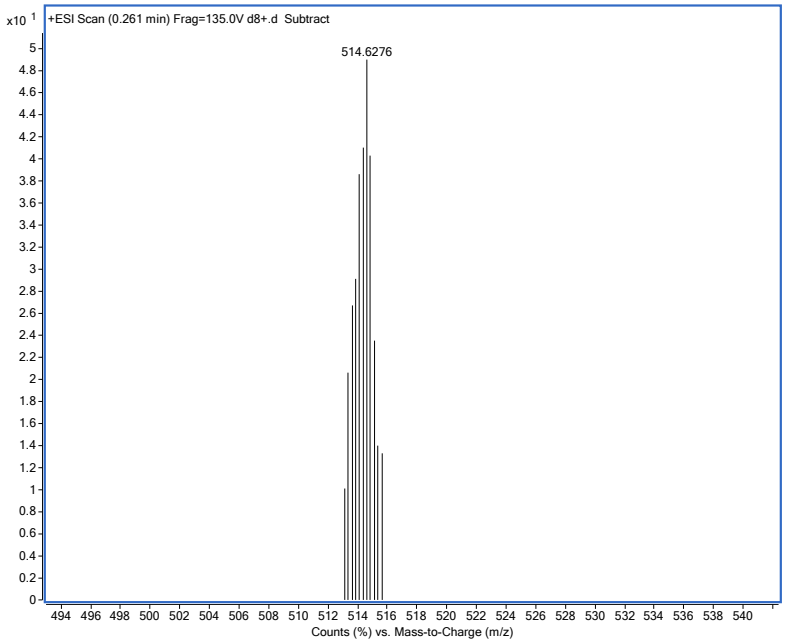

4+
Ru
Os
(PF6-)4
RuOs7


3.3',3'',3'''
6,6',6''
a',b
d d'
f1 (ppm)


+ESI Scan (0.160-0.177 min, 2 scans) Frag=135.0V d7+.d Subtract
394.6262
Counts (%) vs. Mass-to-Charge (m/z)


RuOs8
4+
$(PF_6^-)_4$


9.84
9.82
9.61
9.59
8.47
8.44
8.40
8.36
8.32
8.28
8.27
8.11
8.00
7.87
7.80
7.70
7.66
d-m,d'-m'
a,a',2,2'
b,b'
5,5',6,6'
3,3'
8,8'
9
9'
c
c'
2.37
2.00
8.35
4.00
8.07
2.34
2.34
4.30
4.31
40.46
f1 (ppm)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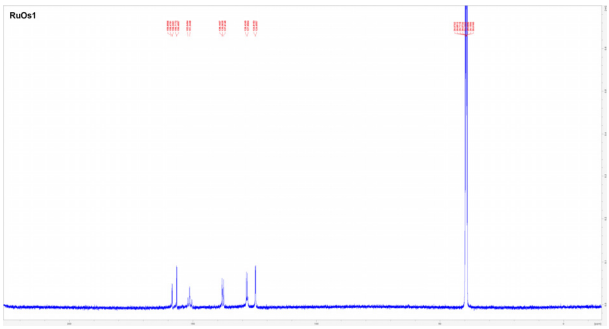
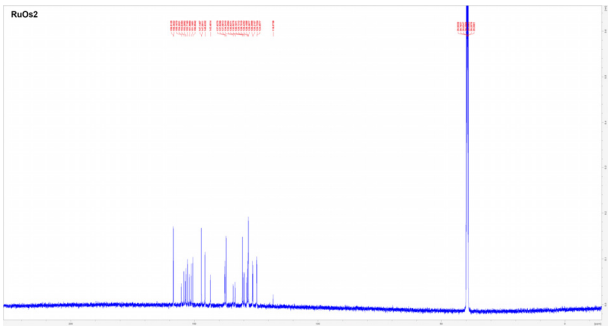
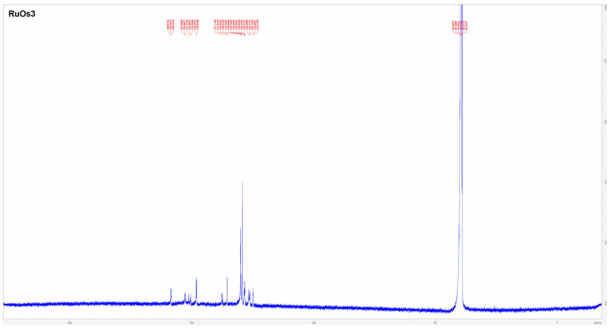
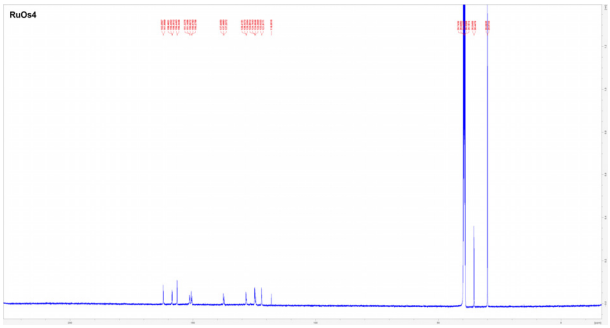
514.6276
Counts (%) vs. Mass-to-Charge (m/z)

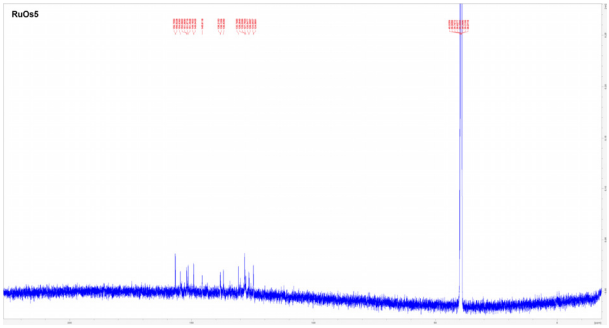
^{13}C NMR spectra of RuOs1−8

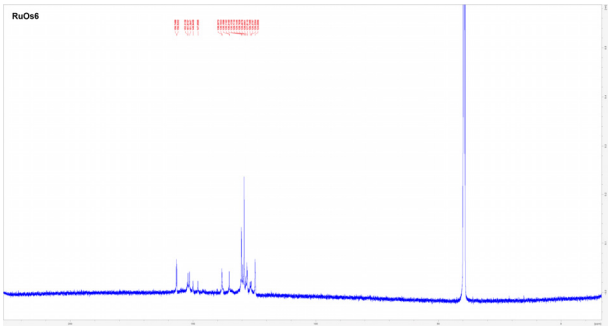


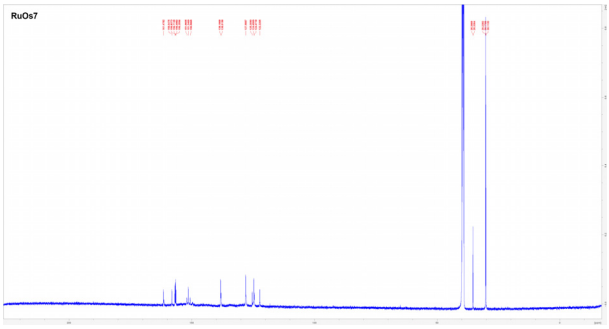


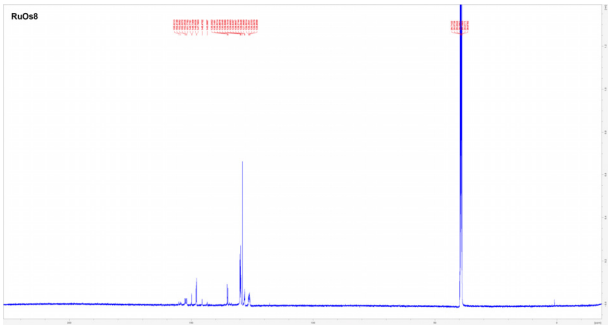




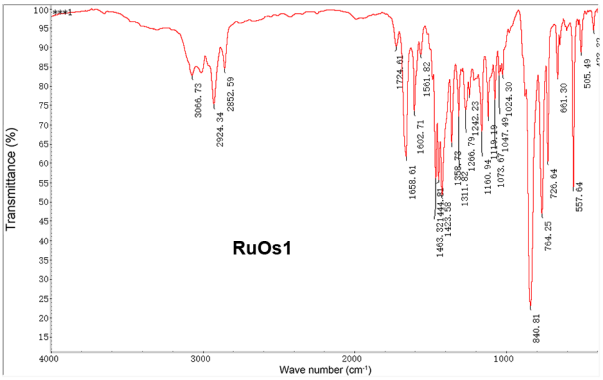


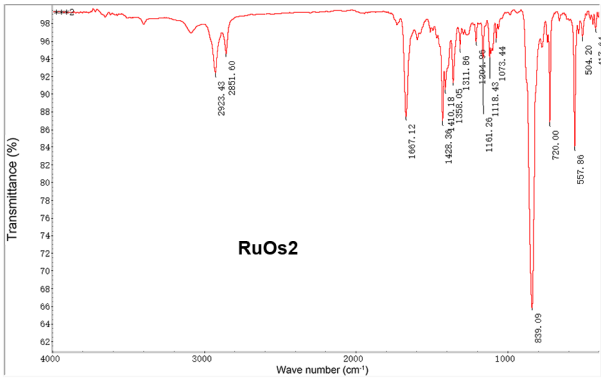


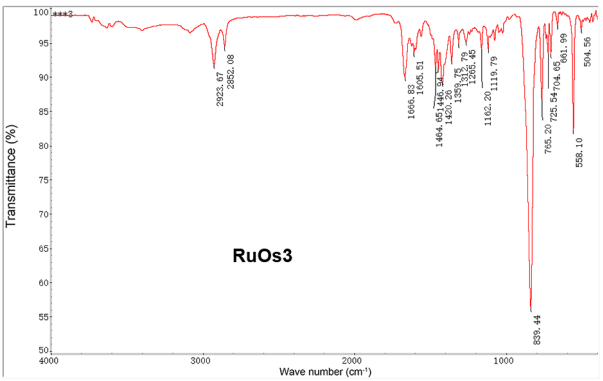


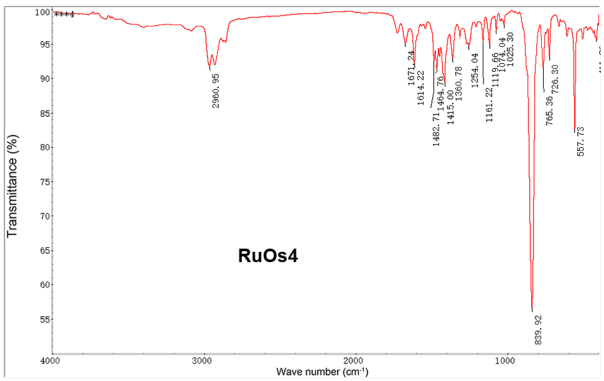


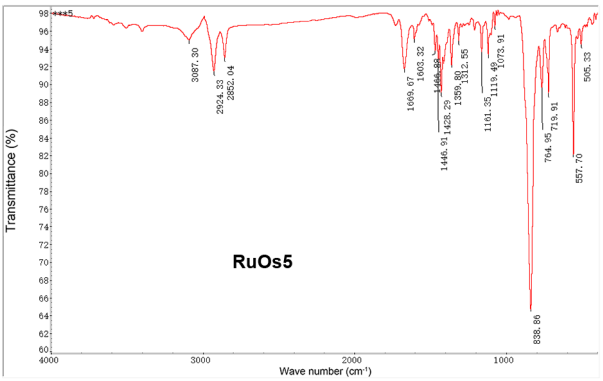
FT-IR spectra of RuOs1−8

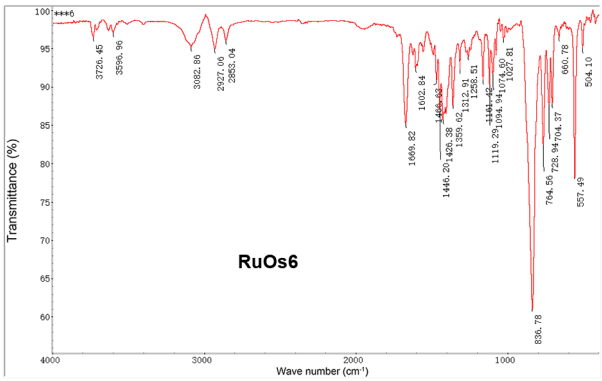


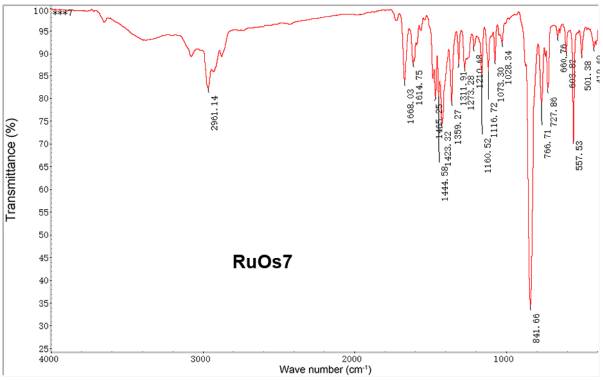


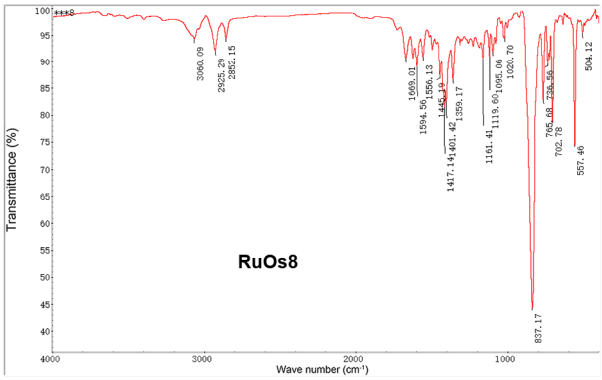




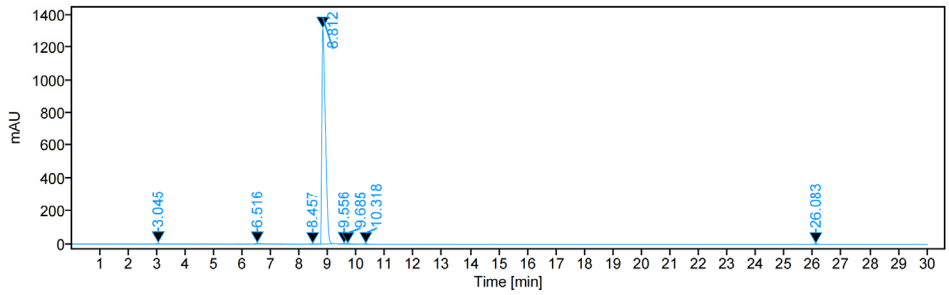






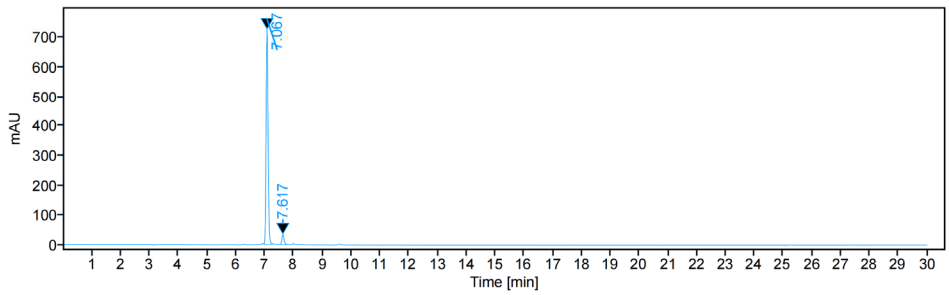


HPLC chromatograms of RuOs1−8



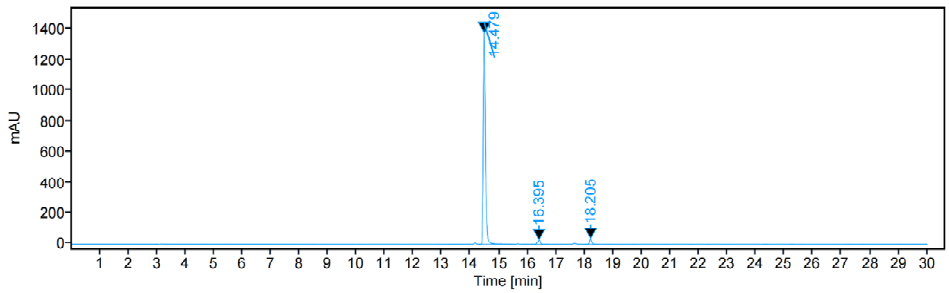
RuOs1

RT [min] Type	Width [min]	Area	Height	Area% Name
3.045 BV	0.1110	19.3049	6.2943	0.1673
6.516 BB	0.3900	48.4955	5.3512	0.4204
8.457 BB	0.2633	10.4697	1.6799	0.0908
8.812 BB	0.5200	11388.8597	1318.2644	98.7237
9.556 BV R	0.3325	20.7475	2.9988	0.1798
9.685 VB T	0.1553	6.4599	1.2390	0.0560
10.318 BB	0.2433	15.3765	2.8995	0.1333
26.083 BB	0.3433	26.3761	3.2513	0.2286
	Sum	11536.0898		



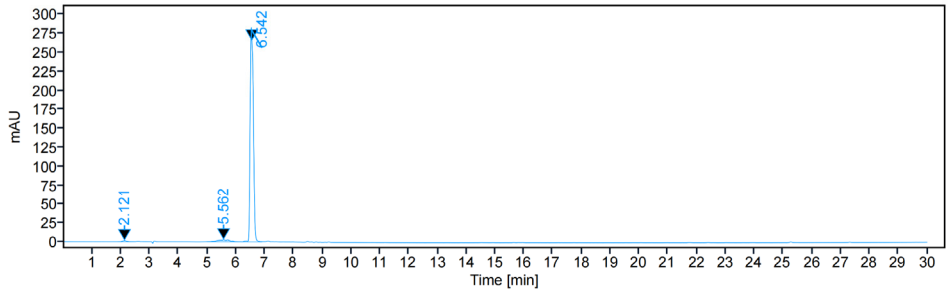
RuOs2

RT [min] Type	Width [min]	Area	Height	Area% Name
7.067 BB	0.2733	3445.5503	726.6991	95.0768
7.617 BB	0.2258	178.4134	34.0174	4.9232
	Sum	3623.9637		



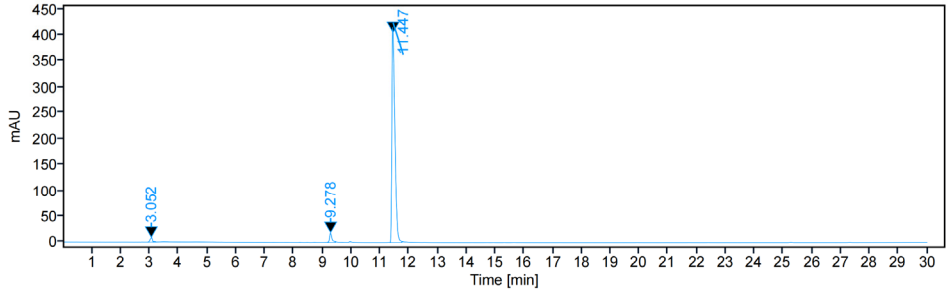
RuOs3

RT [min] Type	Width [min]	Area	Height	Area% Name
14.479 BB	1.2006	7466.0061	1370.2811	95.8081
16.395 BB	0.6593	161.6066	22.8348	2.0738
18.205 BB	0.5400	165.0509	30.9519	2.1180
	Sum	7792.6636		



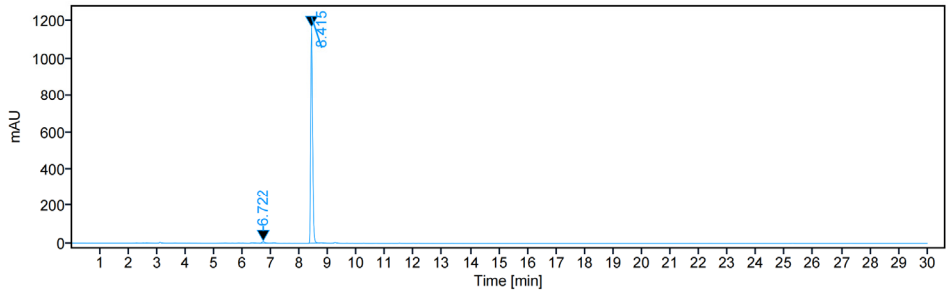
RuOs4

RT [min] Type	Width [min]	Area	Height	Area% Name
2.121 BB	0.5601	19.5612	1.6112	0.8388
5.562 BV X	1.0867	80.1480	2.7387	3.4369
6.542 VB R	1.9170	2232.2895	265.6059	95.7243
	Sum	2331.9987		



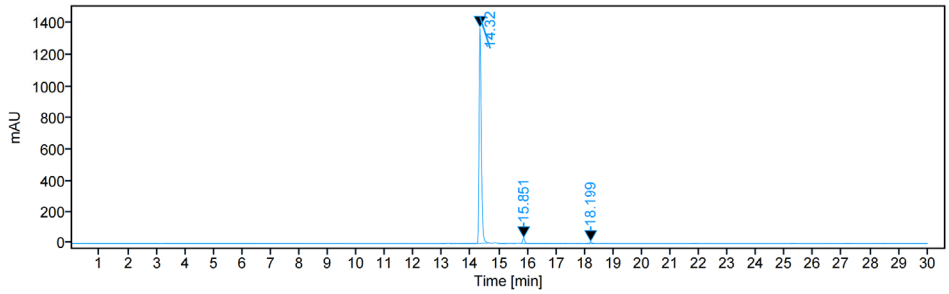
RuOs5

RT [min] Type	Width [min]	Area	Height	Area% Name
3.052 BB	0.3347	51.9143	7.9920	1.6439
9.278 BB	0.2892	105.2132	17.6188	3.3317
11.447 BB	0.4257	3000.8411	404.2573	95.0244
	Sum	3157.9686		



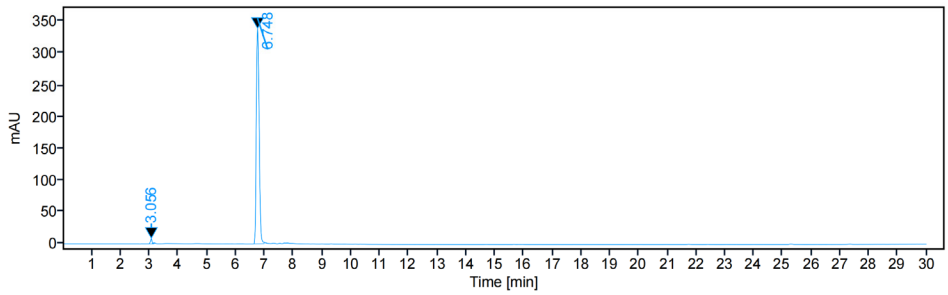
RuOs6

RT [min] Type	Width [min]	Area	Height	Area% Name
6.722 BB	0.3205	54.2637	8.5694	1.0046
8.415 BB	0.2800	5347.2275	1168.1857	98.9954
	Sum	5401.4911		



RuOs7

RT [min] Type	Width [min]	Area	Height	Area% Name
14.320 BB	0.3933	7405.0707	1373.9086	97.1849
15.851 BB	0.2178	162.2294	33.8685	2.1291
18.199 BB	0.2119	52.2652	10.7606	0.6859
	Sum	7619.5654		



RuOs8

RT [min] Type	Width [min]	Area	Height	Area% Name
3.056 BB	0.1783	29.0270	7.6015	1.2349
6.748 BB	0.3478	2321.5091	337.9494	98.7651
	Sum	2350.5361		

4. Experimental Procedures

4.1. DFT Calculations

The density functional theory (DFT) calculations were carried out with the Gaussian16 quantum chemistry program package.[5] MN15,[6] a Kohn–Sham global-hybrid exchange-correlation density functional with simultaneous accuracy for photochemistry application, was selected because the theoretical data calculated by this functional were much closer to the experimental data than the other tested density functions, such as Becke's three-parameter hybrid functional (B3LYP), CAM-B3LYP,[7] global-hybrid meta-GGA (generalized gradient approximation) M06,[8] and MN15-L.[9] For the same reason, LanL2DZ basis set (a double-zeta basis set containing effective core potential) for all atoms was selected from a number of benchmarks, including SDD (Stuttgart/Dresden effective core potential) for all atoms, def2TZVP (Coulomb-fitting basis set) for all atoms, LanL2DZ for Os and Ru/6-31G(d) for the others, LanL2DZ for Os and Ru/6-311G(d,p) for the others, SDD for Os and Ru/6-31G(d) for the others, and SDD for Os and Ru/6-311G(d,p) for the others. DFT-D3 dispersion correction[10] containing Becke-Johnson (BJ) damping[11] was used in all calculations to improve accuracy. The full geometry optimization was carried out for the heteronuclear complexes in aqueous solution, using the conductor polarized continuum model (CPCM)[12]. The stability of the optimized conformation of the heteronuclear complexes was confirmed by the frequency analysis, which shows no imaginary frequency for each energy minimum. For absorption spectral calculations, 80 lowest singlet excited states (ESs) were calculated using the analytical time-dependent DFT (TDDFT) theory to reproduce the experimental spectra. The discrete optical transitions with their corresponding oscillator strength were broadened by a Gaussian function with the full width at half maxima (FWHM) of 2200 cm^{-1} to represent an experimental inhomogeneous spectral broadening. For fluorescence emission spectral calculations, the lowest singlet excited states (S1) were structurally optimized for the lowest 10 states and the theoretical emission spectra were generated as described for absorption spectra above with FWHM of 0.2 eV. The structures of the excited triplet states were also optimized to reveal their transition properties. A compact representation of an ES *via* photoexcited hole–electron pair, which fits for chemical intuition, can be obtained using natural transition orbital (NTO) analysis.[13] By performing NTO calculations, a hole–electron pair transition from a ground state to an ES could be realized through unitary transformation of transition density matrix. NTO pairs contributing to the most important optical transitions were visualized for plotting excited charge densities (isovalue = 0.02).

4.2. Singlet oxygen ($^1O_2$) Quantum Yields

The $^1O_2$ quantum yields of **RuOs1**−**8** have been measured according to the reported method using 9,10-anthracenediyl-bis(methylene)dimalonic acid (ABDA) as an $^1O_2$ indicator.[3] The absorbance of ABDA was adjusted to 0.4 at 378 nm in air-saturated water, and the absorbance of the heteronuclear complex was adjusted to 0.1 at 400 nm. The photo-oxidation of ABDA was monitored at certain intervals under irradiation at 400 nm (LED), 450 nm (LED) and 808 nm (LPL) with external air-cooling devices. The irradiances of LED array light sources were measured by an optical power meter (PM100D, Thorlabs) equipped with a thermal power sensor (S425C, Thorlabs), using the standard 5-point method, and unified to 50 mW cm^{-2} by adjusting the distance between light source and sample. The power of 808 nm LPL was modified by a tunable controller, until the output irradiance reached 100 mW cm^{-2}, as indicated by the optical power meter. The $^1O_2$ generation rates were measured and calculated by the following method. The light intensity (I, einstein s^{-1}) of a light source with a power P (W) and a wavelength λ (nm) can be calculated as follows[14]:

$$I \text{ (einstein s}^{-1}) = P \text{ (W)} \times \lambda \text{ (nm)} \times 8359 \times 10^{-9} \quad \text{(Eq 1)}$$

Therefore, the photon flux (photons obtained by the test compound at one time interval) can be calculated by the I reduction (ΔI) after sample penetration (light absorption). The aqueous solution **Ir1**–**6** or $[Ru(bpy)_3]^{2+}$ (2.5 mL, 1 mM) was put into the standard cuvette. Optical powers in the front (P_f) and back (P_b) of the cuvette toward the light irradiation were measured respectively. Water was used as blank to obtain $P_{f,0}$ and $P_{b,0}$, so as to eliminate the possible influence of light scattering. The optical power decrease (ΔP) caused by light absorption of the test compound was expressed as $\Delta P = (P_f - P_b) - (P_{f,0} - P_{b,0})$. The ΔP of the test heteronuclear complex at the concentration C_M (mM) used in ABDA experiment was calculated as:

$$\Delta P_M = \Delta P \times C_M / 1 \text{ mM} \quad \text{(Eq 2)}$$

$$\Delta I \text{ (einstein min}^{-1}) = \Delta P_M \text{ (W)} \times \lambda \text{ (nm)} \times 5.0154 \times 10^{-4} \quad \text{(Eq 3)}$$

The $^1O_2$ generation rate (per minute) was obtained by the slope (*Slope*) of a linear fit of ΔOD (absorbance of ABDA at 378 nm) versus time (min). The molar extinction coefficient of ABDA (ε_{ABDA}) in aqueous solution at 378 nm was tested to be 12000. The $^1O_2$ quantum yield ($\Phi_{\Delta,\lambda}$) at a wavelength λ (nm) can be calculated as follows:

$$\Phi_{\Delta,\lambda} = \frac{\text{moles of } ^1O_2 \text{ generated per minute}}{\text{moles of photons absorbed per minute}} = \frac{2.5 \times 10^{-3} \times Slope}{\Delta P_M \text{ (W)} \times \lambda \text{ (nm)} \times 5.0154 \times 10^{-4} \times \varepsilon_{ABDA}}$$

$$= \frac{0.0004154 \times Slope}{\Delta P_M \text{ (W)} \times \lambda \text{ (nm)}} \quad \text{(Eq 4)}$$

The maximum permissible measurement uncertainty is 5%. The calculated Φ_Δ for $[Ru(bpy)_3](PF_6)_2$ (0.392) is very close to the reported value (0.42).[15]

4.3. Two-photon Absorption Cross-Section (TPACS)

TPACSs of **RuOs1**−**8** (50 μM) in dry THF (water ≤ 30 ppm by Karl Fischer) were measured by the well-established method involving two-photon-induced fluorescence.[16] Two-photon photoluminescence were recorded on a SpectroPro300i instrument, and the pump laser beam came from a Ti:sapphire laser system (pulse duration, 200 fs; repetition rate, 76 MHz; Coherent Mira900-D).

4.4. Determination of oil/water distribution coefficient (log $K_{O/W}$)

Aqueous solution of heteronuclear complex (5 mL, 100 μM) was mixed thoroughly with *n*-octanol (5 mL) in a 15 mL centrifuge tube. The tube was wrapped in aluminium foil, shaken for 24 h in a thermostatic shaker incubator and allowed to settle until the two phases were completely separated. The oil/water distribution coefficients (log $K_{O/W}$) were calculated using the relative concentrations of complex in the two phases.[3, 17] For absorbance below 0.002, it is used as < 0.002 for log $P_{O/W}$ calculation. The error of log $K_{O/W}$ is ± 0.04.

4.5. Photothermal Conversion Efficiency (PCE)

The temperature changes of **RuOs1**–**8** aqueous solution (1 mL) in different concentrations (10, 50 and 100 μM) under 808 nm LPL (100 mW cm^{-2}) irradiation were monitored using an IR camera for living body (HIKvision). The photothermal conversion efficiencies (η_{808}) of heteronuclear complexes were calculated as described in the literature.[3, 18] The formula is listed below:

$$\eta = \frac{h\,S\,(T_{max} - T_{surr}) - Q_{Dis}}{I\,(1-10^{-A_\lambda})} \qquad \text{(Eq 5)}$$

where η is PCE, h represents heat-transfer coefficient, S represents the surface area of the container, T_{max} represents the equilibrium temperature (the highest temperature the sample can reach with a laser irradiation), T_{surr} represents the surrounding temperature, Q_{Dis} is the baseline energy input of the sample cell, A_λ is the absorbance of compound at λ of the excitation wavelength and I is the power of excitation laser.

4.6. Cell line and culture conditions

Human malignant melanoma A375 cell lines and human normal liver HL-7702 cell lines (STR authentication,

Animal Research and Resource Center) were cultured in Roswell Park Memorial Institute 1640 medium (RPMI 1640, Adamas Life) Human normal kidney HK-2 cell lines were grown Dulbecco's modified Eagle medium/nutrient mixture (DMEM-F12, Gibco). Human lung adenocarcinoma A549 and cisplatin-resistant A549 (A549R) cell lines were cultured in high glucose Dulbecco's Modified Eagle's Medium (DMEM, Gibco). All mediums were supplemented with 10% (v/v) fetal bovine serum (FBS, Gibco), 100 units/mL penicillin and 100 mg/mL streptomycin (Sangon). All cell lines were maintained at 37 °C in a CO_2 incubator with a humidified atmosphere (95% air and 5% CO_2). The cells were routinely subcultured when reached about 80% confluency by trypsin-EDTA treatment. The cells in an exponential growth phase were harvested and counted for tumor inoculation.

4.7. Subcellular Colocalization by Confocal Laser Scanning Microscopy

Human malignant melanoma cells A375 were grown on 8-Chamber Glass Slide (Thermo Scientific) at a density of 6×10^4 cell/ml and incubated for 1 h with the heteronuclear complexes at 2.5 μM. The cells were washed with PBS twice. Nuclei and mitochondria were counterstained with Hoechst 33342 (Invitrogen) and MitoTracker Green (MTG, Invitrogen), respectively. Fluorescence images were collected on a Leica TCS SP8 DIVE two-photon confocal laser scanning microscope (CLSM) at three detection channels (MTG: λ_{ex} = 488 nm, λ_{em} = 510−520 nm; Heteronuclear complex: λ_{ex} = 808 nm, λ_{em} = 610−630 nm; Hoechst: λ_{ex} = 405 nm, λ_{em} = 460−500 nm) and processed by LAS X (Leica) software.

4.8. Cell Uptake and Endocytic Pathways

Exponentially growing A375, A549 and A549R cells (2×10^7 cell ml^{-1}) were harvested, and the resulting single-cell suspension was plated into 100 mm tissue culture plates (Adamas). After 24 h of incubation (37 °C, 5% CO_2), the cells were incubated with **RuOs6** (5 μM) for 2 h at 37 °C in RPMI 1640 medium with 10% (v/v) FBS. The cells were rinsed with PBS, detached with trypsin, counted and divided into three portions: (1) in portion 1, the nuclei were extracted using a nucleus extraction kit (Thermo); (2) in portion 2, the cytoplasm was extracted using a cytoplasm extraction kit (Thermo); (3) in portion 3, the mitochondria were extracted using a mitochondrial extraction kit (Thermo). All extraction procedures followed the manufacturer's protocols. The samples were digested with 60% HNO_3 at room temperature for one day. Each sample was diluted with water to obtain 2% HNO_3 sample solutions. The Ru and Os contents were quantified using the corresponding ruthenium

and osmium ICP standard (Supelco, Merck) on a PlasmaQuant PQ9000 inductively coupled plasma mass spectrometry (ICP-MS).

For the endocytic pathways study, A375, A549 and A549R cells were plated in 6-well plates at a density of 2.0×10^5 cells per well and incubated overnight in the RPMI 1640 culture medium containing 10% FBS. Chlorpromazine (CPZ, 10.0 μg mL^{-1}), amiloride (100.0 μg mL^{-1}) or nystatin (50.0 μg mL^{-1}) was added and further incubated at 37 °C or 4 °C for 1 h. Then, **RuOs6** (10.0 μM) was added. After 4 h of incubation, all wells were washed with PBS three times, and then the cells were collected by treatment with 0.5 mL trypsin. The counted cells were suspended in 1.0 mL PBS and lysed by ultrasonication. Methanol (3 mL) was added to each sample to extract the complexes. The internalized **RuOs6** amount was measured using a fluorescence spectrophotometer.[19]

4.9. In vitro Cell Viability Test (CCK-8 Assay)

The cell viability was determined by the CCK-8 assay. For cytotoxicity to A375, A549, and A549R cells, exponentially grown cells were seeded in 96-well plates, followed by a 24-hour incubation for attachment. Cells were incubated with different concentrations of heteronuclear complex or cisplatin (CP). For phototoxicity studies, after 12 h of incubation, supernatant was replaced with fresh culture medium and cells were subjected to irradiation by the 808 nm LPL (100 mW cm^{-2}, light dose = 30.0 J cm^{-2}), and incubated for an additional 48 h. Cells without irradiation were replaced with fresh culture medium and maintained in the dark. Then 10 μL of CCK-8 (Adamas Life) working solution was added and incubated for 1 h. Absorbance at 450 nm was measured on a microplate reader (iMark, Bio-rad), before and after CCK-8 incubation. IC_{50} values were determined by plotting the percentage of viability versus concentration on a logarithmic graph. For cytotoxicity to normal cells, exponentially grown HL-7702 and HK-2 cells were used instead. The cell viabilities in the presence of different concentrations of **RuOs6** and CP were measured by the same CCK-8 protocol. All data were reported as the mean ± standard deviation (n = 3).

4.10. Flow Cytometry Analysis

Cell apoptosis were measured by Annexin V-FITC (fluorescein isothiocyanate, AV) and propidium iodide (PI) based on the manufacturer's guide (Beyotime). Complex-treated human melanoma cells A375 at a density of 1×10^5 cell mL^{-1} in 1 mL of RPMI 1640 medium containing 10% FBS and 1×10^3 units penicillin/streptomycin were incubated at 37 °C (5% CO_2) for 2 h. The complex-containing medium were replaced with fresh RPMI

1640 medium. Cells were irradiated by the 808 nm LPL (100 mW cm^{-2}, light dose = 30.0 J cm^{-2}) or kept away from light, stained with AV and PI, and examined immediately with a BD FACSCalibur flow cytometer.

4.11. Caspase-3 and -9 Activation

Caspase-3 and -9 activities were measured through cleavage of a colorless substrate specific for caspase-3 (Ac-DEVD-*p*NA) or caspase-9 (Ac-LEHD-*p*NA) releasing *p*-nitroaniline (*p*NA). A375 cells were seeded in 96-well plates (1×10^5 cells/well) and allowed to incubate for 6 h. The cells were then incubated respectively with control (PBS) or heteronuclear complex in the dark. After 12 h incubation, the cells were divided into two groups. The dark groups were incubated for an additional 12 h, and the irradiation groups were exposed to laser irradiation (100 mW cm^{-2}, light dose = 30.0 J cm^{-2}) before they were incubated for 12 h in the dark. The cells were lysed and treated with caspase-3 or -9 activity kit (Beyotime) according to the manufacturer's protocol. Absorbance at 405 nm was measured on an iMark (Bio-rad) microplate reader. The caspase-3 and -9 activities in drug-treated cells were determined as relative values to control groups (PBS). Data were reported as the mean ± standard deviation (n = 3). To reveal the effect of PDT and PTT, caspase activities of **RuOs6**-incubated A375 cells were further examined in the presence of 1.0 mM Asc (**RuOs6**+Asc) and on an ice bath (**RuOs6**+Ice) during laser irradiation.

4.12. In vivo Dual Photodynamic and Photothermal Therapy (PDT/PTT) and Residue Detection

Animal experiments for A375 and A549R tumor cells were reviewed and approved by the Institutional Animal Care and Use Committee (IACUC) at Yunnan University, Kunming, China (Approval No: YNU20220269 and YNU20230422).

For A375 tumor assay, BALB/c female nude mice aged 6−8 weeks (body weight 18−20 g) were purchased from GemPharmatech. The mice were kept in individually ventilated cage (IVC) systems at constant temperature (20−26 ºC) and humidity (40−70%) with five animals in each cage. Each mouse was inoculated subcutaneously at the posterior right flank region with A375 tumor cells (5×10^6) in 0.1 ml of PBS for tumor development (Day 0). The drug treatments were started when the mean tumor size reached 66 mm^3 (Day 10). The mice were randomly allocated into four groups (5 mice for each group): Group I, PBS injection only; Group II, PBS injection and subsequent irradiation with 808 nm LPL (100 mW cm^{-2}, light dose = 30.0 J cm^{-2}); Group III, **RuOs6** (20 μL, 10 μM) injection only; Group 4, **RuOs6** (20 μL, 10 μM) injection and subsequent irradiation with 808 nm LPL (100 mW cm^{-2}, light dose = 30.0 J cm^{-2}). The injection-to-irradiation lag period

is 0.5 h. The temperature changes and photothermal imaging of tumor sites were monitored using an IR camera for living body (Hikvision). The body weight and tumor volume data were recorded every 2 or 3 days in the therapeutic regimen. Tumor volumes were expressed in mm^3 using the formula: $V = 0.5\ a \times b^2$, where a and b are the long and short diameters of the tumor, respectively. Tumor weight was measured at study termination. The entire procedure of dosing, as well as tumor and bodyweight measurement, were conducted in a Laminar Flow Cabinet. The relative tumor volume is calculated by V/V_0 (V is the tumor volume on the day when data were recorded, V_0 is the tumor volume on the day when treatment was started). After 14 days of therapy, the survival rate of mice was 95% (Day 24). The mice were sacrificed when the mean volumes of tumor in Group I, II and III reached 2000 mm^3 (Day 24), and the tumors and primary organs (heart, lung, kidney, spleen, liver, intestine and brain) were collected and separated into two halves. One half of the organs was used for eosin-hematoxylin staining, while the other half was homogenized, digested by 60% nitric acid for 24 h, and diluted with water to generate 2% nitric acid samples for ICP-MS analysis. The Ru and Os contents were expressed as picomoles of Ru and Os per gram of organ weight. The data is reported as the mean value ± standard deviation (n = 5). The injected Ru and Os amounts were calculated by the whole-body weights (Day 10).

For A549R tumor assay, BALB/c female nude mice aged 6−8 weeks (body weight 18−20 g) were purchased and maintained in the same conditions as described above. Each mouse was inoculated subcutaneously at the posterior right flank region with A549R tumor cells (5×10^6) in 0.1 ml of PBS for tumor development (Day 0). The drug treatments were started when the mean tumor size reached 144 mm^3 (Day 41). The mice were randomly allocated into two groups (3 mice for each group): Group V, PBS injection and subsequent irradiation with 808 nm LPL (100 mW cm^{-2}, light dose = 30.0 J cm^{-2}); Group VI, **RuOs6** (20 μL, 10 μM) injection and subsequent irradiation with 808 nm LPL (100 mW cm^{-2}, light dose = 30.0 J cm^{-2}). The injection-to-irradiation lag period is 0.5 h. The temperature changes and photothermal imaging of tumor sites were monitored using an IR camera for living body (Hikvision). The body weight and tumor volume data were recorded every 2 or 3 days in the therapeutic regimen. Tumor volumes and body weights were measured as described above. After 28 days of therapy, the survival rate of mice was 100% (Day 69). The mice were sacrificed at Day 69 and the tumors and primary organs (heart, lung, kidney, spleen, liver, intestine and brain) were collected and separated into two halves. H&E stating and residue analysis were carried out as described above. The injected Ru and Os amounts were calculated by the whole-body weights (Day 41).

5. Supplementary Figures

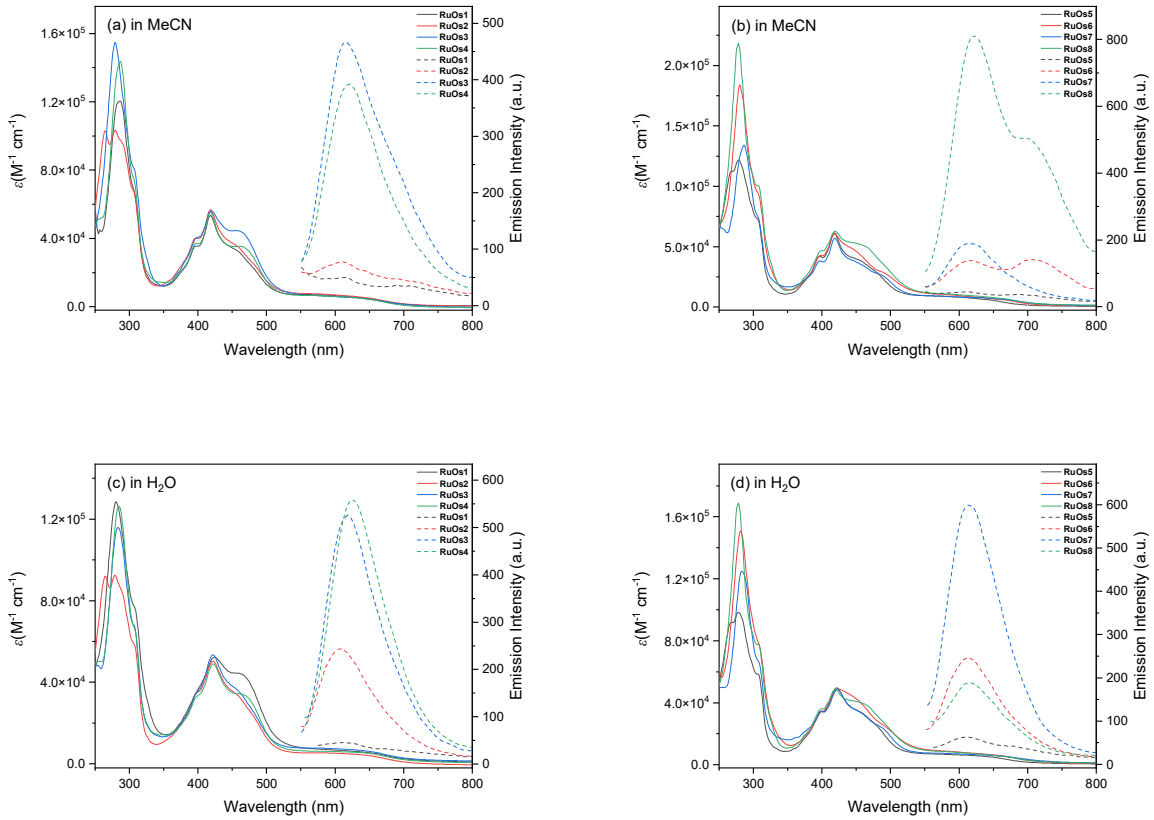


Fig S1. Absorption and emission spectra of **RuOs1–8** (10 μM) in acetonitrile (MeCN, a and b) and aqueous solution (c and d). Each Ru(II)-Os(II) complex was excited by its $MLCT_{Ru\text{-}Os} \rightarrow MLCT_{Ru^{*}\text{-}Os}$ transition wavelength.

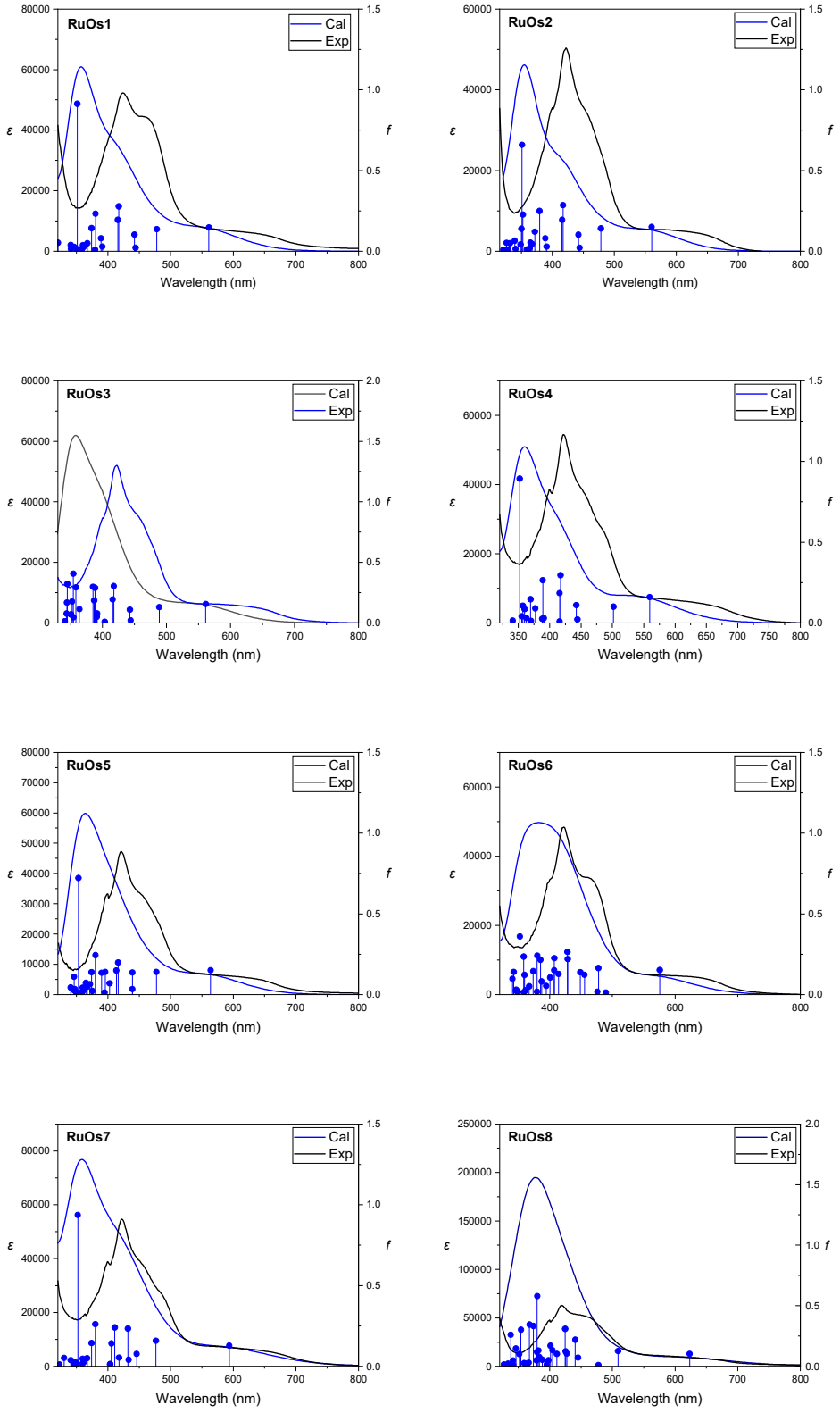


Figure S2. Simulated (Cal) and experimental (Exp) UV-Vis absorption spectra and oscillator strengths (blue spikes) of **RuOs1–8** by MN15-D3(BJ)/Lanl2DZ (CPCM for water).

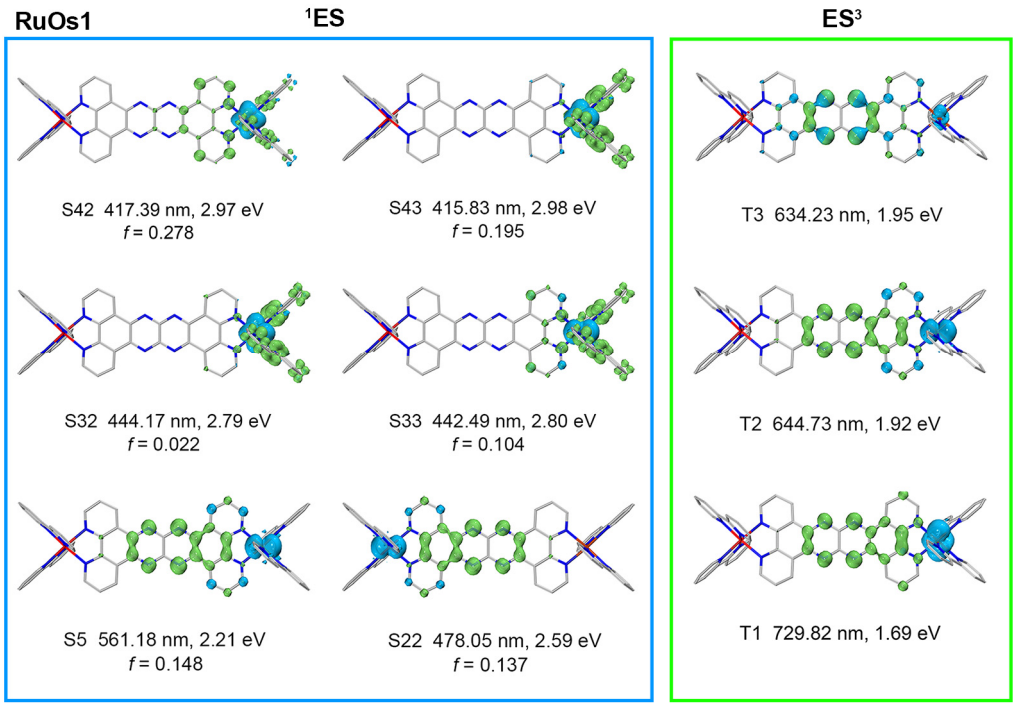


Figure S3. Real space representation of hole (blue) and electron (green) distributions of **RuOs1** for excited singlet (^{1}ES) and triplet states (^{3}ES). Excitation wavelength (nm), excitation energy (eV), and oscillator strength (*f*) for each hole-to-electron transition are presented.

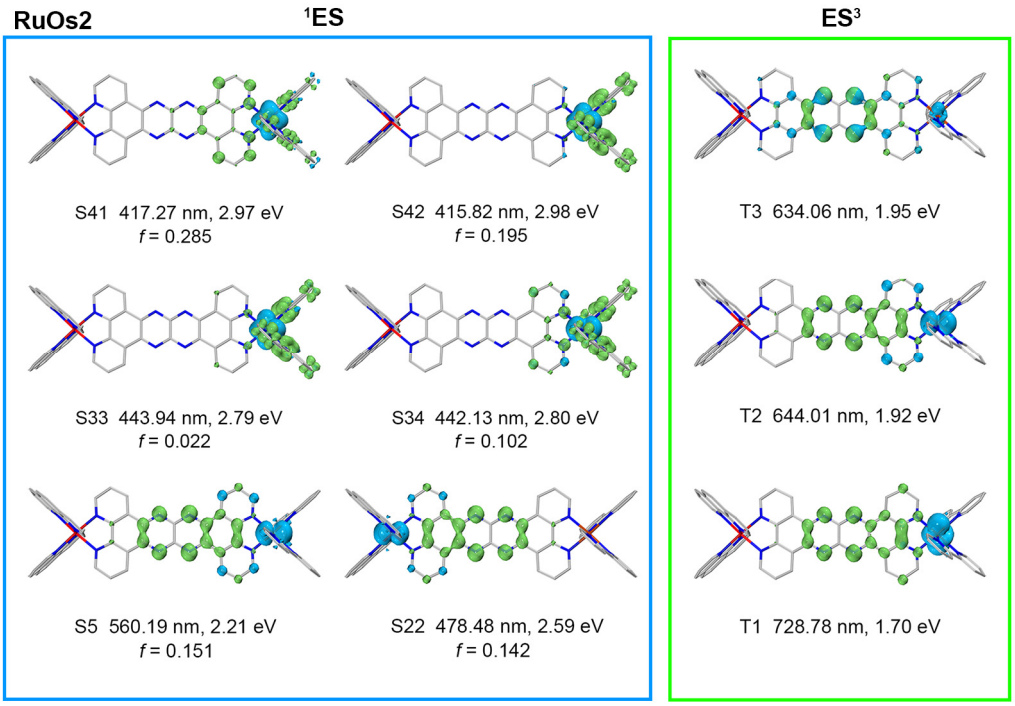


Figure S4. Real space representation of hole (blue) and electron (green) distributions of **RuOs2** for excited singlet (^{1}ES) and triplet states (^{3}ES). Excitation wavelength (nm), excitation energy (eV), and oscillator strength (*f*) for each hole-to-electron transition are presented.

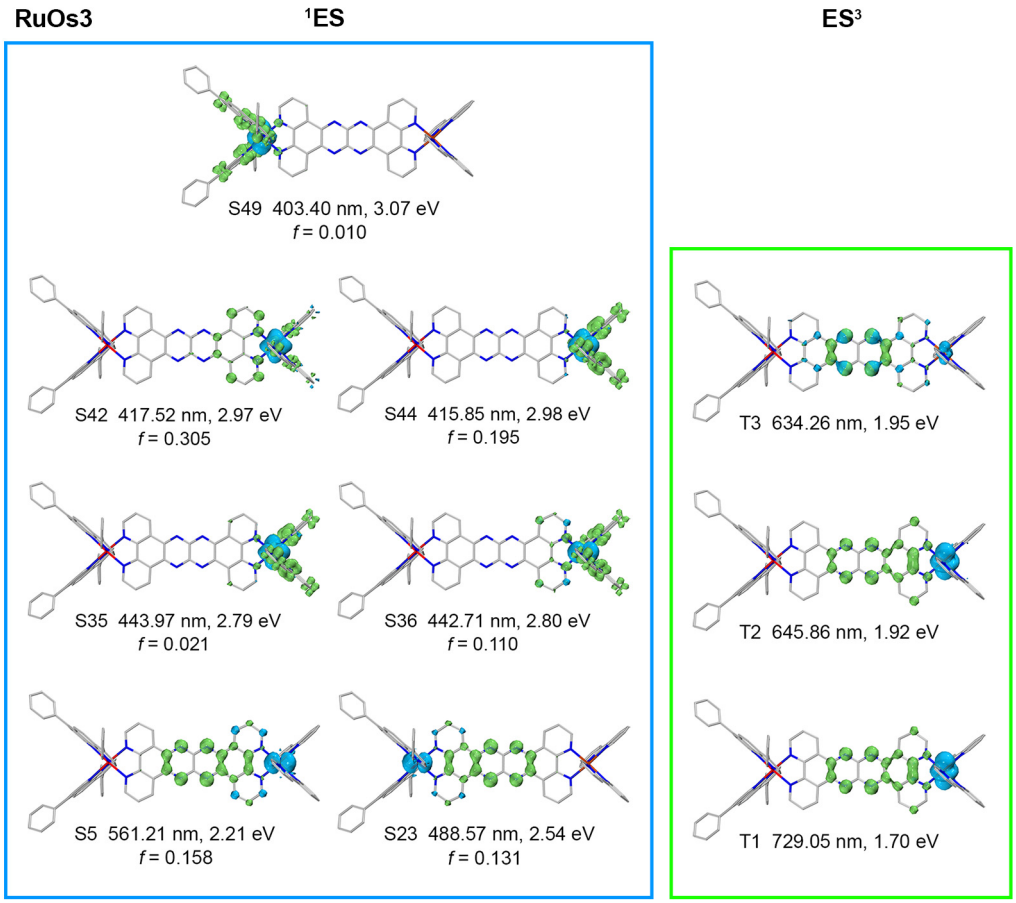


Figure S5. Real space representation of hole (blue) and electron (green) distributions of **RuOs3** for excited singlet (^{1}ES) and triplet states (^{3}ES). Excitation wavelength (nm), excitation energy (eV), and oscillator strength (*f*) for each hole-to-electron transition are presented.

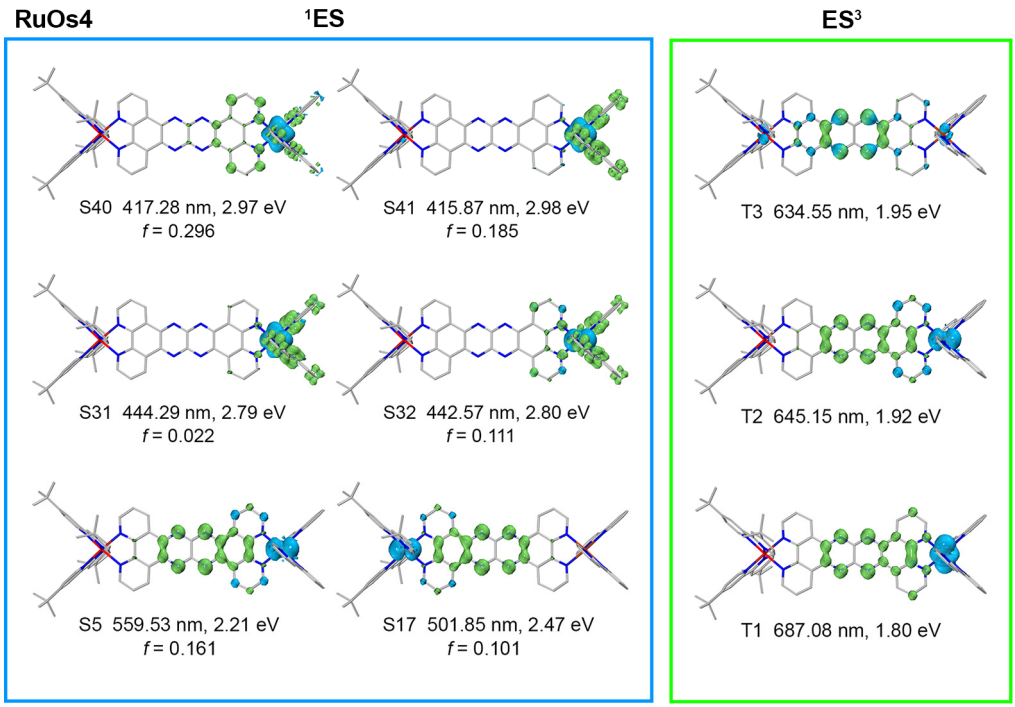


Figure S6. Real space representation of hole (blue) and electron (green) distributions of **RuOs4** for excited singlet (^{1}ES) and triplet states (^{3}ES). Excitation wavelength (nm), excitation energy (eV), and oscillator strength (*f*) for each hole-to-electron transition are presented.

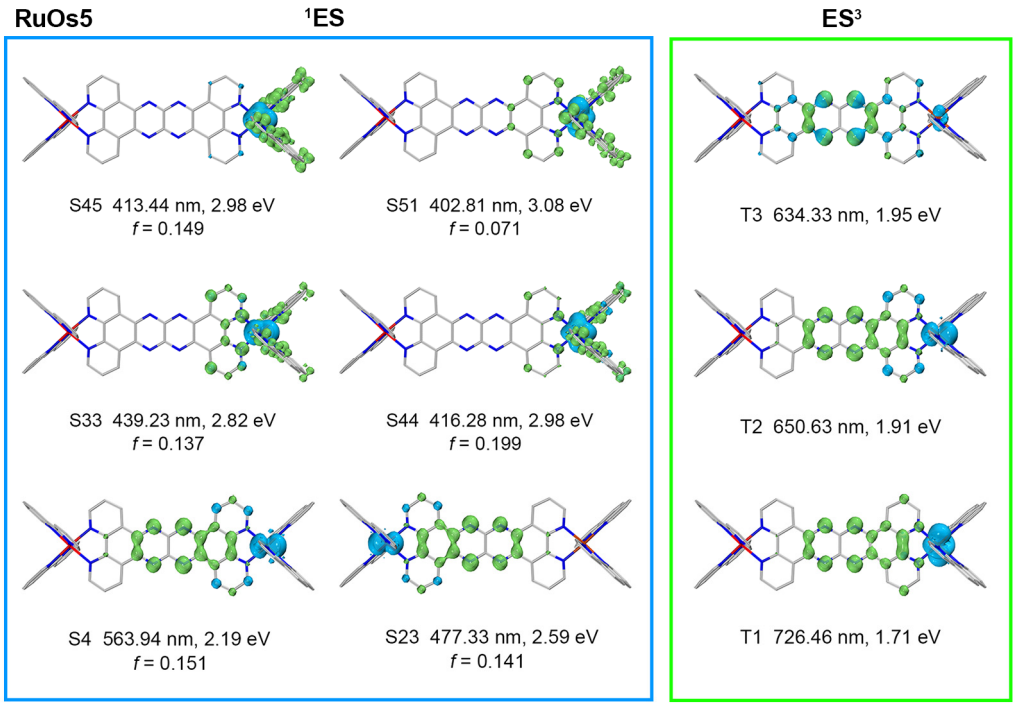


Figure S7. Real space representation of hole (blue) and electron (green) distributions of **RuOs5** for excited singlet (^{1}ES) and triplet states (^{3}ES). Excitation wavelength (nm), excitation energy (eV), and oscillator strength (*f*) for each hole-to-electron transition are presented.

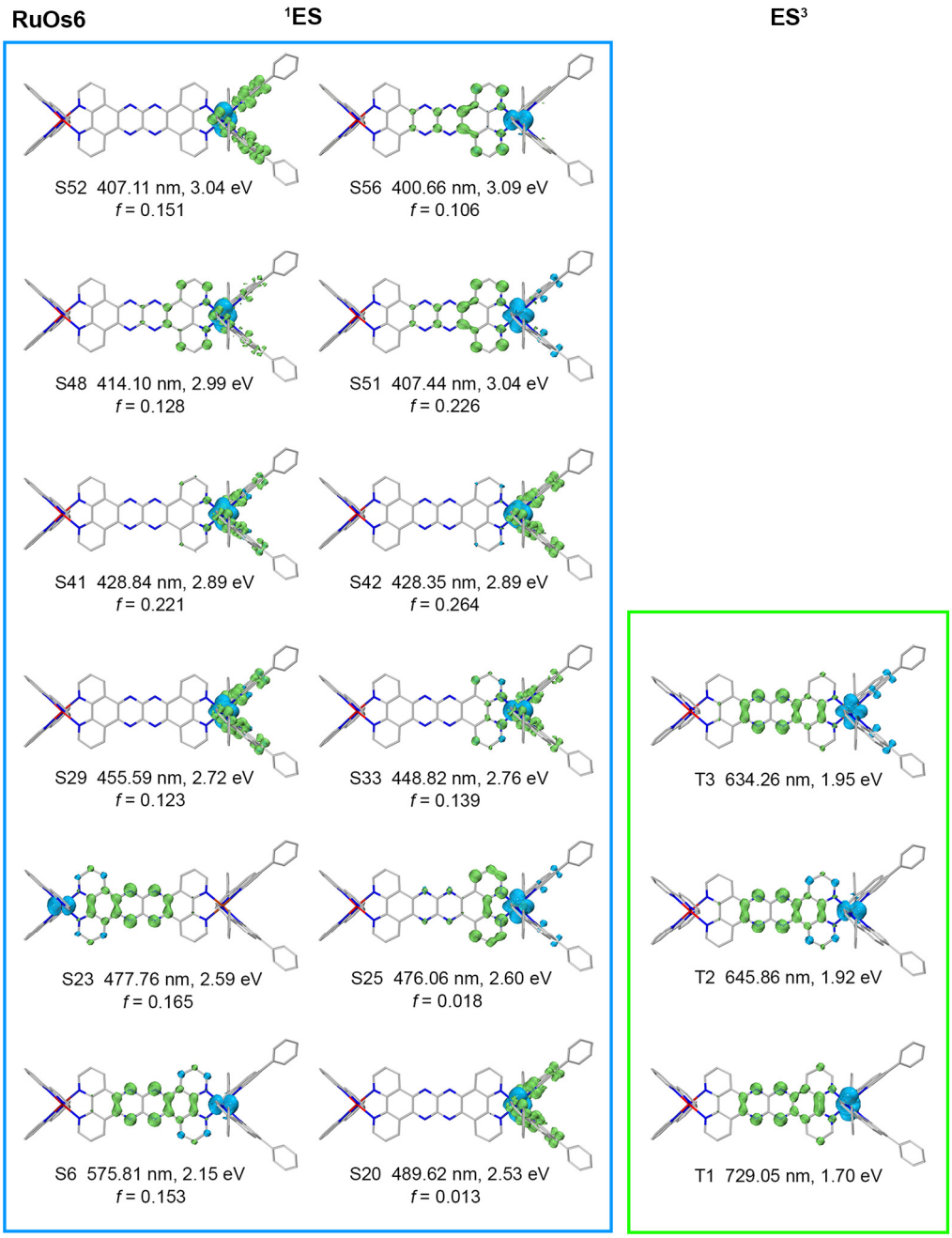


Figure S8. Real space representation of hole (blue) and electron (green) distributions of **RuOs6** for excited singlet (^{1}ES) and triplet states (^{3}ES). Excitation wavelength (nm), excitation energy (eV), and oscillator strength (*f*) for each hole-to-electron transition are presented.

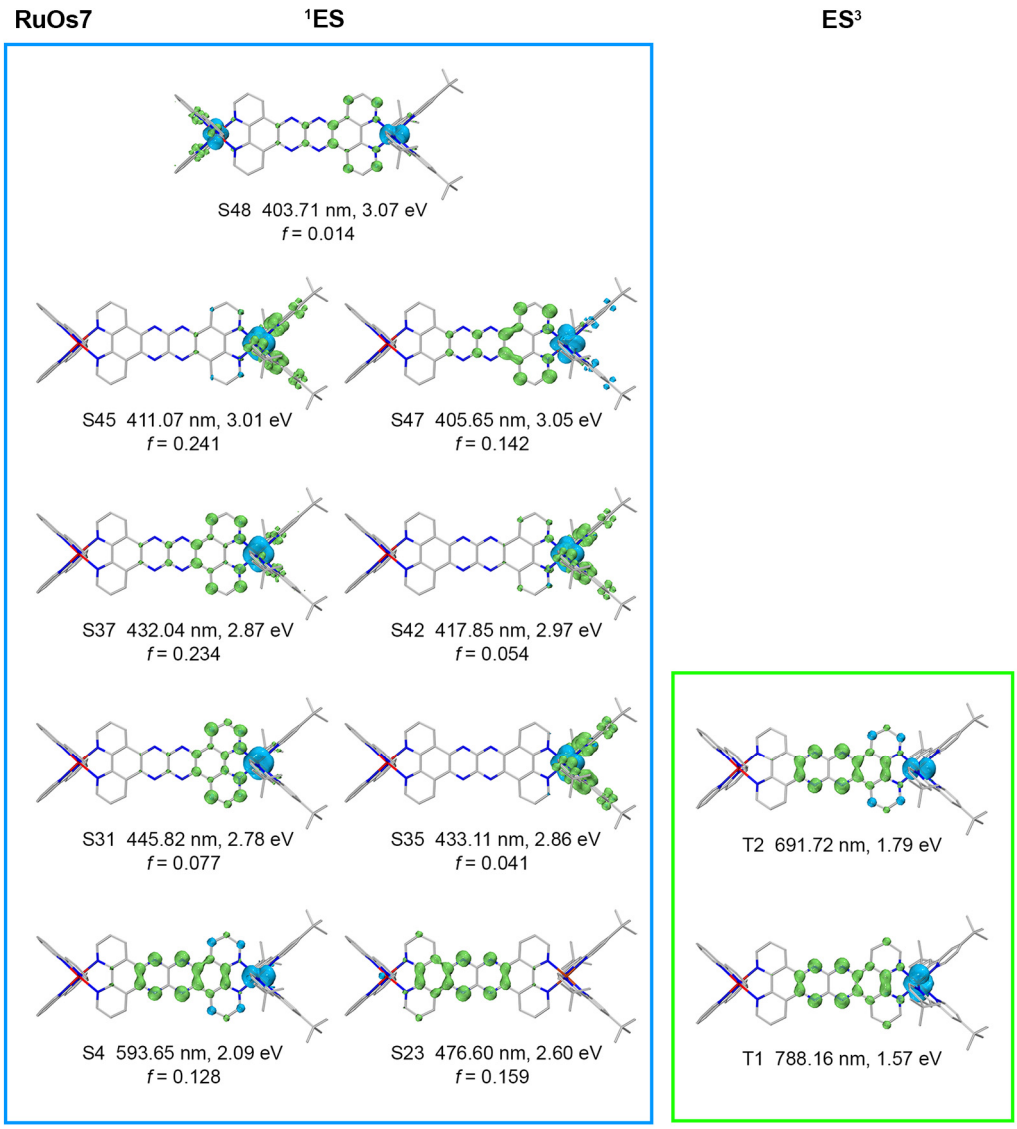


Figure S9. Real space representation of hole (blue) and electron (green) distributions of **RuOs7** for excited singlet (^{1}ES) and triplet states (^{3}ES). Excitation wavelength (nm), excitation energy (eV), and oscillator strength (*f*) for each hole-to-electron transition are presented.

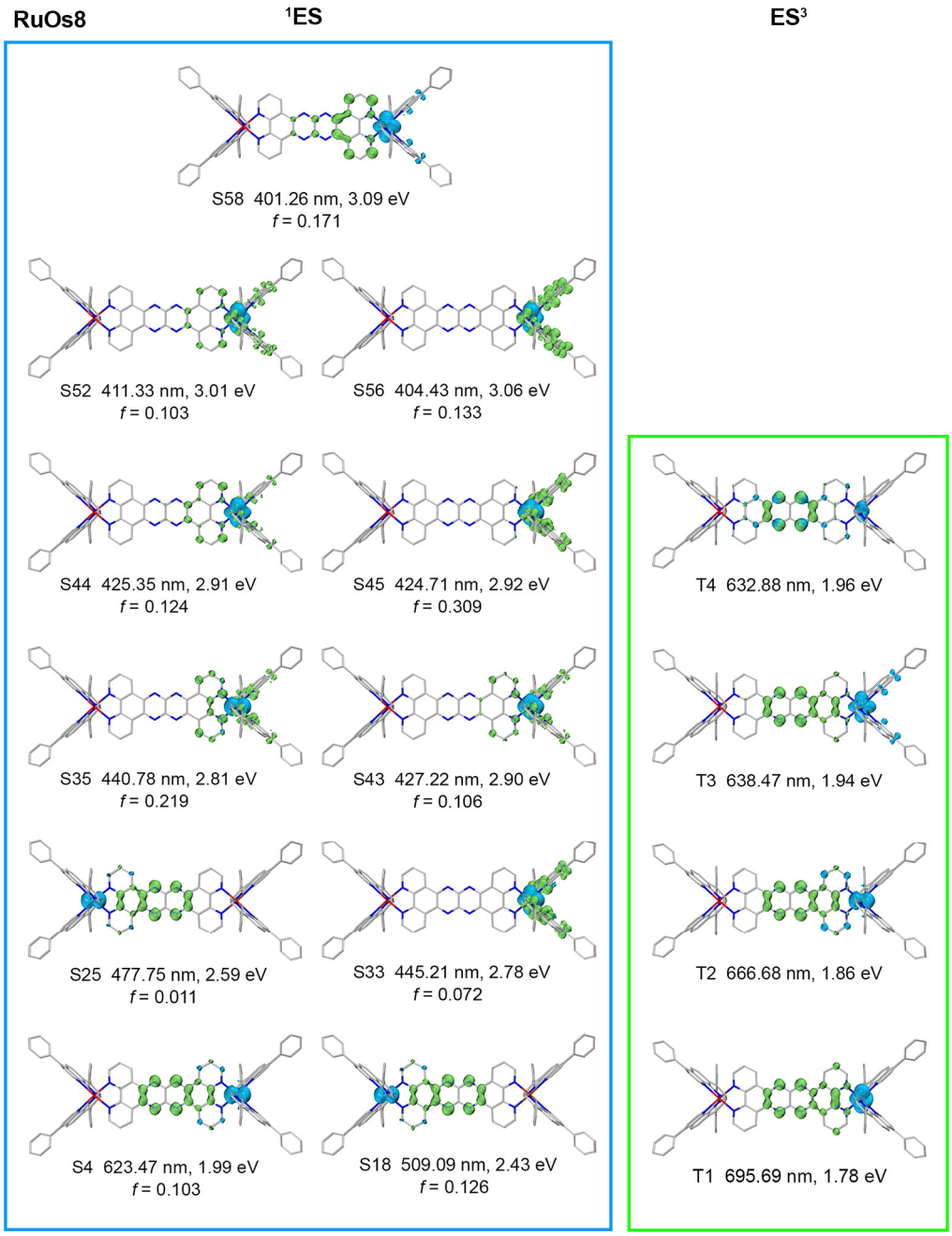


Figure S10. Real space representation of hole (blue) and electron (green) distributions of **RuOs8** for excited singlet (^{1}ES) and triplet states (^{3}ES). Excitation wavelength (nm), excitation energy (eV), and oscillator strength (*f*) for each hole-to-electron transition are presented.

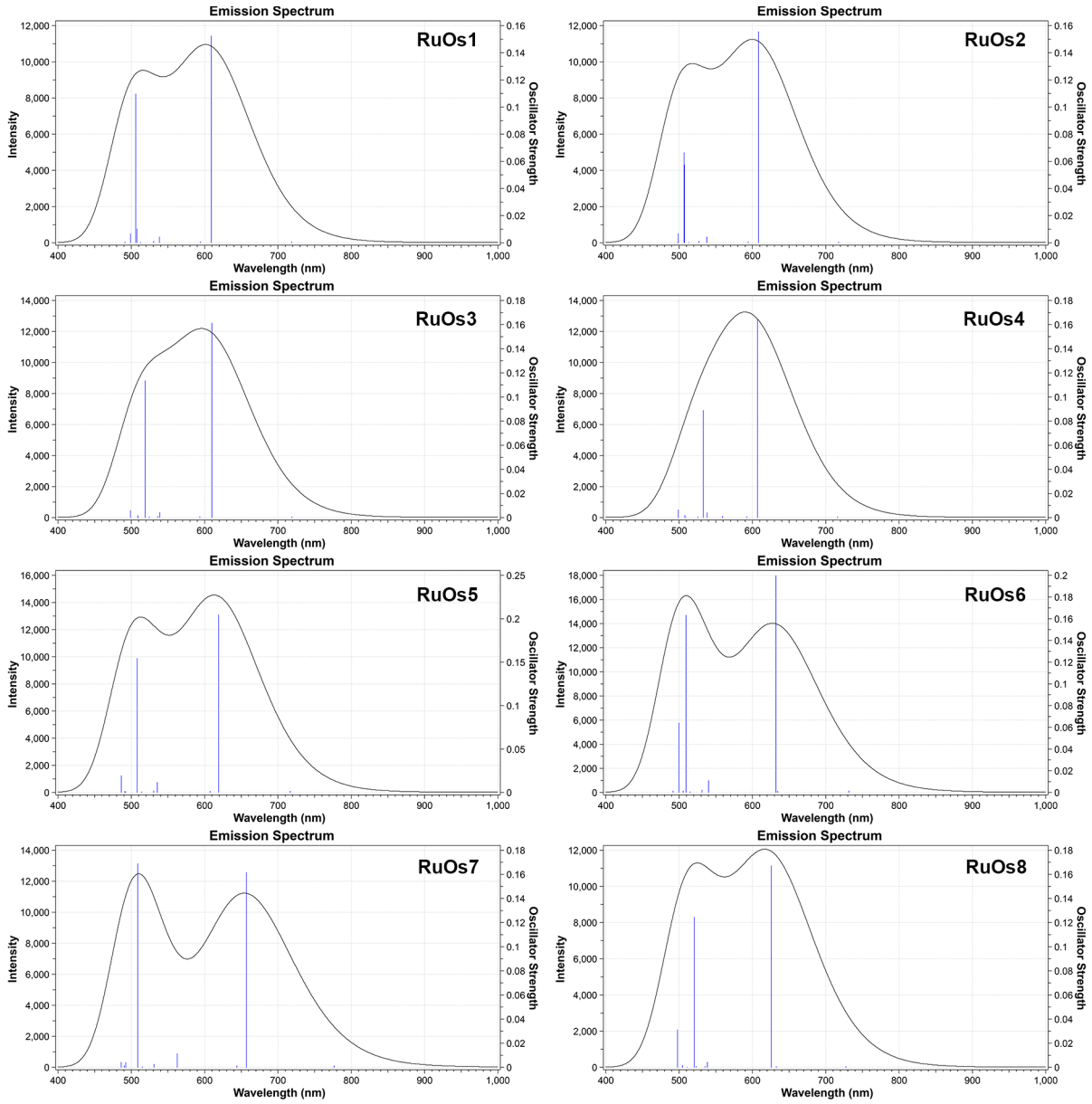


Figure S11 Simulated emission spectra and oscillator strengths (blue spikes) of **RuOs1–8** by MN15-D3(BJ)/Lanl2DZ (CPCM for water).

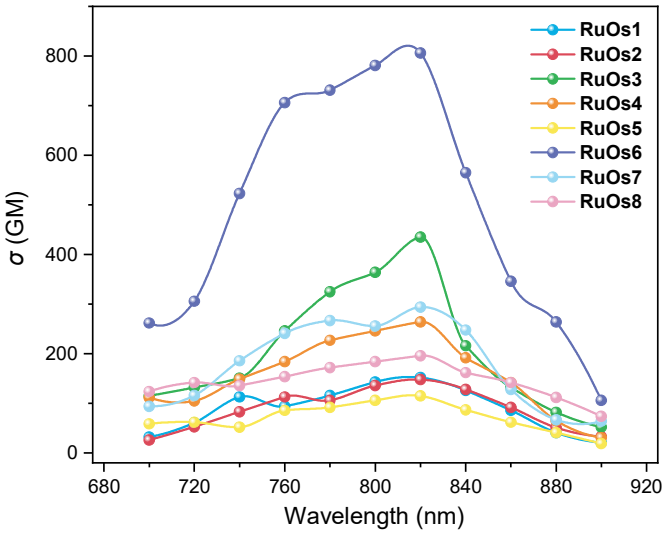


Fig. S12 TPASCs (σ) of **RuOs1−8** (50 μM) in dry THF in the range of 700−900 nm.

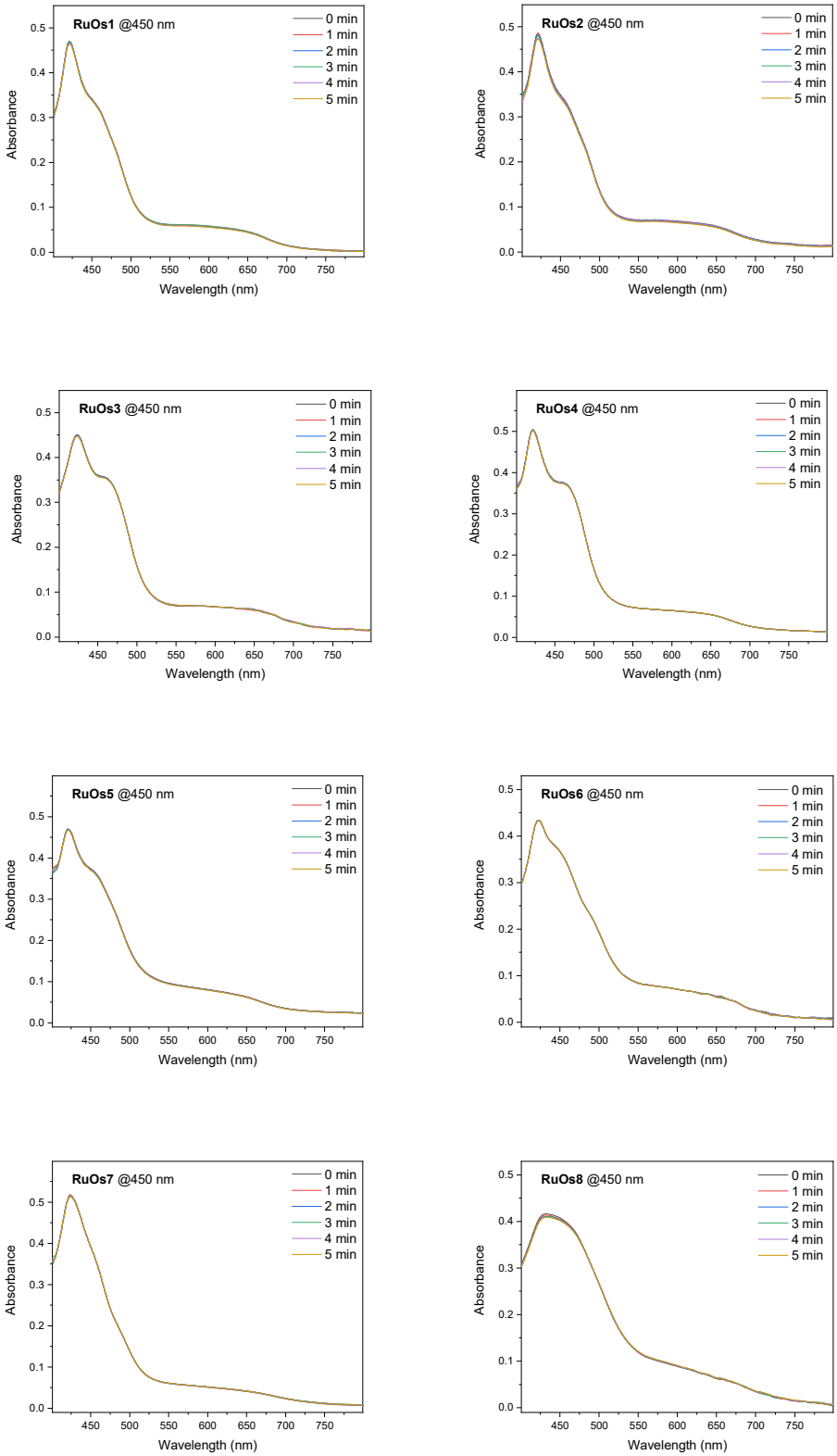


Figure S13. Photostability examined by the absorption spectra of **RuOs1**−**8** (10 μM) in aqueous solution upon 450 nm LED (50 mW cm^{-2}) irradiation for 5 min.

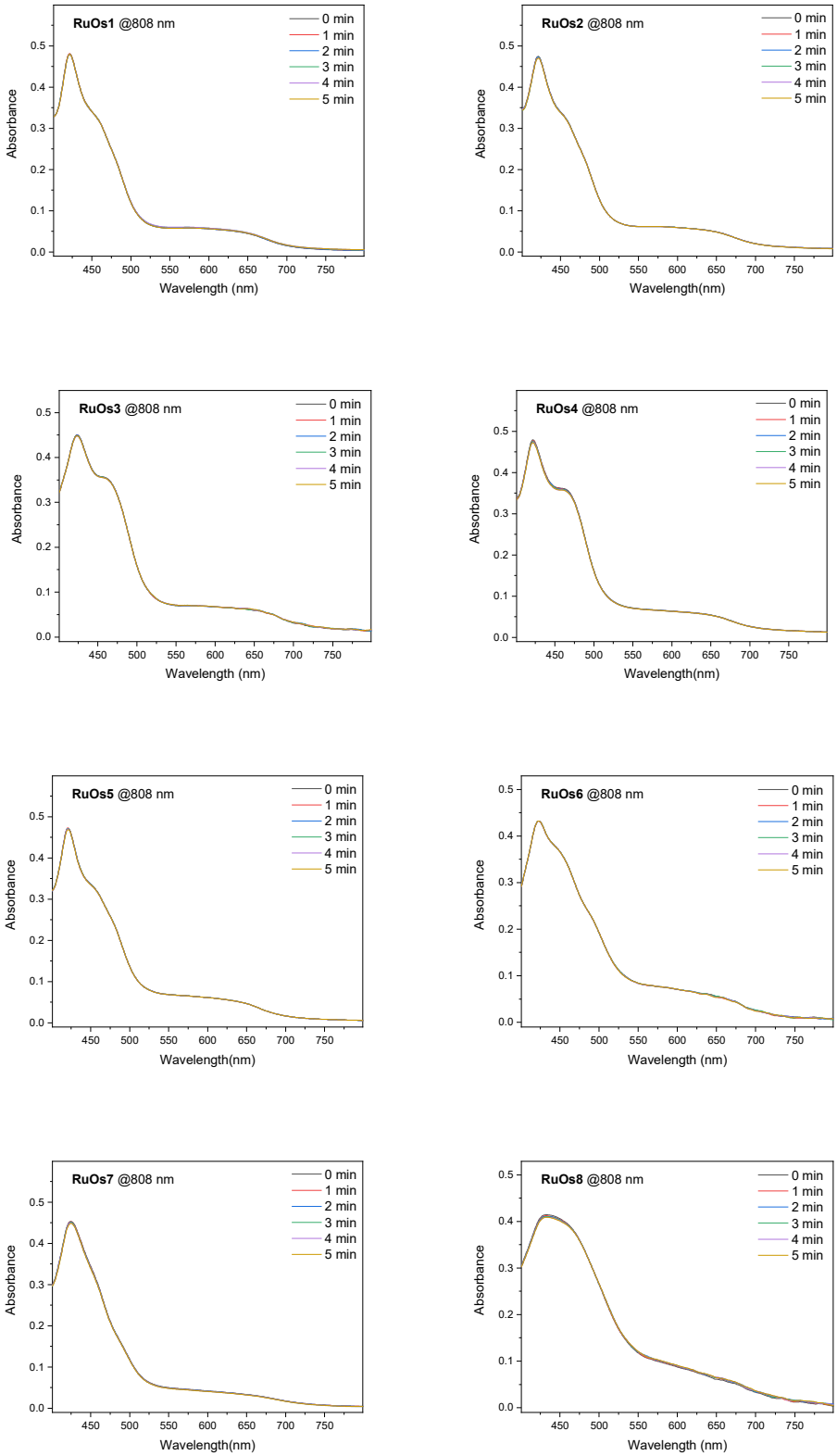


Figure S14. Photostability examined by the absorption spectra of **RuOs1**−**8** (10 μM) in aqueous solution upon 808 nm LED (100 mW cm^{-2}) irradiation for 5 min.

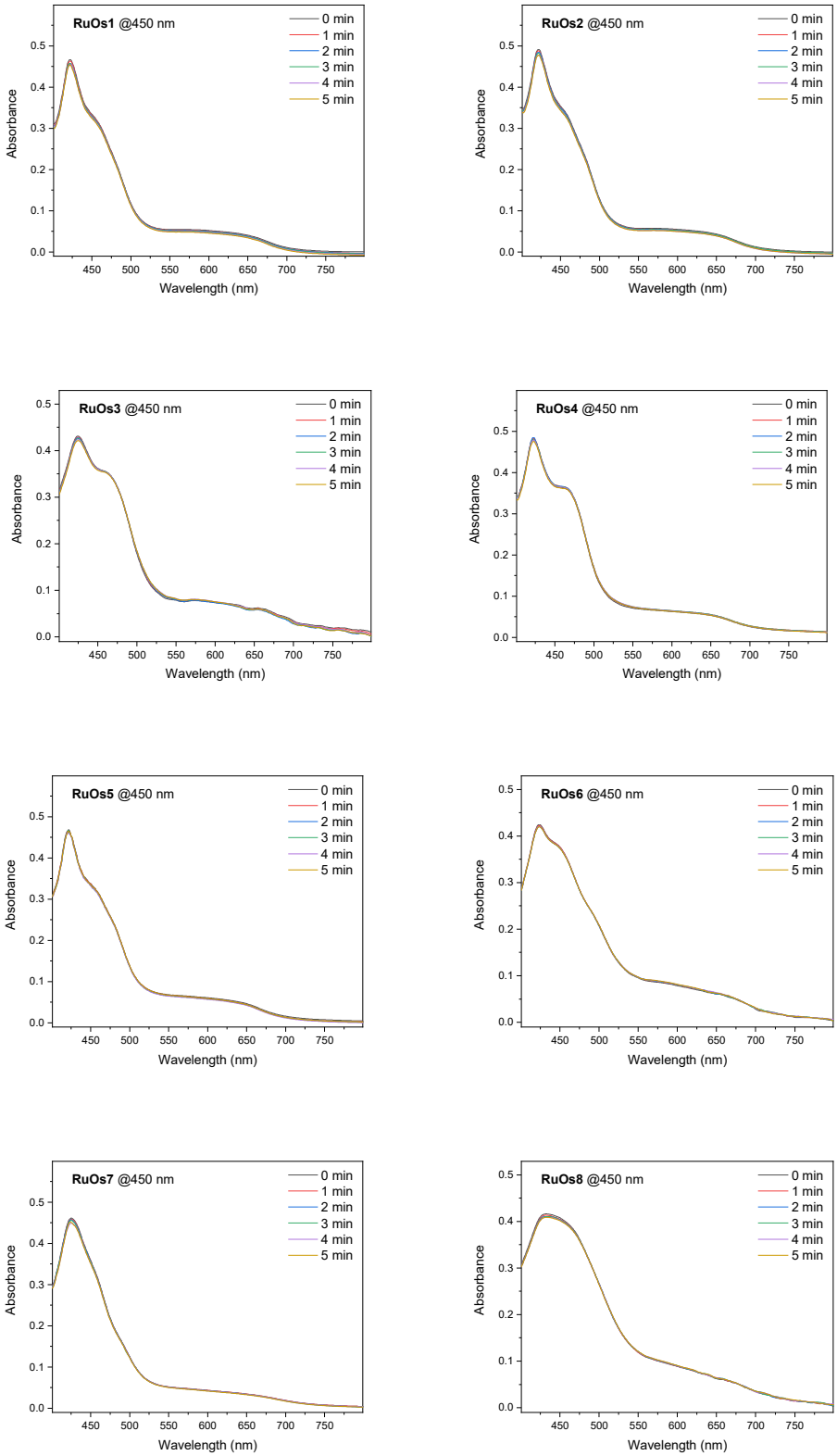


Figure S15. Photostability examined by the absorption spectra of **RuOs1**−**8** (10 μM) in RPMI-1640 medium upon 450 nm LED (50 mW cm^{-2}) irradiation for 5 min.

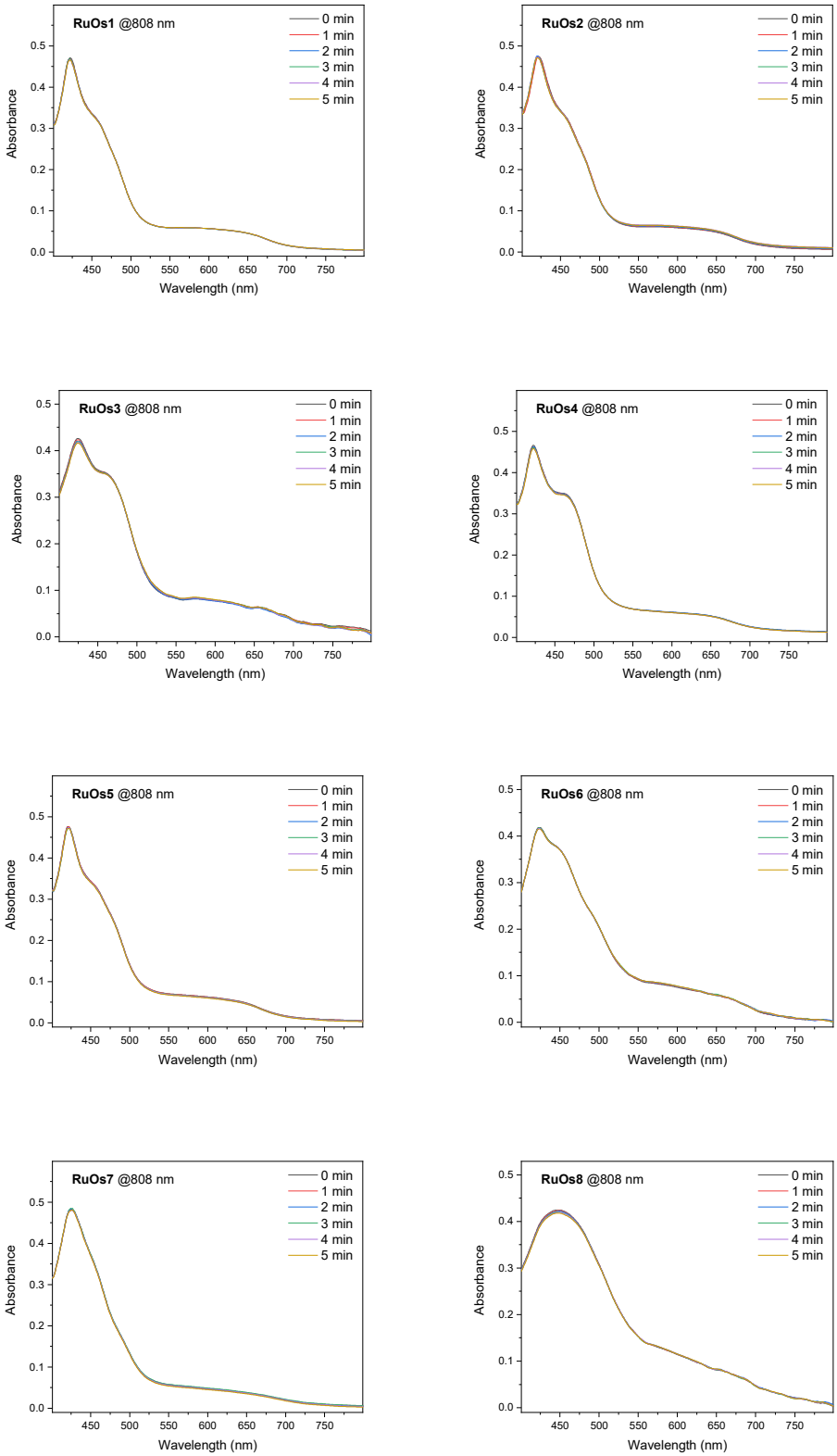


Figure S16. Photostability examined by the absorption spectra of **RuOs1**−**8** (10 μM) in RPMI-1640 medium upon 808 nm LED (100 mW cm^{-2}) irradiation for 5 min.

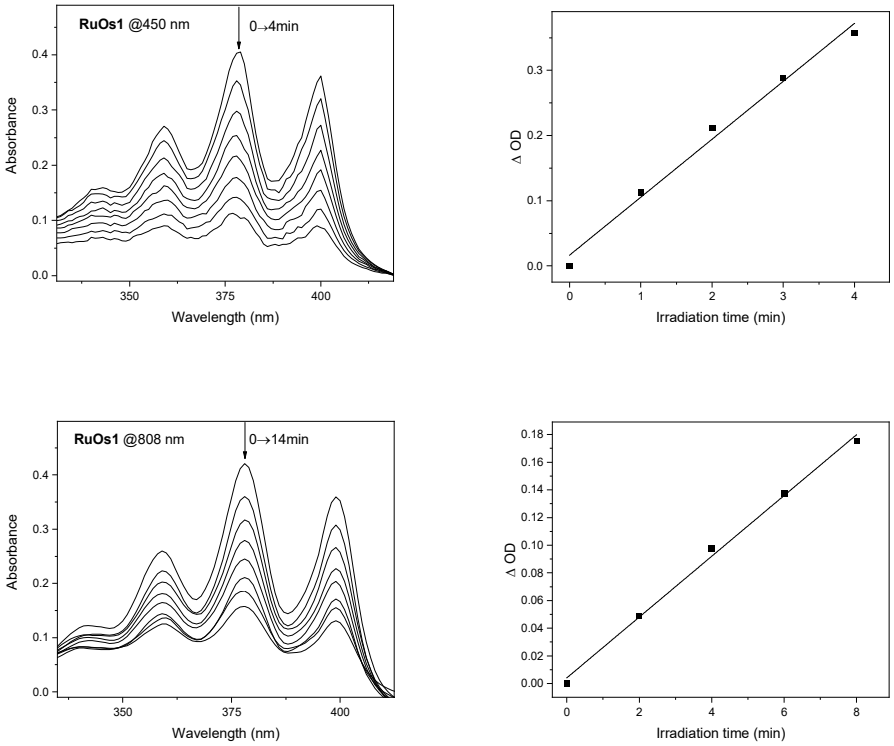


Figure S17. Absorption spectral changes of ABDA in aqueous solution upon irradiation of different light sources in the presence of **RuOs1**.

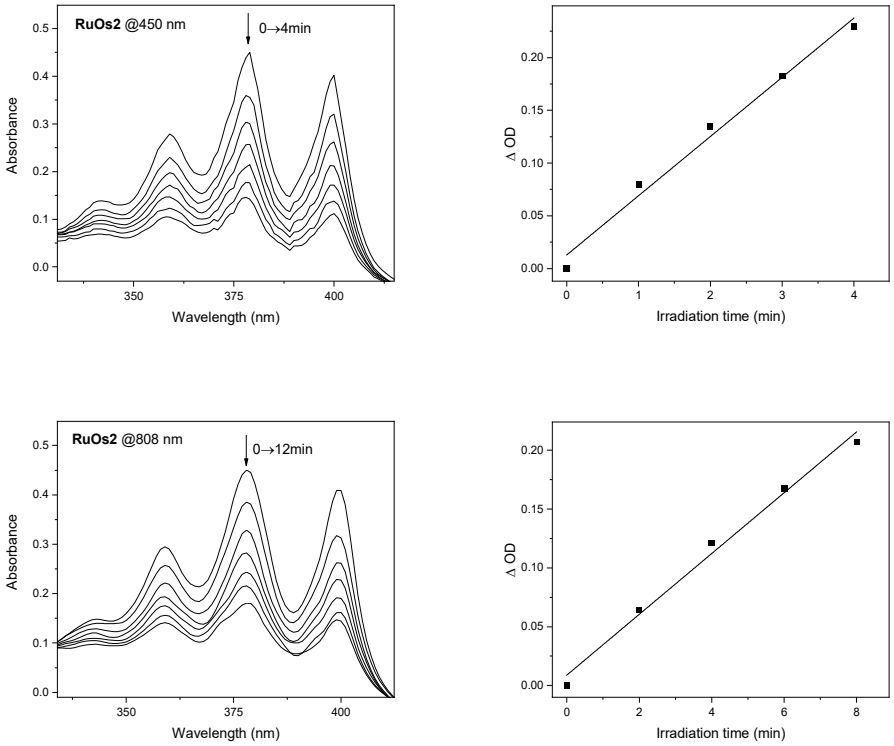


Figure S18. Absorption spectral changes of ABDA in aqueous solution upon irradiation of different light sources in the presence of **RuOs2**.

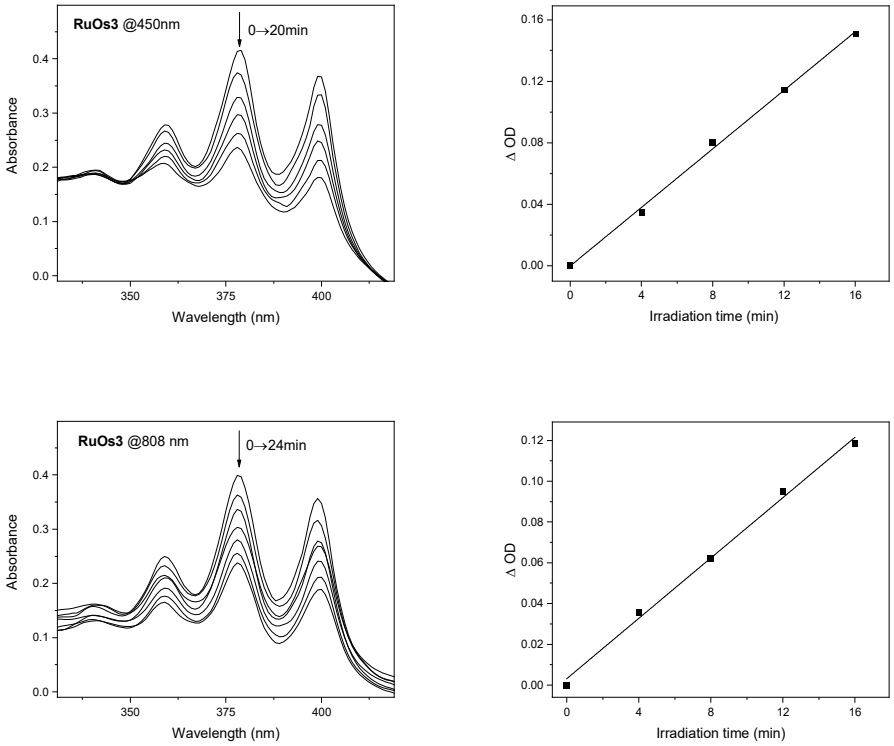


Figure S19. Absorption spectral changes of ABDA in aqueous solution upon irradiation of different light sources in the presence of **RuOs3**.

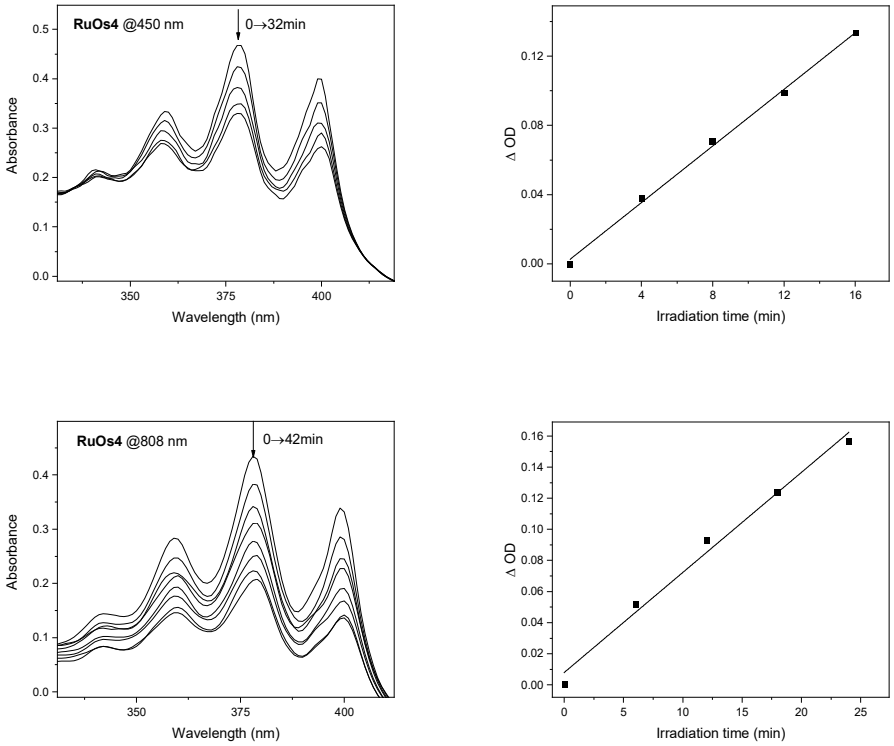


Figure S20. Absorption spectral changes of ABDA in aqueous solution upon irradiation of different light sources in the presence of **RuOs4**.

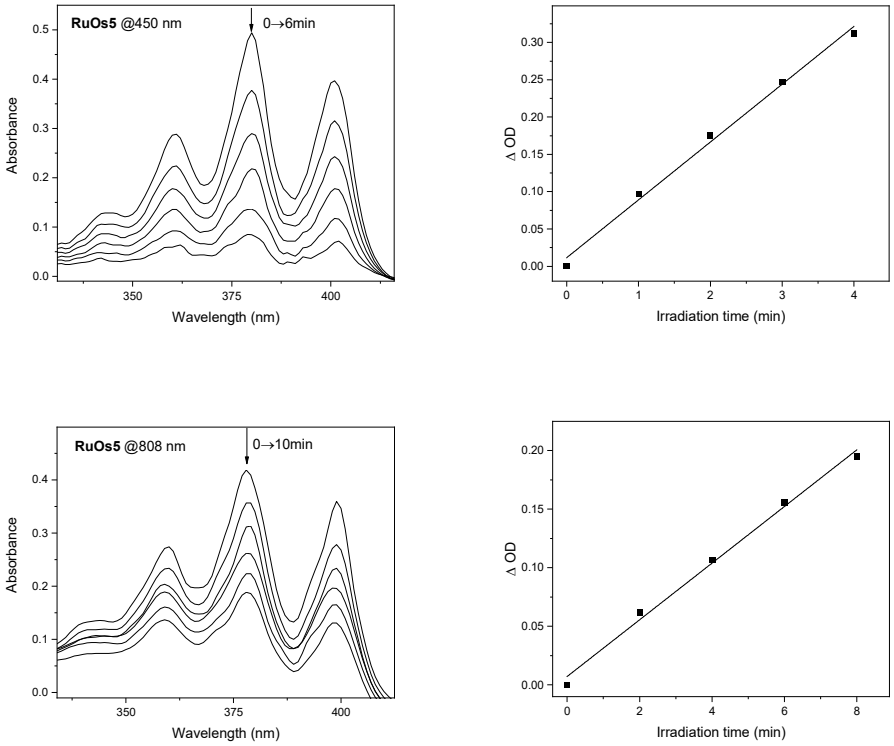


Figure S21. Absorption spectral changes of ABDA in aqueous solution upon irradiation of different light sources in the presence of **RuOs5**.

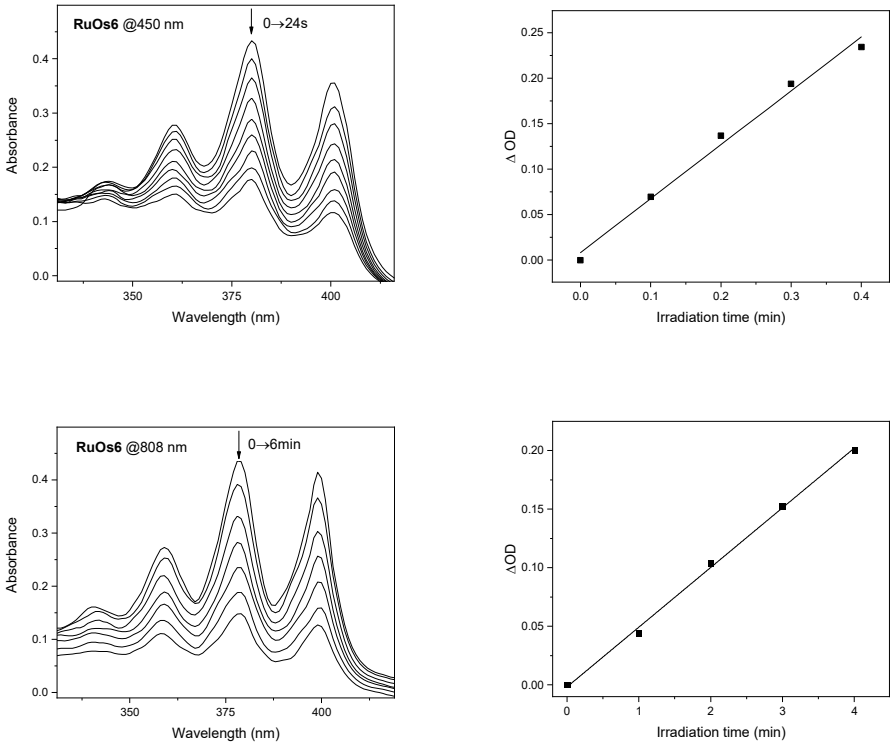


Figure S22. Absorption spectral changes of ABDA in aqueous solution upon irradiation of different light sources in the presence of **RuOs6**.

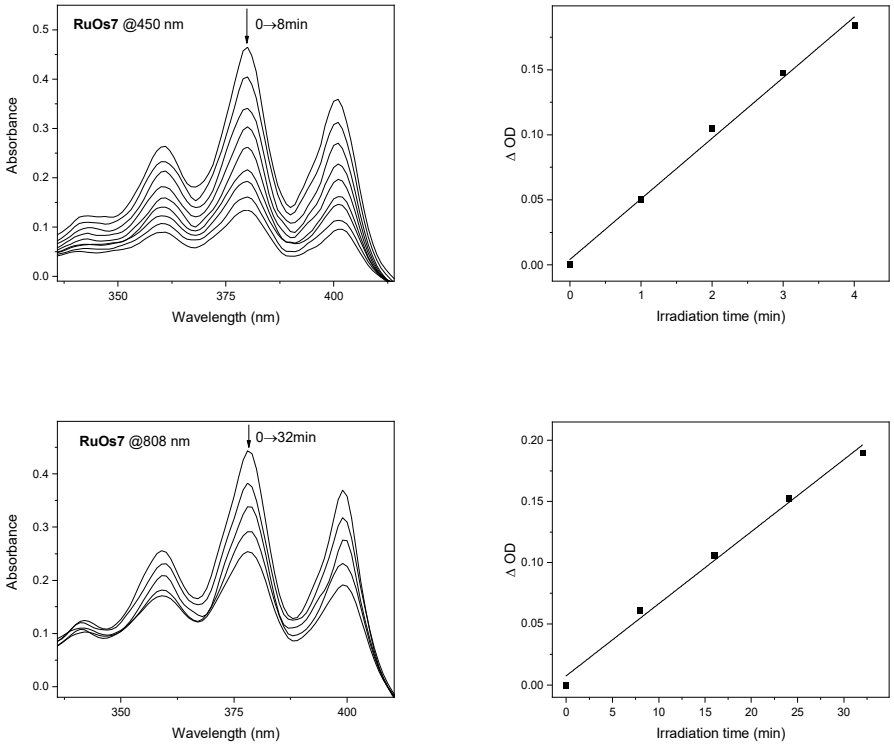


Figure S23. Absorption spectral changes of ABDA in aqueous solution upon irradiation of different light sources in the presence of **RuOs7**.

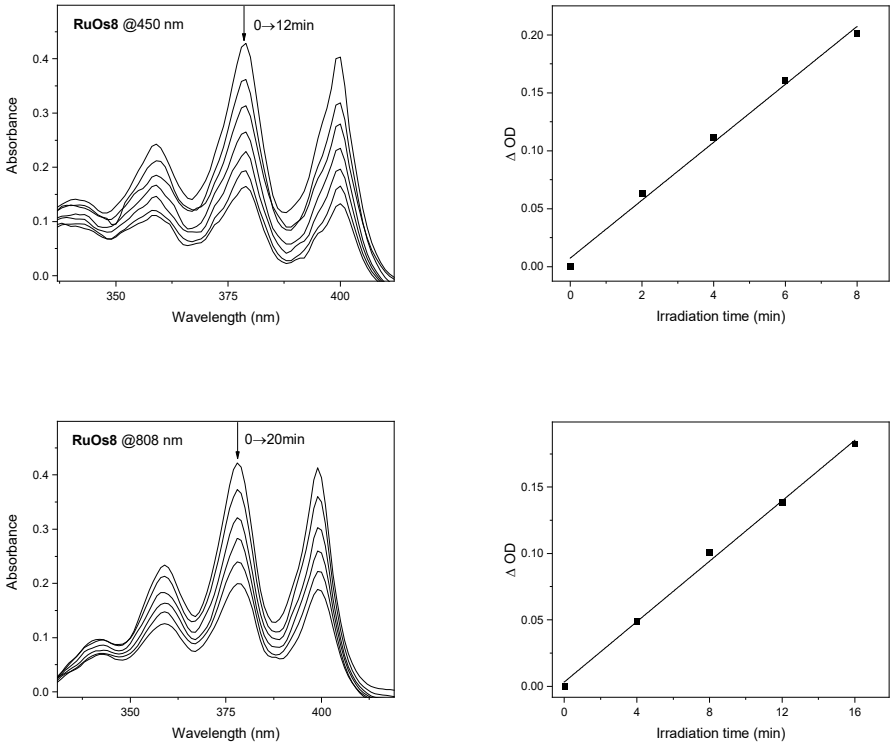


Figure S24. Absorption spectral changes of ABDA in aqueous solution upon irradiation of different light sources in the presence of **RuOs8**.

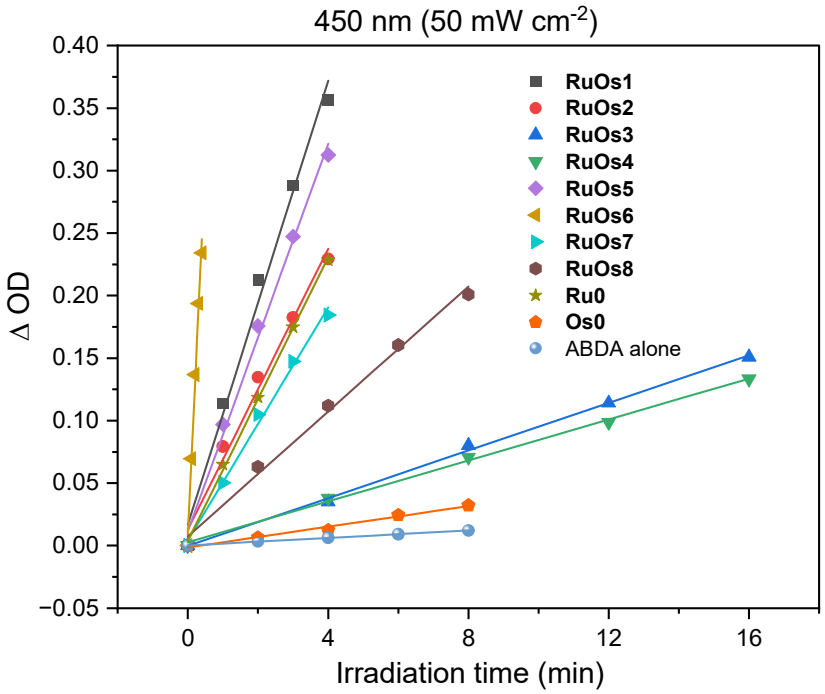


Figure S25. Linear fittings of ΔOD at 378 nm versus time (min) based on the time-dependent changes in absorption spectra of ABDA (100 μM) in the absence and presence of **RuOs1–8**, **Ru0** and **Os0** (10 μM) upon 450 nm LED (50 mW cm^{-2}) irradiation. Same volume of DMSO as complex solution was added for "ABDA alone".

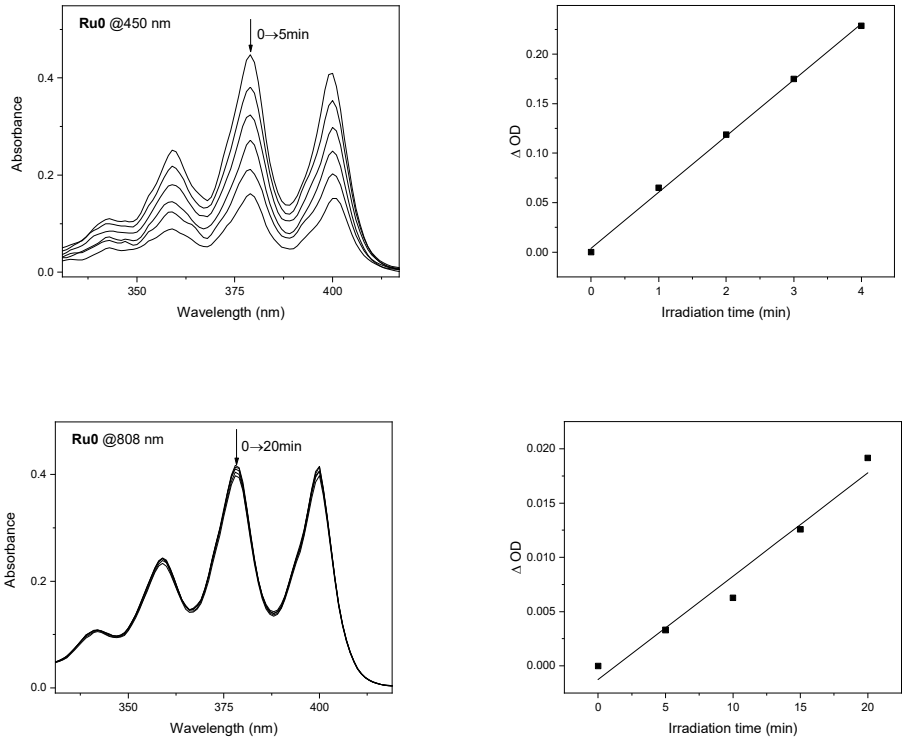


Figure S26. Absorption spectral changes of ABDA in aqueous solution upon irradiation of different light sources in the presence of $[Ru(bpy)_3]^{2+}$ (**Ru0**).

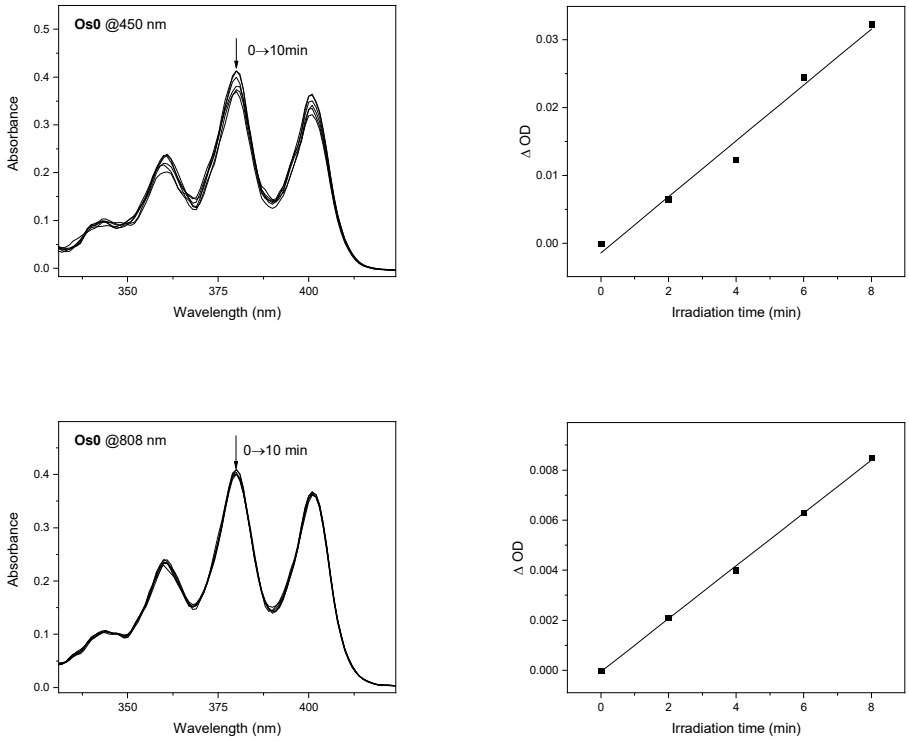


Figure S27. Absorption spectral changes of ABDA in aqueous solution upon irradiation of different light sources in the presence of $[Os(bpy)_3]^{2+}$ (**Os0**).

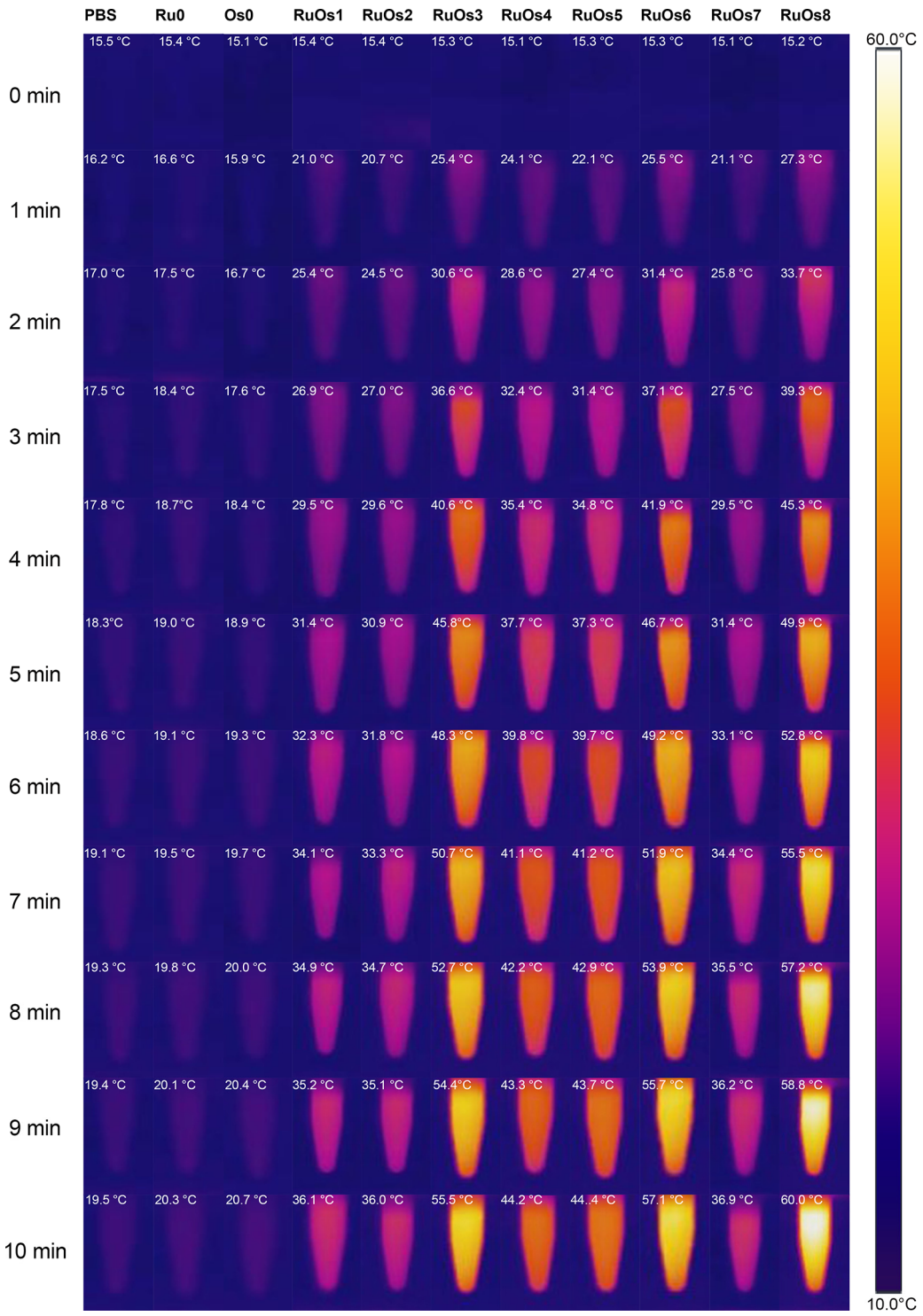


Figure S28. Thermal images of PBS, **RuOs1**−**8**, $[Ru(bpy)_3]^{2+}$ (**Ru0**) and $[Os(bpy)_3]^{2+}$ (**Os0**) in aqueous solution (100 μM) upon 808 nm LPL (100 mW cm^{-2}) irradiation for 10 min at 1-min intervals.

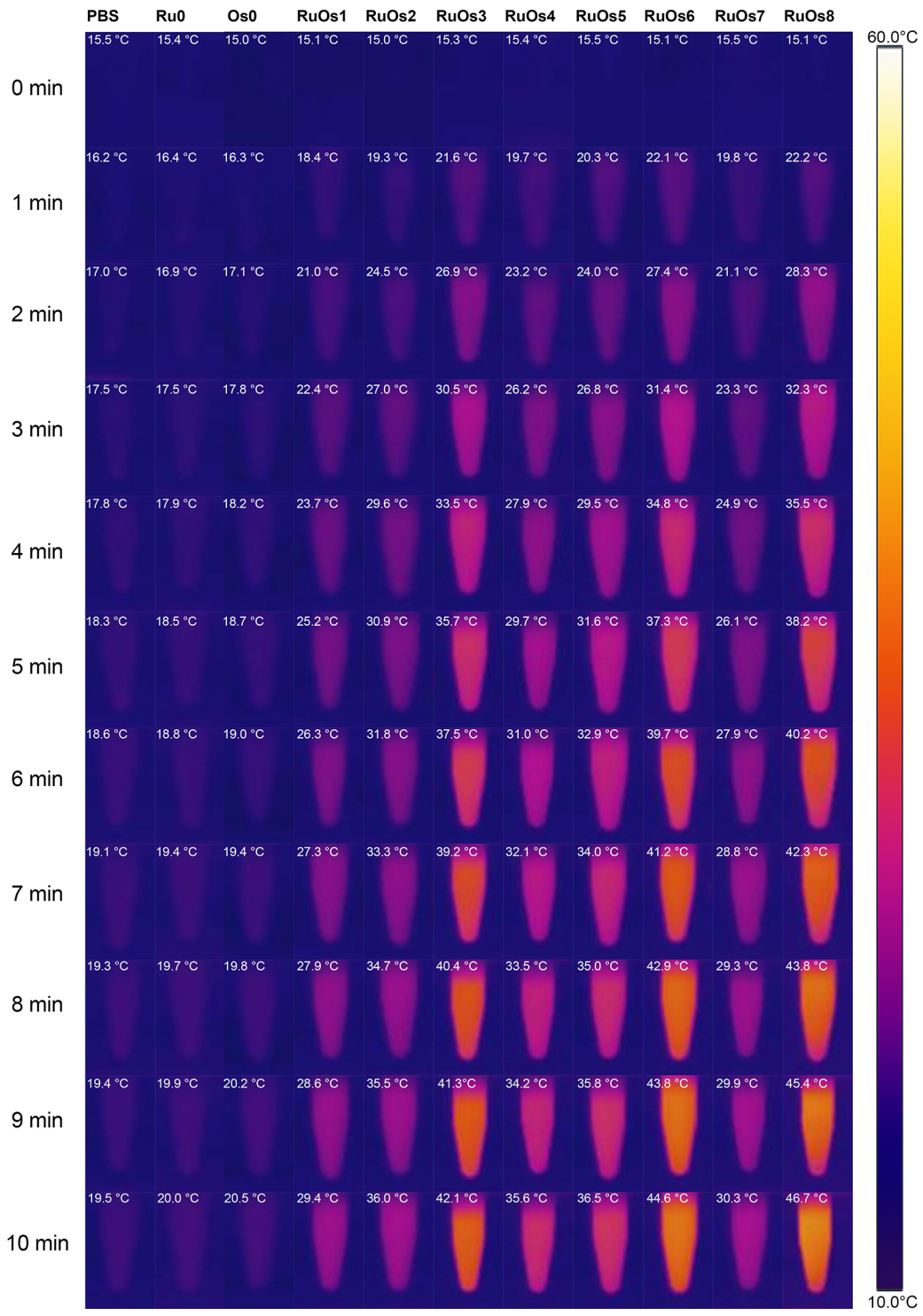


Figure S29. Thermal images of PBS, **RuOs1**−**8**, $[Ru(bpy)_3]^{2+}$ (**Ru0**) and $[Os(bpy)_3]^{2+}$ (**Os0**) in aqueous solution (50 μM) upon 808 nm LPL (100 mW cm^{-2}) irradiation for 10 min at 1-min intervals.

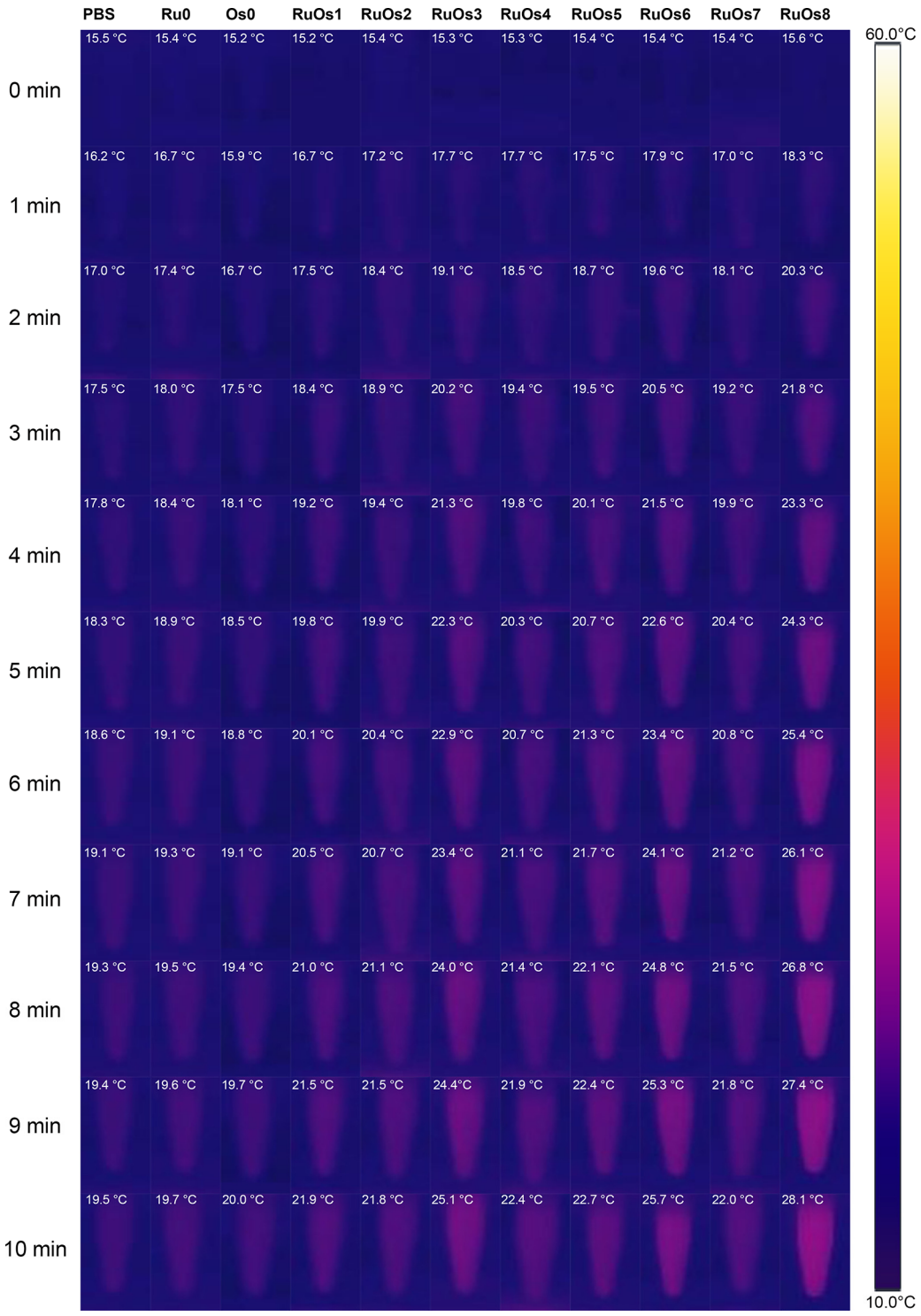


Figure S30. Thermal images of PBS, **RuOs1**−**8**, $[Ru(bpy)_3]^{2+}$ (**Ru0**) and $[Os(bpy)_3]^{2+}$ (**Os0**) in aqueous solution (10 μM) upon 808 nm LPL (100 mW cm^{-2}) irradiation for 10 min at 1-min intervals.

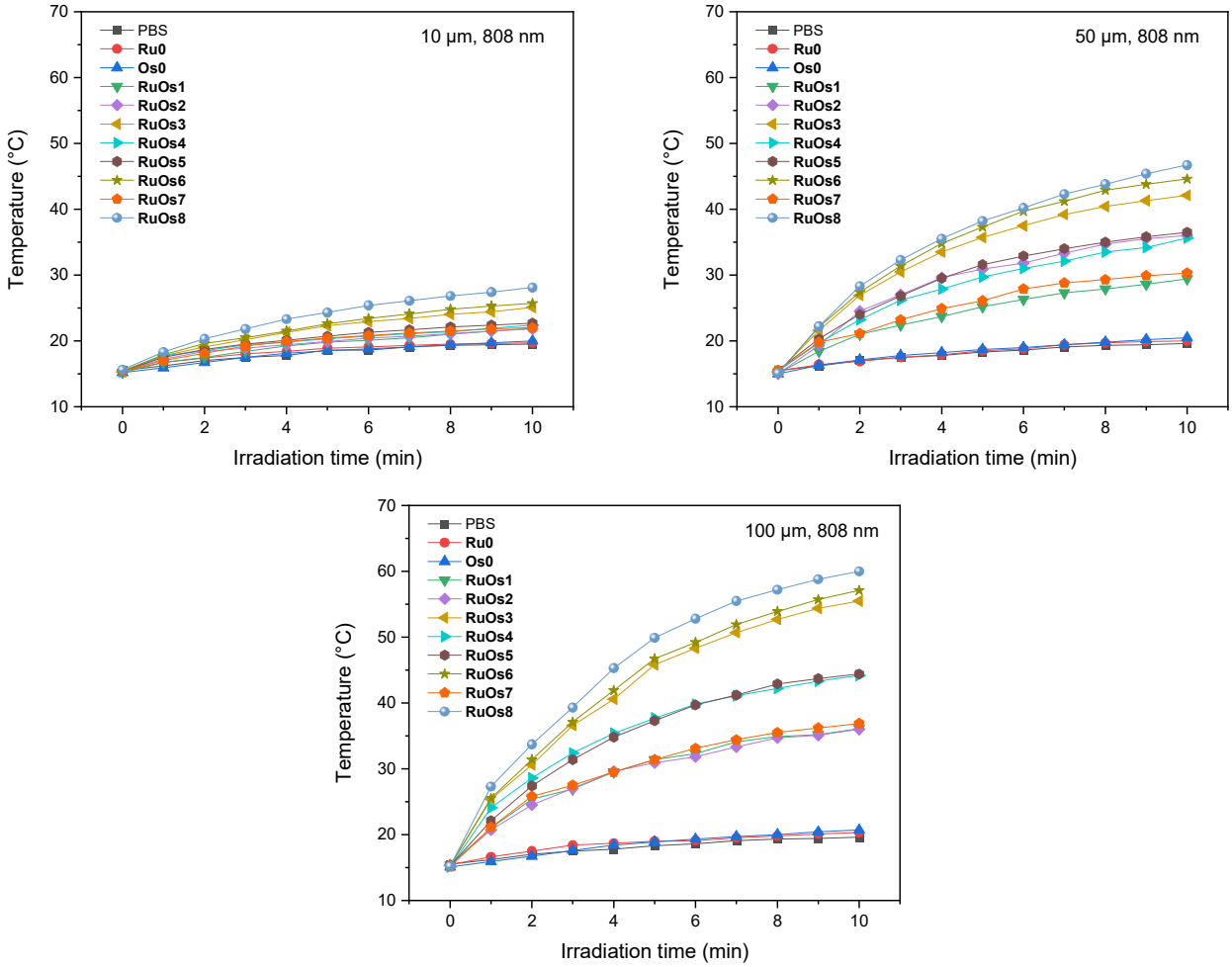


Fig S31. The temperature-rising curves of PBS, **RuOs1**−**8**, $[Ru(bpy)_3]^{2+}$ (**Ru0**) and $[Os(bpy)_3]^{2+}$ (**Os0**) in aqueous solution (10, 50, and 100 μM) upon irradiation of 808 nm LPL (100 mW cm^{-2}) for 10 min at 1-min intervals.

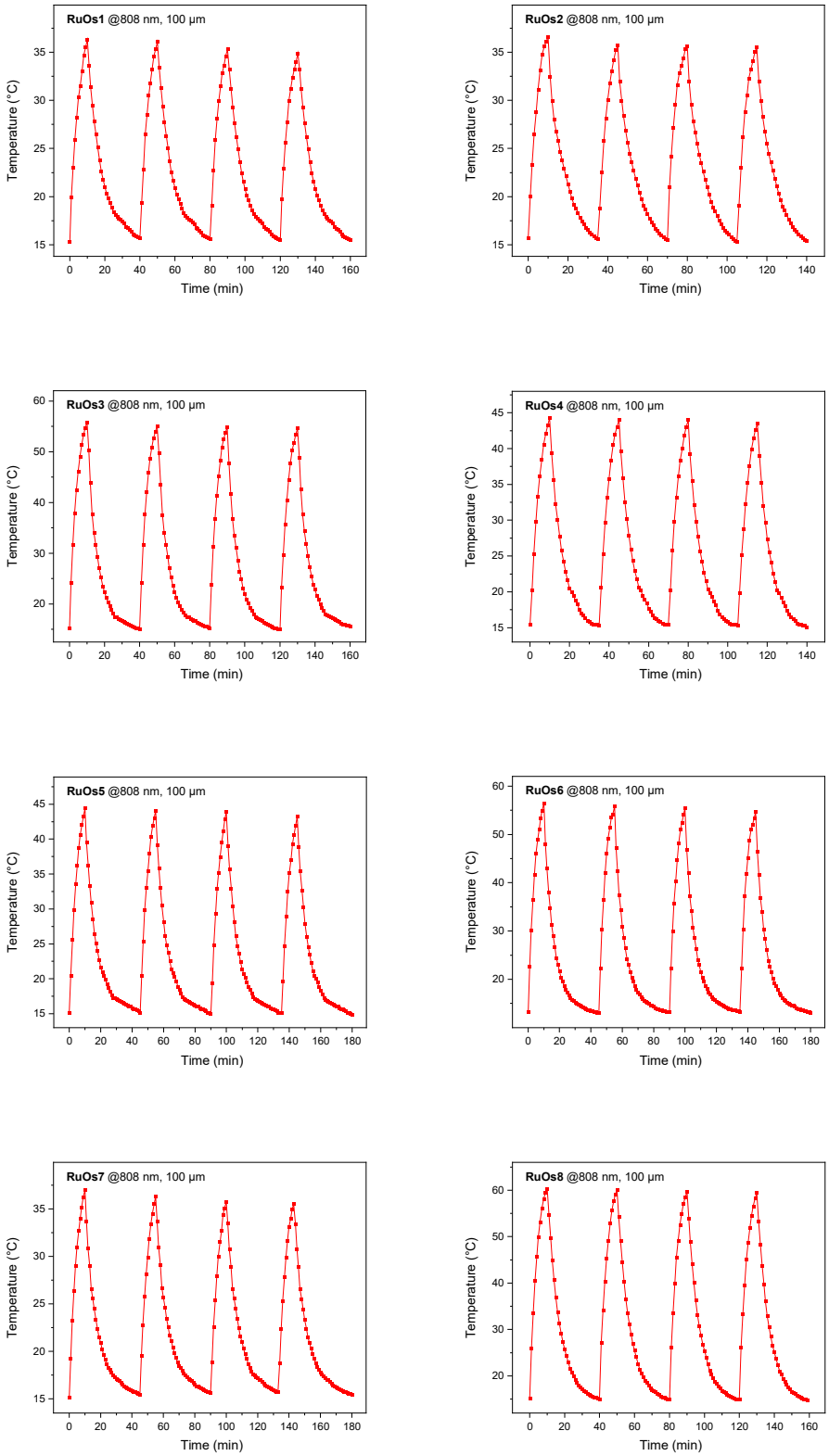


Fig S32. Temperature changes of the aqueous solution of **RuOs1**−**8** (100 μM) during four "irradiating/cooling" cycles by 808 nm LPL (100 mW cm^{-2}).

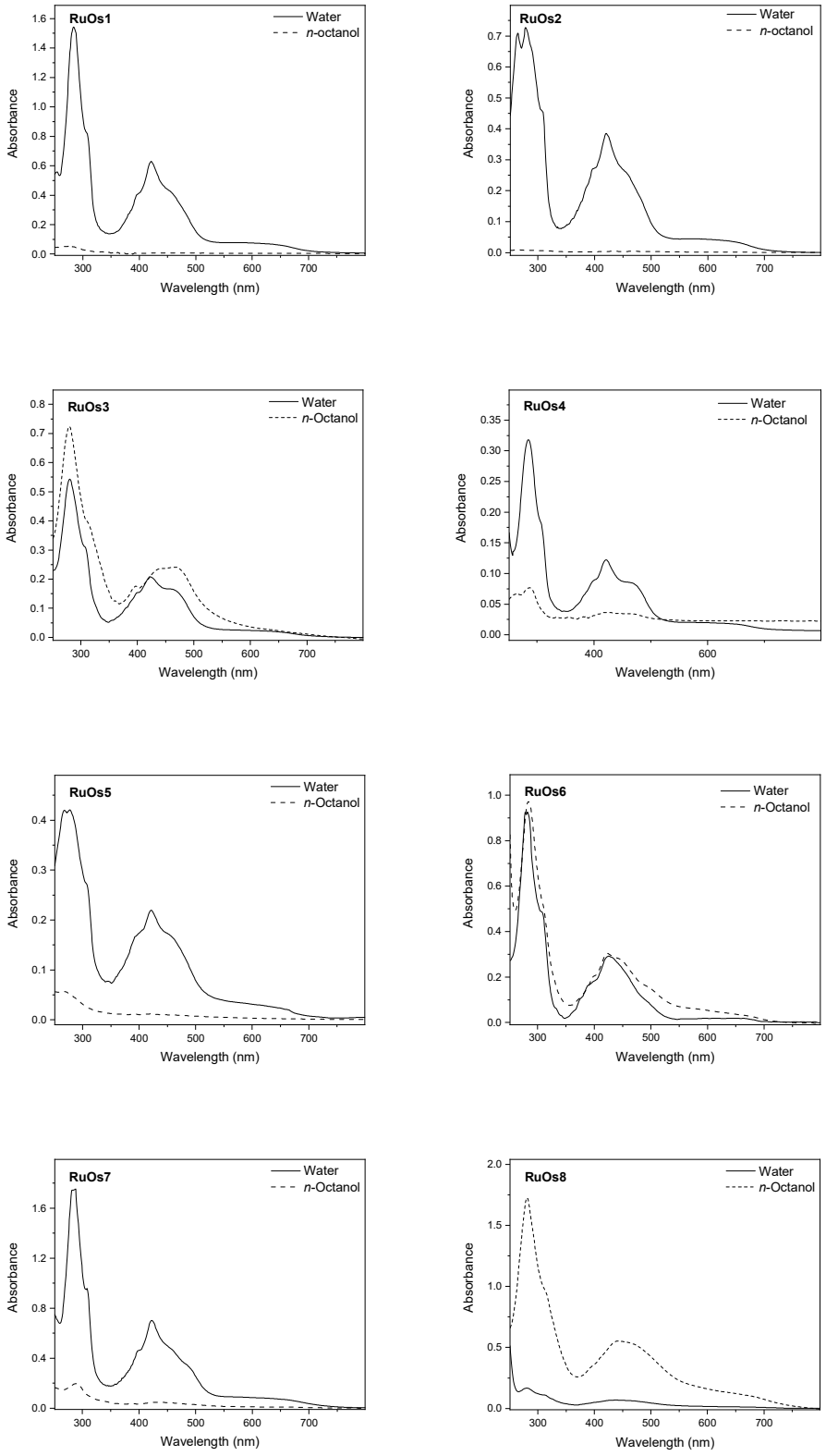


Figure S33. Absorption spectra of **RuOs1−8** in the *n*-octanol and water phase (10 μM in total), by which the partition coefficients (log $K_{O/W}$) were calculated.

Figure S34. Octanol/water partition of **RuOs1−8** (10 μM in total) at 25 ºC.

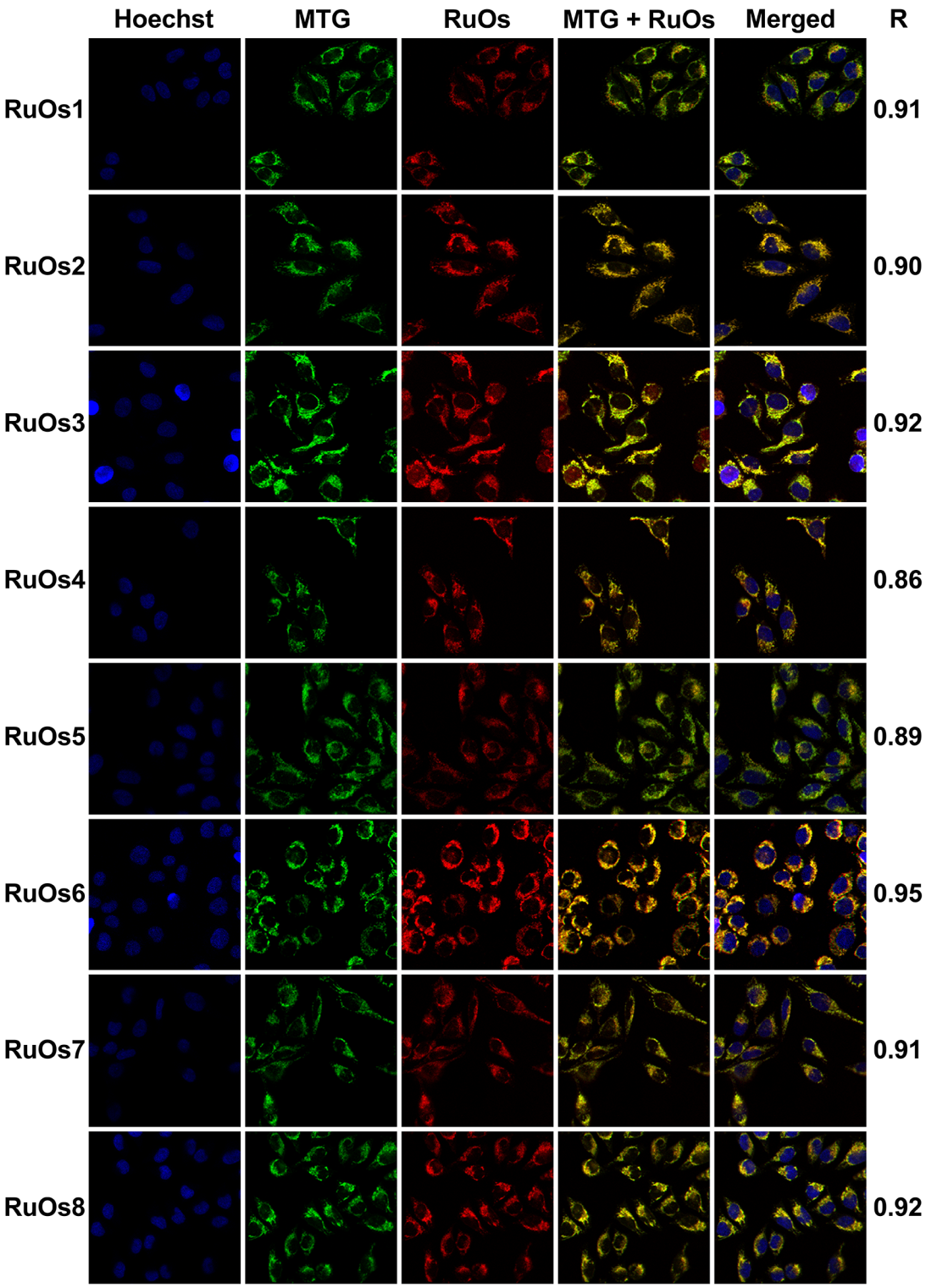


Figure S35. Cellular colocalization of **RuOs1-8** with Hoechst 33342 (Hoechst) and MitoTracker Green (MTG) in A375 cells by CLSM.

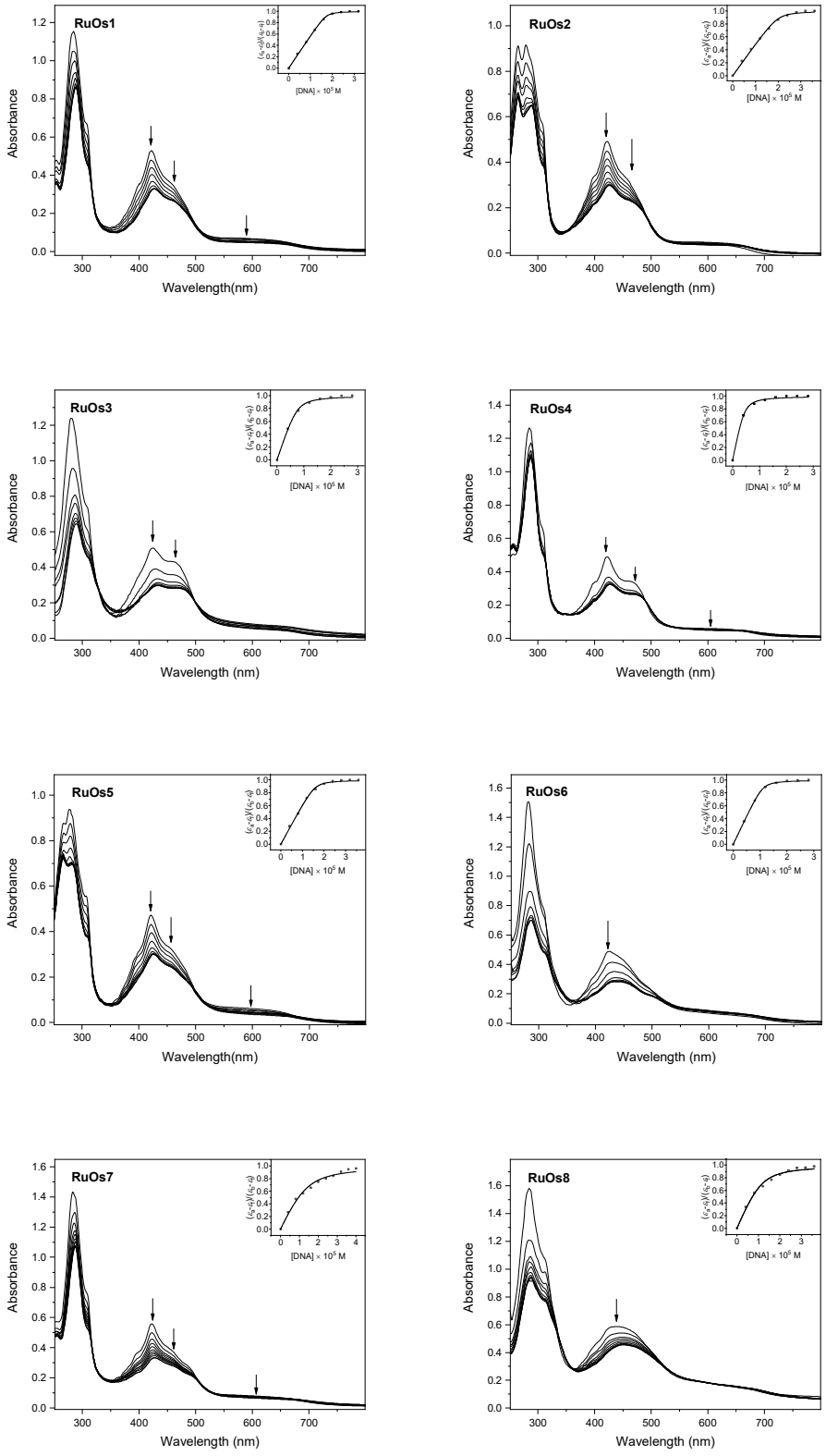


Figure S36. Absorption spectra of **RuOs1-8** in 5 mM Tris–HCl and 50 mM NaCl buffer (pH 7.0) in the presence of increasing amounts of CT-DNA. Insets show the nonlinear fitting by which the binding constants K_b were calculated.

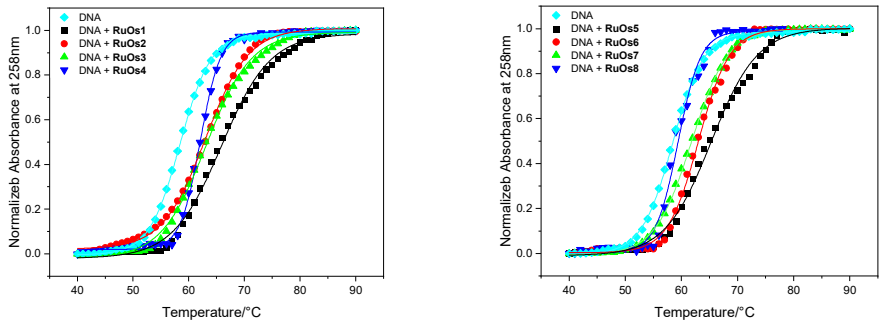


Figure S37. The melting curves of CT-DNA (100 μM) at 260 nm in the absence and the presence of **RuOs1**–**RuOs8** (10 μM) in PBS

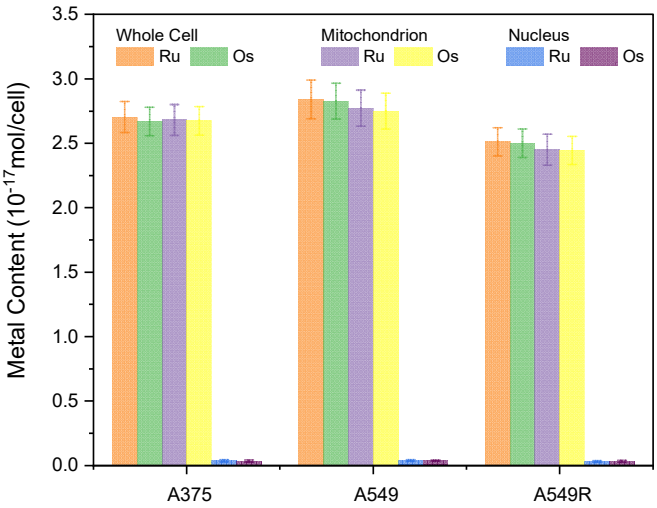


Figure S38. The distribution of ruthenium and osmium for **RuOs6** in various regions of A375, A549 and A549R cells as determined by inductively coupled plasma mass spectrometry (ICP-MS).

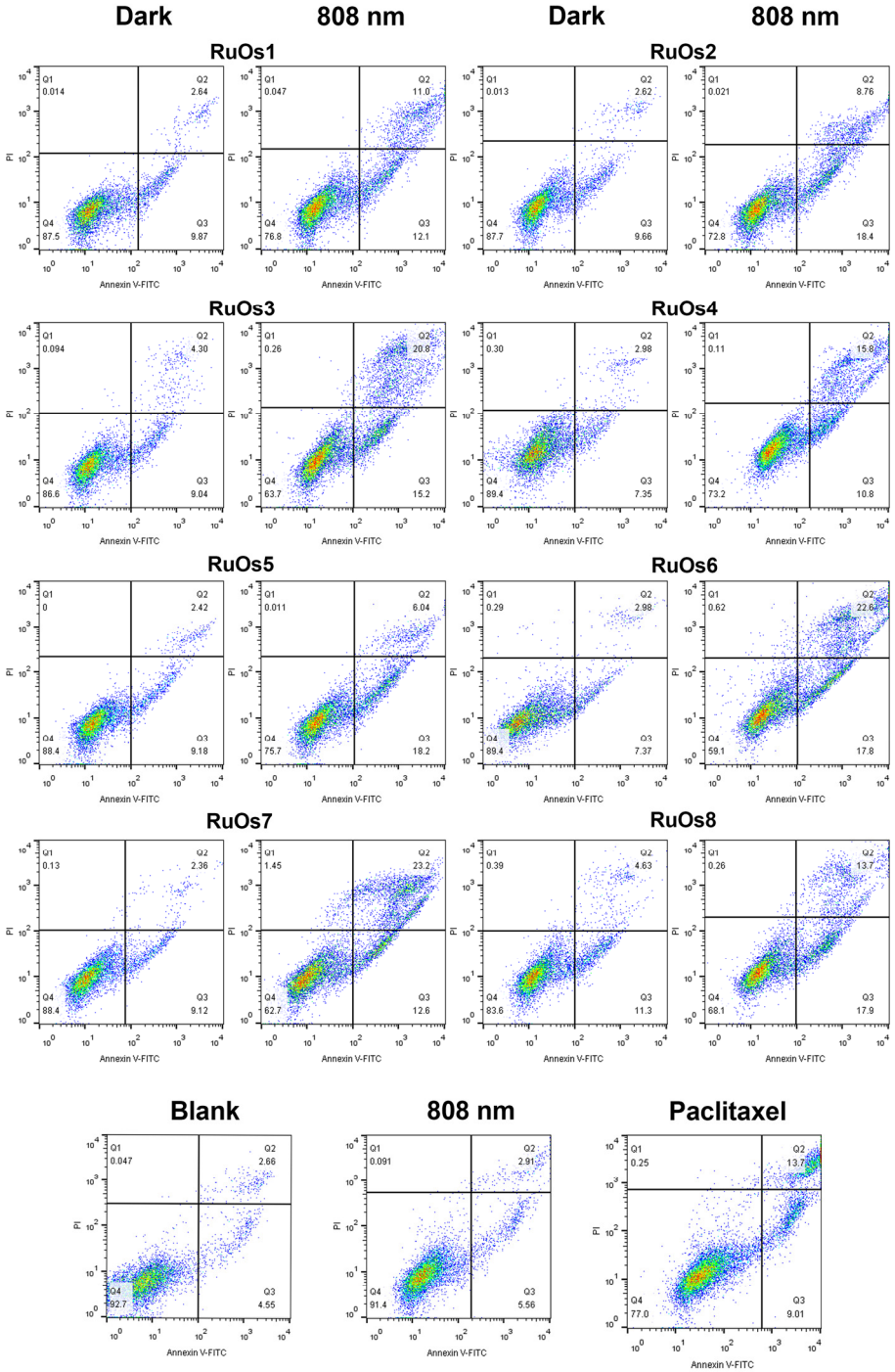


Figure S39. Detection of A375 cells apoptosis with Annexin V-FITC and PI by flow cytometry in the presence of **RuOs1**–**8** (5 μM) in the dark and under 808 nm LPL (100 mW cm^{-2}) irradiation. Paclitaxel was the positive control.

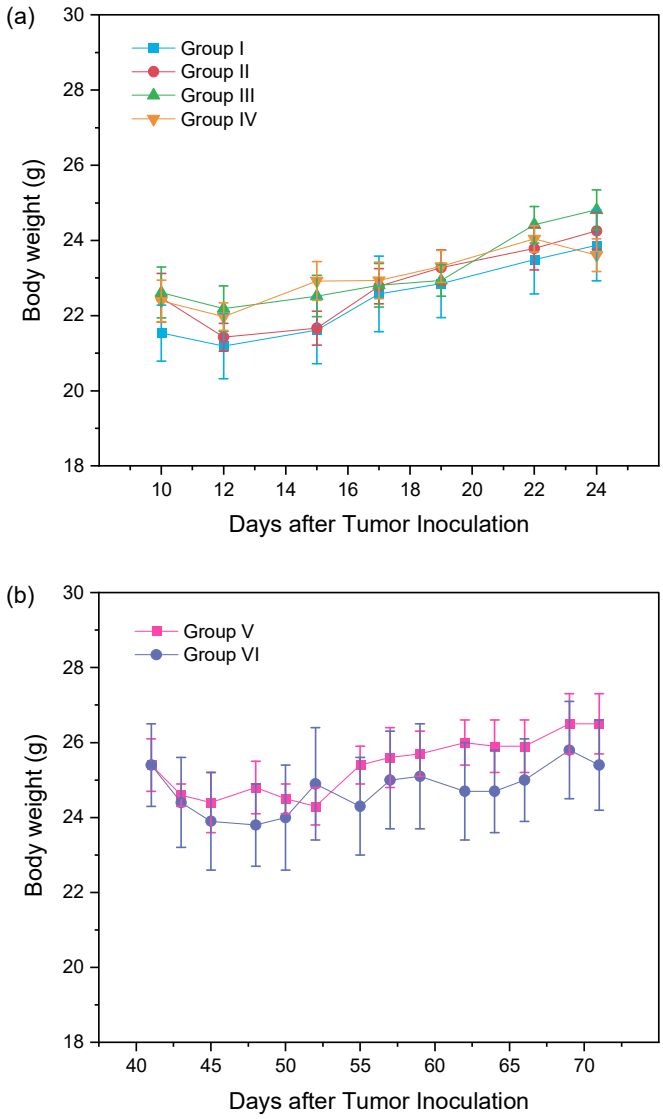


Figure S40. Body weight curves of mice in Group I–IV (a) and Group V–VI (b) after various treatments.

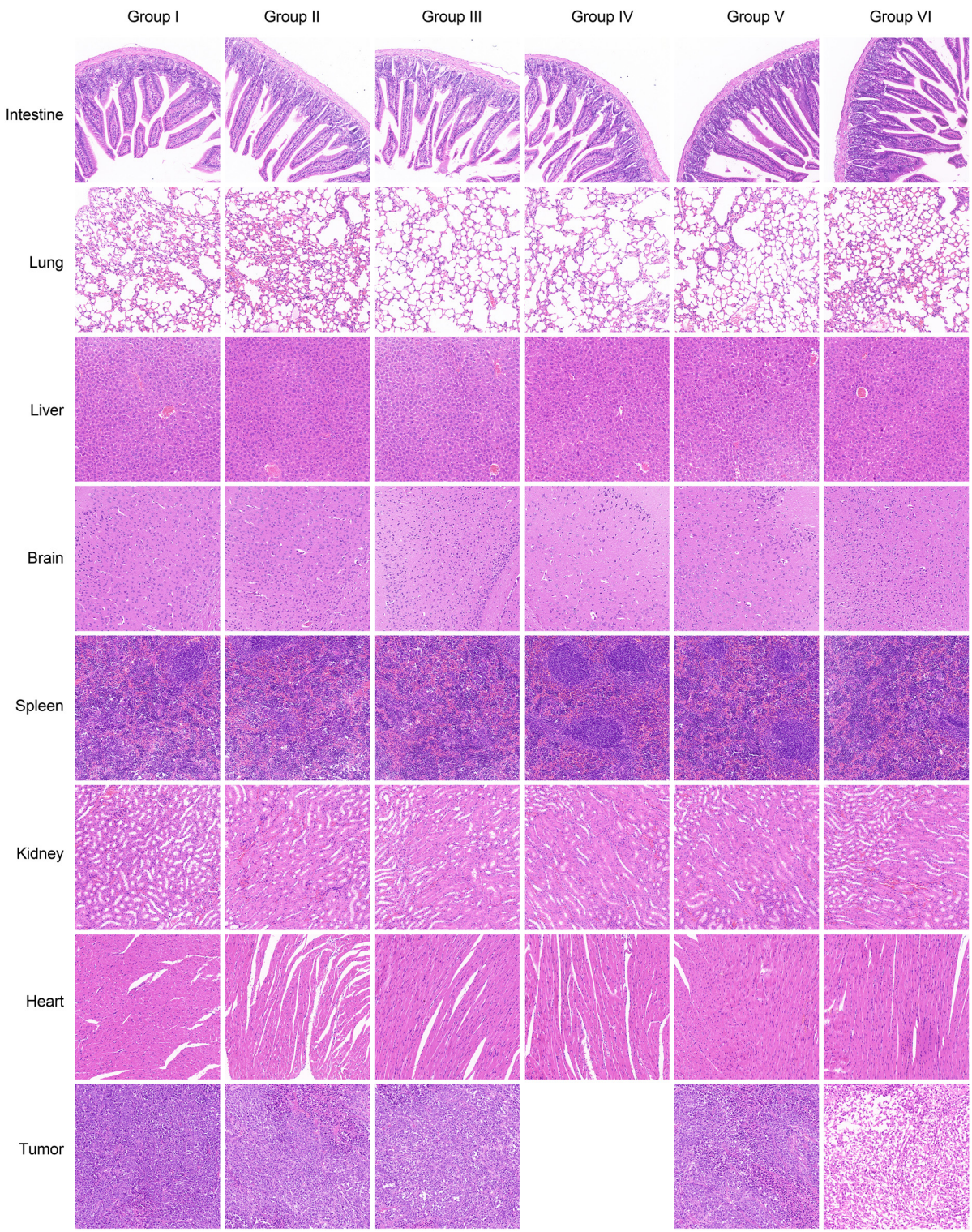


Figure S41. H&E staining of organ slices from different groups.

Table S1. Experimental and computational absorption spectral data of **RuOs1**−**8**, together with the calculated excitation energies (ΔE), oscillator strengths ($f > 0.01$), by TDDFT Method at MN15-D3(BJ)/Lanl2DZ level in aqueous solution (CPCM for water, Gaussian 16).

Compound	λ_{exp}/nm ($\varepsilon/\times10^4 M^{-1}$ cm^{-1})	λ_{cal}/nm	f	ΔE/eV	Excied State	Character
RuOs1	657(0.51)	561.19	0.1480	2.21	S5	MLCT / IL(pppp)
		478.05	0.1372	2.59	S22	MLCT / IL(pppp)
	466(4.36)	444.17	0.0223	2.79	S32	MLCT
		442.49	0.1037	2.80	S33	MLCT / IL(pppp)
	424(5.22)	417.40	0.2785	2.97	S42	MLCT / IL(bpy)
		415.83	0.1953	2.98	S43	MLCT
RuOs2	638(0.44)	560.19	0.1508	2.21	S5	MLCT / IL(pppp)
		478.48	0.1419	2.59	S22	MLCT / IL(pppp)
	458(3.36)	443.94	0.0223	2.79	S33	MLCT
		442.13	0.1025	2.80	S34	MLCT / IL(pppp)
	422(5.03)	417.27	0.2855	2.97	S41	MLCT / IL(bpy)
		415.82	0.1946	2.98	S42	MLCT
RuOs3	649(0.61)	561.21	0.1582	2.21	S5	MLCT / IL(pppp)
		488.57	0.1309	2.54	S23	MLCT / IL(pppp)
	458(3.60)	443.97	0.0215	2.79	S35	MLCT
		442.72	0.1102	2.80	S36	MLCT / IL(pppp)
	422(5.35)	417.52	0.3052	2.97	S42	MLCT
		415.85	0.1948	2.98	S44	MLCT
		403.40	0.0105	3.07	S49	MLCT
RuOs4	649(0.51)	559.53	0.1607	2.22	S5	MLCT / IL(pppp)
		501.85	0.1009	2.47	S17	MLCT / IL(pppp)
	467(3.38)	444.30	0.0224	2.79	S31	MLCT
		442.57	0.1108	2.80	S32	MLCT/ IL(pppp)
	421(4.88)	417.28	0.2959	2.97	S40	MLCT/ IL(pppp)
		415.87	0.1851	2.98	S41	MLCT
RuOs5	643(0.62)	563.94	0.1509	2.20	S4	MLCT / IL(pppp)
		477.33	0.1411	2.60	S23	MLCT / IL(pppp)
	456(3.41)	439.23	0.1373	2.82	S33	MLCT
		439.15	0.0350	2.82	S44	MLCT /IL(bpy)
	422(4.95)	416.28	0.1990	2.98	S45	MLCT
		413.44	0.1498	3.00	S51	MLCT
RuOs6	655(0.41)	575.81	0.1529	2.15	S6	MLCT / IL(pppp)
		489.62	0.0131	2.53	S20	MLCT
		477.76	0.1652	2.60	S23	MLCT / IL(pppp)
		476.06	0.0180	2.60	S25	MLCT / LLCT
	456(4.03)	455.59	0.1234	2.72	S29	MLCT

		448.82	0.1398	2.76	S33	MLCT / IL(pppp)
		428.84	0.2202	2.89	S41	MLCT
		428.35	0.2645	2.89	S42	MLCT
	423(4.88)	414.10	0.1282	2.99	S48	MLCT
		407.44	0.2262	3.04	S51	MLCT / LLCT
		407.11	0.1514	3.05	S52	MLCT
		400.67	0.1061	3.09	S56	MLCT
RuOs7	666(0.62)	593.66	0.1281	2.09	S4	MLCT / IL(pppp)
		476.60	0.1592	2.60	S23	MLCT
	458(3.32)	445.82	0.0773	2.78	S31	MLCT
		433.11	0.0407	2.86	S35	MLCT
		432.04	0.2339	2.87	S37	MLCT
	423(4.87)	417.86	0.0543	2.97	S42	MLCT
		411.07	0.2410	3.02	S45	MLCT / IL(pppp)
		405.65	0.1418	3.06	S47	MLCT/LLCT
		403.71	0.0144	3.07	S48	MLCT
RuOs8	667(1.40)	623.47	0.1036	1.99	S4	MLCT / IL(pppp)
		509.09	0.1264	2.44	S18	MLCT / IL(pppp)
		477.75	0.0106	2.60	S25	MLCT / IL(pppp)
	462(3.92)	445.22	0.0727	2.78	S33	MLCT
		440.78	0.2193	2.81	S35	MLCT
		427.22	0.1060	2.90	S43	MLCT
	420(4.85)	425.35	0.1241	2.91	S44	MLCT
		424.71	0.3097	2.92	S45	MLCT
		411.33	0.1027	3.01	S52	MLCT
		404.43	0.1336	3.07	S56	MLCT
		401.26	0.1706	3.09	S58	MLCT/LLCT

Table S2. Cartesian coordinates of optimized **RuOs1**–**8** for the ground state (S0), first excited singlet state (F1) and first excited triplet state (T1), by MN15-D3(BJ)/Lanl2DZ (CPCM for water, Gaussian 16).

RuOs1		S0			S1			T1	
Atom	X	Y	Z	X	Y	Z	X	Y	Z
Os	0	0	7.24517	0	0	7.251018	0	0	7.259506
Ru	0	0	-7.973187	0	0	-7.983622	0	0	-7.989991
N	0.005017	1.417183	0.808594	0.004635	1.426203	0.812102	-0.025027	1.427439	0.806386
N	-0.005017	-1.417183	0.808594	-0.004635	-1.426203	0.812102	0.025027	-1.427439	0.806386
N	-0.007003	1.314452	5.654475	-0.011433	1.335139	5.678042	-0.093564	1.325899	5.66638
N	0.007003	-1.314452	5.654475	0.011433	-1.335139	5.678042	0.093564	-1.325899	5.66638
N	2.035542	0.30988	7.350062	2.02376	0.394201	7.304424	1.988773	0.560227	7.31544
N	0.126574	1.416397	8.734199	0.105136	1.383463	8.78295	-0.00109	1.385094	8.792875
N	-2.035542	-0.30988	7.350062	-2.02376	-0.394201	7.304424	-1.988773	-0.560227	7.31544
N	-0.126574	-1.416397	8.734199	-0.105136	-1.383463	8.78295	0.00109	-1.385094	8.792875
N	-2.049976	0.286571	-8.073522	-2.049215	0.284651	-8.077861	-2.020311	0.444981	-8.081078
N	-0.127871	1.42796	-9.463393	-0.133437	1.430077	-9.47121	-0.023966	1.433042	-9.48069
N	2.049976	-0.286571	-8.073522	2.049215	-0.284651	-8.077861	2.020311	-0.444981	-8.081078
N	0.127871	-1.42796	-9.463393	0.133437	-1.430077	-9.47121	0.023966	-1.433042	-9.48069
N	-0.005033	1.417199	-1.537056	-0.004688	1.417394	-1.530709	0.024369	1.423124	-1.534146
N	0.005033	-1.417199	-1.537056	0.004688	-1.417394	-1.530709	-0.024369	-1.423124	-1.534146
N	-0.004206	-1.331167	-6.376902	-0.003708	-1.335301	-6.389815	-0.092759	-1.3332	-6.396058
N	0.004206	1.331167	-6.376902	0.003708	1.335301	-6.389815	0.092759	1.3332	-6.396058
C	-0.004936	-0.728203	1.951738	-0.004352	-0.725028	1.964333	0.021812	-0.713692	1.965791
C	0.004936	0.728203	1.951738	0.004352	0.725028	1.964333	-0.021812	0.713692	1.965791
C	0.010715	1.457284	3.222236	0.008236	1.439265	3.229444	-0.064948	1.435359	3.227042
C	0.00252	0.722477	4.41714	-0.004305	0.708284	4.443623	-0.043815	0.714441	4.43498
C	-0.00252	-0.722477	4.41714	0.004305	-0.708284	4.443623	0.043815	-0.714441	4.43498
C	-0.010715	-1.457284	3.222236	-0.008236	-1.439265	3.229444	0.064948	-1.435359	3.227042
C	0.020298	2.864395	3.299205	0.024551	2.847504	3.315839	-0.133532	2.848077	3.312408
C	0.021255	3.466454	4.56276	0.035039	3.469048	4.57016	-0.173621	3.459881	4.565811
C	0.007068	2.669274	5.72058	0.021962	2.680417	5.738355	-0.14746	2.672076	5.735929
C	-0.007068	-2.669274	5.72058	-0.021962	-2.680417	5.738355	0.14746	-2.672076	5.735929
C	-0.021255	-3.466454	4.56276	-0.035039	-3.469048	4.57016	0.173621	-3.459881	4.565811
C	-0.020298	-2.864395	3.299205	-0.024551	-2.847504	3.315839	0.133532	-2.848077	3.312408
C	4.764083	0.901396	7.587615	4.718962	1.086031	7.479499	4.617739	1.470626	7.482452
C	4.31472	-0.042446	6.646303	4.27995	0.174625	6.504496	4.25408	0.519203	6.514114
C	2.946978	-0.312181	6.553538	2.920992	-0.144558	6.438319	2.926521	0.088552	6.452533
C	2.465306	1.233509	8.270649	2.438794	1.295584	8.253281	2.329228	1.496116	8.259817
C	3.825757	1.54406	8.406027	3.785989	1.656701	8.358541	3.64274	1.966843	8.360681
C	1.388779	1.84144	9.068681	1.35969	1.84209	9.094234	1.211248	1.947568	9.103943
C	-0.945205	1.909365	9.412556	-0.969474	1.796647	9.502482	-1.108277	1.70499	9.513033
C	-0.801467	2.845643	10.43966	-0.835879	2.707517	10.554298	-1.050596	2.619602	10.567419
C	1.59159	2.778163	10.091918	1.552471	2.74888	10.14258	1.326748	2.863435	10.155386
C	0.487439	3.289334	10.786816	0.443046	3.190519	10.878509	0.184178	3.206817	10.89323
C	-4.764083	-0.901396	7.587615	-4.718962	-1.086031	7.479499	-4.617739	-1.470626	7.482452
C	-4.31472	0.042446	6.646303	-4.27995	-0.174625	6.504496	-4.25408	-0.519203	6.514114
C	-2.946978	0.312181	6.553538	-2.920992	0.144558	6.438319	-2.926521	-0.088552	6.452533

C	-2.465306	-1.233509	8.270649	-2.438794	-1.295584	8.253281	-2.329228	-1.496116	8.259817
C	-3.825757	-1.54406	8.406027	-3.785989	-1.656701	8.358541	-3.64274	-1.966843	8.360681
C	-1.388779	-1.84144	9.068681	-1.35969	-1.84209	9.094234	-1.211248	-1.947568	9.103943
C	0.945205	-1.909365	9.412556	0.969474	-1.796647	9.502482	1.108277	-1.70499	9.513033
C	0.801467	-2.845643	10.43966	0.835879	-2.707517	10.554298	1.050596	-2.619602	10.567419
C	-1.59159	-2.778163	10.091918	-1.552471	-2.74888	10.14258	-1.326748	-2.863435	10.155386
C	-0.487439	-3.289334	10.786816	-0.443046	-3.190519	10.878509	-0.184178	-3.206817	10.89323
C	-4.772764	0.861847	-8.325844	-4.772863	0.863778	-8.313233	-4.687838	1.248358	-8.299559
C	-4.328095	-0.086067	-7.388124	-4.323795	-0.087084	-7.380439	-4.312721	0.266016	-7.366661
C	-2.95679	-0.347014	-7.2892	-2.95221	-0.349762	-7.289693	-2.967015	-0.109384	-7.2841
C	-2.471189	1.212059	-8.990189	-2.47453	1.213701	-8.988998	-2.373444	1.403489	-8.992696
C	-3.83248	1.51697	-9.134114	-3.836398	1.520463	-9.12462	-3.705893	1.822795	-9.119579
C	-1.394527	1.837518	-9.783883	-1.401126	1.841173	-9.78547	-1.256733	1.937483	-9.797813
C	0.935343	1.93498	-10.135206	0.927242	1.938869	-10.145754	1.07201	1.854086	-10.159438
C	0.780399	2.880736	-11.154991	0.76874	2.887692	-11.162129	0.98542	2.803216	-11.184196
C	-1.612464	2.781723	-10.797631	-1.622804	2.78844	-10.795782	-1.406649	2.88838	-10.817851
C	-0.514624	3.311217	-11.491208	-0.527569	3.319654	-11.492069	-0.274738	3.328146	-11.519204
C	4.772764	-0.861847	-8.325844	4.772863	-0.863778	-8.313233	4.687838	-1.248358	-8.299559
C	4.328095	0.086067	-7.388124	4.323795	0.087084	-7.380439	4.312721	-0.266016	-7.366661
C	2.95679	0.347014	-7.2892	2.95221	0.349762	-7.289693	2.967015	0.109384	-7.2841
C	2.471189	-1.212059	-8.990189	2.47453	-1.213701	-8.988998	2.373444	-1.403489	-8.992696
C	3.83248	-1.51697	-9.134114	3.836398	-1.520463	-9.12462	3.705893	-1.822795	-9.119579
C	1.394527	-1.837518	-9.783883	1.401126	-1.841173	-9.78547	1.256733	-1.937483	-9.797813
C	-0.935343	-1.93498	-10.135206	-0.927242	-1.938869	-10.145754	-1.07201	-1.854086	-10.159438
C	-0.780399	-2.880736	-11.154991	-0.76874	-2.887692	-11.162129	-0.98542	-2.803216	-11.184196
C	1.612464	-2.781723	-10.797631	1.622804	-2.78844	-10.795782	1.406649	-2.88838	-10.817851
C	0.514624	-3.311217	-11.491208	0.527569	-3.319654	-11.492069	0.274738	-3.328146	-11.519204
C	0	0.719682	-0.364304	0	0.728847	-0.366314	0	0.733426	-0.36544
C	0	-0.719682	-0.364304	0	-0.728847	-0.366314	0	-0.733426	-0.36544
C	0.004937	-0.727645	-2.680016	0.004347	-0.713817	-2.692768	-0.021492	-0.712346	-2.697338
C	-0.004937	0.727645	-2.680016	-0.004347	0.713817	-2.692768	0.021492	0.712346	-2.697338
C	0.011159	-1.454635	-3.951147	0.009772	-1.442687	-3.955393	-0.063767	-1.437851	-3.959059
C	0.002919	-0.725618	-5.1506	0.002743	-0.721717	-5.163516	-0.040162	-0.719397	-5.170087
C	-0.002919	0.725618	-5.1506	-0.002743	0.721717	-5.163516	0.040162	0.719397	-5.170087
C	-0.011159	1.454635	-3.951147	-0.009772	1.442687	-3.955393	0.063767	1.437851	-3.959059
C	0.020724	-2.863638	-4.021792	0.018019	-2.8557	-4.02738	-0.136096	-2.850302	-4.031714
C	0.021648	-3.476066	-5.278281	0.018939	-3.472046	-5.279307	-0.183055	-3.466181	-5.282421
C	0.008506	-2.680761	-6.440312	0.007638	-2.681509	-6.4488	-0.159832	-2.677197	-6.453796
C	-0.020724	2.863638	-4.021792	-0.018019	2.8557	-4.02738	0.136096	2.850302	-4.031714
C	-0.021648	3.476066	-5.278281	-0.018939	3.472046	-5.279307	0.183055	3.466181	-5.282421
C	-0.008506	2.680761	-6.440312	-0.007638	2.681509	-6.4488	0.159832	2.677197	-6.453796
H	0.026235	3.451466	2.387485	0.032522	3.42837	2.399193	-0.152712	3.427735	2.395774
H	0.029672	4.544713	4.667647	0.051105	4.547809	4.662608	-0.224995	4.537509	4.661897
H	-0.004233	3.111385	6.710403	0.022307	3.134807	6.723436	-0.182795	3.123426	6.721174
H	0.004233	-3.111385	6.710403	-0.022307	-3.134807	6.723436	0.182795	-3.123426	6.721174
H	-0.029672	-4.544713	4.667647	-0.051105	-4.547809	4.662608	0.224995	-4.537509	4.661897
H	-0.026235	-3.451466	2.387485	-0.032522	-3.42837	2.399193	0.152712	-3.427735	2.395774
H	5.00673	-0.562724	5.994422	4.970291	-0.280674	5.805056	4.97858	0.117213	5.816549
H	2.56156	-1.038553	5.847435	2.539449	-0.843342	5.703545	2.603982	-0.645862	5.724125

H	4.149772	2.277006	9.135803	4.107765	2.372402	9.105302	3.906032	2.708564	9.104975
H	-1.920822	1.545322	9.1119	-1.936894	1.399343	9.217976	-2.03936	1.229785	9.22628
H	-1.682257	3.214176	10.952441	-1.714991	3.023305	11.102581	-1.952751	2.858781	11.117038
H	2.594154	3.102827	10.345689	2.545949	3.104918	10.387147	2.286467	3.302283	10.40025
H	-5.00673	0.562724	5.994422	-4.970291	0.280674	5.805056	-4.97858	-0.117213	5.816549
H	-2.56156	1.038553	5.847435	-2.539449	0.843342	5.703545	-2.603982	0.645862	5.724125
H	-4.149772	-2.277006	9.135803	-4.107765	-2.372402	9.105302	-3.906032	-2.708564	9.104975
H	1.920822	-1.545322	9.1119	1.936894	-1.399343	9.217976	2.03936	-1.229785	9.22628
H	1.682257	-3.214176	10.952441	1.714991	-3.023305	11.102581	1.952751	-2.858781	11.117038
H	-2.594154	-3.102827	10.345689	-2.545949	-3.104918	10.387147	-2.286467	-3.302283	10.40025
H	-5.022705	-0.614485	-6.745661	-5.015465	-0.616139	-6.735254	-5.041229	-0.201537	-6.714531
H	-2.570482	-1.074736	-6.584645	-2.561459	-1.078684	-6.588729	-2.632279	-0.865363	-6.582827
H	-4.158484	2.251935	-9.860838	-4.165503	2.258359	-9.847019	-3.977736	2.585132	-9.840472
H	1.915312	1.57685	-9.840885	1.90803	1.579	-9.855907	2.022898	1.423468	-9.866294
H	1.654625	3.264486	-11.667798	1.641029	3.272782	-11.677317	1.884126	3.116789	-11.702493
H	-2.618104	3.100323	-11.046469	-2.629383	3.107963	-11.039815	-2.386261	3.27999	-11.066265
H	5.022705	0.614485	-6.745661	5.015465	0.616139	-6.735254	5.041229	0.201537	-6.714531
H	2.570482	1.074736	-6.584645	2.561459	1.078684	-6.588729	2.632279	0.865363	-6.582827
H	4.158484	-2.251935	-9.860838	4.165503	-2.258359	-9.847019	3.977736	-2.585132	-9.840472
H	-1.915312	-1.57685	-9.840885	-1.90803	-1.579	-9.855907	-2.022898	-1.423468	-9.866294
H	-1.654625	-3.264486	-11.667798	-1.641029	-3.272782	-11.677317	-1.884126	-3.116789	-11.702493
H	2.618104	-3.100323	-11.046469	2.629383	-3.107963	-11.039815	2.386261	-3.27999	-11.066265
H	0.026543	-3.44341	-3.105215	0.022923	-3.431059	-3.107981	-0.155878	-3.424039	-3.111475
H	0.029607	-4.554957	-5.375868	0.0257	-4.551632	-5.372857	-0.239776	-4.544524	-5.374807
H	-0.000693	-3.126558	-7.428766	-0.000907	-3.133157	-7.434838	-0.203496	-3.128785	-7.439038
H	-0.026543	3.44341	-3.105215	-0.022923	3.431059	-3.107981	0.155878	3.424039	-3.111475
H	-0.029607	4.554957	-5.375868	-0.0257	4.551632	-5.372857	0.239776	4.544524	-5.374807
H	0.000693	3.126558	-7.428766	0.000907	3.133157	-7.434838	0.203496	3.128785	-7.439038
H	-5.829185	1.086308	-8.425977	-5.829637	1.089574	-8.406785	-5.722699	1.561618	-8.385988
H	5.820023	1.130383	7.680706	5.767385	1.353245	7.550744	5.640701	1.823705	7.549947
H	5.829185	-1.086308	-8.425977	5.829637	-1.089574	-8.406785	5.722699	-1.561618	-8.385988
H	-5.820023	-1.130383	7.680706	-5.767385	-1.353245	7.550744	-5.640701	-1.823705	7.549947
H	-0.666852	4.042836	-12.27734	-0.682581	4.053639	-12.275488	-0.374413	4.063634	-12.310191
H	0.627679	4.014911	11.580535	0.575364	3.895085	11.691972	0.25743	3.916832	11.709478
H	0.666852	-4.042836	-12.27734	0.682581	-4.053639	-12.275488	0.374413	-4.063634	-12.310191
H	-0.627679	-4.014911	11.580535	-0.575364	-3.895085	11.691972	-0.25743	-3.916832	11.709478

RuOs2		S0			S1			T1	
Atom	X	Y	Z	X	Y	Z	X	Y	Z
Os	0	0	7.623826	0	0	7.62752	0	0	7.636674
Ru	0	0	-7.591047	0	0	-7.603501	0	0	-7.609058
N	-0.000287	1.41717	1.18714	-0.009696	1.426181	1.188841	-0.024795	1.427511	1.183555
N	0.000287	-1.41717	1.18714	0.009696	-1.426181	1.188841	0.024795	-1.427511	1.183555
N	-0.023844	1.314258	6.033063	-0.053102	1.334297	6.054849	-0.092664	1.325945	6.04356
N	0.023844	-1.314258	6.033063	0.053102	-1.334297	6.054849	0.092664	-1.325945	6.04356
N	2.031003	0.33894	7.728197	2.010622	0.454712	7.682943	1.989258	0.558501	7.692785
N	0.107016	1.416643	9.114192	0.062433	1.385852	9.15995	0	1.385217	9.169978
N	-2.031003	-0.33894	7.728197	-2.010622	-0.454712	7.682943	-1.989258	-0.558501	7.692785
N	-0.107016	-1.416643	9.114192	-0.062433	-1.385852	9.15995	0	-1.385217	9.169978
N	-2.060388	0.252898	-7.692799	-2.054918	0.286076	-7.698812	-2.041299	0.370156	-7.702589
N	-0.106608	1.434242	-9.089367	-0.087821	1.439291	-9.098529	-0.03046	1.441914	-9.103913
N	2.060388	-0.252898	-7.692799	2.054918	-0.286076	-7.698812	2.041299	-0.370156	-7.702589
N	0.106608	-1.434242	-9.089367	0.087821	-1.439291	-9.098529	0.03046	-1.441914	-9.103913
N	0.000349	1.417233	-1.158535	0.008485	1.417331	-1.153998	0.024164	1.423102	-1.156967
N	-0.000349	-1.417233	-1.158535	-0.008485	-1.417331	-1.153998	-0.024164	-1.423102	-1.156967
N	-0.020729	-1.330315	-5.998323	-0.04188	-1.334096	-6.013045	-0.088091	-1.33304	-6.018914
N	0.020729	1.330315	-5.998323	0.04188	1.334096	-6.013045	0.088091	1.33304	-6.018914
C	0.000251	-0.728187	2.330319	0.009185	-0.725016	2.341058	0.02153	-0.713726	2.342943
C	-0.000251	0.728187	2.330319	-0.009185	0.725016	2.341058	-0.02153	0.713726	2.342943
C	-0.004329	1.457298	3.600804	-0.030245	1.439014	3.606141	-0.064294	1.435393	3.604204
C	-0.006022	0.722451	4.795711	-0.025082	0.707832	4.820382	-0.043395	0.714458	4.812146
C	0.006022	-0.722451	4.795711	0.025082	-0.707832	4.820382	0.043395	-0.714458	4.812146
C	0.004329	-1.457298	3.600804	0.030245	-1.439014	3.606141	0.064294	-1.435393	3.604204
C	-0.011329	2.86443	3.677791	-0.058068	2.847	3.69253	-0.132192	2.848152	3.689607
C	-0.019542	3.466436	4.941334	-0.071747	3.468544	4.946887	-0.171787	3.45997	4.943018
C	-0.025842	2.669145	6.099165	-0.062626	2.679925	6.115102	-0.145857	2.672137	6.11313
C	0.025842	-2.669145	6.099165	0.062626	-2.679925	6.115102	0.145857	-2.672137	6.11313
C	0.019542	-3.466436	4.941334	0.071747	-3.468544	4.946887	0.171787	-3.45997	4.943018
C	0.011329	-2.86443	3.677791	0.058068	-2.847	3.69253	0.132192	-2.848152	3.689607
C	4.750493	0.972052	7.962712	4.686297	1.21586	7.869324	4.619314	1.465599	7.860881
C	4.314322	0.022642	7.020799	4.274182	0.29745	6.889132	4.254786	0.514868	6.892187
C	2.95073	-0.267875	6.92949	2.924332	-0.057158	6.817588	2.926717	0.085872	6.830083
C	2.447959	1.267442	8.649829	2.399076	1.362794	8.636638	2.330567	1.493763	8.637486
C	3.80361	1.598996	8.783474	3.736074	1.758412	8.747751	3.644628	1.962857	8.738879
C	1.363326	1.857542	9.450288	1.30327	1.877213	9.476223	1.21286	1.946419	9.48132
C	-0.971467	1.893163	9.793636	-1.025199	1.768908	9.87639	-1.107005	1.706285	9.889885
C	-0.840537	2.827963	10.823814	-0.919402	2.680525	10.930778	-1.04863	2.620899	10.94423
C	1.553389	2.792981	10.477125	1.468391	2.786271	10.527278	1.329072	2.862183	10.532776
C	0.442296	3.287105	11.173303	0.345201	3.196239	11.260657	0.186688	3.206797	11.270338
C	-4.750493	-0.972052	7.962712	-4.686297	-1.21586	7.869324	-4.619314	-1.465599	7.860881
C	-4.314322	-0.022642	7.020799	-4.274182	-0.29745	6.889132	-4.254786	-0.514868	6.892187
C	-2.95073	0.267875	6.92949	-2.924332	0.057158	6.817588	-2.926717	-0.085872	6.830083
C	-2.447959	-1.267442	8.649829	-2.399076	-1.362794	8.636638	-2.330567	-1.493763	8.637486
C	-3.80361	-1.598996	8.783474	-3.736074	-1.758412	8.747751	-3.644628	-1.962857	8.738879
C	-1.363326	-1.857542	9.450288	-1.30327	-1.877213	9.476223	-1.21286	-1.946419	9.48132
C	0.971467	-1.893163	9.793636	1.025199	-1.768908	9.87639	1.107005	-1.706285	9.889885

C	0.840537	-2.827963	10.823814	0.919402	-2.680525	10.930778	1.04863	-2.620899	10.94423
C	-1.553389	-2.792981	10.477125	-1.468391	-2.786271	10.527278	-1.329072	-2.862183	10.532776
C	-0.442296	-3.287105	11.173303	-0.345201	-3.196239	11.260657	-0.186688	-3.206797	11.270338
C	-4.780512	0.862921	-8.085814	-4.765797	0.947473	-8.07344	-4.722792	1.145699	-8.070923
C	-4.382225	-0.066826	-7.12891	-4.378779	0.007221	-7.122034	-4.373373	0.190647	-7.119667
C	-3.006611	-0.352372	-6.955039	-3.007576	-0.304257	-6.957204	-3.016191	-0.178794	-6.958028
C	-2.442679	1.1787	-8.635959	-2.425812	1.2227	-8.635773	-2.374664	1.321691	-8.638695
C	-3.79374	1.515996	-8.87359	-3.771824	1.585357	-8.864571	-3.704708	1.740463	-8.86496
C	-1.39711	1.804468	-9.389944	-1.372887	1.833376	-9.392048	-1.298497	1.888231	-9.396675
C	0.906119	1.988302	-9.77748	0.931278	1.979664	-9.788145	1.009405	1.940549	-9.793958
C	0.678344	2.947545	-10.79353	0.715895	2.947636	-10.798654	0.833009	2.916183	-10.804641
C	-1.707676	2.756072	-10.386587	-1.671275	2.7951	-10.382769	-1.558088	2.861289	-10.387245
C	-0.623284	3.335738	-11.099869	-0.580152	3.359677	-11.097826	-0.445338	3.380505	-11.103343
C	4.780512	-0.862921	-8.085814	4.765797	-0.947473	-8.07344	4.722792	-1.145699	-8.070923
C	4.382225	0.066826	-7.12891	4.378779	-0.007221	-7.122034	4.373373	-0.190647	-7.119667
C	3.006611	0.352372	-6.955039	3.007576	0.304257	-6.957204	3.016191	0.178794	-6.958028
C	2.442679	-1.1787	-8.635959	2.425812	-1.2227	-8.635773	2.374664	-1.321691	-8.638695
C	3.79374	-1.515996	-8.87359	3.771824	-1.585357	-8.864571	3.704708	-1.740463	-8.86496
C	1.39711	-1.804468	-9.389944	1.372887	-1.833376	-9.392048	1.298497	-1.888231	-9.396675
C	-0.906119	-1.988302	-9.77748	-0.931278	-1.979664	-9.788145	-1.009405	-1.940549	-9.793958
C	-0.678344	-2.947545	-10.79353	-0.715895	-2.947636	-10.798654	-0.833009	-2.916183	-10.804641
C	1.707676	-2.756072	-10.386587	1.671275	-2.7951	-10.382769	1.558088	-2.861289	-10.387245
C	0.623284	-3.335738	-11.099869	0.580152	-3.359677	-11.097826	0.445338	-3.380505	-11.103343
C	0	0.719675	0.01426	0	0.7288	0.010419	0.000013	0.733431	0.01171
C	0	-0.719675	0.01426	0	-0.7288	0.010419	-0.000013	-0.733431	0.01171
C	-0.000341	-0.727753	-2.301512	-0.007708	-0.713831	-2.316041	-0.02124	-0.712358	-2.320207
C	0.000341	0.727753	-2.301512	0.007708	0.713831	-2.316041	0.02124	0.712358	-2.320207
C	-0.003783	-1.454812	-3.572644	-0.024302	-1.442641	-3.578704	-0.06234	-1.438018	-3.581981
C	-0.005923	-0.725542	-4.771823	-0.016835	-0.721505	-4.786582	-0.038996	-0.719437	-4.792806
C	0.005923	0.725542	-4.771823	0.016835	0.721505	-4.786582	0.038996	0.719437	-4.792806
C	0.003783	1.454812	-3.572644	0.024302	1.442641	-3.578704	0.06234	1.438018	-3.581981
C	-0.009335	-2.863815	-3.643891	-0.052861	-2.855326	-3.651009	-0.132084	-2.850545	-3.654868
C	-0.016218	-3.475632	-4.900689	-0.071922	-3.470948	-4.903176	-0.176241	-3.46622	-4.905794
C	-0.021849	-2.679901	-6.062505	-0.065394	-2.680127	-6.072478	-0.152421	-2.677118	-6.077019
C	0.009335	2.863815	-3.643891	0.052861	2.855326	-3.651009	0.132084	2.850545	-3.654868
C	0.016218	3.475632	-4.900689	0.071922	3.470948	-4.903176	0.176241	3.46622	-4.905794
C	0.021849	2.679901	-6.062505	0.065394	2.680127	-6.072478	0.152421	2.677118	-6.077019
C	-4.096187	2.49331	-9.894474	-4.061803	2.572162	-9.880079	-3.955008	2.737865	-9.880733
C	4.096187	-2.49331	-9.894474	4.061803	-2.572162	-9.880079	3.955008	-2.737865	-9.880733
C	-3.094589	3.086916	-10.622657	-3.053415	3.151109	-10.610747	-2.924665	3.274077	-10.613417
C	3.094589	-3.086916	-10.622657	3.053415	-3.151109	-10.610747	2.924665	-3.274077	-10.613417
H	-0.01109	3.451541	2.766076	-0.065997	3.427907	2.775904	-0.151192	3.427823	2.772976
H	-0.024232	4.544718	5.046224	-0.090859	4.547263	5.039247	-0.222583	4.537624	5.039122
H	-0.043594	3.111104	7.088975	-0.078616	3.134253	7.100092	-0.180924	3.123492	7.098389
H	0.043594	-3.111104	7.088975	0.078616	-3.134253	7.100092	0.180924	-3.123492	7.098389
H	0.024232	-4.544718	5.046224	0.090859	-4.547263	5.039247	0.222583	-4.537624	5.039122
H	0.01109	-3.451541	2.766076	0.065997	-3.427907	2.775904	0.151192	-3.427823	2.772976
H	5.013276	-0.486082	6.367209	4.978316	-0.136865	6.190108	4.979015	0.112125	6.194774
H	2.57551	-0.999216	6.223016	2.563519	-0.763204	6.079323	2.603534	-0.64802	6.101425

H	4.117387	2.336387	9.513261	4.037026	2.478669	9.498803	3.908605	2.704082	9.483423
H	-1.941983	1.517036	9.491394	-1.980766	1.347191	9.587076	-2.038537	1.232114	9.602884
H	-1.726302	3.183244	11.337375	-1.808452	2.971849	11.476593	-1.950665	2.861052	11.493622
H	2.551507	3.129431	10.732985	2.451113	3.168435	10.775746	2.289201	3.299972	10.777907
H	-5.013276	0.486082	6.367209	-4.978316	0.136865	6.190108	-4.979015	-0.112125	6.194774
H	-2.57551	0.999216	6.223016	-2.563519	0.763204	6.079323	-2.603534	0.64802	6.101425
H	-4.117387	-2.336387	9.513261	-4.037026	-2.478669	9.498803	-3.908605	-2.704082	9.483423
H	1.941983	-1.517036	9.491394	1.980766	-1.347191	9.587076	2.038537	-1.232114	9.602884
H	1.726302	-3.183244	11.337375	1.808452	-2.971849	11.476593	1.950665	-2.861052	11.493622
H	-2.551507	-3.129431	10.732985	-2.451113	-3.168435	10.775746	-2.289201	-3.299972	10.777907
H	-5.107289	-0.583023	-6.510655	-5.109631	-0.497496	-6.501035	-5.123405	-0.281911	-6.496232
H	-2.674883	-1.078709	-6.221011	-2.683537	-1.03865	-6.227626	-2.721426	-0.925798	-6.228791
H	1.911922	1.67612	-9.517768	1.932585	1.64889	-9.533831	1.996618	1.569612	-9.539943
H	1.52835	3.367743	-11.318251	1.570876	3.355933	-11.324789	1.703685	3.289226	-11.331244
H	5.107289	0.583023	-6.510655	5.109631	0.497496	-6.501035	5.123405	0.281911	-6.496232
H	2.674883	1.078709	-6.221011	2.683537	1.03865	-6.227626	2.721426	0.925798	-6.228791
H	-1.911922	-1.67612	-9.517768	-1.932585	-1.64889	-9.533831	-1.996618	-1.569612	-9.539943
H	-1.52835	-3.367743	-11.318251	-1.570876	-3.355933	-11.324789	-1.703685	-3.289226	-11.331244
H	-0.008529	-3.444101	-2.727614	-0.06039	-3.43101	-2.73183	-0.151662	-3.424546	-2.734788
H	-0.019465	-4.554513	-4.998664	-0.093645	-4.550307	-4.997065	-0.230631	-4.544657	-4.998492
H	-0.035026	-3.124899	-7.051255	-0.086649	-3.131071	-7.058615	-0.192413	-3.128748	-7.062345
H	0.008529	3.444101	-2.727614	0.06039	3.43101	-2.73183	0.151662	3.424546	-2.734788
H	0.019465	4.554513	-4.998664	0.093645	4.550307	-4.997065	0.230631	4.544657	-4.998492
H	0.035026	3.124899	-7.051255	0.086649	3.131071	-7.058615	0.192413	3.128748	-7.062345
H	-5.831263	1.092843	-8.235685	-5.813049	1.197299	-8.216085	-5.75891	1.43979	-8.210852
H	5.802897	1.217313	8.054391	5.72723	1.509767	7.945188	5.642711	1.817325	7.928843
H	5.831263	-1.092843	-8.235685	5.813049	-1.197299	-8.216085	5.75891	-1.43979	-8.210852
H	-5.802897	-1.217313	8.054391	-5.72723	-1.509767	7.945188	-5.642711	-1.817325	7.928843
H	-0.817831	4.072665	-11.873523	-0.765151	4.103827	-11.86693	-0.60028	4.131409	-11.872539
H	0.572696	4.011465	11.969805	0.45617	3.902082	12.076213	0.260501	3.916733	12.086603
H	0.817831	-4.072665	-11.873523	0.765151	-4.103827	-11.86693	0.60028	-4.131409	-11.872539
H	-0.572696	-4.011465	11.969805	-0.45617	-3.902082	12.076213	-0.260501	-3.916733	12.086603
H	-5.137252	2.746851	-10.0743	-5.099074	2.844904	-10.053784	-4.980301	3.05327	-10.053148
H	-3.326924	3.819079	-11.390931	-3.276579	3.890542	-11.374818	-3.118185	4.021768	-11.377568
H	3.326924	-3.819079	-11.390931	3.276579	-3.890542	-11.374818	3.118185	-4.021768	-11.377568
H	5.137252	-2.746851	-10.0743	5.099074	-2.844904	-10.053784	4.980301	-3.05327	-10.053148

RuOs3		S0			S1			T1	
Atom	X	Y	Z	X	Y	Z	X	Y	Z
Os	0	0	9.656221	0	0	9.659865	0	0	9.668614
Ru	0	0	-5.559693	0	0	-5.57118	0	0	-5.576285
N	0.583459	-1.291584	3.219292	0.524285	-1.326371	3.221649	0.51165	-1.33288	3.216962
N	-0.583459	1.291584	3.219292	-0.524285	1.326371	3.221649	-0.51165	1.33288	3.216962
N	0.572912	-1.183648	8.065296	0.484754	-1.244152	8.087653	0.466656	-1.244677	8.077088
N	-0.572912	1.183648	8.065296	-0.484754	1.244152	8.087653	-0.466656	1.244677	8.077088
N	-1.691771	-1.173442	9.763685	-1.751331	-1.088701	9.706658	-1.752048	-1.097392	9.716546
N	0.512502	-1.331406	11.140273	0.392673	-1.334709	11.186949	0.391298	-1.336049	11.193797
N	1.691771	1.173442	9.763685	1.751331	1.088701	9.706658	1.752048	1.097392	9.716546
N	-0.512502	1.331406	11.140273	-0.392673	1.334709	11.186949	-0.391298	1.336049	11.193797
N	1.976051	0.615103	-5.667155	1.977332	0.607874	-5.672746	1.977569	0.606011	-5.676481
N	0.698267	-1.247257	-7.056733	0.698727	-1.251122	-7.064959	0.698819	-1.25216	-7.069233
N	-1.976051	-0.615103	-5.667155	-1.977332	-0.607874	-5.672746	-1.977569	-0.606011	-5.676481
N	-0.698267	1.247257	-7.056733	-0.698727	1.251122	-7.064959	-0.698819	1.25216	-7.069233
N	0.582888	-1.291925	0.873545	0.545338	-1.308311	0.87879	0.539939	-1.31696	0.876198
N	-0.582888	1.291925	0.873545	-0.545338	1.308311	0.87879	-0.539939	1.31696	0.876198
N	-0.536201	1.218103	-3.966347	-0.528279	1.225956	-3.980188	-0.52612	1.227831	-3.985899
N	0.536201	-1.218103	-3.966347	0.528279	-1.225956	-3.980188	0.52612	-1.227831	-3.985899
C	-0.300088	0.663592	4.362519	-0.261161	0.676539	4.373933	-0.2503	0.66884	4.376485
C	0.300088	-0.663592	4.362519	0.261161	-0.676539	4.373933	0.2503	-0.66884	4.376485
C	0.605809	-1.325393	5.633038	0.511144	-1.345783	5.638976	0.496512	-1.348545	5.637789
C	0.306133	-0.654503	6.828194	0.257475	-0.659859	6.853167	0.251063	-0.670347	6.845728
C	-0.306133	0.654503	6.828194	-0.257475	0.659859	6.853167	-0.251063	0.670347	6.845728
C	-0.605809	1.325393	5.633038	-0.511144	1.345783	5.638976	-0.496512	1.348545	5.637789
C	1.194431	-2.603518	5.709638	0.999391	-2.666654	5.725683	0.977898	-2.678521	5.723664
C	1.454722	-3.146646	6.973048	1.205865	-3.252892	6.980181	1.177614	-3.258058	6.977145
C	1.135546	-2.416381	8.13102	0.931971	-2.513317	8.148392	0.908064	-2.517493	8.147355
C	-1.135546	2.416381	8.13102	-0.931971	2.513317	8.148392	-0.908064	2.517493	8.147355
C	-1.454722	3.146646	6.973048	-1.205865	3.252892	6.980181	-1.177614	3.258058	6.977145
C	-1.194431	2.603518	5.709638	-0.999391	2.666654	5.725683	-0.977898	2.678521	5.723664
C	-3.882319	-2.903986	10.002567	-4.011208	-2.715356	9.85231	-3.999645	-2.741699	9.846568
C	-3.896813	-1.854653	9.065791	-3.934334	-1.687073	8.897937	-3.933499	-1.698741	8.906841
C	-2.786792	-1.011402	8.972297	-2.784747	-0.89412	8.846551	-2.790475	-0.896673	8.863113
C	-1.668663	-2.195599	10.680191	-1.810806	-2.096019	10.63722	-1.802201	-2.115913	10.634833
C	-2.754016	-3.072667	10.816187	-2.934905	-2.923678	10.72799	-2.920162	-2.953152	10.717053
C	-0.431817	-2.270959	11.473805	-0.608797	-2.225392	11.479074	-0.601931	-2.239771	11.477373
C	1.696353	-1.307804	11.811002	1.537868	-1.334036	11.916393	1.535503	-1.326685	11.927358
C	1.984848	-2.217694	12.831216	1.739637	-2.245401	12.956916	1.743973	-2.242338	12.961679
C	-0.196446	-3.207089	12.490526	-0.462823	-3.155593	12.514059	-0.447616	-3.174495	12.506721
C	1.023746	-3.184186	13.17905	0.725829	-3.170317	13.258625	0.739443	-3.181011	13.254001
C	3.882319	2.903986	10.002567	4.011208	2.715356	9.85231	3.999645	2.741699	9.846568
C	3.896813	1.854653	9.065791	3.934334	1.687073	8.897937	3.933499	1.698741	8.906841
C	2.786792	1.011402	8.972297	2.784747	0.89412	8.846551	2.790475	0.896673	8.863113
C	1.668663	2.195599	10.680191	1.810806	2.096019	10.63722	1.802201	2.115913	10.634833
C	2.754016	3.072667	10.816187	2.934905	2.923678	10.72799	2.920162	2.953152	10.717053
C	0.431817	2.270959	11.473805	0.608797	2.225392	11.479074	0.601931	2.239771	11.477373
C	-1.696353	1.307804	11.811002	-1.537868	1.334036	11.916393	-1.535503	1.326685	11.927358

C	-1.984848	2.217694	12.831216	-1.739637	2.245401	12.956916	-1.743973	2.242338	12.961679
C	0.196446	3.207089	12.490526	0.462823	3.155593	12.514059	0.447616	3.174495	12.506721
C	-1.023746	3.184186	13.17905	-0.725829	3.170317	13.258625	-0.739443	3.181011	13.254001
C	4.740482	1.166738	-5.995998	4.74639	1.145625	-5.986821	4.747713	1.140466	-5.986919
C	3.94811	1.855392	-5.071145	3.951987	1.83975	-5.067794	3.95278	1.835909	-5.069329
C	2.577804	1.560568	-4.926315	2.579406	1.55176	-4.930027	2.579665	1.549543	-4.933288
C	2.721077	-0.060422	-6.606549	2.724766	-0.073328	-6.606058	2.725621	-0.076576	-6.608273
C	4.098198	0.182946	-6.818512	4.104307	0.162945	-6.8106	4.105731	0.158004	-6.810985
C	2.018846	-1.042904	-7.385235	2.022193	-1.0544	-7.386375	2.022989	-1.057341	-7.388932
C	0	-2.171149	-7.737977	0	-2.173188	-7.748261	0	-2.173843	-7.752993
C	0.577844	-2.908943	-8.790607	0.580148	-2.916289	-8.795953	0.58072	-2.918312	-8.799409
C	2.673164	-1.748547	-8.421524	2.679042	-1.76569	-8.417324	2.680462	-1.770071	-8.418522
C	1.908116	-2.702012	-9.171458	1.913723	-2.717019	-9.169458	1.915096	-2.720941	-9.171129
C	-4.740482	-1.166738	-5.995998	-4.74639	-1.145625	-5.986821	-4.747713	-1.140466	-5.986919
C	-3.94811	-1.855392	-5.071145	-3.951987	-1.83975	-5.067794	-3.95278	-1.835909	-5.069329
C	-2.577804	-1.560568	-4.926315	-2.579406	-1.55176	-4.930027	-2.579665	-1.549543	-4.933288
C	-2.721077	0.060422	-6.606549	-2.724766	0.073328	-6.606058	-2.725621	0.076576	-6.608273
C	-4.098198	-0.182946	-6.818512	-4.104307	-0.162945	-6.8106	-4.105731	-0.158004	-6.810985
C	-2.018846	1.042904	-7.385235	-2.022193	1.0544	-7.386375	-2.022989	1.057341	-7.388932
C	0	2.171149	-7.737977	0	2.173188	-7.748261	0	2.173843	-7.752993
C	-0.577844	2.908943	-8.790607	-0.580148	2.916289	-8.795953	-0.58072	2.918312	-8.799409
C	-2.673164	1.748547	-8.421524	-2.679042	1.76569	-8.417324	-2.680462	1.770071	-8.418522
C	-1.908116	2.702012	-9.171458	-1.913723	2.717019	-9.169458	-1.915096	2.720941	-9.171129
C	0.29613	-0.656083	2.046382	0.2743	-0.675309	2.043184	0.270556	-0.681818	2.044966
C	-0.29613	0.656083	2.046382	-0.2743	0.675309	2.043184	-0.270556	0.681818	2.044966
C	-0.299423	0.663468	-0.269488	-0.27947	0.656968	-0.283304	-0.276015	0.657145	-0.287164
C	0.299423	-0.663468	-0.269488	0.27947	-0.656968	-0.283304	0.276015	-0.657145	-0.287164
C	-0.596946	1.32678	-1.540641	-0.572632	1.32452	-1.54595	-0.566712	1.323367	-1.548992
C	-0.29574	0.662694	-2.740068	-0.286993	0.662289	-2.753885	-0.284711	0.661935	-2.759789
C	0.29574	-0.662694	-2.740068	0.286993	-0.662289	-2.753885	0.284711	-0.661935	-2.759789
C	0.596946	-1.32678	-1.540641	0.572632	-1.32452	-1.54595	0.566712	-1.323367	-1.548992
C	-1.175001	2.61176	-1.611765	-1.13593	2.620337	-1.618379	-1.126348	2.622165	-1.622381
C	-1.425829	3.169955	-2.86858	-1.386267	3.183092	-2.870647	-1.376353	3.186234	-2.873569
C	-1.095525	2.446469	-4.030613	-1.071275	2.457898	-4.040016	-1.065094	2.460811	-4.044766
C	1.175001	-2.61176	-1.611765	1.13593	-2.620337	-1.618379	1.126348	-2.622165	-1.622381
C	1.425829	-3.169955	-2.86858	1.386267	-3.183092	-2.870647	1.376353	-3.186234	-2.873569
C	1.095525	-2.446469	-4.030613	1.071275	-2.457898	-4.040016	1.065094	-2.460811	-4.044766
C	4.753647	-0.557389	-7.871555	4.762238	-0.58335	-7.85801	4.764282	-0.589792	-7.856972
C	-4.753647	0.557389	-7.871555	-4.762238	0.58335	-7.85801	-4.764282	0.589792	-7.856972
C	4.076299	-1.477595	-8.632721	4.084811	-1.502064	-8.620911	4.086863	-1.508211	-8.620242
C	-4.076299	1.477595	-8.632721	-4.084811	1.502064	-8.620911	-4.086863	1.508211	-8.620242
C	2.461837	-3.456613	-10.326427	2.47047	-3.47707	-10.319529	2.472576	-3.482407	-10.319941
C	3.144889	-2.795321	-11.370321	3.162476	-2.82154	-11.361166	3.166803	-2.828381	-11.36105
C	2.246307	-4.848346	-10.418488	2.249268	-4.868042	-10.409559	2.249956	-4.873192	-10.409398
C	3.613137	-3.516257	-12.480268	3.633912	-3.547283	-12.466651	3.639018	-3.555384	-12.465381
C	2.72305	-5.570686	-11.524142	2.728958	-5.595253	-11.510777	2.730365	-5.601678	-11.509469
C	3.408793	-4.90656	-12.558018	3.423701	-4.936834	-12.54229	3.427341	-4.944746	-12.540423
C	6.192725	1.473449	-6.080749	6.200489	1.44595	-6.064414	6.202245	1.439277	-6.062749
C	7.161261	0.44666	-6.048446	7.164605	0.415327	-6.023439	7.165305	0.407755	-6.019671

C	6.617531	2.818571	-6.128721	6.631331	2.789075	-6.114438	6.63453	2.781922	-6.113271
C	8.529413	0.76101	-6.07441	8.534222	0.72384	-6.043044	8.535262	0.71488	-6.03773
C	7.985654	3.132272	-6.164137	8.000953	3.096996	-6.143311	8.0045	3.088472	-6.14055
C	8.945767	2.103862	-6.137787	8.956621	2.064711	-6.108463	8.959104	2.055274	-6.103637
C	-2.461837	3.456613	-10.326427	-2.47047	3.47707	-10.319529	-2.472576	3.482407	-10.319941
C	-3.144889	2.795321	-11.370321	-3.162476	2.82154	-11.361166	-3.166803	2.828381	-11.36105
C	-2.246307	4.848346	-10.418488	-2.249268	4.868042	-10.409559	-2.249956	4.873192	-10.409398
C	-3.613137	3.516257	-12.480268	-3.633912	3.547283	-12.466651	-3.639018	3.555384	-12.465381
C	-2.72305	5.570686	-11.524142	-2.728958	5.595253	-11.510777	-2.730365	5.601678	-11.509469
C	-3.408793	4.90656	-12.558018	-3.423701	4.936834	-12.54229	-3.427341	4.944746	-12.540423
C	-6.192725	-1.473449	-6.080749	-6.200489	-1.44595	-6.064414	-6.202245	-1.439277	-6.062749
C	-7.161261	-0.44666	-6.048446	-7.164605	-0.415327	-6.023439	-7.165305	-0.407755	-6.019671
C	-6.617531	-2.818571	-6.128721	-6.631331	-2.789075	-6.114438	-6.63453	-2.781922	-6.113271
C	-8.529413	-0.76101	-6.07441	-8.534222	-0.72384	-6.043044	-8.535262	-0.71488	-6.03773
C	-7.985654	-3.132272	-6.164137	-8.000953	-3.096996	-6.143311	-8.0045	-3.088472	-6.14055
C	-8.945767	-2.103862	-6.137787	-8.956621	-2.064711	-6.108463	-8.959104	-2.055274	-6.103637
H	1.434389	-3.139145	4.797798	1.203325	-3.210799	4.809179	1.17854	-3.222929	4.80722
H	1.904775	-4.126582	7.077641	1.575173	-4.266597	7.072709	1.54001	-4.274226	7.073263
H	1.33735	-2.810708	9.120495	1.089325	-2.939775	9.133413	1.06297	-2.942724	9.132696
H	-1.33735	2.810708	9.120495	-1.089325	2.939775	9.133413	-1.06297	2.942724	9.132696
H	-1.904775	4.126582	7.077641	-1.575173	4.266597	7.072709	-1.54001	4.274226	7.073263
H	-1.434389	3.139145	4.797798	-1.203325	3.210799	4.809179	-1.17854	3.222929	4.80722
H	-4.749386	-1.688023	8.417781	-4.743473	-1.499819	8.202719	-4.746142	-1.507318	8.216864
H	-2.761244	-0.186885	8.269255	-2.684491	-0.090061	8.12744	-2.700261	-0.081078	8.155425
H	-2.720928	-3.875797	11.543334	-2.974571	-3.720119	11.461317	-2.9522	-3.758387	11.441146
H	2.41131	-0.55141	11.509058	2.293679	-0.604972	11.647961	2.283566	-0.586647	11.66727
H	2.941466	-2.165204	13.337923	2.668556	-2.224273	13.513524	2.67061	-2.214096	13.52171
H	-0.952148	-3.941778	12.743458	-1.258275	-3.855026	12.740915	-1.236092	-3.883905	12.726931
H	4.749386	1.688023	8.417781	4.743473	1.499819	8.202719	4.746142	1.507318	8.216864
H	2.761244	0.186885	8.269255	2.684491	0.090061	8.12744	2.700261	0.081078	8.155425
H	2.720928	3.875797	11.543334	2.974571	3.720119	11.461317	2.9522	3.758387	11.441146
H	-2.41131	0.55141	11.509058	-2.293679	0.604972	11.647961	-2.283566	0.586647	11.66727
H	-2.941466	2.165204	13.337923	-2.668556	2.224273	13.513524	-2.67061	2.214096	13.52171
H	0.952148	3.941778	12.743458	1.258275	3.855026	12.740915	1.236092	3.883905	12.726931
H	4.391115	2.606655	-4.425723	4.395022	2.590225	-4.421397	4.395794	2.586211	-4.422698
H	1.968026	2.085708	-4.199339	1.967483	2.080652	-4.207491	1.967131	2.07926	-4.211852
H	-1.035798	-2.320982	-7.453214	-1.038216	-2.316849	-7.468854	-1.0388	-2.315994	-7.474907
H	-0.03986	-3.619101	-9.330467	-0.037875	-3.624696	-9.337827	-0.037374	-3.626334	-9.341728
H	-4.391115	-2.606655	-4.425723	-4.395022	-2.590225	-4.421397	-4.395794	-2.586211	-4.422698
H	-1.968026	-2.085708	-4.199339	-1.967483	-2.080652	-4.207491	-1.967131	-2.07926	-4.211852
H	1.035798	2.320982	-7.453214	1.038216	2.316849	-7.468854	1.0388	2.315994	-7.474907
H	0.03986	3.619101	-9.330467	0.037875	3.624696	-9.337827	0.037374	3.626334	-9.341728
H	-1.413646	3.140605	-0.695426	-1.362577	3.149492	-0.699153	-1.350042	3.151279	-0.702405
H	-1.870083	4.153202	-2.966159	-1.818771	4.172293	-2.964295	-1.80587	4.176968	-2.966168
H	-1.271924	2.85487	-5.019494	-1.24875	2.872092	-5.026533	-1.242652	2.876424	-5.030761
H	1.413646	-3.140605	-0.695426	1.362577	-3.149492	-0.699153	1.350042	-3.151279	-0.702405
H	1.870083	-4.153202	-2.966159	1.818771	-4.172293	-2.964295	1.80587	-4.176968	-2.966168
H	1.271924	-2.85487	-5.019494	1.24875	-2.872092	-5.026533	1.242652	-2.876424	-5.030761
H	-4.730152	-3.573736	10.096194	-4.890342	-3.347314	9.910728	-4.873747	-3.381189	9.898088

H	4.730152	3.573736	10.096194	4.890342	3.347314	9.910728	4.873747	3.381189	9.898088
H	1.220975	-3.902021	13.967689	0.855757	-3.887184	14.061653	0.875233	-3.901748	14.052601
H	-1.220975	3.902021	13.967689	-0.855757	3.887184	14.061653	-0.875233	3.901748	14.052601
H	5.802495	-0.365858	-8.07117	5.813243	-0.397621	-8.051873	5.815801	-0.40547	-8.049433
H	4.605491	-2.028845	-9.402591	4.61579	-2.057771	-9.386375	4.618295	-2.06505	-9.384578
H	-4.605491	2.028845	-9.402591	-4.61579	2.057771	-9.386375	-4.618295	2.06505	-9.384578
H	-5.802495	0.365858	-8.07117	-5.813243	0.397621	-8.051873	-5.815801	0.40547	-8.049433
H	3.28071	-1.716722	-11.331735	3.303028	-1.74347	-11.32431	3.308528	-1.750444	-11.324688
H	1.723406	-5.365584	-9.616674	1.71942	-5.380918	-9.609495	1.718393	-5.384935	-9.609745
H	4.128938	-2.995682	-13.282095	4.156739	-3.030984	-13.26671	4.163586	-3.040198	-13.265023
H	2.561515	-6.643497	-11.578768	2.562811	-6.667457	-11.563737	2.563065	-6.67373	-11.561958
H	3.775226	-5.464215	-13.415434	3.792534	-5.49824	-13.396232	3.796761	-5.507135	-13.393468
H	6.848553	-0.592217	-5.969276	6.847028	-0.621959	-5.942623	6.846566	-0.629148	-5.938463
H	5.87715	3.615372	-6.157706	5.894383	3.588807	-6.149883	5.898407	3.582345	-6.150294
H	9.265947	-0.036669	-6.039621	9.267195	-0.076821	-6.001669	9.26738	-0.086484	-5.994761
H	8.300573	4.170776	-6.212659	8.320458	4.134044	-6.193348	8.325095	4.12517	-6.190956
H	10.004722	2.345602	-6.162067	10.016705	2.301954	-6.127751	10.01945	2.291447	-6.121713
H	-3.28071	1.716722	-11.331735	-3.303028	1.74347	-11.32431	-3.308528	1.750444	-11.324688
H	-1.723406	5.365584	-9.616674	-1.71942	5.380918	-9.609495	-1.718393	5.384935	-9.609745
H	-4.128938	2.995682	-13.282095	-4.156739	3.030984	-13.26671	-4.163586	3.040198	-13.265023
H	-2.561515	6.643497	-11.578768	-2.562811	6.667457	-11.563737	-2.563065	6.67373	-11.561958
H	-3.775226	5.464215	-13.415434	-3.792534	5.49824	-13.396232	-3.796761	5.507135	-13.393468
H	-6.848553	0.592217	-5.969276	-6.847028	0.621959	-5.942623	-6.846566	0.629148	-5.938463
H	-5.87715	-3.615372	-6.157706	-5.894383	-3.588807	-6.149883	-5.898407	-3.582345	-6.150294
H	-9.265947	0.036669	-6.039621	-9.267195	0.076821	-6.001669	-9.26738	0.086484	-5.994761
H	-8.300573	-4.170776	-6.212659	-8.320458	-4.134044	-6.193348	-8.325095	-4.12517	-6.190956
H	-10.004722	-2.345602	-6.162067	-10.016705	-2.301954	-6.127751	-10.01945	-2.291447	-6.121713

RuOs4		S0			S1			T1	
Symbol	X	Y	Z	X	Y	Z	X	Y	Z
Os	0	0	8.97489	0	0	8.97917	0	0	8.98698
Ru	0	0	-6.242511	0	0	-6.254342	0	0	-6.257201
N	0.014715	1.417054	2.538237	0.018525	1.425954	2.540492	0.005951	1.423451	2.529276
N	-0.014715	-1.417054	2.538237	-0.018525	-1.425954	2.540492	-0.005951	-1.423451	2.529276
N	0.006335	1.314479	7.384193	0.010935	1.33527	7.406785	-0.008389	1.320674	7.397028
N	-0.006335	-1.314479	7.384193	-0.010935	-1.33527	7.406785	0.008389	-1.320674	7.397028
N	2.038508	0.289478	9.079743	2.029965	0.360876	9.031167	2.033578	0.311582	9.081104
N	0.140746	1.41576	10.463208	0.128434	1.38223	10.510115	0.132233	1.4187	10.470555
N	-2.038508	-0.289478	9.079743	-2.029965	-0.360876	9.031167	-2.033578	-0.311582	9.081104
N	-0.140746	-1.41576	10.463208	-0.128434	-1.38223	10.510115	-0.132233	-1.4187	10.470555
N	-2.049535	0.278077	-6.35131	-2.049869	0.269059	-6.357113	-2.021966	0.421045	-6.321192
N	-0.132674	1.427099	-7.731389	-0.143181	1.428541	-7.740858	-0.069621	1.39057	-7.779203
N	2.049535	-0.278077	-6.35131	2.049869	-0.269059	-6.357113	2.021966	-0.421045	-6.321192
N	0.132674	-1.427099	-7.731389	0.143181	-1.428541	-7.740858	0.069621	-1.39057	-7.779203
N	0	1.417208	0.192567	0	1.417191	0.197568	0	1.427537	0.188452
N	0	-1.417208	0.192567	0	-1.417191	0.197568	0	-1.427537	0.188452
N	-0.001473	-1.330379	-4.64775	0.002828	-1.334542	-4.661802	-0.021811	-1.339697	-4.667634
N	0.001473	1.330379	-4.64775	-0.002828	1.334542	-4.661802	0.021811	1.339697	-4.667634
C	-0.010978	-0.72805	3.681457	-0.013525	-0.725142	3.692578	-0.004272	-0.713105	3.692694
C	0.010978	0.72805	3.681457	0.013525	0.725142	3.692578	0.004272	0.713105	3.692694
C	0.024572	1.457064	4.951937	0.030264	1.439174	4.957821	0.007969	1.441596	4.953855
C	0.009719	0.722407	6.146872	0.007144	0.70799	6.172158	0.001496	0.71786	6.160598
C	-0.009719	-0.722407	6.146872	-0.007144	-0.70799	6.172158	-0.001496	-0.71786	6.160598
C	-0.024572	-1.457064	4.951937	-0.030264	-1.439174	4.957821	-0.007969	-1.441596	4.953855
C	0.048311	2.864019	5.028925	0.070202	2.846614	5.044171	0.014346	2.854483	5.033243
C	0.055958	3.466046	6.29246	0.092759	3.468114	6.298713	0.013993	3.461955	6.290447
C	0.034081	2.669058	7.450308	0.067342	2.679904	7.466736	0.002451	2.670716	7.4581
C	-0.034081	-2.669058	7.450308	-0.067342	-2.679904	7.466736	-0.002451	-2.670716	7.4581
C	-0.055958	-3.466046	6.29246	-0.092759	-3.468114	6.298713	-0.013993	-3.461955	6.290447
C	-0.048311	-2.864019	5.028925	-0.070202	-2.846614	5.044171	-0.014346	-2.854483	5.033243
C	4.772927	0.852877	9.317574	4.734963	1.014625	9.198597	4.762081	0.91732	9.290725
C	4.314085	-0.086955	8.376815	4.281118	0.10612	8.227678	4.308371	-0.035369	8.360034
C	2.943656	-0.342605	8.283927	2.917586	-0.19373	8.165166	2.941187	-0.311683	8.28061
C	2.477484	1.209589	9.999465	2.459606	1.259195	9.976334	2.467549	1.244236	9.990898
C	3.841073	1.505977	10.135111	3.812056	1.601381	10.077652	3.827973	1.561926	10.112174
C	1.407045	1.829437	10.796507	1.390144	1.823331	10.81801	1.394855	1.852117	10.793495
C	-0.926047	1.919876	11.141265	-0.93849	1.811793	11.231561	-0.936719	1.908867	11.156071
C	-0.773066	2.85651	12.166697	-0.789494	2.722206	12.281686	-0.789918	2.850206	12.177859
C	1.61907	2.766276	11.817777	1.598223	2.729018	11.864403	1.600629	2.794602	11.811246
C	0.520082	3.288984	12.512274	0.4969	3.187636	12.602115	0.499493	3.302977	12.512638
C	-4.772927	-0.852877	9.317574	-4.734963	-1.014625	9.198597	-4.762081	-0.91732	9.290725
C	-4.314085	0.086955	8.376815	-4.281118	-0.10612	8.227678	-4.308371	0.035369	8.360034
C	-2.943656	0.342605	8.283927	-2.917586	0.19373	8.165166	-2.941187	0.311683	8.28061
C	-2.477484	-1.209589	9.999465	-2.459606	-1.259195	9.976334	-2.467549	-1.244236	9.990898
C	-3.841073	-1.505977	10.135111	-3.812056	-1.601381	10.077652	-3.827973	-1.561926	10.112174
C	-1.407045	-1.829437	10.796507	-1.390144	-1.823331	10.81801	-1.394855	-1.852117	10.793495
C	0.926047	-1.919876	11.141265	0.93849	-1.811793	11.231561	0.936719	-1.908867	11.156071

C	0.773066	-2.85651	12.166697	0.789494	-2.722206	12.281686	0.789918	-2.850206	12.177859
C	-1.61907	-2.766276	11.817777	-1.598223	-2.729018	11.864403	-1.600629	-2.794602	11.811246
C	-0.520082	-3.288984	12.512274	-0.4969	-3.187636	12.602115	-0.499493	-3.302977	12.512638
C	-4.806363	0.8339	-6.632212	-4.809655	0.818823	-6.621693	-4.727133	1.175849	-6.514913
C	-4.335548	-0.102737	-5.691244	-4.331275	-0.118467	-5.685122	-4.290609	0.244083	-5.552001
C	-2.963532	-0.352618	-5.577895	-2.957971	-0.365201	-5.579618	-2.939923	-0.104965	-5.476436
C	-2.478045	1.196094	-7.273979	-2.485674	1.188577	-7.274802	-2.411396	1.339326	-7.262954
C	-3.837373	1.483071	-7.426494	-3.846674	1.47244	-7.4195	-3.746824	1.723759	-7.372629
C	-1.399871	1.830917	-8.062272	-1.412899	1.82901	-8.065937	-1.314399	1.871178	-8.09584
C	0.920241	1.949595	-8.402063	0.905326	1.956586	-8.414087	1.009048	1.793345	-8.491656
C	0.759613	2.896875	-9.419383	0.737758	2.905984	-9.42837	0.893802	2.712468	-9.537485
C	-1.614624	2.772731	-9.072152	-1.634748	2.772683	-9.072804	-1.480147	2.783075	-9.137138
C	-0.530218	3.33404	-9.779248	-0.554994	3.339561	-9.7824	-0.369066	3.232484	-9.885325
C	4.806363	-0.8339	-6.632212	4.809655	-0.818823	-6.621693	4.727133	-1.175849	-6.514913
C	4.335548	0.102737	-5.691244	4.331275	0.118467	-5.685122	4.290609	-0.244083	-5.552001
C	2.963532	0.352618	-5.577895	2.957971	0.365201	-5.579618	2.939923	0.104965	-5.476436
C	2.478045	-1.196094	-7.273979	2.485674	-1.188577	-7.274802	2.411396	-1.339326	-7.262954
C	3.837373	-1.483071	-7.426494	3.846674	-1.47244	-7.4195	3.746824	-1.723759	-7.372629
C	1.399871	-1.830917	-8.062272	1.412899	-1.82901	-8.065937	1.314399	-1.871178	-8.09584
C	-0.920241	-1.949595	-8.402063	-0.905326	-1.956586	-8.414087	-1.009048	-1.793345	-8.491656
C	-0.759613	-2.896875	-9.419383	-0.737758	-2.905984	-9.42837	-0.893802	-2.712468	-9.537485
C	1.614624	-2.772731	-9.072152	1.634748	-2.772683	-9.072804	1.480147	-2.783075	-9.137138
C	0.530218	-3.33404	-9.779248	0.554994	-3.339561	-9.7824	0.369066	-3.232484	-9.885325
C	0.003785	0.719651	1.365379	0.004684	0.728617	1.36194	0.001465	0.733467	1.360166
C	-0.003785	-0.719651	1.365379	-0.004684	-0.728617	1.36194	-0.001465	-0.733467	1.360166
C	0.003425	-0.72786	-0.950533	0.003768	-0.714	-0.964508	0.000996	-0.713669	-0.971243
C	-0.003425	0.72786	-0.950533	-0.003768	0.714	-0.964508	-0.000996	0.713669	-0.971243
C	0.010743	-1.454926	-2.221617	0.012282	-1.443142	-2.227203	-0.000662	-1.435844	-2.233154
C	0.003579	-0.725554	-3.421047	0.005168	-0.72178	-3.435127	-0.007658	-0.717332	-3.443576
C	-0.003579	0.725554	-3.421047	-0.005168	0.72178	-3.435127	0.007658	0.717332	-3.443576
C	-0.010743	1.454926	-2.221617	-0.012282	1.443142	-2.227203	0.000662	1.435844	-2.233154
C	0.021478	-2.863819	-2.29255	0.024895	-2.855972	-2.29936	0.00213	-2.851081	-2.314333
C	0.025278	-3.475693	-3.549545	0.030759	-3.47172	-3.551833	0.003617	-3.470548	-3.564011
C	0.013366	-2.680105	-4.711322	0.019452	-2.680851	-4.720992	-0.004642	-2.684101	-4.736563
C	-0.021478	2.863819	-2.29255	-0.024895	2.855972	-2.29936	-0.00213	2.851081	-2.314333
C	-0.025278	3.475693	-3.549545	-0.030759	3.47172	-3.551833	-0.003617	3.470548	-3.564011
C	-0.013366	2.680105	-4.711322	-0.019452	2.680851	-4.720992	0.004642	2.684101	-4.736563
C	-6.28781	1.161123	-6.81875	-6.293071	1.142392	-6.799692	-6.184591	1.60882	-6.65432
C	-6.508984	2.668326	-6.552823	-6.517289	2.648485	-6.530281	-6.275741	3.137061	-6.431058
C	-6.695984	0.833246	-8.273873	-6.708441	0.815602	-8.252987	-6.673181	1.267791	-8.081995
C	-7.182913	0.35602	-5.863029	-7.180741	0.333392	-5.840304	-7.097777	0.90536	-5.637707
C	6.28781	-1.161123	-6.81875	6.293071	-1.142392	-6.799692	6.184591	-1.60882	-6.65432
C	6.508984	-2.668326	-6.552823	6.517289	-2.648485	-6.530281	6.275741	-3.137061	-6.431058
C	6.695984	-0.833246	-8.273873	6.708441	-0.815602	-8.252987	6.673181	-1.267791	-8.081995
C	7.182913	-0.35602	-5.863029	7.180741	-0.333392	-5.840304	7.097777	-0.90536	-5.637707
C	-0.789426	4.364783	-10.877886	-0.821787	4.372045	-10.877724	-0.57431	4.235688	-11.017799
C	-1.673935	3.722844	-11.972051	-1.707066	3.729383	-11.970799	-1.524489	3.614551	-12.069045
C	-1.530734	5.576969	-10.267655	-1.565945	5.579909	-10.262501	-1.217378	5.518453	-10.439831
C	0.514042	4.859345	-11.525248	0.477676	4.873389	-11.527949	0.747782	4.611231	-11.70562

C	0.789426	-4.364783	-10.877886	0.821787	-4.372045	-10.877724	0.57431	-4.235688	-11.017799
C	1.673935	-3.722844	-11.972051	1.707066	-3.729383	-11.970799	1.524489	-3.614551	-12.069045
C	1.530734	-5.576969	-10.267655	1.565945	-5.579909	-10.262501	1.217378	-5.518453	-10.439831
C	-0.514042	-4.859345	-11.525248	-0.477676	-4.873389	-11.527949	-0.747782	-4.611231	-11.70562
H	0.059828	3.450992	4.117196	0.087164	3.427342	4.127542	0.018895	3.435874	4.117828
H	0.075425	4.544167	6.397328	0.127447	4.546446	6.391042	0.019589	4.541174	6.389912
H	0.027514	3.111255	8.440126	0.076291	3.134238	8.451833	-0.009091	3.120094	8.444959
H	-0.027514	-3.111255	8.440126	-0.076291	-3.134238	8.451833	0.009091	-3.120094	8.444959
H	-0.075425	-4.544167	6.397328	-0.127447	-4.546446	6.391042	-0.019589	-4.541174	6.389912
H	-0.059828	-3.450992	4.117196	-0.087164	-3.427342	4.127542	-0.018895	-3.435874	4.117828
H	5.000866	-0.614816	7.7255	4.96354	-0.361341	7.528477	4.997104	-0.556865	7.705534
H	2.550823	-1.065324	7.578164	2.524353	-0.889369	7.433547	2.551349	-1.043137	7.582086
H	4.172426	2.235868	10.864644	4.145477	2.315035	10.821258	4.154625	2.302374	10.833251
H	-1.905204	1.564549	10.841654	-1.912249	1.428081	10.949868	-1.912325	1.537147	10.864369
H	-1.650134	3.23407	12.679294	-1.662777	3.051183	12.83153	-1.668516	3.216043	12.696441
H	2.624724	3.082343	12.070209	2.597278	3.071106	12.106227	2.603589	3.125317	12.055812
H	-5.000866	0.614816	7.7255	-4.96354	0.361341	7.528477	-4.997104	0.556865	7.705534
H	-2.550823	1.065324	7.578164	-2.524353	0.889369	7.433547	-2.551349	1.043137	7.582086
H	-4.172426	-2.235868	10.864644	-4.145477	-2.315035	10.821258	-4.154625	-2.302374	10.833251
H	1.905204	-1.564549	10.841654	1.912249	-1.428081	10.949868	1.912325	-1.537147	10.864369
H	1.650134	-3.23407	12.679294	1.662777	-3.051183	12.83153	1.668516	-3.216043	12.696441
H	-2.624724	-3.082343	12.070209	-2.597278	-3.071106	12.106227	-2.603589	-3.125317	12.055812
H	-5.016027	-0.643215	-5.044044	-5.00693	-0.661667	-5.035079	-4.982612	-0.214813	-4.856767
H	-2.583801	-1.074773	-4.863528	-2.571383	-1.086901	-4.868369	-2.587199	-0.821391	-4.743389
H	-4.147734	2.214879	-8.165709	-4.162751	2.205581	-8.155016	-4.031312	2.454735	-8.122177
H	1.905326	1.60306	-8.109546	1.892503	1.612235	-8.125678	1.971644	1.381923	-8.209808
H	1.643832	3.279085	-9.915582	1.618774	3.292639	-9.926894	1.79085	3.008057	-10.06745
H	-2.629312	3.07348	-9.313198	-2.651441	3.07038	-9.309406	-2.474319	3.147447	-9.373387
H	5.016027	0.643215	-5.044044	5.00693	0.661667	-5.035079	4.982612	0.214813	-4.856767
H	2.583801	1.074773	-4.863528	2.571383	1.086901	-4.868369	2.587199	0.821391	-4.743389
H	4.147734	-2.214879	-8.165709	4.162751	-2.205581	-8.155016	4.031312	-2.454735	-8.122177
H	-1.905326	-1.60306	-8.109546	-1.892503	-1.612235	-8.125678	-1.971644	-1.381923	-8.209808
H	-1.643832	-3.279085	-9.915582	-1.618774	-3.292639	-9.926894	-1.79085	-3.008057	-10.06745
H	2.629312	-3.07348	-9.313198	2.651441	-3.07038	-9.309406	2.474319	-3.147447	-9.373387
H	0.026457	-3.44404	-1.376252	0.029846	-3.431808	-1.380261	0.005661	-3.426666	-1.394888
H	0.034775	-4.554615	-3.647294	0.041572	-4.551315	-3.6456	0.009038	-4.549841	-3.655451
H	0.007244	-3.124696	-5.700434	0.015499	-3.13125	-5.70772	-0.01168	-3.137858	-5.721452
H	-0.026457	3.44404	-1.376252	-0.029846	3.431808	-1.380261	-0.005661	3.426666	-1.394888
H	-0.034775	4.554615	-3.647294	-0.041572	4.551315	-3.6456	-0.009038	4.549841	-3.655451
H	-0.007244	3.124696	-5.700434	-0.015499	3.13125	-5.70772	0.01168	3.137858	-5.721452
H	5.831165	1.070894	9.410904	5.787194	1.26728	9.266728	5.817803	1.151682	9.372703
H	-5.831165	-1.070894	9.410904	-5.787194	-1.26728	9.266728	-5.817803	-1.151682	9.372703
H	0.667445	4.014811	13.304474	0.64107	3.891517	13.414158	0.641967	4.032892	13.30202
H	-0.667445	-4.014811	13.304474	-0.64107	-3.891517	13.414158	-0.641967	-4.032892	13.30202
H	-6.234762	2.929583	-5.522551	-6.237894	2.908953	-5.501189	-5.937481	3.40838	-5.422895
H	-5.921014	3.293895	-7.236655	-5.934963	3.276772	-7.216468	-5.675345	3.695054	-7.160819
H	-7.569343	2.911069	-6.70154	-7.579191	2.888459	-6.672573	-7.320587	3.45388	-6.54294
H	-6.556873	-0.234058	-8.48952	-6.567366	-0.250978	-8.471023	-6.625679	0.187022	-8.266431
H	-7.755907	1.080741	-8.418142	-7.769857	1.060234	-8.391253	-7.715918	1.592405	-8.191352

H	-6.112384	1.412309	-9.001078	-6.130335	1.397425	-8.982401	-6.07981	1.777791	-8.851509
H	-8.230513	0.63074	-6.03923	-8.230106	0.605378	-6.010276	-8.127439	1.253401	-5.785644
H	-7.086597	-0.725136	-6.030497	-7.08219	-0.747248	-6.009831	-7.090544	-0.184745	-5.770176
H	-6.951516	0.57151	-4.811195	-6.944006	0.547984	-4.789476	-6.811264	1.138059	-4.603408
H	6.234762	-2.929583	-5.522551	6.237894	-2.908953	-5.501189	5.937481	-3.40838	-5.422895
H	5.921014	-3.293895	-7.236655	5.934963	-3.276772	-7.216468	5.675345	-3.695054	-7.160819
H	7.569343	-2.911069	-6.70154	7.579191	-2.888459	-6.672573	7.320587	-3.45388	-6.54294
H	6.556873	0.234058	-8.48952	6.567366	0.250978	-8.471023	6.625679	-0.187022	-8.266431
H	7.755907	-1.080741	-8.418142	7.769857	-1.060234	-8.391253	7.715918	-1.592405	-8.191352
H	6.112384	-1.412309	-9.001078	6.130335	-1.397425	-8.982401	6.07981	-1.777791	-8.851509
H	8.230513	-0.63074	-6.03923	8.230106	-0.605378	-6.010276	8.127439	-1.253401	-5.785644
H	7.086597	0.725136	-6.030497	7.08219	0.747248	-6.009831	7.090544	0.184745	-5.770176
H	6.951516	-0.57151	-4.811195	6.944006	-0.547984	-4.789476	6.811264	-1.138059	-4.603408
H	-1.169282	2.862368	-12.430072	-1.200213	2.87224	-12.432662	-1.092684	2.702301	-12.49998
H	-2.638223	3.385288	-11.570727	-2.668515	3.386546	-11.567126	-2.503872	3.366672	-11.640288
H	-1.87604	4.46405	-12.756407	-1.914978	4.471702	-12.752619	-1.685185	4.337802	-12.878779
H	-0.923078	6.058084	-9.490337	-0.957733	6.061567	-9.485939	-0.56242	5.985517	-9.693398
H	-1.731533	6.313958	-11.056337	-1.772214	6.318013	-11.048762	-1.381237	6.235667	-11.254306
H	-2.492369	5.286634	-9.825181	-2.524968	5.284676	-9.817593	-2.188535	5.314682	-9.971069
H	0.270124	5.594195	-12.302728	0.228486	5.609309	-12.302769	0.539875	5.334553	-12.503607
H	1.169999	5.349578	-10.793389	1.134033	5.364187	-10.79682	1.452504	5.078673	-11.004999
H	1.068119	4.038833	-12.000661	1.033455	4.056239	-12.007164	1.231	3.73779	-12.163379
H	1.169282	-2.862368	-12.430072	1.200213	-2.87224	-12.432662	1.092684	-2.702301	-12.49998
H	2.638223	-3.385288	-11.570727	2.668515	-3.386546	-11.567126	2.503872	-3.366672	-11.640288
H	1.87604	-4.46405	-12.756407	1.914978	-4.471702	-12.752619	1.685185	-4.337802	-12.878779
H	0.923078	-6.058084	-9.490337	0.957733	-6.061567	-9.485939	0.56242	-5.985517	-9.693398
H	1.731533	-6.313958	-11.056337	1.772214	-6.318013	-11.048762	1.381237	-6.235667	-11.254306
H	2.492369	-5.286634	-9.825181	2.524968	-5.284676	-9.817593	2.188535	-5.314682	-9.971069
H	-0.270124	-5.594195	-12.302728	-0.228486	-5.609309	-12.302769	-0.539875	-5.334553	-12.503607
H	-1.169999	-5.349578	-10.793389	-1.134033	-5.364187	-10.79682	-1.452504	-5.078673	-11.004999
H	-1.068119	-4.038833	-12.000661	-1.033455	-4.056239	-12.007164	-1.231	-3.73779	-12.163379

RuOs5		S0			S1			T1	
Atom	X	Y	Z	X	Y	Z	X	Y	Z
Os	0	0	6.88838	0	0	6.8929	0	0	6.902633
Ru	0	0	-8.327407	0	0	-8.33695	0	0	-8.341965
N	-0.001057	1.417181	-1.89113	-0.006347	1.41748	-1.883825	-0.022235	1.42318	-1.886543
N	0.001057	-1.417181	-1.89113	0.006347	-1.41748	-1.883825	0.022235	-1.42318	-1.886543
N	0.018212	1.331088	-6.731025	0.005193	1.335398	-6.743143	-0.02511	1.335912	-6.748782
N	-0.018212	-1.331088	-6.731025	-0.005193	-1.335398	-6.743143	0.02511	-1.335912	-6.748782
N	-2.046651	0.309982	-8.427448	-2.048764	0.287952	-8.43085	-2.054772	0.238237	-8.434729
N	-0.111907	1.428636	-9.818228	-0.131414	1.430288	-9.824466	-0.166661	1.429116	-9.827011
N	2.046651	-0.309982	-8.427448	2.048764	-0.287952	-8.43085	2.054772	-0.238237	-8.434729
N	0.111907	-1.428636	-9.818228	0.131414	-1.430288	-9.824466	0.166661	-1.429116	-9.827011
N	2.046766	0.264252	6.996812	2.037932	0.334378	6.948996	2.040949	0.35665	6.96183
N	0.112469	1.423069	8.382659	0.098372	1.391202	8.431835	0.087306	1.392952	8.435407
N	-2.046766	-0.264252	6.996812	-2.037932	-0.334378	6.948996	-2.040949	-0.35665	6.96183
N	-0.112469	-1.423069	8.382659	-0.098372	-1.391202	8.431835	-0.087306	-1.392952	8.435407
N	0	1.417204	0.454551	0	1.426415	0.458927	0.000102	1.427621	0.454196
N	0	-1.417204	0.454551	0	-1.426415	0.458927	-0.000102	-1.427621	0.454196
N	0.019796	-1.314026	5.300524	0.016453	-1.334101	5.32485	0.002639	-1.328707	5.314599
N	-0.019796	1.314026	5.300524	-0.016453	1.334101	5.32485	-0.002639	1.328707	5.314599
C	0.000818	-0.727619	-3.034128	0.004619	-0.713694	-3.046059	0.015554	-0.712525	-3.049832
C	-0.000818	0.727619	-3.034128	-0.004619	0.713694	-3.046059	-0.015554	0.712525	-3.049832
C	0.001024	1.454645	-4.305251	-0.0092	1.442528	-4.308613	-0.036796	1.438862	-4.311664
C	0.004061	0.72561	-5.504726	-0.002178	0.721678	-5.516872	-0.017375	0.720288	-5.522684
C	-0.004061	-0.72561	-5.504726	0.002178	-0.721678	-5.516872	0.017375	-0.720288	-5.522684
C	-0.001024	-1.454645	-4.305251	0.0092	-1.442528	-4.308613	0.036796	-1.438862	-4.311664
C	0.005129	2.863678	-4.375875	-0.016399	2.855604	-4.380608	-0.073746	2.852721	-4.384696
C	0.012011	3.476107	-5.632336	-0.016238	3.472037	-5.632452	-0.089494	3.469861	-5.635575
C	0.018755	2.680745	-6.794391	-0.005048	2.681572	-6.802051	-0.063947	2.680921	-6.806885
C	-0.018755	-2.680745	-6.794391	0.005048	-2.681572	-6.802051	0.063947	-2.680921	-6.806885
C	-0.012011	-3.476107	-5.632336	0.016238	-3.472037	-5.632452	0.089494	-3.469861	-5.635575
C	-0.005129	-2.863678	-4.375875	0.016399	-2.855604	-4.380608	0.073746	-2.852721	-4.384696
C	-4.762331	0.919246	-8.6768	-4.771337	0.872822	-8.664383	-4.791004	0.756705	-8.665518
C	-4.328513	-0.034371	-7.739778	-4.323703	-0.079476	-7.732361	-4.319778	-0.1878	-7.737146
C	-2.960452	-0.312394	-7.642289	-2.952606	-0.345021	-7.642504	-2.942541	-0.419822	-7.648576
C	-2.45736	1.240399	-9.343937	-2.472691	1.218264	-9.341351	-2.501666	1.161594	-9.341254
C	-3.814852	1.562518	-9.486192	-3.83399	1.527959	-9.476006	-3.870299	1.437953	-9.474654
C	-1.373884	1.851987	-10.139183	-1.398439	1.843779	-10.138228	-1.443229	1.816025	-10.136056
C	0.956881	1.92242	-10.491017	0.929968	1.937012	-10.499452	0.881749	1.962663	-10.501718
C	0.812494	2.86808	-11.512443	0.772876	2.886139	-11.51576	0.701506	2.913362	-11.512686
C	-1.581322	2.796472	-11.154873	-1.618721	2.791419	-11.1485	-1.686582	2.764406	-11.140389
C	-0.477654	3.31229	-11.849511	-0.522744	3.320558	-11.845199	-0.60414	3.32129	-11.836596
C	4.762331	-0.919246	-8.6768	4.771337	-0.872822	-8.664383	4.791004	-0.756705	-8.665518
C	4.328513	0.034371	-7.739778	4.323703	0.079476	-7.732361	4.319778	0.1878	-7.737146
C	2.960452	0.312394	-7.642289	2.952606	0.345021	-7.642504	2.942541	0.419822	-7.648576
C	2.45736	-1.240399	-9.343937	2.472691	-1.218264	-9.341351	2.501666	-1.161594	-9.341254
C	3.814852	-1.562518	-9.486192	3.83399	-1.527959	-9.476006	3.870299	-1.437953	-9.474654
C	1.373884	-1.851987	-10.139183	1.398439	-1.843779	-10.138228	1.443229	-1.816025	-10.136056
C	-0.956881	-1.92242	-10.491017	-0.929968	-1.937012	-10.499452	-0.881749	-1.962663	-10.501718

C	-0.812494	-2.86808	-11.512443	-0.772876	-2.886139	-11.51576	-0.701506	-2.913362	-11.512686
C	1.581322	-2.796472	-11.154873	1.618721	-2.791419	-11.1485	1.686582	-2.764406	-11.140389
C	0.477654	-3.31229	-11.849511	0.522744	-3.320558	-11.845199	0.60414	-3.32129	-11.836596
C	4.776822	0.874723	7.380305	4.74172	1.029978	7.26793	4.734209	1.095339	7.272808
C	4.368911	-0.048662	6.419525	4.339533	0.135458	6.278436	4.344937	0.183254	6.293892
C	2.995106	-0.33532	6.248978	2.972519	-0.192533	6.134946	2.983421	-0.167468	6.154649
C	2.44335	1.186488	7.942667	2.423598	1.23449	7.919664	2.413225	1.272762	7.921836
C	3.794133	1.522338	8.175961	3.766053	1.613433	8.121885	3.750314	1.673113	8.120693
C	1.400087	1.803859	8.697922	1.382837	1.798942	8.717113	1.36533	1.824955	8.716055
C	-0.906155	1.971796	9.074964	-0.919281	1.866986	9.171169	-0.939412	1.8558	9.174308
C	-0.683941	2.925123	10.095136	-0.698059	2.794664	10.215516	-0.732406	2.793982	10.210142
C	1.702664	2.751419	9.699046	1.684534	2.719795	9.741478	1.651611	2.757828	9.733733
C	0.614018	3.321826	10.411433	0.59484	3.225638	10.501735	0.554018	3.249788	10.491358
C	-4.776822	-0.874723	7.380305	-4.74172	-1.029978	7.26793	-4.734209	-1.095339	7.272808
C	-4.368911	0.048662	6.419525	-4.339533	-0.135458	6.278436	-4.344937	-0.183254	6.293892
C	-2.995106	0.33532	6.248978	-2.972519	0.192533	6.134946	-2.983421	0.167468	6.154649
C	-2.44335	-1.186488	7.942667	-2.423598	-1.23449	7.919664	-2.413225	-1.272762	7.921836
C	-3.794133	-1.522338	8.175961	-3.766053	-1.613433	8.121885	-3.750314	-1.673113	8.120693
C	-1.400087	-1.803859	8.697922	-1.382837	-1.798942	8.717113	-1.36533	-1.824955	8.716055
C	0.906155	-1.971796	9.074964	0.919281	-1.866986	9.171169	0.939412	-1.8558	9.174308
C	0.683941	-2.925123	10.095136	0.698059	-2.794664	10.215516	0.732406	-2.793982	10.210142
C	-1.702664	-2.751419	9.699046	-1.684534	-2.719795	9.741478	-1.651611	-2.757828	9.733733
C	-0.614018	-3.321826	10.411433	-0.59484	-3.225638	10.501735	-0.554018	-3.249788	10.491358
C	-0.000253	0.719675	-0.718395	-0.001601	0.729023	-0.719373	-0.005696	0.733412	-0.717685
C	0.000253	-0.719675	-0.718395	0.001601	-0.729023	-0.719373	0.005696	-0.733412	-0.717685
C	-0.000227	-0.728292	1.597724	-0.001351	-0.724769	1.611376	-0.004146	-0.713978	1.613761
C	0.000227	0.728292	1.597724	0.001351	0.724769	1.611376	0.004146	0.713978	1.613761
C	0.002083	-1.457382	2.868239	-0.001445	-1.439112	2.876331	-0.011755	-1.436834	2.875174
C	0.004849	-0.722459	4.063044	0.007811	-0.708353	4.090072	0	-0.715666	4.082976
C	-0.004849	0.722459	4.063044	-0.007811	0.708353	4.090072	0	0.715666	4.082976
C	-0.002083	1.457382	2.868239	0.001445	1.439112	2.876331	0.011755	1.436834	2.875174
C	0.00509	-2.864503	2.945362	-0.011893	-2.847722	2.963379	-0.030558	-2.851049	2.96084
C	0.010144	-3.466289	4.209066	-0.020178	-3.468428	4.217855	-0.044206	-3.463777	4.21438
C	0.01748	-2.668914	5.366755	-0.011036	-2.679392	5.386061	-0.03189	-2.675657	5.384314
C	-0.00509	2.864503	2.945362	0.011893	2.847722	2.963379	0.030558	2.851049	2.96084
C	-0.010144	3.466289	4.209066	0.020178	3.468428	4.217855	0.044206	3.463777	4.21438
C	-0.01748	2.668914	5.366755	0.011036	2.679392	5.386061	0.03189	2.675657	5.384314
C	4.092872	2.495607	9.202407	4.064546	2.561822	9.169843	4.033571	2.634451	9.161154
C	-4.092872	-2.495607	9.202407	-4.064546	-2.561822	9.169843	-4.033571	-2.634451	9.161154
C	3.089929	3.083031	9.934692	3.065074	3.090235	9.950662	3.026086	3.152542	9.938714
C	-3.089929	-3.083031	9.934692	-3.065074	-3.090235	9.950662	-3.026086	-3.152542	9.938714
H	0.003862	3.443456	-3.459284	-0.021261	3.430881	-3.461157	-0.089146	3.426897	-3.464665
H	0.01492	4.555027	-5.729895	-0.022076	4.551638	-5.725926	-0.118619	4.54929	-5.728082
H	0.03346	3.1265	-7.782807	0.004306	3.133322	-7.788039	-0.066214	3.133936	-7.792408
H	-0.03346	-3.1265	-7.782807	-0.004306	-3.133322	-7.788039	0.066214	-3.133936	-7.792408
H	-0.01492	-4.555027	-5.729895	0.022076	-4.551638	-5.725926	0.118619	-4.54929	-5.728082
H	-0.003862	-3.443456	-3.459284	0.021261	-3.430881	-3.461157	0.089146	-3.426897	-3.464665
H	-5.028952	-0.554215	-7.09665	-5.0161	-0.607435	-7.087058	-4.998841	-0.734988	-7.093674
H	-2.582517	-1.045098	-6.938349	-2.562912	-1.075084	-6.942132	-2.534367	-1.14234	-6.95089

H	-4.132453	2.301879	-10.21219	-4.161967	2.266976	-10.197776	-4.216574	2.17105	-10.193905
H	1.93273	1.553633	-10.196212	1.910154	1.575171	-10.210024	1.870316	1.621144	-10.215985
H	1.690925	3.241086	-12.025988	1.645689	3.269553	-12.03131	1.564438	3.318589	-12.028216
H	-2.583373	3.125517	-11.404551	-2.624799	3.112762	-11.39221	-2.699982	3.065372	-11.379809
H	5.028952	0.554215	-7.09665	5.0161	0.607435	-7.087058	4.998841	0.734988	-7.093674
H	2.582517	1.045098	-6.938349	2.562912	1.075084	-6.942132	2.534367	1.14234	-6.95089
H	4.132453	-2.301879	-10.21219	4.161967	-2.266976	-10.197776	4.216574	-2.17105	-10.193905
H	-1.93273	-1.553633	-10.196212	-1.910154	-1.575171	-10.210024	-1.870316	-1.621144	-10.215985
H	-1.690925	-3.241086	-12.025988	-1.645689	-3.269553	-12.03131	-1.564438	-3.318589	-12.028216
H	2.583373	-3.125517	-11.404551	2.624799	-3.112762	-11.39221	2.699982	-3.065372	-11.379809
H	5.089708	-0.561396	5.793393	5.058448	-0.320775	5.609102	5.070269	-0.26984	5.62935
H	2.661316	-1.058333	5.512954	2.639212	-0.889868	5.374767	2.662288	-0.87972	5.402749
H	-1.909954	1.658147	8.810368	-1.918984	1.524522	8.927974	-1.933275	1.493194	8.936659
H	-1.538955	3.337109	10.618309	-1.548565	3.158572	10.778841	-1.588015	3.146642	10.772818
H	-5.089708	0.561396	5.793393	-5.058448	0.320775	5.609102	-5.070269	0.26984	5.62935
H	-2.661316	1.058333	5.512954	-2.639212	0.889868	5.374767	-2.662288	0.87972	5.402749
H	1.909954	-1.658147	8.810368	1.918984	-1.524522	8.927974	1.933275	-1.493194	8.936659
H	1.538955	-3.337109	10.618309	1.548565	-3.158572	10.778841	1.588015	-3.146642	10.772818
H	0.003609	-3.451772	2.033747	-0.01732	-3.429063	2.047029	-0.037824	-3.431262	2.044407
H	0.010978	-4.544567	4.314131	-0.031911	-4.547214	4.310775	-0.063158	-4.542441	4.310608
H	0.031077	-3.110604	6.356726	-0.010834	-3.132686	6.371506	-0.034474	-3.127425	6.369862
H	-0.003609	3.451772	2.033747	0.01732	3.429063	2.047029	0.037824	3.431262	2.044407
H	-0.010978	4.544567	4.314131	0.031911	4.547214	4.310775	0.063158	4.542441	4.310608
H	-0.031077	3.110604	6.356726	0.010834	3.132686	6.371506	0.034474	3.127425	6.369862
H	5.828774	1.101806	7.524679	5.789379	1.288256	7.388693	5.778008	1.370373	7.38981
H	-5.815957	1.157067	-8.775547	-5.82769	1.1009	-8.757156	-5.852695	0.958923	-8.757384
H	-5.828774	-1.101806	7.524679	-5.789379	-1.288256	7.388693	-5.778008	-1.370373	7.38981
H	5.815957	-1.157067	-8.775547	5.82769	-1.1009	-8.757156	5.852695	-0.958923	-8.757384
H	0.799403	4.05593	11.189752	0.777067	3.940464	11.298252	0.7242	3.973286	11.282707
H	-0.621734	4.04395	-12.637138	-0.676658	4.05482	-12.628576	-0.775969	4.056495	-12.615362
H	-0.799403	-4.05593	11.189752	-0.777067	-3.940464	11.298252	-0.7242	-3.973286	11.282707
H	0.621734	-4.04395	-12.637138	0.676658	-4.05482	-12.628576	0.775969	-4.056495	-12.615362
H	5.13303	2.751886	9.383284	5.099914	2.848533	9.327382	5.064252	2.938586	9.316675
H	3.322021	3.811816	10.706179	3.295851	3.800019	10.739403	3.245896	3.871622	10.72211
H	-3.322021	-3.811816	10.706179	-3.295851	-3.800019	10.739403	-3.245896	-3.871622	10.72211
H	-5.13303	-2.751886	9.383284	-5.099914	-2.848533	9.327382	-5.064252	-2.938586	9.316675

RuOs6		S0			S1			T1	
Atom	X	Y	Z	X	Y	Z	X	Y	Z
Os	0	0	4.987801	0	0	4.986495	0	0	5.019043
Ru	0	0	-10.228991	0	0	-10.244284	0	0	-10.220687
N	-0.588818	-1.289183	-3.792316	-0.609793	-1.2799	-3.790659	-0.647707	-1.272734	-3.777253
N	0.588818	1.289183	-3.792316	0.609793	1.2799	-3.790659	0.647707	1.272734	-3.777253
N	-0.582909	-1.197285	-8.632279	-0.590886	-1.19802	-8.650325	-0.647521	-1.172865	-8.632767
N	0.582909	1.197285	-8.632279	0.590886	1.19802	-8.650325	0.647521	1.172865	-8.632767
N	1.709799	-1.166676	-10.331324	1.709398	-1.165227	-10.340743	1.586649	-1.328392	-10.268779
N	-0.52112	-1.338314	-11.716119	-0.518384	-1.343097	-11.727998	-0.586711	-1.263139	-11.749006
N	-1.709799	1.166676	-10.331324	-1.709398	1.165227	-10.340743	-1.586649	1.328392	-10.268779
N	0.52112	1.338314	-11.716119	0.518384	1.343097	-11.727998	0.586711	1.263139	-11.749006
N	-1.967417	0.605199	5.102168	-1.969687	0.592081	5.04942	-1.964673	0.610557	5.118945
N	-0.701882	-1.234591	6.480921	-0.706645	-1.188117	6.53128	-0.715797	-1.231603	6.504934
N	1.967417	-0.605199	5.102168	1.969687	-0.592081	5.04942	1.964673	-0.610557	5.118945
N	0.701882	1.234591	6.480921	0.706645	1.188117	6.53128	0.715797	1.231603	6.504934
N	-0.588905	-1.289156	-1.446569	-0.619336	-1.28529	-1.447977	-0.628339	-1.277253	-1.436396
N	0.588905	1.289156	-1.446569	0.619336	1.28529	-1.447977	0.628339	1.277253	-1.436396
N	0.534352	1.200857	3.399543	0.572295	1.204613	3.417442	0.55	1.200719	3.430856
N	-0.534352	-1.200857	3.399543	-0.572295	-1.204613	3.417442	-0.55	-1.200719	3.430856
C	0.302474	0.661906	-4.935354	0.305859	0.644636	-4.953192	0.327055	0.634561	-4.936492
C	-0.302474	-0.661906	-4.935354	-0.305859	-0.644636	-4.953192	-0.327055	-0.634561	-4.936492
C	-0.609408	-1.320874	-6.206496	-0.619876	-1.302339	-6.215613	-0.667746	-1.271142	-6.198195
C	-0.309759	-0.656268	-7.406183	-0.313544	-0.649958	-7.424189	-0.341701	-0.630455	-7.408296
C	0.309759	0.656268	-7.406183	0.313544	0.649958	-7.424189	0.341701	0.630455	-7.408296
C	0.609408	1.320874	-6.206496	0.619876	1.302339	-6.215613	0.667746	1.271142	-6.198195
C	-1.204112	-2.598274	-6.276861	-1.229584	-2.577217	-6.287377	-1.326812	-2.52365	-6.279627
C	-1.471462	-3.14945	-7.533237	-1.500275	-3.131275	-7.53906	-1.619504	-3.069244	-7.529513
C	-1.149655	-2.422327	-8.695376	-1.168331	-2.414141	-8.7089	-1.261907	-2.368949	-8.702163
C	1.149655	2.422327	-8.695376	1.168331	2.414141	-8.7089	1.261907	2.368949	-8.702163
C	1.471462	3.14945	-7.533237	1.500275	3.131275	-7.53906	1.619504	3.069244	-7.529513
C	1.204112	2.598274	-6.276861	1.229584	2.577217	-6.287377	1.326812	2.52365	-6.279627
C	3.891457	-2.894748	-10.579575	3.891366	-2.895127	-10.575302	3.574053	-3.26874	-10.410809
C	3.916976	-1.843443	-9.64702	3.914795	-1.839062	-9.64789	3.660106	-2.232401	-9.466055
C	2.805114	-0.999298	-9.549819	2.802886	-0.994237	-9.557303	2.640382	-1.276653	-9.416607
C	1.674014	-2.18609	-11.244533	1.675171	-2.1898	-11.248175	1.48484	-2.336409	-11.190969
C	2.756729	-3.066296	-11.385686	2.758215	-3.070894	-11.382663	2.473027	-3.323198	-11.279581
C	0.431085	-2.268285	-12.037505	0.433267	-2.27603	-12.042278	0.277186	-2.287105	-12.035456
C	-1.701822	-1.323244	-12.382855	-1.698009	-1.331053	-12.396802	-1.717061	-1.089479	-12.477775
C	-1.985756	-2.240959	-13.400415	-1.9815	-2.254723	-13.409064	-2.046121	-1.958004	-13.523066
C	0.204984	-3.211642	-13.05022	0.20763	-3.225631	-13.049499	0	-3.182821	-13.074392
C	-1.016058	-3.20007	-13.739964	-1.012323	-3.217244	-13.741077	-1.175843	-3.019463	-13.82307
C	-3.891457	2.894748	-10.579575	-3.891366	2.895127	-10.575302	-3.574053	3.26874	-10.410809
C	-3.916976	1.843443	-9.64702	-3.914795	1.839062	-9.64789	-3.660106	2.232401	-9.466055
C	-2.805114	0.999298	-9.549819	-2.802886	0.994237	-9.557303	-2.640382	1.276653	-9.416607
C	-1.674014	2.18609	-11.244533	-1.675171	2.1898	-11.248175	-1.48484	2.336409	-11.190969
C	-2.756729	3.066296	-11.385686	-2.758215	3.070894	-11.382663	-2.473027	3.323198	-11.279581
C	-0.431085	2.268285	-12.037505	-0.433267	2.27603	-12.042278	-0.277186	2.287105	-12.035456
C	1.701822	1.323244	-12.382855	1.698009	1.331053	-12.396802	1.717061	1.089479	-12.477775

C	1.985756	2.240959	-13.400415	1.9815	2.254723	-13.409064	2.046121	1.958004	-13.523066
C	-0.204984	3.211642	-13.05022	-0.20763	3.225631	-13.049499	0	3.182821	-13.074392
C	1.016058	3.20007	-13.739964	1.012323	3.217244	-13.741077	1.175843	3.019463	-13.82307
C	-4.738014	1.169756	5.426866	-4.738183	1.142368	5.310038	-4.745549	1.15423	5.392502
C	-3.938819	1.847662	4.497953	-3.94067	1.764008	4.339786	-3.932308	1.844926	4.485117
C	-2.571314	1.54975	4.353567	-2.571627	1.469519	4.222441	-2.559876	1.557422	4.365744
C	-2.724412	-0.059898	6.044626	-2.722419	-0.022751	6.028664	-2.736093	-0.064926	6.0422
C	-4.099626	0.189178	6.254265	-4.099564	0.224392	6.210443	-4.116581	0.174009	6.227173
C	-2.023726	-1.037077	6.822914	-2.026819	-0.963072	6.854694	-2.04404	-1.04306	6.826825
C	0	-2.160947	7.163995	0	-2.066566	7.263879	-0.019365	-2.155416	7.197516
C	-0.573689	-2.896374	8.217774	-0.576862	-2.740911	8.356703	-0.60558	-2.897351	8.239612
C	-2.671794	-1.742124	7.861915	-2.677326	-1.605691	7.930075	-2.705153	-1.756429	7.851966
C	-1.903168	-2.693746	8.608333	-1.906333	-2.513256	8.730771	-1.943255	-2.705652	8.60784
C	4.738014	-1.169756	5.426866	4.738183	-1.142368	5.310038	4.745549	-1.15423	5.392502
C	3.938819	-1.847662	4.497953	3.94067	-1.764008	4.339786	3.932308	-1.844926	4.485117
C	2.571314	-1.54975	4.353567	2.571627	-1.469519	4.222441	2.559876	-1.557422	4.365744
C	2.724412	0.059898	6.044626	2.722419	0.022751	6.028664	2.736093	0.064926	6.0422
C	4.099626	-0.189178	6.254265	4.099564	-0.224392	6.210443	4.116581	-0.174009	6.227173
C	2.023726	1.037077	6.822914	2.026819	0.963072	6.854694	2.04404	1.04306	6.826825
C	0	2.160947	7.163995	0	2.066566	7.263879	0.019365	2.155416	7.197516
C	0.573689	2.896374	8.217774	0.576862	2.740911	8.356703	0.60558	2.897351	8.239612
C	2.671794	1.742124	7.861915	2.677326	1.605691	7.930075	2.705153	1.756429	7.851966
C	1.903168	2.693746	8.608333	1.906333	2.513256	8.730771	1.943255	2.705652	8.60784
C	-0.299017	-0.654769	-2.619556	-0.315112	-0.657802	-2.626131	-0.328269	-0.655997	-2.605355
C	0.299017	0.654769	-2.619556	0.315112	0.657802	-2.626131	0.328269	0.655997	-2.605355
C	0.302913	0.662475	-0.303335	0.315821	0.651967	-0.29514	0.311677	0.641427	-0.272993
C	-0.302913	-0.662475	-0.303335	-0.315821	-0.651967	-0.29514	-0.311677	-0.641427	-0.272993
C	0.60465	1.326149	0.967201	0.627961	1.29482	0.969536	0.621868	1.301041	0.988075
C	0.297788	0.658311	2.162194	0.30391	0.640548	2.18285	0.305309	0.649857	2.194521
C	-0.297788	-0.658311	2.162194	-0.30391	-0.640548	2.18285	-0.305309	-0.649857	2.194521
C	-0.60465	-1.326149	0.967201	-0.627961	-1.29482	0.969536	-0.621868	-1.301041	0.988075
C	1.189237	2.606035	1.044302	1.250894	2.559034	1.057004	1.228312	2.577043	1.067091
C	1.439791	3.153206	2.308142	1.531951	3.111416	2.311408	1.483366	3.12821	2.324538
C	1.104242	2.430297	3.46596	1.18383	2.402811	3.480013	1.134418	2.417986	3.492034
C	-1.189237	-2.606035	1.044302	-1.250894	-2.559034	1.057004	-1.228312	-2.577043	1.067091
C	-1.439791	-3.153206	2.308142	-1.531951	-3.111416	2.311408	-1.483366	-3.12821	2.324538
C	-1.104242	-2.430297	3.46596	-1.18383	-2.402811	3.480013	-1.134418	-2.417986	3.492034
C	-4.75224	-0.547698	7.31202	-4.756032	-0.449059	7.305871	-4.783566	-0.573502	7.268912
C	4.75224	0.547698	7.31202	4.756032	0.449059	7.305871	4.783566	0.573502	7.268912
C	-4.074346	-1.467156	8.074397	-4.079214	-1.320741	8.123731	-4.11332	-1.491466	8.039951
C	4.074346	1.467156	8.074397	4.079214	1.320741	8.123731	4.11332	1.491466	8.039951
C	-2.448068	-3.449823	9.76573	-2.453357	-3.197034	9.929743	-2.502612	-3.469484	9.753306
C	-3.13573	-2.79246	10.809263	-3.142888	-2.474903	10.928133	-3.213267	-2.820481	10.786604
C	-2.220931	-4.839719	9.860605	-2.225142	-4.578331	10.108386	-2.266803	-4.857941	9.848564
C	-3.59718	-3.515228	11.920865	-3.605549	-3.128054	12.081084	-3.688457	-3.549754	11.888181
C	-2.690476	-5.563833	10.96807	-2.699151	-5.232707	11.256194	-2.749588	-5.588641	10.946025
C	-3.381128	-4.903591	12.001226	-3.390871	-4.509207	12.245351	-3.463046	-4.936627	11.968864
C	-6.188116	1.484464	5.508106	-6.190569	1.441819	5.355552	-6.200947	1.450951	5.442448
C	-7.162141	0.462312	5.491361	-7.14911	0.406043	5.411287	-7.159726	0.415336	5.395555

C	-6.606523	2.832298	5.538504	-6.625046	2.782845	5.276861	-6.63942	2.792313	5.472583
C	-8.528651	0.783848	5.515603	-8.519202	0.709907	5.399615	-8.530955	0.716791	5.390537
C	-7.972929	3.15329	5.571699	-7.995376	3.085606	5.278953	-8.010866	3.093345	5.476216
C	-8.938293	2.129463	5.561251	-8.946012	2.049723	5.340669	-8.960985	2.056044	5.436235
C	2.448068	3.449823	9.76573	2.453357	3.197034	9.929743	2.502612	3.469484	9.753306
C	3.13573	2.79246	10.809263	3.142888	2.474903	10.928133	3.213267	2.820481	10.786604
C	2.220931	4.839719	9.860605	2.225142	4.578331	10.108386	2.266803	4.857941	9.848564
C	3.59718	3.515228	11.920865	3.605549	3.128054	12.081084	3.688457	3.549754	11.888181
C	2.690476	5.563833	10.96807	2.699151	5.232707	11.256194	2.749588	5.588641	10.946025
C	3.381128	4.903591	12.001226	3.390871	4.509207	12.245351	3.463046	4.936627	11.968864
C	6.188116	-1.484464	5.508106	6.190569	-1.441819	5.355552	6.200947	-1.450951	5.442448
C	7.162141	-0.462312	5.491361	7.14911	-0.406043	5.411287	7.159726	-0.415336	5.395555
C	6.606523	-2.832298	5.538504	6.625046	-2.782845	5.276861	6.63942	-2.792313	5.472583
C	8.528651	-0.783848	5.515603	8.519202	-0.709907	5.399615	8.530955	-0.716791	5.390537
C	7.972929	-3.15329	5.571699	7.995376	-3.085606	5.278953	8.010866	-3.093345	5.476216
C	8.938293	-2.129463	5.561251	8.946012	-2.049723	5.340669	8.960985	-2.056044	5.436235
H	-1.443067	-3.126353	-5.360164	-1.474735	-3.097145	-5.367627	-1.589376	-3.035561	-5.359938
H	-1.926255	-4.127877	-7.630558	-1.965401	-4.105604	-7.632258	-2.120176	-4.025323	-7.62144
H	-1.353298	-2.819603	-9.683562	-1.374549	-2.816586	-9.694709	-1.483533	-2.766778	-9.686318
H	1.353298	2.819603	-9.683562	1.374549	2.816586	-9.694709	1.483533	2.766778	-9.686318
H	1.926255	4.127877	-7.630558	1.965401	4.105604	-7.632258	2.120176	4.025323	-7.62144
H	1.443067	3.126353	-5.360164	1.474735	3.097145	-5.367627	1.589376	3.035561	-5.359938
H	4.775183	-1.676108	-9.006705	4.771568	-1.668872	-9.006328	4.494289	-2.161303	-8.778831
H	2.783518	-0.172962	-8.848416	2.778269	-0.164711	-8.859681	2.666788	-0.458542	-8.706166
H	2.720597	-3.873005	-12.108565	2.723353	-3.881521	-12.101282	2.39159	-4.122191	-12.006569
H	-2.420857	-0.568501	-12.085703	-2.416212	-0.573237	-12.10505	-2.359799	-0.258612	-12.210625
H	-2.94185	-2.199061	-13.909035	-2.936767	-2.215081	-13.919503	-2.959205	-1.799159	-14.083594
H	0.964267	-3.943141	-13.301181	0.966568	-3.959546	-13.294574	0.684127	-3.990884	-13.303905
H	-4.775183	1.676108	-9.006705	-4.771568	1.668872	-9.006328	-4.494289	2.161303	-8.778831
H	-2.783518	0.172962	-8.848416	-2.778269	0.164711	-8.859681	-2.666788	0.458542	-8.706166
H	-2.720597	3.873005	-12.108565	-2.723353	3.881521	-12.101282	-2.39159	4.122191	-12.006569
H	2.420857	0.568501	-12.085703	2.416212	0.573237	-12.10505	2.359799	0.258612	-12.210625
H	2.94185	2.199061	-13.909035	2.936767	2.215081	-13.919503	2.959205	1.799159	-14.083594
H	-0.964267	3.943141	-13.301181	-0.966568	3.959546	-13.294574	-0.684127	3.990884	-13.303905
H	-4.377391	2.596619	3.846802	-4.383091	2.458471	3.634129	-4.363324	2.594818	3.829823
H	-1.960337	2.069434	3.624015	-1.961036	1.939871	3.460368	-1.936792	2.085235	3.652145
H	1.034086	-2.311723	6.87449	1.035132	-2.233376	6.986944	1.020198	-2.29808	6.92381
H	0.048687	-3.605323	8.753873	0.043717	-3.417596	8.933882	0.01252	-3.603841	8.784004
H	4.377391	-2.596619	3.846802	4.383091	-2.458471	3.634129	4.363324	-2.594818	3.829823
H	1.960337	-2.069434	3.624015	1.961036	-1.939871	3.460368	1.936792	-2.085235	3.652145
H	-1.034086	2.311723	6.87449	-1.035132	2.233376	6.986944	-1.020198	2.29808	6.92381
H	-0.048687	3.605323	8.753873	-0.043717	3.417596	8.933882	-0.01252	3.603841	8.784004
H	1.433556	3.140136	0.132721	1.506331	3.081316	0.14069	1.482021	3.099838	0.151441
H	1.890059	4.133042	2.412915	2.013165	4.077064	2.404517	1.947544	4.102541	2.424116
H	1.280519	2.835065	4.456097	1.385913	2.807128	4.466257	1.315194	2.829333	4.479009
H	-1.433556	-3.140136	0.132721	-1.506331	-3.081316	0.14069	-1.482021	-3.099838	0.151441
H	-1.890059	-4.133042	2.412915	-2.013165	-4.077064	2.404517	-1.947544	-4.102541	2.424116
H	-1.280519	-2.835065	4.456097	-1.385913	-2.807128	4.466257	-1.315194	-2.829333	4.479009
H	4.737184	-3.566757	-10.677697	4.737336	-3.567626	-10.668173	4.348968	-4.025001	-10.469134

H	-4.737184	3.566757	-10.677697	-4.737336	3.567626	-10.668173	-4.348968	4.025001	-10.469134
H	-1.20585	-3.923883	-14.525157	-1.201818	-3.945907	-14.521882	-1.404817	-3.705946	-14.630618
H	1.20585	3.923883	-14.525157	1.201818	3.945907	-14.521882	1.404817	3.705946	-14.630618
H	-5.800267	-0.354417	7.514238	-5.804846	-0.246624	7.49191	-5.836752	-0.389143	7.452167
H	-4.603365	-2.015221	8.846651	-4.60974	-1.823947	8.924409	-4.652595	-2.046464	8.800165
H	4.603365	2.015221	8.846651	4.60974	1.823947	8.924409	4.652595	2.046464	8.800165
H	5.800267	0.354417	7.514238	5.804846	0.246624	7.49191	5.836752	0.389143	7.452167
H	-3.279642	-1.71497	10.769593	-3.285706	-1.401745	10.823168	-3.364809	-1.744003	10.747114
H	-1.69501	-5.354459	9.059147	-1.698068	-5.141509	9.341132	-1.723278	-5.366477	9.054924
H	-4.116535	-2.997384	12.722173	-4.125181	-2.562116	12.848733	-4.225659	-3.038036	12.681647
H	-2.519867	-6.635147	11.024585	-2.530435	-6.29863	11.378463	-2.571594	-6.65877	11.002714
H	-3.742181	-5.462659	12.86	-3.754143	-5.014543	13.135775	-3.834465	-5.500779	12.819865
H	-6.855039	-0.579085	5.424669	-6.828253	-0.633087	5.424809	-6.835744	-0.62095	5.328748
H	-5.862363	3.625896	5.556196	-5.892298	3.586074	5.238208	-5.907368	3.596298	5.512842
H	-9.269174	-0.01057	5.492864	-9.249097	-0.093692	5.430926	-9.259103	-0.088063	5.345029
H	-8.282548	4.193939	5.606556	-8.319715	4.121072	5.232885	-8.33626	4.129191	5.511048
H	-9.995984	2.376806	5.584032	-10.006948	2.28332	5.337732	-10.022384	2.288148	5.436363
H	3.279642	1.71497	10.769593	3.285706	1.401745	10.823168	3.364809	1.744003	10.747114
H	1.69501	5.354459	9.059147	1.698068	5.141509	9.341132	1.723278	5.366477	9.054924
H	4.116535	2.997384	12.722173	4.125181	2.562116	12.848733	4.225659	3.038036	12.681647
H	2.519867	6.635147	11.024585	2.530435	6.29863	11.378463	2.571594	6.65877	11.002714
H	3.742181	5.462659	12.86	3.754143	5.014543	13.135775	3.834465	5.500779	12.819865
H	6.855039	0.579085	5.424669	6.828253	0.633087	5.424809	6.835744	0.62095	5.328748
H	5.862363	-3.625896	5.556196	5.892298	-3.586074	5.238208	5.907368	-3.596298	5.512842
H	9.269174	0.01057	5.492864	9.249097	0.093692	5.430926	9.259103	0.088063	5.345029
H	8.282548	-4.193939	5.606556	8.319715	-4.121072	5.232885	8.33626	-4.129191	5.511048
H	9.995984	-2.376806	5.584032	10.006948	-2.28332	5.337732	10.022384	-2.288148	5.436363

RuOs7		S0			S1			T1	
Atom	X	Y	Z	X	Y	Z	X	Y	Z
Os	0	0	5.621328	0	0	5.646895	0	0	5.657973
Ru	0	0	-9.595162	0	0	-9.589351	0	0	-9.591383
N	-0.638503	-1.265324	-3.158868	-0.73214	-1.214267	-3.135679	-0.746248	-1.212344	-3.135985
N	0.638503	1.265324	-3.158868	0.73214	1.214267	-3.135679	0.746248	1.212344	-3.135985
N	-0.625616	-1.175284	-7.998901	-0.725207	-1.121639	-7.995319	-0.731223	-1.118626	-7.997972
N	0.625616	1.175284	-7.998901	0.725207	1.121639	-7.995319	0.731223	1.118626	-7.997972
N	1.670658	-1.22178	-9.699105	1.560217	-1.358747	-9.682681	1.555549	-1.363653	-9.683716
N	-0.565769	-1.318927	-11.083234	-0.671986	-1.272699	-11.074026	-0.676098	-1.271656	-11.075161
N	-1.670658	1.22178	-9.699105	-1.560217	1.358747	-9.682681	-1.555549	1.363653	-9.683716
N	0.565769	1.318927	-11.083234	0.671986	1.272699	-11.074026	0.676098	1.271656	-11.075161
N	-1.963806	0.616749	5.73618	-1.968688	0.604976	5.703369	-1.97506	0.602642	5.717444
N	-0.734307	-1.211704	7.116051	-0.744528	-1.170316	7.172659	-0.748088	-1.17175	7.180252
N	1.963806	-0.616749	5.73618	1.968688	-0.604976	5.703369	1.97506	-0.602642	5.717444
N	0.734307	1.211704	7.116051	0.744528	1.170316	7.172659	0.748088	1.17175	7.180252
N	-0.639224	-1.264908	-0.813158	-0.716824	-1.233662	-0.793138	-0.731538	-1.225919	-0.795153
N	0.639224	1.264908	-0.813158	0.716824	1.233662	-0.793138	0.731538	1.225919	-0.795153
N	0.576877	1.179241	4.033886	0.629143	1.17759	4.07096	0.64465	1.161497	4.064765
N	-0.576877	-1.179241	4.033886	-0.629143	-1.17759	4.07096	-0.64465	-1.161497	4.064765
C	0.327713	0.649718	-4.301929	0.372055	0.608728	-4.298296	0.376629	0.605061	-4.299143
C	-0.327713	-0.649718	-4.301929	-0.372055	-0.608728	-4.298296	-0.376629	-0.605061	-4.299143
C	-0.658763	-1.296918	-5.573074	-0.761264	-1.224892	-5.560535	-0.768204	-1.217107	-5.56089
C	-0.33366	-0.644324	-6.772644	-0.385497	-0.609987	-6.769114	-0.388543	-0.606805	-6.77197
C	0.33366	0.644324	-6.772644	0.385497	0.609987	-6.769114	0.388543	0.606805	-6.77197
C	0.658763	1.296918	-5.573074	0.761264	1.224892	-5.560535	0.768204	1.217107	-5.56089
C	-1.301403	-2.550917	-5.643647	-1.51206	-2.422202	-5.632112	-1.527219	-2.410538	-5.63328
C	-1.588678	-3.091792	-6.900081	-1.847145	-2.93978	-6.883755	-1.865049	-2.927436	-6.884028
C	-1.238354	-2.377857	-8.062208	-1.437561	-2.263911	-8.053697	-1.450585	-2.255888	-8.055531
C	1.238354	2.377857	-8.062208	1.437561	2.263911	-8.053697	1.450585	2.255888	-8.055531
C	1.588678	3.091792	-6.900081	1.847145	2.93978	-6.883755	1.865049	2.927436	-6.884028
C	1.301403	2.550917	-5.643647	1.51206	2.422202	-5.632112	1.527219	2.410538	-5.63328
C	3.798972	-3.013488	-9.959709	3.518602	-3.338968	-9.909669	3.507805	-3.350243	-9.908758
C	3.856783	-1.969334	-9.020581	3.668966	-2.289719	-8.986471	3.661314	-2.30061	-8.986473
C	2.771047	-1.092395	-8.917365	2.666684	-1.31677	-8.899676	2.662088	-1.324446	-8.900609
C	1.603187	-2.234686	-10.617752	1.402423	-2.376235	-10.584957	1.394574	-2.381608	-10.584902
C	2.658868	-3.145994	-10.765517	2.372243	-3.380912	-10.716236	2.361326	-3.389397	-10.71527
C	0.357404	-2.276283	-11.409182	0.159644	-2.316431	-11.380111	0.151838	-2.31874	-11.379845
C	-1.746703	-1.266171	-11.747656	-1.837566	-1.118554	-11.749925	-1.841318	-1.114654	-11.75108
C	-2.060154	-2.17184	-12.767323	-2.227613	-2.005606	-12.759606	-2.234679	-2.001939	-12.759255
C	0.101115	-3.209131	-12.424411	-0.177167	-3.237276	-12.382954	-0.188412	-3.240052	-12.38116
C	-1.120311	-3.15851	-13.111756	-1.383732	-3.082877	-13.080684	-1.394597	-3.082671	-13.078835
C	-3.798972	3.013488	-9.959709	-3.518602	3.338968	-9.909669	-3.507805	3.350243	-9.908758
C	-3.856783	1.969334	-9.020581	-3.668966	2.289719	-8.986471	-3.661314	2.30061	-8.986473
C	-2.771047	1.092395	-8.917365	-2.666684	1.31677	-8.899676	-2.662088	1.324446	-8.900609
C	-1.603187	2.234686	-10.617752	-1.402423	2.376235	-10.584957	-1.394574	2.381608	-10.584902
C	-2.658868	3.145994	-10.765517	-2.372243	3.380912	-10.716236	-2.361326	3.389397	-10.71527
C	-0.357404	2.276283	-11.409182	-0.159644	2.316431	-11.380111	-0.151838	2.31874	-11.379845
C	1.746703	1.266171	-11.747656	1.837566	1.118554	-11.749925	1.841318	1.114654	-11.75108

C	2.060154	2.17184	-12.767323	2.227613	2.005606	-12.759606	2.234679	2.001939	-12.759255
C	-0.101115	3.209131	-12.424411	0.177167	3.237276	-12.382954	0.188412	3.240052	-12.38116
C	1.120311	3.15851	-13.111756	1.383732	3.082877	-13.080684	1.394597	3.082671	-13.078835
C	-4.695941	1.313575	6.008448	-4.707581	1.257288	5.872071	-4.717464	1.240667	5.875121
C	-3.867244	1.930381	5.049344	-3.86596	1.854052	4.912261	-3.8728	1.849337	4.924963
C	-2.523838	1.562769	4.93923	-2.515403	1.504753	4.848537	-2.520502	1.50769	4.866611
C	-2.751697	-0.00513	6.674513	-2.766896	-0.002121	6.643058	-2.77508	-0.015318	6.647783
C	-4.10045	0.328003	6.822165	-4.121618	0.309523	6.740292	-4.132028	0.289633	6.739569
C	-2.048338	-1.025998	7.472443	-2.07092	-0.996452	7.482463	-2.077455	-1.007762	7.48557
C	0	-2.131876	7.792225	0	-2.037374	7.901136	0	-2.040264	7.905836
C	-0.537079	-2.896751	8.830943	-0.549833	-2.780768	8.947893	-0.549405	-2.793141	8.944792
C	-2.629217	-1.764942	8.50597	-2.662811	-1.711416	8.522507	-2.66779	-1.732857	8.519072
C	-1.882071	-2.726395	9.216815	-1.910051	-2.631906	9.284166	-1.912146	-2.653963	9.277348
C	4.695941	-1.313575	6.008448	4.707581	-1.257288	5.872071	4.717464	-1.240667	5.875121
C	3.867244	-1.930381	5.049344	3.86596	-1.854052	4.912261	3.8728	-1.849337	4.924963
C	2.523838	-1.562769	4.93923	2.515403	-1.504753	4.848537	2.520502	-1.50769	4.866611
C	2.751697	0.00513	6.674513	2.766896	0.002121	6.643058	2.77508	0.015318	6.647783
C	4.10045	-0.328003	6.822165	4.121618	-0.309523	6.740292	4.132028	-0.289633	6.739569
C	2.048338	1.025998	7.472443	2.07092	0.996452	7.482463	2.077455	1.007762	7.48557
C	0	2.131876	7.792225	0	2.037374	7.901136	0	2.040264	7.905836
C	0.537079	2.896751	8.830943	0.549833	2.780768	8.947893	0.549405	2.793141	8.944792
C	2.629217	1.764942	8.50597	2.662811	1.711416	8.522507	2.66779	1.732857	8.519072
C	1.882071	2.726395	9.216815	1.910051	2.631906	9.284166	1.912146	2.653963	9.277348
C	-0.324535	-0.642449	-1.986184	-0.372036	-0.627573	-1.971182	-0.380451	-0.627188	-1.967008
C	0.324535	0.642449	-1.986184	0.372036	0.627573	-1.971182	0.380451	0.627188	-1.967008
C	0.328893	0.650166	0.330234	0.359443	0.628603	0.359782	0.362723	0.615025	0.364575
C	-0.328893	-0.650166	0.330234	-0.359443	-0.628603	0.359782	-0.362723	-0.615025	0.364575
C	0.655934	1.302167	1.60062	0.70236	1.255512	1.624343	0.720645	1.243645	1.62588
C	0.322565	0.646241	2.79539	0.337281	0.624339	2.837983	0.351343	0.623796	2.83352
C	-0.322565	-0.646241	2.79539	-0.337281	-0.624339	2.837983	-0.351343	-0.623796	2.83352
C	-0.655934	-1.302167	1.60062	-0.70236	-1.255512	1.624343	-0.720645	-1.243645	1.62588
C	1.289616	2.558181	1.678078	1.393479	2.484254	1.710549	1.430519	2.466892	1.711547
C	1.560418	3.094429	2.942821	1.696658	3.025468	2.963886	1.736122	2.997344	2.965536
C	1.195218	2.385564	4.100117	1.303749	2.340588	4.133023	1.334082	2.318633	4.135244
C	-1.289616	-2.558181	1.678078	-1.393479	-2.484254	1.710549	-1.430519	-2.466892	1.711547
C	-1.560418	-3.094429	2.942821	-1.696658	-3.025468	2.963886	-1.736122	-2.997344	2.965536
C	-1.195218	-2.385564	4.100117	-1.303749	-2.340588	4.133023	-1.334082	-2.318633	4.135244
C	-6.172477	1.663546	6.190263	-6.194105	1.582003	5.99609	-6.206235	1.55748	5.992677
C	-7.023747	0.395155	5.949397	-7.007469	0.286975	5.760862	-7.012205	0.260112	5.745253
C	-6.397662	2.163038	7.636371	-6.474174	2.113037	7.421633	-6.496672	2.078534	7.419857
C	-6.631483	2.758405	5.213868	-6.64301	2.640466	4.976203	-6.654402	2.619922	4.976613
C	6.172477	-1.663546	6.190263	6.194105	-1.582003	5.99609	6.206235	-1.55748	5.992677
C	7.023747	-0.395155	5.949397	7.007469	-0.286975	5.760862	7.012205	-0.260112	5.745253
C	6.397662	-2.163038	7.636371	6.474174	-2.113037	7.421633	6.496672	-2.078534	7.419857
C	6.631483	-2.758405	5.213868	6.64301	-2.640466	4.976203	6.654402	-2.619922	4.976613
C	-2.536715	-3.519206	10.347684	-2.578326	-3.404358	10.419212	-2.579526	-3.437329	10.40504
C	-3.017318	-2.533066	11.437853	-3.118734	-2.394078	11.458808	-3.127679	-2.436429	11.449832
C	-3.752337	-4.293011	9.787049	-3.755189	-4.225788	9.842471	-3.75098	-4.260378	9.819358
C	-1.564958	-4.524669	10.986024	-1.602524	-4.362116	11.120985	-1.601047	-4.395164	11.10292

C	2.536715	3.519206	10.347684	2.578326	3.404358	10.419212	2.579526	3.437329	10.40504
C	3.017318	2.533066	11.437853	3.118734	2.394078	11.458808	3.127679	2.436429	11.449832
C	3.752337	4.293011	9.787049	3.755189	4.225788	9.842471	3.75098	4.260378	9.819358
C	1.564958	4.524669	10.986024	1.602524	4.362116	11.120985	1.601047	4.395164	11.10292
H	-1.560762	-3.069283	-4.726937	-1.812271	-2.91201	-4.712103	-1.830698	-2.897027	-4.712553
H	-2.080313	-4.052241	-6.997502	-2.420855	-3.854386	-6.977228	-2.444644	-3.838549	-6.976577
H	-1.456228	-2.767309	-9.050448	-1.690748	-2.639524	-9.039118	-1.705796	-2.631406	-9.040557
H	1.456228	2.767309	-9.050448	1.690748	2.639524	-9.039118	1.705796	2.631406	-9.040557
H	2.080313	4.052241	-6.997502	2.420855	3.854386	-6.977228	2.444644	3.838549	-6.976577
H	1.560762	3.069283	-4.726937	1.812271	2.91201	-4.712103	1.830698	2.897027	-4.712553
H	4.720128	-1.831985	-8.380027	4.540314	-2.221502	-8.345579	4.532812	-2.23458	-8.345537
H	2.774998	-0.269769	-8.211218	2.742371	-0.486967	-8.205929	2.740009	-0.494306	-8.207507
H	2.597733	-3.9467	-11.493366	2.240328	-4.184075	-11.431902	2.226923	-4.192809	-11.430203
H	-2.441845	-0.490698	-11.447083	-2.458291	-0.276011	-11.466669	-2.459003	-0.269465	-11.468962
H	-3.015485	-2.099592	-13.273966	-3.167637	-1.850339	-13.276188	-3.17431	-1.844285	-13.275852
H	0.837429	-3.96251	-12.679099	0.486303	-4.060687	-12.620671	0.472152	-4.066157	-12.617681
H	-4.720128	1.831985	-8.380027	-4.540314	2.221502	-8.345579	-4.532812	2.23458	-8.345537
H	-2.774998	0.269769	-8.211218	-2.742371	0.486967	-8.205929	-2.740009	0.494306	-8.207507
H	-2.597733	3.9467	-11.493366	-2.240328	4.184075	-11.431902	-2.226923	4.192809	-11.430203
H	2.441845	0.490698	-11.447083	2.458291	0.276011	-11.466669	2.459003	0.269465	-11.468962
H	3.015485	2.099592	-13.273966	3.167637	1.850339	-13.276188	3.17431	1.844285	-13.275852
H	-0.837429	3.96251	-12.679099	-0.486303	4.060687	-12.620671	-0.472152	4.066157	-12.617681
H	-4.248626	2.695534	4.383517	-4.243459	2.586052	4.208977	-4.249624	2.58478	4.224921
H	-1.872518	2.033028	4.210981	-1.853299	1.954331	4.117574	-1.857004	1.967291	4.142767
H	-4.6937	-0.183892	7.573628	-4.730188	-0.187558	7.488623	-4.741866	-0.215217	7.48172
H	1.031472	-2.253486	7.481191	1.044053	-2.139626	7.627422	1.046068	-2.133986	7.636724
H	0.104399	-3.615881	9.326496	0.092573	-3.465025	9.488289	0.094977	-3.477015	9.483262
H	-3.669608	-1.590628	8.76234	-3.712262	-1.553023	8.747765	-3.719065	-1.582363	8.741204
H	4.248626	-2.695534	4.383517	4.243459	-2.586052	4.208977	4.249624	-2.58478	4.224921
H	1.872518	-2.033028	4.210981	1.853299	-1.954331	4.117574	1.857004	-1.967291	4.142767
H	4.6937	0.183892	7.573628	4.730188	0.187558	7.488623	4.741866	0.215217	7.48172
H	-1.031472	2.253486	7.481191	-1.044053	2.139626	7.627422	-1.046068	2.133986	7.636724
H	-0.104399	3.615881	9.326496	-0.092573	3.465025	9.488289	-0.094977	3.477015	9.483262
H	3.669608	1.590628	8.76234	3.712262	1.553023	8.747765	3.719065	1.582363	8.741204
H	1.555132	3.082854	0.766965	1.681661	2.987885	0.793493	1.72549	2.966492	0.795025
H	2.04879	4.05586	3.048237	2.22842	3.964267	3.056771	2.280734	3.928698	3.062055
H	1.385436	2.783213	5.090637	1.521508	2.738222	5.118597	1.554254	2.712236	5.121341
H	-1.555132	-3.082854	0.766965	-1.681661	-2.987885	0.793493	-1.72549	-2.966492	0.795025
H	-2.04879	-4.05586	3.048237	-2.22842	-3.964267	3.056771	-2.280734	-3.928698	3.062055
H	-1.385436	-2.783213	5.090637	-1.521508	-2.738222	5.118597	-1.554254	-2.712236	5.121341
H	4.624101	-3.709887	-10.063107	4.277806	-4.108366	-10.000144	4.264659	-4.122046	-9.998503
H	-4.624101	3.709887	-10.063107	-4.277806	4.108366	-10.000144	-4.264659	4.122046	-9.998503
H	-1.333333	-3.873656	-13.898944	-1.658555	-3.787065	-13.858573	-1.672077	-3.787175	-13.855502
H	1.333333	3.873656	-13.898944	1.658555	3.787065	-13.858573	1.672077	3.787175	-13.855502
H	-6.890948	0.021828	4.925736	-6.83277	-0.109374	4.752514	-6.830341	-0.129305	4.735497
H	-6.761716	-0.409827	6.64809	-6.753921	-0.493864	6.489188	-6.75904	-0.523944	6.470238
H	-8.084758	0.636555	6.095691	-8.076983	0.510405	5.86501	-8.083284	0.477969	5.845035
H	-5.810328	3.068919	7.834744	-5.914182	3.036909	7.61457	-5.942551	3.004082	7.621397
H	-7.460225	2.401018	7.777038	-7.545502	2.330341	7.519779	-7.569623	2.289676	7.513481

H	-6.121529	1.402339	8.377898	-6.208083	1.37866	8.192489	-6.230888	1.340866	8.187676
H	-7.694013	2.969603	5.388164	-7.713578	2.835425	5.114622	-7.726742	2.808574	5.109867
H	-6.07464	3.693502	5.361573	-6.10889	3.590109	5.113566	-6.126115	3.571472	5.122961
H	-6.519211	2.442884	4.167875	-6.496077	2.298341	3.943097	-6.49966	2.284913	3.942308
H	6.890948	-0.021828	4.925736	6.83277	0.109374	4.752514	6.830341	0.129305	4.735497
H	6.761716	0.409827	6.64809	6.753921	0.493864	6.489188	6.75904	0.523944	6.470238
H	8.084758	-0.636555	6.095691	8.076983	-0.510405	5.86501	8.083284	-0.477969	5.845035
H	5.810328	-3.068919	7.834744	5.914182	-3.036909	7.61457	5.942551	-3.004082	7.621397
H	7.460225	-2.401018	7.777038	7.545502	-2.330341	7.519779	7.569623	-2.289676	7.513481
H	6.121529	-1.402339	8.377898	6.208083	-1.37866	8.192489	6.230888	-1.340866	8.187676
H	7.694013	-2.969603	5.388164	7.713578	-2.835425	5.114622	7.726742	-2.808574	5.109867
H	6.07464	-3.693502	5.361573	6.10889	-3.590109	5.113566	6.126115	-3.571472	5.122961
H	6.519211	-2.442884	4.167875	6.496077	-2.298341	3.943097	6.49966	-2.284913	3.942308
H	-2.172482	-1.975298	11.862153	-2.303296	-1.800066	11.890779	-2.316212	-1.84238	11.889097
H	-3.744396	-1.811957	11.042516	-3.853122	-1.707355	11.01882	-3.863287	-1.749531	11.012192
H	-3.50371	-3.094086	12.246661	-3.614689	-2.943159	12.269493	-3.624277	-2.993528	12.254609
H	-3.440815	-5.007118	9.013832	-3.401654	-4.954514	9.101961	-3.392227	-4.981628	9.07409
H	-4.233693	-4.851289	10.600754	-4.246166	-4.771461	10.658467	-4.240502	-4.814737	10.630317
H	-4.501062	-3.617755	9.353305	-4.50784	-3.584326	9.366591	-4.506223	-3.619343	9.347088
H	-2.085757	-5.065753	11.786006	-2.136121	-4.888906	11.921663	-2.134418	-4.929887	11.898434
H	-1.209147	-5.26443	10.256335	-1.205507	-5.117341	10.429597	-1.198596	-5.14382	10.407559
H	-0.695507	-4.022753	11.431398	-0.761495	-3.823555	11.577691	-0.763942	-3.855824	11.565811
H	2.172482	1.975298	11.862153	2.303296	1.800066	11.890779	2.316212	1.84238	11.889097
H	3.744396	1.811957	11.042516	3.853122	1.707355	11.01882	3.863287	1.749531	11.012192
H	3.50371	3.094086	12.246661	3.614689	2.943159	12.269493	3.624277	2.993528	12.254609
H	3.440815	5.007118	9.013832	3.401654	4.954514	9.101961	3.392227	4.981628	9.07409
H	4.233693	4.851289	10.600754	4.246166	4.771461	10.658467	4.240502	4.814737	10.630317
H	4.501062	3.617755	9.353305	4.50784	3.584326	9.366591	4.506223	3.619343	9.347088
H	2.085757	5.065753	11.786006	2.136121	4.888906	11.921663	2.134418	4.929887	11.898434
H	1.209147	5.26443	10.256335	1.205507	5.117341	10.429597	1.198596	5.14382	10.407559
H	0.695507	4.022753	11.431398	0.761495	3.823555	11.577691	0.763942	3.855824	11.565811

RuOs8		S0			S1			T1	
Atom	X	Y	Z	X	Y	Z	X	Y	Z
Os	0	0	7.363789	0	0	7.343743	0	0	7.391924
Ru	0	0	-7.850853	0	0	-7.885061	0	0	-7.845509
N	0	1.417191	-1.416657	0.010813	1.417567	-1.433588	0.023963	1.427448	-1.404691
N	0	-1.417191	-1.416657	-0.010813	-1.417567	-1.433588	-0.023963	-1.427448	-1.404691
N	0.061173	1.33008	-6.25626	0.049474	1.334718	-6.293027	0.09362	1.336348	-6.260389
N	-0.061173	-1.33008	-6.25626	-0.049474	-1.334718	-6.293027	-0.09362	-1.336348	-6.260389
N	-2.04086	0.348997	-7.955452	-2.044293	0.320186	-7.982352	-2.008792	0.490132	-7.909691
N	-0.058758	1.435895	-9.339273	-0.083397	1.438449	-9.369998	0.013333	1.400218	-9.366162
N	2.04086	-0.348997	-7.955452	2.044293	-0.320186	-7.982352	2.008792	-0.490132	-7.909691
N	0.058758	-1.435895	-9.339273	0.083397	-1.438449	-9.369998	-0.013333	-1.400218	-9.366162
N	2.017011	0.414329	7.476126	2.017829	0.400668	7.40827	2.017508	0.403585	7.491575
N	0.024878	1.425041	8.851336	0.067203	1.382113	8.887402	0.039795	1.429983	8.871651
N	-2.017011	-0.414329	7.476126	-2.017829	-0.400668	7.40827	-2.017508	-0.403585	7.491575
N	-0.024878	-1.425041	8.851336	-0.067203	-1.382113	8.887402	-0.039795	-1.429983	8.871651
N	-0.032493	1.416805	0.928921	-0.012116	1.426524	0.909069	-0.023223	1.423209	0.935871
N	0.032493	-1.416805	0.928921	0.012116	-1.426524	0.909069	0.023223	-1.423209	0.935871
N	0.091545	-1.311763	5.774669	0.057133	-1.332513	5.774565	0.086047	-1.31849	5.803261
N	-0.091545	1.311763	5.774669	-0.057133	1.332513	5.774565	-0.086047	1.31849	5.803261
C	-0.007438	-0.727621	-2.559632	-0.009804	-0.713465	-2.596061	-0.020851	-0.713373	-2.564201
C	0.007438	0.727621	-2.559632	0.009804	0.713465	-2.596061	0.020851	0.713373	-2.564201
C	0.032996	1.454186	-3.830737	0.030465	1.442013	-3.858558	0.062593	1.434366	-3.825973
C	0.024492	0.725224	-5.030265	0.020383	0.721364	-5.066966	0.04297	0.71588	-5.036176
C	-0.024492	-0.725224	-5.030265	-0.020383	-0.721364	-5.066966	-0.04297	-0.71588	-5.036176
C	-0.032996	-1.454186	-3.830737	-0.030465	-1.442013	-3.858558	-0.062593	-1.434366	-3.825973
C	0.073089	2.862622	-3.901051	0.065704	2.854686	-3.930315	0.127922	2.848003	-3.907181
C	0.103776	3.4746	-5.157353	0.088972	3.470904	-5.182017	0.167242	3.46608	-5.156963
C	0.096942	2.679329	-6.319393	0.079692	2.680601	-6.351727	0.144631	2.680048	-6.329531
C	-0.096942	-2.679329	-6.319393	-0.079692	-2.680601	-6.351727	-0.144631	-2.680048	-6.329531
C	-0.103776	-3.4746	-5.157353	-0.088972	-3.470904	-5.182017	-0.167242	-3.46608	-5.156963
C	-0.073089	-2.862622	-3.901051	-0.065704	-2.854686	-3.930315	-0.127922	-2.848003	-3.907181
C	-4.750149	1.14197	-8.249331	-4.764527	1.081946	-8.255998	-4.651357	1.468759	-8.15228
C	-4.359413	0.143539	-7.350473	-4.356492	0.083438	-7.364875	-4.305267	0.479456	-7.222837
C	-3.006523	-0.230086	-7.222532	-2.998355	-0.274396	-7.24663	-2.982493	0.013056	-7.114817
C	-2.396909	1.310424	-8.873568	-2.417272	1.282405	-8.892673	-2.316595	1.444684	-8.852821
C	-3.732072	1.734599	-9.067406	-3.758574	1.691521	-9.076461	-3.620783	1.957707	-9.024579
C	-1.326219	1.872654	-9.649672	-1.357536	1.862089	-9.671051	-1.230285	1.909607	-9.663452
C	0.982603	1.944278	-10.018924	0.947893	1.962584	-10.053097	1.077545	1.798451	-10.084774
C	0.804482	2.889466	-11.048753	0.752851	2.911255	-11.076772	0.940367	2.718546	-11.139696
C	-1.587214	2.824048	-10.663205	-1.635596	2.815818	-10.67792	-1.446656	2.838525	-10.704713
C	-0.472646	3.333993	-11.408039	-0.531493	3.343049	-11.426011	-0.312526	3.23931	-11.489031
C	4.750149	-1.14197	-8.249331	4.764527	-1.081946	-8.255998	4.651357	-1.468759	-8.15228
C	4.359413	-0.143539	-7.350473	4.356492	-0.083438	-7.364875	4.305267	-0.479456	-7.222837
C	3.006523	0.230086	-7.222532	2.998355	0.274396	-7.24663	2.982493	-0.013056	-7.114817
C	2.396909	-1.310424	-8.873568	2.417272	-1.282405	-8.892673	2.316595	-1.444684	-8.852821
C	3.732072	-1.734599	-9.067406	3.758574	-1.691521	-9.076461	3.620783	-1.957707	-9.024579
C	1.326219	-1.872654	-9.649672	1.357536	-1.862089	-9.671051	1.230285	-1.909607	-9.663452
C	-0.982603	-1.944278	-10.018924	-0.947893	-1.962584	-10.053097	-1.077545	-1.798451	-10.084774

C	-0.804482	-2.889466	-11.048753	-0.752851	-2.911255	-11.076772	-0.940367	-2.718546	-11.139696
C	1.587214	-2.824048	-10.663205	1.635596	-2.815818	-10.67792	1.446656	-2.838525	-10.704713
C	0.472646	-3.333993	-11.408039	0.531493	-3.343049	-11.426011	0.312526	-3.23931	-11.489031
C	4.71535	1.26756	7.779578	4.721558	1.212736	7.67132	4.7194	1.259603	7.75872
C	4.341536	0.27502	6.865077	4.309801	0.287171	6.702892	4.336425	0.254715	6.861364
C	3.000283	-0.129124	6.731018	2.962305	-0.093869	6.583924	2.993826	-0.150575	6.744772
C	2.360932	1.373617	8.406283	2.394152	1.296747	8.38762	2.371031	1.375337	8.40523
C	3.685162	1.824951	8.605142	3.726181	1.724029	8.570647	3.697281	1.828561	8.586017
C	1.277731	1.897703	9.183273	1.338379	1.801756	9.212688	1.295192	1.908543	9.185952
C	-1.035791	1.903627	9.531812	-0.969964	1.829418	9.616689	-1.014182	1.912863	9.560114
C	-0.887573	2.841346	10.570381	-0.778178	2.695748	10.709606	-0.856426	2.861068	10.587569
C	1.506006	2.844079	10.207658	1.610403	2.674493	10.288231	1.532752	2.865885	10.198142
C	-4.71535	-1.26756	7.779578	-4.721558	-1.212736	7.67132	-4.7194	-1.259603	7.75872
C	-4.341536	-0.27502	6.865077	-4.309801	-0.287171	6.702892	-4.336425	-0.254715	6.861364
C	-3.000283	0.129124	6.731018	-2.962305	0.093869	6.583924	-2.993826	0.150575	6.744772
C	-2.360932	-1.373617	8.406283	-2.394152	-1.296747	8.38762	-2.371031	-1.375337	8.40523
C	-3.685162	-1.824951	8.605142	-3.726181	-1.724029	8.570647	-3.697281	-1.828561	8.586017
C	-1.277731	-1.897703	9.183273	-1.338379	-1.801756	9.212688	-1.295192	-1.908543	9.185952
C	1.035791	-1.903627	9.531812	0.969964	-1.829418	9.616689	1.014182	-1.912863	9.560114
C	0.887573	-2.841346	10.570381	0.778178	-2.695748	10.709606	0.856426	-2.861068	10.587569
C	-1.506006	-2.844079	10.207658	-1.610403	-2.674493	10.288231	-1.532752	-2.865885	10.198142
C	-0.374131	-3.31716	10.948513	-0.502819	-3.114725	11.087553	-0.408313	-3.344518	10.946208
C	-0.008358	0.719622	-0.243955	0	0.729207	-0.269117	0	0.733446	-0.23304
C	0.008358	-0.719622	-0.243955	0	-0.729207	-0.269117	0	-0.733446	-0.23304
C	0.024027	-0.727843	2.07209	0.01136	-0.72442	2.061803	0.020358	-0.712758	2.099252
C	-0.024027	0.727843	2.07209	-0.01136	0.72442	2.061803	-0.020358	0.712758	2.099252
C	0.065848	-1.455725	3.34255	0.035809	-1.438605	3.326511	0.060023	-1.440282	3.360359
C	0.040726	-0.72135	4.537607	0.027514	-0.708287	4.539931	0.037512	-0.716952	4.567176
C	-0.040726	0.72135	4.537607	-0.027514	0.708287	4.539931	-0.037512	0.716952	4.567176
C	-0.065848	1.455725	3.34255	-0.035809	1.438605	3.326511	-0.060023	1.440282	3.360359
C	0.135629	-2.86108	3.418941	0.069403	-2.84737	3.41394	0.125916	-2.851561	3.438883
C	0.17811	-3.462045	4.682332	0.085536	-3.467218	4.668391	0.167324	-3.458141	4.695873
C	0.155014	-2.665351	5.840184	0.072867	-2.67775	5.836785	0.145881	-2.667415	5.863575
C	-0.135629	2.86108	3.418941	-0.069403	2.84737	3.41394	-0.125916	2.851561	3.438883
C	-0.17811	3.462045	4.682332	-0.085536	3.467218	4.668391	-0.167324	3.458141	4.695873
C	-0.155014	2.665351	5.840184	-0.072867	2.67775	5.836785	-0.145881	2.667415	5.863575
C	3.902778	2.799197	9.649777	3.989266	2.62691	9.666137	3.924123	2.816172	9.616347
C	-3.978704	2.716194	-10.098121	-4.022611	2.676168	-10.100127	-3.82454	2.917372	-10.083674
C	3.978704	-2.716194	-10.098121	4.022611	-2.676168	-10.100127	3.82454	-2.917372	-10.083674
C	-3.902778	-2.799197	9.649777	-3.989266	-2.62691	9.666137	-3.924123	-2.816172	9.616347
C	2.86705	3.28557	10.409316	2.982218	3.07952	10.483375	2.895618	3.310866	10.380406
C	-2.958356	3.236306	-10.855363	-3.012788	3.21264	-10.860098	-2.789224	3.338525	-10.881884
C	2.958356	-3.236306	-10.855363	3.012788	-3.21264	-10.860098	2.789224	-3.338525	-10.881884
C	-2.86705	-3.28557	10.409316	-2.982218	-3.07952	10.483375	-2.895618	-3.310866	10.380406
C	0.374131	3.31716	10.948513	0.502819	3.114725	11.087553	0.408313	3.344518	10.946208
C	-6.178636	1.549011	-8.311167	-6.198064	1.472838	-8.306937	-6.046329	1.974122	-8.187196
C	-6.553659	2.90856	-8.243739	-6.587765	2.82761	-8.227996	-6.320968	3.359352	-8.181305
C	-7.183873	0.56023	-8.372563	-7.192771	0.47355	-8.369426	-7.118567	1.056254	-8.15879
C	-7.909801	3.27168	-8.249777	-7.947818	3.17591	-8.22398	-7.647578	3.816771	-8.158973

C	-8.539935	0.924165	-8.387953	-8.552886	0.822638	-8.37454	-8.444783	1.515358	-8.149783
C	-8.906772	2.28138	-8.32791	-8.934323	2.175265	-8.303201	-8.712669	2.896918	-8.150151
C	6.135377	1.70029	7.847445	6.143182	1.6349	7.713022	6.140246	1.692792	7.80733
C	6.486221	3.067605	7.810764	6.497443	3.001088	7.766916	6.491123	3.059377	7.749163
C	7.158662	0.728681	7.88521	7.160479	0.659496	7.629392	7.163997	0.721812	7.848818
C	7.83573	3.454548	7.823621	7.847906	3.382314	7.748748	7.840711	3.446357	7.745048
C	8.507926	1.116222	7.907121	8.510746	1.041738	7.625148	8.51349	1.109344	7.85327
C	8.850449	2.480832	7.87773	8.857966	2.404304	7.684797	8.855923	2.473366	7.802927
C	6.178636	-1.549011	-8.311167	6.198064	-1.472838	-8.306937	6.046329	-1.974122	-8.187196
C	6.553659	-2.90856	-8.243739	6.587765	-2.82761	-8.227996	6.320968	-3.359352	-8.181305
C	7.183873	-0.56023	-8.372563	7.192771	-0.47355	-8.369426	7.118567	-1.056254	-8.15879
C	7.909801	-3.27168	-8.249777	7.947818	-3.17591	-8.22398	7.647578	-3.816771	-8.158973
C	8.539935	-0.924165	-8.387953	8.552886	-0.822638	-8.37454	8.444783	-1.515358	-8.149783
C	8.906772	-2.28138	-8.32791	8.934323	-2.175265	-8.303201	8.712669	-2.896918	-8.150151
C	-6.135377	-1.70029	7.847445	-6.143182	-1.6349	7.713022	-6.140246	-1.692792	7.80733
C	-6.486221	-3.067605	7.810764	-6.497443	-3.001088	7.766916	-6.491123	-3.059377	7.749163
C	-7.158662	-0.728681	7.88521	-7.160479	-0.659496	7.629392	-7.163997	-0.721812	7.848818
C	-7.83573	-3.454548	7.823621	-7.847906	-3.382314	7.748748	-7.840711	-3.446357	7.745048
C	-8.507926	-1.116222	7.907121	-8.510746	-1.041738	7.625148	-8.51349	-1.109344	7.85327
C	-8.850449	-2.480832	7.87773	-8.857966	-2.404304	7.684797	-8.855923	-2.473366	7.802927
C	-0.617733	4.296549	-12.531813	-0.694606	4.310411	-12.543321	-0.413906	4.166658	-12.643376
C	-1.535126	4.068234	-13.580457	-1.614111	4.076399	-13.588856	-1.380933	3.976588	-13.654792
C	0.222595	5.429226	-12.587603	0.130219	5.454542	-12.596344	0.515743	5.222192	-12.765103
C	-1.616752	4.963537	-14.658989	-1.712997	4.977035	-14.661517	-1.422472	4.83679	-14.76312
C	0.134597	6.329054	-13.661717	0.024996	6.359621	-13.664523	0.464502	6.089293	-13.867312
C	-0.786488	6.099144	-14.700415	-0.898068	6.123803	-14.700139	-0.505307	5.898986	-14.869138
C	0.48365	4.270356	12.083394	0.665286	3.968899	12.290942	0.527742	4.310108	12.069729
C	-0.392445	5.375263	12.149342	-0.18322	5.081193	12.477396	-0.350249	5.413666	12.133674
C	1.405105	4.060112	13.132443	1.612457	3.646422	13.287317	1.460725	4.113244	13.111174
C	-0.335707	6.265632	13.233354	-0.070663	5.873205	13.630821	-0.284511	6.315294	13.20787
C	1.455936	4.945972	14.220579	1.715566	4.431926	14.445772	1.520878	5.010456	14.189533
C	0.589998	6.054191	14.271932	0.879342	5.550767	14.617728	0.652596	6.116946	14.2388
C	0.617733	-4.296549	-12.531813	0.694606	-4.310411	-12.543321	0.413906	-4.166658	-12.643376
C	-0.222595	-5.429226	-12.587603	-0.130219	-5.454542	-12.596344	-0.515743	-5.222192	-12.765103
C	1.535126	-4.068234	-13.580457	1.614111	-4.076399	-13.588856	1.380933	-3.976588	-13.654792
C	-0.134597	-6.329054	-13.661717	-0.024996	-6.359621	-13.664523	-0.464502	-6.089293	-13.867312
C	1.616752	-4.963537	-14.658989	1.712997	-4.977035	-14.661517	1.422472	-4.83679	-14.76312
C	0.786488	-6.099144	-14.700415	0.898068	-6.123803	-14.700139	0.505307	-5.898986	-14.869138
C	-0.48365	-4.270356	12.083394	-0.665286	-3.968899	12.290942	-0.527742	-4.310108	12.069729
C	-1.405105	-4.060112	13.132443	-1.612457	-3.646422	13.287317	-1.460725	-4.113244	13.111174
C	0.392445	-5.375263	12.149342	0.18322	-5.081193	12.477396	0.350249	-5.413666	12.133674
C	-1.455936	-4.945972	14.220579	-1.715566	-4.431926	14.445772	-1.520878	-5.010456	14.189533
C	0.335707	-6.265632	13.233354	0.070663	-5.873205	13.630821	0.284511	-6.315294	13.20787
C	-0.589998	-6.054191	14.271932	-0.879342	-5.550767	14.617728	-0.652596	-6.116946	14.2388
H	0.081007	3.442243	-2.984399	0.075157	3.429688	-3.010726	0.145388	3.423347	-2.987725
H	0.134934	4.553096	-5.254781	0.115986	4.550212	-5.275349	0.216445	4.544222	-5.248717
H	0.127956	3.124572	-7.307695	0.104235	3.132005	-7.337647	0.180625	3.133367	-7.313891
H	-0.127956	-3.124572	-7.307695	-0.104235	-3.132005	-7.337647	-0.180625	-3.133367	-7.313891
H	-0.134934	-4.553096	-5.254781	-0.115986	-4.550212	-5.275349	-0.216445	-4.544222	-5.248717

H	-0.081007	-3.442243	-2.984399	-0.075157	-3.429688	-3.010726	-0.145388	-3.423347	-2.987725
H	-5.094849	-0.332411	-6.710264	-5.082504	-0.404718	-6.723004	-5.051688	0.086008	-6.541688
H	-2.703076	-0.994029	-6.515083	-2.679992	-1.037505	-6.544765	-2.713959	-0.740849	-6.383433
H	1.971968	1.590593	-9.750288	1.942676	1.618466	-9.791749	2.045383	1.383879	-9.825725
H	1.67714	3.245008	-11.586674	1.618072	3.280084	-11.617831	1.822417	2.992096	-11.70815
H	5.094849	0.332411	-6.710264	5.082504	0.404718	-6.723004	5.051688	-0.086008	-6.541688
H	2.703076	0.994029	-6.515083	2.679992	1.037505	-6.544765	2.713959	0.740849	-6.383433
H	-1.971968	-1.590593	-9.750288	-1.942676	-1.618466	-9.791749	-2.045383	-1.383879	-9.825725
H	-1.67714	-3.245008	-11.586674	-1.618072	-3.280084	-11.617831	-1.822417	-2.992096	-11.70815
H	5.085674	-0.174901	6.216163	5.027126	-0.119656	5.998679	5.074511	-0.204222	6.211716
H	2.714923	-0.889639	6.01279	2.644715	-0.795921	5.821757	2.699888	-0.919992	6.039447
H	-2.014191	1.529665	9.251516	-1.962292	1.493292	9.337094	-1.99449	1.533124	9.294332
H	-1.774462	3.168299	11.103222	-1.644487	3.003678	11.284815	-1.737966	3.191267	11.127371
H	-5.085674	0.174901	6.216163	-5.027126	0.119656	5.998679	-5.074511	0.204222	6.211716
H	-2.714923	0.889639	6.01279	-2.644715	0.795921	5.821757	-2.699888	0.919992	6.039447
H	2.014191	-1.529665	9.251516	1.962292	-1.493292	9.337094	1.99449	-1.533124	9.294332
H	1.774462	-3.168299	11.103222	1.644487	-3.003678	11.284815	1.737966	-3.191267	11.127371
H	0.156327	-3.447521	2.507043	0.079677	-3.428848	2.497731	0.14448	-3.432092	2.523081
H	0.231411	-4.539056	4.787005	0.108533	-4.545859	4.761514	0.218223	-4.536207	4.795104
H	0.196607	-3.106264	6.829774	0.088414	-3.128974	6.823154	0.186145	-3.115997	6.85007
H	-0.156327	3.447521	2.507043	-0.079677	3.428848	2.497731	-0.14448	3.432092	2.523081
H	-0.231411	4.539056	4.787005	-0.108533	4.545859	4.761514	-0.218223	4.536207	4.795104
H	-0.196607	3.106264	6.829774	-0.088414	3.128974	6.823154	-0.186145	3.115997	6.85007
H	4.913983	3.140259	9.844011	5.010427	2.93979	9.853064	4.936879	3.160462	9.796546
H	3.067476	4.031644	11.170735	3.214699	3.772289	11.284526	3.10322	4.066035	11.130939
H	-3.067476	-4.031644	11.170735	-3.214699	-3.772289	11.284526	-3.10322	-4.066035	11.130939
H	-4.913983	-3.140259	9.844011	-5.010427	-2.93979	9.853064	-4.936879	-3.160462	9.796546
H	-4.998822	3.034631	-10.283985	-5.047459	2.983734	-10.278407	-4.823914	3.299919	-10.25845
H	-3.179003	3.986186	-11.607421	-3.246652	3.963986	-11.606744	-2.975803	4.076548	-11.653949
H	4.998822	-3.034631	-10.283985	5.047459	-2.983734	-10.278407	4.823914	-3.299919	-10.25845
H	3.179003	-3.986186	-11.607421	3.246652	-3.963986	-11.606744	2.975803	-4.076548	-11.653949
H	-5.790165	3.678136	-8.153106	-5.832153	3.604851	-8.136548	-5.503834	4.07672	-8.155628
H	-6.903057	-0.489532	-8.427606	-6.900668	-0.572648	-8.433149	-6.914629	-0.01238	-8.167083
H	-8.186896	4.320218	-8.188465	-8.236045	4.220908	-8.153928	-7.848886	4.883874	-8.143056
H	-9.304804	0.155098	-8.447364	-9.309575	0.045553	-8.434762	-9.26316	0.801375	-8.142352
H	-9.955899	2.563623	-8.337134	-9.986545	2.445934	-8.304565	-9.739077	3.252625	-8.138678
H	5.709273	3.82544	7.73753	5.72305	3.764519	7.78375	5.713506	3.81623	7.67283
H	6.896941	-0.326945	7.917377	6.895416	-0.39491	7.591724	6.902498	-0.333256	7.897365
H	8.093903	4.509019	7.78586	8.110287	4.435763	7.778443	8.09849	4.500247	7.691084
H	9.286466	0.359772	7.948086	9.286485	0.283287	7.575333	9.292309	0.353306	7.897096
H	9.894354	2.781605	7.892047	9.903023	2.700864	7.67663	9.899941	2.774138	7.804002
H	5.790165	-3.678136	-8.153106	5.832153	-3.604851	-8.136548	5.503834	-4.07672	-8.155628
H	6.903057	0.489532	-8.427606	6.900668	0.572648	-8.433149	6.914629	0.01238	-8.167083
H	8.186896	-4.320218	-8.188465	8.236045	-4.220908	-8.153928	7.848886	-4.883874	-8.143056
H	9.304804	-0.155098	-8.447364	9.309575	-0.045553	-8.434762	9.26316	-0.801375	-8.142352
H	9.955899	-2.563623	-8.337134	9.986545	-2.445934	-8.304565	9.739077	-3.252625	-8.138678
H	-5.709273	-3.82544	7.73753	-5.72305	-3.764519	7.78375	-5.713506	-3.81623	7.67283
H	-6.896941	0.326945	7.917377	-6.895416	0.39491	7.591724	-6.902498	0.333256	7.897365
H	-8.093903	-4.509019	7.78586	-8.110287	-4.435763	7.778443	-8.09849	-4.500247	7.691084

H	-9.286466	-0.359772	7.948086	-9.286485	-0.283287	7.575333	-9.292309	-0.353306	7.897096
H	-9.894354	-2.781605	7.892047	-9.903023	-2.700864	7.67663	-9.899941	-2.774138	7.804002
H	-2.158901	3.177114	-13.571715	-2.226153	3.177143	-13.582163	-2.073099	3.139619	-13.597312
H	0.929437	5.614273	-11.781425	0.838467	5.644001	-11.792418	1.261047	5.377097	-11.987864
H	-2.319619	4.772854	-15.464948	-2.417362	4.781938	-15.465131	-2.162404	4.675949	-15.541647
H	0.778733	7.203359	-13.688	0.657326	7.242581	-13.688551	1.175116	6.906943	-13.944626
H	-0.8535	6.793261	-15.53355	-0.978418	6.821999	-15.528684	-0.542881	6.5672	-15.724842
H	-1.102678	5.547069	11.343199	-0.913004	5.336795	11.712078	-1.069399	5.57532	11.333335
H	2.056148	3.188837	13.11667	2.240898	2.765594	13.176367	2.113778	3.243434	13.097327
H	-1.007438	7.118656	13.267323	-0.718932	6.735108	13.759277	-0.958133	7.166921	13.240156
H	2.162536	4.768878	15.026378	2.439534	4.169709	15.211722	2.236492	4.843449	14.98954
H	0.63304	6.741176	15.112527	0.963637	6.161139	15.512464	0.702646	6.812634	15.071832
H	-0.929437	-5.614273	-11.781425	-0.838467	-5.644001	-11.792418	-1.261047	-5.377097	-11.987864
H	2.158901	-3.177114	-13.571715	2.226153	-3.177143	-13.582163	2.073099	-3.139619	-13.597312
H	-0.778733	-7.203359	-13.688	-0.657326	-7.242581	-13.688551	-1.175116	-6.906943	-13.944626
H	2.319619	-4.772854	-15.464948	2.417362	-4.781938	-15.465131	2.162404	-4.675949	-15.541647
H	0.8535	-6.793261	-15.53355	0.978418	-6.821999	-15.528684	0.542881	-6.5672	-15.724842
H	-2.056148	-3.188837	13.11667	-2.240898	-2.765594	13.176367	-2.113778	-3.243434	13.097327
H	1.102678	-5.547069	11.343199	0.913004	-5.336795	11.712078	1.069399	-5.57532	11.333335
H	-2.162536	-4.768878	15.026378	-2.439534	-4.169709	15.211722	-2.236492	-4.843449	14.98954
H	1.007438	-7.118656	13.267323	0.718932	-6.735108	13.759277	0.958133	-7.166921	13.240156
H	-0.63304	-6.741176	15.112527	-0.963637	-6.161139	15.512464	-0.702646	-6.812634	15.071832

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