Supplementary data (ESI) for *Dalton Transactions*

Supplementary Data

To accompany, "Synthesis and structure of two tetranuclear osmium carbonyl isotopomers: A crystallographic isotope effect." by John P. Canal,[*,a] Michael Jennings,[b] Glenn P. A. Yap,[c] and Roland K. Pomeroy[a]

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Captions

Figure S1. (a) IR (KBr) spectrum of $[Os_4(\mu\text{-H})(\mu\text{-OH})(\mu\text{-CO})(CO)_{12}\cdot H_2O]$ (**1·H$_2$O**) (* stretches due to CO_2). (b) IR (hexanes) spectrum (ν(CO) region) of **1·H$_2$O**.

Figure S2. ^{1}H NMR spectra of (A) $Os_4(\mu\text{-H})(\mu\text{-OD})(\mu\text{-CO})(CO)_{12}$ (**2**) and (B) **1·H$_2$O**.

Table S1. Summary of Crystal Data and Details of Intensity Collection for $[Os_4(\mu\text{-H})(\mu\text{-OH})(\mu\text{-CO})(CO)_{12}\cdot H_2O]$ (**1.H$_2$O**)

Table S2. Atomic Coordinates for **1.H$_2$O**

Table S3. Bond Lengths and Angles for **1.H$_2$O**

Table S4. Anisotropic Thermal Parameters for **1.H$_2$O**

Table S5. Hydrogen Atom Coordinates for **1.H$_2$O**

Table S6. Summary of Crystal Data and Details of Intensity Collection for $[Os_4(\mu\text{-H})(\mu\text{-OD})(\mu\text{-CO})(CO)_{12}]$ (**2**)

Table S7. Atomic Coordinates for **2**

Table S8. Bond Lengths and Angles for **2**

Table S9. Anisotropic Thermal Parameters for **2**

Table S10. Hydrogen Atom Coordinates for **2**

Figures

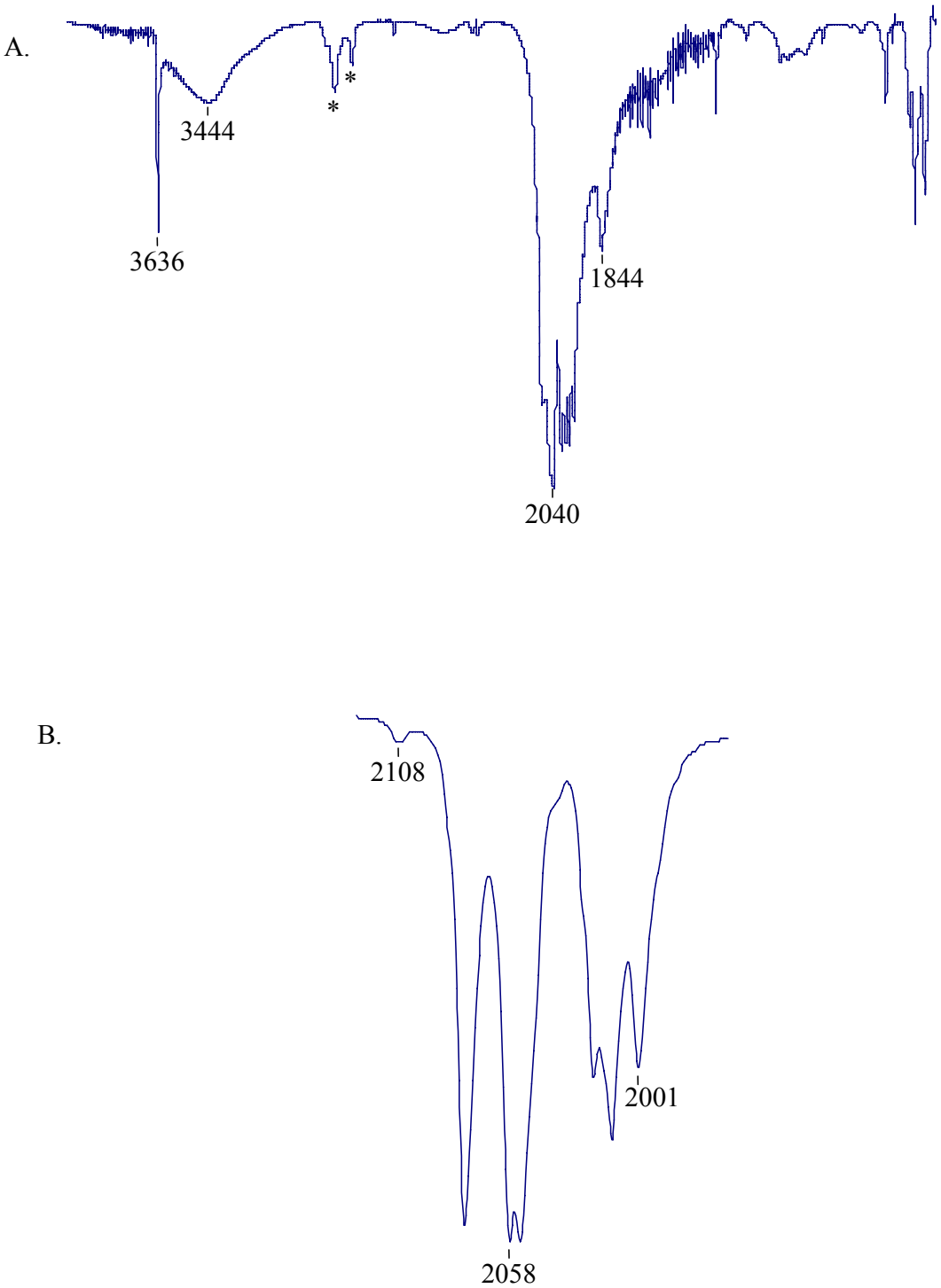

Figure S1.

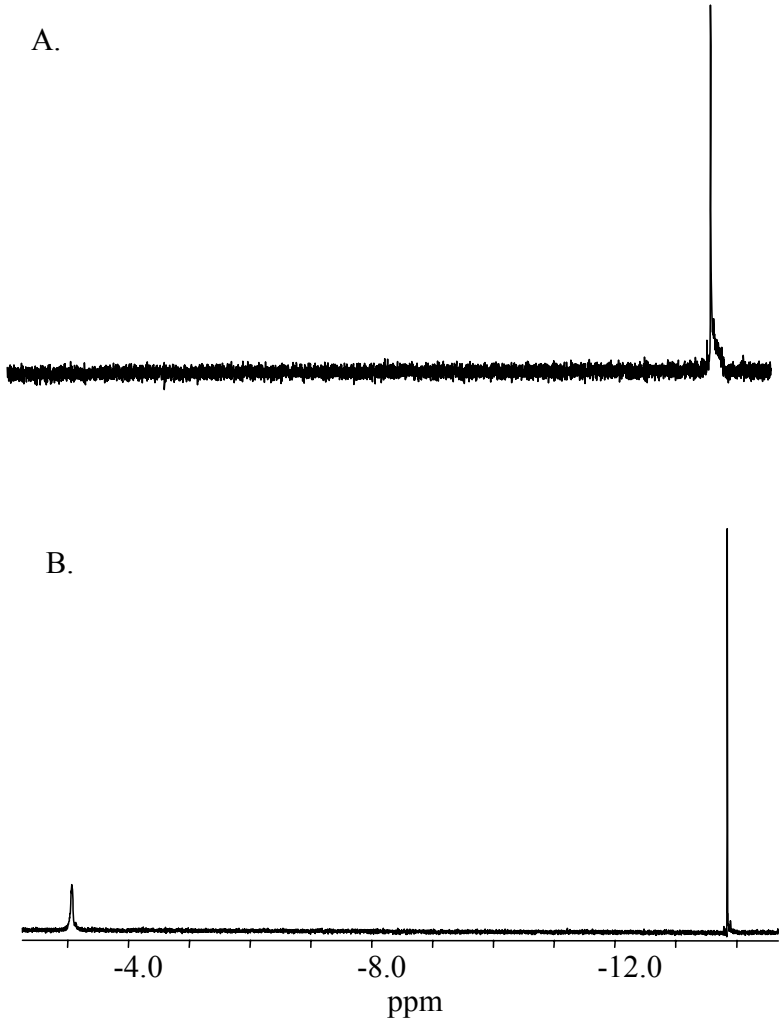

Figure S2.

Tables

Table S1. Summary of Crystal Data and Details of Intensity Collection for $[Os_4(\mu\text{-}H)(\mu\text{-}OH)(\mu\text{-}CO)(CO)_{12}\cdot H_2O]$ (**1.H$_2$O**)

Identification code	rp013 (**1.H$_2$O**)
Empirical formula	C13 H4 O15 Os4
Formula weight	1160.96
Temperature	203(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, C2/c
Unit cell dimensions	a = 29.882(2) A alpha = 90 deg.
	b = 9.4147(7) A beta = 105.2270(10) deg.
	c = 15.2741(12) A gamma = 90 deg.
Volume	4146.3(6) A^3
Z, Calculated density	8, 3.720 Mg/m^3
Absorption coefficient	24.512 mm^-1
F(000)	4048
Crystal size	0.1 x 0.1 x 0.1 mm
Theta range for data collection	1.41 to 28.76 deg.
Limiting indices	-38<=h<=37, 0<=k<=12, 0<=l<=20
Reflections collected / unique	4932 / 4932 [R(int) = 0.0000]
Completeness to theta = 28.76	91.4 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.928075 and 0.735427
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4932 / 1 / 292
Goodness-of-fit on F^2	1.034
Final R indices [I>2sigma(I)]	R1 = 0.0286, wR2 = 0.0633
R indices (all data)	R1 = 0.0358, wR2 = 0.0644
Largest diff. peak and hole	2.231 and -1.711 e.A^-3

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for **1.H$_2$O** U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Os(1)	687(1)	-3140(1)	10475(1)	17(1)
Os(2)	1668(1)	-2516(1)	10527(1)	16(1)
Os(3)	1387(1)	-2923(1)	12131(1)	15(1)
Os(4)	1322(1)	-168(1)	11324(1)	17(1)
C(1)	264(3)	-3103(8)	9259(5)	24(2)
O(1)	25(2)	-3184(8)	8557(4)	45(2)
C(2)	754(3)	-5101(9)	10401(5)	24(2)
O(2)	792(2)	-6316(7)	10342(4)	39(2)
C(3)	234(3)	-3358(9)	11143(5)	25(2)
O(3)	-37(2)	-3506(8)	11532(4)	41(2)
C(4)	1696(3)	-1404(8)	9514(5)	22(2)
O(4)	1727(2)	-749(7)	8902(4)	40(2)
C(5)	1834(3)	-4243(9)	10015(5)	27(2)
O(5)	1940(3)	-5265(7)	9720(4)	43(2)
C(6)	2291(3)	-2069(8)	11154(5)	20(2)
O(6)	2665(2)	-1782(7)	11500(4)	34(1)
C(7)	1660(3)	-4609(9)	11723(5)	22(2)
O(7)	1775(2)	-5761(6)	11635(4)	29(1)
C(8)	1937(3)	-2487(9)	13088(5)	22(2)
O(8)	2261(2)	-2255(7)	13663(4)	39(2)
C(9)	1107(3)	-4139(9)	12833(5)	25(2)
O(9)	935(2)	-4856(7)	13248(4)	42(2)
C(10)	1924(3)	302(8)	12018(5)	23(2)
O(10)	2285(2)	582(7)	12442(4)	37(2)
C(11)	1067(3)	1360(9)	11896(5)	26(2)
O(11)	956(2)	2261(7)	12277(4)	40(2)
C(12)	1400(3)	987(9)	10358(5)	26(2)
O(12)	1445(3)	1755(7)	9802(4)	45(2)
C(13)	1004(3)	-1418(9)	12451(5)	21(2)
O(13)	739(2)	-917(7)	12788(4)	37(2)
O(14)	651(2)	-900(6)	10602(3)	24(1)
O(15)	164(2)	146(7)	9013(4)	44(2)

Table S3. Bond lengths [Å] and angles [deg] for **1.H_2O**

Os(1)-C(2)	1.864(9)
Os(1)-C(3)	1.910(8)
Os(1)-C(1)	1.953(8)
Os(1)-O(14)	2.123(5)
Os(1)-Os(3)	2.8343(4)
Os(1)-Os(2)	2.9701(5)
Os(2)-C(4)	1.887(7)
Os(2)-C(6)	1.904(8)
Os(2)-C(5)	1.924(9)
Os(2)-Os(3)	2.8170(4)
Os(2)-Os(4)	2.8466(4)
Os(3)-C(9)	1.906(8)
Os(3)-C(8)	1.935(8)
Os(3)-C(7)	1.959(8)
Os(3)-C(13)	1.963(8)
Os(3)-Os(4)	2.8569(4)
Os(4)-C(10)	1.887(8)
Os(4)-C(12)	1.895(8)
Os(4)-C(11)	1.940(8)
Os(4)-O(14)	2.132(5)
Os(4)-C(13)	2.472(7)
C(1)-O(1)	1.124(9)
C(2)-O(2)	1.154(10)
C(3)-O(3)	1.132(9)
C(4)-O(4)	1.144(9)
C(5)-O(5)	1.141(10)
C(6)-O(6)	1.136(9)
C(7)-O(7)	1.155(10)
C(8)-O(8)	1.144(10)
C(9)-O(9)	1.138(10)
C(10)-O(10)	1.133(10)
C(11)-O(11)	1.126(10)
C(12)-O(12)	1.150(10)
C(13)-O(13)	1.152(9)
O(14)-O(15)	2.669(8)
H(1)-Os(1)	1.75(4)
H(1)-Os(2)	1.76(4)
C(2)-Os(1)-C(3)	91.6(4)
C(2)-Os(1)-C(1)	90.7(3)
C(3)-Os(1)-C(1)	97.8(3)
C(2)-Os(1)-O(14)	176.7(3)
C(3)-Os(1)-O(14)	89.9(3)

C(1)-Os(1)-O(14)	91.9(3)
C(2)-Os(1)-Os(3)	93.4(2)
C(3)-Os(1)-Os(3)	89.5(2)
C(1)-Os(1)-Os(3)	171.5(2)
O(14)-Os(1)-Os(3)	83.70(14)
C(2)-Os(1)-Os(2)	94.4(2)
C(3)-Os(1)-Os(2)	147.2(2)
C(1)-Os(1)-Os(2)	114.2(2)
O(14)-Os(1)-Os(2)	82.79(15)
Os(3)-Os(1)-Os(2)	58.011(10)
C(4)-Os(2)-C(6)	92.5(3)
C(4)-Os(2)-C(5)	93.7(3)
C(6)-Os(2)-C(5)	94.0(3)
C(4)-Os(2)-Os(3)	151.1(2)
C(6)-Os(2)-Os(3)	93.9(2)
C(5)-Os(2)-Os(3)	114.0(2)
C(4)-Os(2)-Os(4)	91.1(2)
C(6)-Os(2)-Os(4)	91.7(2)
C(5)-Os(2)-Os(4)	172.4(2)
Os(3)-Os(2)-Os(4)	60.582(10)
C(4)-Os(2)-Os(1)	110.0(2)
C(6)-Os(2)-Os(1)	152.3(2)
C(5)-Os(2)-Os(1)	100.4(2)
Os(3)-Os(2)-Os(1)	58.578(10)
Os(4)-Os(2)-Os(1)	72.415(11)
C(9)-Os(3)-C(8)	96.5(3)
C(9)-Os(3)-C(7)	88.5(3)
C(8)-Os(3)-C(7)	94.0(3)
C(9)-Os(3)-C(13)	85.6(3)
C(8)-Os(3)-C(13)	95.4(3)
C(7)-Os(3)-C(13)	169.4(3)
C(9)-Os(3)-Os(2)	147.8(2)
C(8)-Os(3)-Os(2)	103.9(2)
C(7)-Os(3)-Os(2)	65.8(2)
C(13)-Os(3)-Os(2)	116.4(2)
C(9)-Os(3)-Os(1)	97.4(2)
C(8)-Os(3)-Os(1)	166.1(2)
C(7)-Os(3)-Os(1)	86.0(2)
C(13)-Os(3)-Os(1)	86.1(2)
Os(2)-Os(3)-Os(1)	63.411(11)
C(9)-Os(3)-Os(4)	142.9(2)
C(8)-Os(3)-Os(4)	94.7(2)
C(7)-Os(3)-Os(4)	125.8(2)
C(13)-Os(3)-Os(4)	58.2(2)
Os(2)-Os(3)-Os(4)	60.222(10)
Os(1)-Os(3)-Os(4)	74.312(11)

C(10)-Os(4)-C(12)	90.5(3)
C(10)-Os(4)-C(11)	90.1(3)
C(12)-Os(4)-C(11)	93.9(3)
C(10)-Os(4)-O(14)	174.3(3)
C(12)-Os(4)-O(14)	94.2(3)
C(11)-Os(4)-O(14)	92.6(3)
C(10)-Os(4)-C(13)	101.8(3)
C(12)-Os(4)-C(13)	164.4(3)
C(11)-Os(4)-C(13)	76.7(3)
O(14)-Os(4)-C(13)	74.0(2)
C(10)-Os(4)-Os(2)	91.3(2)
C(12)-Os(4)-Os(2)	88.8(2)
C(11)-Os(4)-Os(2)	176.9(2)
O(14)-Os(4)-Os(2)	85.72(14)
C(13)-Os(4)-Os(2)	100.22(18)
C(10)-Os(4)-Os(3)	91.3(2)
C(12)-Os(4)-Os(3)	148.0(2)
C(11)-Os(4)-Os(3)	118.0(2)
O(14)-Os(4)-Os(3)	82.97(14)
C(13)-Os(4)-Os(3)	42.47(18)
Os(2)-Os(4)-Os(3)	59.196(11)
O(1)-C(1)-Os(1)	175.1(8)
O(2)-C(2)-Os(1)	179.0(8)
O(3)-C(3)-Os(1)	178.9(8)
O(4)-C(4)-Os(2)	177.6(7)
O(5)-C(5)-Os(2)	178.8(8)
O(6)-C(6)-Os(2)	177.6(7)
O(7)-C(7)-Os(3)	163.3(6)
O(8)-C(8)-Os(3)	178.5(7)
O(9)-C(9)-Os(3)	179.1(8)
O(10)-C(10)-Os(4)	179.5(8)
O(11)-C(11)-Os(4)	174.0(8)
O(12)-C(12)-Os(4)	176.0(7)
O(13)-C(13)-Os(3)	157.0(7)
O(13)-C(13)-Os(4)	123.5(6)
Os(3)-C(13)-Os(4)	79.3(2)
Os(1)-O(14)-Os(4)	107.8(2)
Os(1)-O(14)-O(15)	108.2(3)
Os(4)-O(14)-O(15)	124.4(3)
Os(1)-H(1)-Os(2)	115(4)

Table S4. Anisotropic displacement parameters ($Å^2$ x 10^3) for **1.H_2O**.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Os(1)	12(1)	21(1)	16(1)	0(1)	0(1)	0(1)
Os(2)	15(1)	20(1)	16(1)	-1(1)	5(1)	1(1)
Os(3)	13(1)	19(1)	14(1)	1(1)	2(1)	0(1)
Os(4)	15(1)	16(1)	19(1)	-1(1)	4(1)	1(1)
C(1)	20(4)	21(4)	27(4)	3(3)	2(3)	1(3)
O(1)	43(4)	59(5)	25(3)	-4(3)	-5(3)	-2(4)
C(2)	18(4)	27(5)	23(4)	2(3)	-3(3)	1(3)
O(2)	34(4)	32(4)	45(4)	-3(3)	4(3)	-1(3)
C(3)	20(4)	30(5)	24(4)	-2(3)	5(3)	-6(3)
O(3)	33(4)	51(4)	41(4)	-5(3)	13(3)	-12(3)
C(4)	26(4)	20(4)	20(3)	-1(3)	7(3)	3(3)
O(4)	55(4)	40(4)	29(3)	10(3)	19(3)	13(3)
C(5)	19(4)	37(5)	25(4)	-2(3)	9(3)	-5(4)
O(5)	55(5)	32(4)	44(4)	-16(3)	20(3)	2(3)
C(6)	18(4)	22(4)	20(3)	6(3)	5(3)	-1(3)
O(6)	18(3)	40(4)	41(3)	-6(3)	2(3)	2(3)
C(7)	8(3)	35(5)	22(3)	6(3)	3(3)	0(3)
O(7)	26(3)	23(3)	36(3)	7(3)	4(3)	7(3)
C(8)	20(4)	28(4)	19(3)	2(3)	9(3)	1(3)
O(8)	29(4)	46(4)	33(3)	1(3)	-10(3)	-6(3)
C(9)	19(4)	33(5)	26(4)	-2(3)	10(3)	2(3)
O(9)	48(4)	41(4)	46(4)	14(3)	29(3)	-5(3)
C(10)	22(4)	18(4)	29(4)	-7(3)	8(3)	0(3)
O(10)	16(3)	39(4)	51(4)	-10(3)	1(3)	-6(3)
C(11)	22(4)	28(5)	26(4)	6(3)	5(3)	7(4)
O(11)	45(4)	36(4)	39(3)	-10(3)	12(3)	11(3)
C(12)	25(4)	23(4)	29(4)	-2(3)	5(3)	3(3)
O(12)	71(5)	33(4)	42(4)	8(3)	33(4)	5(4)
C(13)	16(4)	28(4)	20(3)	0(3)	6(3)	2(3)
O(13)	38(4)	41(4)	40(3)	2(3)	25(3)	3(3)
O(14)	24(3)	19(3)	25(3)	-1(2)	3(2)	-1(2)
O(15)	41(4)	57(5)	36(3)	19(3)	12(3)	17(3)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for **1.H_2O**.

	x	y	z	U(eq)
H(1)	1101(10)	-2870(80)	9860(50)	20

Table S6. Summary of Crystal Data and Details of Intensity Collection for $[Os_4(\mu\text{-}H)(\mu\text{-}OD)(\mu\text{-}CO)(CO)_{12}]$ (**2**)

Identification code	03110	
Empirical formula	C13 H D O14 Os4	
Formula weight	1142.95	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/n	
Unit cell dimensions	a = 9.2448(2) Å	alpha= 90°.
	b = 14.2439(3) Å	beta= 97.040(10)°.
	c = 15.2035(4) Å	gamma = 90°.
Volume	1986.93(8) $Å^3$	
Z, Calculated Density	4, 3.821 Mg/m^3	
Absorption coefficient	25.568 mm^{-1}	
F(000)	1984	
Crystal size	0.28 x 0.25 x 0.13 mm^3	
Theta range for data collection	2.64 to 25.35°.	
Index ranges	-11<=h<=11, -16<=k<=17, -18<=l<=18	
Reflections collected	24430	
Independent reflections	3632 [R(int) = 0.121]	
Completeness to theta = 25.00°	99.9 %	
Absorption correction	Integration	
Max. and min. transmission	0.1423 and 0.0538	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3632 / 4 / 153	
Goodness-of-fit on F^2	1.011	
Final R indices [I>2sigma(I)]	R1 = 0.0448, wR2 = 0.1029	
R indices (all data)	R1 = 0.0615, wR2 = 0.1090	
Extinction coefficient	0.00119(7)	
Largest diff. peak and hole	3.062 and -3.355 $e.Å^{-3}$	

Table S7. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for **2**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Os(1)	7537(1)	8029(1)	-997(1)	8(1)
Os(2)	7401(1)	8445(1)	891(1)	8(1)
Os(3)	7756(1)	6593(1)	300(1)	8(1)
Os(4)	4912(1)	7332(1)	278(1)	9(1)
O(1)	6948(11)	9607(8)	-2356(7)	23(3)
C(1)	7152(14)	9051(10)	-1835(9)	10(3)

O(2)	10778(12)	8360(8)	-797(7)	25(3)
C(2)	9565(15)	8225(10)	-886(10)	14(3)
O(3)	7792(12)	6616(8)	-2453(8)	30(3)
C(3)	7677(16)	7140(11)	-1899(10)	18(3)
O(4)	5776(11)	10252(7)	1179(7)	21(3)
C(4)	6375(17)	9576(12)	1057(10)	21(4)
O(5)	10239(12)	9505(8)	1271(8)	32(3)
C(5)	9208(15)	9104(11)	1139(10)	16(3)
O(6)	7392(12)	7741(8)	2769(7)	30(3)
C(6)	7409(15)	8007(10)	2076(9)	10(3)
O(7)	10751(12)	7266(8)	1130(7)	28(3)
C(7)	9576(15)	7130(10)	848(9)	12(3)
O(8)	7729(12)	5279(9)	1904(8)	32(3)
C(8)	7703(15)	5782(10)	1323(10)	13(3)
O(9)	9297(10)	5298(7)	-892(7)	19(2)
C(9)	8777(16)	5783(11)	-423(10)	20(4)
O(10)	4706(12)	6504(8)	2092(7)	26(3)
C(10)	4793(14)	6828(10)	1396(9)	7(3)
O(11)	2169(11)	6228(8)	-420(7)	21(3)
C(11)	3228(15)	6640(10)	-189(10)	11(3)
O(12)	3164(11)	9069(8)	658(7)	25(3)
C(12)	3865(16)	8423(11)	522(10)	20(4)
O(13)	5365(11)	5475(8)	-851(7)	23(3)
C(13)	5975(13)	6017(10)	-349(8)	6(3)
O(14)	5278(10)	7761(7)	-1006(6)	13(2)

Table S8. Bond lengths [Å] and angles [deg] for **2**.

Os(1)-C(2)	1.882(14)
Os(1)-C(3)	1.883(16)
Os(1)-C(1)	1.938(14)
Os(1)-O(14)	2.122(9)
Os(1)-Os(3)	2.8309(8)
Os(1)-Os(2)	2.9482(8)
Os(2)-C(4)	1.903(16)
Os(2)-C(6)	1.907(14)
Os(2)-C(5)	1.913(15)
Os(2)-Os(3)	2.8188(8)
Os(2)-Os(4)	2.8547(8)
Os(3)-C(9)	1.919(15)
Os(3)-C(7)	1.941(15)
Os(3)-C(8)	1.942(15)
Os(3)-C(13)	1.990(13)
Os(3)-Os(4)	2.8288(7)
Os(4)-C(10)	1.861(13)

Os(4)-C(12)	1.890(16)
Os(4)-C(11)	1.905(14)
Os(4)-O(14)	2.112(10)
Os(4)-C(13)	2.370(13)
O(1)-C(1)	1.119(16)
O(2)-C(2)	1.130(17)
O(3)-C(3)	1.140(18)
O(4)-C(4)	1.137(18)
O(5)-C(5)	1.108(17)
O(6)-C(6)	1.121(16)
O(7)-C(7)	1.134(17)
O(8)-C(8)	1.135(17)
O(9)-C(9)	1.141(17)
O(10)-C(10)	1.165(17)
O(11)-C(11)	1.158(17)
O(12)-C(12)	1.159(17)
O(13)-C(13)	1.179(16)

C(2)-Os(1)-C(3)	90.5(6)
C(2)-Os(1)-C(1)	92.7(6)
C(3)-Os(1)-C(1)	92.8(6)
C(2)-Os(1)-O(14)	174.9(5)
C(3)-Os(1)-O(14)	91.7(5)
C(1)-Os(1)-O(14)	91.7(5)
C(2)-Os(1)-Os(3)	93.4(5)
C(3)-Os(1)-Os(3)	90.9(5)
C(1)-Os(1)-Os(3)	172.8(4)
O(14)-Os(1)-Os(3)	82.0(3)
C(2)-Os(1)-Os(2)	92.5(4)
C(3)-Os(1)-Os(2)	149.2(5)
C(1)-Os(1)-Os(2)	117.6(4)
O(14)-Os(1)-Os(2)	83.3(3)
Os(3)-Os(1)-Os(2)	58.344(19)
C(4)-Os(2)-C(6)	95.5(6)
C(4)-Os(2)-C(5)	89.7(6)
C(6)-Os(2)-C(5)	94.1(6)
C(4)-Os(2)-Os(3)	156.1(5)
C(6)-Os(2)-Os(3)	90.4(4)
C(5)-Os(2)-Os(3)	112.9(5)
C(4)-Os(2)-Os(4)	96.8(5)
C(6)-Os(2)-Os(4)	92.1(4)
C(5)-Os(2)-Os(4)	170.5(4)
Os(3)-Os(2)-Os(4)	59.811(19)
C(4)-Os(2)-Os(1)	112.4(5)
C(6)-Os(2)-Os(1)	149.2(4)
C(5)-Os(2)-Os(1)	98.6(4)

Os(3)-Os(2)-Os(1)	58.746(19)
Os(4)-Os(2)-Os(1)	72.52(2)
C(9)-Os(3)-C(7)	91.2(6)
C(9)-Os(3)-C(8)	99.4(6)
C(7)-Os(3)-C(8)	89.8(6)
C(9)-Os(3)-C(13)	84.4(6)
C(7)-Os(3)-C(13)	175.2(5)
C(8)-Os(3)-C(13)	92.9(6)
C(9)-Os(3)-Os(2)	146.1(5)
C(7)-Os(3)-Os(2)	67.9(4)
C(8)-Os(3)-Os(2)	106.6(4)
C(13)-Os(3)-Os(2)	115.0(4)
C(9)-Os(3)-Os(4)	137.6(5)
C(7)-Os(3)-Os(4)	127.9(4)
C(8)-Os(3)-Os(4)	96.7(4)
C(13)-Os(3)-Os(4)	55.7(4)
Os(2)-Os(3)-Os(4)	60.724(19)
C(9)-Os(3)-Os(1)	91.9(5)
C(7)-Os(3)-Os(1)	89.9(4)
C(8)-Os(3)-Os(1)	168.7(4)
C(13)-Os(3)-Os(1)	88.2(4)
Os(2)-Os(3)-Os(1)	62.91(2)
Os(4)-Os(3)-Os(1)	74.68(2)
C(10)-Os(4)-C(12)	92.8(6)
C(10)-Os(4)-C(11)	90.2(6)
C(12)-Os(4)-C(11)	94.8(6)
C(10)-Os(4)-O(14)	171.9(5)
C(12)-Os(4)-O(14)	95.0(5)
C(11)-Os(4)-O(14)	91.2(5)
C(10)-Os(4)-C(13)	97.8(5)
C(12)-Os(4)-C(13)	167.4(6)
C(11)-Os(4)-C(13)	78.5(5)
O(14)-Os(4)-C(13)	74.7(4)
C(10)-Os(4)-Os(3)	90.3(4)
C(12)-Os(4)-Os(3)	143.2(5)
C(11)-Os(4)-Os(3)	121.8(4)
O(14)-Os(4)-Os(3)	82.2(3)
C(13)-Os(4)-Os(3)	43.9(3)
C(10)-Os(4)-Os(2)	93.0(4)
C(12)-Os(4)-Os(2)	83.8(5)
C(11)-Os(4)-Os(2)	176.6(4)
O(14)-Os(4)-Os(2)	85.8(3)
C(13)-Os(4)-Os(2)	102.3(3)
Os(3)-Os(4)-Os(2)	59.465(19)
O(1)-C(1)-Os(1)	176.0(13)
O(2)-C(2)-Os(1)	177.9(14)

O(3)-C(3)-Os(1)	178.1(14)
O(4)-C(4)-Os(2)	178.2(14)
O(5)-C(5)-Os(2)	178.2(15)
O(6)-C(6)-Os(2)	178.8(14)
O(7)-C(7)-Os(3)	165.7(13)
O(8)-C(8)-Os(3)	176.3(13)
O(9)-C(9)-Os(3)	175.3(14)
O(10)-C(10)-Os(4)	179.2(14)
O(11)-C(11)-Os(4)	175.4(12)
O(12)-C(12)-Os(4)	176.8(14)
O(13)-C(13)-Os(3)	153.1(11)
O(13)-C(13)-Os(4)	126.0(10)
Os(3)-C(13)-Os(4)	80.4(5)
Os(4)-O(14)-Os(1)	108.4(4)

Table S9. Anisotropic displacement parameters ($Å^2$ x 10^3) for **2**.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Os(1)	6(1)	6(1)	12(1)	0(1)	5(1)	1(1)
Os(2)	7(1)	7(1)	13(1)	-2(1)	4(1)	0(1)
Os(3)	6(1)	5(1)	13(1)	1(1)	5(1)	2(1)
Os(4)	4(1)	10(1)	15(1)	1(1)	5(1)	0(1)

Table S10. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for **2**.

	x	y	z	U(eq)
H	6940(140)	9000(90)	-260(30)	13
H(14)	5120(110)	8350(20)	-1010(90)	20