Experimental Details for Synthesis and Structural Analyses of Compounds 1 - 5.

General Data. Reagent grade solvents were dried by using sodium-benzophenone followed by distillation and were either used immediately or stored over 4Å molecular sieves. 2-vinylthiacyclohexane,[1] $Os_3(CO)_{10}(NCMe)_2$[2] were prepared by the published procedures. All reactions were performed under a nitrogen atmosphere unless specified otherwise. Infrared spectra were recorded on a Nicolet 5DXB FTIR spectrophotometer. ^1H NMR spectra were run on either a Brüker AM-300 or Varian Mercury-400 spectrometer operating at 300 and 400 MHz, respectively. Chromatographic separations were performed in air on silica gel by using Analtech (0.25 mm) F_{254} uniplates. Elemental analyses were performed by Oneida Research Services, Whitesboro, NY.

Reaction of $Os_3(CO)_{10}(NCMe)_2$ with 2-vinylthiacyclohexane. A 20.5-mg amount of $Os_3(CO)_{10}(NCMe)_2$ (0.022 mmol) and 2.5 µL (0.039 mmol) 2-vinylthiacyclohexane were dissolved in 10mL of CH_2Cl_2 at 25°C. After stirring for 19 h at 25 °C, the solvent was removed *in vacuo.* and the residue was separated by TLC using pure hexane solvent as eluent. The following compounds were isolated in order of elution: $Os_3(CO)_{10}(\mu\text{-}H)(\mu\text{-}S(CH_2)_3CH{=}CHCH{=}CH_2)$, **3**, (1.8 mg, 8%), $Os_3(CO)_{10}(\mu\text{-}\eta^4\text{-}S(CH_2)_4CHCHCH_2)$, **2**, (3.4 mg, 16%), $Os_3(CO)_{10}(\eta^3\text{-}S(CH_2)_4CHCHCH_2)$, **1**, (11.6 mg, 54%). Analytical and spectral data for **3**: IR νCO (cm^{-1}) in hexane: 2109(m), 2067(vs), 2059(s), 2025(vs), 2019(s), 2005(w), 1999(s), 1990(m), 1983(m). ^1H NMR (δ in $CDCl_3$): 6.27(dt, $J_{H\text{-}H}$= 19 Hz, $J_{H\text{-}H}$= 21 Hz, 1H), 6.04(dd, $J_{H\text{-}H}$= 10Hz, $J_{H\text{-}H}$= 15 Hz, 1H), 5.61(dt, $J_{H\text{-}H}$= 15 Hz, $J_{H\text{-}H}$= 15 Hz, 1H), 5.10(d, $J_{H\text{-}H}$= 17 Hz, 1H), 4.98(d, $J_{H\text{-}H}$= 10 Hz, 1H), 2.34(t, $J_{H\text{-}H}$= 16Hz, 2H), 2.18(q, $J_{H\text{-}H}$= 7 Hz, 2H), 1.68(m, 2H), -17.40(s, 1H). For **2**: IR νCO (cm^{-1}) in hexane: 2123(m), 2066(s),

2047(vs), 2018(s), 2004(w), 1995(s), 1983(m), 1927(m). ^{1}H NMR (δ in $CDCl_3$): 4.66(dt, J_{H-H}= 12 Hz, J_{H-H}= 15 Hz, 1H), 4.17(m, 1H), 3.62(dt, J_{H-H}= 7 Hz, J_{H-H}=4 Hz, 1H), 2.78(m, 1H) 2.46(m, 2H), 2.13(m, 1H), 1.65(m, 2H), 1.51(dd, J_{H-H}=12 Hz, J_{H-H}=2 Hz, 1H), 1.32(m, 2H). Anal. calcd (found) for **2**: C 20.84 (21.37), H 1.24(1.04). For **1**: IR νCO (cm^{-1}) in hexane: 2105(m), 2044(m), 2032(s), 2017(vs), 1997(m), 1983(w), 1969(m), 1962(m). ^{1}H NMR (δ in $CDCl_3$): 2.91(dd, J_{H-H}= 23 Hz, J_{H-H}= 23 Hz, 2H), 2.77(bm, 1H), 2.64(m, 1H), 2.31(m, 1H) 2.11(dd, J_{H-H}= 2 Hz, J_{H-H}= 11Hz, 1H), 2.07-1.66(bm, 5H), 1.42(bm, 1H). Anal. calcd (found) for **3**: C, 20.84 (20.65); H, 1.24 (1.09).

Thermolysis of 2. A 8.6-mg amount of **2** (0.0088 mmol) was dissolved in 5 mL hexane. The solution was heated to 50 °C in a constant temperature oil-bath for 48 h. The solvent was removed *in vacuo* and the residue was separated by TLC using pure hexane solvent as eluent. The following compounds were isolated in order of elution: **3**, (3.8mg, 44%), $Os_3(CO)_9(\mu\text{-}\eta^4\text{-cis-}S(CH_2)_4CHCHCH_2)$, **4**, (1.7mg, 20%), $Os_3(CO)_9(\mu\text{-}\eta^4\text{-trans-}S(CH_2)_4CHCHCH_2)$, **5**, (1.1mg, 13%), unreacted **2**, (1.1mg). Analytical and spectral data for **4**: IR νCO (cm^{-1}) in hexane: 2098(m), 2049(s), 2021(vs), 2014(m), 1999(m), 1976(m), 1928(w). ^{1}H NMR (δ in $CDCl_3$): 4.87(m, 1H), 4.66(m, 1H), 4.29(dt, J_{H-H}= 7 Hz, J_{H-H}= 3 Hz, 1H), 3.68(bd, J_{H-H}= 12 Hz, 1H), 2.95(m, 1H), 2.44(dd, J_{H-H}= 2 Hz, J_{H-H}= 13 Hz, 1H), 2.15(m, 1H), 1.79(m, 1H), 1.68(m, 4H). Anal. calc (found) for **4:** C,20.20 (20.22); H,1.28 (1.13). For **5**: IR νCO (cm^{-1}) in hexane: 2097(m), 2050(s), 2019(vs), 2013(m), 1998(m), 1978(m), 1908(w). ^{1}H NMR (δ in $CDCl_3$): 4.59(dt, J_{H-H}= 8 Hz, J_{H-H}= 22 Hz, 1H), 4.18(dt, J_{H-H}= 9 Hz, J_{H-H}= 6 Hz, 1H), 3.15(dd, J_{H-H}= 3 Hz, J_{H-H}= 8 Hz, 1H), 3.07(dt, J_{H-H}= 18 Hz, J_{H-H}= 5 Hz, 1H), 2.87(ddd, J_{H-H}= 1 Hz, J_{H-H}= 10 Hz, J_{H-H}= 14 Hz, 1H), 2.34(m, 2H), 2.09(m, 1H), 1.80(m, 2H), 1.23(m, 1H), 0.78(m, 1H).

Thermolysis of 1. A 10.2-mg amount of **1** (0.010 mmol) was dissolved in 5 mL of hexane and the solution was heated to 45 °C in a constant temperature oil-bath for 40 h in the presence of a slow nitrogen purge. The solvent was removed *in vacuo* and the residue was separated by TLC using pure hexane solvent as eluent. Five products separated by TLC were found to be **3** (1.6 mg, 16%), **2** (0.8 mg, 8%), unreacted **1** (7.9 mg) **4** (0.9 mg, 10%), and **5** (0.3 mg, 3%).

Thermolysis of 4. A 20.0-mg amount of **4** (0.021 mmol) was dissolved in 5 mL of hexane and the solution was refluxed for 24h in the presence of a slow nitrogen purge. The solvent was removed *in vacuo* and the residue was separated by TLC using pure hexane solvent as eluent. Two products separated by TLC were found to be unreacted **4** (11.3mg), and **5** (8.2 mg, 41%).

Thermolysis of 4 in the Presence of CO. A solution of **4** (10 mg, 0.010 mmol) in 10mL of hexane was heated to 45 °C for 40 h under an atmosphere of carbon monoxide. The reaction was monitored by IR and ^{1}H-NMR spectroscopy. At the end of the time period most of the **2** was unchanged. There was no spectroscopic evidence for the formation of any of the compound **2**.

Crystallographic Analyses. Crystals of **1**, **2**, **4** and **5** suitable for x-ray diffraction measurements were obtained by slow evaporation of solvent from solutions in a pure hexane solvent at -17°C. The crystals used in data collection were mounted in thin-walled glass capillaries. Diffraction measurements were made on a Rigaku AFC6S fully automated four-circle diffractometer using graphite-monochromated Mo Kα radiation. Unit cells were determined and refined from 15 randomly selected reflections obtained by using the AFC6 automatic search, center, index, and least-squares

routines. Crystal data, data collection parameters, and results of the analyses are listed in Table 1. All data processing was performed on a Digital Equipment Corp. VAXstation 3520 computer by using the TEXSAN structure solving program library obtained from the Molecular Structure Corp., The Woodlands, TX. Neutral atom scattering factors were calculated by the standard procedures.[3a] Anomalous dispersion corrections were applied to all non-hydrogen atoms.[3b] Full matrix least-squares refinements minimized the function: $\Sigma_{hkl}\ w(|F_o|-|F_c|)^2$, *where* $w = 1/\sigma(F)^2$, $\sigma(F) = \sigma(F_o^2)/2F_o$ *and* $\sigma(F_o^2) = [\sigma(I_{raw})^2+(0.06\ I_{net})^2]^{1/2}/L_p$.

Compounds **1**, **2**, **4** and **5** crystallized in the monoclinic crystal system. The space group settings $P2_1/n$, $P2_1/n$, $P2_1/n$ and $P2_1/a$ were identified for the compounds **1**, **2**, **4** and **5**, respectively, on the basis of the patterns of systematic absences observed in the data. All structures were solved by a combination of direct methods (SIR92) and difference Fourier syntheses. Compound **1** crystallized with two independent formula units in the asymmetric crystal unit. Both molecules are structurally similar. All nonhydrogen atoms were refined with anisotropic thermal parameters. All hydrogen atom positions on the ligands were calculated by assuming idealized geometries with C - H distances of 0.95Å. The contributions of the hydrogen atoms were included in the structure factor calculations, but their positions were not refined.

1. D. L. Tuleen, R. H. Bennett, *J. Heterocycl. Chem.* 6 (1969) 115, 1969.
2. 2. J. N. Nicholls, M. D. Vargas, *Inorg. Syn.* 28 (1998) 232.
3. *International Tables for X-ray Crystallography*; Kynoch Press: Birmingham, England, 1975; Vol. IV, pp 99-101, Table 2.2B. (b) *Ibid.* pp 149-150, Table 2.3.1.

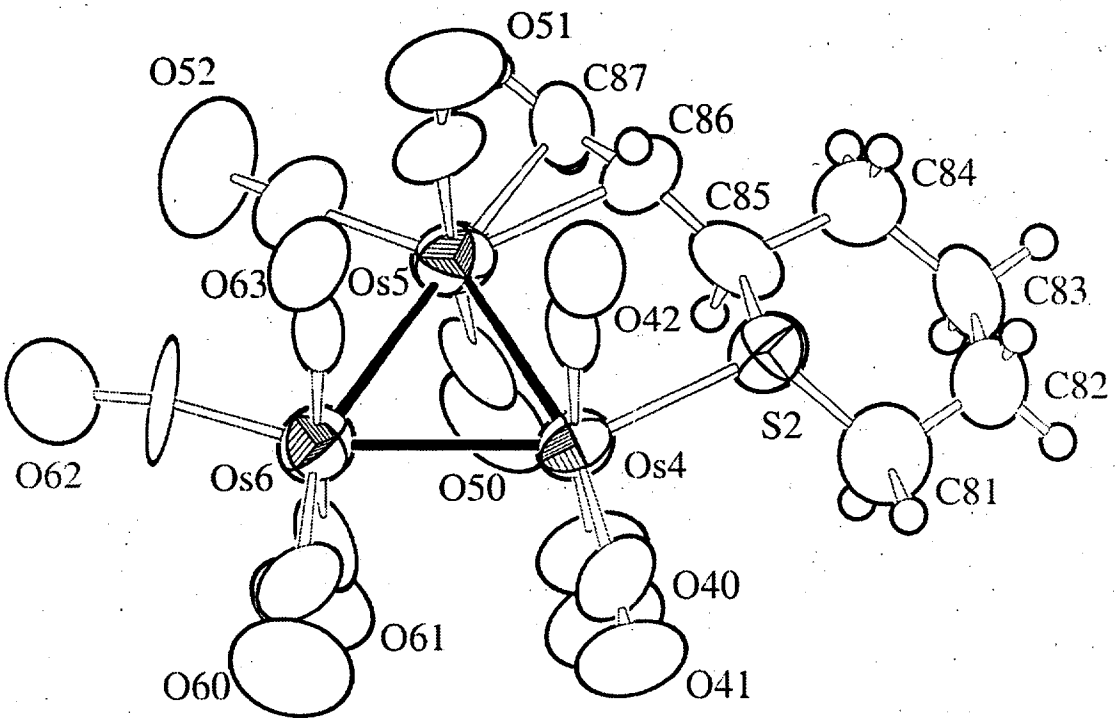

Figure 1.

An ORTEP diagram of the molecular structure $Os_3(CO)_{10}(\mu\text{-}\eta^3\text{-}S(CH_2)_4CHCHCH_2)$, **1** showing 50% probability thermal ellipsoids.

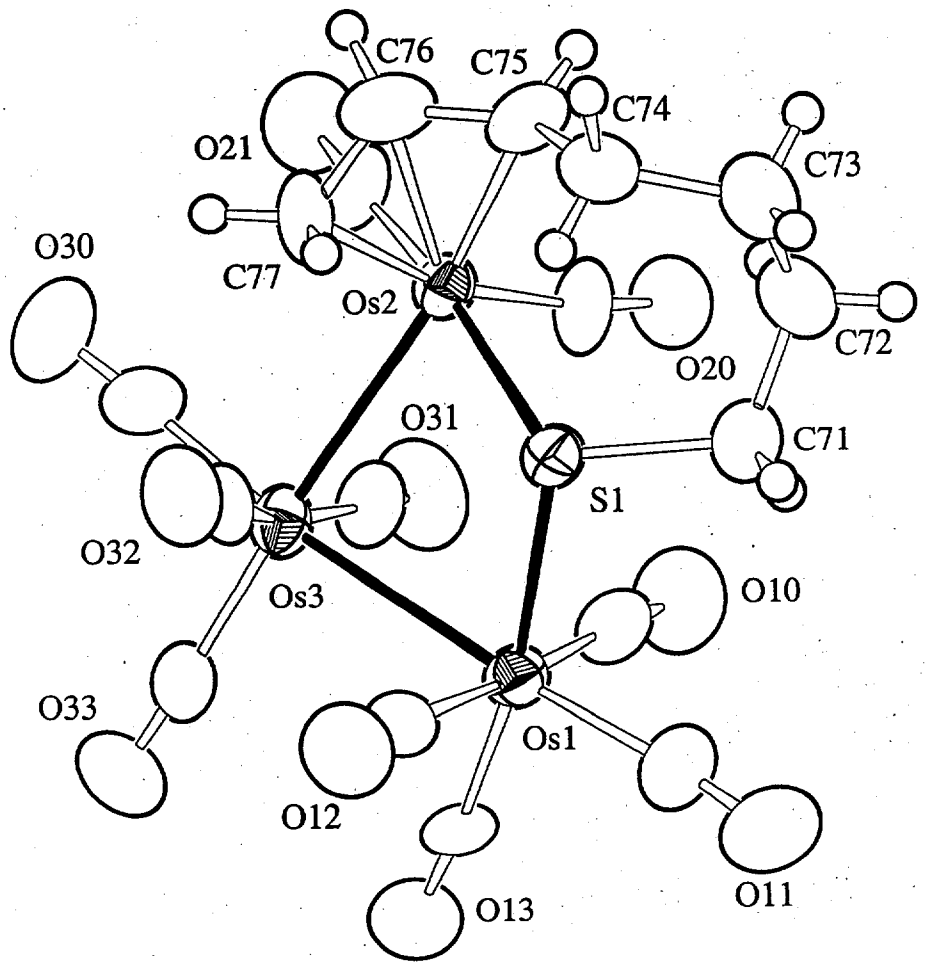

Figure 2.

An ORTEP diagram of the molecular structure of $Os_3(CO)_{10}(\mu\text{-}\eta^4\text{-}S(CH_2)_4CHCHCH_2)$, **2** showing 50% probability thermal ellipsoids.

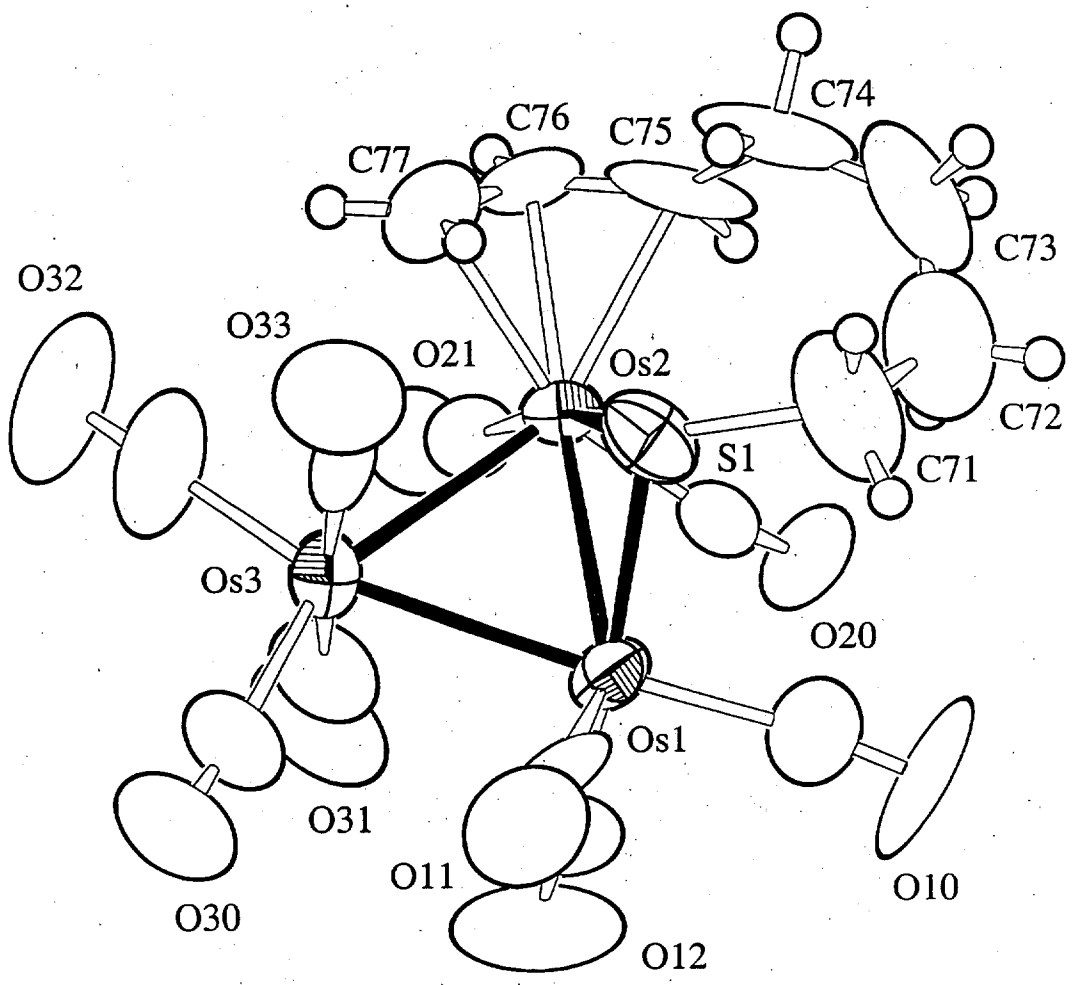

Figure 3.

An ORTEP diagram of the molecular structure of $Os_3(CO)_9(\mu\text{-}\eta^4\text{-cis-}S(CH_2)_4CHCHCH_2)$, **4** showing 50% probability thermal ellipsoids.

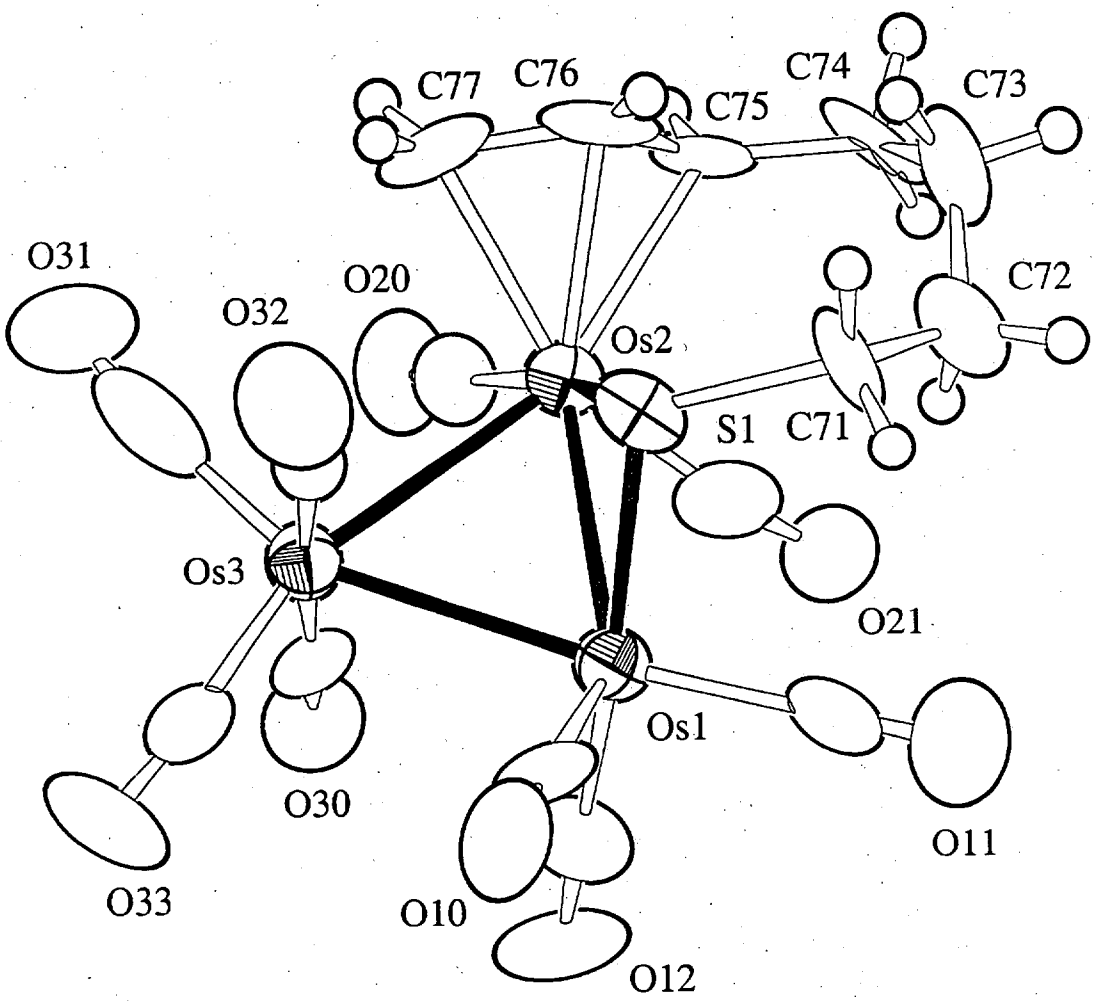

Figure 4.

An ORTEP diagram of the molecular structure of $Os_3(CO)_9(\mu\text{-}\eta^4\text{-trans-}S(CH_2)_4CHCHCH_2)$, **5** showing 50% probability thermal ellipsoids.

Table S1. Crystallographic Data for Compounds **1**, **2**, **4** and **5**.

Compound	**1**	**2**	**4**	**5**
Formula	$Os_3SO_{10}C_{17}H_{12}$	$Os_3SO_{10}C_{17}H_{12}$	$Os_3SO_9C_{16}H_{12}$	$Os_3SO_9C_{16}H_{12}$
Formula weight	978.94	978.94	950.93	950.93
Crystal system	Monoclinic	Monoclinic	Monoclinic	Monoclinic
Lattice parameters				
a (Å)	12.368(6)	14.770(5)	15.553(5)	13.385(4)
b (Å)	12.692(3)	10.015(4)	14.966(9)	21.51(1)
c (Å)	29.490(9)	16.402(7)	9.238(4)	14.635(8)
α (°)	90	90	90	90
β (°)	100.08(4)	113.80(3)	90.664(9)	93.76(4)
γ (°)	90	90	90	90
V ($Å^3$)	4558(3)	2220(2)	2150(2)	4205(3)
Space group	$P2_1/c$(# 14)	$P2_1/n$(# 14)	$P2_1/n$(# 14)	$P2_1/a$(# 14)
Z value	8	4	4	8
ρcalc. (g/cm^3)	2.85	2.93	2.94	3.00
μ (Mo Kα) (cm^{-1})	168.15	172.63	178.15	182.19
Temperature (°C)	20	20	20	20
$2\Theta_{max}$ (°)	43	44	42.1	42.0
No. Obs. (I>3σ(I))	3410	1812	1661	2990
No. Variables	555	281	263	519
Goodness of Fit	1.488	1.032	1.181	1.074
Max shift in final cycle	0.01	0.01	0.01	0.01
Residuals: R; R_w	0.055; 0.073	0.031; 0.033	0.036; 0.046	0.037; 0.045
Abs. Cor.	DIFABS	DIFABS	DIFABS	PSI
Transmiss. coeff, Max/Min	1.00-0.305	1.00-0.571	1.00-0.520	1.00-0.235
Largest peak in Final Diff. Map ($e^-/Å^3$)	2.09	0.80	1.63	2.00

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*$R = \Sigma_{hkl}(||F_{obs}| - |F_{calc}||)/\Sigma_{hkl}|F_{obs}|$; $R_w = [\Sigma_{hkl}w(|F_{obs}| - |F_{calc}|)^2/\Sigma_{hkl}wF_{obs}^2]^{1/2}$, $w = 1/\sigma^2(F_{obs})$; $GOF = [\Sigma_{hkl}w(|F_{obs}| - |F_{calc}|)^2/(n_{data} - n_{vari})]^{1/2}$.

Table S2. Atomic Positional Parameters for Compound **1**.

atom	x	y	z	B(eq)
Os(1)	0.4237(1)	0.48193(9)	0.09994(3)	3.93(3)
Os(2)	0.4728(1)	0.5959(1)	0.18515(4)	4.52(3)
Os(3)	0.6445(1)	0.5398(1)	0.13406(4)	4.78(3)
Os(4)	-0.0916(1)	0.1496(1)	0.08867(4)	4.70(3)
Os(5)	-0.0505(1)	0.0211(1)	0.16982(4)	5.70(4)
Os(6)	0.1289(1)	0.0953(1)	0.12647(4)	5.38(4)
S(1)	0.2360(7)	0.4720(6)	0.1084(2)	4.3(2)
S(2)	-0.2835(8)	0.1508(7)	0.0923(3)	5.3(2)
O(10)	0.374(2)	0.683(2)	0.0446(8)	7.3(8)
O(11)	0.440(2)	0.273(2)	0.1506(7)	6.6(7)
O(12)	0.431(3)	0.370(2)	0.0090(8)	10(1)
O(20)	0.412(3)	0.801(2)	0.1321(9)	8.2(9)
O(21)	0.504(3)	0.394(2)	0.2446(8)	8.8(9)
O(22)	0.646(3)	0.706(2)	0.252(1)	8.9(9)
O(30)	0.853(3)	0.628(3)	0.1965(9)	11(1)
O(31)	0.678(3)	0.326(2)	0.1872(8)	8.0(8)
O(32)	0.734(2)	0.442(2)	0.0536(8)	7.9(8)
O(33)	0.615(2)	0.754(2)	0.0839(9)	7.2(8)
O(40)	-0.126(3)	-0.036(2)	0.0210(8)	10(1)
O(41)	-0.065(2)	0.290(2)	0.0069(7)	7.7(8)
O(42)	-0.089(2)	0.350(2)	0.1492(8)	6.8(7)
O(50)	-0.100(3)	-0.171(2)	0.107(1)	9(1)
O(51)	-0.037(3)	0.210(3)	0.2368(8)	10(1)
O(52)	0.124(3)	-0.095(3)	0.237(1)	12(1)
O(60)	0.226(3)	0.217(2)	0.053(1)	10(1)

Table S2. Atomic Positional Parameters for Compound **1.** (continued)

atom	x	y	z	B(eq)
O(61)	0.116(3)	-0.110(2)	0.070(1)	10(1)
O(62)	0.334(3)	0.011(3)	0.183(1)	11(1)
O(63)	0.145(2)	0.291(2)	0.1915(8)	7.8(8)
C(10)	0.394(3)	0.608(2)	0.0669(9)	4.6(8)
C(11)	0.439(3)	0.353(3)	0.1316(9)	4.6(8)
C(12)	0.427(2)	0.410(3)	0.044(1)	5.7(9)
C(20)	0.438(3)	0.722(3)	0.152(1)	6(1)
C(21)	0.504(4)	0.468(3)	0.222(1)	7(1)
C(22)	0.584(3)	0.663(3)	0.228(1)	5.9(9)
C(30)	0.769(3)	0.592(3)	0.175(1)	5.9(9)
C(31)	0.666(3)	0.406(3)	0.169(1)	6(1)
C(32)	0.711(4)	0.478(3)	0.085(1)	8(1)
C(33)	0.621(3)	0.673(3)	0.103(1)	7(1)
C(40)	-0.113(4)	0.033(3)	0.047(1)	8(1)
C(41)	-0.081(3)	0.234(3)	0.037(1)	7(1)
C(42)	-0.083(3)	0.274(3)	0.130(1)	4.6(8)
C(50)	-0.078(4)	-0.093(3)	0.129(1)	7(1)
C(51)	-0.031(4)	0.141(3)	0.211(1)	7(1)
C(52)	0.059(4)	-0.051(3)	0.211(1)	8(1)
C(60)	0.191(3)	0.174(3)	0.082(1)	7(1)
C(61)	0.110(3)	-0.031(3)	0.090(1)	6(1)
C(62)	0.244(3)	0.039(3)	0.164(1)	7(1)
C(63)	0.135(3)	0.225(3)	0.166(1)	5.5(9)
C(71)	0.141(3)	0.509(3)	0.057(1)	6.1(9)
C(72)	0.018(3)	0.520(2)	0.068(1)	6(1)

Table S2. Atomic Positional Parameters for Compound **1**. (continued)

atom	x	y	z	B(eq)
C(73)	0.022(4)	0.601(3)	0.105(1)	7.8(9)
C(74)	0.091(3)	0.586(3)	0.150(1)	6(1)
C(75)	0.214(3)	0.586(2)	0.147(1)	5.4(9)
C(76)	0.291(3)	0.571(3)	0.187(1)	5.5(9)
C(77)	0.340(3)	0.650(3)	0.221(1)	6(1)
C(81)	-0.374(4)	0.119(3)	0.040(1)	8(1)
C(82)	-0.483(3)	0.115(4)	0.049(1)	8(1)
C(83)	-0.507(3)	0.018(3)	0.082(1)	6(1)
C(84)	-0.425(3)	0.029(3)	0.130(1)	7(1)
C(85)	-0.303(3)	0.032(3)	0.128(1)	6(1)
C(86)	-0.231(3)	0.043(3)	0.171(1)	5.7(9)
C(87)	-0.191(3)	-0.043(3)	0.199(1)	7(1)
H(1)	0.1605	0.5713	0.0428	6.6515
H(2)	0.1419	0.4526	0.0318	6.6515
H(3)	-0.0318	0.5309	0.0398	8.1792
H(4)	0.0000	0.4483	0.0787	8.1792
H(5)	0.0402	0.6697	0.0929	9.7581
H(6)	-0.0541	0.6118	0.1113	9.7581
H(7)	0.0813	0.6409	0.1724	8.4726
H(8)	0.0784	0.5206	0.1631	8.4726
H(9)	0.2349	0.6547	0.1332	6.3520
H(10)	-0.3704	0.1716	0.0155	9.7353
H(11)	-0.3555	0.0526	0.0268	9.7353
H(12)	-0.5030	0.1784	0.0611	8.6545
H(13)	-0.5361	0.1054	0.0187	8.6545

Table S2. Atomic Positional Parameters for Compound **1**. (continued)

atom	x	y	z	B(eq)
H(14)	-0.5818	0.0127	0.0897	8.2973
H(15)	-0.4961	-0.0549	0.0700	8.2973
H(16)	-0.4420	0.0881	0.1439	8.4656
H(17)	-0.4374	-0.0333	0.1499	8.4656
H(18)	-0.2842	-0.0374	0.1125	6.7601
H(19)	0.3063	0.4962	0.1949	7.7325
H(20)	0.3896	0.6358	0.2488	7.8165
H(21)	0.3242	0.7265	0.2145	7.8165
H(22)	-0.2131	0.1171	0.1827	7.4593
H(23)	-0.1416	-0.0403	0.2282	7.7250
H(24)	-0.2091	-0.1160	0.1874	7.7250

Table S3. Atomic Positional Parameters for Compound **2**.

atom	x	y	z	B(eq)
Os(1)	-1.05305(5)	-0.39265(7)	-0.71298(5)	3.23(2)
Os(2)	-0.93572(5)	-0.07432(7)	-0.77514(5)	3.07(2)
Os(3)	-0.95401(5)	-0.15328(8)	-0.61070(5)	3.35(2)
S(1)	-0.9576(3)	-0.3183(4)	-0.7964(3)	3.1(1)
O(10)	-1.236(1)	-0.222(2)	-0.827(1)	6.9(4)
O(11)	-1.148(1)	-0.640(2)	-0.824(1)	6.6(5)
O(12)	-0.868(1)	-0.560(2)	-0.5990(9)	5.9(4)
O(13)	-1.148(1)	-0.439(2)	-0.582(1)	7.8(5)
O(20)	-1.1474(9)	-0.014(1)	-0.9050(9)	5.6(4)
O(21)	-0.933(1)	0.220(1)	-0.734(1)	6.7(5)
O(30)	-0.829(1)	0.092(2)	-0.523(1)	7.2(5)
O(31)	-1.150(1)	0.006(2)	-0.696(1)	7.6(5)
O(32)	-0.757(1)	-0.299(2)	-0.5671(9)	5.9(4)
O(33)	-0.974(1)	-0.254(2)	-0.4431(9)	6.8(5)
C(10)	-1.165(1)	-0.283(2)	-0.783(1)	4.8(6)
C(11)	-1.111(1)	-0.547(2)	-0.786(1)	4.5(5)
C(12)	-0.932(2)	-0.496(2)	-0.635(1)	3.8(5)
C(13)	-1.115(1)	-0.425(2)	-0.635(1)	5.3(6)
C(20)	-1.068(1)	-0.044(2)	-0.852(1)	4.7(5)
C(21)	-0.932(1)	0.105(2)	-0.747(1)	3.9(5)
C(30)	-0.880(1)	0.001(2)	-0.559(1)	4.6(6)
C(31)	-1.078(2)	-0.053(2)	-0.665(1)	4.5(5)
C(32)	-0.832(1)	-0.247(2)	-0.588(1)	4.3(5)
C(33)	-0.967(1)	-0.220(2)	-0.507(1)	4.6(5)
C(71)	-1.034(1)	-0.369(2)	-0.914(1)	4.5(5)
C(72)	-1.021(2)	-0.280(2)	-0.983(1)	5.8(6)
C(73)	-0.925(2)	-0.270(2)	-0.988(1)	5.4(6)
C(74)	-0.839(1)	-0.215(2)	-0.902(1)	4.6(5)
C(75)	-0.857(1)	-0.078(2)	-0.872(1)	3.9(5)
C(76)	-0.798(1)	-0.020(2)	-0.791(1)	4.9(6)
C(77)	-0.768(1)	-0.101(2)	-0.714(1)	4.2(5)
H(1)	-1.0158	-0.4581	-0.9223	5.3700
H(2)	-1.1016	-0.3672	-0.9235	5.3700
H(3)	-1.0657	-0.3120	-1.0398	6.8890
H(4)	-1.0388	-0.1925	-0.9738	6.8890
H(5)	-0.9073	-0.3566	-0.9995	6.3949
H(6)	-0.9327	-0.2116	-1.0358	6.3949
H(7)	-0.7812	-0.2098	-0.9145	5.4472
H(8)	-0.8279	-0.2766	-0.8553	5.4472
H(9)	-0.8829	-0.0153	-0.9194	4.6579
H(10)	-0.7769	0.0703	-0.7874	5.8520
H(11)	-0.7310	-0.0610	-0.6574	5.0228
H(12)	-0.7420	-0.1879	-0.7153	5.0228

Table S4. Atomic Positional Parameters for Compound **4**.

atom	x	y	z	B(eq)
Os(2)	0.28388(5)	0.30566(6)	0.47289(8)	3.51(2)
Os(1)	0.42591(5)	0.19039(6)	0.50337(9)	4.01(2)
Os(3)	0.32100(5)	0.21798(7)	0.74348(8)	4.19(2)
S(1)	0.4351(4)	0.3501(4)	0.5051(7)	5.1(2)
O(10)	0.529(1)	0.158(2)	0.232(2)	11.9(8)
O(11)	0.576(1)	0.158(2)	0.705(2)	9.2(6)
O(12)	0.371(2)	-0.005(2)	0.496(3)	13(1)
O(20)	0.300(1)	0.209(1)	0.187(2)	6.5(5)
O(21)	0.109(1)	0.216(1)	0.481(2)	6.8(5)
O(30)	0.422(1)	0.098(1)	0.955(2)	8.6(6)
O(31)	0.203(1)	0.067(2)	0.629(2)	9.7(7)
O(32)	0.177(1)	0.282(2)	0.940(2)	12.9(9)
O(33)	0.430(1)	0.380(1)	0.845(2)	8.0(6)
C(10)	0.486(2)	0.173(2)	0.322(3)	6.5(8)
C(11)	0.520(1)	0.168(2)	0.628(3)	5.9(7)
C(12)	0.391(2)	0.067(2)	0.502(3)	7.5(9)
C(20)	0.301(1)	0.238(2)	0.294(3)	5.0(6)
C(21)	0.176(1)	0.246(2)	0.478(2)	4.9(6)
C(30)	0.386(1)	0.139(2)	0.874(3)	5.5(7)
C(31)	0.247(2)	0.122(2)	0.669(3)	6.8(8)
C(32)	0.231(2)	0.258(3)	0.867(3)	10(1)
C(33)	0.391(2)	0.322(2)	0.799(3)	5.6(7)
C(71)	0.494(2)	0.390(3)	0.345(3)	10(1)
C(72)	0.448(2)	0.409(3)	0.211(4)	12(1)
C(73)	0.389(3)	0.483(3)	0.205(3)	10(1)
C(74)	0.327(2)	0.501(2)	0.315(4)	9(1)
C(75)	0.252(2)	0.438(2)	0.345(4)	7.6(9)
C(76)	0.202(2)	0.427(2)	0.473(3)	6.8(8)
C(77)	0.242(2)	0.424(2)	0.611(2)	6.4(7)
H(1)	0.5214	0.4474	0.3730	10.7362
H(2)	0.5401	0.3493	0.3273	10.7362
H(3)	0.4911	0.4160	0.1335	13.0484
H(4)	0.4170	0.3545	0.1852	13.0484
H(5)	0.4280	0.5307	0.1891	10.8173
H(6)	0.3600	0.4703	0.1134	10.8173
H(7)	0.3605	0.5092	0.3995	10.5031
H(8)	0.3049	0.5585	0.2844	10.5031
H(9)	0.2388	0.3975	0.2627	9.1327
H(10)	0.1393	0.4200	0.4655	8.3118
H(11)	0.2083	0.4155	0.6999	6.9278
H(12)	0.3026	0.4277	0.6234	6.9278

Table S5. Atomic Positional Parameters for Compound 5.

atom	x	y	z	B(eq)
Os(1)	0.35195(7)	-0.17268(5)	0.68181(8)	3.25(3)
Os(2)	0.43898(7)	-0.07774(4)	0.79075(8)	3.16(3)
Os(3)	0.35582(7)	-0.18424(5)	0.87419(8)	3.43(3)
Os(4)	0.03886(7)	0.12053(4)	0.61264(8)	2.95(3)
Os(5)	0.01219(7)	0.12920(5)	0.80124(8)	3.35(3)
Os(6)	0.16558(7)	0.19897(5)	0.72154(8)	3.51(3)
S(1)	0.5290(4)	-0.1569(3)	0.7126(5)	3.8(2)
S(2)	0.0881(5)	0.0432(3)	0.7247(5)	3.8(2)
O(10)	0.355(2)	-0.3120(9)	0.664(1)	6.5(7)
O(11)	0.358(2)	-0.145(1)	0.478(2)	7.3(8)
O(12)	0.123(1)	-0.166(1)	0.668(2)	6.7(7)
O(20)	0.312(2)	-0.003(1)	0.915(2)	6.0(6)
O(21)	0.316(1)	-0.0191(9)	0.630(2)	5.1(6)
O(30)	0.156(1)	-0.1127(9)	0.869(1)	5.4(6)
O(31)	0.405(2)	-0.134(1)	1.065(2)	7.9(9)
O(32)	0.553(1)	-0.258(1)	0.878(2)	7.4(7)
O(33)	0.254(2)	-0.310(1)	0.901(2)	8.3(8)
O(40)	0.203(1)	0.0904(9)	0.490(2)	5.5(6)
O(41)	-0.125(1)	0.048(1)	0.509(2)	6.1(6)
O(42)	-0.014(1)	0.2341(9)	0.495(1)	5.5(6)
O(50)	-0.193(1)	0.1369(8)	0.702(1)	4.6(5)
O(51)	-0.032(2)	0.254(1)	0.890(2)	7.9(8)
O(60)	0.318(1)	0.096(1)	0.767(2)	6.8(7)
O(61)	0.288(1)	0.2438(9)	0.569(2)	6.4(7)
O(62)	0.007(1)	0.3037(9)	0.689(1)	5.2(6)
O(63)	0.255(2)	0.272(1)	0.888(2)	8.2(8)
C(10)	0.354(2)	-0.259(1)	0.672(2)	3.8(7)
C(11)	0.354(2)	-0.153(1)	0.552(3)	4.6(8)
C(12)	0.209(2)	-0.169(1)	0.674(2)	4.6(8)
C(20)	0.355(2)	-0.032(1)	0.871(2)	4.6(8)
C(21)	0.360(2)	-0.047(2)	0.687(2)	5(1)
C(30)	0.231(2)	-0.140(1)	0.869(2)	4.9(9)
C(31)	0.382(2)	-0.155(2)	0.997(3)	7(1)
C(32)	0.480(2)	-0.228(1)	0.871(2)	3.0(5)
C(33)	0.294(2)	-0.262(2)	0.886(2)	4.9(8)
C(40)	0.137(2)	0.102(1)	0.535(2)	4.7(8)
C(41)	-0.065(2)	0.072(1)	0.552(2)	3.8(7)
C(42)	0.003(2)	0.191(1)	0.542(2)	3.4(7)
C(50)	-0.108(2)	0.132(1)	0.730(2)	3.2(7)
C(51)	-0.017(2)	0.207(2)	0.853(2)	5.3(9)
C(60)	0.256(2)	0.131(1)	0.747(2)	5.5(9)
C(61)	0.240(2)	0.227(1)	0.622(2)	3.8(7)
C(62)	0.064(2)	0.265(2)	0.701(2)	6(1)
C(63)	0.224(2)	0.244(2)	0.829(2)	5(1)
C(71)	0.592(2)	-0.130(1)	0.609(2)	4.6(8)
C(72)	0.570(2)	-0.062(1)	0.574(2)	5.0(8)
C(73)	0.625(2)	-0.009(1)	0.624(2)	5.2(8)
C(74)	0.571(2)	0.033(1)	0.689(2)	5.2(8)
C(75)	0.540(2)	0.010(1)	0.778(2)	3.9(7)
C(76)	0.593(2)	-0.040(1)	0.825(3)	5.5(9)

Table S5. Atomic Positional Parameters for Compound 5.

atom	x	y	z	B(eq)
C(77)	0.561(2)	-0.069(1)	0.907(2)	5.5(9)
C(81)	0.007(2)	-0.027(1)	0.710(2)	4.3(7)
C(82)	-0.102(2)	-0.022(1)	0.737(2)	5.8(9)
C(83)	-0.116(2)	-0.029(1)	0.842(2)	6(1)
C(84)	-0.152(2)	0.028(1)	0.889(2)	5.3(9)
C(85)	-0.075(2)	0.077(1)	0.911(2)	6.0(9)
C(86)	0.031(2)	0.066(1)	0.923(2)	4.2(8)
C(87)	0.104(2)	0.111(2)	0.935(2)	6(1)
H(1)	0.6624	-0.1329	0.6234	5.5644
H(2)	0.5730	-0.1573	0.5606	5.5644
H(3)	0.5871	-0.0601	0.5121	5.8700
H(4)	0.5007	-0.0545	0.5772	5.8700
H(5)	0.6792	-0.0280	0.6593	6.3872
H(6)	0.6499	0.0165	0.5786	6.3872
H(7)	0.6148	0.0674	0.7025	6.3005
H(8)	0.5121	0.0474	0.6566	6.3005
H(9)	0.5244	0.0432	0.8179	4.8336
H(10)	0.6472	-0.0586	0.7959	6.7724
H(11)	0.5492	-0.0424	0.9573	6.4382
H(12)	0.5951	-0.1051	0.9285	6.4382
H(13)	0.0048	-0.0384	0.6475	5.2566
H(14)	0.0380	-0.0592	0.7463	5.2566
H(15)	-0.1277	0.0168	0.7168	6.9200
H(16)	-0.1392	-0.0546	0.7061	6.9200
H(17)	-0.1641	-0.0604	0.8495	7.6156
H(18)	-0.0541	-0.0399	0.8713	7.6156
H(19)	-0.2032	0.0466	0.8495	6.4414
H(20)	-0.1793	0.0152	0.9438	6.4414
H(21)	-0.0965	0.1048	0.9574	7.3259
H(22)	0.0531	0.0252	0.9121	5.1571
H(23)	0.1726	0.0984	0.9341	7.1780
H(24)	0.0995	0.1397	0.9855	7.1780

Table S6. Selected Bond Distances for 1.

atom	atom	distance	atom	atom	distance
Os(1)	Os(2)	2.871(2)	Os(5)	C(86)	2.26(4)
Os(1)	Os(3)	2.837(2)	Os(5)	C(87)	2.23(3)
Os(1)	S(1)	2.381(8)	Os(6)	C(60)	1.92(4)
Os(1)	C(10)	1.88(3)	Os(6)	C(61)	1.92(5)
Os(1)	C(11)	1.87(3)	Os(6)	C(62)	1.79(3)
Os(1)	C(12)	1.88(4)	Os(6)	C(63)	2.01(4)
Os(2)	Os(3)	2.900(2)	S(1)	C(71)	1.82(3)
Os(2)	C(20)	1.89(4)	S(1)	C(75)	1.88(3)
Os(2)	C(21)	1.95(4)	S(2)	C(81)	1.80(4)
Os(2)	C(22)	1.90(4)	S(2)	C(85)	1.88(3)
Os(2)	C(76)	2.28(3)	O(10)	C(10)	1.16(3)
Os(2)	C(77)	2.21(3)	O(11)	C(11)	1.16(4)
Os(3)	C(30)	1.90(4)	O(12)	C(12)	1.17(4)
Os(3)	C(31)	1.98(4)	O(20)	C(20)	1.18(4)
Os(3)	C(32)	1.96(4)	O(21)	C(21)	1.16(4)
Os(3)	C(33)	1.92(5)	O(22)	C(22)	1.10(4)
Os(4)	Os(5)	2.867(2)	O(30)	C(30)	1.21(4)
Os(4)	Os(6)	2.844(2)	O(31)	C(31)	1.14(4)
Os(4)	S(2)	2.39(1)	O(32)	C(32)	1.10(4)
Os(4)	C(40)	1.91(4)	O(33)	C(33)	1.16(4)
Os(4)	C(41)	1.88(4)	O(40)	C(40)	1.16(4)
Os(4)	C(42)	1.98(3)	O(41)	C(41)	1.18(4)
Os(5)	Os(6)	2.905(2)	O(42)	C(42)	1.14(3)
Os(5)	C(50)	1.88(5)	O(50)	C(50)	1.19(5)
Os(5)	C(51)	1.94(4)	O(51)	C(51)	1.17(4)
Os(5)	C(52)	1.90(4)	O(52)	C(52)	1.14(5)

Distances are in angstroms. Estimated standard deviations in the least significant figure are given in parentheses.

Table S6. Selected Bond Distances for 1. (cont)

atom	atom	distance	atom	atom	distance
O(60)	C(60)	1.15(4)			
O(61)	C(61)	1.18(4)			
O(62)	C(62)	1.21(4)			
O(63)	C(63)	1.11(4)			
C(71)	C(72)	1.62(4)			
C(72)	C(73)	1.49(5)			
C(73)	C(74)	1.47(5)			
C(74)	C(75)	1.53(5)			
C(75)	C(76)	1.41(4)			
C(76)	C(77)	1.46(4)			
C(81)	C(82)	1.43(6)			
C(82)	C(83)	1.63(5)			
C(83)	C(84)	1.59(5)			
C(84)	C(85)	1.52(6)			
C(85)	C(86)	1.43(5)			
C(86)	C(87)	1.41(4)			

Distances are in angstroms. Estimated standard deviations in the least significant figure are given in parentheses.

Table S7. Selected Bond Distances for 2.

atom	atom	distance	atom	atom	distance
Os(1)	Os(3)	2.953(1)	Os(3)	C(30)	1.89(2)
Os(1)	S(1)	2.443(5)	Os(3)	C(31)	1.96(2)
Os(1)	C(10)	1.93(2)	Os(3)	C(32)	1.94(2)
Os(1)	C(11)	1.93(2)	Os(3)	C(33)	1.91(2)
Os(1)	C(12)	2.02(2)	S(1)	C(71)	1.87(2)
Os(1)	C(13)	1.88(3)	O	C(av)	1.15(3)
Os(2)	Os(3)	2.926(1)	C(71)	C(72)	1.51(3)
Os(2)	S(1)	2.471(5)	C(72)	C(73)	1.44(4)
Os(2)	C(20)	1.87(2)	C(73)	C(74)	1.57(2)
Os(2)	C(21)	1.85(2)	C(74)	C(75)	1.51(3)
Os(2)	C(75)	2.32(2)	C(75)	C(76)	1.39(3)
Os(2)	C(76)	2.22(2)	C(76)	C(77)	1.41(3)
Os(2)	C(77)	2.28(2)			

Table S8. Selected Bond Distances for 4.

atom	atom	distance	atom	atom	distance
Os(2)	Os(1)	2.814(1)	S(1)	C(71)	1.85(3)
Os(2)	Os(3)	2.876(1)	O(10)	C(10)	1.10(3)
Os(2)	S(1)	2.459(6)	O(11)	C(11)	1.13(3)
Os(2)	C(20)	1.96(3)	O(12)	C(12)	1.13(4)
Os(2)	C(21)	1.90(2)	O(20)	C(20)	1.07(3)
Os(2)	C(75)	2.35(3)	O(21)	C(21)	1.14(3)
Os(2)	C(76)	2.22(3)	O(30)	C(30)	1.10(3)
Os(2)	C(77)	2.28(3)	O(31)	C(31)	1.13(4)
Os(1)	Os(3)	2.799(1)	O(32)	C(32)	1.14(4)
Os(1)	S(1)	2.394(7)	O(33)	C(33)	1.13(3)
Os(1)	C(10)	1.94(3)	C(71)	C(72)	1.45(5)
Os(1)	C(11)	1.88(2)	C(72)	C(73)	1.44(6)
Os(1)	C(12)	1.92(3)	C(73)	C(74)	1.44(5)
Os(3)	C(30)	1.97(2)	C(74)	C(75)	1.52(4)
Os(3)	C(31)	1.96(3)	C(75)	C(76)	1.43(4)
Os(3)	C(32)	1.91(3)	C(76)	C(77)	1.41(4)
Os(3)	C(33)	1.97(3)			

Distances are in angstroms. Estimated standard deviations in the least significant figure are given in parentheses.

Table S9. Selected Bond Distances for 5.

atom	atom	distance	atom	atom	distance
Os(1)	Os(2)	2.798(1)	Os(5)	C(51)	1.89(3)
Os(1)	Os(3)	2.824(2)	Os(5)	C(85)	2.33(3)
Os(1)	S(1)	2.408(6)	Os(5)	C(86)	2.24(3)
Os(1)	C(10)	1.87(3)	Os(5)	C(87)	2.28(3)
Os(1)	C(11)	1.95(4)	Os(6)	C(60)	1.91(3)
Os(1)	C(12)	1.91(3)	Os(6)	C(61)	1.92(3)
Os(2)	Os(3)	2.856(2)	Os(6)	C(62)	1.97(3)
Os(2)	S(1)	2.417(7)	Os(6)	C(63)	1.97(3)
Os(2)	C(20)	1.94(3)	S(1)	C(71)	1.87(3)
Os(2)	C(21)	1.90(3)	S(2)	C(81)	1.86(2)
Os(2)	C(75)	2.34(2)	O	C(av)	1.14(4)
Os(2)	C(76)	2.24(3)	C(71)	C(72)	1.57(4)
Os(2)	C(77)	2.28(3)	C(72)	C(73)	1.51(4)
Os(3)	C(30)	1.92(3)	C(73)	C(74)	1.54(4)
Os(3)	C(31)	1.91(5)	C(74)	C(75)	1.47(4)
Os(3)	C(32)	1.92(2)	C(75)	C(76)	1.44(4)
Os(3)	C(33)	1.87(3)	C(76)	C(77)	1.44(5)
Os(4)	Os(5)	2.812(2)	C(81)	C(82)	1.54(4)
Os(4)	Os(6)	2.813(2)	C(82)	C(83)	1.56(5)
Os(4)	S(2)	2.397(7)	C(83)	C(84)	1.49(4)
Os(4)	C(40)	1.84(3)	C(84)	C(85)	1.49(4)
Os(4)	C(41)	1.91(3)	C(85)	C(86)	1.44(4)
Os(4)	C(42)	1.88(3)	C(86)	C(87)	1.38(4)
Os(5)	Os(6)	2.854(2)			
Os(5)	S(2)	2.420(7)			
Os(5)	C(50)	1.86(3)			

Distances are in angstroms. Estimated standard deviations in the least significant figure are given in parentheses.

Table S10. Selected Bond Angles for 1.

atom	atom	atom	angle	atom	atom	atom	angle
Os(2)	Os(1)	Os(3)	61.07(4)	C(20)	Os(2)	C(21)	177(1)
Os(2)	Os(1)	S(1)	89.8(2)	C(20)	Os(2)	C(22)	93(2)
Os(2)	Os(1)	C(10)	91.0(8)	C(20)	Os(2)	C(76)	90(1)
Os(2)	Os(1)	C(11)	90.9(8)	C(20)	Os(2)	C(77)	82(1)
Os(2)	Os(1)	C(12)	167(1)	C(21)	Os(2)	C(22)	87(2)
Os(3)	Os(1)	S(1)	150.7(2)	C(21)	Os(2)	C(76)	88(2)
Os(3)	Os(1)	C(10)	93(1)	C(21)	Os(2)	C(77)	95(2)
Os(3)	Os(1)	C(11)	92(1)	C(22)	Os(2)	C(76)	130(1)
Os(3)	Os(1)	C(12)	106(1)	C(22)	Os(2)	C(77)	93(1)
S(1)	Os(1)	C(10)	90(1)	C(76)	Os(2)	C(77)	38(1)
S(1)	Os(1)	C(11)	85(1)	Os(1)	Os(3)	Os(2)	60.04(5)
S(1)	Os(1)	C(12)	104(1)	Os(1)	Os(3)	C(30)	159(1)
C(10)	Os(1)	C(11)	174(1)	Os(1)	Os(3)	C(31)	90(1)
C(10)	Os(1)	C(12)	90(1)	Os(1)	Os(3)	C(32)	98(1)
C(11)	Os(1)	C(12)	90(1)	Os(1)	Os(3)	C(33)	90(1)
Os(1)	Os(2)	Os(3)	58.89(5)	Os(2)	Os(3)	C(30)	100(1)
Os(1)	Os(2)	C(20)	89(1)	Os(2)	Os(3)	C(31)	89(1)
Os(1)	Os(2)	C(21)	93(1)	Os(2)	Os(3)	C(32)	158(1)
Os(1)	Os(2)	C(22)	146(1)	Os(2)	Os(3)	C(33)	88(1)
Os(1)	Os(2)	C(76)	84.0(7)	C(30)	Os(3)	C(31)	87(1)
Os(1)	Os(2)	C(77)	120.7(9)	C(30)	Os(3)	C(32)	102(2)
Os(3)	Os(2)	C(20)	93(1)	C(30)	Os(3)	C(33)	92(1)
Os(3)	Os(2)	C(21)	90(1)	C(31)	Os(3)	C(32)	90(1)
Os(3)	Os(2)	C(22)	87(1)	C(31)	Os(3)	C(33)	177(1)
Os(3)	Os(2)	C(76)	142.7(7)	C(32)	Os(3)	C(33)	93(1)
Os(3)	Os(2)	C(77)	175(1)	Os(5)	Os(4)	Os(6)	61.14(5)

Angles are in degrees. Estimated standard deviations in the least significant figure are given in parentheses.

Table S10. Selected Bond Angles for 1. (cont)

atom	atom	atom	angle	atom	atom	atom	angle
Os(5)	Os(4)	S(2)	89.9(2)	C(50)	Os(5)	C(52)	94(2)
Os(5)	Os(4)	C(40)	94(1)	C(50)	Os(5)	C(86)	92(1)
Os(5)	Os(4)	C(41)	166(1)	C(50)	Os(5)	C(87)	84(1)
Os(5)	Os(4)	C(42)	87.8(9)	C(51)	Os(5)	C(52)	89(2)
Os(6)	Os(4)	S(2)	150.9(2)	C(51)	Os(5)	C(86)	84(2)
Os(6)	Os(4)	C(40)	95(1)	C(51)	Os(5)	C(87)	94(2)
Os(6)	Os(4)	C(41)	105(1)	C(52)	Os(5)	C(86)	130(1)
Os(6)	Os(4)	C(42)	91(1)	C(52)	Os(5)	C(87)	95(1)
S(2)	Os(4)	C(40)	90(1)	C(86)	Os(5)	C(87)	37(1)
S(2)	Os(4)	C(41)	104(1)	Os(4)	Os(6)	Os(5)	59.82(5)
S(2)	Os(4)	C(42)	85(1)	Os(4)	Os(6)	C(60)	94(1)
C(40)	Os(4)	C(41)	87(1)	Os(4)	Os(6)	C(61)	88(1)
C(40)	Os(4)	C(42)	175(2)	Os(4)	Os(6)	C(62)	161(1)
C(41)	Os(4)	C(42)	92(1)	Os(4)	Os(6)	C(63)	88(1)
Os(4)	Os(5)	Os(6)	59.04(5)	Os(5)	Os(6)	C(60)	154(1)
Os(4)	Os(5)	C(50)	85(1)	Os(5)	Os(6)	C(61)	87(1)
Os(4)	Os(5)	C(51)	93.3(9)	Os(5)	Os(6)	C(62)	101(1)
Os(4)	Os(5)	C(52)	145(1)	Os(5)	Os(6)	C(63)	88(1)
Os(4)	Os(5)	C(86)	85.2(7)	C(60)	Os(6)	C(61)	94(1)
Os(4)	Os(5)	C(87)	119.8(9)	C(60)	Os(6)	C(62)	105(2)
Os(6)	Os(5)	C(50)	92(1)	C(60)	Os(6)	C(63)	89(1)
Os(6)	Os(5)	C(51)	90(1)	C(61)	Os(6)	C(62)	91(2)
Os(6)	Os(5)	C(52)	86(1)	C(61)	Os(6)	C(63)	175(1)
Os(6)	Os(5)	C(86)	143.5(7)	C(62)	Os(6)	C(63)	91(1)
Os(6)	Os(5)	C(87)	176(1)	Os(1)	S(1)	C(71)	113(1)
C(50)	Os(5)	C(51)	176(2)	Os(1)	S(1)	C(75)	106(1)

Angles are in degrees. Estimated standard deviations in the least significant figure are given in parentheses.

Table S10. Selected Bond Angles for 1. (cont)

atom	atom	atom	angle	atom	atom	atom	angle
C(71)	S(1)	C(75)	99(2)	C(72)	C(73)	C(74)	121(4)
Os(4)	S(2)	C(81)	116(1)	C(73)	C(74)	C(75)	111(3)
Os(4)	S(2)	C(85)	104(1)	S(1)	C(75)	C(74)	107(2)
C(81)	S(2)	C(85)	100(2)	S(1)	C(75)	C(76)	105(2)
Os(1)	C(10)	O(10)	177(3)	C(74)	C(75)	C(76)	118(3)
Os(1)	C(11)	O(11)	175(3)	Os(2)	C(76)	C(75)	119(2)
Os(1)	C(12)	O(12)	177(3)	Os(2)	C(76)	C(77)	68(2)
Os(2)	C(20)	O(20)	177(3)	C(75)	C(76)	C(77)	128(3)
Os(2)	C(21)	O(21)	168(4)	Os(2)	C(77)	C(76)	74(2)
Os(2)	C(22)	O(22)	176(3)	S(2)	C(81)	C(82)	108(3)
Os(3)	C(30)	O(30)	172(3)	C(81)	C(82)	C(83)	115(3)
Os(3)	C(31)	O(31)	177(3)	C(82)	C(83)	C(84)	108(3)
Os(3)	C(32)	O(32)	170(4)	C(83)	C(84)	C(85)	117(3)
Os(3)	C(33)	O(33)	175(3)	S(2)	C(85)	C(84)	105(2)
Os(4)	C(40)	O(40)	178(3)	S(2)	C(85)	C(86)	108(3)
Os(4)	C(41)	O(41)	174(3)	C(84)	C(85)	C(86)	115(3)
Os(4)	C(42)	O(42)	172(3)	Os(5)	C(86)	C(85)	115(2)
Os(5)	C(50)	O(50)	173(3)	Os(5)	C(86)	C(87)	70(2)
Os(5)	C(51)	O(51)	169(4)	C(85)	C(86)	C(87)	123(3)
Os(5)	C(52)	O(52)	178(4)	Os(5)	C(87)	C(86)	73(2)
Os(6)	C(60)	O(60)	176(3)				
Os(6)	C(61)	O(61)	170(4)				
Os(6)	C(62)	O(62)	167(4)				
Os(6)	C(63)	O(63)	172(3)				
S(1)	C(71)	C(72)	110(2)				
C(71)	C(72)	C(73)	107(3)				

Angles are in degrees. Estimated standard deviations in the least significant figure are given in parentheses.

Table S11. Selected Bond Angles for 2.

atom	atom	atom	angle	atom	atom	atom	angle
Os(3)	Os(1)	S(1)	78.8(1)	C(20)	Os(2)	C(21)	85.9(7)
Os(3)	Os(1)	C(10)	89.0(6)	C(20)	Os(2)	C(75)	102.7(8)
Os(3)	Os(1)	C(11)	175.2(7)	C(20)	Os(2)	C(76)	129.8(9)
Os(3)	Os(1)	C(12)	87.1(5)	C(20)	Os(2)	C(77)	165.4(8)
Os(3)	Os(1)	C(13)	91.0(6)	C(21)	Os(2)	C(75)	102.5(8)
S(1)	Os(1)	C(10)	92.5(7)	C(21)	Os(2)	C(76)	81.8(8)
S(1)	Os(1)	C(11)	96.4(7)	C(21)	Os(2)	C(77)	95.1(7)
S(1)	Os(1)	C(12)	86.9(7)	C(75)	Os(2)	C(76)	35.6(7)
S(1)	Os(1)	C(13)	169.8(6)	C(75)	Os(2)	C(77)	62.9(6)
C(10)	Os(1)	C(11)	91.8(8)	C(76)	Os(2)	C(77)	36.6(7)
C(10)	Os(1)	C(12)	176.1(8)	Os(1)	Os(3)	Os(2)	84.53(3)
C(10)	Os(1)	C(13)	88.2(9)	Os(1)	Os(3)	C(30)	170.3(8)
C(11)	Os(1)	C(12)	92.1(8)	Os(1)	Os(3)	C(31)	90.0(5)
C(11)	Os(1)	C(13)	94(1)	Os(1)	Os(3)	C(32)	85.7(6)
C(12)	Os(1)	C(13)	91.8(9)	Os(1)	Os(3)	C(33)	91.0(6)
Os(3)	Os(2)	S(1)	78.9(1)	Os(2)	Os(3)	C(30)	86.7(7)
Os(3)	Os(2)	C(20)	101.7(7)	Os(2)	Os(3)	C(31)	82.0(7)
Os(3)	Os(2)	C(21)	92.2(7)	Os(2)	Os(3)	C(32)	83.4(6)
Os(3)	Os(2)	C(75)	152.3(4)	Os(2)	Os(3)	C(33)	175.2(7)
Os(3)	Os(2)	C(76)	127.1(5)	C(30)	Os(3)	C(31)	92.9(8)
Os(3)	Os(2)	C(77)	92.8(5)	C(30)	Os(3)	C(32)	89.1(9)
S(1)	Os(2)	C(20)	91.2(6)	C(30)	Os(3)	C(33)	97.6(9)
S(1)	Os(2)	C(21)	169.9(7)	C(31)	Os(3)	C(32)	165.1(9)
S(1)	Os(2)	C(75)	87.7(4)	C(31)	Os(3)	C(33)	99.8(9)
S(1)	Os(2)	C(76)	107.4(6)	C(32)	Os(3)	C(33)	94.5(9)
S(1)	Os(2)	C(77)	90.1(5)	Os(1)	S(1)	Os(2)	107.1(2)

Angles are in degrees. Estimated standard deviations in the least significant figure are given in parentheses.

Table S11. Selected Bond Angles for 2. cont

atom	atom	atom	angle	atom	atom	atom	angle
Os(1)	S(1)	C(71)	104.7(7)				
Os(2)	S(1)	C(71)	113.8(7)				
Os(1)	C(10)	O(10)	176(2)				
Os(1)	C(11)	O(11)	175(2)				
Os(1)	C(12)	O(12)	174(2)				
Os(1)	C(13)	O(13)	175(2)				
Os(2)	C(20)	O(20)	172(2)				
Os(2)	C(21)	O(21)	176(1)				
Os(3)	C(30)	O(30)	176(2)				
Os(3)	C(31)	O(31)	180(2)				
Os(3)	C(32)	O(32)	175(2)				
Os(3)	C(33)	O(33)	177(2)				
S(1)	C(71)	C(72)	114(1)				
C(71)	C(72)	C(73)	120(2)				
C(72)	C(73)	C(74)	116(2)				
C(73)	C(74)	C(75)	115(2)				
Os(2)	C(75)	C(74)	116(1)				
Os(2)	C(75)	C(76)	68(1)				
C(74)	C(75)	C(76)	125(2)				
Os(2)	C(76)	C(75)	76(1)				
Os(2)	C(76)	C(77)	74(1)				
C(75)	C(76)	C(77)	118(2)				
Os(2)	C(77)	C(76)	69(1)				

Angles are in degrees. Estimated standard deviations in the least significant figure are given in parentheses.

Table S12. Selected Bond Angles for 4.

atom	atom	atom	angle	atom	atom	atom	angle
Os(1)	Os(2)	Os(3)	58.93(3)	C(75)	Os(2)	C(77)	64(1)
Os(1)	Os(2)	S(1)	53.5(2)	C(76)	Os(2)	C(77)	37(1)
Os(1)	Os(2)	C(20)	69.8(7)	Os(2)	Os(1)	Os(3)	61.63(3)
Os(1)	Os(2)	C(21)	113.7(7)	Os(2)	Os(1)	S(1)	55.6(1)
Os(1)	Os(2)	C(75)	136.4(8)	Os(2)	Os(1)	C(10)	112.3(8)
Os(1)	Os(2)	C(76)	162.1(7)	Os(2)	Os(1)	C(11)	140.8(8)
Os(1)	Os(2)	C(77)	130.5(6)	Os(2)	Os(1)	C(12)	111(1)
Os(3)	Os(2)	S(1)	80.6(1)	Os(3)	Os(1)	S(1)	83.3(1)
Os(3)	Os(2)	C(20)	118.0(7)	Os(3)	Os(1)	C(10)	172.8(7)
Os(3)	Os(2)	C(21)	86.1(7)	Os(3)	Os(1)	C(11)	90.0(7)
Os(3)	Os(2)	C(75)	149.1(8)	Os(3)	Os(1)	C(12)	88.7(9)
Os(3)	Os(2)	C(76)	118.9(8)	S(1)	Os(1)	C(10)	96.4(9)
Os(3)	Os(2)	C(77)	85.7(6)	S(1)	Os(1)	C(11)	97.3(9)
S(1)	Os(2)	C(20)	96.0(6)	S(1)	Os(1)	C(12)	167(1)
S(1)	Os(2)	C(21)	165.2(7)	C(10)	Os(1)	C(11)	97(1)
S(1)	Os(2)	C(75)	91.5(7)	C(10)	Os(1)	C(12)	90(1)
S(1)	Os(2)	C(76)	109.1(7)	C(11)	Os(1)	C(12)	93(1)
S(1)	Os(2)	C(77)	90.2(6)	Os(2)	Os(3)	Os(1)	59.44(3)
C(20)	Os(2)	C(21)	84.5(9)	Os(2)	Os(3)	C(30)	155.0(7)
C(20)	Os(2)	C(75)	92(1)	Os(2)	Os(3)	C(31)	85.3(8)
C(20)	Os(2)	C(76)	120(1)	Os(2)	Os(3)	C(32)	103(1)
C(20)	Os(2)	C(77)	156.2(9)	Os(2)	Os(3)	C(33)	88.3(7)
C(21)	Os(2)	C(75)	103(1)	Os(1)	Os(3)	C(30)	95.5(7)
C(21)	Os(2)	C(76)	83(1)	Os(1)	Os(3)	C(31)	87.6(8)
C(21)	Os(2)	C(77)	95(1)	Os(1)	Os(3)	C(32)	162.9(9)
C(75)	Os(2)	C(76)	36(1)	Os(1)	Os(3)	C(33)	89.8(7)

Angles are in degrees. Estimated standard deviations in the least significant figure are given in parentheses.

Table S12. Selected Bond Angles for 4. cont

atom	atom	atom	angle	atom	atom	atom	angle
C(30)	Os(3)	C(31)	94(1)	Os(2)	C(76)	C(77)	74(2)
C(30)	Os(3)	C(32)	102(1)	C(75)	C(76)	C(77)	121(2)
C(30)	Os(3)	C(33)	92(1)	Os(2)	C(77)	C(76)	69(2)
C(31)	Os(3)	C(32)	90(1)				
C(31)	Os(3)	C(33)	174(1)				
C(32)	Os(3)	C(33)	90(1)				
Os(2)	S(1)	Os(1)	70.9(2)				
Os(2)	S(1)	C(71)	118.5(9)				
Os(1)	S(1)	C(71)	111(1)				
Os(1)	C(10)	O(10)	170(2)				
Os(1)	C(11)	O(11)	177(3)				
Os(1)	C(12)	O(12)	177(3)				
Os(2)	C(20)	O(20)	168(2)				
Os(2)	C(21)	O(21)	175(2)				
Os(3)	C(30)	O(30)	175(2)				
Os(3)	C(31)	O(31)	178(2)				
Os(3)	C(32)	O(32)	180(3)				
Os(3)	C(33)	O(33)	173(2)				
S(1)	C(71)	C(72)	120(2)				
C(71)	C(72)	C(73)	119(3)				
C(72)	C(73)	C(74)	124(3)				
C(73)	C(74)	C(75)	122(3)				
Os(2)	C(75)	C(74)	118(2)				
Os(2)	C(75)	C(76)	67(2)				
C(74)	C(75)	C(76)	130(3)				
Os(2)	C(76)	C(75)	77(2)				

Angles are in degrees. Estimated standard deviations in the least

Table S14. Anisotropic Thermal Parameters. U-values for 1.

atom	U11	U22	U33	U12	U13	U23
Os(1)	0.0492(9)	0.0543(8)	0.0464(6)	0.0021(7)	0.0097(5)	0.0016(5)
Os(2)	0.058(1)	0.0620(8)	0.0530(7)	-0.0103(7)	0.0124(6)	-0.0074(6)
Os(3)	0.0487(9)	0.0681(9)	0.0650(7)	0.0009(8)	0.0103(6)	0.0034(6)
Os(4)	0.070(1)	0.0552(8)	0.0523(7)	-0.0012(8)	0.0091(6)	0.0057(5)
Os(5)	0.091(1)	0.0652(9)	0.0616(8)	0.0132(9)	0.0184(7)	0.0150(6)
Os(6)	0.072(1)	0.0654(9)	0.0647(7)	0.0059(8)	0.0064(7)	-0.0026(6)
S(1)	0.046(5)	0.061(5)	0.056(4)	-0.004(4)	0.005(4)	0.002(3)
S(2)	0.068(7)	0.065(5)	0.066(4)	-0.013(5)	0.006(4)	0.003(4)
O(10)	0.11(2)	0.07(2)	0.10(2)	0.01(2)	0.03(2)	0.01(1)
O(11)	0.06(2)	0.09(2)	0.09(2)	0.01(2)	0.00(1)	0.02(1)
O(12)	0.18(4)	0.13(2)	0.07(1)	0.02(2)	0.05(2)	-0.03(2)
O(20)	0.12(3)	0.08(2)	0.12(2)	0.02(2)	0.03(2)	0.02(2)
O(21)	0.15(3)	0.11(2)	0.07(2)	-0.03(2)	-0.01(2)	0.01(1)
O(22)	0.09(2)	0.13(2)	0.11(2)	-0.02(2)	0.00(2)	-0.05(2)
O(30)	0.12(3)	0.18(3)	0.09(2)	-0.03(3)	-0.03(2)	-0.02(2)
O(31)	0.12(3)	0.08(2)	0.10(2)	0.02(2)	0.00(2)	0.02(1)
O(32)	0.07(2)	0.15(3)	0.08(1)	0.03(2)	0.02(1)	-0.01(2)
O(33)	0.09(2)	0.07(2)	0.13(2)	-0.02(2)	0.05(2)	0.01(1)
O(40)	0.15(3)	0.12(2)	0.08(2)	-0.06(2)	0.00(2)	-0.04(2)
O(41)	0.15(3)	0.08(2)	0.06(1)	-0.01(2)	0.03(2)	0.02(1)

Table S14. Anisotropic Thermal Parameters. U-values for 1.

atom	U11	U22	U33	U12	U13	U23
O(42)	0.09(2)	0.07(2)	0.10(2)	0.02(2)	0.00(1)	0.00(1)
O(50)	0.11(3)	0.08(2)	0.17(3)	0.01(2)	0.07(2)	-0.02(2)
O(51)	0.18(4)	0.13(3)	0.07(2)	0.00(2)	0.03(2)	0.01(2)
O(52)	0.15(4)	0.12(3)	0.18(3)	0.03(3)	-0.02(3)	0.10(2)
O(60)	0.16(3)	0.10(2)	0.14(2)	-0.03(2)	0.06(2)	0.01(2)
O(61)	0.14(3)	0.10(2)	0.15(2)	-0.02(2)	0.07(2)	-0.04(2)
O(62)	0.12(3)	0.17(3)	0.13(2)	0.06(3)	0.02(2)	-0.02(2)
O(63)	0.10(2)	0.10(2)	0.08(2)	0.04(2)	-0.01(1)	-0.02(1)
C(10)	0.07(3)	0.04(2)	0.06(2)	0.01(2)	0.02(2)	0.00(1)
C(11)	0.05(2)	0.07(2)	0.05(2)	0.01(2)	0.00(1)	-0.01(2)
C(12)	0.02(2)	0.09(3)	0.10(2)	-0.01(2)	-0.01(2)	0.01(2)
C(20)	0.08(3)	0.08(3)	0.09(2)	0.00(2)	0.04(2)	-0.04(2)
C(21)	0.11(4)	0.10(3)	0.06(2)	0.02(3)	0.01(2)	-0.02(2)
C(22)	0.06(3)	0.09(3)	0.06(2)	0.01(2)	-0.03(2)	-0.03(2)
C(30)	0.05(2)	0.07(2)	0.09(2)	0.05(2)	-0.01(2)	0.00(2)
C(31)	0.02(2)	0.08(3)	0.12(3)	0.00(2)	0.01(2)	0.01(2)
C(32)	0.11(4)	0.12(3)	0.08(2)	0.11(3)	0.03(2)	0.04(2)
C(33)	0.07(3)	0.11(3)	0.09(2)	-0.08(3)	0.04(2)	-0.04(2)
C(40)	0.14(5)	0.08(3)	0.07(2)	-0.03(3)	0.02(2)	0.00(2)
C(41)	0.08(3)	0.09(3)	0.06(2)	0.00(3)	-0.02(2)	-0.01(2)

Table S14. Anisotropic Thermal Parameters. U-values for 1.

atom	U11	U22	U33	U12	U13	U23
C(42)	0.03(2)	0.07(2)	0.08(2)	0.00(2)	0.01(2)	0.01(2)
C(50)	0.08(3)	0.10(3)	0.13(3)	0.07(3)	0.06(3)	0.07(3)
C(51)	0.12(4)	0.09(3)	0.04(2)	0.04(3)	0.01(2)	0.01(2)
C(52)	0.11(4)	0.10(3)	0.08(2)	-0.01(3)	0.00(2)	0.04(2)
C(60)	0.08(3)	0.10(3)	0.05(2)	-0.03(3)	-0.02(2)	-0.05(2)
C(61)	0.04(2)	0.10(3)	0.12(3)	0.01(2)	0.03(2)	0.04(2)
C(62)	0.04(2)	0.05(2)	0.13(3)	0.01(2)	-0.06(2)	0.00(2)
C(63)	0.04(2)	0.10(3)	0.07(2)	0.02(2)	0.00(2)	0.01(2)
C(71)	0.02(2)	0.11(3)	0.10(2)	0.03(2)	0.00(2)	0.05(2)
C(72)	0.06(2)	0.06(2)	0.12(3)	-0.02(2)	0.04(2)	-0.03(2)
C(74)	0.06(3)	0.10(3)	0.08(2)	0.01(2)	0.03(2)	-0.03(2)
C(75)	0.08(3)	0.06(2)	0.06(2)	-0.01(2)	0.03(2)	-0.02(2)
C(76)	0.03(2)	0.09(3)	0.08(2)	-0.01(2)	0.00(2)	-0.06(2)
C(77)	0.06(3)	0.11(3)	0.08(2)	-0.02(2)	0.04(2)	-0.03(2)
C(81)	0.09(3)	0.10(3)	0.12(3)	-0.02(3)	0.03(3)	0.06(2)
C(82)	0.07(3)	0.13(4)	0.09(2)	0.01(3)	0.01(2)	0.01(2)
C(83)	0.05(3)	0.08(2)	0.11(3)	0.01(2)	0.02(2)	0.01(2)
C(84)	0.09(3)	0.08(3)	0.09(2)	-0.02(2)	0.02(2)	0.03(2)
C(85)	0.10(3)	0.06(2)	0.09(2)	0.03(2)	0.05(2)	0.01(2)
C(86)	0.08(3)	0.08(2)	0.05(2)	-0.01(2)	0.00(2)	0.03(2)
C(87)	0.04(2)	0.13(3)	0.08(2)	0.01(2)	0.01(2)	0.03(2)

Table S15. Anisotropic Thermal Parameters. U-values for 2.

atom	U11	U22	U33	U12	U13	U23
Os(1)	0.0405(4)	0.0419(5)	0.0424(4)	-0.0053(3)	0.0191(3)	-0.0041(3)
Os(2)	0.0390(4)	0.0349(4)	0.0409(4)	-0.0012(3)	0.0141(3)	-0.0033(3)
Os(3)	0.0410(4)	0.0458(5)	0.0403(4)	-0.0010(4)	0.0163(3)	-0.0090(4)
S(1)	0.041(2)	0.038(3)	0.039(2)	-0.007(2)	0.016(2)	-0.004(2)
O(10)	0.056(9)	0.09(1)	0.10(1)	0.021(9)	0.007(9)	0.012(9)
O(11)	0.09(1)	0.07(1)	0.10(1)	-0.02(1)	0.05(1)	-0.01(1)
O(12)	0.07(1)	0.07(1)	0.08(1)	0.017(9)	0.020(8)	0.013(8)
O(13)	0.10(1)	0.13(2)	0.08(1)	-0.04(1)	0.05(1)	0.00(1)
O(20)	0.040(8)	0.09(1)	0.067(9)	0.012(8)	0.009(7)	0.010(8)
O(21)	0.12(1)	0.04(1)	0.09(1)	0.014(9)	0.04(1)	-0.010(8)
O(30)	0.08(1)	0.09(1)	0.10(1)	-0.02(1)	0.025(9)	-0.03(1)
O(31)	0.06(1)	0.12(2)	0.09(1)	0.03(1)	0.010(9)	0.02(1)
O(32)	0.052(8)	0.10(1)	0.062(9)	0.009(9)	0.010(7)	0.004(8)
O(33)	0.11(1)	0.10(1)	0.057(9)	-0.01(1)	0.041(9)	0.007(9)
C(10)	0.05(1)	0.07(2)	0.06(1)	-0.02(1)	0.03(1)	-0.01(1)
C(11)	0.06(1)	0.04(1)	0.07(1)	0.00(1)	0.01(1)	-0.01(1)
C(12)	0.07(1)	0.05(1)	0.04(1)	-0.01(1)	0.04(1)	-0.01(1)
C(13)	0.07(1)	0.09(2)	0.06(1)	-0.05(1)	0.04(1)	0.00(1)
C(20)	0.05(1)	0.06(1)	0.05(1)	0.00(1)	0.00(1)	-0.02(1)
C(21)	0.020(9)	0.05(1)	0.06(1)	0.005(9)	-0.001(8)	-0.01(1)
C(30)	0.06(1)	0.05(1)	0.07(1)	-0.01(1)	0.04(1)	0.00(1)
C(31)	0.07(1)	0.04(1)	0.06(1)	0.00(1)	0.02(1)	-0.02(1)
C(32)	0.06(1)	0.07(2)	0.03(1)	-0.01(1)	0.01(1)	-0.01(1)
C(33)	0.04(1)	0.08(2)	0.04(1)	-0.01(1)	0.01(1)	-0.01(1)
C(71)	0.05(1)	0.07(2)	0.05(1)	-0.01(1)	0.03(1)	-0.02(1)
C(72)	0.08(2)	0.09(2)	0.05(1)	-0.01(1)	0.03(1)	0.00(1)
C(73)	0.09(2)	0.06(2)	0.05(1)	0.00(1)	0.03(1)	0.00(1)
C(74)	0.06(1)	0.08(2)	0.06(1)	-0.01(1)	0.04(1)	-0.01(1)
C(75)	0.06(1)	0.02(1)	0.07(1)	-0.003(9)	0.03(1)	-0.01(1)
C(76)	0.07(1)	0.06(1)	0.09(2)	-0.01(1)	0.06(1)	-0.01(1)
C(77)	0.04(1)	0.09(2)	0.03(1)	0.00(1)	0.018(8)	-0.03(1)

Table S16. Anisotropic Thermal Parameters. U-values for 4.

atom	U11	U22	U33	U12	U13	U23
Os(2)	0.0448(5)	0.0357(6)	0.0527(5)	0.0034(4)	-0.0046(4)	-0.0042(4)
Os(1)	0.0490(5)	0.0541(7)	0.0491(5)	0.0133(4)	0.0019(4)	-0.0088(4)
Os(3)	0.0509(5)	0.0654(7)	0.0430(5)	-0.0021(5)	0.0028(4)	-0.0001(5)
S(1)	0.056(3)	0.060(4)	0.078(4)	-0.015(3)	-0.011(3)	0.018(3)
O(10)	0.12(2)	0.28(3)	0.06(1)	0.06(2)	0.03(1)	-0.07(2)
O(11)	0.07(1)	0.17(2)	0.10(1)	0.05(1)	-0.03(1)	0.00(1)
O(12)	0.23(3)	0.06(2)	0.22(3)	0.03(2)	-0.04(2)	-0.04(2)
O(20)	0.09(1)	0.11(2)	0.047(9)	0.02(1)	-0.006(9)	-0.04(1)
O(21)	0.05(1)	0.09(1)	0.11(1)	-0.02(1)	-0.003(9)	0.01(1)
O(30)	0.14(2)	0.10(2)	0.08(1)	0.01(1)	-0.04(1)	0.03(1)
O(31)	0.13(2)	0.11(2)	0.13(2)	-0.05(2)	-0.06(1)	0.03(1)
O(32)	0.07(1)	0.33(4)	0.09(1)	0.07(2)	0.01(1)	-0.02(2)
O(33)	0.12(2)	0.08(2)	0.11(1)	-0.03(1)	-0.04(1)	-0.02(1)
C(10)	0.07(2)	0.12(3)	0.06(2)	0.02(2)	-0.01(1)	0.00(2)
C(11)	0.05(1)	0.10(2)	0.08(2)	0.05(1)	0.00(1)	-0.02(1)
C(12)	0.14(3)	0.05(2)	0.09(2)	0.01(2)	-0.04(2)	-0.03(2)
C(20)	0.06(1)	0.05(2)	0.08(2)	0.00(1)	0.02(1)	0.02(1)
C(21)	0.05(1)	0.07(2)	0.07(1)	0.01(1)	-0.01(1)	0.00(1)
C(30)	0.06(2)	0.07(2)	0.08(2)	-0.02(1)	-0.02(1)	0.02(2)
C(31)	0.09(2)	0.09(2)	0.08(2)	-0.01(2)	-0.03(2)	0.02(2)
C(32)	0.07(2)	0.24(5)	0.05(2)	0.05(2)	-0.01(1)	0.00(2)
C(33)	0.06(2)	0.10(2)	0.05(1)	0.00(2)	0.03(1)	0.00(1)
C(71)	0.07(2)	0.18(4)	0.11(2)	-0.03(2)	-0.01(2)	0.06(3)
C(72)	0.11(3)	0.24(5)	0.10(3)	0.05(3)	0.00(2)	0.05(3)
C(73)	0.12(3)	0.14(4)	0.10(2)	-0.08(3)	-0.02(2)	0.05(2)
C(74)	0.11(2)	0.03(2)	0.20(4)	0.00(2)	-0.06(2)	0.02(2)
C(75)	0.11(2)	0.02(1)	0.16(3)	0.00(2)	-0.05(2)	0.02(2)
C(76)	0.09(2)	0.07(2)	0.10(2)	0.05(2)	0.01(2)	0.00(2)
C(77)	0.08(2)	0.10(2)	0.06(2)	0.02(2)	-0.02(1)	-0.02(1)

Table S17. Anisotropic Thermal Parameters. U-values for 5.

atom	U11	U22	U33	U12	U13	U23
Os(1)	0.0413(6)	0.0415(6)	0.0413(8)	-0.0026(5)	0.0059(5)	-0.0045(5)
Os(2)	0.0377(6)	0.0377(6)	0.0448(8)	0.0006(4)	0.0050(5)	-0.0044(5)
Os(3)	0.0391(6)	0.0471(6)	0.0441(8)	0.0027(5)	0.0042(5)	0.0055(6)
Os(4)	0.0410(6)	0.0371(6)	0.0351(8)	0.0010(4)	0.0092(5)	0.0010(5)
Os(5)	0.0394(6)	0.0517(6)	0.0370(8)	-0.0047(5)	0.0092(5)	-0.0050(6)
Os(6)	0.0357(6)	0.0431(6)	0.0556(9)	-0.0040(5)	0.0109(5)	-0.0021(6)
S(1)	0.041(4)	0.037(4)	0.068(6)	0.000(3)	0.014(4)	-0.005(4)
S(2)	0.045(4)	0.042(4)	0.060(6)	0.005(3)	0.009(4)	0.003(4)
O(10)	0.15(2)	0.05(1)	0.05(2)	0.00(1)	0.01(1)	-0.01(1)
O(11)	0.10(2)	0.11(2)	0.07(2)	0.01(1)	0.02(2)	0.00(2)
O(12)	0.04(1)	0.10(2)	0.11(2)	0.00(1)	-0.03(1)	-0.02(1)
O(20)	0.10(2)	0.08(1)	0.06(2)	0.01(1)	0.04(1)	-0.02(1)
O(21)	0.06(1)	0.07(1)	0.06(2)	0.01(1)	0.00(1)	0.00(1)
O(30)	0.05(1)	0.10(2)	0.06(2)	0.01(1)	0.02(1)	-0.01(1)
O(31)	0.10(2)	0.09(2)	0.11(3)	-0.03(1)	-0.03(2)	-0.01(2)
O(32)	0.06(1)	0.10(2)	0.12(2)	0.03(1)	0.01(1)	0.03(2)
O(33)	0.07(1)	0.09(2)	0.16(3)	-0.04(1)	0.00(2)	0.04(2)
O(40)	0.05(1)	0.08(1)	0.08(2)	0.01(1)	0.04(1)	0.01(1)
O(41)	0.07(1)	0.09(2)	0.07(2)	-0.04(1)	0.00(1)	0.00(1)
O(42)	0.09(2)	0.06(1)	0.05(2)	0.01(1)	-0.02(1)	0.01(1)
O(50)	0.05(1)	0.06(1)	0.07(2)	0.015(9)	0.01(1)	-0.01(1)
O(51)	0.07(1)	0.10(2)	0.14(3)	-0.01(1)	0.02(1)	-0.05(2)
O(60)	0.05(1)	0.08(1)	0.13(2)	-0.01(1)	0.00(1)	-0.01(1)
O(61)	0.05(1)	0.08(1)	0.12(2)	-0.01(1)	0.04(1)	0.01(1)
O(62)	0.08(1)	0.09(1)	0.03(1)	0.04(1)	0.00(1)	0.00(1)
O(63)	0.07(2)	0.21(3)	0.03(2)	-0.01(2)	0.00(1)	-0.06(2)
C(10)	0.05(2)	0.04(2)	0.05(2)	0.01(1)	-0.02(1)	-0.02(1)
C(11)	0.07(2)	0.03(1)	0.08(3)	-0.03(1)	0.01(2)	0.00(2)
C(12)	0.04(2)	0.05(2)	0.09(3)	0.00(1)	0.01(2)	0.00(2)
C(20)	0.09(2)	0.03(2)	0.05(2)	-0.01(2)	0.00(2)	0.00(2)
C(21)	0.04(2)	0.11(3)	0.05(3)	-0.02(2)	0.02(2)	-0.05(2)
C(30)	0.07(2)	0.09(2)	0.02(2)	-0.03(2)	0.00(2)	-0.02(2)
C(31)	0.05(2)	0.05(2)	0.15(5)	0.00(2)	0.02(3)	0.05(3)
C(33)	0.02(1)	0.12(3)	0.04(2)	0.00(2)	0.00(1)	0.00(2)
C(40)	0.07(2)	0.05(2)	0.06(3)	-0.01(1)	0.02(2)	0.00(2)
C(41)	0.05(2)	0.03(1)	0.07(2)	-0.01(1)	0.03(2)	-0.02(1)
C(42)	0.04(1)	0.03(1)	0.06(2)	0.00(1)	0.01(1)	0.02(1)
C(50)	0.08(2)	0.02(1)	0.03(2)	0.01(1)	0.03(2)	0.00(1)
C(51)	0.06(2)	0.09(2)	0.05(3)	-0.01(2)	0.03(2)	-0.01(2)
C(60)	0.03(2)	0.06(2)	0.12(3)	0.01(1)	0.01(2)	0.03(2)

Table S17. Anisotropic Thermal Parameters. U-values for 5.

atom	U11	U22	U33	U12	U13	U23
C(61)	0.05(2)	0.03(1)	0.07(2)	-0.01(1)	0.01(2)	0.01(1)
C(62)	0.05(2)	0.09(2)	0.08(3)	-0.03(2)	0.01(2)	-0.05(2)
C(63)	0.04(2)	0.12(3)	0.05(3)	0.01(2)	0.02(2)	-0.01(2)
C(71)	0.07(2)	0.05(2)	0.05(2)	-0.02(1)	0.05(2)	0.00(1)
C(72)	0.06(2)	0.06(2)	0.08(3)	0.00(1)	0.03(2)	0.01(2)
C(73)	0.09(2)	0.05(2)	0.07(3)	0.00(2)	0.03(2)	0.02(2)
C(74)	0.07(2)	0.02(1)	0.11(3)	-0.04(1)	0.03(2)	-0.01(2)
C(75)	0.04(1)	0.04(2)	0.07(2)	-0.02(1)	-0.01(1)	-0.02(2)
C(76)	0.04(2)	0.06(2)	0.11(3)	-0.03(1)	-0.03(2)	0.00(2)
C(77)	0.07(2)	0.07(2)	0.06(3)	0.00(2)	-0.04(2)	-0.02(2)
C(81)	0.07(2)	0.03(1)	0.06(2)	-0.02(1)	-0.01(2)	0.01(1)
C(82)	0.05(2)	0.07(2)	0.10(3)	-0.01(1)	-0.01(2)	0.03(2)
C(83)	0.09(2)	0.08(2)	0.07(3)	-0.04(2)	0.03(2)	0.04(2)
C(84)	0.03(1)	0.07(2)	0.10(3)	-0.02(1)	0.00(2)	0.02(2)
C(85)	0.06(2)	0.11(2)	0.07(3)	-0.02(2)	0.04(2)	0.04(2)
C(86)	0.06(2)	0.06(2)	0.04(2)	-0.02(1)	0.02(2)	0.02(1)
C(87)	0.08(2)	0.13(3)	0.02(2)	-0.01(2)	0.00(2)	0.00(2)