STUDIES OF THE ROLE OF LIGANDS IN DETERMINING THE STRUCTURES OF POLYNUCLEAR METAL COMPOUNDS

(Volume 2)

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APPENDIX

Crystallographic Tables for $[AgRu_3(CO)_9(C_2Bu^t)(PPh_3)]$, {X-ray study presented in section 1.2, Vol.1}.

TABLE 1 Fractional atomic coordinates and thermal parameters ($Å^2$) for $[AgRu_3(CO)_9(C_2Bu^t)(PPh_3)]$

Atom	x	y	z	U_{iso} or U_{eq}
Ru(1)	-0.20798(14)	0.20314(15)	0.27652(11)	0.0381(13)
Ru(2)	-0.2575(2)	0.1216(1)	0.0951(1)	0.045(1)
Ru(3)	-0.29154(14)	0.28481(14)	0.09836(12)	0.0382(13)
Ag	-0.36910(14)	0.28103(14)	0.24198(12)	0.0503(13)
P(1)	-0.4960(5)	0.2935(5)	0.2913(4)	0.056(5)
C(11)	-0.1919(19)	0.2806(19)	0.3781(17)	0.058(7)
O(11)	-0.1784(15)	0.3225(14)	0.4447(14)	0.078(6)
C(12)	-0.2858(18)	0.1339(18)	0.3056(16)	0.050(6)
O(12)	-0.3299(17)	0.0958(16)	0.3305(14)	0.092(7)
C(13)	-0.1144(24)	0.1403(23)	0.3417(21)	0.078(9)
O(13)	-0.0494(18)	0.0951(16)	0.3849(15)	0.096(7)
C(21)	-0.1970(26)	0.0258(26)	0.1351(22)	0.089(10)
O(21)	-0.1509(18)	-0.0312(18)	0.1628(15)	0.098(7)
C(22)	-0.2691(20)	0.1094(20)	-0.0376(19)	0.054(7)
O(22)	-0.2706(14)	0.1084(14)	-0.1190(13)	0.068(6)
C(23)	-0.3711(26)	0.0808(22)	0.0794(21)	0.080(9)
O(23)	-0.4405(18)	0.0560(16)	0.0752(14)	0.095(7)
C(31)	-0.2860(19)	0.3035(21)	-0.0244(19)	0.057(8)
O(31)	-0.2844(15)	0.3141(14)	-0.1047(14)	0.080(7)
C(32)	-0.4107(19)	0.2563(16)	0.0469(16)	0.048(6)
O(32)	-0.4876(16)	0.2431(13)	0.0102(13)	0.073(5)
C(33)	-0.3029(23)	0.3908(24)	0.1273(20)	0.077(9)
O(33)	-0.3118(18)	0.4576(19)	0.1446(15)	0.101(7)
C(111)	-0.4697(14)	0.3282(12)	0.4174(10)	0.055(7)
C(112)	-0.3852(14)	0.3121(12)	0.4860(10)	0.086(10)

table 1 continued

C(113)	-0.3605(14)	0.3414(12)	0.5822(10)	0.093(10)
C(114)	-0.4203(14)	0.3870(12)	0.6098(10)	0.098(11)
C(115)	-0.5047(14)	0.4031(12)	0.5411(10)	0.085(9)
C(116)	-0.5294(14)	0.3738(12)	0.4450(10)	0.089(10)
C(121)	-0.5467(14)	0.1970(10)	0.2858(12)	0.052(6)
C(122)	-0.5615(14)	0.1623(10)	0.3660(12)	0.091(10)
C(123)	-0.5995(14)	0.0867(10)	0.3567(12)	0.094(10)
C(124)	-0.6228(14)	0.0458(10)	0.2672(12)	0.087(9)
C(125)	-0.6080(14)	0.0805(10)	0.1870(12)	0.062(8)
C(126)	-0.5700(14)	0.1561(10)	0.1963(12)	0.086(10)
C(131)	-0.5852(15)	0.3555(13)	0.2129(13)	0.073(8)
C(132)	-0.6739(15)	0.3365(13)	0.1946(13)	0.092(10)
C(133)	-0.7415(15)	0.3836(13)	0.1307(13)	0.119(13)
C(134)	-0.7203(15)	0.4496(13)	0.0850(13)	0.106(12)
C(135)	-0.6316(15)	0.4687(13)	0.1033(13)	0.138(15)
C(136)	-0.5640(15)	0.4216(13)	0.1673(13)	0.097(11)
C(1)	-0.1687(17)	0.2109(19)	0.1461(15)	0.049(6)
C(2)	-0.1458(16)	0.2786(16)	0.1890(14)	0.043(6)
C(3)	-0.0648(20)	0.3318(19)	0.2149(17)	0.058(7)
C(4)	-0.0701(24)	0.3975(24)	0.2868(21)	0.084(9)
C(5)	-0.0684(24)	0.3740(24)	0.1130(21)	0.084(9)
C(6)	0.0200(29)	0.2750(28)	0.2581(26)	0.110(12)

TABLE 2 Fractional atomic coordinates for the hydrogen atoms for $[AgRu_3(CO)_9(C_2Bu^t)(PPh_3)]$

Atom	x	y	z
H(112)	-0.3390	0.2768	0.4647
H(113)	-0.2952	0.3289	0.6353
H(114)	-0.4011	0.4097	0.6842
H(115)	-0.5509	0.4384	0.5625
H(116)	-0.5948	0.3863	0.3918
H(122)	-0.5435	0.1939	0.4353
H(123)	-0.6110	0.0598	0.4189
H(124)	-0.6522	-0.0127	0.2600
H(125)	-0.6260	0.0489	0.1177
H(126)	-0.5585	0.1830	0.1341
H(132)	-0.6903	0.2854	0.2300
H(133)	-0.8102	0.3689	0.1165
H(134)	-0.7726	0.4861	0.0355
H(135)	-0.6152	0.5198	0.0680
H(136)	-0.4953	0.4363	0.1814

TABLE 3 Anisotropic thermal parameters (Å ^{2}) for $[AgRu_3(CO)_9(C_2Bu^t)(PPh_3)]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ru(1)	0.037(1)	0.041(2)	0.037(1)	0.001(1)	0.009(1)	0.004(1)
Ru(2)	0.048(1)	0.040(2)	0.048(1)	-0.009(1)	0.011(1)	-0.004(1)
Ru(3)	0.039(1)	0.037(1)	0.038(1)	0.001(1)	0.010(1)	0.000(1)
Ag	0.042(1)	0.057(2)	0.052(1)	0.003(1)	0.022(1)	0.006(1)
P(1)	0.055(5)	0.054(5)	0.058(4)	0.000(4)	0.028(3)	-0.005(5)

TABLE 4 Bond lengths (A°) for $[AgRu_3(CO)_9(C_2Bu^t)(PPh_3)]$

Ru(1) -Ru(2)	2.814(3)	Ru(1) -Ru(3)	2.805(2)
Ru(1) -Ag	2.788(3)	Ru(1) -C(11)	1.91(3)
Ru(1) -C(12)	1.87(3)	Ru(1) -C(13)	1.81(3)
Ru(1) -C(1)	2.20(3)	Ru(1) -C(2)	2.27(3)
Ru(2) -Ru(3)	2.799(3)	Ru(2) -C(21)	1.86(4)
Ru(2) -C(22)	1.88(3)	Ru(2) -C(23)	1.89(4)
Ru(2) -C(1)	2.02(3)	Ru(3) -Ag	2.785(3)
Ru(3) -C(31)	1.84(3)	Ru(3) -C(32)	1.86(3)
Ru(3) -C(33)	1.85(4)	Ru(3) -C(1)	2.23(3)
Ru(3) -C(2)	2.247(22)	Ag -P(1)	2.405(9)
Ag -C(11)	2.831(25)	Ag -C(12)	2.81(3)
Ag -C(32)	2.694(23)	P(1) -C(111)	1.817(17)
P(1) -C(121)	1.804(20)	P(1) -C(131)	1.809(21)
C(11) -O(11)	1.15(3)	C(12) -O(12)	1.11(4)
C(13) -O(13)	1.26(4)	C(21) -O(21)	1.19(5)
C(22) -O(22)	1.17(4)	C(23) -O(23)	1.17(5)
C(31) -O(31)	1.19(4)	C(32) -O(32)	1.18(4)
C(33) -O(33)	1.17(5)	C(111)-C(112)	1.395(24)
C(111)-C(116)	1.39(3)	C(112)-C(113)	1.395(21)
C(113)-C(114)	1.39(3)	C(114)-C(115)	1.395(24)
C(115)-C(116)	1.395(21)	C(121)-C(122)	1.39(3)
C(121)-C(126)	1.395(24)	C(122)-C(123)	1.395(25)
C(123)-C(124)	1.395(24)	C(124)-C(125)	1.39(3)
C(125)-C(126)	1.395(25)	C(131)-C(132)	1.39(3)
C(131)-C(136)	1.39(3)	C(132)-C(133)	1.39(3)

table 4 continued

C(133)-C(134)	1.39(3)	C(134)-C(135)	1.39(3)
C(135)-C(136)	1.39(3)	C(1) -C(2)	1.28(4)
C(2) -C(3)	1.51(4)	C(3) -C(4)	1.54(5)
C(3) -C(5)	1.62(4)	C(3) -C(6)	1.60(5)

TABLE 5 Bond angles (°) for $[AgRu_3(CO)_9(C_2Bu^t)(PPh_3)]$

Ru(3)	-Ru(1)	-Ru(2)	59.8(1)	Ag	-Ru(1)	-Ru(2)	97.2(1)
Ag	-Ru(1)	-Ru(3)	59.7(1)	C(11)	-Ru(1)	-Ru(2)	164.9(8)
C(11)	-Ru(1)	-Ru(3)	105.3(8)	C(11)	-Ru(1)	-Ag	71.3(8)
C(12)	-Ru(1)	-Ru(2)	85.3(7)	C(12)	-Ru(1)	-Ru(3)	111.9(7)
C(12)	-Ru(1)	-Ag	71.0(9)	C(12)	-Ru(1)	-C(11)	100(1)
C(13)	-Ru(1)	-Ru(2)	96(1)	C(13)	-Ru(1)	-Ru(3)	143(1)
C(13)	-Ru(1)	-Ag	157(1)	C(13)	-Ru(1)	-C(11)	98(1)
C(13)	-Ru(1)	-C(12)	91(1)	C(1)	-Ru(1)	-Ru(2)	45.5(7)
C(1)	-Ru(1)	-Ru(3)	51.1(7)	C(1)	-Ru(1)	-Ag	110.7(7)
C(1)	-Ru(1)	-C(11)	128(1)	C(1)	-Ru(1)	-C(12)	131(1)
C(1)	-Ru(1)	-C(13)	92(1)	C(2)	-Ru(1)	-Ru(2)	77.5(6)
C(2)	-Ru(1)	-Ru(3)	51.3(5)	C(2)	-Ru(1)	-Ag	102.0(7)
C(2)	-Ru(1)	-C(11)	95(1)	C(2)	-Ru(1)	-C(12)	160.6(8)
C(2)	-Ru(1)	-C(13)	99(1)	C(2)	-Ru(1)	-C(1)	33(1)
Ru(3)	-Ru(2)	-Ru(1)	60.0(1)	C(21)	-Ru(2)	-Ru(1)	101(1)
C(21)	-Ru(2)	-Ru(3)	158(1)	C(22)	-Ru(2)	-Ru(1)	154(1)
C(22)	-Ru(2)	-Ru(3)	100(1)	C(22)	-Ru(2)	-C(21)	94(1)
C(23)	-Ru(2)	-Ru(1)	103(1)	C(23)	-Ru(2)	-Ru(3)	100(1)
C(23)	-Ru(2)	-C(21)	96(2)	C(23)	-Ru(2)	-C(22)	96(1)
C(1)	-Ru(2)	-Ru(1)	51.0(7)	C(1)	-Ru(2)	-Ru(3)	52.0(8)
C(1)	-Ru(2)	-C(21)	108(1)	C(1)	-Ru(2)	-C(22)	105(1)
C(1)	-Ru(2)	-C(23)	147(1)	Ru(2)	-Ru(3)	-Ru(1)	60.3(1)
Ag	-Ru(3)	-Ru(1)	59.8(1)	Ag	-Ru(3)	-Ru(2)	97.7(1)
C(31)	-Ru(3)	-Ru(1)	143(1)	C(31)	-Ru(3)	-Ru(2)	94(1)
C(31)	-Ru(3)	-Ag	156.4(9)	C(32)	-Ru(3)	-Ru(1)	109.3(8)

table 5 continued

C(32) -Ru(3) -Ru(2)	85.5(9)	C(32) -Ru(3) -Ag	67.5(8)
C(32) -Ru(3) -C(31)	93(1)	C(33) -Ru(3) -Ru(1)	108.4(8)
C(33) -Ru(3) -Ru(2)	168.7(8)	C(33) -Ru(3) -Ag	75(1)
C(33) -Ru(3) -C(31)	96(1)	C(33) -Ru(3) -C(32)	100(1)
C(1) -Ru(3) -Ru(1)	50.3(6)	C(1) -Ru(3) -Ru(2)	45.7(8)
C(1) -Ru(3) -Ag	110.0(7)	C(1) -Ru(3) -C(31)	93(1)
C(1) -Ru(3) -C(32)	131(1)	C(1) -Ru(3) -C(33)	128(1)
C(2) -Ru(3) -Ru(1)	51.8(7)	C(2) -Ru(3) -Ru(2)	78.1(7)
C(2) -Ru(3) -Ag	102.6(6)	C(2) -Ru(3) -C(31)	100(1)
C(2) -Ru(3) -C(32)	160(1)	C(2) -Ru(3) -C(33)	95(1)
C(2) -Ru(3) -C(1)	33(1)	Ru(3) -Ag -Ru(1)	60.4(1)
P(1) -Ag -Ru(1)	145.5(2)	P(1) -Ag -Ru(3)	151.3(2)
C(11) -Ag -Ru(1)	39.8(6)	C(11) -Ag -Ru(3)	84.8(6)
C(11) -Ag -P(1)	123.1(6)	C(12) -Ag -Ru(1)	39.0(6)
C(12) -Ag -Ru(3)	88.6(6)	C(12) -Ag -P(1)	109.7(7)
C(12) -Ag -C(11)	61.6(8)	C(32) -Ag -Ru(1)	89.0(6)
C(32) -Ag -Ru(3)	39.6(7)	C(32) -Ag -P(1)	114.0(7)
C(32) -Ag -C(11)	122.8(9)	C(32) -Ag -C(12)	96.9(8)
C(111)-P(1) -Ag	114.2(8)	C(121)-P(1) -Ag	109.2(8)
C(121)-P(1) -C(111)	106(1)	C(131)-P(1) -Ag	115.6(9)
C(131)-P(1) -C(111)	107(1)	C(131)-P(1) -C(121)	104(1)
Ag -C(11) -Ru(1)	68.9(7)	O(11) -C(11) -Ru(1)	174(2)
O(11) -C(11) -Ag	115(2)	Ag -C(12) -Ru(1)	70.0(9)
O(12) -C(12) -Ru(1)	174(2)	O(12) -C(12) -Ag	109(2)
O(13) -C(13) -Ru(1)	178(3)	O(21) -C(21) -Ru(2)	174(4)
O(22) -C(22) -Ru(2)	173(3)	O(23) -C(23) -Ru(2)	176(2)
O(31) -C(31) -Ru(3)	178(3)	Ag -C(32) -Ru(3)	72.9(7)
O(32) -C(32) -Ru(3)	175(2)	O(32) -C(32) -Ag	109(2)

table 5 continued

O(33) -C(33) -Ru(3)	179(3)	C(112)-C(111)-P(1)	118(2)
C(116)-C(111)-P(1)	122(1)	C(116)-C(111)-C(112)	120(1)
C(113)-C(112)-C(111)	120(2)	C(114)-C(113)-C(112)	120(2)
C(115)-C(114)-C(113)	120(1)	C(116)-C(115)-C(114)	120(2)
C(115)-C(116)-C(111)	120(2)	C(122)-C(121)-P(1)	123(1)
C(126)-C(121)-P(1)	117(1)	C(126)-C(121)-C(122)	120(2)
C(123)-C(122)-C(121)	120(2)	C(124)-C(123)-C(122)	120(2)
C(125)-C(124)-C(123)	120(2)	C(126)-C(125)-C(124)	120(2)
C(125)-C(126)-C(121)	120(2)	C(132)-C(131)-P(1)	121(2)
C(136)-C(131)-P(1)	119(2)	C(136)-C(131)-C(132)	120(2)
C(133)-C(132)-C(131)	120(2)	C(134)-C(133)-C(132)	120(2)
C(135)-C(134)-C(133)	120(2)	C(136)-C(135)-C(134)	120(2)
C(135)-C(136)-C(131)	120(2)	Ru(2) -C(1) -Ru(1)	83(1)
Ru(3) -C(1) -Ru(1)	79(1)	Ru(3) -C(1) -Ru(2)	82.3(9)
C(2) -C(1) -Ru(1)	76(2)	C(2) -C(1) -Ru(2)	151(2)
C(2) -C(1) -Ru(3)	74(2)	Ru(3) -C(2) -Ru(1)	76.9(9)
C(1) -C(2) -Ru(1)	71(2)	C(1) -C(2) -Ru(3)	72(1)
C(3) -C(2) -Ru(1)	135(1)	C(3) -C(2) -Ru(3)	138(2)
C(3) -C(2) -C(1)	136(3)	C(4) -C(3) -C(2)	110(3)
C(5) -C(3) -C(2)	107(2)	C(5) -C(3) -C(4)	108(3)
C(6) -C(3) -C(2)	106(3)	C(6) -C(3) -C(4)	114(2)
C(6) -C(3) -C(5)	111(3)		

TABLE 6 Intermolecular distances (A°) for $[AgRu_3(CO)_9(C_2Bu^t)(PPh_3)]$

atom1	atom2	dist	S	a	b	c
O(32)	...Ru(1)	4.03	-2	0.0	1.0	0.0
H(115)	...Ru(2)	3.67	-2	0.0	1.0	1.0
O(21)	...Ag	3.41	2	-1.0	-1.0	0.0
O(21)	...P(1)	3.68	2	-1.0	-1.0	0.0
O(32)	...C(11)	3.19	-2	0.0	1.0	0.0
O(32)	...O(11)	3.08	-2	0.0	1.0	0.0
H(126)	...O(11)	2.73	-2	0.0	1.0	0.0
O(33)	...C(12)	3.31	2	-1.0	0.0	0.0
O(33)	...O(12)	3.18	2	-1.0	0.0	0.0
O(33)	...C(13)	3.32	2	-1.0	0.0	0.0
O(32)	...C(13)	3.22	-2	0.0	1.0	0.0
O(33)	...O(13)	3.13	2	-1.0	0.0	0.0
H(135)	...O(13)	2.79	2	-1.0	0.0	0.0
O(32)	...O(13)	3.22	-2	0.0	1.0	0.0
O(33)	...C(21)	3.35	2	-1.0	0.0	0.0
H(115)	...C(21)	2.96	-2	0.0	1.0	1.0
O(33)	...O(21)	3.06	2	-1.0	0.0	0.0
H(136)	...O(21)	2.67	2	-1.0	0.0	0.0
H(115)	...O(21)	2.97	-2	0.0	1.0	1.0
C(124)	...O(22)	3.41	-1	-1.0	0.0	0.0
H(124)	...O(22)	2.55	-1	-1.0	0.0	0.0
H(116)	...O(22)	2.78	-2	0.0	1.0	1.0
O(23)	...O(23)	2.99	-1	-1.0	0.0	0.0
C(4)	...O(23)	3.30	2	-1.0	0.0	0.0
C(6)	...O(31)	3.41	-2	1.0	1.0	1.0

table 6 continued

H(135)...C(33)	3.05	-1	-1.0	1.0	0.0
H(135)...O(33)	2.90	-1	-1.0	1.0	0.0
C(115)...C(115)	3.49	-1	-1.0	1.0	1.0
C(5) ...H(122)	2.97	-2	1.0	1.0	0.0
C(5) ...H(123)	2.87	-2	1.0	1.0	0.0

Symmetry Transformations:

The second atom is related to the first atom, at (x,y,z), by the symmetry operation S with (a,b,c) added to the (x',y',z') of S.

Where S =

1	x, y, z
2	0.5-x, 0.5+y, 0.5-z

TABLE 7 Intramolecular distances (A°) for $[AgRu_3(CO)_9(C_2Bu^t)(PPh_3)]$

O(11) ...Ru(1)	3.06	O(12) ...Ru(1)	2.97
O(13) ...Ru(1)	3.07	C(21) ...Ru(1)	3.65
C(23) ...Ru(1)	3.73	C(32) ...Ru(1)	3.84
C(33) ...Ru(1)	3.82	C(3) ...Ru(1)	3.50
C(4) ...Ru(1)	3.92	C(6) ...Ru(1)	3.97
Ag ...Ru(2)	4.20	C(12) ...Ru(2)	3.25
O(12) ...Ru(2)	4.00	C(13) ...Ru(2)	3.51
O(21) ...Ru(2)	3.05	O(22) ...Ru(2)	3.04
O(23) ...Ru(2)	3.07	C(31) ...Ru(2)	3.46
C(32) ...Ru(2)	3.24	O(32) ...Ru(2)	4.02
C(2) ...Ru(2)	3.21	C(11) ...Ru(3)	3.79
C(12) ...Ru(3)	3.90	C(22) ...Ru(3)	3.63
C(23) ...Ru(3)	3.63	O(31) ...Ru(3)	3.03
O(32) ...Ru(3)	3.04	O(33) ...Ru(3)	3.02
C(3) ...Ru(3)	3.52	C(4) ...Ru(3)	4.10
C(5) ...Ru(3)	3.83	O(11) ...Ag	3.48
O(12) ...Ag	3.34	C(23) ...Ag	4.10
O(32) ...Ag	3.28	C(33) ...Ag	2.93
O(33) ...Ag	3.55	C(111)...Ag	3.56
C(112)...Ag	3.67	H(112)...Ag	3.09
C(121)...Ag	3.45	C(126)...Ag	3.71
H(126)...Ag	3.33	C(131)...Ag	3.58
C(136)...Ag	3.77	H(136)...Ag	3.23
C(1) ...Ag	4.12	C(2) ...Ag	3.94
C(112)...P(1)	2.76	C(116)...P(1)	2.81

table 7 continued

H(112)...P(1)	2.87	H(116)...P(1)	2.96
C(122)...P(1)	2.82	C(126)...P(1)	2.73
H(122)...P(1)	2.98	H(126)...P(1)	2.83
C(132)...P(1)	2.80	C(136)...P(1)	2.77
H(132)...P(1)	2.94	H(136)...P(1)	2.88
C(12) ...C(11)	2.89	C(13) ...C(11)	2.81
H(112)...C(11)	3.05	C(2) ...C(11)	3.09
C(4) ...C(11)	3.36	H(112)...O(11)	2.81
C(13) ...C(12)	2.62	C(23) ...C(12)	3.19
C(21) ...C(13)	3.40	C(1) ...C(13)	2.90
C(2) ...C(13)	3.12	C(22) ...C(21)	2.74
C(23) ...C(21)	2.79	C(1) ...C(21)	3.14
C(23) ...C(22)	2.79	C(31) ...C(22)	3.28
C(1) ...C(22)	3.09	C(32) ...C(23)	3.02
O(32) ...C(23)	3.26	O(32) ...O(23)	3.29
C(32) ...C(31)	2.69	C(33) ...C(31)	2.73
C(1) ...C(31)	2.96	C(2) ...C(31)	3.14
C(33) ...C(32)	2.83	H(126)...O(32)	2.65
C(2) ...C(33)	3.02	C(113)...C(111)	2.42
C(114)...C(111)	2.79	C(115)...C(111)	2.42
H(112)...C(111)	2.15	H(116)...C(111)	2.15
C(121)...C(111)	2.89	C(122)...C(111)	3.12
H(122)...C(111)	2.61	C(131)...C(111)	2.92
C(114)...C(112)	2.42	C(115)...C(112)	2.79
C(116)...C(112)	2.42	H(113)...C(112)	2.15
C(115)...C(113)	2.42	C(116)...C(113)	2.79
H(112)...C(113)	2.15	H(114)...C(113)	2.15
C(116)...C(114)	2.42	H(113)...C(114)	2.15

table 7 continued

H(115)...C(114)	2.15	H(114)...C(115)	2.15
H(116)...C(115)	2.15	H(115)...C(116)	2.15
H(122)...C(116)	3.03	C(131)...C(116)	3.17
C(131)...H(116)	2.70	C(132)...H(116)	2.81
C(123)...C(121)	2.42	C(124)...C(121)	2.79
C(125)...C(121)	2.42	H(122)...C(121)	2.15
H(126)...C(121)	2.15	C(131)...C(121)	2.85
C(132)...C(121)	3.08	H(132)...C(121)	2.62
C(124)...C(122)	2.42	C(125)...C(122)	2.79
C(126)...C(122)	2.42	H(123)...C(122)	2.15
C(125)...C(123)	2.42	C(126)...C(123)	2.79
H(122)...C(123)	2.15	H(124)...C(123)	2.15
C(126)...C(124)	2.42	H(123)...C(124)	2.15
H(125)...C(124)	2.15	H(124)...C(125)	2.15
H(126)...C(125)	2.15	H(125)...C(126)	2.15
C(131)...C(126)	3.37	C(132)...C(126)	3.46
H(132)...C(126)	3.07	C(133)...C(131)	2.42
C(134)...C(131)	2.79	C(135)...C(131)	2.42
H(132)...C(131)	2.15	H(136)...C(131)	2.15
C(134)...C(132)	2.42	C(135)...C(132)	2.79
C(136)...C(132)	2.42	H(133)...C(132)	2.15
C(135)...C(133)	2.42	C(136)...C(133)	2.79
H(132)...C(133)	2.15	H(134)...C(133)	2.15
C(136)...C(134)	2.42	H(133)...C(134)	2.15
H(135)...C(134)	2.15	H(134)...C(135)	2.15
H(136)...C(135)	2.15	H(135)...C(136)	2.15
C(3) ...C(1)	2.59	C(5) ...C(1)	3.30
C(6) ...C(1)	3.08	C(4) ...C(2)	2.50

table 7 continued

C(5)	...C(2)	2.51	C(6)	...C(2)	2.50
C(5)	...C(4)	2.56	C(6)	...C(4)	2.64
C(6)	...C(5)	2.66			

Crystallographic Tables for $[Cu_2Ru_4(\mu_3\text{-}H)_2(CO)_{12}\{P(C_6H_{11})_3\}_2]$, {X-ray study presented in section 1.3, Vol.1}.

TABLE 1 Fractional atomic coordinates and thermal parameters ($Å^2$) for $[Cu_2Ru_4(\mu_3\text{-}H)_2(CO)_{12}(P\{C_6H_{11}\}_3)_2]$

Atom	x	y	z	U_{iso} or U_{eq}
Ru(1)	0.1589(2)	0.2378(2)	-0.1069(5)	0.041(3)
Ru(2)	0.2566(2)	0.1701(2)	-0.1262(3)	0.040(3)
Ru(3)	0.1592(2)	0.1107(2)	-0.0683(3)	0.037(3)
Ru(4)	0.2251(2)	0.1938(1)	0.1197(4)	0.038(3)
Cu(1)	0.0834(3)	0.1828(3)	0.0016(7)	0.051(5)
Cu(2)	0.2640(2)	0.0921(2)	0.0675(7)	0.061(5)
P(1)	-0.0067(6)	0.1861(6)	0.0470(13)	0.039(9)
P(2)	0.3243(6)	0.0190(6)	0.1772(14)	0.043(10)
C(11)	0.1106(30)	0.2418(29)	-0.2593(72)	0.086(24)
O(11)	0.0739(17)	0.2453(16)	-0.3679(40)	0.069(13)
C(12)	0.1096(23)	0.2860(24)	-0.0362(53)	0.088(17)
O(12)	0.0910(14)	0.3243(15)	0.0248(33)	0.091(10)
C(13)	0.2000(32)	0.2995(35)	-0.1474(73)	0.083(27)
O(13)	0.2243(22)	0.3400(23)	-0.1794(50)	0.090(19)
C(21)	0.3023(23)	0.1076(24)	-0.1378(51)	0.051(16)
O(21)	0.3318(17)	0.0708(18)	-0.1791(39)	0.063(14)
C(22)	0.2145(28)	0.1748(31)	-0.2980(70)	0.067(24)
O(22)	0.2045(17)	0.1696(18)	-0.3997(43)	0.062(13)
C(23)	0.3090(24)	0.2261(24)	-0.1418(52)	0.039(17)
O(23)	0.3406(15)	0.2652(15)	-0.1594(33)	0.075(11)
C(31)	0.0981(25)	0.0668(24)	-0.0136(54)	0.098(17)
O(31)	0.0701(15)	0.0387(15)	0.0414(34)	0.090(11)
C(32)	0.2047(24)	0.0394(25)	-0.1077(55)	0.094(18)
O(32)	0.2120(15)	-0.0027(16)	-0.1572(33)	0.083(11)
C(33)	0.1145(25)	0.1094(25)	-0.2259(58)	0.062(18)

table 1 continued

O(33)	0.0826(19)	0.1098(19)	-0.3267(44)	0.090(15)
C(41)	0.1763(26)	0.2046(27)	0.2373(59)	0.066(20)
O(41)	0.1488(18)	0.2103(18)	0.3083(41)	0.085(15)
C(42)	0.2791(20)	0.1719(21)	0.2554(48)	0.029(13)
O(42)	0.3198(16)	0.1719(17)	0.3665(39)	0.080(13)
C(43)	0.2430(34)	0.2830(35)	0.1118(80)	0.075(30)
O(43)	0.2605(18)	0.3263(20)	0.1340(42)	0.090(14)
C(51)	-0.0160(20)	0.1235(19)	0.1687(42)	0.037(13)
C(52)	0.0330(18)	0.1123(19)	0.2693(42)	0.039(13)
C(53)	0.0220(24)	0.0560(24)	0.3387(55)	0.067(18)
C(54)	-0.0332(23)	0.0531(26)	0.3773(55)	0.079(20)
C(55)	-0.0833(28)	0.0686(27)	0.2721(63)	0.087(23)
C(56)	-0.0761(25)	0.1238(26)	0.2056(59)	0.075(21)
C(61)	-0.0641(25)	0.1753(28)	-0.1106(59)	0.093(20)
C(62)	-0.0490(25)	0.2255(25)	-0.1999(59)	0.076(20)
C(63)	-0.0900(29)	0.2170(30)	-0.3145(68)	0.092(24)
C(64)	-0.0971(31)	0.1521(31)	-0.3932(72)	0.093(26)
C(65)	-0.1012(28)	0.1075(28)	-0.2593(66)	0.088(21)
C(66)	-0.0682(31)	0.1079(33)	-0.1548(72)	0.123(25)
C(71)	-0.0280(28)	0.2630(27)	0.0957(60)	0.093(20)
C(72)	0.0119(22)	0.2716(23)	0.2488(49)	0.057(16)
C(73)	-0.0058(29)	0.3292(30)	0.3046(66)	0.127(24)
C(74)	-0.0454(29)	0.3627(28)	0.2605(66)	0.113(24)
C(75)	-0.0890(27)	0.3449(26)	0.1309(61)	0.081(22)
C(76)	-0.0860(29)	0.2765(28)	0.0998(70)	0.114(25)
C(81)	0.3185(27)	0.0214(27)	0.3582(60)	0.080(21)
C(82)	0.2426(20)	0.0267(21)	0.3395(44)	0.039(14)
C(83)	0.2436(30)	0.0339(28)	0.4869(59)	0.099(24)

table 1 continued

C(84)	0.2664(22)	-0.0231(22)	0.5647(53)	0.061(16)
C(85)	0.3187(29)	-0.0287(31)	0.5487(63)	0.086(25)
C(86)	0.3391(19)	-0.0379(17)	0.4338(40)	0.037(12)
C(91)	0.4033(26)	0.0381(26)	0.1921(58)	0.058(19)
C(92)	0.4495(26)	0.0012(25)	0.2763(58)	0.095(18)
C(93)	0.5175(26)	0.0257(26)	0.2655(58)	0.093(19)
C(94)	0.5007(30)	0.0847(31)	0.3039(71)	0.093(24)
C(95)	0.4886(32)	0.1237(31)	0.1754(71)	0.084(24)
C(96)	0.4160(30)	0.0956(32)	0.1789(67)	0.098(24)
C(01)	0.3213(26)	-0.0612(24)	0.1244(58)	0.065(19)
C(02)	0.3432(30)	-0.0748(28)	0.0217(63)	0.065(23)
C(03)	0.3405(27)	-0.1420(25)	0.0018(62)	0.094(21)
C(04)	0.2735(28)	-0.1616(29)	-0.0363(63)	0.116(24)
C(05)	0.2565(35)	-0.1534(31)	0.0634(77)	0.085(29)
C(06)	0.2529(28)	-0.0897(27)	0.1128(67)	0.094(24)

TABLE 2 Fractional atomic coordinates for the hydrogen atoms for $[Cu_2Ru_4(\mu_3\text{-}H)_2(CO)_{12}(P\{C_6H_{11}\}_3)_2]$

Atom	x	y	z
H(346)	0.2011	0.1155	0.0956
H(246)	0.2829	0.1615	0.0460
H(52a)	0.0729	0.1101	0.2340
H(52b)	0.0353	0.1490	0.3345
H(53a)	0.0247	0.0198	0.2747
H(53b)	0.0567	0.0523	0.4204
H(54a)	-0.0370	0.0082	0.4103
H(54b)	-0.0331	0.0839	0.4539
H(55a)	-0.0888	0.0318	0.2067
H(55b)	-0.1211	0.0720	0.3148
H(56a)	-0.1083	0.1240	0.1191
H(56b)	-0.0817	0.1627	0.2607
H(72a)	0.0087	0.2307	0.2994
H(72b)	0.0566	0.2789	0.2413
H(73a)	0.0320	0.3559	0.3419
H(73b)	-0.0231	0.3106	0.3815
H(74a)	-0.0749	0.3724	0.3230
H(74b)	-0.0222	0.4026	0.2450
H(75a)	-0.0749	0.3705	0.0580
H(75b)	-0.1333	0.3566	0.1346
H(76a)	-0.1082	0.2673	0.0043
H(76b)	-0.1058	0.2508	0.1646
H(82a)	0.2235	0.0614	0.2754
H(82b)	0.2226	-0.0155	0.3081
H(83a)	0.2690	0.0725	0.5225

table 2 continued

H(83b)	0.1985	0.0415	0.4913
H(84a)	0.2456	-0.0624	0.5194
H(84b)	0.2585	-0.0201	0.6595
H(85a)	0.3392	-0.0650	0.6062
H(85b)	0.3397	0.0126	0.5828
H(86a)	0.3834	-0.0454	0.4230
H(86b)	0.3129	-0.0762	0.3995
H(02a)	0.3154	-0.0533	-0.0574
H(02b)	0.3871	-0.0584	0.0307
H(03a)	0.3523	-0.1516	-0.0877
H(03b)	0.3710	-0.1634	0.0766
H(04a)	0.2719	-0.2094	-0.0477
H(04b)	0.2431	-0.1412	-0.1127
H(05a)	0.2139	-0.1713	0.0657
H(05b)	0.2883	-0.1732	0.1379
H(06a)	0.2374	-0.0815	0.1988
H(06b)	0.2246	-0.0680	0.0350

TABLE 3 Anisotropic thermal parameters ($Å^2$) for $[Cu_2Ru_4(\mu_3\text{-}H)_2(CO)_{12}(P\{C_6H_{11}\}_3)_2]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ru(1)	0.041(3)	0.031(3)	0.051(4)	0.012(3)	0.009(3)	0.004(2)
Ru(2)	0.036(3)	0.040(3)	0.044(3)	-0.002(3)	0.010(3)	-0.004(3)
Ru(3)	0.035(3)	0.029(3)	0.047(3)	-0.002(3)	0.012(3)	-0.001(2)
Ru(4)	0.038(3)	0.029(3)	0.045(3)	-0.005(2)	0.006(3)	-0.001(2)
Cu(1)	0.041(4)	0.039(5)	0.072(6)	0.008(4)	0.016(4)	-0.004(4)
Cu(2)	0.057(5)	0.062(4)	0.065(6)	-0.002(4)	0.000(5)	0.003(4)
P(1)	0.042(8)	0.030(9)	0.046(10)	0.000(7)	-0.005(8)	0.004(7)
P(2)	0.049(10)	0.030(8)	0.049(10)	-0.005(8)	0.005(9)	0.003(7)

TABLE 4 Bond lengths (Å) for $[Cu_2Ru_4(\mu_3\text{-}H)_2(CO)_{12}(P\{C_6H_{11}\}_3)_2]$

Ru(1) -Ru(2)	2.792(2)	Ru(1) -Ru(3)	2.885(2)
Ru(1) -Ru(4)	2.807(2)	Ru(1) -Cu(1)	2.619(3)
Ru(1) -C(11)	1.81(7)	Ru(1) -C(12)	1.86(6)
Ru(1) -C(13)	1.79(8)	Ru(2) -Ru(3)	2.822(2)
Ru(2) -Ru(4)	2.946(2)	Ru(2) -Cu(2)	2.711(3)
Ru(2) -C(21)	1.79(5)	Ru(2) -C(22)	1.93(7)
Ru(2) -C(23)	1.79(6)	Ru(3) -Ru(4)	2.960(2)
Ru(3) -Cu(1)	2.625(3)	Ru(3) -Cu(2)	2.634(3)
Ru(3) -C(31)	1.93(6)	Ru(3) -C(32)	2.02(6)
Ru(3) -C(33)	1.82(6)	Ru(4) -Cu(2)	2.565(3)
Ru(4) -C(41)	1.89(7)	Ru(4) -C(42)	1.81(4)
Ru(4) -C(43)	2.05(8)	Cu(1) -C(12)	2.45(5)
Cu(1) -P(1)	2.263(9)	Cu(2) -C(32)	2.43(5)
Cu(2) -P(2)	2.333(9)	C(11) -O(11)	1.31(8)
C(12) -O(12)	1.22(7)	C(13) -O(13)	1.16(9)
C(21) -O(21)	1.22(7)	C(22) -O(22)	1.08(9)
C(23) -O(23)	1.19(7)	C(31) -O(31)	1.16(7)
C(32) -O(32)	1.12(7)	C(33) -O(33)	1.19(7)
C(41) -O(41)	1.10(8)	C(42) -O(42)	1.38(6)
C(43) -O(43)	1.07(9)	P(1) -C(51)	1.97(5)
P(1) -C(61)	1.97(6)	P(1) -C(71)	1.90(6)
P(2) -C(81)	1.99(7)	P(2) -C(91)	1.88(6)
P(2) -C(01)	1.89(6)	C(51) -C(52)	1.44(6)
C(51) -C(56)	1.54(8)	C(52) -C(53)	1.52(7)
C(53) -C(54)	1.44(8)	C(54) -C(55)	1.51(8)

table 4 continued

C(55) -C(56)	1.46(9)	C(61) -C(62)	1.57(9)
C(61) -C(66)	1.59(9)	C(62) -C(63)	1.42(9)
C(63) -C(64)	1.68(9)	C(64) -C(65)	1.78(9)
C(65) -C(66)	1.24(9)	C(71) -C(72)	1.74(8)
C(71) -C(76)	1.40(9)	C(72) -C(73)	1.52(9)
C(73) -C(74)	1.22(9)	C(74) -C(75)	1.61(9)
C(75) -C(76)	1.58(9)	C(81) -C(82)	1.76(8)
C(81) -C(86)	1.59(7)	C(82) -C(83)	1.60(8)
C(83) -C(84)	1.57(8)	C(84) -C(85)	1.28(9)
C(85) -C(86)	1.43(9)	C(91) -C(92)	1.52(8)
C(91) -C(96)	1.34(9)	C(92) -C(93)	1.71(9)
C(93) -C(94)	1.46(9)	C(94) -C(95)	1.62(9)
C(95) -C(96)	1.82(9)	C(01) -C(02)	1.35(9)
C(01) -C(06)	1.71(9)	C(02) -C(03)	1.53(8)
C(03) -C(04)	1.61(9)	C(04) -C(05)	1.24(9)
C(05) -C(06)	1.53(9)		

TABLE 5 Bond angles (°) for $[Cu_2Ru_4(\mu_3\text{-}H)_2(CO)_{12}(P\{C_6H_{11}\}_3)_2]$

Ru(3) -Ru(1) -Ru(2)	59.6(2)	Ru(4) -Ru(1) -Ru(2)	63.5(1)
Ru(4) -Ru(1) -Ru(3)	62.7(1)	Cu(1) -Ru(1) -Ru(2)	114.5(2)
Cu(1) -Ru(1) -Ru(3)	56.7(2)	Cu(1) -Ru(1) -Ru(4)	75.5(2)
C(11) -Ru(1) -Ru(2)	109(2)	C(11) -Ru(1) -Ru(3)	99(2)
C(11) -Ru(1) -Ru(4)	162(2)	C(11) -Ru(1) -Cu(1)	94(2)
C(12) -Ru(1) -Ru(2)	159(2)	C(12) -Ru(1) -Ru(3)	120(2)
C(12) -Ru(1) -Ru(4)	97(2)	C(12) -Ru(1) -Cu(1)	64(2)
C(12) -Ru(1) -C(11)	91(3)	C(13) -Ru(1) -Ru(2)	85(2)
C(13) -Ru(1) -Ru(3)	145(2)	C(13) -Ru(1) -Ru(4)	105(2)
C(13) -Ru(1) -Cu(1)	157(3)	C(13) -Ru(1) -C(11)	90(3)
C(13) -Ru(1) -C(12)	93(3)	Ru(3) -Ru(2) -Ru(1)	61.9(2)
Ru(4) -Ru(2) -Ru(1)	58.5(1)	Ru(4) -Ru(2) -Ru(3)	61.7(1)
Cu(2) -Ru(2) -Ru(1)	102.8(2)	Cu(2) -Ru(2) -Ru(3)	56.8(2)
Cu(2) -Ru(2) -Ru(4)	53.7(2)	C(21) -Ru(2) -Ru(1)	161(2)
C(21) -Ru(2) -Ru(3)	100(2)	C(21) -Ru(2) -Ru(4)	118(2)
C(21) -Ru(2) -Cu(2)	66(2)	C(22) -Ru(2) -Ru(1)	77(2)
C(22) -Ru(2) -Ru(3)	88(2)	C(22) -Ru(2) -Ru(4)	133(2)
C(22) -Ru(2) -Cu(2)	136(2)	C(22) -Ru(2) -C(21)	100(3)
C(23) -Ru(2) -Ru(1)	102(2)	C(23) -Ru(2) -Ru(3)	163(2)
C(23) -Ru(2) -Ru(4)	105(2)	C(23) -Ru(2) -Cu(2)	126(2)
C(23) -Ru(2) -C(21)	96(2)	C(23) -Ru(2) -C(22)	96(3)
Ru(2) -Ru(3) -Ru(1)	58.6(2)	Ru(4) -Ru(3) -Ru(1)	57.4(1)
Ru(4) -Ru(3) -Ru(2)	61.2(1)	Cu(1) -Ru(3) -Ru(1)	56.5(2)
Cu(1) -Ru(3) -Ru(2)	113.3(2)	Cu(1) -Ru(3) -Ru(4)	72.8(2)
Cu(2) -Ru(3) -Ru(1)	102.3(2)	Cu(2) -Ru(3) -Ru(2)	59.5(2)

table 5 continued

Cu(2) -Ru(3) -Ru(4)	54.2(1)	Cu(2) -Ru(3) -Cu(1)	123.2(2)
C(31) -Ru(3) -Ru(1)	125(2)	C(31) -Ru(3) -Ru(2)	174(2)
C(31) -Ru(3) -Ru(4)	115(2)	C(31) -Ru(3) -Cu(1)	69(2)
C(31) -Ru(3) -Cu(2)	115(2)	C(32) -Ru(3) -Ru(1)	138(2)
C(32) -Ru(3) -Ru(2)	81(2)	C(32) -Ru(3) -Ru(4)	115(1)
C(32) -Ru(3) -Cu(1)	165(2)	C(32) -Ru(3) -Cu(2)	61(1)
C(32) -Ru(3) -C(31)	97(2)	C(33) -Ru(3) -Ru(1)	84(2)
C(33) -Ru(3) -Ru(2)	98(2)	C(33) -Ru(3) -Ru(4)	141(2)
C(33) -Ru(3) -Cu(1)	89(2)	C(33) -Ru(3) -Cu(2)	145(2)
C(33) -Ru(3) -C(31)	87(2)	C(33) -Ru(3) -C(32)	91(2)
Ru(2) -Ru(4) -Ru(1)	58.0(2)	Ru(3) -Ru(4) -Ru(1)	60.0(1)
Ru(3) -Ru(4) -Ru(2)	57.1(1)	Cu(2) -Ru(4) -Ru(1)	106.3(2)
Cu(2) -Ru(4) -Ru(2)	58.4(2)	Cu(2) -Ru(4) -Ru(3)	56.4(2)
C(41) -Ru(4) -Ru(1)	104(2)	C(41) -Ru(4) -Ru(2)	158(2)
C(41) -Ru(4) -Ru(3)	104(2)	C(41) -Ru(4) -Cu(2)	123(2)
C(42) -Ru(4) -Ru(1)	169(2)	C(42) -Ru(4) -Ru(2)	115(2)
C(42) -Ru(4) -Ru(3)	125(1)	C(42) -Ru(4) -Cu(2)	73(2)
C(42) -Ru(4) -C(41)	85(2)	C(43) -Ru(4) -Ru(1)	73(2)
C(43) -Ru(4) -Ru(2)	93(2)	C(43) -Ru(4) -Ru(3)	132(2)
C(43) -Ru(4) -Cu(2)	141(2)	C(43) -Ru(4) -C(41)	93(3)
C(43) -Ru(4) -C(42)	101(3)	Ru(3) -Cu(1) -Ru(1)	66.8(2)
C(12) -Cu(1) -Ru(1)	43(1)	C(12) -Cu(1) -Ru(3)	109(1)
P(1) -Cu(1) -Ru(1)	145.6(5)	P(1) -Cu(1) -Ru(3)	142.9(4)
P(1) -Cu(1) -C(12)	106(1)	Ru(3) -Cu(2) -Ru(2)	63.7(2)
Ru(4) -Cu(2) -Ru(2)	67.8(2)	Ru(4) -Cu(2) -Ru(3)	69.4(2)
C(32) -Cu(2) -Ru(2)	77(1)	C(32) -Cu(2) -Ru(3)	47(1)
C(32) -Cu(2) -Ru(4)	116(1)	P(2) -Cu(2) -Ru(2)	142.0(5)
P(2) -Cu(2) -Ru(3)	143.1(4)	P(2) -Cu(2) -Ru(4)	136.2(5)

table 5 continued

P(2) -Cu(2) -C(32)	104(1)	O(11) -C(11) -Ru(1)	178(6)
Cu(1) -C(12) -Ru(1)	73(2)	O(12) -C(12) -Ru(1)	163(4)
O(12) -C(12) -Cu(1)	117(4)	O(13) -C(13) -Ru(1)	176(6)
O(21) -C(21) -Ru(2)	162(5)	O(22) -C(22) -Ru(2)	160(6)
O(23) -C(23) -Ru(2)	175(4)	O(31) -C(31) -Ru(3)	166(4)
Cu(2) -C(32) -Ru(3)	72(2)	O(32) -C(32) -Ru(3)	156(4)
O(32) -C(32) -Cu(2)	132(4)	O(33) -C(33) -Ru(3)	176(6)
O(41) -C(41) -Ru(4)	178(5)	O(42) -C(42) -Ru(4)	164(4)
O(43) -C(43) -Ru(4)	163(7)	C(51) -P(1) -Cu(1)	111(1)
C(61) -P(1) -Cu(1)	108(2)	C(61) -P(1) -C(51)	110(2)
C(71) -P(1) -Cu(1)	113(2)	C(71) -P(1) -C(51)	113(3)
C(71) -P(1) -C(61)	100(3)	C(81) -P(2) -Cu(2)	109(2)
C(91) -P(2) -Cu(2)	112(2)	C(91) -P(2) -C(81)	100(3)
C(01) -P(2) -Cu(2)	122(2)	C(01) -P(2) -C(81)	108(3)
C(01) -P(2) -C(91)	103(3)	C(52) -C(51) -P(1)	117(3)
C(56) -C(51) -P(1)	113(3)	C(56) -C(51) -C(52)	116(4)
C(53) -C(52) -C(51)	109(4)	C(54) -C(53) -C(52)	116(4)
C(55) -C(54) -C(53)	112(5)	C(56) -C(55) -C(54)	115(5)
C(55) -C(56) -C(51)	109(5)	C(62) -C(61) -P(1)	104(4)
C(66) -C(61) -P(1)	112(4)	C(66) -C(61) -C(62)	120(6)
C(63) -C(62) -C(61)	104(5)	C(64) -C(63) -C(62)	123(5)
C(65) -C(64) -C(63)	95(5)	C(66) -C(65) -C(64)	128(6)
C(65) -C(66) -C(61)	106(6)	C(72) -C(71) -P(1)	104(3)
C(76) -C(71) -P(1)	121(5)	C(76) -C(71) -C(72)	107(5)
C(73) -C(72) -C(71)	110(4)	C(74) -C(73) -C(72)	128(6)
C(75) -C(74) -C(73)	119(6)	C(76) -C(75) -C(74)	112(5)
C(75) -C(76) -C(71)	108(5)	C(82) -C(81) -P(2)	99(3)
C(86) -C(81) -P(2)	114(4)	C(86) -C(81) -C(82)	108(4)

table 5 continued

C(83) -C(82) -C(81)	94(4)	C(84) -C(83) -C(82)	113(5)
C(85) -C(84) -C(83)	104(5)	C(86) -C(85) -C(84)	129(5)
C(85) -C(86) -C(81)	102(4)	C(92) -C(91) -P(2)	120(4)
C(96) -C(91) -P(2)	117(5)	C(96) -C(91) -C(92)	116(5)
C(93) -C(92) -C(91)	110(5)	C(94) -C(93) -C(92)	88(5)
C(95) -C(94) -C(93)	105(6)	C(96) -C(95) -C(94)	78(5)
C(95) -C(96) -C(91)	124(6)	C(02) -C(01) -P(2)	118(5)
C(06) -C(01) -P(2)	111(4)	C(06) -C(01) -C(02)	111(5)
C(03) -C(02) -C(01)	109(6)	C(04) -C(03) -C(02)	109(5)
C(05) -C(04) -C(03)	102(6)	C(06) -C(05) -C(04)	119(7)
C(05) -C(06) -C(01)	105(5)		

TABLE 6 Intermolecular distances (Å) for $[Cu_2Ru_4(u_3\text{-}H)_2(CO)_{12}(P\{C_6H_{11}\}_3)_2]$

atom1	atom2	dist	S	a	b	c
H(55a)	Ru(3)	3.78	-1	0.0	0.0	0.0
H(03a)	O(11)	2.99	-2	1.0	0.0	0.0
C(84)	O(13)	3.31	-2	1.0	0.0	1.0
H(84a)	O(13)	2.80	-2	1.0	0.0	1.0
H(85a)	O(13)	2.81	-2	1.0	0.0	1.0
H(03a)	O(13)	2.79	-2	1.0	0.0	0.0
C(04)	O(13)	3.09	-2	1.0	0.0	0.0
H(04b)	O(13)	2.55	-2	1.0	0.0	0.0
H(74a)	C(21)	3.03	2	-1.0	0.0	0.0
H(84b)	O(21)	3.00	1	0.0	0.0	1.0
H(85b)	O(21)	2.93	1	0.0	0.0	1.0
C(74)	O(21)	3.42	2	-1.0	0.0	0.0
H(74a)	O(21)	2.53	2	-1.0	0.0	0.0
H(75b)	O(21)	2.84	2	-1.0	0.0	0.0
O(41)	O(22)	3.30	1	0.0	0.0	1.0
H(83a)	O(22)	2.88	1	0.0	0.0	1.0
H(04a)	O(22)	2.86	-2	1.0	0.0	0.0
H(56b)	O(23)	2.70	2	-1.0	0.0	0.0
H(76b)	O(23)	2.51	2	-1.0	0.0	0.0
H(55a)	C(31)	3.02	-1	0.0	0.0	0.0
H(84b)	O(32)	2.48	1	0.0	0.0	1.0
C(55)	O(32)	3.37	-1	0.0	0.0	0.0
H(55a)	O(32)	2.91	-1	0.0	0.0	0.0
H(55b)	O(32)	2.90	-1	0.0	0.0	0.0
H(53b)	O(33)	2.98	1	0.0	0.0	1.0

table 6 continued

H(54a)...O(33)	2.93	-1	0.0	0.0	0.0
C(75) ...O(42)	3.24	2	-1.0	0.0	-1.0
H(75b)...O(42)	2.96	2	-1.0	0.0	-1.0
C(76) ...O(42)	3.22	2	-1.0	0.0	-1.0
H(76a)...O(42)	2.44	2	-1.0	0.0	-1.0
H(84a)...O(43)	2.99	-2	1.0	0.0	1.0
H(86b)...O(43)	2.77	-2	1.0	0.0	1.0
C(05) ...O(43)	3.40	-2	1.0	0.0	1.0
H(05b)...O(43)	2.92	-2	1.0	0.0	1.0
C(06) ...O(43)	3.39	-2	1.0	0.0	1.0
H(06a)...O(43)	2.74	-2	1.0	0.0	1.0
H(54a)...C(53)	3.03	-1	0.0	0.0	1.0
H(54a)...C(54)	2.90	-1	0.0	0.0	1.0
C(64) ...H(54b)	2.88	1	0.0	0.0	-1.0
C(92) ...H(74b)	2.83	-2	1.0	0.0	1.0
C(93) ...H(74b)	2.77	-2	1.0	0.0	1.0

Symmetry Transformations:

The second atom is related to the first atom, at (x,y,z), by the symmetry operation S with (a,b,c) added to the (x',y',z') of S.

Where S =

1	x, y, z
2	0.5+x, 0.5-y, 0.5+z

TABLE 7 Intramolecular distances (Å) for $[Cu_2Ru_4(u_3\text{-}H)_2(CO)_{12}(P\{C_6H_{11}\}_3)_2]$

Cu(2) ...Ru(1)	4.30	O(11) ...Ru(1)	3.12
O(12) ...Ru(1)	3.04	O(13) ...Ru(1)	2.95
C(22) ...Ru(1)	3.01	O(22) ...Ru(1)	3.85
C(23) ...Ru(1)	3.63	C(33) ...Ru(1)	3.24
O(33) ...Ru(1)	3.93	C(41) ...Ru(1)	3.74
C(43) ...Ru(1)	2.94	O(43) ...Ru(1)	3.74
H(346)...Ru(1)	3.53	H(246)...Ru(1)	3.49
Cu(1) ...Ru(2)	4.55	C(11) ...Ru(2)	3.80
C(13) ...Ru(2)	3.19	O(13) ...Ru(2)	3.91
O(21) ...Ru(2)	2.97	O(22) ...Ru(2)	2.97
O(23) ...Ru(2)	2.97	C(32) ...Ru(2)	3.20
O(32) ...Ru(2)	4.02	C(33) ...Ru(2)	3.56
C(42) ...Ru(2)	4.05	C(43) ...Ru(2)	3.67
H(346)...Ru(2)	3.19	C(11) ...Ru(3)	3.65
C(12) ...Ru(3)	4.14	C(21) ...Ru(3)	3.58
C(22) ...Ru(3)	3.35	O(22) ...Ru(3)	4.15
O(31) ...Ru(3)	3.06	O(32) ...Ru(3)	3.07
O(33) ...Ru(3)	3.01	C(41) ...Ru(3)	3.88
H(246)...Ru(3)	3.13	Cu(1) ...Ru(4)	3.32
C(12) ...Ru(4)	3.56	C(13) ...Ru(4)	3.69
C(21) ...Ru(4)	4.10	C(23) ...Ru(4)	3.82
C(31) ...Ru(4)	4.17	C(32) ...Ru(4)	4.23
O(41) ...Ru(4)	2.99	O(42) ...Ru(4)	3.15
O(43) ...Ru(4)	3.09	P(2) ...Ru(4)	4.55
H(82a)...Ru(4)	3.42	C(11) ...Cu(1)	3.29

table 7 continued

O(12) ...Cu(1)	3.19	C(31) ...Cu(1)	2.64
O(31) ...Cu(1)	3.29	C(33) ...Cu(1)	3.16
O(33) ...Cu(1)	3.91	C(41) ...Cu(1)	3.05
O(41) ...Cu(1)	3.42	H(346)...Cu(1)	3.13
C(51) ...Cu(1)	3.49	C(52) ...Cu(1)	3.69
H(52a)...Cu(1)	3.05	C(61) ...Cu(1)	3.44
C(62) ...Cu(1)	3.55	C(66) ...Cu(1)	3.99
C(71) ...Cu(1)	3.49	C(72) ...Cu(1)	3.96
H(72b)...Cu(1)	3.53	C(21) ...Cu(2)	2.58
O(21) ...Cu(2)	3.40	C(23) ...Cu(2)	4.03
C(31) ...Cu(2)	3.86	O(32) ...Cu(2)	3.28
C(41) ...Cu(2)	3.94	C(42) ...Cu(2)	2.68
O(42) ...Cu(2)	3.70	C(81) ...Cu(2)	3.53
C(82) ...Cu(2)	3.41	H(82a)...Cu(2)	2.70
C(91) ...Cu(2)	3.49	C(96) ...Cu(2)	3.53
C(01) ...Cu(2)	3.71	C(12) ...C(11)	2.61
C(13) ...C(11)	2.56	C(22) ...C(11)	2.96
O(22) ...C(11)	3.33	C(33) ...C(11)	3.00
O(33) ...C(11)	3.09	O(33) ...O(11)	3.08
C(13) ...C(12)	2.65	C(43) ...C(12)	3.22
P(1) ...C(12)	3.78	C(71) ...O(12)	3.34
H(72b)...O(12)	2.82	C(22) ...C(13)	3.29
C(23) ...C(13)	3.03	O(23) ...C(13)	3.41
C(43) ...C(13)	2.81	O(43) ...C(13)	3.15
C(23) ...O(13)	3.22	O(23) ...O(13)	3.17
C(43) ...O(13)	3.35	C(22) ...C(21)	2.85
C(23) ...C(21)	2.67	C(32) ...C(21)	2.83
O(32) ...C(21)	3.24	H(246)...C(21)	2.45

table 7 continued

C(32) ...O(21)	3.30	O(32) ...O(21)	3.31
C(23) ...C(22)	2.76	C(33) ...C(22)	3.00
O(33) ...C(22)	3.38	C(33) ...O(22)	3.37
H(246)...C(23)	2.66	C(32) ...C(31)	2.94
C(33) ...C(31)	2.59	H(346)...C(31)	2.70
P(1) ...C(31)	3.78	H(52a)...C(31)	3.02
C(51) ...O(31)	3.27	C(52) ...O(31)	3.23
H(52a)...O(31)	2.62	H(53a)...O(31)	2.96
C(33) ...C(32)	2.74	H(346)...C(32)	2.80
P(2) ...C(32)	3.76	H(06b)...C(32)	2.85
C(33) ...O(32)	3.38	H(02a)...O(32)	2.70
H(06b)...O(32)	2.51	C(42) ...C(41)	2.49
C(43) ...C(41)	2.87	H(346)...C(41)	2.66
C(42) ...O(41)	3.33	H(52a)...O(41)	2.89
H(72b)...O(41)	2.64	C(43) ...C(42)	2.97
H(346)...C(42)	2.59	H(246)...C(42)	2.30
P(2) ...C(42)	3.74	H(82a)...C(42)	2.83
C(81) ...O(42)	3.38	H(246)...C(43)	3.02
C(52) ...P(1)	2.92	H(52a)...P(1)	3.00
H(52b)...P(1)	3.18	C(56) ...P(1)	2.94
H(56a)...P(1)	3.00	H(56b)...P(1)	3.21
C(62) ...P(1)	2.80	C(66) ...P(1)	2.95
C(72) ...P(1)	2.88	H(72a)...P(1)	2.86
H(72b)...P(1)	3.12	C(76) ...P(1)	2.89
H(76a)...P(1)	2.96	H(76b)...P(1)	3.21
C(82) ...P(2)	2.85	H(82a)...P(2)	2.93
H(82b)...P(2)	3.10	C(86) ...P(2)	3.01
H(86a)...P(2)	3.10	H(86b)...P(2)	3.27

table 7 continued

C(92) ...P(2)	2.94	C(96) ...P(2)	2.75
C(02) ...P(2)	2.79	H(02a)...P(2)	2.99
H(02b)...P(2)	2.94	C(06) ...P(2)	2.97
H(06a)...P(2)	3.08	H(06b)...P(2)	3.20
H(52a)...C(51)	2.09	H(52b)...C(51)	2.03
C(53) ...C(51)	2.41	H(53a)...C(51)	2.69
C(54) ...C(51)	2.85	C(55) ...C(51)	2.44
H(55a)...C(51)	2.76	H(56a)...C(51)	2.13
H(56b)...C(51)	2.18	C(61) ...C(51)	3.22
C(66) ...C(51)	3.49	C(71) ...C(51)	3.23
C(72) ...C(51)	3.47	H(72a)...C(51)	2.80
H(53a)...C(52)	2.09	H(53b)...C(52)	2.11
C(54) ...C(52)	2.50	H(54b)...C(52)	2.83
C(55) ...C(52)	2.90	C(56) ...C(52)	2.53
H(56b)...C(52)	2.90	H(72a)...C(52)	2.75
C(53) ...H(52a)	2.17	C(53) ...H(52b)	2.12
C(54) ...H(52b)	2.78	C(56) ...H(52b)	2.76
C(72) ...H(52b)	2.92	H(54a)...C(53)	2.02
H(54b)...C(53)	2.06	C(55) ...C(53)	2.45
H(55a)...C(53)	2.76	C(56) ...C(53)	2.89
C(54) ...H(53a)	2.06	C(55) ...H(53a)	2.76
C(54) ...H(53b)	2.07	H(55a)...C(54)	2.09
H(55b)...C(54)	2.08	C(56) ...C(54)	2.50
H(56b)...C(54)	2.90	C(55) ...H(54a)	2.15
C(55) ...H(54b)	2.11	C(56) ...H(54b)	2.82
H(56a)...C(55)	2.06	H(56b)...C(55)	2.12
C(56) ...H(55a)	2.09	C(56) ...H(55b)	2.09
H(76b)...C(56)	2.95	C(63) ...C(61)	2.36

table 7 continued

C(64) ...C(61)	3.05	C(65) ...C(61)	2.26
C(71) ...C(61)	2.97	C(76) ...C(61)	3.33
H(76a)...C(61)	2.72	C(64) ...C(62)	2.73
C(65) ...C(62)	2.94	C(66) ...C(62)	2.74
C(71) ...C(62)	3.25	H(76a)...C(62)	2.98
C(65) ...C(63)	2.56	C(66) ...C(63)	2.98
C(66) ...C(64)	2.72	H(72a)...C(71)	2.32
H(72b)...C(71)	2.30	C(73) ...C(71)	2.67
C(74) ...C(71)	2.94	C(75) ...C(71)	2.41
H(75a)...C(71)	2.65	H(76a)...C(71)	1.95
H(76b)...C(71)	2.12	H(73a)...C(72)	2.15
H(73b)...C(72)	1.99	C(74) ...C(72)	2.46
H(74b)...C(72)	3.05	C(75) ...C(72)	2.96
C(76) ...C(72)	2.53	H(76b)...C(72)	2.77
C(73) ...H(72a)	2.24	C(76) ...H(72a)	2.96
C(73) ...H(72b)	2.07	H(74a)...C(73)	1.93
H(74b)...C(73)	1.78	C(75) ...C(73)	2.45
H(75a)...C(73)	2.98	C(76) ...C(73)	2.86
H(76b)...C(73)	3.08	C(74) ...H(73a)	1.86
C(74) ...H(73b)	1.76	C(75) ...H(73b)	2.94
H(75a)...C(74)	2.17	H(75b)...C(74)	2.24
C(76) ...C(74)	2.65	H(76b)...C(74)	2.97
C(75) ...H(74a)	2.13	C(75) ...H(74b)	2.21
H(76a)...C(75)	2.21	H(76b)...C(75)	2.19
C(76) ...H(75a)	2.19	C(76) ...H(75b)	2.19
H(82a)...C(81)	2.40	H(82b)...C(81)	2.36
C(83) ...C(81)	2.46	H(83a)...C(81)	2.58
C(84) ...C(81)	2.93	C(85) ...C(81)	2.35

table 7 continued

H(85b)...C(81)	2.39	H(86a)...C(81)	2.15
H(86b)...C(81)	2.25	C(91) ...C(81)	2.96
C(92) ...C(81)	3.39	C(01) ...C(81)	3.15
H(83a)...C(82)	2.21	H(83b)...C(82)	2.13
C(84) ...C(82)	2.64	H(84a)...C(82)	2.78
C(85) ...C(82)	2.87	C(86) ...C(82)	2.71
H(86b)...C(82)	2.84	H(06a)...C(82)	2.86
C(83) ...H(82a)	2.33	C(83) ...H(82b)	2.20
C(84) ...H(82b)	2.77	C(86) ...H(82b)	2.84
C(06) ...H(82b)	2.89	H(84a)...C(83)	2.19
H(84b)...C(83)	2.19	C(85) ...C(83)	2.25
H(85b)...C(83)	2.34	C(86) ...C(83)	2.91
C(84) ...H(83a)	2.20	C(85) ...H(83a)	2.54
C(84) ...H(83b)	2.18	H(85a)...C(84)	1.92
H(85b)...C(84)	1.87	C(86) ...C(84)	2.44
H(86b)...C(84)	2.57	C(85) ...H(84a)	1.85
C(86) ...H(84a)	2.60	C(85) ...H(84b)	2.04
H(86a)...C(85)	2.26	H(86b)...C(85)	1.92
C(86) ...H(85a)	1.96	C(86) ...H(85b)	1.97
C(92) ...C(86)	3.48	C(01) ...C(86)	3.33
C(92) ...H(86a)	2.64	C(01) ...H(86b)	3.04
C(93) ...C(91)	2.65	C(94) ...C(91)	2.58
C(95) ...C(91)	2.81	C(01) ...C(91)	2.94
C(02) ...C(91)	3.29	H(02b)...C(91)	2.76
C(94) ...C(92)	2.22	C(95) ...C(92)	3.16
C(96) ...C(92)	2.43	C(01) ...C(92)	3.42
H(02b)...C(92)	3.07	C(95) ...C(93)	2.45
C(96) ...C(93)	2.85	C(96) ...C(94)	2.18

table 7 continued

H(02a)...C(01)	1.95	H(02b)...C(01)	2.01
C(03) ...C(01)	2.34	H(03b)...C(01)	2.67
C(04) ...C(01)	2.93	C(05) ...C(01)	2.58
H(05b)...C(01)	2.65	H(06a)...C(01)	2.31
H(06b)...C(01)	2.29	H(03a)...C(02)	2.13
H(03b)...C(02)	2.14	C(04) ...C(02)	2.54
H(04b)...C(02)	2.91	C(05) ...C(02)	2.80
H(05b)...C(02)	2.96	C(06) ...C(02)	2.53
H(06b)...C(02)	2.82	C(03) ...H(02a)	2.14
C(04) ...H(02a)	2.65	C(05) ...H(02a)	3.07
C(06) ...H(02a)	2.70	C(03) ...H(02b)	2.16
H(04a)...C(03)	2.20	H(04b)...C(03)	2.37
C(05) ...C(03)	2.22	H(05b)...C(03)	2.21
C(06) ...C(03)	2.83	C(04) ...H(03a)	2.05
C(05) ...H(03a)	3.03	C(04) ...H(03b)	2.37
C(05) ...H(03b)	2.67	H(05a)...C(04)	1.96
H(05b)...C(04)	1.87	C(06) ...C(04)	2.40
H(06b)...C(04)	2.59	C(05) ...H(04a)	1.83
C(05) ...H(04b)	1.89	C(06) ...H(04b)	2.67
H(06a)...C(05)	2.28	H(06b)...C(05)	2.06
C(06) ...H(05a)	2.07	C(06) ...H(05b)	2.05

Crystallographic Tables for $[Cu_2Ru_4(\mu_3\text{-}H)_2(CO)_{12}\{P(CHMe_2)_3\}_2]$, {X-ray study presented in section 1.3, Vol.1}.

TABLE 1 Fractional atomic coordinates and thermal parameters ($Å^2$) for $[Cu_2Ru_4(\mu_3\text{-}H)_2(CO)_{12}(P\{CHMe_2\}_3)_2]$

Atom	x	y	z	U_{iso} or U_{eq}
Ru(1)	0.2701(2)	0.2537(7)	0.0479(2)	0.065(2)
Ru(2)	0.0431(2)	0.2500	0.0324(2)	0.065(2)
Ru(3)	0.2318(3)	0.3471(2)	0.2212(3)	0.058(2)
Ru(4)	0.2283(3)	0.1549(2)	0.2196(3)	0.059(2)
Cu(1)	0.3199(4)	0.2567(9)	0.4208(4)	0.067(3)
Cu(2)	0.0874(3)	0.2506(10)	0.2871(4)	0.069(2)
P(1)	0.4630(8)	0.2505(16)	0.6121(9)	0.077(4)
P(2)	-0.0421(7)	0.2526(15)	0.3666(7)	0.057(3)
C(11)	0.4250(24)	0.2363(28)	0.0924(25)	0.059(4)
O(11)	0.5240(20)	0.2530(36)	0.1266(21)	0.101(4)
C(12)	0.2680(28)	0.1590(25)	-0.0507(29)	0.066(4)
O(12)	0.2386(24)	0.1015(22)	-0.1349(26)	0.103(4)
C(13m)	0.2467(23)	0.3350(21)	-0.0634(24)	0.061(4)
O(13m)	0.2534(19)	0.3935(18)	-0.1214(20)	0.088(3)
C(21)	-0.1092(24)	0.2658(29)	0.0220(24)	0.060(4)
O(21)	-0.2077(20)	0.2253(17)	0.0009(21)	0.072(4)
C(22)	0.0189(29)	0.1722(26)	-0.0793(30)	0.072(4)
O(22)	-0.0225(25)	0.1118(23)	-0.1576(27)	0.115(4)
C(23m)	0.0118(24)	0.3414(23)	-0.0879(25)	0.071(4)
O(23m)	0.0033(20)	0.3983(18)	-0.1462(21)	0.096(3)
C(31)	0.3830(23)	0.3498(21)	0.2775(24)	0.063(4)
O(31)	0.4906(19)	0.3636(17)	0.3198(20)	0.083(3)
C(32)	0.2032(24)	0.4139(20)	0.3399(22)	0.066(4)
O(32)	0.1890(20)	0.4569(18)	0.4033(20)	0.093(3)
C(33)	0.2063(24)	0.4471(23)	0.1200(25)	0.073(4)

table 1 continued

O(33)	0.2259(20)	0.5181(18)	0.0797(21)	0.092(3)
C(41)	0.3940(29)	0.1460(26)	0.2829(29)	0.067(4)
O(41)	0.4776(25)	0.1368(22)	0.3167(25)	0.101(4)
C(42)	0.2099(28)	0.0943(25)	0.3427(26)	0.072(4)
O(42)	0.1836(25)	0.0383(21)	0.3976(25)	0.109(4)
C(43)	0.2229(29)	0.0548(27)	0.1374(30)	0.077(4)
O(43)	0.1827(25)	-0.0115(24)	0.0651(27)	0.112(4)
C(11p)	0.4873(27)	0.1442(19)	0.6925(25)	0.088(4)
C(111)	0.3878(28)	0.0788(21)	0.6572(26)	0.083(4)
C(112)	0.4982(30)	0.1529(27)	0.8281(23)	0.092(4)
C(12p)	0.4339(23)	0.3294(19)	0.7325(23)	0.062(4)
C(121)	0.3822(28)	0.4099(20)	0.6892(25)	0.077(4)
C(122)	0.5402(27)	0.3387(27)	0.8328(26)	0.092(4)
C(13p)	0.5999(21)	0.3018(19)	0.6094(25)	0.070(4)
C(131)	0.7064(21)	0.2869(22)	0.6971(26)	0.072(4)
C(132)	0.5775(23)	0.4008(18)	0.5750(27)	0.065(4)
C(21p)	-0.1574(23)	0.1731(18)	0.3044(22)	0.051(4)
C(211)	-0.1975(27)	0.1288(24)	0.4075(26)	0.078(4)
C(212)	-0.1491(23)	0.1029(20)	0.2241(24)	0.052(4)
C(22p)	-0.1117(23)	0.3634(17)	0.3630(26)	0.061(4)
C(221)	-0.1125(26)	0.4354(19)	0.2848(29)	0.085(4)
C(222)	-0.2372(22)	0.3475(24)	0.3737(30)	0.077(4)
C(23p)	0.0073(24)	0.2266(18)	0.5202(21)	0.062(4)
C(231)	0.0633(27)	0.1343(19)	0.5537(24)	0.075(4)
C(232)	0.0832(28)	0.2993(21)	0.5882(22)	0.081(4)

TABLE 2 Anisotropic thermal parameters ($Å^2$) for $[Cu_2Ru_4(\mu_3\text{-}H)_2(CO)_{12}(P\{CHMe_2\}_3)_2]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ru(1)	0.068(2)	0.067(2)	0.061(2)	0.003(3)	0.045(1)	0.000(4)
Ru(2)	0.055(2)	0.087(2)	0.053(2)	-0.001(4)	0.027(1)	-0.004(4)
Ru(3)	0.063(2)	0.051(2)	0.061(2)	-0.004(2)	0.027(1)	-0.001(2)
Ru(4)	0.070(2)	0.038(2)	0.069(2)	0.000(2)	0.056(2)	0.002(2)
Cu(1)	0.071(2)	0.069(3)	0.061(2)	0.004(4)	0.036(2)	-0.005(4)
Cu(2)	0.062(2)	0.068(2)	0.075(2)	0.004(4)	0.049(2)	0.006(4)
P(1)	0.067(4)	0.090(4)	0.074(4)	0.001(4)	0.029(3)	-0.004(4)
P(2)	0.050(3)	0.063(3)	0.058(3)	-0.001(4)	0.031(3)	0.002(4)

TABLE 3 Bond lengths (Å) for $[Cu_2Ru_4(\mu_3\text{-}H)_2(CO)_{12}(P\{CHMe_2\}_3)_2]$

Ru(1) -Ru(2)	2.835(4)	Ru(1) -Ru(3)	2.699(7)
Ru(1) -Ru(4)	2.743(8)	Ru(1) -C(11)	1.92(3)
Ru(1) -C(12)	1.87(4)	Ru(1) -C(13m)	1.81(3)
Ru(2) -Ru(3)	3.253(4)	Ru(2) -Ru(4)	3.204(4)
Ru(2) -Cu(2)	3.050(5)	Ru(2) -C(21)	1.92(3)
Ru(2) -C(22)	1.78(4)	Ru(2) -C(23m)	1.99(3)
Ru(3) -Ru(4)	2.906(5)	Ru(3) -Cu(1)	2.798(8)
Ru(3) -Cu(2)	2.617(10)	Ru(3) -C(31)	1.87(3)
Ru(3) -C(32)	1.88(3)	Ru(3) -C(33)	1.94(3)
Ru(4) -Cu(1)	2.910(9)	Ru(4) -Cu(2)	2.586(10)
Ru(4) -C(41)	2.06(3)	Ru(4) -C(42)	1.84(3)
Ru(4) -C(43)	1.81(4)	Cu(1) -Cu(2)	3.008(6)
Cu(1) -P(1)	2.603(10)	Cu(1) -C(31)	2.53(3)
Cu(2) -P(2)	2.104(11)	P(1) -C(11p)	1.87(4)
P(1) -C(12p)	2.01(3)	P(1) -C(13p)	1.91(3)
P(2) -C(21p)	1.90(3)	P(2) -C(22p)	1.89(3)
P(2) -C(23p)	1.88(3)	C(11) -O(11)	1.25(4)
C(12) -O(12)	1.34(5)	C(13m)-O(13m)	1.15(4)
C(21) -O(21)	1.36(4)	C(22) -O(22)	1.34(5)
C(23m)-O(23m)	1.11(4)	C(31) -O(31)	1.35(3)
C(32) -O(32)	1.07(4)	C(33) -O(33)	1.23(4)
C(41) -O(41)	1.05(5)	C(42) -O(42)	1.18(5)
C(43) -O(43)	1.36(5)	C(11p)-C(111)	1.58(4)
C(11p)-C(112)	1.65(4)	C(12p)-C(121)	1.42(4)
C(12p)-C(122)	1.60(4)	C(13p)-C(131)	1.53(3)

table 3 continued

C(13p)-C(132)	1.56(4)	C(21p)-C(211)	1.62(5)
C(21p)-C(212)	1.47(4)	C(22p)-C(221)	1.45(4)
C(22p)-C(222)	1.64(4)	C(23p)-C(231)	1.58(4)
C(23p)-C(232)	1.56(4)		

TABLE 4 Bond angles (°) for $[Cu_2Ru_4(\mu_3\text{-}H)_2(CO)_{12}(P\{CHMe_2\}_3)_2]$

Ru(3) -Ru(1) -Ru(2)	72.0(1)	Ru(4) -Ru(1) -Ru(2)	70.1(1)
Ru(4) -Ru(1) -Ru(3)	64.5(1)	C(11) -Ru(1) -Ru(2)	165(1)
C(11) -Ru(1) -Ru(3)	102(1)	C(11) -Ru(1) -Ru(4)	95(1)
C(12) -Ru(1) -Ru(2)	95(1)	C(12) -Ru(1) -Ru(3)	159(1)
C(12) -Ru(1) -Ru(4)	96(1)	C(12) -Ru(1) -C(11)	86(2)
C(13m)-Ru(1) -Ru(2)	89(1)	C(13m)-Ru(1) -Ru(3)	102(1)
C(13m)-Ru(1) -Ru(4)	158(1)	C(13m)-Ru(1) -C(11)	106(1)
C(13m)-Ru(1) -C(12)	93(1)	Ru(3) -Ru(2) -Ru(1)	52.1(2)
Ru(4) -Ru(2) -Ru(1)	53.6(2)	Ru(4) -Ru(2) -Ru(3)	53.5(1)
Cu(2) -Ru(2) -Ru(1)	90.0(1)	Cu(2) -Ru(2) -Ru(3)	48.9(2)
Cu(2) -Ru(2) -Ru(4)	48.8(2)	C(21) -Ru(2) -Ru(1)	172(1)
C(21) -Ru(2) -Ru(3)	123(1)	C(21) -Ru(2) -Ru(4)	131(1)
C(21) -Ru(2) -Cu(2)	90.0(9)	C(22) -Ru(2) -Ru(1)	93(1)
C(22) -Ru(2) -Ru(3)	144(1)	C(22) -Ru(2) -Ru(4)	103(1)
C(22) -Ru(2) -Cu(2)	139(1)	C(22) -Ru(2) -C(21)	93(2)
C(23m)-Ru(2) -Ru(1)	93.0(9)	C(23m)-Ru(2) -Ru(3)	101.4(9)
C(23m)-Ru(2) -Ru(4)	145.6(9)	C(23m)-Ru(2) -Cu(2)	136(1)
C(23m)-Ru(2) -C(21)	81(1)	C(23m)-Ru(2) -C(22)	85(1)
Ru(2) -Ru(3) -Ru(1)	56.0(1)	Ru(4) -Ru(3) -Ru(1)	58.4(2)
Ru(4) -Ru(3) -Ru(2)	62.4(1)	Cu(1) -Ru(3) -Ru(1)	109.2(3)
Cu(1) -Ru(3) -Ru(2)	118.4(2)	Cu(1) -Ru(3) -Ru(4)	61.3(3)
Cu(2) -Ru(3) -Ru(1)	103.1(3)	Cu(2) -Ru(3) -Ru(2)	61.5(1)
Cu(2) -Ru(3) -Ru(4)	55.6(3)	Cu(2) -Ru(3) -Cu(1)	67.4(2)
C(31) -Ru(3) -Ru(1)	87(1)	C(31) -Ru(3) -Ru(2)	141(1)
C(31) -Ru(3) -Ru(4)	92(1)	C(31) -Ru(3) -Cu(1)	62(1)

table 4 continued

C(31) -Ru(3) -Cu(2)	129(1)	C(32) -Ru(3) -Ru(1)	178.8(9)
C(32) -Ru(3) -Ru(2)	123.5(9)	C(32) -Ru(3) -Ru(4)	122(1)
C(32) -Ru(3) -Cu(1)	72.0(9)	C(32) -Ru(3) -Cu(2)	77(1)
C(32) -Ru(3) -C(31)	94(1)	C(33) -Ru(3) -Ru(1)	86(1)
C(33) -Ru(3) -Ru(2)	85.0(9)	C(33) -Ru(3) -Ru(4)	141(1)
C(33) -Ru(3) -Cu(1)	156.3(9)	C(33) -Ru(3) -Cu(2)	128(1)
C(33) -Ru(3) -C(31)	102(1)	C(33) -Ru(3) -C(32)	93(1)
Ru(2) -Ru(4) -Ru(1)	56.3(1)	Ru(3) -Ru(4) -Ru(1)	57.0(2)
Ru(3) -Ru(4) -Ru(2)	64.1(1)	Cu(1) -Ru(4) -Ru(1)	104.9(3)
Cu(1) -Ru(4) -Ru(2)	116.6(2)	Cu(1) -Ru(4) -Ru(3)	57.5(2)
Cu(2) -Ru(4) -Ru(1)	102.7(3)	Cu(2) -Ru(4) -Ru(2)	62.5(1)
Cu(2) -Ru(4) -Ru(3)	56.6(3)	Cu(2) -Ru(4) -Cu(1)	66.1(2)
C(41) -Ru(4) -Ru(1)	88(1)	C(41) -Ru(4) -Ru(2)	143(1)
C(41) -Ru(4) -Ru(3)	93(1)	C(41) -Ru(4) -Cu(1)	63(1)
C(41) -Ru(4) -Cu(2)	129(1)	C(42) -Ru(4) -Ru(1)	175(1)
C(42) -Ru(4) -Ru(2)	127(1)	C(42) -Ru(4) -Ru(3)	120(1)
C(42) -Ru(4) -Cu(1)	70(1)	C(42) -Ru(4) -Cu(2)	77(1)
C(42) -Ru(4) -C(41)	89(1)	C(43) -Ru(4) -Ru(1)	91(1)
C(43) -Ru(4) -Ru(2)	93(1)	C(43) -Ru(4) -Ru(3)	147(1)
C(43) -Ru(4) -Cu(1)	151(1)	C(43) -Ru(4) -Cu(2)	135(1)
C(43) -Ru(4) -C(41)	93(1)	C(43) -Ru(4) -C(42)	93(2)
Ru(4) -Cu(1) -Ru(3)	61.2(1)	Cu(2) -Cu(1) -Ru(3)	53.4(2)
Cu(2) -Cu(1) -Ru(4)	51.8(2)	P(1) -Cu(1) -Ru(3)	148.8(7)
P(1) -Cu(1) -Ru(4)	143.0(7)	P(1) -Cu(1) -Cu(2)	150.4(4)
C(31) -Cu(1) -Ru(3)	40.7(6)	C(31) -Cu(1) -Ru(4)	80.1(7)
C(31) -Cu(1) -Cu(2)	93.9(6)	C(31) -Cu(1) -P(1)	112.5(7)
Ru(3) -Cu(2) -Ru(2)	69.6(2)	Ru(4) -Cu(2) -Ru(2)	68.7(2)
Ru(4) -Cu(2) -Ru(3)	67.9(2)	Cu(1) -Cu(2) -Ru(2)	118.4(2)

table 4 continued

Cu(1) -Cu(2) -Ru(3)	59.2(2)	Cu(1) -Cu(2) -Ru(4)	62.1(2)
P(2) -Cu(2) -Ru(2)	120.6(3)	P(2) -Cu(2) -Ru(3)	144.9(9)
P(2) -Cu(2) -Ru(4)	146.5(9)	P(2) -Cu(2) -Cu(1)	121.0(3)
C(11p)-P(1) -Cu(1)	120(1)	C(12p)-P(1) -Cu(1)	116(1)
C(12p)-P(1) -C(11p)	111(1)	C(13p)-P(1) -Cu(1)	114(1)
C(13p)-P(1) -C(11p)	109(1)	C(13p)-P(1) -C(12p)	112(1)
C(21p)-P(2) -Cu(2)	114(1)	C(22p)-P(2) -Cu(2)	114(1)
C(22p)-P(2) -C(21p)	104(1)	C(23p)-P(2) -Cu(2)	111(1)
C(23p)-P(2) -C(21p)	108(1)	C(23p)-P(2) -C(22p)	104(1)
O(11) -C(11) -Ru(1)	160(4)	O(12) -C(12) -Ru(1)	163(3)
O(13m)-C(13m)-Ru(1)	165(2)	O(21) -C(21) -Ru(2)	145(3)
O(22) -C(22) -Ru(2)	166(3)	O(23m)-C(23m)-Ru(2)	172(3)
Cu(1) -C(31) -Ru(3)	77(1)	O(31) -C(31) -Ru(3)	172(2)
O(31) -C(31) -Cu(1)	106(2)	O(32) -C(32) -Ru(3)	175(3)
O(33) -C(33) -Ru(3)	157(2)	O(41) -C(41) -Ru(4)	176(4)
O(42) -C(42) -Ru(4)	160(3)	O(43) -C(43) -Ru(4)	160(3)
C(111)-C(11p)-P(1)	112(2)	C(112)-C(11p)-P(1)	115(2)
C(112)-C(11p)-C(111)	101(3)	C(121)-C(12p)-P(1)	112(2)
C(122)-C(12p)-P(1)	111(2)	C(122)-C(12p)-C(121)	116(3)
C(131)-C(13p)-P(1)	115(2)	C(132)-C(13p)-P(1)	107(2)
C(132)-C(13p)-C(131)	114(2)	C(211)-C(21p)-P(2)	107(2)
C(212)-C(21p)-P(2)	113(2)	C(212)-C(21p)-C(211)	108(2)
C(221)-C(22p)-P(2)	117(3)	C(222)-C(22p)-P(2)	109(2)
C(222)-C(22p)-C(221)	108(2)	C(231)-C(23p)-P(2)	118(2)
C(232)-C(23p)-P(2)	114(2)	C(232)-C(23p)-C(231)	108(2)

TABLE 5 Intermolecular distances (A°) for $[Cu_2Ru_4(\mu_3\text{-}H)_2(CO)_{12}(P\{CHMe_2\}_3)_2]$

atom1	atom2	dist	S	a	b	c
C(221)	O(12)	3.29	2	0.0	0.0	0.0
C(12p)	O(13m)	3.38	1	0.0	0.0	1.0
C(121)	O(13m)	3.16	1	0.0	0.0	1.0
O(33)	O(21)	3.28	2	0.0	0.0	0.0
O(33)	O(22)	3.28	2	0.0	0.0	0.0
O(43)	C(23m)	3.38	2	0.0	-1.0	0.0
O(43)	O(23m)	3.09	2	0.0	-1.0	0.0
C(222)	O(31)	3.36	1	-1.0	0.0	0.0

Symmetry Transformations:

The second atom is related to the first atom, at (x,y,z), by the symmetry operation S with (a,b,c) added to the (x',y',z') of S.

Where S =

1	x, y, z
2	-x, 0.5+y, -z

TABLE 6 Intramolecular distances (A°) for $[Cu_2Ru_4(\mu_3\text{-}H)_2(CO)_{12}(P\{CHMe_2\}_3)_2]$

Cu(1) ...Ru(1)	4.48	Cu(2) ...Ru(1)	4.16
O(11) ...Ru(1)	3.13	O(12) ...Ru(1)	3.18
O(13m)...Ru(1)	2.94	C(22) ...Ru(1)	3.42
C(23m)...Ru(1)	3.55	C(31) ...Ru(1)	3.19
O(31) ...Ru(1)	4.15	C(33) ...Ru(1)	3.21
O(33) ...Ru(1)	4.07	C(41) ...Ru(1)	3.36
O(41) ...Ru(1)	4.10	C(43) ...Ru(1)	3.31
P(2) ...Ru(2)	4.50	C(12) ...Ru(2)	3.53
C(13m)...Ru(2)	3.34	O(21) ...Ru(2)	3.13
O(22) ...Ru(2)	3.10	O(23m)...Ru(2)	3.09
C(33) ...Ru(2)	3.64	C(43) ...Ru(2)	3.76
P(2) ...Ru(3)	4.50	C(11) ...Ru(3)	3.63
C(13m)...Ru(3)	3.56	C(23m)...Ru(3)	4.14
O(31) ...Ru(3)	3.22	O(32) ...Ru(3)	2.94
O(33) ...Ru(3)	3.11	C(41) ...Ru(3)	3.64
C(42) ...Ru(3)	4.14	P(2) ...Ru(4)	4.49
C(11) ...Ru(4)	3.47	C(12) ...Ru(4)	3.49
C(22) ...Ru(4)	3.99	C(31) ...Ru(4)	3.52
C(32) ...Ru(4)	4.22	O(41) ...Ru(4)	3.11
O(42) ...Ru(4)	2.97	O(43) ...Ru(4)	3.12
O(31) ...Cu(1)	3.18	C(32) ...Cu(1)	2.85
O(32) ...Cu(1)	3.43	C(41) ...Cu(1)	2.71
O(41) ...Cu(1)	3.19	C(42) ...Cu(1)	2.87
O(42) ...Cu(1)	3.70	C(11p)...Cu(1)	3.89
C(111)...Cu(1)	3.90	C(12p)...Cu(1)	3.92

table 6 continued

C(121)...Cu(1)	3.96	C(13p)...Cu(1)	3.80
C(132)...Cu(1)	4.00	C(232)...Cu(1)	4.08
C(21) ...Cu(2)	3.60	C(31) ...Cu(2)	4.06
C(32) ...Cu(2)	2.87	O(32) ...Cu(2)	3.54
C(33) ...Cu(2)	4.10	C(42) ...Cu(2)	2.82
O(42) ...Cu(2)	3.58	C(43) ...Cu(2)	4.08
C(21p)...Cu(2)	3.37	C(212)...Cu(2)	3.66
C(22p)...Cu(2)	3.36	C(221)...Cu(2)	3.77
C(23p)...Cu(2)	3.29	C(231)...Cu(2)	3.80
C(232)...Cu(2)	3.80	C(111)...P(1)	2.87
C(112)...P(1)	2.98	C(121)...P(1)	2.87
C(122)...P(1)	2.97	C(131)...P(1)	3.06
C(132)...P(1)	2.79	C(211)...P(2)	2.85
C(212)...P(2)	2.98	C(221)...P(2)	3.00
C(222)...P(2)	2.88	C(231)...P(2)	2.97
C(232)...P(2)	2.89	C(12) ...C(11)	2.59
C(13m)...C(11)	2.98	C(31) ...C(11)	3.00
O(31) ...C(11)	3.33	C(41) ...C(11)	2.82
O(41) ...C(11)	3.07	C(31) ...O(11)	3.22
O(31) ...O(11)	3.02	C(41) ...O(11)	3.25
O(41) ...O(11)	3.10	C(13m)...C(12)	2.67
C(22) ...C(12)	3.10	C(43) ...C(12)	2.97
O(43) ...C(12)	3.26	C(22) ...O(12)	3.21
O(22) ...O(12)	3.26	O(43) ...O(12)	3.22
C(23m)...C(13m)	2.92	O(23m)...C(13m)	3.15
C(33) ...C(13m)	2.97	O(33) ...C(13m)	3.33
C(23m)...O(13m)	3.28	O(23m)...O(13m)	3.11
C(33) ...O(13m)	3.27	O(33) ...O(13m)	3.20

table 6 continued

C(22) ...C(21)	2.68	C(23m)...C(21)	2.55
C(22) ...O(21)	3.35	C(212)...O(21)	3.25
C(23m)...C(22)	2.56	C(33) ...C(23m)	3.48
C(32) ...C(31)	2.75	C(33) ...C(31)	2.97
C(41) ...C(31)	3.08	C(132)...O(31)	3.12
C(33) ...C(32)	2.76	C(42) ...C(41)	2.72
C(43) ...C(41)	2.82	C(43) ...C(42)	2.64
C(43) ...O(42)	3.37	C(231)...O(42)	3.09
C(12p)...C(11p)	2.95	C(122)...C(11p)	3.39
C(13p)...C(11p)	3.08	C(112)...C(111)	2.49
C(12p)...C(112)	2.95	C(122)...C(112)	2.86
C(13p)...C(12p)	2.90	C(132)...C(12p)	3.15
C(122)...C(121)	2.57	C(132)...C(121)	3.13
C(13p)...C(122)	3.08	C(131)...C(122)	3.09
C(132)...C(122)	3.45	C(132)...C(131)	2.59
C(22p)...C(21p)	2.99	C(222)...C(21p)	3.02
C(23p)...C(21p)	3.06	C(212)...C(211)	2.51
C(222)...C(211)	3.35	C(23p)...C(211)	3.02
C(231)...C(211)	3.36	C(23p)...C(22p)	2.98
C(232)...C(22p)	3.38	C(222)...C(221)	2.51
C(232)...C(231)	2.53		

Crystallographic Tables for $[Cu_2Ru_4(\mu\text{-}CO)_3(CO)_{10}(PPh_3)_2]$, {X-ray study presented in section 1.4, Vol.1}.

TABLE 1 Fractional atomic coordinates and thermal parameters ($Å^2$) for $[Cu_2Ru_4(\mu\text{-}CO)_3(CO)_{10}(PPh_3)_2]$

Atom	x	y	z	U_{iso} or U_{eq}
Ru(1)	0.32019(8)	0.20905(10)	0.09351(12)	0.0462(11)
Ru(2)	0.29707(7)	0.07893(9)	0.19845(13)	0.0415(11)
Ru(3)	0.23670(7)	0.22894(10)	0.22989(12)	0.0431(10)
Ru(4)	0.20045(7)	0.12916(10)	0.07974(12)	0.0383(11)
Cu(1)	0.3499(1)	0.1991(1)	0.2853(2)	0.045(1)
Cu(2)	0.2958(1)	0.0782(1)	0.0007(2)	0.047(2)
P(1)	0.4254(2)	0.2280(3)	0.3892(4)	0.044(3)
P(2)	0.3344(2)	0.0182(3)	-0.1200(4)	0.046(3)
C(11)	0.3219(9)	0.2259(12)	-0.0333(16)	0.065(6)
O(11)	0.3232(7)	0.2443(9)	-0.1120(13)	0.094(5)
C(12)	0.3862(12)	0.2715(16)	0.1115(19)	0.097(9)
O(12)	0.4306(9)	0.3092(12)	0.1258(14)	0.089(7)
C(13)	0.2654(9)	0.3016(13)	0.1236(15)	0.064(6)
O(13)	0.2538(7)	0.3626(10)	0.0901(11)	0.093(5)
C(21)	0.3811(10)	0.1182(13)	0.1343(16)	0.076(7)
O(21)	0.4300(6)	0.0972(8)	0.1275(10)	0.074(4)
C(22)	0.3144(10)	0.0564(13)	0.3190(17)	0.071(6)
O(22)	0.3254(7)	0.0361(9)	0.3975(12)	0.090(5)
C(23)	0.3245(10)	-0.0184(14)	0.1667(16)	0.078(7)
O(23)	0.3449(7)	-0.0784(10)	0.1541(12)	0.093(5)
C(24)	0.2093(8)	0.0434(11)	0.1875(14)	0.053(5)
O(24)	0.1784(6)	-0.0014(8)	0.2278(10)	0.074(4)
C(31)	0.1637(10)	0.2772(13)	0.2064(16)	0.075(7)
O(31)	0.1177(8)	0.3111(10)	0.1873(13)	0.089(6)
C(32)	0.2687(9)	0.3027(13)	0.3166(15)	0.064(6)

table 1 continued

O(32)	0.2830(6)	0.3488(8)	0.3710(10)	0.073(4)
C(33)	0.2108(9)	0.1644(12)	0.3243(16)	0.064(6)
O(33)	0.1900(7)	0.1345(9)	0.3871(12)	0.093(5)
C(41)	0.1901(9)	0.2074(12)	-0.0085(15)	0.057(6)
O(41)	0.1795(7)	0.2532(9)	-0.0667(12)	0.087(5)
C(42)	0.1874(9)	0.0475(13)	-0.0013(15)	0.064(6)
O(42)	0.1721(7)	-0.0049(10)	-0.0490(12)	0.095(5)
C(43)	0.1209(11)	0.1324(13)	0.1121(16)	0.078(7)
O(43)	0.0694(8)	0.1316(10)	0.1326(13)	0.108(6)
C(111)	0.4785(5)	0.1489(6)	0.4151(9)	0.049(5)
C(112)	0.4796(5)	0.0888(6)	0.3504(9)	0.067(6)
C(113)	0.5230(5)	0.0303(6)	0.3617(9)	0.073(7)
C(114)	0.5652(5)	0.0319(6)	0.4376(9)	0.070(6)
C(115)	0.5640(5)	0.0919(6)	0.5023(9)	0.079(7)
C(116)	0.5207(5)	0.1504(6)	0.4911(9)	0.063(6)
C(121)	0.3981(6)	0.2585(8)	0.5001(8)	0.055(5)
C(122)	0.3465(6)	0.2221(8)	0.5304(8)	0.076(7)
C(123)	0.3218(6)	0.2462(8)	0.6124(8)	0.093(8)
C(124)	0.3487(6)	0.3067(8)	0.6643(8)	0.092(8)
C(125)	0.4003(6)	0.3431(8)	0.6340(8)	0.098(8)
C(126)	0.4250(6)	0.3190(8)	0.5520(8)	0.073(7)
C(131)	0.4727(6)	0.3088(7)	0.3537(9)	0.047(5)
C(132)	0.5345(6)	0.2997(7)	0.3420(9)	0.071(6)
C(133)	0.5683(6)	0.3619(7)	0.3111(9)	0.085(7)
C(134)	0.5403(6)	0.4331(7)	0.2918(9)	0.093(8)
C(135)	0.4785(6)	0.4421(7)	0.3035(9)	0.096(8)
C(136)	0.4447(6)	0.3799(7)	0.3344(9)	0.081(7)
C(211)	0.3579(6)	-0.0821(6)	-0.1044(10)	0.056(5)

table 1 continued

C(212)	0.3203(6)	-0.1312(6)	-0.0570(10)	0.083(7)
C(213)	0.3353(6)	-0.2093(6)	-0.0454(10)	0.095(8)
C(214)	0.3880(6)	-0.2383(6)	-0.0812(10)	0.092(8)
C(215)	0.4257(6)	-0.1891(6)	-0.1286(10)	0.087(8)
C(216)	0.4106(6)	-0.1110(6)	-0.1402(10)	0.068(6)
C(221)	0.2875(6)	0.0177(9)	-0.2273(10)	0.064(6)
C(222)	0.2945(6)	-0.0383(9)	-0.2956(10)	0.062(9)
C(223)	0.2587(6)	-0.0355(9)	-0.3787(10)	0.062(10)
C(224)	0.2159(6)	0.0233(9)	-0.3933(10)	0.075(10)
C(225)	0.2089(6)	0.0793(9)	-0.3250(10)	0.075(9)
C(226)	0.2447(6)	0.0765(9)	-0.2419(10)	0.079(7)
C(231)	0.4025(5)	0.0682(7)	-0.1503(10)	0.052(5)
C(232)	0.4519(5)	0.0666(7)	-0.0854(10)	0.075(7)
C(233)	0.5031(5)	0.1113(7)	-0.0996(10)	0.090(8)
C(234)	0.5049(5)	0.1576(7)	-0.1788(10)	0.087(8)
C(235)	0.4556(5)	0.1592(7)	-0.2438(10)	0.083(7)
C(236)	0.4043(5)	0.1145(7)	-0.2296(10)	0.069(6)

TABLE 2 Fractional atomic coordinates for the hydrogen atoms for $[Cu_2Ru_4(\mu\text{-}CO)_3(CO)_{10}(PPh_3)_2]$

Atom	x	y	z
H(112)	0.4470	0.0876	0.2916
H(113)	0.5240	-0.0162	0.3116
H(114)	0.5988	-0.0134	0.4463
H(115)	0.5967	0.0931	0.5611
H(116)	0.5197	0.1969	0.5412
H(122)	0.3257	0.1753	0.4902
H(123)	0.2819	0.2181	0.6358
H(124)	0.3296	0.3253	0.7278
H(125)	0.4212	0.3899	0.6741
H(126)	0.4650	0.3472	0.5286
H(132)	0.5562	0.2446	0.3569
H(133)	0.6161	0.3549	0.3021
H(134)	0.5665	0.4812	0.2679
H(135)	0.4569	0.4972	0.2886
H(136)	0.3969	0.3869	0.3434
H(212)	0.2794	-0.1088	-0.0293
H(213)	0.3061	-0.2473	-0.0087
H(214)	0.3997	-0.2987	-0.0722
H(215)	0.4665	-0.2115	-0.1563
H(216)	0.4398	-0.0730	-0.1769
H(222)	0.3277	-0.0838	-0.2843
H(223)	0.2641	-0.0789	-0.4316
H(224)	0.1882	0.0255	-0.4576
H(225)	0.1757	0.1249	-0.3363
H(226)	0.2393	0.1199	-0.1890

table 2 continued

H(232)	0.4505	0.0308	-0.0240
H(233)	0.5413	0.1101	-0.0493
H(234)	0.5446	0.1922	-0.1898
H(235)	0.4570	0.1950	-0.3051
H(236)	0.3661	0.1157	-0.2799

TABLE 3 Anisotropic thermal parameters ($Å^2$) for $[Cu_2Ru_4(\mu\text{-}CO)_3(CO)_{10}(PPh_3)_2]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ru(1)	0.047(1)	0.047(1)	0.044(1)	0.002(1)	0.012(1)	-0.007(1)
Ru(2)	0.043(1)	0.037(1)	0.045(1)	0.006(1)	-0.012(1)	-0.002(1)
Ru(3)	0.038(1)	0.046(1)	0.044(1)	-0.008(1)	0.000(1)	0.009(1)
Ru(4)	0.032(1)	0.042(1)	0.040(1)	-0.010(1)	-0.006(1)	0.004(1)
Cu(1)	0.043(1)	0.049(1)	0.042(2)	0.001(1)	-0.009(1)	-0.001(1)
Cu(2)	0.050(1)	0.052(2)	0.041(2)	-0.003(1)	0.006(1)	0.005(1)
P(1)	0.040(3)	0.044(3)	0.049(4)	0.002(3)	-0.005(3)	-0.002(2)
P(2)	0.049(3)	0.042(3)	0.047(4)	-0.003(3)	0.005(3)	0.006(3)

TABLE 4 Bond lengths (Å) for $[Cu_2Ru_4(\mu\text{-}CO)_3(CO)_{10}(PPh_3)_2]$

Ru(1) -Ru(2)	2.771(2)	Ru(1) -Ru(3)	2.797(2)
Ru(1) -Ru(4)	2.981(2)	Ru(1) -Cu(1)	2.806(2)
Ru(1) -Cu(2)	2.662(2)	Ru(1) -C(11)	1.853(3)
Ru(1) -C(12)	1.820(4)	Ru(1) -C(13)	2.065(4)
Ru(1) -C(21)	2.126(5)	Ru(2) -Ru(3)	2.958(2)
Ru(2) -Ru(4)	2.793(2)	Ru(2) -Cu(1)	2.656(2)
Ru(2) -Cu(2)	2.848(2)	Ru(2) -C(21)	2.230(3)
Ru(2) -C(22)	1.798(5)	Ru(2) -C(23)	1.852(5)
Ru(2) -C(24)	2.031(4)	Ru(3) -Ru(4)	2.842(2)
Ru(3) -Cu(1)	2.633(2)	Ru(3) -C(13)	2.105(4)
Ru(3) -C(31)	1.829(5)	Ru(3) -C(32)	1.891(3)
Ru(3) -C(33)	1.873(4)	Ru(4) -Cu(2)	2.608(2)
Ru(4) -C(24)	2.145(4)	Ru(4) -C(41)	1.859(3)
Ru(4) -C(42)	1.841(4)	Ru(4) -C(43)	1.846(3)
Cu(1) -P(1)	2.231(6)	Cu(1) -C(22)	2.639(4)
Cu(1) -C(32)	2.593(3)	Cu(2) -P(2)	2.236(6)
Cu(2) -C(42)	2.452(4)	P(1) -C(111)	1.823(8)
P(1) -C(121)	1.820(9)	P(1) -C(131)	1.833(9)
P(2) -C(211)	1.816(8)	P(2) -C(221)	1.808(9)
P(2) -C(231)	1.812(9)	C(11) -O(11)	1.180(6)
C(12) -O(12)	1.185(7)	C(13) -O(13)	1.180(4)
C(21) -O(21)	1.150(6)	C(22) -O(22)	1.195(6)
C(23) -O(23)	1.148(6)	C(24) -O(24)	1.204(5)
C(31) -O(31)	1.192(4)	C(32) -O(32)	1.147(7)
C(33) -O(33)	1.161(6)	C(41) -O(41)	1.165(7)

table 4 continued

C(42) -O(42)	1.173(4)	C(43) -O(43)	1.195(6)
C(111)-C(112)	1.395(18)	C(111)-C(116)	1.395(17)
C(112)-C(113)	1.395(16)	C(113)-C(114)	1.395(17)
C(114)-C(115)	1.395(18)	C(115)-C(116)	1.395(16)
C(121)-C(122)	1.395(19)	C(121)-C(126)	1.395(19)
C(122)-C(123)	1.395(18)	C(123)-C(124)	1.395(19)
C(124)-C(125)	1.395(19)	C(125)-C(126)	1.395(18)
C(131)-C(132)	1.395(18)	C(131)-C(136)	1.395(17)
C(132)-C(133)	1.395(17)	C(133)-C(134)	1.395(17)
C(134)-C(135)	1.395(18)	C(135)-C(136)	1.395(17)
C(211)-C(212)	1.395(19)	C(211)-C(216)	1.395(19)
C(212)-C(213)	1.395(16)	C(213)-C(214)	1.395(19)
C(214)-C(215)	1.395(19)	C(215)-C(216)	1.395(16)
C(221)-C(222)	1.395(21)	C(221)-C(226)	1.395(21)
C(222)-C(223)	1.395(19)	C(223)-C(224)	1.395(21)
C(224)-C(225)	1.395(21)	C(225)-C(226)	1.395(19)
C(231)-C(232)	1.395(17)	C(231)-C(236)	1.395(19)
C(232)-C(233)	1.395(17)	C(233)-C(234)	1.395(19)
C(234)-C(235)	1.395(17)	C(235)-C(236)	1.395(17)

TABLE 5 Bond angles (°) for $[Cu_2Ru_4(\mu\text{-}CO)_3(CO)_{10}(PPh_3)_2]$

Ru(3) -Ru(1) -Ru(2)	64.2(1)	Ru(4) -Ru(1) -Ru(2)	58.0(1)
Ru(4) -Ru(1) -Ru(3)	58.8(1)	Cu(1) -Ru(1) -Ru(2)	56.9(1)
Cu(1) -Ru(1) -Ru(3)	56.1(1)	Cu(1) -Ru(1) -Ru(4)	101.1(1)
Cu(2) -Ru(1) -Ru(2)	63.2(1)	Cu(2) -Ru(1) -Ru(3)	109.5(1)
Cu(2) -Ru(1) -Ru(4)	54.7(1)	Cu(2) -Ru(1) -Cu(1)	118.1(1)
C(11) -Ru(1) -Ru(2)	132.9(7)	C(11) -Ru(1) -Ru(3)	136.7(7)
C(11) -Ru(1) -Ru(4)	94.4(6)	C(11) -Ru(1) -Cu(1)	164.3(7)
C(11) -Ru(1) -Cu(2)	69.7(7)	C(12) -Ru(1) -Ru(2)	125.1(9)
C(12) -Ru(1) -Ru(3)	112.6(9)	C(12) -Ru(1) -Ru(4)	169.9(9)
C(12) -Ru(1) -Cu(1)	75.9(9)	C(12) -Ru(1) -Cu(2)	135.3(9)
C(12) -Ru(1) -C(11)	89(1)	C(13) -Ru(1) -Ru(2)	112.4(6)
C(13) -Ru(1) -Ru(3)	48.5(6)	C(13) -Ru(1) -Ru(4)	80.8(6)
C(13) -Ru(1) -Cu(1)	86.9(6)	C(13) -Ru(1) -Cu(2)	131.0(6)
C(13) -Ru(1) -C(11)	97.7(9)	C(13) -Ru(1) -C(12)	89(1)
C(21) -Ru(1) -Ru(2)	52.2(6)	C(21) -Ru(1) -Ru(3)	109.3(6)
C(21) -Ru(1) -Ru(4)	102.9(6)	C(21) -Ru(1) -Cu(1)	64.9(6)
C(21) -Ru(1) -Cu(2)	67.6(6)	C(21) -Ru(1) -C(11)	109.7(9)
C(21) -Ru(1) -C(12)	85(1)	C(21) -Ru(1) -C(13)	151.8(9)
Ru(3) -Ru(2) -Ru(1)	58.3(1)	Ru(4) -Ru(2) -Ru(1)	64.8(1)
Ru(4) -Ru(2) -Ru(3)	59.1(1)	Cu(1) -Ru(2) -Ru(1)	62.2(1)
Cu(1) -Ru(2) -Ru(3)	55.6(1)	Cu(1) -Ru(2) -Ru(4)	110.2(1)
Cu(2) -Ru(2) -Ru(1)	56.6(1)	Cu(2) -Ru(2) -Ru(3)	100.4(1)
Cu(2) -Ru(2) -Ru(4)	55.1(1)	Cu(2) -Ru(2) -Cu(1)	116.9(1)
C(21) -Ru(2) -Ru(1)	48.9(6)	C(21) -Ru(2) -Ru(3)	101.1(6)
C(21) -Ru(2) -Ru(4)	106.1(6)	C(21) -Ru(2) -Cu(1)	66.7(6)

table 5 continued

C(21) -Ru(2) -Cu(2)	62.9(6)	C(22) -Ru(2) -Ru(1)	131.8(7)
C(22) -Ru(2) -Ru(3)	96.5(7)	C(22) -Ru(2) -Ru(4)	140.3(7)
C(22) -Ru(2) -Cu(1)	69.6(7)	C(22) -Ru(2) -Cu(2)	162.5(7)
C(22) -Ru(2) -C(21)	109.4(9)	C(23) -Ru(2) -Ru(1)	121.7(8)
C(23) -Ru(2) -Ru(3)	171.2(7)	C(23) -Ru(2) -Ru(4)	112.3(7)
C(23) -Ru(2) -Cu(1)	133.0(7)	C(23) -Ru(2) -Cu(2)	74.5(7)
C(23) -Ru(2) -C(21)	83.1(9)	C(23) -Ru(2) -C(22)	89(1)
C(24) -Ru(2) -Ru(1)	114.1(6)	C(24) -Ru(2) -Ru(3)	80.7(6)
C(24) -Ru(2) -Ru(4)	49.8(6)	C(24) -Ru(2) -Cu(1)	131.6(6)
C(24) -Ru(2) -Cu(2)	88.2(6)	C(24) -Ru(2) -C(21)	151.0(8)
C(24) -Ru(2) -C(22)	99.0(9)	C(24) -Ru(2) -C(23)	91.9(9)
Ru(2) -Ru(3) -Ru(1)	57.5(1)	Ru(4) -Ru(3) -Ru(1)	63.8(1)
Ru(4) -Ru(3) -Ru(2)	57.5(1)	Cu(1) -Ru(3) -Ru(1)	62.2(1)
Cu(1) -Ru(3) -Ru(2)	56.4(1)	Cu(1) -Ru(3) -Ru(4)	109.4(1)
C(13) -Ru(3) -Ru(1)	47.3(6)	C(13) -Ru(3) -Ru(2)	104.5(6)
C(13) -Ru(3) -Ru(4)	83.7(6)	C(13) -Ru(3) -Cu(1)	90.8(6)
C(31) -Ru(3) -Ru(1)	122.6(7)	C(31) -Ru(3) -Ru(2)	140.4(7)
C(31) -Ru(3) -Ru(4)	86.0(7)	C(31) -Ru(3) -Cu(1)	163.2(7)
C(31) -Ru(3) -C(13)	84.0(9)	C(32) -Ru(3) -Ru(1)	108.1(7)
C(32) -Ru(3) -Ru(2)	122.4(6)	C(32) -Ru(3) -Ru(4)	171.1(7)
C(32) -Ru(3) -Cu(1)	67.7(6)	C(32) -Ru(3) -C(13)	87.9(9)
C(32) -Ru(3) -C(31)	96.1(9)	C(33) -Ru(3) -Ru(1)	132.9(7)
C(33) -Ru(3) -Ru(2)	75.6(7)	C(33) -Ru(3) -Ru(4)	96.2(7)
C(33) -Ru(3) -Cu(1)	89.4(6)	C(33) -Ru(3) -C(13)	179.7(4)
C(33) -Ru(3) -C(31)	96(1)	C(33) -Ru(3) -C(32)	92.2(9)
Ru(2) -Ru(4) -Ru(1)	57.2(1)	Ru(3) -Ru(4) -Ru(1)	57.4(1)
Ru(3) -Ru(4) -Ru(2)	63.3(1)	Cu(2) -Ru(4) -Ru(1)	56.4(1)
Cu(2) -Ru(4) -Ru(2)	63.5(1)	Cu(2) -Ru(4) -Ru(3)	109.8(1)

table 5 continued

C(24) -Ru(4) -Ru(1)	103.2(5)	C(24) -Ru(4) -Ru(2)	46.3(5)
C(24) -Ru(4) -Ru(3)	81.8(5)	C(24) -Ru(4) -Cu(2)	92.4(5)
C(41) -Ru(4) -Ru(1)	77.4(6)	C(41) -Ru(4) -Ru(2)	134.6(6)
C(41) -Ru(4) -Ru(3)	95.7(6)	C(41) -Ru(4) -Cu(2)	90.9(6)
C(41) -Ru(4) -C(24)	176.4(8)	C(42) -Ru(4) -Ru(1)	120.0(6)
C(42) -Ru(4) -Ru(2)	103.6(6)	C(42) -Ru(4) -Ru(3)	166.5(7)
C(42) -Ru(4) -Cu(2)	64.2(6)	C(42) -Ru(4) -C(24)	86.3(9)
C(42) -Ru(4) -C(41)	96.5(9)	C(43) -Ru(4) -Ru(1)	145.5(7)
C(43) -Ru(4) -Ru(2)	124.1(7)	C(43) -Ru(4) -Ru(3)	91.1(7)
C(43) -Ru(4) -Cu(2)	158.0(7)	C(43) -Ru(4) -C(24)	83.5(9)
C(43) -Ru(4) -C(41)	94.0(9)	C(43) -Ru(4) -C(42)	94(1)
Ru(2) -Cu(1) -Ru(1)	60.9(1)	Ru(3) -Cu(1) -Ru(1)	61.8(1)
Ru(3) -Cu(1) -Ru(2)	68.0(1)	P(1) -Cu(1) -Ru(1)	140.3(2)
P(1) -Cu(1) -Ru(2)	141.3(2)	P(1) -Cu(1) -Ru(3)	145.0(2)
C(22) -Cu(1) -Ru(1)	100.6(5)	C(22) -Cu(1) -Ru(2)	39.7(5)
C(22) -Cu(1) -Ru(3)	87.1(5)	C(22) -Cu(1) -P(1)	107.7(5)
C(32) -Cu(1) -Ru(1)	90.3(5)	C(32) -Cu(1) -Ru(2)	109.3(5)
C(32) -Cu(1) -Ru(3)	42.4(5)	C(32) -Cu(1) -P(1)	103.2(5)
C(32) -Cu(1) -C(22)	113.2(7)	Ru(2) -Cu(2) -Ru(1)	60.3(1)
Ru(4) -Cu(2) -Ru(1)	68.9(1)	Ru(4) -Cu(2) -Ru(2)	61.4(1)
P(2) -Cu(2) -Ru(1)	135.0(2)	P(2) -Cu(2) -Ru(2)	143.0(2)
P(2) -Cu(2) -Ru(4)	148.4(2)	C(42) -Cu(2) -Ru(1)	110.9(5)
C(42) -Cu(2) -Ru(2)	87.9(5)	C(42) -Cu(2) -Ru(4)	42.5(5)
C(42) -Cu(2) -P(2)	108.0(5)	C(111)-P(1) -Cu(1)	114.6(5)
C(121)-P(1) -Cu(1)	112.3(5)	C(121)-P(1) -C(111)	106.2(7)
C(131)-P(1) -Cu(1)	113.5(5)	C(131)-P(1) -C(111)	104.8(6)
C(131)-P(1) -C(121)	104.5(6)	C(211)-P(2) -Cu(2)	117.7(5)
C(221)-P(2) -Cu(2)	116.2(5)	C(221)-P(2) -C(211)	104.3(7)

table 5 continued

C(231)-P(2) -Cu(2)	109.2(5)	C(231)-P(2) -C(211)	104.3(6)
C(231)-P(2) -C(221)	103.8(7)	O(11) -C(11) -Ru(1)	173(2)
O(12) -C(12) -Ru(1)	177(2)	Ru(3) -C(13) -Ru(1)	84.2(8)
O(13) -C(13) -Ru(1)	136(2)	O(13) -C(13) -Ru(3)	139(2)
Ru(2) -C(21) -Ru(1)	79.0(8)	O(21) -C(21) -Ru(1)	142(2)
O(21) -C(21) -Ru(2)	139(2)	Cu(1) -C(22) -Ru(2)	70.7(7)
O(22) -C(22) -Ru(2)	175(2)	O(22) -C(22) -Cu(1)	114(2)
O(23) -C(23) -Ru(2)	174(2)	Ru(4) -C(24) -Ru(2)	83.9(7)
O(24) -C(24) -Ru(2)	136(1)	O(24) -C(24) -Ru(4)	140(1)
O(31) -C(31) -Ru(3)	176(2)	Cu(1) -C(32) -Ru(3)	69.9(7)
O(32) -C(32) -Ru(3)	174(2)	O(32) -C(32) -Cu(1)	115(1)
O(33) -C(33) -Ru(3)	169(2)	O(41) -C(41) -Ru(4)	174(2)
Cu(2) -C(42) -Ru(4)	73.3(7)	O(42) -C(42) -Ru(4)	172(2)
O(42) -C(42) -Cu(2)	115(1)	O(43) -C(43) -Ru(4)	178(2)
C(112)-C(111)-P(1)	117.2(9)	C(116)-C(111)-P(1)	122.5(9)
C(116)-C(111)-C(112)	120(1)	C(113)-C(112)-C(111)	120(1)
C(114)-C(113)-C(112)	120(1)	C(115)-C(114)-C(113)	120(1)
C(116)-C(115)-C(114)	120(1)	C(115)-C(116)-C(111)	120(1)
C(122)-C(121)-P(1)	118(1)	C(126)-C(121)-P(1)	122(1)
C(126)-C(121)-C(122)	120(1)	C(123)-C(122)-C(121)	120(1)
C(124)-C(123)-C(122)	120(1)	C(125)-C(124)-C(123)	120(1)
C(126)-C(125)-C(124)	120(1)	C(125)-C(126)-C(121)	120(1)
C(132)-C(131)-P(1)	121.9(9)	C(136)-C(131)-P(1)	118(1)
C(136)-C(131)-C(132)	120(1)	C(133)-C(132)-C(131)	120(1)
C(134)-C(133)-C(132)	120(1)	C(135)-C(134)-C(133)	120(1)
C(136)-C(135)-C(134)	120(1)	C(135)-C(136)-C(131)	120(1)
C(212)-C(211)-P(2)	118(1)	C(216)-C(211)-P(2)	122(1)
C(216)-C(211)-C(212)	120(1)	C(213)-C(212)-C(211)	120(1)

table 5 continued

C(214)-C(213)-C(212)	120(1)	C(215)-C(214)-C(213)	120(1)
C(216)-C(215)-C(214)	120(1)	C(215)-C(216)-C(211)	120(1)
C(222)-C(221)-P(2)	122(1)	C(226)-C(221)-P(2)	118(1)
C(226)-C(221)-C(222)	120(1)	C(223)-C(222)-C(221)	120(1)
C(224)-C(223)-C(222)	120(1)	C(225)-C(224)-C(223)	120(1)
C(226)-C(225)-C(224)	120(1)	C(225)-C(226)-C(221)	120(1)
C(232)-C(231)-P(2)	117(1)	C(236)-C(231)-P(2)	122.4(9)
C(236)-C(231)-C(232)	120(1)	C(233)-C(232)-C(231)	120(1)
C(234)-C(233)-C(232)	120(1)	C(235)-C(234)-C(233)	120(1)
C(236)-C(235)-C(234)	120(1)	C(235)-C(236)-C(231)	120(1)

TABLE 6 Intermolecular distances (Å) for $[Cu_2Ru_4(\mu\text{-}CO)_3(CO)_{10}(PPh_3)_2]$

atom1	atom2	dist	S	a	b	c
H(124)	O(11)	2.71	1	0.0	0.0	1.0
H(215)	O(12)	2.84	-1	1.0	0.0	0.0
H(223)	O(13)	2.51	-2	1.0	0.0	0.0
H(216)	O(21)	2.95	-1	1.0	0.0	0.0
H(114)	O(22)	2.75	-1	1.0	0.0	1.0
H(115)	O(22)	2.86	-1	1.0	0.0	1.0
O(32)	C(23)	3.32	-2	1.0	1.0	1.0
C(31)	O(23)	3.21	-2	1.0	1.0	1.0
O(31)	O(23)	3.05	-2	1.0	1.0	1.0
C(32)	O(23)	3.29	-2	1.0	1.0	1.0
O(32)	O(23)	3.10	-2	1.0	1.0	1.0
O(32)	O(24)	3.09	-2	1.0	1.0	1.0
H(135)	O(24)	2.99	-2	1.0	1.0	1.0
H(136)	O(24)	2.71	-2	1.0	1.0	1.0
C(115)	O(31)	3.31	2	0.0	0.0	0.0
H(115)	O(31)	2.48	2	0.0	0.0	0.0
H(116)	O(31)	2.93	2	0.0	0.0	0.0
C(234)	O(31)	3.29	2	0.0	0.0	-1.0
H(234)	O(31)	2.47	2	0.0	0.0	-1.0
H(212)	O(32)	2.83	-2	1.0	0.0	1.0
H(224)	O(33)	2.92	1	0.0	0.0	-1.0
H(213)	O(33)	2.68	-2	1.0	0.0	1.0
H(132)	O(41)	2.88	2	0.0	0.0	0.0
H(133)	O(41)	2.95	2	0.0	0.0	0.0
C(125)	O(42)	3.27	-2	1.0	1.0	1.0

table 6 continued

H(126)...O(43)	2.70	2	0.0	0.0	0.0
H(135)...O(43)	2.66	-2	1.0	1.0	1.0
H(216)...C(113)	2.93	-1	1.0	0.0	0.0
C(231)...H(113)	3.05	-1	1.0	0.0	0.0
C(235)...H(113)	2.70	-1	1.0	0.0	0.0
C(236)...H(113)	2.65	-1	1.0	0.0	0.0
H(236)...C(123)	2.87	1	0.0	0.0	-1.0
H(235)...C(125)	2.95	1	0.0	0.0	-1.0
H(235)...C(126)	3.02	1	0.0	0.0	-1.0
C(225)...H(123)	2.96	1	0.0	0.0	-1.0
H(215)...C(132)	3.08	-1	1.0	0.0	0.0
C(225)...H(133)	3.05	2	-1.0	0.0	-1.0
H(225)...C(214)	2.96	-2	1.0	1.0	0.0
H(233)...C(215)	2.96	-1	1.0	0.0	0.0
H(233)...C(216)	2.87	-1	1.0	0.0	0.0

Symmetry Transformations:

The second atom is related to the first atom, at (x,y,z), by the symmetry operation S with (a,b,c) added to the (x',y',z') of S.

Where S =

1	x, y, z
2	0.5+x, 0.5-y, 0.5+z

TABLE 7 Intramolecular distances (Å) for $[Cu_2Ru_4(\mu\text{-}CO)_3(CO)_{10}(PPh_3)_2]$

P(2) ...Ru(1)	4.53	O(11) ...Ru(1)	3.03
O(12) ...Ru(1)	3.00	O(13) ...Ru(1)	3.03
O(21) ...Ru(1)	3.12	C(22) ...Ru(1)	4.19
C(23) ...Ru(1)	4.06	C(24) ...Ru(1)	4.05
C(31) ...Ru(1)	4.08	C(32) ...Ru(1)	3.83
C(41) ...Ru(1)	3.15	O(41) ...Ru(1)	3.84
C(42) ...Ru(1)	4.22	C(12) ...Ru(2)	4.10
C(13) ...Ru(2)	4.04	O(21) ...Ru(2)	3.18
O(22) ...Ru(2)	2.99	O(23) ...Ru(2)	3.00
O(24) ...Ru(2)	3.02	C(33) ...Ru(2)	3.08
O(33) ...Ru(2)	3.83	C(42) ...Ru(2)	3.69
C(43) ...Ru(2)	4.12	H(112)...Ru(2)	3.50
Cu(2) ...Ru(3)	4.46	C(12) ...Ru(3)	3.88
O(13) ...Ru(3)	3.10	C(21) ...Ru(3)	4.03
C(22) ...Ru(3)	3.63	C(24) ...Ru(3)	3.31
O(31) ...Ru(3)	3.02	O(32) ...Ru(3)	3.03
O(33) ...Ru(3)	3.02	C(41) ...Ru(3)	3.55
C(43) ...Ru(3)	3.42	Cu(1) ...Ru(4)	4.47
C(11) ...Ru(4)	3.63	C(13) ...Ru(4)	3.35
C(21) ...Ru(4)	4.03	C(23) ...Ru(4)	3.89
O(24) ...Ru(4)	3.16	C(31) ...Ru(4)	3.27
O(31) ...Ru(4)	3.99	C(33) ...Ru(4)	3.57
O(41) ...Ru(4)	3.02	O(42) ...Ru(4)	3.01
O(43) ...Ru(4)	3.04	Cu(2) ...Cu(1)	4.69
C(12) ...Cu(1)	2.95	O(12) ...Cu(1)	3.54

table 7 continued

C(13) ...Cu(1)	3.39	C(21) ...Cu(1)	2.71
O(21) ...Cu(1)	3.44	O(22) ...Cu(1)	3.31
C(23) ...Cu(1)	4.15	O(32) ...Cu(1)	3.26
C(33) ...Cu(1)	3.22	O(33) ...Cu(1)	4.07
C(111)...Cu(1)	3.42	C(112)...Cu(1)	3.52
H(112)...Cu(1)	2.88	C(121)...Cu(1)	3.37
C(122)...Cu(1)	3.56	H(122)...Cu(1)	3.06
C(131)...Cu(1)	3.40	C(136)...Cu(1)	3.80
H(136)...Cu(1)	3.49	C(11) ...Cu(2)	2.66
O(11) ...Cu(2)	3.37	C(21) ...Cu(2)	2.70
O(21) ...Cu(2)	3.41	C(23) ...Cu(2)	2.95
O(23) ...Cu(2)	3.62	C(24) ...Cu(2)	3.45
C(41) ...Cu(2)	3.23	O(41) ...Cu(2)	4.05
O(42) ...Cu(2)	3.13	C(211)...Cu(2)	3.47
C(212)...Cu(2)	3.75	H(212)...Cu(2)	3.27
C(221)...Cu(2)	3.44	C(226)...Cu(2)	3.61
H(226)...Cu(2)	3.02	C(231)...Cu(2)	3.31
C(232)...Cu(2)	3.74	H(232)...Cu(2)	3.55
C(32) ...P(1)	3.79	C(112)...P(1)	2.76
C(116)...P(1)	2.83	H(112)...P(1)	2.86
H(116)...P(1)	2.98	C(122)...P(1)	2.76
C(126)...P(1)	2.82	H(122)...P(1)	2.86
H(126)...P(1)	2.97	C(132)...P(1)	2.83
C(136)...P(1)	2.78	H(132)...P(1)	2.97
H(136)...P(1)	2.88	C(42) ...P(2)	3.80
C(212)...P(2)	2.76	C(216)...P(2)	2.82
H(212)...P(2)	2.86	H(216)...P(2)	2.97
C(222)...P(2)	2.80	C(226)...P(2)	2.76

table 7 continued

H(222)...P(2)	2.95	H(226)...P(2)	2.87
C(232)...P(2)	2.75	C(236)...P(2)	2.82
H(232)...P(2)	2.85	H(236)...P(2)	2.97
C(12) ...C(11)	2.58	C(13) ...C(11)	2.95
O(13) ...C(11)	3.36	C(21) ...C(11)	3.26
C(41) ...C(11)	2.97	O(41) ...C(11)	3.19
O(41) ...O(11)	3.29	C(236)...O(11)	3.38
C(13) ...C(12)	2.74	O(13) ...C(12)	3.32
C(21) ...C(12)	2.67	O(21) ...C(12)	3.16
C(131)...O(12)	3.36	C(136)...O(12)	3.24
C(31) ...C(13)	2.64	C(32) ...C(13)	2.78
C(41) ...C(13)	2.94	O(41) ...C(13)	3.35
C(31) ...O(13)	3.06	C(32) ...O(13)	3.42
C(41) ...O(13)	3.31	O(41) ...O(13)	3.30
C(22) ...C(21)	3.30	C(23) ...C(21)	2.72
H(112)...C(21)	2.67	C(23) ...O(21)	3.14
C(112)...O(21)	3.33	H(112)...O(21)	2.38
C(232)...O(21)	3.18	H(232)...O(21)	2.53
C(23) ...C(22)	2.57	C(24) ...C(22)	2.92
O(24) ...C(22)	3.36	C(33) ...C(22)	2.96
O(33) ...C(22)	3.27	H(112)...C(22)	3.03
H(122)...O(22)	2.75	C(24) ...C(23)	2.79
O(24) ...C(23)	3.41	C(212)...O(23)	3.19
H(212)...O(23)	2.98	C(33) ...C(24)	2.87
O(33) ...C(24)	3.33	C(42) ...C(24)	2.73
C(43) ...C(24)	2.66	C(33) ...O(24)	3.24
O(33) ...O(24)	3.28	C(43) ...O(24)	3.08
C(32) ...C(31)	2.77	C(33) ...C(31)	2.75

table 7 continued

C(41) ...C(31)	3.41	C(43) ...C(31)	2.97
O(43) ...C(31)	3.39	C(43) ...O(31)	3.27
C(33) ...C(32)	2.71	C(122)...O(32)	3.41
H(136)...O(32)	2.65	C(42) ...C(41)	2.76
C(43) ...C(41)	2.71	C(43) ...C(42)	2.69
H(212)...O(42)	2.97	C(113)...C(111)	2.42
C(114)...C(111)	2.79	C(115)...C(111)	2.42
H(112)...C(111)	2.15	H(116)...C(111)	2.15
C(121)...C(111)	2.91	C(131)...C(111)	2.90
C(132)...C(111)	3.09	H(132)...C(111)	2.56
C(114)...C(112)	2.42	C(115)...C(112)	2.79
C(116)...C(112)	2.42	H(113)...C(112)	2.15
C(115)...C(113)	2.42	C(116)...C(113)	2.79
H(112)...C(113)	2.15	H(114)...C(113)	2.15
C(116)...C(114)	2.42	H(113)...C(114)	2.15
H(115)...C(114)	2.15	H(114)...C(115)	2.15
H(116)...C(115)	2.15	H(115)...C(116)	2.15
C(121)...C(116)	3.30	C(131)...C(116)	3.50
C(132)...C(116)	3.38	H(132)...C(116)	2.68
C(121)...H(116)	2.92	C(126)...H(116)	2.98
C(123)...C(121)	2.42	C(124)...C(121)	2.79
C(125)...C(121)	2.42	H(122)...C(121)	2.15
H(126)...C(121)	2.15	C(131)...C(121)	2.89
C(136)...C(121)	3.38	C(124)...C(122)	2.42
C(125)...C(122)	2.79	C(126)...C(122)	2.42
H(123)...C(122)	2.15	C(125)...C(123)	2.42
C(126)...C(123)	2.79	H(122)...C(123)	2.15
H(124)...C(123)	2.15	C(126)...C(124)	2.42

table 7 continued

H(123)...C(124)	2.15	H(125)...C(124)	2.15
H(124)...C(125)	2.15	H(126)...C(125)	2.15
H(125)...C(126)	2.15	C(131)...C(126)	3.11
C(136)...C(126)	3.36	C(131)...H(126)	2.62
C(136)...H(126)	2.86	C(133)...C(131)	2.42
C(134)...C(131)	2.79	C(135)...C(131)	2.42
H(132)...C(131)	2.15	H(136)...C(131)	2.15
C(134)...C(132)	2.42	C(135)...C(132)	2.79
C(136)...C(132)	2.42	H(133)...C(132)	2.15
C(135)...C(133)	2.42	C(136)...C(133)	2.79
H(132)...C(133)	2.15	H(134)...C(133)	2.15
C(136)...C(134)	2.42	H(133)...C(134)	2.15
H(135)...C(134)	2.15	H(134)...C(135)	2.15
H(136)...C(135)	2.15	H(135)...C(136)	2.15
C(213)...C(211)	2.42	C(214)...C(211)	2.79
C(215)...C(211)	2.42	H(212)...C(211)	2.15
H(216)...C(211)	2.15	C(221)...C(211)	2.86
C(222)...C(211)	3.11	H(222)...C(211)	2.64
C(231)...C(211)	2.87	C(232)...C(211)	3.30
H(232)...C(211)	3.01	C(214)...C(212)	2.42
C(215)...C(212)	2.79	C(216)...C(212)	2.42
H(213)...C(212)	2.15	C(215)...C(213)	2.42
C(216)...C(213)	2.79	H(212)...C(213)	2.15
H(214)...C(213)	2.15	C(216)...C(214)	2.42
H(213)...C(214)	2.15	H(215)...C(214)	2.15
H(214)...C(215)	2.15	H(216)...C(215)	2.15
H(215)...C(216)	2.15	H(222)...C(216)	2.73
C(231)...C(216)	3.10	C(232)...C(216)	3.28

table 7 continued

H(232)...C(216)	3.06	C(231)...H(216)	2.61
C(232)...H(216)	2.75	C(223)...C(221)	2.42
C(224)...C(221)	2.79	C(225)...C(221)	2.42
H(222)...C(221)	2.15	H(226)...C(221)	2.15
C(231)...C(221)	2.85	C(236)...C(221)	3.08
H(236)...C(221)	2.57	C(224)...C(222)	2.42
C(225)...C(222)	2.79	C(226)...C(222)	2.42
H(223)...C(222)	2.15	C(225)...C(223)	2.42
C(226)...C(223)	2.79	H(222)...C(223)	2.15
H(224)...C(223)	2.15	C(226)...C(224)	2.42
H(223)...C(224)	2.15	H(225)...C(224)	2.15
H(224)...C(225)	2.15	H(226)...C(225)	2.15
H(225)...C(226)	2.15	H(236)...C(226)	2.85
C(233)...C(231)	2.42	C(234)...C(231)	2.79
C(235)...C(231)	2.42	H(232)...C(231)	2.15
H(236)...C(231)	2.15	C(234)...C(232)	2.42
C(235)...C(232)	2.79	C(236)...C(232)	2.42
H(233)...C(232)	2.15	C(235)...C(233)	2.42
C(236)...C(233)	2.79	H(232)...C(233)	2.15
H(234)...C(233)	2.15	C(236)...C(234)	2.42
H(233)...C(234)	2.15	H(235)...C(234)	2.15
H(234)...C(235)	2.15	H(236)...C(235)	2.15
H(235)...C(236)	2.15		

Crystallographic Tables for $[Ag_2Ru_4(\mu\text{-}CO)_3(CO)_{10}(PPh_3)_2]$, {X-ray study presented in section 1.4, Vol.1}.

TABLE 1 Fractional atomic coordinates and thermal parameters ($Å^2$) for $[Ag_2Ru_4(\mu\text{-}CO)_3(CO)_{10}(PPh_3)_2]$

Atom	x	y	z	U_{iso} or U_{eq}
Ru(1)	0.27949(4)	0.06267(8)	-0.20321(11)	0.0395(6)
Ru(2)	0.20781(4)	-0.13737(8)	-0.24581(11)	0.0383(6)
Ru(3)	0.28840(4)	-0.07638(9)	0.01010(10)	0.0445(6)
Ru(4)	0.18970(4)	0.07077(9)	-0.02446(11)	0.0434(6)
Ag(1)	0.32167(4)	-0.20751(8)	-0.23948(11)	0.0437(6)
Ag(2)	0.16924(4)	0.11158(8)	-0.29688(10)	0.0469(6)
P(1)	0.3981(1)	-0.3287(3)	-0.3404(3)	0.040(2)
P(2)	0.1164(1)	0.2465(3)	-0.4310(3)	0.050(2)
C(11)	0.2742(5)	0.2270(13)	-0.2201(14)	0.067(4)
O(11)	0.2735(4)	0.3364(10)	-0.2278(10)	0.086(3)
C(12)	0.3331(5)	0.0459(12)	-0.3167(14)	0.067(4)
O(12)	0.3668(4)	0.0398(10)	-0.3896(11)	0.100(3)
C(13)	0.3303(5)	0.0802(11)	0.9606(12)	0.055(3)
O(13)	0.3683(4)	0.1400(9)	0.0179(10)	0.080(3)
C(21)	0.2398(6)	-0.1072(13)	-0.4054(16)	0.075(4)
O(21)	0.2463(4)	-0.1219(10)	-0.5178(11)	0.091(3)
C(22)	0.2190(6)	-0.3074(14)	-0.2439(14)	0.073(4)
O(22)	0.2224(4)	-0.4179(10)	-0.2414(11)	0.100(3)
C(23)	0.1424(6)	-0.1758(12)	-0.3488(14)	0.068(4)
O(23)	0.1021(4)	-0.2020(10)	-0.4143(11)	0.092(3)
C(24)	0.1547(5)	-0.1029(13)	-0.0804(14)	0.067(4)
O(24)	0.1208(4)	-0.1645(9)	-0.0513(10)	0.084(3)
C(31)	0.2995(5)	0.0157(13)	0.1890(15)	0.068(4)
O(31)	0.3084(4)	0.0753(11)	0.2972(12)	0.104(3)
C(32)	0.3573(5)	-0.1624(12)	0.0262(13)	0.061(3)

table 1 continued

O(32)	0.4001(4)	-0.2062(9)	0.0534(10)	0.081(3)
C(33)	0.2475(6)	-0.2077(15)	0.0518(16)	0.087(5)
O(33)	0.2266(5)	-0.2828(12)	0.0930(13)	0.088(4)
C(41)	0.1801(6)	0.0571(13)	0.1541(16)	0.076(4)
O(41)	0.1735(4)	0.0435(10)	0.2620(12)	0.100(3)
C(42)	0.1221(5)	0.1592(12)	-0.0488(13)	0.059(3)
O(42)	0.0799(4)	0.2129(9)	-0.0540(10)	0.082(3)
C(43)	0.2268(6)	0.2266(14)	0.0251(15)	0.075(4)
O(43)	0.2440(4)	0.3281(10)	0.0686(11)	0.095(3)
C(111)	0.3828(3)	-0.4095(8)	-0.5176(7)	0.056(3)
C(112)	0.3579(3)	-0.3382(8)	-0.6094(7)	0.077(4)
C(113)	0.3453(3)	-0.3968(8)	-0.7448(7)	0.089(5)
C(114)	0.3577(3)	-0.5267(8)	-0.7883(7)	0.090(5)
C(115)	0.3827(3)	-0.5981(8)	-0.6964(7)	0.076(4)
C(116)	0.3953(3)	-0.5395(8)	-0.5610(7)	0.061(3)
C(121)	0.4543(3)	-0.2274(7)	-0.3410(9)	0.049(3)
C(122)	0.4820(3)	-0.2352(7)	-0.4556(9)	0.071(4)
C(123)	0.5245(3)	-0.1543(7)	-0.4520(9)	0.083(4)
C(124)	0.5394(3)	-0.0656(7)	-0.3338(9)	0.095(5)
C(125)	0.5118(3)	-0.0578(7)	-0.2192(9)	0.097(5)
C(126)	0.4692(3)	-0.1387(7)	-0.2228(9)	0.084(4)
C(131)	0.4258(3)	-0.4532(6)	-0.2537(8)	0.046(3)
C(132)	0.4816(3)	-0.4829(6)	-0.2394(8)	0.056(3)
C(133)	0.5012(3)	-0.5844(6)	-0.1784(8)	0.075(4)
C(134)	0.4649(3)	-0.6562(6)	-0.1318(8)	0.071(4)
C(135)	0.4090(3)	-0.6265(6)	-0.1461(8)	0.068(4)
C(136)	0.3895(3)	-0.5251(6)	-0.2071(8)	0.064(3)
C(211)	0.0724(3)	0.3592(8)	-0.3284(8)	0.054(3)

table 1 continued

C(212)	0.0157(3)	0.3543(8)	-0.3445(8)	0.074(4)
C(213)	-0.0155(3)	0.4378(8)	-0.2551(8)	0.080(5)
C(214)	0.0099(3)	0.5264(8)	-0.1494(8)	0.099(5)
C(215)	0.0667(3)	0.5313(8)	-0.1333(8)	0.082(5)
C(216)	0.0979(3)	0.4477(8)	-0.2228(8)	0.081(4)
C(221)	0.1568(3)	0.3461(8)	-0.5028(9)	0.058(3)
C(222)	0.1363(3)	0.4623(8)	-0.5328(9)	0.070(4)
C(223)	0.1686(3)	0.5347(8)	-0.5906(9)	0.094(5)
C(224)	0.2213(3)	0.4910(8)	-0.6184(9)	0.103(5)
C(225)	0.2419(3)	0.3747(8)	-0.5883(9)	0.094(5)
C(226)	0.2096(3)	0.3023(8)	-0.5305(9)	0.072(4)
C(231)	0.0717(3)	0.1635(8)	-0.5728(8)	0.051(3)
C(232)	0.0639(3)	0.0340(8)	-0.5818(8)	0.093(5)
C(233)	0.0317(3)	-0.0339(8)	-0.6919(8)	0.076(7)
C(234)	0.0073(3)	0.0277(8)	-0.7928(8)	0.094(5)
C(235)	0.0151(3)	0.1572(8)	-0.7838(8)	0.107(6)
C(236)	0.0472(3)	0.2252(8)	-0.6737(8)	0.081(4)

TABLE 2 Fractional atomic coordinates for the hydrogen atoms for $[Ag_2Ru_4(\mu\text{-}CO)_3(CO)_{10}(PPh_3)_2]$

Atom	x	y	z
H(112)	0.3483	-0.2376	-0.5758
H(113)	0.3260	-0.3416	-0.8159
H(114)	0.3480	-0.5721	-0.8931
H(115)	0.3923	-0.6987	-0.7301
H(116)	0.4146	-0.5947	-0.4899
H(122)	0.4705	-0.3039	-0.5470
H(123)	0.5460	-0.1604	-0.5407
H(124)	0.5724	-0.0030	-0.3310
H(125)	0.5233	0.0109	-0.1277
H(126)	0.4478	-0.1326	-0.1342
H(132)	0.5098	-0.4273	-0.2754
H(133)	0.5444	-0.6073	-0.1673
H(134)	0.4800	-0.7347	-0.0847
H(135)	0.3809	-0.6821	-0.1101
H(136)	0.3462	-0.5021	-0.2182
H(212)	-0.0041	0.2857	-0.4263
H(213)	-0.0595	0.4340	-0.2675
H(214)	-0.0142	0.5911	-0.0802
H(215)	0.0864	0.5999	-0.0516
H(216)	0.1418	0.4516	-0.2103
H(222)	0.0954	0.4962	-0.5113
H(223)	0.1527	0.6247	-0.6139
H(224)	0.2463	0.5470	-0.6631
H(225)	0.2827	0.3408	-0.6098
H(226)	0.2255	0.2123	-0.5073

table 2 continued

H(232)	0.0828	-0.0137	-0.5037
H(233)	0.0257	-0.1342	-0.6989
H(234)	-0.0176	-0.0249	-0.8780
H(235)	-0.0038	0.2050	-0.8619
H(236)	0.0532	0.3255	-0.6667

TABLE 3 Anisotropic thermal parameters ($Å^2$) for $[Ag_2Ru_4(u\text{-}CO)_3(CO)_{10}(PPh_3)_2]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ru(1)	0.037(1)	0.036(1)	0.045(1)	0.020(1)	-0.001(1)	0.000(1)
Ru(2)	0.038(1)	0.030(1)	0.047(1)	0.007(1)	-0.001(1)	0.002(1)
Ru(3)	0.040(1)	0.044(1)	0.049(1)	0.020(1)	0.002(1)	0.005(1)
Ru(4)	0.038(1)	0.043(1)	0.049(1)	0.008(1)	0.004(1)	0.005(1)
Ag(1)	0.044(1)	0.045(1)	0.042(1)	0.010(1)	0.009(1)	0.012(1)
Ag(2)	0.045(1)	0.048(1)	0.048(1)	0.017(1)	-0.006(1)	0.009(1)
P(1)	0.038(2)	0.042(2)	0.040(2)	0.014(2)	0.006(1)	0.004(1)
P(2)	0.042(2)	0.049(2)	0.058(2)	0.015(2)	0.004(2)	0.006(1)

TABLE 4 Bond lengths (Å) for $[Ag_2Ru_4(\mu\text{-}CO)_3(CO)_{10}(PPh_3)_2]$

Ru(1) -Ru(2)	2.797(1)	Ru(1) -Ru(3)	2.853(2)
Ru(1) -Ru(4)	2.997(1)	Ru(1) -Ag(1)	2.977(1)
Ru(1) -Ag(2)	2.838(1)	Ru(1) -C(11)	1.799(3)
Ru(1) -C(12)	1.823(4)	Ru(1) -C(13)	1.953(3)
Ru(1) -C(21)	2.589(3)	Ru(2) -Ru(3)	3.074(1)
Ru(2) -Ru(4)	2.866(1)	Ru(2) -Ag(1)	2.861(1)
Ru(2) -Ag(2)	2.905(1)	Ru(2) -C(21)	1.967(4)
Ru(2) -C(22)	1.828(4)	Ru(2) -C(23)	1.846(3)
Ru(2) -C(24)	2.196(3)	Ru(3) -Ru(4)	2.849(1)
Ru(3) -Ag(1)	2.806(1)	Ru(3) -C(13)	2.193(3)
Ru(3) -C(31)	1.875(3)	Ru(3) -C(32)	1.890(3)
Ru(3) -C(33)	1.922(4)	Ru(4) -Ag(2)	2.872(2)
Ru(4) -C(24)	2.044(3)	Ru(4) -C(41)	1.887(4)
Ru(4) -C(42)	1.886(3)	Ru(4) -C(43)	1.902(4)
Ag(1) -P(1)	2.419(3)	Ag(1) -C(21)	2.796(4)
Ag(1) -C(22)	2.803(3)	Ag(1) -C(32)	2.694(3)
Ag(2) -P(2)	2.417(3)	Ag(2) -C(42)	2.822(3)
P(1) -C(111)	1.834(7)	P(1) -C(121)	1.816(9)
P(1) -C(131)	1.807(8)	P(2) -C(211)	1.811(8)
P(2) -C(221)	1.809(4)	P(2) -C(231)	1.822(8)
C(11) -O(11)	1.189(4)	C(12) -O(12)	1.160(5)
C(13) -O(13)	1.197(4)	C(21) -O(21)	1.145(5)
C(22) -O(22)	1.187(5)	C(23) -O(23)	1.149(4)
C(24) -O(24)	1.194(4)	C(31) -O(31)	1.155(4)
C(32) -O(32)	1.160(4)	C(33) -O(33)	1.151(5)

table 4 continued

C(41) -O(41)	1.162(5)	C(42) -O(42)	1.160(4)
C(43) -O(43)	1.171(4)	C(111)-C(112)	1.395(11)
C(111)-C(116)	1.395(11)	C(112)-C(113)	1.395(9)
C(113)-C(114)	1.395(11)	C(114)-C(115)	1.395(11)
C(115)-C(116)	1.395(9)	C(121)-C(122)	1.395(13)
C(121)-C(126)	1.395(11)	C(122)-C(123)	1.395(11)
C(123)-C(124)	1.395(11)	C(124)-C(125)	1.395(13)
C(125)-C(126)	1.395(11)	C(131)-C(132)	1.395(10)
C(131)-C(136)	1.395(11)	C(132)-C(133)	1.395(10)
C(133)-C(134)	1.395(11)	C(134)-C(135)	1.395(10)
C(135)-C(136)	1.395(10)	C(211)-C(212)	1.395(11)
C(211)-C(216)	1.395(10)	C(212)-C(213)	1.395(11)
C(213)-C(214)	1.395(10)	C(214)-C(215)	1.395(11)
C(215)-C(216)	1.395(11)	C(221)-C(222)	1.395(12)
C(221)-C(226)	1.395(11)	C(222)-C(223)	1.395(13)
C(223)-C(224)	1.395(11)	C(224)-C(225)	1.395(12)
C(225)-C(226)	1.395(13)	C(231)-C(232)	1.395(13)
C(231)-C(236)	1.395(12)	C(232)-C(233)	1.395(10)
C(233)-C(234)	1.395(12)	C(234)-C(235)	1.395(13)
C(235)-C(236)	1.395(10)		

TABLE 5 Bond angles (°) for $[Ag_2Ru_4(\mu\text{-}CO)_3(CO)_{10}(PPh_3)_2]$

Ru(3) -Ru(1) -Ru(2)	65.9(1)	Ru(4) -Ru(1) -Ru(2)	59.2(1)
Ru(4) -Ru(1) -Ru(3)	58.2(1)	Ag(1) -Ru(1) -Ru(2)	59.3(1)
Ag(1) -Ru(1) -Ru(3)	57.5(1)	Ag(1) -Ru(1) -Ru(4)	103.1(1)
Ag(2) -Ru(1) -Ru(2)	62.1(1)	Ag(2) -Ru(1) -Ru(3)	112.1(1)
Ag(2) -Ru(1) -Ru(4)	58.9(1)	Ag(2) -Ru(1) -Ag(1)	118.4(1)
C(11) -Ru(1) -Ru(2)	135.6(4)	C(11) -Ru(1) -Ru(3)	137.7(4)
C(11) -Ru(1) -Ru(4)	98.4(4)	C(11) -Ru(1) -Ag(1)	158.6(4)
C(11) -Ru(1) -Ag(2)	73.6(4)	C(12) -Ru(1) -Ru(2)	116.9(4)
C(12) -Ru(1) -Ru(3)	120.1(4)	C(12) -Ru(1) -Ru(4)	175.9(4)
C(12) -Ru(1) -Ag(1)	73.4(4)	C(12) -Ru(1) -Ag(2)	120.8(4)
C(12) -Ru(1) -C(11)	85.2(6)	C(13) -Ru(1) -Ru(2)	115.9(4)
C(13) -Ru(1) -Ru(3)	50.1(4)	C(13) -Ru(1) -Ru(4)	87.3(4)
C(13) -Ru(1) -Ag(1)	81.9(3)	C(13) -Ru(1) -Ag(2)	142.7(4)
C(13) -Ru(1) -C(11)	98.8(5)	C(13) -Ru(1) -C(12)	94.1(6)
C(21) -Ru(1) -Ru(2)	42.6(4)	C(21) -Ru(1) -Ru(3)	101.0(4)
C(21) -Ru(1) -Ru(4)	97.6(4)	C(21) -Ru(1) -Ag(1)	59.8(3)
C(21) -Ru(1) -Ag(2)	65.1(3)	C(21) -Ru(1) -C(11)	117.8(5)
C(21) -Ru(1) -C(12)	78.9(5)	C(21) -Ru(1) -C(13)	141.6(5)
Ru(3) -Ru(2) -Ru(1)	57.9(1)	Ru(4) -Ru(2) -Ru(1)	63.9(1)
Ru(4) -Ru(2) -Ru(3)	57.2(1)	Ag(1) -Ru(2) -Ru(1)	63.5(1)
Ag(1) -Ru(2) -Ru(3)	56.3(1)	Ag(1) -Ru(2) -Ru(4)	109.5(1)
Ag(2) -Ru(2) -Ru(1)	59.7(1)	Ag(2) -Ru(2) -Ru(3)	104.3(1)
Ag(2) -Ru(2) -Ru(4)	59.7(1)	Ag(2) -Ru(2) -Ag(1)	120.0(1)
C(21) -Ru(2) -Ru(1)	63.0(4)	C(21) -Ru(2) -Ru(3)	111.1(4)
C(21) -Ru(2) -Ru(4)	120.2(4)	C(21) -Ru(2) -Ag(1)	67.9(4)

table 5 continued

C(21) -Ru(2) -Ag(2)	70.9(4)	C(22) -Ru(2) -Ru(1)	132.1(4)
C(22) -Ru(2) -Ru(3)	89.0(4)	C(22) -Ru(2) -Ru(4)	128.7(5)
C(22) -Ru(2) -Ag(1)	69.4(4)	C(22) -Ru(2) -Ag(2)	166.5(4)
C(22) -Ru(2) -C(21)	107.0(6)	C(23) -Ru(2) -Ru(1)	135.3(5)
C(23) -Ru(2) -Ru(3)	158.1(5)	C(23) -Ru(2) -Ru(4)	109.1(4)
C(23) -Ru(2) -Ag(1)	141.3(4)	C(23) -Ru(2) -Ag(2)	78.4(4)
C(23) -Ru(2) -C(21)	90.5(6)	C(23) -Ru(2) -C(22)	88.4(6)
C(24) -Ru(2) -Ru(1)	108.8(3)	C(24) -Ru(2) -Ru(3)	76.7(3)
C(24) -Ru(2) -Ru(4)	45.3(3)	C(24) -Ru(2) -Ag(1)	129.2(3)
C(24) -Ru(2) -Ag(2)	87.0(4)	C(24) -Ru(2) -C(21)	157.7(6)
C(24) -Ru(2) -C(22)	93.7(6)	C(24) -Ru(2) -C(23)	81.8(6)
Ru(2) -Ru(3) -Ru(1)	56.2(1)	Ru(4) -Ru(3) -Ru(1)	63.4(1)
Ru(4) -Ru(3) -Ru(2)	57.7(1)	Ag(1) -Ru(3) -Ru(1)	63.5(1)
Ag(1) -Ru(3) -Ru(2)	58.0(1)	Ag(1) -Ru(3) -Ru(4)	111.6(1)
C(13) -Ru(3) -Ru(1)	43.1(3)	C(13) -Ru(3) -Ru(2)	99.2(3)
C(13) -Ru(3) -Ru(4)	86.8(3)	C(13) -Ru(3) -Ag(1)	82.3(3)
C(31) -Ru(3) -Ru(1)	118.0(5)	C(31) -Ru(3) -Ru(2)	146.0(4)
C(31) -Ru(3) -Ru(4)	89.0(4)	C(31) -Ru(3) -Ag(1)	154.7(4)
C(31) -Ru(3) -C(13)	84.4(6)	C(32) -Ru(3) -Ru(1)	111.7(4)
C(32) -Ru(3) -Ru(2)	122.5(4)	C(32) -Ru(3) -Ru(4)	174.5(4)
C(32) -Ru(3) -Ag(1)	66.7(4)	C(32) -Ru(3) -C(13)	87.7(5)
C(32) -Ru(3) -C(31)	91.3(5)	C(33) -Ru(3) -Ru(1)	134.6(5)
C(33) -Ru(3) -Ru(2)	78.8(5)	C(33) -Ru(3) -Ru(4)	89.6(5)
C(33) -Ru(3) -Ag(1)	99.0(5)	C(33) -Ru(3) -C(13)	176.4(6)
C(33) -Ru(3) -C(31)	95.6(7)	C(33) -Ru(3) -C(32)	95.9(6)
Ru(2) -Ru(4) -Ru(1)	56.9(1)	Ru(3) -Ru(4) -Ru(1)	58.4(1)
Ru(3) -Ru(4) -Ru(2)	65.1(1)	Ag(2) -Ru(4) -Ru(1)	57.8(1)
Ag(2) -Ru(4) -Ru(2)	60.8(1)	Ag(2) -Ru(4) -Ru(3)	111.3(1)

table 5 continued

C(24) -Ru(4) -Ru(1)	106.3(4)	C(24) -Ru(4) -Ru(2)	49.8(4)
C(24) -Ru(4) -Ru(3)	84.4(4)	C(24) -Ru(4) -Ag(2)	90.8(4)
C(41) -Ru(4) -Ru(1)	139.7(4)	C(41) -Ru(4) -Ru(2)	126.1(4)
C(41) -Ru(4) -Ru(3)	85.4(4)	C(41) -Ru(4) -Ag(2)	162.4(4)
C(41) -Ru(4) -C(24)	85.2(6)	C(42) -Ru(4) -Ru(1)	123.4(4)
C(42) -Ru(4) -Ru(2)	113.0(4)	C(42) -Ru(4) -Ru(3)	176.6(4)
C(42) -Ru(4) -Ag(2)	69.2(4)	C(42) -Ru(4) -C(24)	92.2(5)
C(42) -Ru(4) -C(41)	93.8(6)	C(43) -Ru(4) -Ru(1)	70.6(4)
C(43) -Ru(4) -Ru(2)	127.3(4)	C(43) -Ru(4) -Ru(3)	91.9(4)
C(43) -Ru(4) -Ag(2)	89.3(5)	C(43) -Ru(4) -C(24)	176.2(6)
C(43) -Ru(4) -C(41)	95.8(6)	C(43) -Ru(4) -C(42)	91.4(6)
Ru(2) -Ag(1) -Ru(1)	57.2(1)	Ru(3) -Ag(1) -Ru(1)	59.0(1)
Ru(3) -Ag(1) -Ru(2)	65.7(1)	P(1) -Ag(1) -Ru(1)	135.7(1)
P(1) -Ag(1) -Ru(2)	151.0(1)	P(1) -Ag(1) -Ru(3)	142.1(1)
C(21) -Ag(1) -Ru(1)	53.2(3)	C(21) -Ag(1) -Ru(2)	40.7(3)
C(21) -Ag(1) -Ru(3)	97.2(3)	C(21) -Ag(1) -P(1)	119.3(3)
C(22) -Ag(1) -Ru(1)	94.5(3)	C(22) -Ag(1) -Ru(2)	37.6(3)
C(22) -Ag(1) -Ru(3)	78.5(3)	C(22) -Ag(1) -P(1)	123.9(3)
C(22) -Ag(1) -C(21)	66.1(5)	C(32) -Ag(1) -Ru(1)	88.5(3)
C(32) -Ag(1) -Ru(2)	104.4(3)	C(32) -Ag(1) -Ru(3)	40.1(3)
C(32) -Ag(1) -P(1)	102.0(3)	C(32) -Ag(1) -C(21)	136.6(4)
C(32) -Ag(1) -C(22)	102.6(4)	Ru(2) -Ag(2) -Ru(1)	58.3(1)
Ru(4) -Ag(2) -Ru(1)	63.3(1)	Ru(4) -Ag(2) -Ru(2)	59.5(1)
P(2) -Ag(2) -Ru(1)	139.5(1)	P(2) -Ag(2) -Ru(2)	152.0(1)
P(2) -Ag(2) -Ru(4)	141.8(1)	C(42) -Ag(2) -Ru(1)	99.8(3)
C(42) -Ag(2) -Ru(2)	88.6(3)	C(42) -Ag(2) -Ru(4)	38.7(3)
C(42) -Ag(2) -P(2)	104.8(3)	C(111)-P(1) -Ag(1)	114.5(3)
C(121)-P(1) -Ag(1)	111.6(3)	C(121)-P(1) -C(111)	105.2(4)

table 5 continued

C(131)-P(1) -Ag(1)	113.8(3)	C(131)-P(1) -C(111)	105.0(4)
C(131)-P(1) -C(121)	106.0(4)	C(211)-P(2) -Ag(2)	111.0(3)
C(221)-P(2) -Ag(2)	114.3(3)	C(221)-P(2) -C(211)	104.0(4)
C(231)-P(2) -Ag(2)	115.6(3)	C(231)-P(2) -C(211)	105.5(4)
C(231)-P(2) -C(221)	105.5(4)	O(11) -C(11) -Ru(1)	176(1)
O(12) -C(12) -Ru(1)	177(1)	Ru(3) -C(13) -Ru(1)	86.8(4)
O(13) -C(13) -Ru(1)	142(1)	O(13) -C(13) -Ru(3)	132(1)
Ru(2) -C(21) -Ru(1)	74.3(5)	Ag(1) -C(21) -Ru(1)	67.0(3)
Ag(1) -C(21) -Ru(2)	71.5(5)	O(21) -C(21) -Ru(1)	129(1)
O(21) -C(21) -Ru(2)	156(1)	O(21) -C(21) -Ag(1)	116(1)
Ag(1) -C(22) -Ru(2)	72.9(5)	O(22) -C(22) -Ru(2)	175(1)
O(22) -C(22) -Ag(1)	112(1)	O(23) -C(23) -Ru(2)	179(1)
Ru(4) -C(24) -Ru(2)	85.0(5)	O(24) -C(24) -Ru(2)	132.9(9)
O(24) -C(24) -Ru(4)	142(1)	O(31) -C(31) -Ru(3)	177(1)
Ag(1) -C(32) -Ru(3)	73.1(4)	O(32) -C(32) -Ru(3)	171(1)
O(32) -C(32) -Ag(1)	115.6(9)	O(33) -C(33) -Ru(3)	171(1)
O(41) -C(41) -Ru(4)	177(1)	Ag(2) -C(42) -Ru(4)	72.1(4)
O(42) -C(42) -Ru(4)	175(1)	O(42) -C(42) -Ag(2)	113(1)
O(43) -C(43) -Ru(4)	170(1)	C(112)-C(111)-P(1)	118.5(6)
C(116)-C(111)-P(1)	121.5(6)	C(116)-C(111)-C(112)	120.0(6)
C(113)-C(112)-C(111)	120.0(7)	C(114)-C(113)-C(112)	120.0(7)
C(115)-C(114)-C(113)	120.0(6)	C(116)-C(115)-C(114)	120.0(7)
C(115)-C(116)-C(111)	120.0(7)	C(122)-C(121)-P(1)	122.0(6)
C(126)-C(121)-P(1)	118.0(7)	C(126)-C(121)-C(122)	120.0(7)
C(123)-C(122)-C(121)	120.0(7)	C(124)-C(123)-C(122)	120.0(8)
C(125)-C(124)-C(123)	120.0(7)	C(126)-C(125)-C(124)	120.0(7)
C(125)-C(126)-C(121)	120.0(8)	C(132)-C(131)-P(1)	121.7(6)
C(136)-C(131)-P(1)	118.2(5)	C(136)-C(131)-C(132)	120.0(7)

table 5 continued

C(133)-C(132)-C(131)	120.0(7)	C(134)-C(133)-C(132)	120.0(7)
C(135)-C(134)-C(133)	120.0(7)	C(136)-C(135)-C(134)	120.0(7)
C(135)-C(136)-C(131)	120.0(7)	C(212)-C(211)-P(2)	123.0(6)
C(216)-C(211)-P(2)	116.8(6)	C(216)-C(211)-C(212)	120.0(7)
C(213)-C(212)-C(211)	120.0(7)	C(214)-C(213)-C(212)	120.0(7)
C(215)-C(214)-C(213)	120.0(7)	C(216)-C(215)-C(214)	120.0(7)
C(215)-C(216)-C(211)	120.0(7)	C(222)-C(221)-P(2)	122.0(6)
C(226)-C(221)-P(2)	118.0(7)	C(226)-C(221)-C(222)	120.0(8)
C(223)-C(222)-C(221)	120.0(7)	C(224)-C(223)-C(222)	120.0(8)
C(225)-C(224)-C(223)	120.0(8)	C(226)-C(225)-C(224)	120.0(7)
C(225)-C(226)-C(221)	120.0(8)	C(232)-C(231)-P(2)	118.4(6)
C(236)-C(231)-P(2)	121.6(7)	C(236)-C(231)-C(232)	120.0(7)
C(233)-C(232)-C(231)	120.0(8)	C(234)-C(233)-C(232)	120.0(8)
C(235)-C(234)-C(233)	120.0(7)	C(236)-C(235)-C(234)	120.0(8)
C(235)-C(236)-C(231)	120.0(8)		

TABLE 6 Intermolecular distances (Å) for $[Ag_2Ru_4(\mu\text{-}CO)_3(CO)_{10}(PPh_3)_2]$

atom1	atom2	dist	S	a	b	c
H(135)	Ru(1)	3.73	1	0.0	-1.0	0.0
C(13)	Ru(2)	4.05	1	0.0	0.0	1.0
H(113)	Ru(3)	3.67	1	0.0	0.0	-1.0
C(13)	Ru(4)	3.50	1	0.0	0.0	1.0
C(13)	Ag(1)	3.32	1	0.0	0.0	1.0
C(13)	C(11)	2.85	1	0.0	0.0	1.0
H(135)	C(11)	2.89	1	0.0	-1.0	0.0
O(22)	O(11)	2.87	1	0.0	-1.0	0.0
C(135)	O(11)	3.38	1	0.0	-1.0	0.0
C(136)	O(11)	3.27	1	0.0	-1.0	0.0
H(135)	O(11)	2.80	1	0.0	-1.0	0.0
H(136)	O(11)	2.55	1	0.0	-1.0	0.0
C(13)	C(12)	2.77	1	0.0	0.0	1.0
H(123)	O(12)	2.80	-1	1.0	0.0	-1.0
C(31)	C(13)	2.74	1	0.0	0.0	-1.0
C(32)	C(13)	2.84	1	0.0	0.0	-1.0
C(43)	C(13)	2.97	1	0.0	0.0	-1.0
O(43)	C(13)	3.37	1	0.0	0.0	-1.0
H(115)	O(13)	2.80	1	0.0	-1.0	-1.0
H(135)	O(13)	2.57	1	0.0	-1.0	0.0
H(216)	O(22)	2.58	1	0.0	1.0	0.0
H(223)	O(23)	2.79	1	0.0	1.0	0.0
H(212)	O(23)	2.85	-1	0.0	0.0	-1.0
H(215)	O(24)	2.71	1	0.0	1.0	0.0
H(235)	O(24)	2.96	-1	0.0	0.0	-1.0

table 6 continued

H(225)...O(31)	2.86	1	0.0	0.0	-1.0
H(124)...O(31)	3.00	-1	1.0	0.0	0.0
H(113)...C(32)	2.93	1	0.0	0.0	-1.0
H(113)...O(32)	2.98	1	0.0	0.0	-1.0
H(125)...O(32)	2.84	-1	1.0	0.0	0.0
H(133)...O(32)	2.73	-1	1.0	-1.0	0.0
H(134)...O(32)	2.98	-1	1.0	-1.0	0.0
H(113)...C(33)	2.74	1	0.0	0.0	-1.0
H(113)...O(33)	2.61	1	0.0	0.0	-1.0
C(226)...O(41)	3.22	1	0.0	0.0	-1.0
H(226)...O(41)	2.87	1	0.0	0.0	-1.0
C(231)...O(41)	3.22	1	0.0	0.0	-1.0
C(232)...O(41)	3.30	1	0.0	0.0	-1.0
H(234)...C(42)	2.98	-1	0.0	0.0	-1.0
H(214)...O(42)	2.78	-1	0.0	1.0	0.0
H(234)...O(42)	2.54	-1	0.0	0.0	-1.0
C(114)...O(43)	3.34	1	0.0	-1.0	-1.0
H(114)...O(43)	2.80	1	0.0	-1.0	-1.0
C(224)...O(43)	3.37	1	0.0	0.0	-1.0
C(225)...O(43)	3.41	1	0.0	0.0	-1.0
H(224)...C(112)	3.03	1	0.0	1.0	0.0
H(224)...C(113)	2.80	1	0.0	1.0	0.0
H(133)...C(113)	2.96	-1	1.0	-1.0	-1.0
H(133)...C(114)	3.00	-1	1.0	-1.0	-1.0
H(225)...C(115)	2.86	1	0.0	1.0	0.0
H(132)...C(115)	2.74	-1	1.0	-1.0	-1.0
H(225)...C(116)	3.08	1	0.0	1.0	0.0
H(132)...C(116)	2.98	-1	1.0	-1.0	-1.0

table 6 continued

C(135)...H(114)	3.05	1	0.0	0.0	1.0
C(122)...H(116)	3.07	-1	1.0	-1.0	-1.0
C(123)...H(116)	2.98	-1	1.0	-1.0	-1.0
C(132)...H(122)	3.08	-1	1.0	-1.0	-1.0
C(133)...H(122)	2.93	-1	1.0	-1.0	-1.0
H(233)...C(212)	2.76	-1	0.0	0.0	-1.0
H(236)...C(213)	2.88	-1	0.0	1.0	-1.0
C(214)...C(214)	3.29	-1	0.0	1.0	0.0
H(214)...C(214)	2.86	-1	0.0	1.0	0.0
H(235)...C(214)	2.85	-1	0.0	1.0	-1.0
H(236)...C(214)	2.95	-1	0.0	1.0	-1.0
C(222)...H(213)	2.96	-1	0.0	1.0	-1.0
C(223)...H(213)	2.95	-1	0.0	1.0	-1.0

Symmetry Transformations:

The second atom is related to the first atom, at (x,y,z), by the symmetry operation S with (a,b,c) added to the (x',y',z') of S.

Where S =

1	x, y, z

TABLE 7 Intramolecular distances (Å) for $[Ag_2Ru_4(\mu\text{-}CO)_3(CO)_{10}(PPh_3)_2]$

O(11) ...Ru(1)	2.99	O(12) ...Ru(1)	2.98
O(13) ...Ru(1)	2.98	O(21) ...Ru(1)	3.43
C(22) ...Ru(1)	4.24	C(24) ...Ru(1)	4.07
C(31) ...Ru(1)	4.08	C(32) ...Ru(1)	3.96
C(43) ...Ru(1)	2.97	O(43) ...Ru(1)	3.66
C(12) ...Ru(2)	3.97	O(21) ...Ru(2)	3.05
O(22) ...Ru(2)	3.01	O(23) ...Ru(2)	2.99
O(24) ...Ru(2)	3.13	C(33) ...Ru(2)	3.29
O(33) ...Ru(2)	4.03	C(42) ...Ru(2)	4.00
Ag(2) ...Ru(3)	4.72	C(12) ...Ru(3)	4.09
O(13) ...Ru(3)	3.12	C(21) ...Ru(3)	4.20
C(22) ...Ru(3)	3.55	C(24) ...Ru(3)	3.34
O(31) ...Ru(3)	3.03	O(32) ...Ru(3)	3.04
O(33) ...Ru(3)	3.06	C(41) ...Ru(3)	3.29
O(41) ...Ru(3)	3.99	C(43) ...Ru(3)	3.48
Ag(1) ...Ru(4)	4.68	C(11) ...Ru(4)	3.71
C(21) ...Ru(4)	4.21	C(23) ...Ru(4)	3.88
O(24) ...Ru(4)	3.08	C(31) ...Ru(4)	3.38
O(31) ...Ru(4)	4.14	C(33) ...Ru(4)	3.42
O(41) ...Ru(4)	3.05	O(42) ...Ru(4)	3.04
O(43) ...Ru(4)	3.06	Ag(2) ...Ag(1)	4.99
C(12) ...Ag(1)	3.01	O(12) ...Ag(1)	3.60
O(13) ...Ag(1)	4.22	O(21) ...Ag(1)	3.46
O(22) ...Ag(1)	3.42	O(32) ...Ag(1)	3.36
C(33) ...Ag(1)	3.64	C(111)...Ag(1)	3.59

table 7 continued

C(112)...Ag(1)	3.90	H(112)...Ag(1)	3.49
C(121)...Ag(1)	3.52	C(126)...Ag(1)	3.74
H(126)...Ag(1)	3.27	C(131)...Ag(1)	3.56
C(136)...Ag(1)	3.76	H(136)...Ag(1)	3.22
C(11) ...Ag(2)	2.90	O(11) ...Ag(2)	3.55
C(12) ...Ag(2)	4.08	C(21) ...Ag(2)	2.93
O(21) ...Ag(2)	3.59	C(23) ...Ag(2)	3.11
O(23) ...Ag(2)	3.75	C(24) ...Ag(2)	3.55
O(42) ...Ag(2)	3.44	C(43) ...Ag(2)	3.42
O(43) ...Ag(2)	4.24	C(211)...Ag(2)	3.50
C(216)...Ag(2)	3.87	H(216)...Ag(2)	3.60
C(221)...Ag(2)	3.57	C(226)...Ag(2)	3.68
H(226)...Ag(2)	3.07	C(231)...Ag(2)	3.60
C(232)...Ag(2)	3.67	H(232)...Ag(2)	2.99
C(112)...P(1)	2.78	C(116)...P(1)	2.83
H(112)...P(1)	2.89	H(116)...P(1)	2.96
C(122)...P(1)	2.82	C(126)...P(1)	2.76
H(122)...P(1)	2.96	H(126)...P(1)	2.87
C(132)...P(1)	2.80	C(136)...P(1)	2.76
H(132)...P(1)	2.95	H(136)...P(1)	2.87
C(212)...P(2)	2.83	C(216)...P(2)	2.74
H(212)...P(2)	2.98	H(216)...P(2)	2.84
C(222)...P(2)	2.81	C(226)...P(2)	2.76
H(222)...P(2)	2.95	H(226)...P(2)	2.86
C(232)...P(2)	2.77	C(236)...P(2)	2.82
H(232)...P(2)	2.88	H(236)...P(2)	2.95
C(12) ...C(11)	2.45	O(12) ...C(11)	3.32
O(13) ...C(11)	3.40	C(43) ...C(11)	2.86

table 7 continued

O(43) ...C(11)	3.06	H(226)...C(11)	3.00
C(12) ...O(11)	3.35	C(43) ...O(11)	3.37
O(43) ...O(11)	3.19	C(226)...O(11)	3.26
O(13) ...C(12)	3.37	C(21) ...C(12)	2.87
O(21) ...C(12)	3.16	C(31) ...O(13)	3.09
C(32) ...O(13)	3.29	C(22) ...C(21)	3.05
C(23) ...C(21)	2.71	C(23) ...O(21)	3.38
H(112)...O(21)	2.80	C(23) ...C(22)	2.56
C(24) ...C(22)	2.95	O(24) ...C(22)	3.37
C(33) ...C(22)	2.99	O(33) ...C(22)	3.36
C(33) ...O(22)	3.36	C(24) ...C(23)	2.66
O(24) ...C(23)	3.10	H(232)...C(23)	2.82
C(232)...O(23)	3.36	H(232)...O(23)	2.38
C(33) ...C(24)	2.82	O(33) ...C(24)	3.20
C(41) ...C(24)	2.66	C(42) ...C(24)	2.84
C(33) ...O(24)	3.22	O(33) ...O(24)	3.18
C(41) ...O(24)	3.13	C(32) ...C(31)	2.69
C(33) ...C(31)	2.81	C(41) ...C(31)	2.95
O(41) ...C(31)	3.26	C(43) ...C(31)	3.39
C(41) ...O(31)	3.34	C(33) ...C(32)	2.83
H(126)...C(32)	2.97	H(126)...O(32)	2.62
C(41) ...C(33)	3.23	C(42) ...C(41)	2.75
C(43) ...C(41)	2.81	C(43) ...C(42)	2.71
C(216)...O(42)	3.40	C(113)...C(111)	2.42
C(114)...C(111)	2.79	C(115)...C(111)	2.42
H(112)...C(111)	2.15	H(116)...C(111)	2.15
C(121)...C(111)	2.90	C(122)...C(111)	3.10
H(122)...C(111)	2.57	C(131)...C(111)	2.89

table 7 continued

C(114)...C(112)	2.42	C(115)...C(112)	2.79
C(116)...C(112)	2.42	H(113)...C(112)	2.15
C(121)...C(112)	3.48	C(122)...C(112)	3.42
H(122)...C(112)	2.81	C(115)...C(113)	2.42
C(116)...C(113)	2.79	H(112)...C(113)	2.15
H(114)...C(113)	2.15	C(116)...C(114)	2.42
H(113)...C(114)	2.15	H(115)...C(114)	2.15
H(114)...C(115)	2.15	H(116)...C(115)	2.15
H(115)...C(116)	2.15	C(131)...C(116)	3.08
C(131)...H(116)	2.55	C(132)...H(116)	2.95
C(136)...H(116)	2.93	C(123)...C(121)	2.42
C(124)...C(121)	2.79	C(125)...C(121)	2.42
H(122)...C(121)	2.15	H(126)...C(121)	2.15
C(131)...C(121)	2.89	C(132)...C(121)	3.13
H(132)...C(121)	2.63	C(124)...C(122)	2.42
C(125)...C(122)	2.79	C(126)...C(122)	2.42
H(123)...C(122)	2.15	H(132)...C(122)	3.03
C(125)...C(123)	2.42	C(126)...C(123)	2.79
H(122)...C(123)	2.15	H(124)...C(123)	2.15
C(126)...C(124)	2.42	H(123)...C(124)	2.15
H(125)...C(124)	2.15	H(124)...C(125)	2.15
H(126)...C(125)	2.15	H(125)...C(126)	2.15
C(133)...C(131)	2.42	C(134)...C(131)	2.79
C(135)...C(131)	2.42	H(132)...C(131)	2.15
H(136)...C(131)	2.15	C(134)...C(132)	2.42
C(135)...C(132)	2.79	C(136)...C(132)	2.42
H(133)...C(132)	2.15	C(135)...C(133)	2.42
C(136)...C(133)	2.79	H(132)...C(133)	2.15

table 7 continued

H(134)...C(133)	2.15	C(136)...C(134)	2.42
H(133)...C(134)	2.15	H(135)...C(134)	2.15
H(134)...C(135)	2.15	H(136)...C(135)	2.15
H(135)...C(136)	2.15	C(213)...C(211)	2.42
C(214)...C(211)	2.79	C(215)...C(211)	2.42
H(212)...C(211)	2.15	H(216)...C(211)	2.15
C(221)...C(211)	2.85	C(222)...C(211)	3.14
H(222)...C(211)	2.72	C(231)...C(211)	2.89
C(236)...C(211)	3.50	C(214)...C(212)	2.42
C(215)...C(212)	2.79	C(216)...C(212)	2.42
H(213)...C(212)	2.15	C(231)...C(212)	3.13
C(236)...C(212)	3.49	C(215)...C(213)	2.42
C(216)...C(213)	2.79	H(212)...C(213)	2.15
H(214)...C(213)	2.15	C(216)...C(214)	2.42
H(213)...C(214)	2.15	H(215)...C(214)	2.15
H(214)...C(215)	2.15	H(216)...C(215)	2.15
H(215)...C(216)	2.15	C(221)...C(216)	3.28
C(222)...C(216)	3.41	H(222)...C(216)	3.07
C(231)...H(212)	2.63	C(236)...H(212)	2.87
C(221)...H(216)	3.00	C(223)...C(221)	2.42
C(224)...C(221)	2.79	C(225)...C(221)	2.42
H(222)...C(221)	2.15	H(226)...C(221)	2.15
C(231)...C(221)	2.89	C(236)...C(221)	3.24
H(236)...C(221)	2.89	C(224)...C(222)	2.42
C(225)...C(222)	2.79	C(226)...C(222)	2.42
H(223)...C(222)	2.15	C(236)...C(222)	3.44
H(236)...C(222)	2.67	C(225)...C(223)	2.42
C(226)...C(223)	2.79	H(222)...C(223)	2.15

table 7 continued

H(224)...C(223)	2.15	C(226)...C(224)	2.42
H(223)...C(224)	2.15	H(225)...C(224)	2.15
H(224)...C(225)	2.15	H(226)...C(225)	2.15
H(225)...C(226)	2.15	C(233)...C(231)	2.42
C(234)...C(231)	2.79	C(235)...C(231)	2.42
H(232)...C(231)	2.15	H(236)...C(231)	2.15
C(234)...C(232)	2.42	C(235)...C(232)	2.79
C(236)...C(232)	2.42	H(233)...C(232)	2.15
C(235)...C(233)	2.42	C(236)...C(233)	2.79
H(232)...C(233)	2.15	H(234)...C(233)	2.15
C(236)...C(234)	2.42	H(233)...C(234)	2.15
H(235)...C(234)	2.15	H(234)...C(235)	2.15
H(236)...C(235)	2.15	H(235)...C(236)	2.15

Crystallographic Tables for $[Au_2Ru_4(\mu\text{-}H)(\mu_3\text{-}H)(CO)_{12}\{\mu\text{-}Ph_2PCH{=}CHPPh_2\}]$, {X-ray study presented in section 2.2, Vol.1}.

TABLE 1 Fractional atomic coordinates and thermal parameters ($Å^2$) for $[Au_2Ru_4(\mu\text{-}H)(\mu_3\text{-}H)(CO)_{12}\{\mu\text{-}Ph_2PCH{=}CHPPh_2\}]$

Atom	x	y	z	U_{iso} or U_{eq}
Au(1)	-0.15949(4)	0.25084(11)	-0.14608(5)	0.0425(8)
Au(2)	-0.08529(4)	0.26026(11)	-0.06934(5)	0.0389(8)
Ru(1)	-0.0815(1)	0.0455(2)	-0.0424(1)	0.043(2)
Ru(2)	-0.1512(1)	-0.0559(2)	-0.0161(1)	0.054(2)
Ru(3)	-0.1544(1)	0.1771(2)	-0.0291(1)	0.042(2)
Ru(4)	-0.1537(1)	0.0296(2)	-0.1336(1)	0.044(2)
P(1)	-0.1673(3)	0.4216(7)	-0.1879(4)	0.044(5)
P(2)	-0.0650(2)	0.4081(7)	-0.1200(4)	0.038(5)
C(11)	-0.0641(10)	-0.0966(27)	-0.0428(14)	0.051(9)
O(11)	-0.0520(8)	-0.1858(22)	-0.0411(11)	0.083(8)
C(12)	-0.0349(12)	0.1012(31)	-0.0677(17)	0.071(11)
O(12)	-0.0046(8)	0.1164(20)	-0.0873(11)	0.079(8)
C(13)	-0.0574(12)	0.0728(34)	0.0333(20)	0.087(13)
O(13)	-0.0462(9)	0.0881(25)	0.0814(14)	0.103(10)
C(21)	-0.1411(11)	-0.2034(34)	-0.0315(17)	0.070(12)
O(21)	-0.1371(9)	-0.2959(27)	-0.0348(13)	0.107(10)
C(22)	-0.1310(11)	-0.0671(29)	0.0630(17)	0.067(11)
O(22)	0.8828(9)	0.9279(24)	0.1115(14)	0.105(10)
C(23)	-0.2062(14)	-0.0812(34)	-0.0115(19)	0.090(14)
O(23)	-0.2386(12)	-0.0823(31)	-0.0026(17)	0.095(14)
C(31)	-0.2083(12)	0.1753(28)	-0.0240(15)	0.062(10)
O(31)	-0.2430(10)	0.1814(27)	-0.0272(14)	0.082(11)
C(32)	-0.1410(12)	0.1707(33)	0.0521(20)	0.082(13)
O(32)	-0.1322(8)	0.1817(24)	0.1025(14)	0.101(9)
C(33)	-0.1515(11)	0.3328(33)	-0.0339(16)	0.067(11)

table 1 continued

O(33)	-0.1598(7)	0.4215(20)	-0.0260(11)	0.073(8)
C(41)	-0.2058(13)	0.0318(33)	-0.1545(18)	0.085(13)
O(41)	-0.2414(10)	0.0354(26)	-0.1713(14)	0.090(11)
C(42)	-0.1504(11)	-0.1164(33)	-0.1480(17)	0.071(12)
O(42)	-0.1494(9)	-0.2074(27)	-0.1668(14)	0.098(11)
C(43)	-0.1418(11)	0.0743(29)	-0.2073(16)	0.062(10)
O(43)	-0.1320(8)	0.0879(23)	-0.2537(13)	0.095(9)
C(1)	-0.1364(8)	0.5282(23)	-0.1471(12)	0.038(8)
C(2)	-0.0982(8)	0.5228(22)	-0.1240(12)	0.034(7)
C(111)	-0.2186(5)	0.4778(20)	-0.1851(10)	0.040(8)
C(112)	-0.2287(5)	0.5860(20)	-0.1985(10)	0.099(15)
C(113)	-0.2671(5)	0.6142(20)	-0.1934(10)	0.109(16)
C(114)	-0.2954(5)	0.5542(20)	-0.1747(10)	0.080(12)
C(115)	-0.2854(5)	0.4460(20)	-0.1613(10)	0.088(16)
C(116)	-0.2470(5)	0.4078(20)	-0.1664(10)	0.078(12)
C(121)	-0.1602(6)	0.4348(20)	-0.2652(8)	0.043(8)
C(122)	-0.1679(6)	0.3449(20)	-0.3020(8)	0.059(10)
C(123)	-0.1674(6)	0.3563(20)	-0.3611(8)	0.102(15)
C(124)	-0.1593(6)	0.4575(20)	-0.3854(8)	0.082(16)
C(125)	-0.1516(6)	0.5474(20)	-0.3485(8)	0.082(16)
C(126)	-0.1521(6)	0.5360(20)	-0.2884(8)	0.089(13)
C(212)	-0.0071(5)	0.5757(15)	-0.1045(8)	0.048(9)
C(213)	0.0307(5)	0.6197(15)	-0.0859(8)	0.055(10)
C(214)	0.0602(5)	0.5561(15)	-0.0538(8)	0.065(11)
C(215)	0.0519(5)	0.4484(15)	-0.0402(8)	0.061(10)
C(216)	0.0141(5)	0.4043(15)	-0.0589(8)	0.048(9)
C(211)	-0.0154(5)	0.4680(15)	-0.0910(8)	0.044(8)
C(221)	-0.0602(6)	0.3714(18)	-0.1944(8)	0.044(9)

table 1 continued

C(222)	-0.0598(6)	0.2621(18)	-0.2110(8)	0.073(11)
C(223)	-0.0561(6)	0.2345(18)	-0.2687(8)	0.071(11)
C(224)	-0.0528(6)	0.3161(18)	-0.3099(8)	0.096(14)
C(225)	-0.0533(6)	0.4254(18)	-0.2933(8)	0.068(11)
C(226)	-0.0570(6)	0.4530(18)	-0.2356(8)	0.073(11)

TABLE 2 Fractional atomic coordinates for the hydrogen atoms for $[Au_2Ru_4(\mu\text{-}H)(\mu_3\text{-}H)(CO)_{12}\{\mu\text{-}Ph_2PCH{=}CHPPh_2\}]$

Atom	x	y	z
H(112)	-0.2056	0.6393	-0.1128
H(113)	-0.2748	0.7080	-0.2038
H(114)	-0.3251	0.5838	-0.1707
H(115)	-0.3073	0.3918	-0.1468
H(116)	-0.2393	0.3240	-0.1560
H(122)	-0.1742	0.2666	-0.2840
H(123)	-0.1734	0.2867	-0.3907
H(124)	-0.1590	0.4663	-0.4319
H(125)	-0.1454	0.6257	-0.3666
H(126)	-0.1461	0.6056	-0.2599
H(212)	-0.0299	0.6249	-0.1294
H(213)	0.0371	0.7031	-0.0964
H(214)	0.0894	0.5901	-0.0393
H(215)	0.0747	0.3991	-0.0153
H(216)	0.0077	0.3210	-0.0484
H(222)	-0.0623	0.1989	-0.1791
H(223)	-0.0557	0.1499	-0.2815
H(224)	-0.0499	0.2948	-0.3545
H(225)	-0.0508	0.4886	-0.3252
H(226)	-0.0573	0.5376	-0.2228
H(14)	-0.0982	0.0297	-0.1217
H(234)	-0.1741	0.0506	-0.0647

TABLE 3 Anisotropic thermal parameters (Å ^{2}) for $[Au_2Ru_4(\mu\text{-}H)(\mu_3\text{-}H)(CO)_{12}\{\mu\text{-}Ph_2PCH{=}CHPPh_2\}]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Au(1)	0.046(1)	0.039(1)	0.043(1)	0.004(1)	0.002(1)	0.001(1)
Au(2)	0.039(1)	0.041(1)	0.037(1)	0.004(1)	0.009(1)	0.000(1)
Ru(1)	0.049(2)	0.041(2)	0.039(2)	0.002(1)	0.004(1)	0.004(1)
Ru(2)	0.064(2)	0.042(2)	0.055(2)	0.007(1)	0.018(2)	-0.003(2)
Ru(3)	0.043(2)	0.041(2)	0.042(2)	-0.001(1)	0.015(1)	0.000(1)
Ru(4)	0.054(2)	0.037(1)	0.041(2)	-0.003(1)	0.003(1)	0.000(1)
P(1)	0.045(5)	0.041(5)	0.047(6)	0.009(4)	-0.004(5)	-0.004(4)
P(2)	0.037(5)	0.045(5)	0.032(5)	0.006(4)	0.004(4)	0.000(4)

TABLE 4 Bond lengths (Å) for $[Au_2Ru_4(\mu\text{-}H)(\mu_3\text{-}H)(CO)_{12}\{\mu\text{-}Ph_2PCH{=}CHPPh_2\}]$

Au(1) -Au(2)	2.861(2)	Au(1) -Ru(3)	2.827(2)
Au(1) -Ru(4)	2.735(2)	Au(1) -P(1)	2.307(9)
Au(1) -C(33)	2.75(4)	Au(1) -C(43)	2.70(4)
Au(2) -Ru(1)	2.707(2)	Au(2) -Ru(3)	2.811(2)
Au(2) -P(2)	2.311(8)	Au(2) -C(12)	2.59(4)
Au(2) -C(33)	2.63(4)	Ru(1) -Ru(2)	2.796(3)
Ru(1) -Ru(3)	2.988(3)	Ru(1) -Ru(4)	2.995(3)
Ru(1) -C(11)	1.84(3)	Ru(1) -C(12)	1.88(4)
Ru(1) -C(13)	1.85(4)	Ru(2) -Ru(3)	2.877(3)
Ru(2) -Ru(4)	2.897(3)	Ru(2) -C(21)	1.88(4)
Ru(2) -C(22)	1.86(4)	Ru(2) -C(23)	1.89(5)
Ru(3) -Ru(4)	3.017(3)	Ru(3) -C(31)	1.84(4)
Ru(3) -C(32)	1.87(4)	Ru(3) -C(33)	1.92(4)
Ru(4) -C(41)	1.76(4)	Ru(4) -C(42)	1.83(4)
Ru(4) -C(43)	1.88(4)	P(1) -C(1)	1.85(3)
P(1) -C(111)	1.872(22)	P(1) -C(121)	1.837(21)
P(2) -C(2)	1.79(3)	P(2) -C(211)	1.864(19)
P(2) -C(221)	1.802(20)	C(11) -O(11)	1.17(4)
C(12) -O(12)	1.18(5)	C(13) -O(13)	1.14(5)
C(21) -O(21)	1.15(5)	C(22) -O(22)	1.15(5)
C(23) -O(23)	1.14(6)	C(31) -O(31)	1.16(5)
C(32) -O(32)	1.17(5)	C(33) -O(33)	1.14(5)
C(41) -O(41)	1.21(5)	C(42) -O(42)	1.20(5)
C(43) -O(43)	1.17(5)	C(1) -C(2)	1.33(4)
C(111)-C(112)	1.39(3)	C(111)-C(116)	1.39(3)

table 4 continued

C(112)-C(113)	1.36(3)	C(113)-C(114)	1.32(3)
C(114)-C(115)	1.39(3)	C(115)-C(116)	1.39(3)
C(121)-C(122)	1.39(3)	C(121)-C(126)	1.39(3)
C(122)-C(123)	1.37(3)	C(123)-C(124)	1.40(3)
C(124)-C(125)	1.39(3)	C(125)-C(126)	1.39(3)
C(212)-C(213)	1.395(25)	C(212)-C(211)	1.39(3)
C(213)-C(214)	1.395(25)	C(214)-C(215)	1.39(3)
C(215)-C(216)	1.395(25)	C(216)-C(211)	1.395(25)
C(221)-C(222)	1.39(3)	C(221)-C(226)	1.39(3)
C(222)-C(223)	1.39(3)	C(223)-C(224)	1.40(3)
C(224)-C(225)	1.40(3)	C(225)-C(226)	1.39(3)

TABLE 5 Bond angles (°) for $[Au_2Ru_4(\mu\text{-}H)(\mu_3\text{-}H)(CO)_{12}\{\mu\text{-}Ph_2PCH{=}CHPPh_2\}]$

Ru(3) -Au(1) -Au(2)	59.2(1)	Ru(4) -Au(1) -Au(2)	86.0(1)
Ru(4) -Au(1) -Ru(3)	65.7(1)	P(1) -Au(1) -Au(2)	105.2(2)
P(1) -Au(1) -Ru(3)	132.7(2)	P(1) -Au(1) -Ru(4)	161.5(2)
C(33) -Au(1) -Au(2)	55.9(8)	C(33) -Au(1) -Ru(3)	40.1(8)
C(33) -Au(1) -Ru(4)	105.5(8)	C(33) -Au(1) -P(1)	93.0(9)
C(43) -Au(1) -Au(2)	96.9(7)	C(43) -Au(1) -Ru(3)	104.7(8)
C(43) -Au(1) -Ru(4)	40.5(8)	C(43) -Au(1) -P(1)	122.1(8)
C(43) -Au(1) -C(33)	142(1)	Ru(1) -Au(2) -Au(1)	96.4(1)
Ru(3) -Au(2) -Au(1)	59.8(1)	Ru(3) -Au(2) -Ru(1)	65.5(1)
P(2) -Au(2) -Au(1)	90.7(2)	P(2) -Au(2) -Ru(1)	150.7(2)
P(2) -Au(2) -Ru(3)	140.1(2)	C(12) -Au(2) -Au(1)	119.7(8)
C(12) -Au(2) -Ru(1)	41.5(9)	C(12) -Au(2) -Ru(3)	107.0(9)
C(12) -Au(2) -P(2)	111.2(9)	C(33) -Au(2) -Au(1)	60.0(8)
C(33) -Au(2) -Ru(1)	105.9(9)	C(33) -Au(2) -Ru(3)	41.1(9)
C(33) -Au(2) -P(2)	102.3(9)	C(33) -Au(2) -C(12)	146(1)
Ru(2) -Ru(1) -Au(2)	118.0(1)	Ru(3) -Ru(1) -Au(2)	58.9(1)
Ru(3) -Ru(1) -Ru(2)	59.5(1)	Ru(4) -Ru(1) -Au(2)	83.9(1)
Ru(4) -Ru(1) -Ru(2)	59.9(1)	Ru(4) -Ru(1) -Ru(3)	60.6(1)
C(11) -Ru(1) -Au(2)	158(1)	C(11) -Ru(1) -Ru(2)	82(1)
C(11) -Ru(1) -Ru(3)	141(1)	C(11) -Ru(1) -Ru(4)	99(1)
C(12) -Ru(1) -Au(2)	66(1)	C(12) -Ru(1) -Ru(2)	173(1)
C(12) -Ru(1) -Ru(3)	125(1)	C(12) -Ru(1) -Ru(4)	116(1)
C(12) -Ru(1) -C(11)	93(2)	C(13) -Ru(1) -Au(2)	92(1)
C(13) -Ru(1) -Ru(2)	99(1)	C(13) -Ru(1) -Ru(3)	94(1)
C(13) -Ru(1) -Ru(4)	152(1)	C(13) -Ru(1) -C(11)	94(2)

table 5 continued

C(13) -Ru(1) -C(12)	87(2)	Ru(3) -Ru(2) -Ru(1)	63.5(1)
Ru(4) -Ru(2) -Ru(1)	63.5(1)	Ru(4) -Ru(2) -Ru(3)	63.0(1)
C(21) -Ru(2) -Ru(1)	102(1)	C(21) -Ru(2) -Ru(3)	160(1)
C(21) -Ru(2) -Ru(4)	99(1)	C(22) -Ru(2) -Ru(1)	92(1)
C(22) -Ru(2) -Ru(3)	100(1)	C(22) -Ru(2) -Ru(4)	154(1)
C(22) -Ru(2) -C(21)	93(2)	C(23) -Ru(2) -Ru(1)	160(1)
C(23) -Ru(2) -Ru(3)	98(1)	C(23) -Ru(2) -Ru(4)	102(1)
C(23) -Ru(2) -C(21)	93(2)	C(23) -Ru(2) -C(22)	99(2)
Au(2) -Ru(3) -Au(1)	61.0(1)	Ru(1) -Ru(3) -Au(1)	91.1(1)
Ru(1) -Ru(3) -Au(2)	55.5(1)	Ru(2) -Ru(3) -Au(1)	114.5(1)
Ru(2) -Ru(3) -Au(2)	112.0(1)	Ru(2) -Ru(3) -Ru(1)	56.9(1)
Ru(4) -Ru(3) -Au(1)	55.7(1)	Ru(4) -Ru(3) -Au(2)	81.8(1)
Ru(4) -Ru(3) -Ru(1)	59.8(1)	Ru(4) -Ru(3) -Ru(2)	58.8(1)
C(31) -Ru(3) -Au(1)	98(1)	C(31) -Ru(3) -Au(2)	154(1)
C(31) -Ru(3) -Ru(1)	146(1)	C(31) -Ru(3) -Ru(2)	90(1)
C(31) -Ru(3) -Ru(4)	99(1)	C(32) -Ru(3) -Au(1)	161(1)
C(32) -Ru(3) -Au(2)	104(1)	C(32) -Ru(3) -Ru(1)	89(1)
C(32) -Ru(3) -Ru(2)	81(1)	C(32) -Ru(3) -Ru(4)	138(1)
C(32) -Ru(3) -C(31)	92(2)	C(33) -Ru(3) -Au(1)	68(1)
C(33) -Ru(3) -Au(2)	64(1)	C(33) -Ru(3) -Ru(1)	119(1)
C(33) -Ru(3) -Ru(2)	175(1)	C(33) -Ru(3) -Ru(4)	123(1)
C(33) -Ru(3) -C(31)	94(2)	C(33) -Ru(3) -C(32)	95(2)
Ru(1) -Ru(4) -Au(1)	92.8(1)	Ru(2) -Ru(4) -Au(1)	116.8(1)
Ru(2) -Ru(4) -Ru(1)	56.6(1)	Ru(3) -Ru(4) -Au(1)	58.6(1)
Ru(3) -Ru(4) -Ru(1)	59.6(1)	Ru(3) -Ru(4) -Ru(2)	58.2(1)
C(41) -Ru(4) -Au(1)	84(1)	C(41) -Ru(4) -Ru(1)	151(1)
C(41) -Ru(4) -Ru(2)	99(1)	C(41) -Ru(4) -Ru(3)	95(1)
C(42) -Ru(4) -Au(1)	164(1)	C(42) -Ru(4) -Ru(1)	97(1)

table 5 continued

C(42) -Ru(4) -Ru(2)	80(1)	C(42) -Ru(4) -Ru(3)	138(1)
C(42) -Ru(4) -C(41)	93(2)	C(43) -Ru(4) -Au(1)	69(1)
C(43) -Ru(4) -Ru(1)	111(1)	C(43) -Ru(4) -Ru(2)	166(1)
C(43) -Ru(4) -Ru(3)	125(1)	C(43) -Ru(4) -C(41)	94(2)
C(43) -Ru(4) -C(42)	95(2)	C(1) -P(1) -Au(1)	114.0(9)
C(111)-P(1) -Au(1)	111.9(9)	C(111)-P(1) -C(1)	100(1)
C(121)-P(1) -Au(1)	117.6(9)	C(121)-P(1) -C(1)	107(1)
C(121)-P(1) -C(111)	104(1)	C(2) -P(2) -Au(2)	115(1)
C(211)-P(2) -Au(2)	116.1(7)	C(211)-P(2) -C(2)	103(1)
C(221)-P(2) -Au(2)	110.9(8)	C(221)-P(2) -C(2)	106(1)
C(221)-P(2) -C(211)	104(1)	O(11) -C(11) -Ru(1)	177(3)
Ru(1) -C(12) -Au(2)	73(1)	O(12) -C(12) -Au(2)	118(3)
O(12) -C(12) -Ru(1)	167(3)	O(13) -C(13) -Ru(1)	173(4)
O(21) -C(21) -Ru(2)	172(4)	O(22) -C(22) -Ru(2)	177(3)
O(23) -C(23) -Ru(2)	169(4)	O(31) -C(31) -Ru(3)	171(3)
O(32) -C(32) -Ru(3)	171(4)	Au(2) -C(33) -Au(1)	64.1(9)
Ru(3) -C(33) -Au(1)	72(1)	Ru(3) -C(33) -Au(2)	74(1)
O(33) -C(33) -Au(1)	120(3)	O(33) -C(33) -Au(2)	127(3)
O(33) -C(33) -Ru(3)	158(3)	O(41) -C(41) -Ru(4)	177(4)
O(42) -C(42) -Ru(4)	169(3)	Ru(4) -C(43) -Au(1)	71(1)
O(43) -C(43) -Au(1)	118(3)	O(43) -C(43) -Ru(4)	171(3)
C(2) -C(1) -P(1)	128(2)	C(1) -C(2) -P(2)	129(2)
C(112)-C(111)-P(1)	123(2)	C(116)-C(111)-P(1)	117(2)
C(116)-C(111)-C(112)	120(2)	C(113)-C(112)-C(111)	115(2)
C(114)-C(113)-C(112)	128(2)	C(115)-C(114)-C(113)	116(2)
C(116)-C(115)-C(114)	120(2)	C(115)-C(116)-C(111)	120(2)
C(122)-C(121)-P(1)	119(2)	C(126)-C(121)-P(1)	121(2)
C(126)-C(121)-C(122)	120(2)	C(123)-C(122)-C(121)	120(2)

table 5 continued

C(124)-C(123)-C(122)	121(2)	C(125)-C(124)-C(123)	119(2)
C(126)-C(125)-C(124)	120(2)	C(125)-C(126)-C(121)	120(2)
C(211)-C(212)-C(213)	120(2)	C(214)-C(213)-C(212)	120(2)
C(215)-C(214)-C(213)	120(2)	C(216)-C(215)-C(214)	120(2)
C(211)-C(216)-C(215)	120(2)	C(212)-C(211)-P(2)	119(1)
C(216)-C(211)-P(2)	120(1)	C(216)-C(211)-C(212)	120(2)
C(222)-C(221)-P(2)	120(1)	C(226)-C(221)-P(2)	120(2)
C(226)-C(221)-C(222)	120(2)	C(223)-C(222)-C(221)	120(2)
C(224)-C(223)-C(222)	120(2)	C(225)-C(224)-C(223)	120(2)
C(226)-C(225)-C(224)	120(2)	C(225)-C(226)-C(221)	120(2)

TABLE 6 Intermolecular distances (Å) for

$[Au_2Ru_4(\mu\text{-}H)(\mu_3\text{-}H)(CO)_{12}\{\mu\text{-}Ph_2PCH{=}CHPPh_2\}]$

atom1	atom2	dist	S	a	b	c
C(213)	Au(2)	4.07	-1	0.0	1.0	0.0
C(214)	Au(2)	3.63	-1	0.0	1.0	0.0
H(214)	Au(2)	3.13	-1	0.0	1.0	0.0
O(22)	Ru(1)	4.16	1	1.0	1.0	0.0
O(22)	Ru(2)	3.02	1	1.0	1.0	0.0
H(214)	Ru(3)	3.81	-1	0.0	1.0	0.0
H(216)	O(11)	2.90	-1	0.0	0.0	0.0
C(13)	O(12)	3.26	-1	0.0	0.0	0.0
O(13)	O(12)	3.03	-1	0.0	0.0	0.0
O(22)	C(13)	3.38	1	1.0	1.0	0.0
O(22)	O(13)	3.24	1	1.0	1.0	0.0
H(213)	O(13)	2.60	-1	0.0	1.0	0.0
C(1)	O(21)	3.37	1	0.0	1.0	0.0
C(2)	O(21)	3.41	1	0.0	1.0	0.0
H(112)	O(21)	2.84	1	0.0	1.0	0.0
H(215)	O(21)	2.59	-1	0.0	0.0	0.0
H(115)	C(22)	3.07	-2	-0.5	0.5	0.5
C(32)	O(22)	3.33	1	-1.0	-1.0	0.0
O(32)	O(22)	3.16	1	-1.0	-1.0	0.0
O(43)	O(22)	3.22	2	-1.0	1.0	-1.0
H(115)	O(22)	2.81	-2	0.5	-0.5	0.5
O(31)	O(23)	3.06	-2	-0.5	0.5	0.5
H(125)	O(32)	2.53	2	0.0	1.0	-1.0
H(114)	O(32)	2.57	-2	-0.5	0.5	0.5
H(214)	C(33)	2.68	-1	0.0	1.0	0.0

table 6 continued

H(214)...O(33)	2.63	-1	0.0	1.0	0.0
H(124)...O(33)	2.57	2	0.0	1.0	-1.0
C(111)...O(41)	3.40	-1	-0.5	0.5	-0.5
C(112)...O(41)	3.38	-1	-0.5	0.5	-0.5
C(122)...O(41)	3.37	-1	-0.5	0.5	-0.5
C(1) ...O(42)	3.30	1	0.0	1.0	0.0
C(114)...O(43)	3.26	-1	-0.5	0.5	-0.5
C(115)...O(43)	3.20	-1	-0.5	0.5	-0.5
H(114)...O(43)	2.98	-1	-0.5	0.5	-0.5
H(115)...O(43)	2.87	-1	-0.5	0.5	-0.5
H(225)...C(212)	2.90	-2	0.0	0.0	0.0
H(225)...C(213)	2.76	-2	0.0	0.0	0.0
H(225)...C(214)	2.89	-2	0.0	0.0	0.0
H(224)...C(215)	3.07	-2	0.0	0.0	0.0
H(224)...C(216)	2.81	-2	0.0	0.0	0.0

Symmetry Transformations:

The second atom is related to the first atom, at (x,y,z), by the symmetry operation S with (a,b,c) added to the (x',y',z') of S.

Where S =

1	x, y, z
2	x, -y, 0.5+z

TABLE 7 Intramolecular distances (Å) for

$[Au_2Ru_4(\mu\text{-}H)(\mu_3\text{-}H)(CO)_{12}\{\mu\text{-}Ph_2PCH{=}CHPPh_2\}]$

Ru(1) ...Au(1)	4.15	Ru(2) ...Au(1)	4.80
P(2) ...Au(1)	3.70	C(31) ...Au(1)	3.57
O(33) ...Au(1)	3.47	C(41) ...Au(1)	3.10
O(41) ...Au(1)	3.81	O(43) ...Au(1)	3.41
C(1) ...Au(1)	3.49	C(2) ...Au(1)	3.92
C(111)...Au(1)	3.47	C(116)...Au(1)	3.50
H(116)...Au(1)	2.81	C(121)...Au(1)	3.55
C(122)...Au(1)	3.75	H(122)...Au(1)	3.16
C(221)...Au(1)	3.95	C(222)...Au(1)	3.86
H(222)...Au(1)	3.52	H(14) ...Au(1)	3.41
H(234)...Au(1)	3.17	Ru(2) ...Au(2)	4.72
Ru(4) ...Au(2)	3.82	P(1) ...Au(2)	4.12
O(12) ...Au(2)	3.31	C(13) ...Au(2)	3.34
O(13) ...Au(2)	4.13	C(32) ...Au(2)	3.74
O(33) ...Au(2)	3.45	C(43) ...Au(2)	4.16
C(1) ...Au(2)	4.02	C(2) ...Au(2)	3.47
C(216)...Au(2)	3.76	C(211)...Au(2)	3.55
H(216)...Au(2)	3.19	C(221)...Au(2)	3.40
C(222)...Au(2)	3.49	H(222)...Au(2)	2.85
H(14) ...Au(2)	3.08	O(11) ...Ru(1)	3.01
O(12) ...Ru(1)	3.04	O(13) ...Ru(1)	2.99
C(21) ...Ru(1)	3.68	C(22) ...Ru(1)	3.42
C(32) ...Ru(1)	3.51	C(42) ...Ru(1)	3.70
C(43) ...Ru(1)	4.07	H(222)...Ru(1)	3.80
H(234)...Ru(1)	3.09	C(11) ...Ru(2)	3.12

table 7 continued

O(11) ...Ru(2)	3.82	C(13) ...Ru(2)	3.58
O(21) ...Ru(2)	3.02	O(23) ...Ru(2)	3.02
C(31) ...Ru(2)	3.42	C(32) ...Ru(2)	3.19
O(32) ...Ru(2)	3.99	C(41) ...Ru(2)	3.62
C(42) ...Ru(2)	3.13	O(42) ...Ru(2)	3.95
H(14) ...Ru(2)	3.38	C(13) ...Ru(3)	3.62
C(22) ...Ru(3)	3.70	C(23) ...Ru(3)	3.67
O(31) ...Ru(3)	2.99	O(32) ...Ru(3)	3.03
O(33) ...Ru(3)	3.01	C(41) ...Ru(3)	3.63
H(14) ...Ru(3)	3.54	C(11) ...Ru(4)	3.76
C(12) ...Ru(4)	4.18	C(21) ...Ru(4)	3.69
C(23) ...Ru(4)	3.78	C(31) ...Ru(4)	3.77
O(41) ...Ru(4)	2.96	O(42) ...Ru(4)	3.02
O(43) ...Ru(4)	3.04	P(2) ...P(1)	3.59
C(33) ...P(1)	3.68	O(33) ...P(1)	3.71
C(2) ...P(1)	2.86	C(112)...P(1)	2.88
C(116)...P(1)	2.80	H(116)...P(1)	2.89
C(122)...P(1)	2.79	C(126)...P(1)	2.82
H(122)...P(1)	2.91	H(126)...P(1)	2.95
C(221)...P(1)	3.68	C(1) ...P(2)	2.82
C(212)...P(2)	2.82	C(216)...P(2)	2.84
H(212)...P(2)	2.93	H(216)...P(2)	2.96
C(222)...P(2)	2.78	C(226)...P(2)	2.77
H(222)...P(2)	2.91	H(226)...P(2)	2.89
C(12) ...C(11)	2.71	C(13) ...C(11)	2.71
C(21) ...C(11)	2.95	H(14) ...C(11)	2.64
C(21) ...O(11)	3.05	O(21) ...O(11)	3.19
C(13) ...C(12)	2.57	H(216)...C(12)	3.06

table 7 continued

H(222)...C(12)	2.87	H(14) ...C(12)	2.68
H(216)...O(12)	2.68	H(222)...O(12)	2.86
C(22) ...C(13)	3.16	C(32) ...C(13)	3.15
C(22) ...O(13)	3.41	C(32) ...O(13)	3.33
O(32) ...O(13)	3.21	C(22) ...C(21)	2.73
C(23) ...C(21)	2.74	C(42) ...C(21)	2.87
O(42) ...C(21)	3.10	C(42) ...O(21)	3.40
O(42) ...O(21)	3.20	C(23) ...C(22)	2.87
C(32) ...C(22)	2.95	O(32) ...C(22)	3.19
C(31) ...C(23)	3.16	H(234)...C(23)	2.68
C(31) ...O(23)	3.38	O(31) ...O(23)	3.29
C(32) ...C(31)	2.67	C(33) ...C(31)	2.75
C(41) ...C(31)	3.50	H(234)...C(31)	2.60
C(33) ...C(32)	2.80	C(1) ...O(33)	3.28
C(42) ...C(41)	2.60	C(43) ...C(41)	2.67
H(234)...C(41)	2.61	C(43) ...C(42)	2.75
H(14) ...C(42)	2.53	H(234)...C(42)	2.99
H(122)...C(43)	3.06	H(222)...C(43)	3.08
H(14) ...C(43)	2.66	H(122)...O(43)	2.65
C(222)...O(43)	3.29	C(223)...O(43)	3.18
H(223)...O(43)	2.83	C(111)...C(1)	2.86
C(112)...C(1)	3.25	H(112)...C(1)	2.90
C(121)...C(1)	2.96	C(126)...C(1)	3.23
H(126)...C(1)	2.75	C(221)...C(1)	3.50
C(212)...C(2)	3.11	C(211)...C(2)	2.87
H(212)...C(2)	2.64	C(221)...C(2)	2.88
C(226)...C(2)	3.20	H(226)...C(2)	2.83
C(113)...C(111)	2.33	C(114)...C(111)	2.79

table 7 continued

C(115)...C(111)	2.42	H(112)...C(111)	2.59
H(116)...C(111)	2.15	C(121)...C(111)	2.92
C(114)...C(112)	2.42	C(115)...C(112)	2.79
C(116)...C(112)	2.42	H(112)...C(112)	2.13
H(113)...C(112)	2.15	C(121)...C(112)	3.48
C(115)...C(113)	2.31	C(116)...C(113)	2.67
H(112)...C(113)	2.61	H(114)...C(113)	2.12
C(116)...C(114)	2.42	H(113)...C(114)	2.15
H(115)...C(114)	2.15	H(114)...C(115)	2.15
H(116)...C(115)	2.15	H(115)...C(116)	2.15
C(123)...C(121)	2.40	C(124)...C(121)	2.79
C(125)...C(121)	2.42	H(122)...C(121)	2.15
H(126)...C(121)	2.15	C(226)...C(121)	3.46
C(124)...C(122)	2.42	C(125)...C(122)	2.79
C(126)...C(122)	2.42	H(123)...C(122)	2.15
C(125)...C(123)	2.41	C(126)...C(123)	2.78
H(122)...C(123)	2.13	H(124)...C(123)	2.17
C(126)...C(124)	2.42	H(123)...C(124)	2.15
H(125)...C(124)	2.15	H(124)...C(125)	2.15
H(126)...C(125)	2.15	H(125)...C(126)	2.15
C(226)...C(126)	3.42	C(214)...C(212)	2.42
C(215)...C(212)	2.79	C(216)...C(212)	2.42
H(213)...C(212)	2.15	H(226)...C(212)	3.04
C(215)...C(213)	2.42	C(216)...C(213)	2.79
C(211)...C(213)	2.42	H(212)...C(213)	2.15
H(214)...C(213)	2.15	C(216)...C(214)	2.42
C(211)...C(214)	2.79	H(213)...C(214)	2.15
H(215)...C(214)	2.15	C(211)...C(215)	2.42

table 7 continued

H(214)...C(215)	2.15	H(216)...C(215)	2.15
H(215)...C(216)	2.15	H(212)...C(211)	2.15
H(216)...C(211)	2.15	C(221)...C(211)	2.90
C(226)...C(211)	3.44	C(223)...C(221)	2.42
C(224)...C(221)	2.79	C(225)...C(221)	2.42
H(222)...C(221)	2.15	H(226)...C(221)	2.15
C(224)...C(222)	2.42	C(225)...C(222)	2.79
C(226)...C(222)	2.42	H(223)...C(222)	2.15
C(225)...C(223)	2.42	C(226)...C(223)	2.79
H(222)...C(223)	2.15	H(224)...C(223)	2.15
C(226)...C(224)	2.42	H(223)...C(224)	2.15
H(225)...C(224)	2.15	H(224)...C(225)	2.15
H(226)...C(225)	2.15	H(225)...C(226)	2.15

Crystallographic Tables for $[AuCuRu_4(\mu\text{-}H)(\mu_3\text{-}H)(CO)_{12}\{\mu\text{-}Ph_2PCH_2CH_2PPh_2\}]$, {X-ray study presented in section 2.3, Vol.1}.

TABLE 1 Fractional atomic coordinates and thermal parameters ($Å^2$) for $[AuCuRu_4(\mu\text{-}H)(\mu_3\text{-}H)(CO)_{12}\{\mu\text{-}Ph_2PCH_2CH_2PPh_2\}]$

Atom	x	y	z	U_{iso} or U_{eq}
Au	0.0296(7)	-0.0677(10)	0.1057(8)	0.047(6)
Cu	0.2373(18)	-0.0040(11)	0.1278(17)	0.038(14)
Ru(1)	0.3590(12)	0.0577(8)	0.2620(13)	0.037(10)
Ru(2)	0.2186(13)	0.1119(8)	0.3403(13)	0.034(10)
Ru(3)	0.1482(12)	0.0886(7)	0.1425(12)	0.037(10)
Ru(4)	0.1651(12)	0.0154(6)	0.3010(11)	0.038(9)
P(1)	-0.0533(36)	-0.0596(18)	0.0291(44)	0.045(20)
P(2)	0.2315(43)	-0.0538(22)	0.0140(37)	0.045(21)
C(11)	0.4234(24)	0.0564(92)	0.4214(24)	0.063(25)
O(11)	0.5095(24)	0.0356(64)	0.5193(24)	0.069(24)
C(12)	0.4406(24)	0.0048(24)	0.2117(24)	0.077(25)
O(12)	0.5217(24)	-0.0262(67)	0.1737(24)	0.089(25)
C(13)	0.4206(24)	0.1098(90)	0.2343(24)	0.049(25)
O(13)	0.4803(24)	0.1389(69)	0.2393(24)	0.079(24)
C(21)	0.2613(24)	0.1715(98)	0.3261(24)	0.068(26)
O(21)	0.2700(24)	0.1993(82)	0.3817(24)	0.096(25)
C(22)	0.1231(24)	0.1308(85)	0.3735(24)	0.042(25)
O(22)	0.0080(24)	0.1595(66)	0.3528(24)	0.069(24)
C(23)	0.2741(24)	0.0877(24)	0.4434(24)	0.080(26)
O(23)	0.3192(98)	0.0993(53)	0.5512(24)	0.088(23)
C(31)	-0.0473(24)	0.1091(79)	0.1541(24)	0.040(24)
O(31)	-0.1269(24)	0.1326(74)	0.1263(24)	0.087(24)
C(32)	0.0746(24)	0.0569(65)	-0.0036(24)	0.062(23)
O(32)	0.1231(24)	0.0840(95)	-0.0633(24)	0.078(25)
C(33)	0.1729(24)	0.1607(81)	0.1045(24)	0.046(25)

table 1 continued

O(33)	C.2331(24)	0.1925(70)	0.1593(24)	0.083(24)
C(41)	0.2180(24)	0.0159(68)	0.4282(24)	0.060(23)
O(41)	0.2589(85)	-0.0109(45)	0.5202(83)	0.097(21)
C(42)	0.1300(24)	0.9502(69)	0.2762(24)	0.079(24)
O(42)	0.1094(88)	-0.0977(47)	0.2759(87)	0.066(21)
C(43)	0.0087(24)	0.0438(87)	0.3277(24)	0.053(25)
O(43)	-0.0756(24)	0.0523(70)	0.3284(24)	0.080(25)
C(1)	0.0219(24)	-0.1228(24)	-0.0265(24)	0.089(26)
C(2)	0.1173(24)	-0.0879(95)	-0.0710(24)	0.062(26)
C(15)	-0.1578(75)	-0.0573(38)	-0.1783(76)	0.008(26)
C(16)	-0.2200(75)	-0.0415(38)	-0.2706(76)	0.064(25)
C(17)	-0.2784(75)	0.0021(38)	-0.2776(76)	0.066(26)
C(18)	-0.2745(75)	0.0299(38)	-0.1922(76)	0.065(26)
C(19)	-0.2124(75)	0.0141(38)	-0.1000(76)	0.072(24)
C(14)	-0.1540(75)	-0.0294(38)	-0.0930(76)	0.090(23)
C(25)	-0.2350(81)	-0.0787(40)	0.1156(72)	0.047(25)
C(26)	-0.3033(81)	-0.1049(40)	0.1619(72)	0.080(26)
C(27)	-0.2753(81)	-0.1521(40)	0.1968(72)	0.062(25)
C(28)	-0.1790(81)	-0.1732(40)	0.1853(72)	0.064(25)
C(29)	-0.1106(81)	-0.1470(40)	0.1390(72)	0.082(26)
C(24)	-0.1386(81)	-0.0998(40)	0.1041(72)	0.073(24)
C(35)	0.3786(90)	-0.1160(50)	0.1547(99)	0.065(26)
C(36)	0.4338(90)	-0.1586(50)	0.1925(99)	0.050(25)
C(37)	0.4442(90)	-0.1965(50)	0.1282(99)	0.070(26)
C(38)	0.3992(90)	-0.1919(50)	0.0260(99)	0.063(25)
C(39)	0.3439(90)	-0.1493(50)	-0.0119(99)	0.070(26)
C(34)	0.3336(90)	-0.1114(50)	0.0524(99)	0.089(26)
C(45)	0.2589(69)	-0.0101(36)	-0.1614(68)	0.071(25)

table 1 continued

C(46)	0.3088(69)	0.0089(36)	-0.2326(68)	0.060(22)
C(47)	0.4176(69)	-0.0016(36)	-0.2274(68)	0.077(26)
C(48)	0.4765(69)	-0.0312(36)	-0.1510(68)	0.081(26)
C(49)	0.4266(69)	-0.0503(36)	-0.0798(68)	0.061(24)
C(44)	0.3178(69)	-0.0397(36)	-0.0850(68)	0.062(25)

TABLE 2 Anisotropic thermal parameters ($Å^2$)

for $[AuCuRu_4(\mu\text{-}H)(\mu_3\text{-}H)(CO)_{12}\{\mu\text{-}Ph_2PCH_2CH_2PPh_2\}]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Au	0.050(6)	0.029(6)	0.062(7)	-0.033(6)	-0.005(5)	0.005(5)
Cu	0.034(13)	0.058(16)	0.022(13)	-0.006(14)	0.029(11)	0.015(14)
Ru(1)	0.036(8)	0.036(12)	0.038(10)	-0.011(10)	-0.008(7)	-0.008(9)
Ru(2)	0.034(9)	0.037(12)	0.031(10)	-0.023(10)	0.001(8)	-0.014(9)
Ru(3)	0.038(9)	0.037(10)	0.038(9)	-0.013(9)	0.012(8)	0.018(8)
Ru(4)	0.038(9)	0.036(9)	0.039(9)	-0.004(8)	0.026(8)	0.017(7)
P(1)	0.045(19)	0.049(20)	0.041(22)	-0.012(20)	0.015(18)	0.005(17)
P(2)	0.048(20)	0.042(22)	0.048(20)	-0.035(19)	0.022(18)	-0.001(20)

TABLE 3 Bond lengths (Å) for $[AuCuRu_4(\mu\text{-}H)(\mu_3\text{-}H)(CO)_{12}\{\mu\text{-}Ph_2PCH_2CH_2PPh_2\}]$

Au	-Cu	2.614(3)	Au	-Ru(3)	2.823(3)
Au	-Ru(4)	2.823(3)	Au	-P(1)	2.21(3)
Au	-C(32)	2.60(3)	Au	-C(42)	2.75(3)
Cu	-Ru(1)	2.674(3)	Cu	-Ru(3)	2.817(3)
Cu	-Ru(4)	2.822(3)	Cu	-P(2)	2.15(4)
Cu	-C(12)	2.57(3)	Ru(1)	-Ru(2)	2.803(3)
Ru(1)	-Ru(3)	2.985(3)	Ru(1)	-Ru(4)	2.930(3)
Ru(1)	-C(11)	1.87(9)	Ru(1)	-C(12)	1.89(9)
Ru(1)	-C(13)	1.72(9)	Ru(2)	-Ru(3)	2.815(3)
Ru(2)	-Ru(4)	2.813(3)	Ru(2)	-C(21)	1.75(9)
Ru(2)	-O(21)	2.51(9)	Ru(2)	-C(22)	1.49(9)
Ru(2)	-C(23)	1.57(9)	Ru(3)	-Ru(4)	2.964(3)
Ru(3)	-C(31)	1.69(9)	Ru(3)	-C(32)	1.91(9)
Ru(3)	-C(33)	1.80(9)	Ru(4)	-C(41)	1.72(9)
Ru(4)	-C(42)	1.85(9)	Ru(4)	-C(43)	1.79(9)
P(1)	-C(1)	1.90(9)	P(1)	-C(14)	1.96(9)
P(1)	-C(24)	1.97(9)	P(2)	-C(2)	1.88(9)
P(2)	-C(34)	1.90(9)	P(2)	-C(44)	1.99(9)
C(11)	-O(11)	1.12(9)	C(12)	-O(12)	1.12(9)
C(13)	-O(13)	1.09(9)	C(21)	-O(21)	1.07(9)
C(22)	-O(22)	1.12(9)	C(23)	-O(23)	1.19(9)
C(31)	-O(31)	1.18(9)	C(32)	-O(32)	1.26(9)
C(33)	-O(33)	1.28(9)	C(41)	-O(41)	1.15(9)
C(42)	-O(42)	1.14(9)	C(43)	-O(43)	1.10(9)
C(1)	-C(2)	1.81(9)	C(15)	-C(16)	1.39(9)

table 3 continued

C(15) -C(14)	1.39(9)	C(16) -C(17)	1.39(9)
C(17) -C(18)	1.39(9)	C(18) -C(19)	1.39(9)
C(19) -C(14)	1.39(9)	C(25) -C(26)	1.39(9)
C(25) -C(24)	1.39(9)	C(26) -C(27)	1.39(9)
C(27) -C(28)	1.39(9)	C(28) -C(29)	1.39(9)
C(29) -C(24)	1.39(9)	C(35) -C(36)	1.39(9)
C(35) -C(34)	1.39(9)	C(36) -C(37)	1.39(9)
C(37) -C(38)	1.39(9)	C(38) -C(39)	1.39(9)
C(39) -C(34)	1.39(9)	C(45) -C(46)	1.39(9)
C(45) -C(44)	1.39(9)	C(46) -C(47)	1.39(9)
C(47) -C(48)	1.39(9)	C(48) -C(49)	1.39(9)
C(49) -C(44)	1.39(9)		

TABLE 4 Bond angles (°) for $[AuCuRu_4(\mu\text{-}H)(\mu_3\text{-}H)(CO)_{12}\{\mu\text{-}Ph_2PCH_2CH_2PPh_2\}]$

Ru(3)	-Au	-Cu	62.1(8)	Ru(4)	-Au	-Cu	62.1(7)
Ru(4)	-Au	-Ru(3)	62.2(5)	P(1)	-Au	-Cu	114(1)
P(1)	-Au	-Ru(3)	160(2)	P(1)	-Au	-Ru(4)	135(1)
C(42)	-Au	-Cu	68(4)	C(42)	-Au	-Ru(3)	99(4)
C(42)	-Au	-Ru(4)	38(4)	C(42)	-Au	-P(1)	97(4)
C(42)	-Au	-C(32)	138(5)	Ru(1)	-Cu	-Au	117(1)
Ru(3)	-Cu	-Au	63.4(7)	Ru(3)	-Cu	-Ru(1)	63.7(8)
Ru(4)	-Cu	-Au	63.8(7)	Ru(4)	-Cu	-Ru(1)	63.1(7)
Ru(4)	-Cu	-Ru(3)	63.1(8)	P(2)	-Cu	-Au	95(2)
P(2)	-Cu	-Ru(1)	147(2)	P(2)	-Cu	-Ru(3)	135(2)
P(2)	-Cu	-Ru(4)	144(2)	C(12)	-Cu	-Au	159(5)
C(12)	-Cu	-Ru(1)	45(6)	C(12)	-Cu	-Ru(3)	105(6)
C(12)	-Cu	-Ru(4)	96(5)	C(12)	-Cu	-P(2)	104(6)
Ru(2)	-Ru(1)	-Cu	107.1(8)	Ru(3)	-Ru(1)	-Cu	59.9(7)
Ru(3)	-Ru(1)	-Ru(2)	58.0(6)	Ru(4)	-Ru(1)	-Cu	60.4(7)
Ru(4)	-Ru(1)	-Ru(2)	58.5(6)	Ru(4)	-Ru(1)	-Ru(3)	61.0(5)
C(11)	-Ru(1)	-Cu	135(7)	C(11)	-Ru(1)	-Ru(2)	74(6)
C(11)	-Ru(1)	-Ru(3)	131(6)	C(11)	-Ru(1)	-Ru(4)	86(6)
C(12)	-Ru(1)	-Cu	64(5)	C(12)	-Ru(1)	-Ru(2)	166(7)
C(12)	-Ru(1)	-Ru(3)	120(5)	C(12)	-Ru(1)	-Ru(4)	108(7)
C(12)	-Ru(1)	-C(11)	104(8)	C(13)	-Ru(1)	-Cu	126(6)
C(13)	-Ru(1)	-Ru(2)	91(8)	C(13)	-Ru(1)	-Ru(3)	92(6)
C(13)	-Ru(1)	-Ru(4)	146(7)	C(13)	-Ru(1)	-C(11)	99(9)

table 4 continued

C(13) -Ru(1) -C(12)	102.8(4)	Ru(3) -Ru(2) -Ru(1)	64.1(6)
Ru(4) -Ru(2) -Ru(1)	63.5(7)	Ru(4) -Ru(2) -Ru(3)	64.8(7)
C(21) -Ru(2) -Ru(1)	102(8)	C(21) -Ru(2) -Ru(3)	98(7)
C(21) -Ru(2) -Ru(4)	161(8)	O(21) -Ru(2) -Ru(1)	117(5)
O(21) -Ru(2) -Ru(3)	117(4)	O(21) -Ru(2) -Ru(4)	178(4)
O(21) -Ru(2) -C(21)	21(9)	C(22) -Ru(2) -Ru(1)	165(8)
C(22) -Ru(2) -Ru(3)	107(7)	C(22) -Ru(2) -Ru(4)	102(9)
C(22) -Ru(2) -C(21)	90(2)	C(22) -Ru(2) -O(21)	77(*)
C(23) -Ru(2) -Ru(1)	86(9)	C(23) -Ru(2) -Ru(3)	140(*)
C(23) -Ru(2) -Ru(4)	79(9)	C(23) -Ru(2) -C(21)	114(1)
C(23) -Ru(2) -O(21)	99.2(3)	C(23) -Ru(2) -C(22)	95(2)
Cu -Ru(3) -Au	54.5(6)	Ru(1) -Ru(3) -Au	103.2(7)
Ru(1) -Ru(3) -Cu	56.4(7)	Ru(2) -Ru(3) -Au	114.1(8)
Ru(2) -Ru(3) -Cu	104.1(8)	Ru(2) -Ru(3) -Ru(1)	57.9(6)
Ru(4) -Ru(3) -Au	59.3(5)	Ru(4) -Ru(3) -Cu	58.7(7)
Ru(4) -Ru(3) -Ru(1)	59.2(6)	Ru(4) -Ru(3) -Ru(2)	57.8(6)
C(31) -Ru(3) -Au	74(5)	C(31) -Ru(3) -Cu	128(5)
C(31) -Ru(3) -Ru(1)	142(4)	C(31) -Ru(3) -Ru(2)	88(4)
C(31) -Ru(3) -Ru(4)	90(4)	C(32) -Ru(3) -Au	54(5)
C(31) -Ru(3) -Cu	139(6)	C(31) -Ru(3) -Ru(1)	104(5)
C(31) -Ru(3) -Ru(2)	90(5)	C(31) -Ru(3) -Ru(4)	148(5)
C(31) -Ru(3) -C(31)	91(7)	C(31) -Ru(3) -C(32)	101(7)
Cu -Ru(4) -Au	54.1(6)	Ru(1) -Ru(4) -Au	103.1(6)
Ru(1) -Ru(4) -Cu	56.5(7)	Ru(2) -Ru(4) -Au	113.0(6)
Ru(2) -Ru(4) -Cu	103.5(9)	Ru(2) -Ru(4) -Ru(1)	58.0(7)

table 4 continued

Ru(3) -Ru(4) -Au	58.5(4)	Ru(3) -Ru(4) -Cu	58.2(8)
Ru(3) -Ru(4) -Ru(1)	59.8(6)	Ru(3) -Ru(4) -Ru(2)	57.4(6)
C(41) -Ru(4) -Au	164(6)	C(41) -Ru(4) -Cu	138(5)
C(41) -Ru(4) -Ru(1)	93(5)	C(41) -Ru(4) -Ru(2)	77(6)
C(41) -Ru(4) -Ru(3)	134(6)	C(42) -Ru(4) -Au	68(5)
C(42) -Ru(4) -Cu	77(6)	C(42) -Ru(4) -Ru(1)	122(6)
C(42) -Ru(4) -Ru(2)	179(5)	C(42) -Ru(4) -Ru(3)	123(5)
C(42) -Ru(4) -C(41)	102(8)	C(43) -Ru(4) -Au	82(5)
C(43) -Ru(4) -Cu	134(5)	C(43) -Ru(4) -Ru(1)	136(6)
C(43) -Ru(4) -Ru(2)	80(6)	C(43) -Ru(4) -Ru(3)	89(6)
C(43) -Ru(4) -C(41)	88(7)	C(43) -Ru(4) -C(42)	100(8)
C(1) -P(1) -Au	116(3)	C(14) -P(1) -Au	104(4)
C(14) -P(1) -C(1)	105(7)	C(24) -P(1) -Au	116(4)
C(24) -P(1) -C(1)	95(8)	C(24) -P(1) -C(14)	110(4)
C(2) -P(2) -Cu	115(3)	C(34) -P(2) -Cu	114(4)
C(34) -P(2) -C(2)	97(9)	C(44) -P(2) -Cu	118(4)
C(44) -P(2) -C(2)	98(8)	C(44) -P(2) -C(34)	85(5)
O(11) -C(11) -Ru(1)	170(5)	Ru(1) -C(12) -Cu	71(6)
O(12) -C(12) -Cu	119(3)	O(12) -C(12) -Ru(1)	167(7)
O(13) -C(13) -Ru(1)	160(7)	O(21) -C(21) -Ru(2)	174(2)
C(21) -O(21) -Ru(2)	95(6)	O(22) -C(22) -Ru(2)	172(5)
O(23) -C(23) -Ru(2)	160(1)	O(31) -C(31) -Ru(3)	179(7)
O(32) -C(32) -Ru(3)	170(2)	O(33) -C(33) -Ru(3)	167(4)
O(41) -C(41) -Ru(4)	169(4)	Ru(4) -C(42) -Au	74(6)
O(42) -C(42) -Au	116(8)	O(42) -C(42) -Ru(4)	170(3)
O(43) -C(43) -Ru(4)	168(9)	C(2) -C(1) -P(1)	95(5)
C(1) -C(2) -P(2)	123(4)	C(14) -C(15) -C(16)	120(9)

table 4 continued

C(17) -C(16) -C(15)	120(9)	C(18) -C(17) -C(16)	120(9)
C(19) -C(18) -C(17)	120(9)	C(14) -C(19) -C(18)	120(9)
C(15) -C(14) -P(1)	111(7)	C(19) -C(14) -P(1)	128(8)
C(19) -C(14) -C(15)	120(9)	C(24) -C(25) -C(26)	120(9)
C(27) -C(26) -C(25)	120.0(1)	C(28) -C(27) -C(26)	120.0(3)
C(29) -C(28) -C(27)	120(9)	C(24) -C(29) -C(28)	120.0(1)
C(25) -C(24) -P(1)	115(8)	C(29) -C(24) -P(1)	124(8)
C(29) -C(24) -C(25)	120.0(3)	C(34) -C(35) -C(36)	120(3)
C(37) -C(36) -C(35)	120(2)	C(38) -C(37) -C(36)	120(2)
C(39) -C(38) -C(37)	120(3)	C(34) -C(39) -C(38)	120(2)
C(35) -C(34) -P(2)	114.4(1)	C(39) -C(34) -P(2)	124(9)
C(39) -C(34) -C(35)	120(2)	C(44) -C(45) -C(46)	120(8)
C(47) -C(46) -C(45)	120(8)	C(48) -C(47) -C(46)	120(9)
C(49) -C(48) -C(47)	120(8)	C(44) -C(49) -C(48)	120(8)
C(45) -C(44) -P(2)	111(7)	C(49) -C(44) -P(2)	129(7)
C(49) -C(44) -C(45)	120(9)		

TABLE 5 Intermolecular distances (Å) for

$[AuCuRu_4(\mu\text{-}H)(\mu_3\text{-}H)(CO)_{12}\{\mu\text{-}Ph_2PCH_2CH_2PPh_2\}]$

atom1	atom2	dist	S	a	b	c
C(42)	...Cu	3.00	1	0.0	1.0	0.0
C(42)	...Ru(1)	4.17	1	0.0	1.0	0.0
C(42)	...Ru(3)	4.25	1	0.0	1.0	0.0
C(42)	...P(1)	3.64	1	0.0	1.0	0.0
C(26)	...O(12)	3.13	1	-1.0	0.0	0.0
C(42)	...C(41)	2.78	1	0.0	1.0	0.0
C(46)	...O(41)	3.37	1	0.0	0.0	-1.0
C(43)	...C(42)	3.16	1	0.0	-1.0	0.0

Symmetry Transformations:

The second atom is related to the first atom, at (x,y,z), by the symmetry operation S with (a,b,c) added to the (x',y',z') of S.

Where S =

1	x, y, z
2	-x, 0.5+y, -z

TABLE 6 Intramolecular distances (Å) for

$[AuCuRu_4(\mu\text{-}H)(\mu_3\text{-}H)(CO)_{12}\{\mu\text{-}Ph_2PCH_2CH_2PPh_2\}]$

Ru(1) ...Au	4.50	Ru(2) ...Au	4.68
P(2) ...Au	3.45	C(31) ...Au	3.26
O(31) ...Au	4.18	O(32) ...Au	3.68
O(42) ...Au	3.55	C(43) ...Au	3.37
O(43) ...Au	3.91	C(1) ...Au	3.82
C(2) ...Au	3.79	C(19) ...Au	3.66
C(14) ...Au	3.24	C(25) ...Au	4.02
C(24) ...Au	3.46	Ru(2) ...Cu	4.37
P(1) ...Cu	3.91	O(12) ...Cu	3.56
C(13) ...Cu	3.95	C(32) ...Cu	2.92
O(32) ...Cu	3.61	O(42) ...Cu	3.88
C(2) ...Cu	3.62	C(35) ...Cu	3.53
C(34) ...Cu	3.44	C(45) ...Cu	4.08
C(44) ...Cu	3.48	O(11) ...Ru(1)	3.66
O(12) ...Ru(1)	3.50	O(13) ...Ru(1)	2.76
C(21) ...Ru(1)	3.54	C(22) ...Ru(1)	4.19
C(23) ...Ru(1)	3.07	C(31) ...Ru(1)	3.97
O(31) ...Ru(1)	4.13	C(41) ...Ru(1)	3.43
C(11) ...Ru(2)	2.98	C(13) ...Ru(2)	3.25
O(13) ...Ru(2)	3.97	O(22) ...Ru(2)	3.02
O(23) ...Ru(2)	2.90	C(31) ...Ru(2)	3.71
C(31) ...Ru(2)	3.44	O(31) ...Ru(2)	3.38
C(41) ...Ru(2)	2.90	O(41) ...Ru(2)	4.14
C(43) ...Ru(2)	3.22	O(43) ...Ru(2)	4.04
P(2) ...Ru(3)	4.52	C(13) ...Ru(3)	3.43

table 6 continued

C(21) ...Ru(3)	3.45	C(22) ...Ru(3)	3.46
C(23) ...Ru(3)	4.08	O(31) ...Ru(3)	3.65
O(32) ...Ru(3)	2.79	O(31) ...Ru(3)	3.03
C(43) ...Ru(3)	3.66	C(11) ...Ru(4)	3.48
C(12) ...Ru(4)	3.99	C(22) ...Ru(4)	3.40
C(23) ...Ru(4)	2.90	C(31) ...Ru(4)	3.91
C(32) ...Ru(4)	4.24	O(41) ...Ru(4)	3.06
O(42) ...Ru(4)	3.18	O(43) ...Ru(4)	3.33
P(2) ...P(1)	3.67	C(32) ...P(1)	3.66
O(42) ...P(1)	3.68	C(2) ...P(1)	2.94
C(15) ...P(1)	2.85	C(19) ...P(1)	3.10
C(25) ...P(1)	2.89	C(29) ...P(1)	3.02
C(12) ...P(2)	3.68	C(32) ...P(2)	3.60
C(1) ...P(2)	3.20	C(35) ...P(2)	2.90
C(39) ...P(2)	3.04	C(45) ...P(2)	2.80
C(49) ...P(2)	3.06	C(12) ...C(11)	3.28
C(13) ...C(11)	2.96	C(23) ...C(11)	2.17
O(23) ...C(11)	2.74	C(41) ...C(11)	2.86
O(41) ...C(11)	3.32	C(23) ...O(11)	3.25
O(23) ...O(11)	3.10	C(13) ...C(12)	2.91
C(35) ...C(12)	3.45	C(35) ...O(12)	3.03
C(21) ...C(13)	3.13	O(31) ...C(13)	3.26
C(21) ...O(13)	3.40	O(31) ...O(13)	3.39
C(22) ...C(21)	2.30	O(22) ...C(21)	3.34
C(23) ...C(21)	2.79	C(31) ...C(21)	3.01
O(31) ...C(21)	2.32	C(22) ...O(21)	2.63
C(23) ...O(21)	3.17	O(31) ...O(21)	3.00
C(23) ...C(22)	2.26	O(23) ...C(22)	3.16

table 6 continued

C(31) ...C(22)	3.32	C(41) ...C(22)	3.39
C(43) ...C(22)	2.78	O(43) ...C(22)	3.26
C(31) ...O(22)	3.00	O(31) ...O(22)	3.27
C(43) ...O(22)	3.19	O(43) ...O(22)	3.11
C(41) ...C(23)	2.09	O(41) ...C(23)	2.93
C(41) ...O(23)	2.95	O(41) ...O(23)	3.12
C(32) ...C(31)	3.29	C(31) ...C(31)	3.35
C(43) ...C(31)	2.94	O(43) ...C(31)	2.96
C(31) ...C(32)	3.31	C(31) ...O(32)	3.08
C(43) ...C(41)	2.79	C(29) ...O(42)	3.26
C(15) ...C(1)	3.24	C(14) ...C(1)	3.37
C(29) ...C(1)	3.22	C(24) ...C(1)	3.10
C(39) ...C(2)	3.26	C(34) ...C(2)	2.93
C(45) ...C(2)	3.23	C(44) ...C(2)	2.91
C(17) ...C(15)	2.42	C(18) ...C(15)	2.79
C(19) ...C(15)	2.42	C(18) ...C(16)	2.42
C(19) ...C(16)	2.79	C(14) ...C(16)	2.42
C(19) ...C(17)	2.42	C(14) ...C(17)	2.79
C(14) ...C(18)	2.42	C(24) ...C(14)	3.30
C(27) ...C(25)	2.42	C(28) ...C(25)	2.79
C(29) ...C(25)	2.42	C(28) ...C(26)	2.42
C(29) ...C(26)	2.79	C(24) ...C(26)	2.42
C(29) ...C(27)	2.42	C(24) ...C(27)	2.79
C(24) ...C(28)	2.42	C(37) ...C(35)	2.42
C(38) ...C(35)	2.79	C(39) ...C(35)	2.42
C(38) ...C(36)	2.42	C(39) ...C(36)	2.79
C(34) ...C(36)	2.42	C(39) ...C(37)	2.42
C(34) ...C(37)	2.79	C(34) ...C(38)	2.42

table 6 continued

C(49) ...C(39)	3.13	C(44) ...C(39)	3.16
C(49) ...C(34)	2.93	C(44) ...C(34)	2.70
C(47) ...C(45)	2.42	C(48) ...C(45)	2.79
C(49) ...C(45)	2.42	C(48) ...C(46)	2.42
C(49) ...C(46)	2.79	C(44) ...C(46)	2.42
C(49) ...C(47)	2.42	C(44) ...C(47)	2.79
C(44) ...C(48)	2.42		

Crystallographic Tables for $[Au_3Ru_4(\mu\text{-}H)(CO)_{12}\{\mu\text{-}Ph_2PCH_2PPh_2\}(PPh_3)]$, {X-ray study presented in section 2.4, Vol.1}.

TABLE 1 Fractional atomic coordinates and thermal parameters ($Å^2$) for $[Au_3Ru_4(\mu\text{-}H)(CO)_{12}\{(\mu\text{-}PPh_2CH_2PPh_2)\}(PPh_3)]$

Atom	x	y	z	U_{iso} or U_{eq}
Au(1)	0.09543(8)	0.16080(4)	0.21592(9)	0.0405(7)
Au(2)	-0.04171(8)	0.09767(5)	0.24657(8)	0.0437(8)
Au(3)	0.24423(8)	0.10603(5)	0.19473(8)	0.0433(8)
Ru(1)	0.12232(15)	0.04820(9)	0.26896(15)	0.0346(14)
Ru(2)	0.22691(16)	0.14212(9)	0.36643(15)	0.0361(14)
Ru(3)	0.07242(16)	0.10450(10)	0.41840(15)	0.0415(15)
Ru(4)	0.23504(17)	0.03997(9)	0.43950(16)	0.0414(15)
P(1)	-0.0051(5)	0.2141(3)	0.1239(5)	0.044(5)
P(2)	-0.1600(5)	0.1501(3)	0.1768(6)	0.049(5)
P(3)	0.3328(5)	0.1170(3)	0.0950(5)	0.042(5)
C(11)	0.0582(21)	-0.0098(12)	0.2968(20)	0.055(9)
O(11)	0.0170(16)	-0.0460(10)	0.3097(15)	0.087(8)
C(12)	0.2213(22)	0.0020(13)	0.2648(20)	0.060(9)
O(12)	0.2742(15)	-0.0269(9)	0.2523(14)	0.069(7)
C(13)	0.0646(22)	0.0424(13)	0.1485(22)	0.061(9)
O(13)	0.0408(16)	0.0342(9)	0.0720(16)	0.085(8)
C(21)	0.3440(25)	0.1534(13)	0.3463(22)	0.071(11)
O(21)	0.4165(16)	0.1617(9)	0.3433(14)	0.079(7)
C(22)	0.2574(22)	0.1594(13)	0.4827(23)	0.069(10)
O(22)	0.2874(18)	0.1725(10)	0.5560(17)	0.099(8)
C(23)	0.1905(20)	0.2140(12)	0.3380(19)	0.051(9)
O(23)	0.1813(16)	0.2608(10)	0.3371(16)	0.091(8)
C(31)	-0.0257(25)	0.0636(14)	0.4214(23)	0.078(11)
O(31)	-0.0945(19)	0.0405(11)	0.4293(17)	0.106(9)
C(32)	0.0942(21)	0.1223(12)	0.5366(21)	0.057(9)

table 1 continued

O(32)	0.1111(16)	0.1323(9)	0.6106(17)	0.088(8)
C(33)	0.0195(20)	0.1726(12)	0.3914(19)	0.052(8)
O(33)	-0.0128(14)	0.2151(8)	0.3804(13)	0.061(6)
C(41)	0.3552(22)	0.0399(12)	0.4203(20)	0.056(9)
O(41)	0.4252(15)	0.0372(9)	0.4100(14)	0.071(7)
C(42)	0.2227(21)	-0.0357(13)	0.4533(20)	0.056(9)
O(42)	0.2171(18)	-0.0823(11)	0.4515(17)	0.102(9)
C(43)	0.2770(23)	0.0463(13)	0.5588(23)	0.068(10)
O(43)	0.2997(17)	0.0515(10)	0.6349(18)	0.099(9)
C(1)	-0.1140(18)	0.2145(10)	0.1575(18)	0.044(8)
C(111)	-0.0264(14)	0.1954(8)	0.0100(10)	0.037(7)
C(112)	-0.0982(14)	0.2146(8)	-0.0533(10)	0.063(9)
C(113)	-0.1110(14)	0.1971(8)	-0.1400(10)	0.100(13)
C(114)	-0.0519(14)	0.1604(8)	-0.1635(10)	0.081(11)
C(115)	0.0200(14)	0.1411(8)	-0.1001(10)	0.084(11)
C(116)	0.0327(14)	0.1586(8)	-0.0134(10)	0.074(10)
C(121)	0.0168(14)	0.2860(7)	0.1201(17)	0.054(9)
C(122)	0.0072(14)	0.3169(7)	0.1919(17)	0.093(13)
C(123)	0.0230(14)	0.3722(7)	0.1927(17)	0.111(15)
C(124)	0.0483(14)	0.3966(7)	0.1217(17)	0.118(16)
C(125)	0.0578(14)	0.3657(7)	0.0498(17)	0.144(19)
C(126)	0.0421(14)	0.3104(7)	0.0490(17)	0.127(17)
C(211)	-0.2235(14)	0.1293(8)	0.0727(10)	0.053(8)
C(212)	-0.3060(14)	0.1523(8)	0.0360(10)	0.073(10)
C(213)	-0.3501(14)	0.1388(8)	-0.0492(10)	0.078(11)
C(214)	-0.3116(14)	0.1024(8)	-0.0978(10)	0.087(12)
C(215)	-0.2291(14)	0.0794(8)	-0.0611(10)	0.098(13)
C(216)	-0.1851(14)	0.0929(8)	0.0241(10)	0.053(9)

table 1 continued

C(221)	-0.2404(14)	0.1700(10)	0.2405(14)	0.064(9)
C(222)	-0.2745(14)	0.1282(10)	0.2827(14)	0.104(14)
C(223)	-0.3383(14)	0.1390(10)	0.3312(14)	0.126(16)
C(224)	-0.3679(14)	0.1916(10)	0.3376(14)	0.112(15)
C(225)	-0.3338(14)	0.2334(10)	0.2953(14)	0.092(13)
C(226)	-0.2700(14)	0.2227(10)	0.2468(14)	0.094(13)
C(311)	0.2822(12)	0.0994(7)	-0.0168(9)	0.040(7)
C(312)	0.2249(12)	0.0553(7)	-0.0341(9)	0.051(8)
C(313)	0.1870(12)	0.0408(7)	-0.1206(9)	0.066(10)
C(314)	0.2064(12)	0.0705(7)	-0.1898(9)	0.068(10)
C(315)	0.2636(12)	0.1146(7)	-0.1726(9)	0.066(10)
C(316)	0.3015(12)	0.1291(7)	-0.0861(9)	0.067(10)
C(321)	0.4335(11)	0.0782(7)	0.1207(14)	0.047(8)
C(322)	0.4890(11)	0.0723(7)	0.0619(14)	0.071(10)
C(323)	0.5648(11)	0.0400(7)	0.0839(14)	0.086(12)
C(324)	0.5851(11)	0.0136(7)	0.1647(14)	0.074(11)
C(325)	0.5296(11)	0.0195(7)	0.2235(14)	0.085(12)
C(326)	0.4539(11)	0.0518(7)	0.2015(14)	0.070(10)
C(331)	0.3672(17)	0.1861(7)	0.0926(14)	0.062(9)
C(332)	0.4554(17)	0.2037(7)	0.1098(14)	0.080(11)
C(333)	0.4743(17)	0.2585(7)	0.1073(14)	0.090(12)
C(334)	0.4050(17)	0.2958(7)	0.0875(14)	0.086(12)
C(335)	0.3169(17)	0.2783(7)	0.0703(14)	0.121(16)
C(336)	0.2980(17)	0.2234(7)	0.0729(14)	0.112(15)
H	0.12125	0.03841	0.45880	0.0800

TABLE 2 Fractional atomic coordinates for the hydrogen atoms for $[Au_3Ru_4(\mu\text{-}H)(CO)_{12}\{(\mu\text{-}PPh_2CH_2PPh_2)\}(PPh_3)]$

Atom	x	y	z
H(1)	-0.1053	0.2384	0.2165
H(2)	-0.1611	0.2340	0.1052
H(112)	-0.1440	0.2431	-0.0352
H(113)	-0.1666	0.2121	-0.1891
H(114)	-0.0617	0.1468	-0.2306
H(115)	0.0657	0.1126	-0.1182
H(116)	0.0883	0.1437	0.0356
H(122)	-0.0124	0.2980	0.2469
H(123)	0.0156	0.3962	0.2483
H(124)	0.0605	0.4395	0.1223
H(125)	0.0774	0.3846	-0.0052
H(126)	0.0494	0.2865	-0.0066
H(212)	-0.3358	0.1804	0.0736
H(213)	-0.4140	0.1566	-0.0777
H(214)	-0.3457	0.0920	-0.1638
H(215)	-0.1994	0.0512	-0.0988
H(216)	-0.1212	0.0751	0.0525
H(222)	-0.2515	0.0875	0.2778
H(223)	-0.3647	0.1066	0.3639
H(224)	-0.4173	0.1999	0.3751
H(225)	-0.3568	0.2742	0.3002
H(226)	-0.2436	0.2550	0.2141
H(312)	0.2100	0.0323	0.0195
H(313)	0.1427	0.0066	-0.1339
H(314)	0.1770	0.0593	-0.2567

table 2 continued

H(315)	0.2786	0.1376	-0.2262
H(316)	0.3458	0.1632	-0.0727
H(322)	0.4733	0.0927	-0.0007
H(323)	0.6077	0.0354	0.0384
H(324)	0.6437	-0.0114	0.1817
H(325)	0.5454	-0.0009	0.2860
H(326)	0.4110	0.0564	0.2470
H(332)	0.5090	0.1748	0.1251
H(333)	0.5426	0.2721	0.1206
H(334)	0.4197	0.3383	0.0856
H(335)	0.2632	0.3071	0.0550
H(336)	0.2297	0.2099	0.0595

Table 3 Anisotropic thermal parameters for $[Au_3Ru_4(\mu\text{-}H)(CO)_{12}\{\mu\text{-}Ph_2PCH_2PPh_2\}(PPh_3)]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Au(1)	0.034(1)	0.033(1)	0.054(1)	0.010(1)	-0.001(1)	0.003(1)
Au(2)	0.035(1)	0.040(1)	0.056(1)	0.010(1)	-0.006(1)	-0.005(1)
Au(3)	0.038(1)	0.046(1)	0.045(1)	0.004(1)	0.006(1)	0.006(1)
Ru(1)	0.034(1)	0.027(1)	0.043(1)	-0.001(1)	-0.003(1)	-0.003(1)
Ru(2)	0.035(1)	0.032(1)	0.040(1)	-0.004(1)	-0.003(1)	-0.004(1)
Ru(3)	0.040(1)	0.044(1)	0.040(1)	0.005(1)	0.008(1)	0.004(1)
Ru(4)	0.044(2)	0.037(1)	0.044(1)	0.007(1)	-0.001(1)	0.005(1)
P(1)	0.040(5)	0.037(5)	0.055(5)	0.008(4)	0.002(4)	0.004(4)
P(2)	0.041(5)	0.044(5)	0.060(6)	0.003(4)	-0.004(5)	-0.004(4)
P(3)	0.043(5)	0.039(5)	0.044(5)	0.001(4)	0.006(4)	0.006(4)

TABLE 4 Bond lengths (A°) for $[Au_3Ru_4(\mu\text{-}H)(CO)_{12}\{(\mu\text{-}PPh_2CH_2PPh_2)\}(PPh_3)]$

Au(1) -Au(2)	2.758(2)	Au(1) -Au(3)	2.749(2)
Au(1) -Ru(1)	2.920(2)	Au(1) -Ru(2)	2.781(2)
Au(1) -P(1)	2.287(8)	Au(1) -C(23)	2.51(3)
Au(2) -Ru(1)	2.762(2)	Au(2) -Ru(3)	2.869(2)
Au(2) -P(2)	2.306(8)	Au(2) -C(13)	2.64(4)
Au(2) -C(31)	2.82(4)	Au(3) -Ru(1)	2.812(2)
Au(3) -Ru(2)	2.898(2)	Au(3) -P(3)	2.306(9)
Au(3) -C(21)	2.78(3)	Ru(1) -Ru(2)	3.044(3)
Ru(1) -Ru(3)	2.967(3)	Ru(1) -Ru(4)	2.847(3)
Ru(1) -C(11)	1.85(3)	Ru(1) -C(12)	1.92(3)
Ru(1) -C(13)	1.90(3)	Ru(2) -Ru(3)	2.840(3)
Ru(2) -Ru(4)	2.773(3)	Ru(2) -C(21)	1.92(4)
Ru(2) -C(22)	1.83(3)	Ru(2) -C(23)	1.89(3)
Ru(3) -Ru(4)	2.931(3)	Ru(3) -C(31)	1.83(4)
Ru(3) -C(32)	1.86(3)	Ru(3) -C(33)	1.88(3)
Ru(3) -H	1.857(2)	Ru(4) -C(41)	1.94(3)
Ru(4) -C(42)	1.91(3)	Ru(4) -C(43)	1.84(3)
Ru(4) -H	1.845(3)	P(1) -C(1)	1.87(3)
P(1) -C(111)	1.798(18)	P(1) -C(121)	1.820(20)
P(2) -C(1)	1.80(3)	P(2) -C(211)	1.779(18)
P(2) -C(221)	1.82(3)	P(3) -C(311)	1.802(16)
P(3) -C(321)	1.796(19)	P(3) -C(331)	1.799(20)
C(11) -O(11)	1.14(4)	C(12) -O(12)	1.14(4)
C(13) -O(13)	1.19(4)	C(21) -O(21)	1.15(5)
C(22) -O(22)	1.18(4)	C(23) -O(23)	1.17(4)

table 4 continued

C(31) -O(31)	1.24(5)	C(32) -O(32)	1.15(4)
C(33) -O(33)	1.16(4)	C(41) -O(41)	1.13(4)
C(42) -O(42)	1.16(4)	C(43) -O(43)	1.17(4)
C(111)-C(112)	1.395(24)	C(111)-C(116)	1.39(3)
C(112)-C(113)	1.395(22)	C(113)-C(114)	1.39(3)
C(114)-C(115)	1.395(24)	C(115)-C(116)	1.395(22)
C(121)-C(122)	1.39(3)	C(121)-C(126)	1.39(4)
C(122)-C(123)	1.395(25)	C(123)-C(124)	1.39(4)
C(124)-C(125)	1.39(3)	C(125)-C(126)	1.395(25)
C(211)-C(212)	1.39(3)	C(211)-C(216)	1.39(3)
C(212)-C(213)	1.395(22)	C(213)-C(214)	1.39(3)
C(214)-C(215)	1.39(3)	C(215)-C(216)	1.395(22)
C(221)-C(222)	1.39(4)	C(221)-C(226)	1.39(4)
C(222)-C(223)	1.39(3)	C(223)-C(224)	1.39(4)
C(224)-C(225)	1.39(4)	C(225)-C(226)	1.39(3)
C(311)-C(312)	1.39(3)	C(311)-C(316)	1.395(24)
C(312)-C(313)	1.395(20)	C(313)-C(314)	1.395(24)
C(314)-C(315)	1.39(3)	C(315)-C(316)	1.395(20)
C(321)-C(322)	1.39(3)	C(321)-C(326)	1.39(3)
C(322)-C(323)	1.395(24)	C(323)-C(324)	1.39(3)
C(324)-C(325)	1.39(3)	C(325)-C(326)	1.395(24)
C(331)-C(332)	1.39(3)	C(331)-C(336)	1.39(3)
C(332)-C(333)	1.39(3)	C(333)-C(334)	1.39(3)
C(334)-C(335)	1.39(3)	C(335)-C(336)	1.39(3)

TABLE 5 Bond angles (°) for $[Au_3Ru_4(\mu\text{-}H)(CO)_{12}\{(\mu\text{-}PPh_2CH_2PPh_2)\}(PPh_3)]$

Au(3) -Au(1) -Au(2)	115.6(1)	Ru(1) -Au(1) -Au(2)	58.1(1)
Ru(1) -Au(1) -Au(3)	59.4(1)	Ru(2) -Au(1) -Au(2)	101.6(1)
Ru(2) -Au(1) -Au(3)	63.2(1)	Ru(2) -Au(1) -Ru(1)	64.5(1)
P(1) -Au(1) -Au(2)	90.0(2)	P(1) -Au(1) -Au(3)	132.6(2)
P(1) -Au(1) -Ru(1)	140.0(2)	P(1) -Au(1) -Ru(2)	153.2(2)
C(23) -Au(1) -Au(2)	120.5(8)	C(23) -Au(1) -Au(3)	89.5(7)
C(23) -Au(1) -Ru(1)	105.5(7)	C(23) -Au(1) -Ru(2)	41.6(7)
C(23) -Au(1) -P(1)	111.9(7)	Ru(1) -Au(2) -Au(1)	63.9(1)
Ru(3) -Au(2) -Au(1)	78.2(1)	Ru(3) -Au(2) -Ru(1)	63.6(1)
P(2) -Au(2) -Au(1)	98.8(2)	P(2) -Au(2) -Ru(1)	156.3(2)
P(2) -Au(2) -Ru(3)	131.6(2)	C(13) -Au(2) -Au(1)	67.9(7)
C(13) -Au(2) -Ru(1)	39.7(6)	C(13) -Au(2) -Ru(3)	103.1(6)
C(13) -Au(2) -P(2)	120.6(7)	C(31) -Au(2) -Au(1)	115.7(7)
C(31) -Au(2) -Ru(1)	82.2(8)	C(31) -Au(2) -Ru(3)	37.6(7)
C(31) -Au(2) -P(2)	121.1(8)	C(31) -Au(2) -C(13)	116(1)
Ru(1) -Au(3) -Au(1)	63.3(1)	Ru(2) -Au(3) -Au(1)	58.9(1)
Ru(2) -Au(3) -Ru(1)	64.4(1)	P(3) -Au(3) -Au(1)	131.1(2)
P(3) -Au(3) -Ru(1)	152.9(2)	P(3) -Au(3) -Ru(2)	141.3(2)
C(21) -Au(3) -Au(1)	90.3(8)	C(21) -Au(3) -Ru(1)	99.1(8)
C(21) -Au(3) -Ru(2)	39.5(8)	C(21) -Au(3) -P(3)	103.2(8)
Au(2) -Ru(1) -Au(1)	58.0(1)	Au(3) -Ru(1) -Au(1)	57.3(1)
Au(3) -Ru(1) -Au(2)	113.4(1)	Ru(2) -Ru(1) -Au(1)	55.5(1)
Ru(2) -Ru(1) -Au(2)	95.2(1)	Ru(2) -Ru(1) -Au(3)	59.2(1)
Ru(3) -Ru(1) -Au(1)	74.2(1)	Ru(3) -Ru(1) -Au(2)	60.0(1)
Ru(3) -Ru(1) -Au(3)	113.5(1)	Ru(3) -Ru(1) -Ru(2)	56.4(1)

table 5 continued

Ru(4) -Ru(1) -Au(1)	110.7(1)	Ru(4) -Ru(1) -Au(2)	120.1(1)
Ru(4) -Ru(1) -Au(3)	95.7(1)	Ru(4) -Ru(1) -Ru(2)	56.1(1)
Ru(4) -Ru(1) -Ru(3)	60.5(1)	C(11) -Ru(1) -Au(1)	140(1)
C(11) -Ru(1) -Au(2)	82(1)	C(11) -Ru(1) -Au(3)	159(1)
C(11) -Ru(1) -Ru(2)	137(1)	C(11) -Ru(1) -Ru(3)	86(1)
C(11) -Ru(1) -Ru(4)	88.3(9)	C(12) -Ru(1) -Au(1)	129(1)
C(12) -Ru(1) -Au(2)	166.5(9)	C(12) -Ru(1) -Au(3)	71(1)
C(12) -Ru(1) -Ru(2)	98.0(9)	C(12) -Ru(1) -Ru(3)	130.9(9)
C(12) -Ru(1) -Ru(4)	70.4(9)	C(12) -Ru(1) -C(11)	91(1)
C(13) -Ru(1) -Au(1)	78(1)	C(13) -Ru(1) -Au(2)	72(1)
C(13) -Ru(1) -Au(3)	81(1)	C(13) -Ru(1) -Ru(2)	129(1)
C(13) -Ru(1) -Ru(3)	132(1)	C(13) -Ru(1) -Ru(4)	167(1)
C(13) -Ru(1) -C(11)	91(1)	C(13) -Ru(1) -C(12)	97(1)
Au(3) -Ru(2) -Au(1)	57.9(1)	Ru(1) -Ru(2) -Au(1)	60.0(1)
Ru(1) -Ru(2) -Au(3)	56.4(1)	Ru(3) -Ru(2) -Au(1)	78.3(1)
Ru(3) -Ru(2) -Au(3)	114.8(1)	Ru(3) -Ru(2) -Ru(1)	60.4(1)
Ru(4) -Ru(2) -Au(1)	117.3(1)	Ru(4) -Ru(2) -Au(3)	95.4(1)
Ru(4) -Ru(2) -Ru(1)	58.4(1)	Ru(4) -Ru(2) -Ru(3)	62.9(1)
C(21) -Ru(2) -Au(1)	112(1)	C(21) -Ru(2) -Au(3)	67(1)
C(21) -Ru(2) -Ru(1)	116(1)	C(21) -Ru(2) -Ru(3)	167(1)
C(21) -Ru(2) -Ru(4)	104(1)	C(22) -Ru(2) -Au(1)	141(1)
C(22) -Ru(2) -Au(3)	160(1)	C(22) -Ru(2) -Ru(1)	132(1)
C(22) -Ru(2) -Ru(3)	81(1)	C(22) -Ru(2) -Ru(4)	80(1)
C(22) -Ru(2) -C(21)	95(1)	C(23) -Ru(2) -Au(1)	61.5(8)
C(23) -Ru(2) -Au(3)	99.1(9)	C(23) -Ru(2) -Ru(1)	120.6(8)
C(23) -Ru(2) -Ru(3)	99(1)	C(23) -Ru(2) -Ru(4)	160(1)
C(23) -Ru(2) -C(21)	94(1)	C(23) -Ru(2) -C(22)	90(1)
Ru(1) -Ru(3) -Au(2)	56.5(1)	Ru(2) -Ru(3) -Au(2)	97.5(1)

table 5 continued

Ru(2) -Ru(3) -Ru(1)	63.2(1)	Ru(4) -Ru(3) -Au(2)	113.8(1)
Ru(4) -Ru(3) -Ru(1)	57.7(1)	Ru(4) -Ru(3) -Ru(2)	57.4(1)
C(31) -Ru(3) -Au(2)	70(1)	C(31) -Ru(3) -Ru(1)	97(1)
C(31) -Ru(3) -Ru(2)	160(1)	C(31) -Ru(3) -Ru(4)	113(1)
C(32) -Ru(3) -Au(2)	152(1)	C(32) -Ru(3) -Ru(1)	151(1)
C(32) -Ru(3) -Ru(2)	103(1)	C(32) -Ru(3) -Ru(4)	93(1)
C(32) -Ru(3) -C(31)	94(1)	C(33) -Ru(3) -Au(2)	72.5(8)
C(33) -Ru(3) -Ru(1)	115.0(9)	C(33) -Ru(3) -Ru(2)	89(1)
C(33) -Ru(3) -Ru(4)	146(1)	C(33) -Ru(3) -C(31)	101(1)
C(33) -Ru(3) -C(32)	89(1)	H -Ru(3) -Au(2)	112.6(1)
H -Ru(3) -Ru(1)	72.2(1)	H -Ru(3) -Ru(2)	94.9(1)
H -Ru(3) -Ru(4)	37.5(1)	H -Ru(3) -C(31)	77(1)
H -Ru(3) -C(32)	84.4(9)	H -Ru(3) -C(33)	173(1)
Ru(2) -Ru(4) -Ru(1)	65.6(1)	Ru(3) -Ru(4) -Ru(1)	61.8(1)
Ru(3) -Ru(4) -Ru(2)	59.6(1)	C(41) -Ru(4) -Ru(1)	105.0(9)
C(41) -Ru(4) -Ru(2)	83.9(9)	C(41) -Ru(4) -Ru(3)	143.6(9)
C(42) -Ru(4) -Ru(1)	97.0(8)	C(42) -Ru(4) -Ru(2)	162.2(9)
C(42) -Ru(4) -Ru(3)	117(1)	C(42) -Ru(4) -C(41)	98(1)
C(43) -Ru(4) -Ru(1)	161(1)	C(43) -Ru(4) -Ru(2)	108(1)
C(43) -Ru(4) -Ru(3)	100(1)	C(43) -Ru(4) -C(41)	91(1)
C(43) -Ru(4) -C(42)	89(1)	H -Ru(4) -Ru(1)	75.6(1)
H -Ru(4) -Ru(2)	97.4(1)	H -Ru(4) -Ru(3)	37.8(1)
H -Ru(4) -C(41)	178.6(9)	H -Ru(4) -C(42)	81(1)
H -Ru(4) -C(43)	88(1)	C(1) -P(1) -Au(1)	110.5(9)
C(111)-P(1) -Au(1)	114.9(7)	C(111)-P(1) -C(1)	108(1)
C(121)-P(1) -Au(1)	118.9(7)	C(121)-P(1) -C(1)	101(1)
C(121)-P(1) -C(111)	102(1)	C(1) -P(2) -Au(2)	106.3(9)
C(211)-P(2) -Au(2)	119.0(8)	C(211)-P(2) -C(1)	105(1)

table 5 continued

C(221)-P(2) -Au(2)	117.2(8)	C(221)-P(2) -C(1)	101(1)
C(221)-P(2) -C(211)	106(1)	C(311)-P(3) -Au(3)	115.7(7)
C(321)-P(3) -Au(3)	113.4(8)	C(321)-P(3) -C(311)	105(1)
C(331)-P(3) -Au(3)	110.4(9)	C(331)-P(3) -C(311)	106(1)
C(331)-P(3) -C(321)	106(1)	O(11) -C(11) -Ru(1)	177(3)
O(12) -C(12) -Ru(1)	172(3)	Ru(1) -C(13) -Au(2)	68(1)
O(13) -C(13) -Au(2)	123(2)	O(13) -C(13) -Ru(1)	169(3)
Ru(2) -C(21) -Au(3)	73(1)	O(21) -C(21) -Au(3)	114(2)
O(21) -C(21) -Ru(2)	173(3)	O(22) -C(22) -Ru(2)	171(3)
Ru(2) -C(23) -Au(1)	77(1)	O(23) -C(23) -Au(1)	118(2)
O(23) -C(23) -Ru(2)	165(2)	Ru(3) -C(31) -Au(2)	73(1)
O(31) -C(31) -Au(2)	110(2)	O(31) -C(31) -Ru(3)	173(3)
O(32) -C(32) -Ru(3)	177(3)	O(33) -C(33) -Ru(3)	176(3)
O(41) -C(41) -Ru(4)	177(3)	O(42) -C(42) -Ru(4)	172(3)
O(43) -C(43) -Ru(4)	177(3)	P(2) -C(1) -P(1)	117(1)
C(112)-C(111)-P(1)	124(1)	C(116)-C(111)-P(1)	116(1)
C(116)-C(111)-C(112)	120(1)	C(113)-C(112)-C(111)	120(2)
C(114)-C(113)-C(112)	120(2)	C(115)-C(114)-C(113)	120(1)
C(116)-C(115)-C(114)	120(2)	C(115)-C(116)-C(111)	120(2)
C(122)-C(121)-P(1)	117(2)	C(126)-C(121)-P(1)	123(2)
C(126)-C(121)-C(122)	120(2)	C(123)-C(122)-C(121)	120(2)
C(124)-C(123)-C(122)	120(2)	C(125)-C(124)-C(123)	120(2)
C(126)-C(125)-C(124)	120(2)	C(125)-C(126)-C(121)	120(2)
C(212)-C(211)-P(2)	122(1)	C(216)-C(211)-P(2)	118(1)
C(216)-C(211)-C(212)	120(1)	C(213)-C(212)-C(211)	120(2)
C(214)-C(213)-C(212)	120(2)	C(215)-C(214)-C(213)	120(1)
C(216)-C(215)-C(214)	120(2)	C(215)-C(216)-C(211)	120(2)
C(222)-C(221)-P(2)	115(2)	C(226)-C(221)-P(2)	125(2)

table 5 continued

C(226)-C(221)-C(222)	120(2)	C(223)-C(222)-C(221)	120(2)
C(224)-C(223)-C(222)	120(2)	C(225)-C(224)-C(223)	120(2)
C(226)-C(225)-C(224)	120(2)	C(225)-C(226)-C(221)	120(2)
C(312)-C(311)-P(3)	120(1)	C(316)-C(311)-P(3)	120(1)
C(316)-C(311)-C(312)	120(1)	C(313)-C(312)-C(311)	120(2)
C(314)-C(313)-C(312)	120(2)	C(315)-C(314)-C(313)	120(1)
C(316)-C(315)-C(314)	120(2)	C(315)-C(316)-C(311)	120(2)
C(322)-C(321)-P(3)	122(1)	C(326)-C(321)-P(3)	118(2)
C(326)-C(321)-C(322)	120(2)	C(323)-C(322)-C(321)	120(2)
C(324)-C(323)-C(322)	120(2)	C(325)-C(324)-C(323)	120(2)
C(326)-C(325)-C(324)	120(2)	C(325)-C(326)-C(321)	120(2)
C(332)-C(331)-P(3)	125(2)	C(336)-C(331)-P(3)	115(2)
C(336)-C(331)-C(332)	120(2)	C(333)-C(332)-C(331)	120(2)
C(334)-C(333)-C(332)	120(2)	C(335)-C(334)-C(333)	120(2)
C(336)-C(335)-C(334)	120(2)	C(335)-C(336)-C(331)	120(2)
Ru(4) -H -Ru(3)	104.7(1)		

TABLE 6 Intermolecular distances (Å) for

$[Au_3Ru_4(\mu\text{-}H)(CO)_{12}\{(\mu\text{-}PPh_2CH_2PPh_2)\}(PPh_3)]$

atom1	atom2	dist	S	a	b	c
C(313)	Au(2)	4.33	-1	0.0	0.0	0.0
H(313)	Au(2)	3.32	-1	0.0	0.0	0.0
H(112)	Ru(2)	3.62	-2	0.0	1.0	0.0
O(31)	Ru(4)	3.86	-1	0.0	0.0	1.0
O(32)	O(11)	3.34	-1	0.0	0.0	1.0
H(114)	O(11)	2.94	-1	0.0	0.0	0.0
H(314)	O(11)	2.94	-1	0.0	0.0	0.0
H(215)	C(12)	2.87	-1	0.0	0.0	0.0
C(214)	O(12)	3.21	-1	0.0	0.0	0.0
C(215)	O(12)	3.19	-1	0.0	0.0	0.0
H(214)	O(12)	2.53	-1	0.0	0.0	0.0
H(215)	O(12)	2.49	-1	0.0	0.0	0.0
H(124)	O(12)	2.97	2	0.0	0.0	0.0
O(13)	O(13)	2.88	-1	0.0	0.0	0.0
H(224)	O(21)	2.67	1	-1.0	0.0	0.0
H(112)	C(22)	2.91	-2	0.0	1.0	0.0
C(1)	O(22)	3.41	-2	0.0	1.0	0.0
H(2)	O(22)	2.52	-2	0.0	1.0	0.0
H(112)	O(22)	2.87	-2	0.0	1.0	0.0
H(112)	C(23)	3.05	-2	0.0	1.0	0.0
H(113)	C(23)	2.97	-2	0.0	1.0	0.0
C(113)	O(23)	3.31	-2	0.0	1.0	0.0
H(112)	O(23)	2.97	-2	0.0	1.0	0.0
H(113)	O(23)	2.56	-2	0.0	1.0	0.0
C(213)	O(23)	3.16	-2	0.0	1.0	0.0

table 6 continued

C(42) ...O(31)	2.98	-1	0.0	0.0	1.0
O(42) ...O(31)	3.11	-1	0.0	0.0	1.0
H ...O(31)	2.72	-1	0.0	0.0	1.0
H(314)...O(32)	2.77	1	0.0	0.0	-1.0
H(333)...O(32)	2.62	-2	1.0	1.0	0.0
H(334)...O(32)	2.98	-2	1.0	1.0	0.0
H(124)...C(41)	2.95	2	0.0	0.0	0.0
H(124)...O(41)	2.50	2	0.0	0.0	0.0
H(334)...O(42)	2.85	2	0.0	0.0	0.0
H(335)...O(42)	2.77	2	0.0	0.0	0.0
C(314)...O(43)	3.40	1	0.0	0.0	-1.0
H(314)...O(43)	2.81	1	0.0	0.0	-1.0
H(324)...O(43)	2.98	-1	1.0	0.0	1.0
H(325)...O(43)	2.74	-1	1.0	0.0	1.0
H(214)...C(123)	2.81	-2	0.0	1.0	0.0
H(224)...C(126)	2.93	-2	0.0	1.0	1.0
C(224)...H(126)	3.04	-2	0.0	1.0	1.0
H(323)...C(213)	3.05	1	1.0	0.0	0.0
H(312)...C(215)	2.85	-1	0.0	0.0	0.0
H(313)...C(216)	3.00	-1	0.0	0.0	0.0
H(324)...C(313)	3.06	-1	1.0	0.0	0.0
H(324)...C(314)	2.72	-1	1.0	0.0	0.0
H(324)...C(315)	2.95	-1	1.0	0.0	0.0

Symmetry Transformations:

The second atom is related to the first atom, at (x,y,z), by the symmetry operation S with (a,b,c) added to the (x',y',z') of S.

Where S =

1	x, y, z
2	0.5-x, 0.5+y, 0.5-z

TABLE 7 Intramolecular distances (Å) for

$[Au_3Ru_4(u\text{-}H)(CO)_{12}\{(u\text{-}PPh_2CH_2PPh_2)\}(PPh_3)]$

Ru(3) ...Au(1)	3.55	Ru(4) ...Au(1)	4.74
P(2) ...Au(1)	3.86	P(3) ...Au(1)	4.61
C(13) ...Au(1)	3.12	O(13) ...Au(1)	3.85
C(21) ...Au(1)	3.92	O(23) ...Au(1)	3.22
C(33) ...Au(1)	3.23	O(33) ...Au(1)	3.62
C(1) ...Au(1)	3.42	H(1) ...Au(1)	3.65
C(111)...Au(1)	3.45	C(116)...Au(1)	3.50
H(116)...Au(1)	2.83	C(121)...Au(1)	3.55
C(122)...Au(1)	4.10	H(122)...Au(1)	3.87
H(336)...Au(1)	3.74	Au(3) ...Au(2)	4.66
Ru(2) ...Au(2)	4.29	Ru(4) ...Au(2)	4.86
P(1) ...Au(2)	3.58	C(11) ...Au(2)	3.10
O(11) ...Au(2)	3.76	O(13) ...Au(2)	3.62
O(31) ...Au(2)	3.45	C(33) ...Au(2)	2.92
O(33) ...Au(2)	3.56	C(1) ...Au(2)	3.30
H(1) ...Au(2)	3.63	C(211)...Au(2)	3.53
C(216)...Au(2)	3.68	H(216)...Au(2)	3.06
C(221)...Au(2)	3.53	C(222)...Au(2)	3.83
H(222)...Au(2)	3.38	Ru(3) ...Au(3)	4.83
Ru(4) ...Au(3)	4.19	P(1) ...Au(3)	4.62
C(12) ...Au(3)	2.86	O(12) ...Au(3)	3.43
C(13) ...Au(3)	3.13	O(13) ...Au(3)	3.74
O(21) ...Au(3)	3.41	C(23) ...Au(3)	3.70
C(41) ...Au(3)	3.92	O(41) ...Au(3)	4.22
C(116)...Au(3)	4.26	H(116)...Au(3)	3.19

table 7 continued

C(311)...Au(3)	3.49	C(312)...Au(3)	3.74
H(312)...Au(3)	3.24	C(321)...Au(3)	3.44
C(326)...Au(3)	3.48	H(326)...Au(3)	2.80
C(331)...Au(3)	3.38	C(336)...Au(3)	3.68
H(336)...Au(3)	3.31	O(11) ...Ru(1)	2.99
O(12) ...Ru(1)	3.05	O(13) ...Ru(1)	3.08
C(31) ...Ru(1)	3.67	C(33) ...Ru(1)	4.13
C(41) ...Ru(1)	3.84	C(42) ...Ru(1)	3.61
H ...Ru(1)	2.98	C(12) ...Ru(2)	3.82
O(21) ...Ru(2)	3.06	O(22) ...Ru(2)	3.00
O(23) ...Ru(2)	3.04	C(32) ...Ru(2)	3.73
C(33) ...Ru(2)	3.39	C(41) ...Ru(2)	3.21
O(41) ...Ru(2)	3.96	C(43) ...Ru(2)	3.78
H ...Ru(2)	3.52	C(11) ...Ru(3)	3.40
C(22) ...Ru(3)	3.12	O(22) ...Ru(3)	3.91
C(23) ...Ru(3)	3.65	O(31) ...Ru(3)	3.06
O(32) ...Ru(3)	3.01	O(33) ...Ru(3)	3.05
C(43) ...Ru(3)	3.71	C(11) ...Ru(4)	3.35
C(12) ...Ru(4)	2.85	O(12) ...Ru(4)	3.53
C(21) ...Ru(4)	3.74	C(22) ...Ru(4)	3.04
O(22) ...Ru(4)	3.76	C(31) ...Ru(4)	4.01
C(32) ...Ru(4)	3.56	O(41) ...Ru(4)	3.07
O(42) ...Ru(4)	3.06	O(43) ...Ru(4)	3.01
P(2) ...P(1)	3.13	H(1) ...P(1)	2.42
H(2) ...P(1)	2.41	C(112)...P(1)	2.82
C(116)...P(1)	2.72	H(112)...P(1)	2.98
H(116)...P(1)	2.82	C(122)...P(1)	2.76
C(126)...P(1)	2.83	H(122)...P(1)	2.85

table 7 continued

H(126)...P(1)	2.98	H(1) ...P(2)	2.38
H(2) ...P(2)	2.36	C(212)...P(2)	2.78
C(216)...P(2)	2.73	H(212)...P(2)	2.93
H(216)...P(2)	2.85	C(222)...P(2)	2.73
C(226)...P(2)	2.85	H(222)...P(2)	2.81
H(226)...P(2)	3.02	C(312)...P(3)	2.77
C(316)...P(3)	2.78	H(312)...P(3)	2.90
H(316)...P(3)	2.91	C(322)...P(3)	2.80
C(326)...P(3)	2.74	H(322)...P(3)	2.95
H(326)...P(3)	2.84	C(332)...P(3)	2.84
C(336)...P(3)	2.70	H(332)...P(3)	3.02
H(336)...P(3)	2.78	C(12) ...C(11)	2.68
C(13) ...C(11)	2.68	C(31) ...C(11)	3.15
C(42) ...C(11)	3.17	H ...C(11)	2.77
C(31) ...O(11)	3.38	C(13) ...C(12)	2.86
C(41) ...C(12)	2.97	C(42) ...C(12)	3.09
C(41) ...O(12)	3.12	C(42) ...O(12)	3.41
H(326)...O(12)	2.97	H(216)...C(13)	3.03
C(116)...O(13)	3.36	H(116)...O(13)	2.90
H(216)...O(13)	2.65	H(312)...O(13)	2.90
C(22) ...C(21)	2.76	C(23) ...C(21)	2.78
C(41) ...C(21)	3.04	O(41) ...C(21)	3.21
O(41) ...O(21)	3.26	C(23) ...C(22)	2.64
C(32) ...C(22)	2.97	O(32) ...C(22)	3.40
C(43) ...C(22)	3.04	C(32) ...O(22)	3.18
O(32) ...O(22)	3.18	C(43) ...O(22)	3.14
O(43) ...O(22)	3.24	C(33) ...C(23)	3.11
O(33) ...C(23)	3.35	C(122)...O(23)	3.40

table 7 continued

C(32) ...C(31)	2.70	C(33) ...C(31)	2.86
H ...C(31)	2.30	C(33) ...C(32)	2.62
C(43) ...C(32)	3.35	H ...C(32)	2.49
H(1) ...O(33)	2.70	H(122)...O(33)	2.93
C(42) ...C(41)	2.90	C(43) ...C(41)	2.71
H(326)...C(41)	3.05	C(326)...O(41)	3.40
H(326)...O(41)	2.55	C(43) ...C(42)	2.63
H ...C(42)	2.43	H ...C(43)	2.56
C(111)...C(1)	2.96	C(112)...C(1)	3.36
H(112)...C(1)	3.03	C(121)...C(1)	2.84
C(122)...C(1)	3.13	H(122)...C(1)	2.78
C(211)...C(1)	2.84	C(221)...C(1)	2.80
C(226)...C(1)	3.04	H(226)...C(1)	2.56
C(121)...H(1)	2.91	C(122)...H(1)	2.69
C(221)...H(1)	2.78	C(226)...H(1)	2.71
C(111)...H(2)	2.97	C(112)...H(2)	2.89
C(121)...H(2)	2.99	C(211)...H(2)	2.78
C(212)...H(2)	3.03	C(226)...H(2)	3.07
C(113)...C(111)	2.42	C(114)...C(111)	2.79
C(115)...C(111)	2.42	H(112)...C(111)	2.15
H(116)...C(111)	2.15	C(121)...C(111)	2.82
C(126)...C(111)	3.06	H(126)...C(111)	2.59
C(114)...C(112)	2.42	C(115)...C(112)	2.79
C(116)...C(112)	2.42	H(113)...C(112)	2.15
C(121)...C(112)	3.39	C(126)...C(112)	3.37
H(126)...C(112)	2.86	C(115)...C(113)	2.42
C(116)...C(113)	2.79	H(112)...C(113)	2.15
H(114)...C(113)	2.15	C(116)...C(114)	2.42

table 7 continued

H(113)...C(114)	2.15	H(115)...C(114)	2.15
H(114)...C(115)	2.15	H(116)...C(115)	2.15
H(115)...C(116)	2.15	C(312)...H(115)	2.89
C(313)...H(115)	2.59	C(314)...H(115)	2.85
C(123)...C(121)	2.42	C(124)...C(121)	2.79
C(125)...C(121)	2.42	H(122)...C(121)	2.15
H(126)...C(121)	2.15	C(124)...C(122)	2.42
C(125)...C(122)	2.79	C(126)...C(122)	2.42
H(123)...C(122)	2.15	C(125)...C(123)	2.42
C(126)...C(123)	2.79	H(122)...C(123)	2.15
H(124)...C(123)	2.15	C(126)...C(124)	2.42
H(123)...C(124)	2.15	H(125)...C(124)	2.15
H(124)...C(125)	2.15	H(126)...C(125)	2.15
H(125)...C(126)	2.15	C(213)...C(211)	2.42
C(214)...C(211)	2.79	C(215)...C(211)	2.42
H(212)...C(211)	2.15	H(216)...C(211)	2.15
C(221)...C(211)	2.88	C(214)...C(212)	2.42
C(215)...C(212)	2.79	C(216)...C(212)	2.42
H(213)...C(212)	2.15	C(221)...C(212)	3.16
C(215)...C(213)	2.42	C(216)...C(213)	2.79
H(212)...C(213)	2.15	H(214)...C(213)	2.15
C(216)...C(214)	2.42	H(213)...C(214)	2.15
H(215)...C(214)	2.15	H(214)...C(215)	2.15
H(216)...C(215)	2.15	H(215)...C(216)	2.15
C(221)...H(212)	2.71	C(226)...H(212)	2.87
C(223)...C(221)	2.42	C(224)...C(221)	2.79
C(225)...C(221)	2.42	H(222)...C(221)	2.15
H(226)...C(221)	2.15	C(224)...C(222)	2.42

table 7 continued

C(225)...C(222)	2.79	C(226)...C(222)	2.42
H(223)...C(222)	2.15	C(225)...C(223)	2.42
C(226)...C(223)	2.79	H(222)...C(223)	2.15
H(224)...C(223)	2.15	C(226)...C(224)	2.42
H(223)...C(224)	2.15	H(225)...C(224)	2.15
H(224)...C(225)	2.15	H(226)...C(225)	2.15
H(225)...C(226)	2.15	C(313)...C(311)	2.42
C(314)...C(311)	2.79	C(315)...C(311)	2.42
H(312)...C(311)	2.15	H(316)...C(311)	2.15
C(321)...C(311)	2.85	C(322)...C(311)	3.22
H(322)...C(311)	2.90	C(331)...C(311)	2.88
C(336)...C(311)	3.37	C(314)...C(312)	2.42
C(315)...C(312)	2.79	C(316)...C(312)	2.42
H(313)...C(312)	2.15	C(315)...C(313)	2.42
C(316)...C(313)	2.79	H(312)...C(313)	2.15
H(314)...C(313)	2.15	C(316)...C(314)	2.42
H(313)...C(314)	2.15	H(315)...C(314)	2.15
H(314)...C(315)	2.15	H(316)...C(315)	2.15
H(315)...C(316)	2.15	H(322)...C(316)	2.83
C(331)...C(316)	3.09	C(336)...C(316)	3.42
C(331)...H(316)	2.59	C(336)...H(316)	2.95
C(323)...C(321)	2.42	C(324)...C(321)	2.79
C(325)...C(321)	2.42	H(322)...C(321)	2.15
H(326)...C(321)	2.15	C(331)...C(321)	2.87
C(332)...C(321)	3.14	H(332)...C(321)	2.66
C(324)...C(322)	2.42	C(325)...C(322)	2.79
C(326)...C(322)	2.42	H(323)...C(322)	2.15
C(331)...C(322)	3.49	C(332)...C(322)	3.41

table 7 continued

H(332)...C(322)	2.72	C(325)...C(323)	2.42
C(326)...C(323)	2.79	H(322)...C(323)	2.15
H(324)...C(323)	2.15	C(326)...C(324)	2.42
H(323)...C(324)	2.15	H(325)...C(324)	2.15
H(324)...C(325)	2.15	H(326)...C(325)	2.15
H(325)...C(326)	2.15	C(333)...C(331)	2.42
C(334)...C(331)	2.79	C(335)...C(331)	2.42
H(332)...C(331)	2.15	H(336)...C(331)	2.15
C(334)...C(332)	2.42	C(335)...C(332)	2.79
C(336)...C(332)	2.42	H(333)...C(332)	2.15
C(335)...C(333)	2.42	C(336)...C(333)	2.79
H(332)...C(333)	2.15	H(334)...C(333)	2.15
C(336)...C(334)	2.42	H(333)...C(334)	2.15
H(335)...C(334)	2.15	H(334)...C(335)	2.15
H(336)...C(335)	2.15	H(335)...C(336)	2.15

Crystallographic Tables for $[Os_3(\mu\text{-}H)_2(C{=}CHOEt)(CO)_9]$, {X-ray study presented in section 3.2, Vol.1}.

TABLE 1 Fractional atomic coordinates and thermal parameters ($Å^2$) for $[Os_3(\mu\text{-}H)_2(C{=}CHOEt)(CO)_9]$

Atom	x	y	z	Uiso or Ueq
Os(1)	-0.13278(4)	-0.17350(6)	-0.51607(9)	0.0274(4)
Os(2)	-0.20208(4)	-0.30960(6)	-0.31606(9)	0.0299(4)
Os(3)	-0.06860(4)	-0.19826(6)	-0.19513(9)	0.0299(4)
C(11)	-0.0453(12)	-0.1444(16)	-0.5730(23)	0.043(12)
O(11)	0.0063(8)	-0.1256(14)	-0.6067(20)	0.067(11)
C(12)	-0.1608(10)	-0.0064(15)	-0.5347(24)	0.035(11)
O(12)	-0.1783(8)	0.0808(11)	-0.5331(21)	0.069(11)
C(13)	-0.1766(10)	-0.2211(21)	-0.7249(30)	0.058(15)
O(13)	-0.1978(9)	-0.2551(14)	-0.8511(18)	0.066(11)
C(21)	-0.1869(10)	-0.4277(18)	-0.1656(28)	0.050(13)
O(21)	-0.1759(9)	-0.4954(14)	-0.0655(21)	0.067(12)
C(22)	-0.2828(12)	-0.2470(14)	-0.2509(24)	0.043(12)
O(22)	-0.3317(9)	-0.2085(13)	-0.2179(23)	0.077(12)
C(23)	-0.2539(10)	-0.4135(17)	-0.4791(29)	0.044(13)
O(23)	-0.2820(8)	-0.4744(14)	-0.5717(21)	0.070(11)
C(31)	-0.0838(10)	-0.0443(19)	-0.1455(23)	0.039(12)
O(31)	-0.0966(8)	0.0538(13)	-0.1221(19)	0.061(10)
C(32)	-0.0346(11)	-0.2604(18)	0.0064(25)	0.042(12)
O(32)	-0.0131(9)	-0.3052(15)	0.1294(20)	0.073(12)
C(33)	0.0220(11)	-0.1583(18)	-0.2279(24)	0.047(12)
O(33)	0.0756(7)	-0.1285(15)	-0.2376(21)	0.069(11)
C(1)	-0.1089(9)	-0.3217(14)	-0.3909(20)	0.026(9)
C(2)	-0.0487(10)	-0.3818(15)	-0.3159(26)	0.038(11)
O(1)	0.0099(7)	-0.3783(10)	-0.3848(17)	0.038(8)
C(3)	0.0716(10)	-0.4303(20)	-0.2881(33)	0.065(15)

table 1 continued

C(4)	0.1328(11)	-0.4050(25)	-0.3550(36)	0.086(20)

TABLE 2 Fractional atomic coordinates for the hydrogen atoms for $[Os_3(\mu\text{-}H)_2(C{=}CHOEt)(CO)_9]$

Atom	x	y	z
H(12)	-0.2189	-0.1881	-0.4608
H(23)	-0.1554	-0.2211	-0.1450

TABLE 3 Anisotropic thermal parameters ($Å^2$) for $[Os_3(\mu\text{-}H)_2(C{=}CHOEt)(CO)_9]$

Atom	U11	U22	U33	U23	U13	U12
Os(1)	0.0284(4)	0.0266(4)	0.0270(4)	-0.0005(3)	0.0066(3)	-0.0008(3)
Os(2)	0.0273(4)	0.0293(4)	0.0329(4)	-0.0029(3)	0.0087(3)	-0.0052(3)
Os(3)	0.0300(4)	0.0332(4)	0.0266(4)	-0.0055(3)	0.0058(3)	-0.0066(3)
C(11)	0.066(14)	0.036(11)	0.028(11)	-0.015(9)	0.011(10)	-0.017(10)
O(11)	0.050(9)	0.085(11)	0.066(11)	-0.021(9)	0.032(9)	-0.023(8)
C(12)	0.048(12)	0.014(10)	0.043(12)	0.006(9)	0.009(10)	-0.009(9)
O(12)	0.080(11)	0.026(8)	0.[illegible](14)	0.006(8)	0.049(10)	0.013(7)
C(13)	0.030(11)	0.078(17)	0.06[illegible]16)	0.036(14)	0.019(11)	0.016(11)
O(13)	0.097(13)	0.074(11)	0.027(9)	-0.008(8)	-0.010(9)	-0.022(9)
C(21)	0.035(11)	0.046(12)	0.067(16)	0.013(12)	0.026(11)	-0.006(10)
O(21)	0.079(12)	0.062(11)	0.061(12)	0.009(9)	0.017(10)	0.007(9)
C(22)	0.074(16)	0.021(9)	0.033(12)	0.006(8)	0.017(11)	0.017(9)
O(22)	0.073(11)	0.055(10)	0.102(15)	0.008(10)	0.052(11)	0.006(9)

table 3 continued

C(23)	0.031(11)	0.038(12)	0.065(16)	0.001(12)	0.017(11)	0.011(9)
O(23)	0.058(10)	0.074(12)	0.076(12)	-0.037(10)	-0.001(9)	-0.019(9)
C(31)	0.033(11)	0.059(14)	0.024(11)	0.002(10)	0.001(9)	-0.012(10)
O(31)	0.073(11)	0.043(9)	0.066(11)	-0.010(8)	0.023(9)	-0.004(8)
C(32)	0.044(12)	0.048(13)	0.034(12)	-0.019(10)	-0.016(10)	-0.016(10)
O(32)	0.079(12)	0.090(13)	0.049(10)	0.002(10)	-0.005(9)	-0.027(10)
C(33)	0.047(12)	0.057(14)	0.037(12)	-0.032(11)	0.014(9)	-0.021(10)
O(33)	0.034(8)	0.101(13)	0.072(12)	-0.021(10)	0.020(8)	-0.018(8)
C(1)	0.036(9)	0.022(9)	0.021(9)	-0.001(8)	0.000(8)	0.010(8)
C(2)	0.034(11)	0.020(9)	0.060(14)	-0.007(9)	0.008(10)	-0.002(8)
O(1)	0.038(8)	0.023(6)	0.055(9)	-0.004(6)	0.010(7)	0.003(5)
C(3)	0.027(11)	0.063(14)	0.105(21)	0.013(15)	0.011(13)	0.008(10)
C(4)	0.034(12)	0.114(23)	0.111(24)	-0.013(19)	0.036(14)	-0.010(13)

TABLE 4 Bond lengths (Å) for $[Os_3(\mu\text{-}H)_2(C{=}CHOEt)(CO)_9]$

Os(1) -Os(2)	2.883(1)	Os(1) -Os(3)	2.774(1)
Os(1) -C(11)	1.903(24)	Os(1) -C(12)	1.996(18)
Os(1) -C(13)	1.887(23)	Os(1) -C(1)	2.014(16)
Os(2) -Os(3)	2.863(1)	Os(2) -C(21)	1.855(22)
Os(2) -C(22)	1.923(24)	Os(2) -C(23)	1.940(21)
Os(2) -C(1)	2.060(18)	Os(3) -C(31)	1.863(22)
Os(3) -C(32)	1.854(20)	Os(3) -C(33)	1.900(22)
Os(3) -C(1)	2.207(16)	Os(3) -C(2)	2.426(19)
C(11) -O(11)	1.13(3)	C(12) -O(12)	1.060(23)
C(13) -O(13)	1.14(3)	C(21) -O(21)	1.15(3)
C(22) -O(22)	1.14(3)	C(23) -O(23)	1.11(3)
C(31) -O(31)	1.18(3)	C(32) -O(32)	1.17(3)
C(33) -O(33)	1.12(3)	C(1) -C(2)	1.384(23)
C(2) -O(1)	1.40(3)	O(1) -C(3)	1.425(24)
C(3) -C(4)	1.46(4)		

TABLE 5 Bond angles (°) for $[Os_3(\mu\text{-}H)_2(C{=}CHOEt)(CO)_9]$

Os(3) -Os(1) -Os(2)	60.8(1)	C(11) -Os(1) -Os(2)	144.9(6)
C(11) -Os(1) -Os(3)	93.1(6)	C(12) -Os(1) -Os(2)	114.5(6)
C(12) -Os(1) -Os(3)	103.3(6)	C(12) -Os(1) -C(11)	93.0(8)
C(13) -Os(1) -Os(2)	104.1(7)	C(13) -Os(1) -Os(3)	157.2(7)
C(13) -Os(1) -C(11)	92.2(9)	C(13) -Os(1) -C(12)	98.6(9)
C(1) -Os(1) -Os(2)	45.6(5)	C(1) -Os(1) -Os(3)	52.0(5)
C(1) -Os(1) -C(11)	100.3(8)	C(1) -Os(1) -C(12)	152.1(8)
C(1) -Os(1) -C(13)	105.2(9)	Os(3) -Os(2) -Os(1)	57.7(1)
C(21) -Os(2) -Os(1)	142.7(7)	C(21) -Os(2) -Os(3)	95.1(6)
C(22) -Os(2) -Os(1)	119.7(5)	C(22) -Os(2) -Os(3)	117.1(5)
C(22) -Os(2) -C(21)	94.5(9)	C(23) -Os(2) -Os(1)	97.9(7)
C(23) -Os(2) -Os(3)	144.5(7)	C(23) -Os(2) -C(21)	91.5(9)
C(23) -Os(2) -C(22)	97.0(8)	C(1) -Os(2) -Os(1)	44.3(4)
C(1) -Os(2) -Os(3)	50.1(4)	C(1) -Os(2) -C(21)	99.2(8)
C(1) -Os(2) -C(22)	161.9(7)	C(1) -Os(2) -C(23)	94.4(8)
Os(2) -Os(3) -Os(1)	61.5(1)	C(31) -Os(3) -Os(1)	94.2(6)
C(31) -Os(3) -Os(2)	109.4(6)	C(32) -Os(3) -Os(1)	162.8(6)
C(32) -Os(3) -Os(2)	105.3(7)	C(32) -Os(3) -C(31)	101.1(9)
C(33) -Os(3) -Os(1)	92.5(6)	C(33) -Os(3) -Os(2)	147.7(6)
C(33) -Os(3) -C(31)	90.3(9)	C(33) -Os(3) -C(32)	95.3(9)
C(1) -Os(3) -Os(1)	46.0(4)	C(1) -Os(3) -Os(2)	45.7(5)
C(1) -Os(3) -C(31)	137.8(7)	C(1) -Os(3) -C(32)	117.1(8)
C(1) -Os(3) -C(33)	102.7(8)	C(2) -Os(3) -Os(1)	75.0(5)
C(2) -Os(3) -Os(2)	71.0(4)	C(2) -Os(3) -C(31)	167.6(8)
C(2) -Os(3) -C(32)	90.5(8)	C(2) -Os(3) -C(33)	84.4(8)

table 5 continued

C(2)	-Os(3)	-C(1)	34.4(6)	O(11)	-C(11)	-Os(1)	179(2)
O(12)	-C(12)	-Os(1)	173(2)	O(13)	-C(13)	-Os(1)	174(2)
O(21)	-C(21)	-Os(2)	176(2)	O(22)	-C(22)	-Os(2)	177(2)
O(23)	-C(23)	-Os(2)	178(2)	O(31)	-C(31)	-Os(3)	176(1)
O(32)	-C(32)	-Os(3)	176(2)	O(33)	-C(33)	-Os(3)	174(2)
Os(2)	-C(1)	-Os(1)	90.1(7)	Os(3)	-C(1)	-Os(1)	82.0(6)
Os(3)	-C(1)	-Os(2)	84.2(7)	C(2)	-C(1)	-Os(1)	138(1)
C(2)	-C(1)	-Os(2)	127(1)	C(2)	-C(1)	-Os(3)	81(1)
C(1)	-C(2)	-Os(3)	64(1)	O(1)	-C(2)	-Os(3)	112(1)
O(1)	-C(2)	-C(1)	118(2)	C(3)	-O(1)	-C(2)	113(2)
C(4)	-C(3)	-O(1)	110(2)				

TABLE 6 Intermolecular distances (Å) for $[Os_3(\mu\text{-}H)_2(C{=}CHOEt)(CO)_9]$

atom1	atom2	dist	S	a	b	c
O(13)	...Os(2)	4.04	1	0.0	0.0	-1.0
O(31)	...Os(2)	4.13	2	-1.0	0.0	-1.0
O(31)	...Os(3)	4.06	-1	0.0	0.0	0.0
O(32)	...C(11)	3.34	1	0.0	0.0	1.0
O(32)	...O(11)	3.03	1	0.0	0.0	1.0
C(12)	...O(11)	3.33	-1	0.0	0.0	-1.0
O(12)	...O(11)	3.32	-1	0.0	0.0	-1.0
O(31)	...O(11)	3.33	-1	0.0	0.0	-1.0
O(33)	...C(12)	3.24	-1	0.0	0.0	-1.0
O(23)	...C(12)	3.34	2	-1.0	-1.0	-2.0
O(33)	...O(12)	3.16	-1	0.0	0.0	-1.0
O(13)	...O(12)	3.04	2	-1.0	-1.0	-2.0
O(21)	...O(12)	3.26	2	-1.0	-1.0	-1.0
C(22)	...O(12)	3.37	2	-1.0	-1.0	-1.0
O(22)	...O(12)	3.23	2	-1.0	-1.0	-1.0
O(23)	...C(13)	3.34	2	-1.0	-1.0	-2.0
C(21)	...O(13)	3.41	1	0.0	0.0	1.0
H(23)	...O(13)	2.87	1	0.0	0.0	1.0
O(23)	...O(13)	3.30	2	-1.0	-1.0	-2.0
C(3)	...O(21)	3.36	-1	0.0	-1.0	0.0
C(22)	...O(21)	3.31	2	-1.0	0.0	-1.0
O(22)	...O(21)	3.11	2	-1.0	0.0	-1.0
O(31)	...C(22)	3.28	2	-1.0	0.0	-1.0
O(31)	...O(22)	3.23	2	-1.0	0.0	-1.0
O(31)	...C(23)	3.24	2	-1.0	0.0	-1.0

table 6 continued

C(4)	...O(23)	3.40	-1	0.0	-1.0	-1.0
O(31)	...O(23)	3.21	2	-1.0	0.0	-1.0
O(33)	...O(23)	3.04	-2	1.0	0.0	1.0
C(33)	...O(31)	3.26	-1	0.0	0.0	0.0
O(33)	...O(31)	3.15	-1	0.0	0.0	0.0

Symmetry Transformations:

The second atom is related to the first atom, at (x,y,z), by the symmetry operation S with (a,b,c) added to the (x',y',z') of S.

Where S =

1	x, y, z
2	0.5-x, 0.5+y, 0.5-z

TABLE 7 Intramolecular distances (Å) for $[Os_3(\mu\text{-}H)_2(C{=}CHOEt)(CO)_9]$

O(11) ...Os(1)	3.03	O(12) ...Os(1)	3.05
O(13) ...Os(1)	3.02	C(22) ...Os(1)	4.18
C(23) ...Os(1)	3.69	C(31) ...Os(1)	3.45
C(33) ...Os(1)	3.43	C(2) ...Os(1)	3.18
O(1) ...Os(1)	3.61	H(23) ...Os(1)	3.37
C(12) ...Os(2)	4.13	C(13) ...Os(2)	3.81
O(21) ...Os(2)	3.00	O(22) ...Os(2)	3.07
O(23) ...Os(2)	3.05	C(31) ...Os(2)	3.90
C(32) ...Os(2)	3.80	C(2) ...Os(2)	3.09
C(11) ...Os(3)	3.45	C(12) ...Os(3)	3.77
C(21) ...Os(3)	3.55	C(22) ...Os(3)	4.11
O(31) ...Os(3)	3.05	O(32) ...Os(3)	3.02
O(33) ...Os(3)	3.02	O(1) ...Os(3)	3.23
C(3) ...Os(3)	4.03	H(12) ...Os(3)	3.27
C(12) ...C(11)	2.83	C(13) ...C(11)	2.73
C(33) ...C(11)	2.96	O(33) ...C(11)	3.28
C(1) ...C(11)	3.01	O(1) ...C(11)	3.20
C(33) ...O(11)	3.23	O(33) ...O(11)	3.15
C(13) ...C(12)	2.94	C(31) ...C(12)	3.37
H(12) ...C(12)	2.53	C(1) ...C(13)	3.10
H(12) ...C(13)	2.62	C(22) ...C(21)	2.78
C(23) ...C(21)	2.72	C(1) ...C(21)	2.98
C(2) ...C(21)	3.28	H(23) ...C(21)	2.45
C(23) ...C(22)	2.89	H(12) ...C(22)	2.51
H(23) ...C(22)	2.45	C(1) ...C(23)	2.94

table 7 continued

H(12)	...C(23)	2.68	C(32)	...C(31)	2.87
C(33)	...C(31)	2.67	H(23)	...C(31)	2.46
C(33)	...C(32)	2.77	C(1)	...C(32)	3.47
C(2)	...C(32)	3.07	H(23)	...C(32)	2.45
C(1)	...C(33)	3.21	C(2)	...C(33)	2.93
O(1)	...C(33)	2.86	C(3)	...C(33)	3.35
O(1)	...O(33)	3.28	O(1)	...C(1)	2.39
H(12)	...C(1)	2.59	H(23)	...C(1)	2.74
C(3)	...C(2)	2.36	C(4)	...O(1)	2.36

Crystallographic Tables for $[Os_3(\mu\text{-}H)_2(HC{=}COEt)(CO)_9]$, {X-ray study presented in section 3.2, Vol.1}.

TABLE 1 Fractional atomic coordinates and thermal parameters ($Å^2$) for $[Os_3(\mu\text{-}H)_2(HC{=}COEt)(CO)_9]$

Atom	x	y	z	Uiso or Ueq
Os(1)	0.00000	0.11443(13)	0.00000	0.0234(7)
Os(2)	0.07573(11)	0.39064(13)	0.04453(15)	0.0288(8)
Os(3)	0.1225(1)	0.2165(1)	-0.1019(2)	0.028(1)
O(11)	-0.0711(24)	0.0432(32)	0.1988(28)	0.071(22)
O(12)	0.0107(20)	-0.1692(30)	-0.0628(31)	0.061(20)
O(13)	-0.1839(20)	0.1720(34)	-0.1719(31)	0.064(21)
O(21)	0.2148(32)	0.6045(36)	0.0584(43)	0.107(35)
O(22)	0.1011(25)	0.4042(45)	0.2951(35)	0.099(30)
O(23)	-0.0925(22)	0.5738(29)	-0.0237(33)	0.072(24)
O(31)	0.2981(33)	0.3703(39)	-0.1338(39)	0.097(32)
O(32)	-0.0108(31)	0.2458(37)	-0.3203(32)	0.084(27)
O(33)	0.1911(27)	-0.0525(27)	-0.1314(24)	0.070(21)
C(11)	-0.0460(34)	0.0802(45)	0.1220(43)	0.055(12)
C(12)	0.0031(25)	-0.0596(37)	-0.0315(33)	0.035(9)
C(13)	-0.1261(31)	0.1432(41)	-0.1028(41)	0.050(12)
C(21)	0.1633(33)	0.5294(47)	0.0556(41)	0.054(12)
C(22)	0.0971(28)	0.4056(39)	0.1992(37)	0.038(9)
C(23)	-0.0272(25)	0.5122(36)	0.0057(32)	0.033(9)
C(31)	0.2335(46)	0.3176(61)	-0.1216(56)	0.077(18)
C(32)	0.0332(31)	0.2237(42)	-0.2438(40)	0.048(11)
C(33)	0.1595(34)	0.0541(49)	-0.1214(45)	0.060(13)
C(1)	0.1771(24)	0.2438(34)	0.0857(32)	0.031(8)
C(2)	0.1264(33)	0.1259(42)	0.0759(44)	0.055(12)
O(1)	0.1925(18)	0.0052(26)	0.1244(23)	0.043(7)
C(3)	0.2930(25)	0.0217(35)	0.1699(32)	0.033(9)
C(4)	0.3279(33)	-0.1172(46)	0.1833(42)	0.057(13)

TABLE 2 Fractional atomic coordinates for the hydrogen atoms for $[Os_3(\mu\text{-}H)_2(HC{=}COEt)(CO)_9]$

Atom	x	y	z
H(12)	0.1189	-0.1891	-0.2608
H(23)	0.1554	-0.1211	-0.1460

TABLE 3 Anisotropic thermal parameters ($Å^2$) for $[Os_3(\mu\text{-}H)_2(HC{=}COEt)(CO)_9]$

Atom	U11	U22	U33	U23	U13	U12
Os(1)	0.021(1)	0.026(1)	0.023(1)	0.002(1)	0.005(1)	-0.005(1)
Os(2)	0.028(1)	0.028(1)	0.031(1)	-0.009(1)	0.008(1)	-0.004(1)
Os(3)	0.032(1)	0.026(1)	0.027(1)	-0.005(1)	0.013(1)	-0.007(1)
O(11)	0.090(24)	0.058(21)	0.064(22)	0.024(18)	0.056(20)	0.018(18)
O(12)	0.048(17)	0.047(17)	0.089(27)	-0.033(19)	0.012(18)	-0.010(14)
O(13)	0.038(16)	0.082(22)	0.073(26)	0.018(22)	-0.010(17)	0.003(15)
O(21)	0.111(34)	0.061(24)	0.149(48)	0.021(27)	-0.060(34)	-0.045(23)
O(22)	0.054(22)	0.150(37)	0.094(31)	-0.092(29)	-0.010(22)	-0.022(21)
O(23)	0.057(19)	0.047(18)	0.114(33)	0.018(20)	0.039(22)	0.000(15)
O(31)	0.103(33)	0.084(28)	0.103(36)	-0.028(25)	0.027(30)	-0.024(24)
O(32)	0.139(35)	0.068(24)	0.047(23)	-0.005(20)	-0.047(24)	-0.004(23)
O(33)	0.143(31)	0.025(14)	0.043(19)	0.003(14)	0.052(21)	0.023(18)

TABLE 4 Bond lengths (Å) for $[Os_3(\mu\text{-}H)_2(HC{=}COEt)(CO)_9]$

Os(1) -Os(2)	3.006(2)	Os(1) -Os(3)	2.770(2)
Os(1) -C(11)	1.93(5)	Os(1) -C(12)	1.81(4)
Os(1) -C(13)	1.98(5)	Os(1) -C(2)	1.86(5)
Os(2) -Os(3)	2.824(2)	Os(2) -C(21)	1.90(5)
Os(2) -C(22)	1.93(4)	Os(2) -C(23)	1.92(4)
Os(2) -C(1)	2.08(3)	Os(3) -C(31)	2.04(6)
Os(3) -C(32)	1.91(5)	Os(3) -C(33)	1.78(5)
Os(3) -C(1)	2.32(4)	Os(3) -C(2)	2.45(5)
C(11) -O(11)	1.22(6)	C(12) -O(12)	1.20(4)
C(13) -O(13)	1.08(5)	C(21) -O(21)	1.08(6)
C(22) -O(22)	1.22(6)	C(23) -O(23)	1.13(4)
C(31) -O(31)	1.16(7)	C(32) -O(32)	1.03(5)
C(33) -O(33)	1.20(5)	C(1) -C(2)	1.40(5)
C(2) -O(1)	1.58(5)	O(1) -C(3)	1.46(4)
C(3) -C(4)	1.49(6)		

TABLE 5 Bond angles (°) for $[Os_3(\mu\text{-}H)_2(HC{=}COEt)(CO)_9]$

Os(3) -Os(1) -Os(2)	58.4(1)	C(11) -Os(1) -Os(2)	103(1)
C(11) -Os(1) -Os(3)	155(1)	C(12) -Os(1) -Os(2)	156(1)
C(12) -Os(1) -Os(3)	101(1)	C(12) -Os(1) -C(11)	93(2)
C(13) -Os(1) -Os(2)	103(1)	C(13) -Os(1) -Os(3)	106(1)
C(13) -Os(1) -C(11)	94(2)	C(13) -Os(1) -C(12)	94(2)
C(2) -Os(1) -Os(2)	65(1)	C(2) -Os(1) -Os(3)	60(2)
C(2) -Os(1) -C(11)	98(2)	C(2) -Os(1) -C(12)	95(2)
C(2) -Os(1) -C(13)	164(2)	Os(3) -Os(2) -Os(1)	56.6(1)
C(21) -Os(2) -Os(1)	156(1)	C(21) -Os(2) -Os(3)	102(1)
C(22) -Os(2) -Os(1)	102(1)	C(22) -Os(2) -Os(3)	138(1)
C(22) -Os(2) -C(21)	88(2)	C(23) -Os(2) -Os(1)	108(1)
C(23) -Os(2) -Os(3)	125(1)	C(23) -Os(2) -C(21)	92(2)
C(23) -Os(2) -C(22)	95(2)	C(1) -Os(2) -Os(1)	65.8(9)
C(1) -Os(2) -Os(3)	54(1)	C(1) -Os(2) -C(21)	94(2)
C(1) -Os(2) -C(22)	85(2)	C(1) -Os(2) -C(23)	174(1)
Os(2) -Os(3) -Os(1)	65.0(1)	C(31) -Os(3) -Os(1)	159(2)
C(31) -Os(3) -Os(2)	99(2)	C(32) -Os(3) -Os(1)	95(1)
C(32) -Os(3) -Os(2)	112(1)	C(32) -Os(3) -C(31)	103(2)
C(33) -Os(3) -Os(1)	90(2)	C(33) -Os(3) -Os(2)	145(2)
C(33) -Os(3) -C(31)	98(2)	C(33) -Os(3) -C(32)	93(2)
C(1) -Os(3) -Os(1)	68.0(9)	C(1) -Os(3) -Os(2)	46.4(8)
C(1) -Os(3) -C(31)	92(2)	C(1) -Os(3) -C(32)	156(2)
C(1) -Os(3) -C(33)	103(2)	C(2) -Os(3) -Os(1)	41(1)
C(2) -Os(3) -Os(2)	63(1)	C(2) -Os(3) -C(31)	121(2)
C(2) -Os(3) -C(32)	136(2)	C(2) -Os(3) -C(33)	82(2)

table 5 continued

C(2)	-Os(3)	-C(1)	34(1)	O(11)	-C(11)	-Os(1)	172(4)
O(12)	-C(12)	-Os(1)	171(4)	O(13)	-C(13)	-Os(1)	164(4)
O(21)	-C(21)	-Os(2)	176(6)	O(22)	-C(22)	-Os(2)	172(4)
O(23)	-C(23)	-Os(2)	173(4)	O(31)	-C(31)	-Os(3)	177(6)
O(32)	-C(32)	-Os(3)	169(4)	O(33)	-C(33)	-Os(3)	175(4)
Os(3)	-C(1)	-Os(2)	80(1)	C(2)	-C(1)	-Os(2)	104(3)
C(2)	-C(1)	-Os(3)	78(3)	Os(3)	-C(2)	-Os(1)	79(2)
C(1)	-C(2)	-Os(1)	123(3)	C(1)	-C(2)	-Os(3)	68(3)
O(1)	-C(2)	-Os(1)	125(3)	O(1)	-C(2)	-Os(3)	119(3)
O(1)	-C(2)	-C(1)	111(3)	C(3)	-O(1)	-C(2)	121(3)
C(4)	-C(3)	-O(1)	103(3)				

TABLE 6 Intermolecular distances (Å) for $[Os_3(\mu\text{-}H)_2(HC{=}COEt)(CO)_9]$

atom1	atom2	dist	S	a	b	c
O(11)	...Os(1)	4.03	2	0.0	0.0	0.0
O(31)	...Os(1)	3.89	1	0.5	0.5	0.0
O(22)	...Os(2)	3.94	2	0.0	1.0	0.0
O(22)	...Os(3)	4.04	2	0.0	1.0	0.0
O(32)	...C(11)	3.38	2	0.0	0.0	-1.0
C(12)	...O(11)	3.32	2	0.0	0.0	-1.0
O(12)	...O(11)	3.21	2	0.0	0.0	-1.0
C(32)	...O(11)	3.10	2	0.0	0.0	-1.0
O(32)	...O(11)	3.09	2	0.0	0.0	-1.0
O(21)	...O(11)	3.24	1	0.5	0.5	0.0
O(32)	...C(12)	3.37	2	0.0	0.0	-1.0
O(31)	...C(12)	3.05	1	0.5	0.5	0.0
O(23)	...O(12)	3.15	1	0.0	1.0	0.0
O(32)	...O(12)	3.33	2	0.0	0.0	-1.0
O(31)	...O(12)	3.08	1	0.5	0.5	0.0
O(31)	...C(13)	2.97	1	0.5	0.5	0.0
O(31)	...O(13)	3.12	1	0.5	0.5	0.0
C(22)	...O(13)	3.30	2	0.5	0.5	0.0
O(22)	...O(13)	3.23	2	0.5	0.5	0.0
C(1)	...O(13)	3.30	2	0.5	0.5	0.0
O(22)	...C(21)	3.27	2	0.0	1.0	0.0
O(22)	...O(21)	3.31	2	0.0	1.0	0.0
O(32)	...C(23)	3.28	2	0.0	1.0	-1.0
O(32)	...O(23)	3.12	2	0.0	1.0	-1.0
O(1)	...O(33)	3.19	2	0.0	0.0	0.0

table 6 continued

C(3) ...O(33)	3.38	2	0.0	0.0	0.0

Symmetry Transformations:

The second atom is related to the first atom, at (x,y,z), by the symmetry operation S with (a,b,c) added to the (x',y',z') of S.

Where S =

1	x, y, z
2	x, -y, 0.5+z

TABLE 7 Intramolecular distances (Å) for $[Os_3(\mu\text{-}H)_2(HC{=}COEt)(CO)_9]$

O(11) ...Os(1)	3.15	O(12) ...Os(1)	3.00
O(13) ...Os(1)	3.03	C(22) ...Os(1)	3.89
C(23) ...Os(1)	4.05	C(32) ...Os(1)	3.51
C(33) ...Os(1)	3.30	C(1) ...Os(1)	2.87
O(1) ...Os(1)	3.06	C(11) ...Os(2)	3.92
C(13) ...Os(2)	3.95	O(21) ...Os(2)	2.98
O(22) ...Os(2)	3.14	O(23) ...Os(2)	3.04
C(31) ...Os(2)	3.73	C(32) ...Os(2)	3.96
C(2) ...Os(2)	2.78	C(12) ...Os(3)	3.59
C(13) ...Os(3)	3.81	C(21) ...Os(3)	3.71
O(31) ...Os(3)	3.20	O(32) ...Os(3)	2.93
O(33) ...Os(3)	2.98	O(1) ...Os(3)	3.51
C(12) ...C(11)	2.71	C(13) ...C(11)	2.85
C(2) ...C(11)	2.87	C(13) ...C(12)	2.78
C(33) ...C(12)	3.14	C(2) ...C(12)	2.70
O(1) ...C(12)	3.02	O(33) ...O(12)	3.32
C(22) ...C(21)	2.67	C(23) ...C(21)	2.75
C(1) ...C(21)	2.91	C(23) ...C(22)	2.84
C(1) ...C(22)	2.71	C(2) ...C(22)	3.34
C(32) ...C(31)	3.10	C(33) ...C(31)	2.89
C(1) ...C(31)	3.13	C(33) ...C(32)	2.69
C(1) ...C(33)	3.23	C(2) ...C(33)	2.83
O(1) ...C(33)	3.10	O(1) ...C(1)	2.46
C(3) ...C(1)	2.85	C(3) ...C(2)	2.65
C(4) ...O(1)	2.31		

Crystallographic Tables for $[Ru_4(\mu\text{-}H)_3(CO)_{12}][PPN]$, {X-ray study presented in section 3.3, Vol.1}.

TABLE 1 Fractional atomic coordinates and thermal parameters ($Å^2$) for $[Ru_4(\mu\text{-}H)_3(CO)_{12}][PPN]$

Atom	x	y	z	U_{iso} or U_{eq}
Ru(1)	-0.07787(18)	0.14243(8)	0.21397(15)	0.0519(15)
Ru(2)	0.0047(2)	0.2145(1)	0.1176(2)	0.063(2)
Ru(3)	0.0018(2)	0.1181(1)	0.0555(1)	0.061(2)
Ru(4)	0.16832(18)	0.14401(7)	0.20562(15)	0.0483(15)
P(1)	0.6183(5)	0.3848(2)	0.1265(4)	0.036(4)
P(2)	0.4359(5)	0.4237(2)	0.2214(4)	0.035(4)
C(11)	-0.0958(25)	0.0851(11)	0.2614(19)	0.078(9)
O(11)	-0.1100(18)	0.0481(7)	0.2881(14)	0.099(7)
C(12)	-0.2264(22)	0.1448(8)	0.1418(16)	0.050(7)
O(12)	-0.3188(18)	0.1464(7)	0.1022(13)	0.092(6)
C(13)	-0.1147(27)	0.1719(11)	0.3188(23)	0.091(11)
O(13)	-0.1324(19)	0.1892(8)	0.3853(16)	0.109(8)
C(21)	-0.0180(27)	0.2487(11)	0.2159(23)	0.087(10)
O(21)	-0.0286(21)	0.2700(8)	0.2816(18)	0.123(8)
C(22)	0.0876(32)	0.2587(12)	0.0597(24)	0.111(13)
O(22)	0.1394(22)	0.2833(9)	0.0237(17)	0.129(9)
C(23)	-0.1438(33)	0.2275(12)	0.0504(24)	0.110(12)
O(23)	-0.2379(22)	0.2385(8)	0.0124(16)	0.120(8)
C(31)	-0.0140(20)	0.0654(8)	0.0859(15)	0.046(7)
O(31)	-0.0360(18)	0.0214(7)	0.1005(13)	0.100(7)
C(32)	-0.1349(36)	0.1206(13)	-0.0298(28)	0.131(14)
O(32)	-0.2149(25)	0.1184(9)	-0.0868(18)	0.144(10)
C(33)	0.1057(31)	0.1053(12)	-0.0291(24)	0.104(12)
O(33)	0.1644(23)	0.4088(9)	0.4246(17)	0.137(9)
C(41)	0.2665(28)	0.1676(11)	0.3137(23)	0.089(10)

table 1 continued

O(41)	0.3270(18)	0.1784(7)	0.3809(14)	0.088(7)
C(42)	0.1910(22)	0.0807(9)	0.2307(17)	0.061(8)
O(42)	0.2066(17)	0.0435(7)	0.2431(13)	0.092(7)
C(43)	0.2767(25)	0.1468(9)	0.1288(19)	0.073(9)
O(43)	0.3506(18)	0.1477(7)	0.0856(14)	0.097(7)
N	0.5561(14)	0.4184(6)	0.1848(11)	0.035(5)
C(111)	0.7687(11)	0.3956(6)	0.1519(11)	0.045(7)
C(112)	0.8454(11)	0.3672(6)	0.1159(11)	0.081(10)
C(113)	0.9629(11)	0.3784(6)	0.1283(11)	0.088(10)
C(114)	1.0037(11)	0.4181(6)	0.1757(11)	0.068(8)
C(115)	0.9270(11)	0.4466(6)	0.2127(11)	0.060(8)
C(116)	0.8095(11)	0.4354(6)	0.2003(11)	0.056(8)
C(121)	0.5962(14)	0.3255(4)	0.1497(11)	0.036(6)
C(122)	0.6658(14)	0.3029(4)	0.2226(11)	0.066(8)
C(123)	0.6383(14)	0.2582(4)	0.2463(11)	0.092(10)
C(124)	0.5411(14)	0.2361(4)	0.1970(11)	0.072(8)
C(125)	0.4715(14)	0.2587(4)	0.1241(11)	0.073(9)
C(126)	0.4990(14)	0.3034(4)	0.1005(11)	0.062(8)
C(131)	0.5774(13)	0.3933(5)	0.0057(8)	0.050(7)
C(132)	0.5089(13)	0.4314(5)	-0.0253(8)	0.044(7)
C(133)	0.4801(13)	0.4405(5)	-0.1190(8)	0.071(9)
C(134)	0.5198(13)	0.4114(5)	-0.1818(8)	0.066(8)
C(135)	0.5883(13)	0.3732(5)	-0.1508(8)	0.080(9)
C(136)	0.6171(13)	0.3642(5)	-0.0570(8)	0.057(8)
C(211)	0.3171(11)	0.4352(5)	0.1289(8)	0.033(6)
C(212)	0.2814(11)	0.4807(5)	0.1105(8)	0.051(7)
C(213)	0.1987(11)	0.4909(5)	0.0331(8)	0.072(9)
C(214)	0.1518(11)	0.4555(5)	-0.0260(8)	0.062(8)

table 1 continued

C(215)	0.1875(11)	0.4100(5)	-0.0077(8)	0.061(8)
C(216)	0.2701(11)	0.3999(5)	0.0698(8)	0.045(7)
C(221)	0.4009(15)	0.3751(4)	0.2833(10)	0.038(6)
C(222)	0.2926(15)	0.3536(4)	0.2699(10)	0.067(8)
C(223)	0.2753(15)	0.3146(4)	0.3209(10)	0.094(10)
C(224)	0.3663(15)	0.2970(4)	0.3853(10)	0.076(9)
C(225)	0.4746(15)	0.3184(4)	0.3987(10)	0.083(10)
C(226)	0.4919(15)	0.3575(4)	0.3477(10)	0.071(8)
C(231)	0.4494(13)	0.4701(4)	0.3016(8)	0.045(6)
C(232)	0.5587(13)	0.4894(4)	0.3312(8)	0.031(6)
C(233)	0.5716(13)	0.5264(4)	0.3922(8)	0.059(8)
C(234)	0.4752(13)	0.5442(4)	0.4236(8)	0.063(8)
C(235)	0.3659(13)	0.5249(4)	0.3940(8)	0.061(8)
C(236)	0.3530(13)	0.4879(4)	0.3329(8)	0.042(7)

TABLE 2 Fractional atomic coordinates for the hydrogen atoms for $[Ru_4(\mu\text{-}H)_3(CO)_{12}][PPN]$

Atom	x	y	z
H(112)	0.8140	0.3365	0.0781
H(113)	1.0223	0.3566	0.1002
H(114)	1.0943	0.4270	0.1868
H(115)	0.9580	0.4771	0.2513
H(116)	0.7496	0.4570	0.2292
H(122)	0.7417	0.3199	0.2603
H(123)	0.6922	0.2407	0.3025
H(124)	0.5183	0.2018	0.2163
H(125)	0.3939	0.2422	0.0878
H(126)	0.4434	0.3214	0.0456
H(132)	0.4785	0.4539	0.0235
H(133)	0.4264	0.4700	-0.1428
H(134)	0.4961	0.4184	-0.2545
H(135)	0.6180	0.3508	-0.1999
H(136)	0.6701	0.3347	-0.0336
H(212)	0.3178	0.5080	0.1563
H(213)	0.1715	0.5261	0.0167
H(214)	0.0879	0.4635	-0.0861
H(215)	0.1507	0.3827	-0.0534
H(216)	0.2971	0.3646	0.0842
H(222)	0.2229	0.3673	0.2193
H(223)	0.1903	0.2982	0.3097
H(224)	0.3501	0.2670	0.4255
H(225)	0.5425	0.3048	0.4509
H(226)	0.5751	0.3738	0.3606

table 2 continued

H(232)	0.6331	0.4756	0.3066
H(233)	0.6570	0.5409	0.4160
H(234)	0.4864	0.5725	0.4724
H(235)	0.2921	0.5387	0.4194
H(236)	0.2682	0.4734	0.3100

TABLE 3 Anisotropic thermal parameters ($Å^2$) for $[Ru_4(u\text{-}H)_3(CO)_{12}][PPN]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ru(1)	0.046(1)	0.053(1)	0.057(2)	0.007(1)	0.013(1)	0.000(1)
Ru(2)	0.058(2)	0.049(1)	0.083(2)	0.023(1)	0.008(1)	0.003(1)
Ru(3)	0.062(2)	0.074(2)	0.046(2)	-0.001(1)	0.005(1)	-0.003(1)
Ru(4)	0.047(1)	0.046(1)	0.052(2)	0.005(1)	0.010(1)	-0.002(1)
P(1)	0.039(4)	0.036(4)	0.033(4)	-0.007(3)	0.012(3)	0.002(3)
P(2)	0.034(4)	0.036(4)	0.034(4)	0.002(3)	0.013(3)	0.003(3)

TABLE 4 Bond lengths (Å) for $[Ru_4(u\text{-}H)_3(CO)_{12}][PPN]$

Ru(1) -Ru(2)	2.799(3)	Ru(1) -Ru(3)	2.769(3)
Ru(1) -Ru(4)	2.911(3)	Ru(1) -C(11)	1.83(3)
Ru(1) -C(12)	1.875(24)	Ru(1) -C(13)	1.89(3)
Ru(2) -Ru(3)	2.941(3)	Ru(2) -Ru(4)	2.943(3)
Ru(2) -C(21)	1.82(3)	Ru(2) -C(22)	1.90(4)
Ru(2) -C(23)	1.88(3)	Ru(3) -Ru(4)	2.788(3)
Ru(3) -C(31)	1.612(24)	Ru(3) -C(32)	1.86(4)
Ru(3) -C(33)	1.93(4)	Ru(4) -C(41)	1.92(3)
Ru(4) -C(42)	1.88(3)	Ru(4) -C(43)	1.85(3)
C(11) -O(11)	1.16(4)	C(12) -O(12)	1.14(3)
C(13) -O(13)	1.16(4)	C(21) -O(21)	1.18(4)
C(22) -O(22)	1.13(5)	C(23) -O(23)	1.19(4)
C(31) -O(31)	1.33(3)	C(32) -O(32)	1.15(5)
C(41) -O(41)	1.16(4)	C(42) -O(42)	1.10(3)
C(43) -O(43)	1.17(4)	N -P(1)	1.567(19)
N -P(2)	1.605(19)	P(1) -C(111)	1.764(14)
P(1) -C(121)	1.779(14)	P(1) -C(131)	1.786(13)
P(2) -C(211)	1.803(13)	P(2) -C(221)	1.769(16)
P(2) -C(231)	1.783(13)	C(111)-C(112)	1.395(22)
C(111)-C(116)	1.395(22)	C(112)-C(113)	1.395(18)
C(113)-C(114)	1.395(22)	C(114)-C(115)	1.395(22)
C(115)-C(116)	1.395(18)	C(121)-C(122)	1.395(20)
C(121)-C(126)	1.395(20)	C(122)-C(123)	1.395(19)
C(123)-C(124)	1.395(20)	C(124)-C(125)	1.395(20)
C(125)-C(126)	1.395(19)	C(131)-C(132)	1.395(21)

table 4 continued

C(131)-C(136)	1.395(21)	C(132)-C(133)	1.395(17)
C(133)-C(134)	1.395(21)	C(134)-C(135)	1.395(21)
C(135)-C(136)	1.395(17)	C(211)-C(212)	1.395(21)
C(211)-C(216)	1.395(19)	C(212)-C(213)	1.395(17)
C(213)-C(214)	1.395(19)	C(214)-C(215)	1.395(21)
C(215)-C(216)	1.395(17)	C(221)-C(222)	1.395(23)
C(221)-C(226)	1.395(21)	C(222)-C(223)	1.395(20)
C(223)-C(224)	1.395(21)	C(224)-C(225)	1.395(23)
C(225)-C(226)	1.395(20)	C(231)-C(232)	1.395(20)
C(231)-C(236)	1.395(22)	C(232)-C(233)	1.395(17)
C(233)-C(234)	1.395(22)	C(234)-C(235)	1.395(20)
C(235)-C(236)	1.395(17)		

TABLE 5 Bond angles (°) for $[Ru_4(\mu\text{-}H)_3(CO)_{12}][PPN]$

Ru(3) -Ru(1) -Ru(2)	63.8(1)	Ru(4) -Ru(1) -Ru(2)	62.0(1)
Ru(4) -Ru(1) -Ru(3)	58.7(1)	C(11) -Ru(1) -Ru(2)	161(1)
C(11) -Ru(1) -Ru(3)	100(1)	C(11) -Ru(1) -Ru(4)	102.3(9)
C(12) -Ru(1) -Ru(2)	93.0(8)	C(12) -Ru(1) -Ru(3)	86.9(8)
C(12) -Ru(1) -Ru(4)	143.3(8)	C(12) -Ru(1) -C(11)	95(1)
C(13) -Ru(1) -Ru(2)	103(1)	C(13) -Ru(1) -Ru(3)	167(1)
C(13) -Ru(1) -Ru(4)	113.7(9)	C(13) -Ru(1) -C(11)	92(1)
C(13) -Ru(1) -C(12)	97(1)	Ru(3) -Ru(2) -Ru(1)	57.6(1)
Ru(4) -Ru(2) -Ru(1)	60.8(1)	Ru(4) -Ru(2) -Ru(3)	56.6(1)
C(21) -Ru(2) -Ru(1)	83(1)	C(21) -Ru(2) -Ru(3)	141(1)
C(21) -Ru(2) -Ru(4)	101.5(9)	C(22) -Ru(2) -Ru(1)	170(1)
C(22) -Ru(2) -Ru(3)	118(1)	C(22) -Ru(2) -Ru(4)	109(1)
C(22) -Ru(2) -C(21)	99(1)	C(23) -Ru(2) -Ru(1)	93(1)
C(23) -Ru(2) -Ru(3)	94(1)	C(23) -Ru(2) -Ru(4)	147(1)
C(23) -Ru(2) -C(21)	93(1)	C(23) -Ru(2) -C(22)	97(1)
Ru(2) -Ru(3) -Ru(1)	58.6(1)	Ru(4) -Ru(3) -Ru(1)	63.2(1)
Ru(4) -Ru(3) -Ru(2)	61.8(1)	C(31) -Ru(3) -Ru(1)	86.1(9)
C(31) -Ru(3) -Ru(2)	143.9(9)	C(31) -Ru(3) -Ru(4)	97.6(8)
C(32) -Ru(3) -Ru(1)	101(1)	C(32) -Ru(3) -Ru(2)	98(1)
C(32) -Ru(3) -Ru(4)	158(1)	C(32) -Ru(3) -C(31)	96(1)
C(33) -Ru(3) -Ru(1)	161(1)	C(33) -Ru(3) -Ru(2)	114(1)
C(33) -Ru(3) -Ru(4)	98(1)	C(33) -Ru(3) -C(31)	97(1)
C(33) -Ru(3) -C(32)	98(2)	Ru(2) -Ru(4) -Ru(1)	57.1(1)
Ru(3) -Ru(4) -Ru(1)	58.1(1)	Ru(3) -Ru(4) -Ru(2)	61.7(1)
C(41) -Ru(4) -Ru(1)	115(1)	C(41) -Ru(4) -Ru(2)	111.6(9)

table 5 continued

C(41) -Ru(4) -Ru(3)	172(1)	C(42) -Ru(4) -Ru(1)	94.7(8)
C(42) -Ru(4) -Ru(2)	145.3(8)	C(42) -Ru(4) -Ru(3)	87.1(7)
C(42) -Ru(4) -C(41)	98(1)	C(43) -Ru(4) -Ru(1)	145.2(8)
C(43) -Ru(4) -Ru(2)	99.3(8)	C(43) -Ru(4) -Ru(3)	88.9(8)
C(43) -Ru(4) -C(41)	97(1)	C(43) -Ru(4) -C(42)	94(1)
O(11) -C(11) -Ru(1)	177(2)	O(12) -C(12) -Ru(1)	176(2)
O(13) -C(13) -Ru(1)	177(3)	O(21) -C(21) -Ru(2)	177(3)
O(22) -C(22) -Ru(2)	177(3)	O(23) -C(23) -Ru(2)	175(3)
O(31) -C(31) -Ru(3)	173(2)	O(32) -C(32) -Ru(3)	173(4)
O(41) -C(41) -Ru(4)	175(3)	O(42) -C(42) -Ru(4)	177(3)
O(43) -C(43) -Ru(4)	175(2)	P(2) -N -P(1)	140(1)
C(111)-P(1) -N	108.4(9)	C(121)-P(1) -N	113.3(9)
C(121)-P(1) -C(111)	107.8(8)	C(131)-P(1) -N	113.5(8)
C(131)-P(1) -C(111)	105.6(8)	C(131)-P(1) -C(121)	107.8(8)
C(211)-P(2) -N	111.5(8)	C(221)-P(2) -N	113.5(9)
C(221)-P(2) -C(211)	108.8(8)	C(231)-P(2) -N	108.5(8)
C(231)-P(2) -C(211)	109.4(7)	C(231)-P(2) -C(221)	104.9(7)
C(112)-C(111)-P(1)	120(1)	C(116)-C(111)-P(1)	120(1)
C(116)-C(111)-C(112)	120(1)	C(113)-C(112)-C(111)	120(1)
C(114)-C(113)-C(112)	120(1)	C(115)-C(114)-C(113)	120(1)
C(116)-C(115)-C(114)	120(1)	C(115)-C(116)-C(111)	120(1)
C(122)-C(121)-P(1)	121(1)	C(126)-C(121)-P(1)	118(1)
C(126)-C(121)-C(122)	120(1)	C(123)-C(122)-C(121)	120(1)
C(124)-C(123)-C(122)	120(1)	C(125)-C(124)-C(123)	120(1)
C(126)-C(125)-C(124)	120(1)	C(125)-C(126)-C(121)	120(1)
C(132)-C(131)-P(1)	118(1)	C(136)-C(131)-P(1)	121(1)
C(136)-C(131)-C(132)	120(1)	C(133)-C(132)-C(131)	120(1)
C(134)-C(133)-C(132)	120(1)	C(135)-C(134)-C(133)	120(1)

table 5 continued

C(136)-C(135)-C(134)	120(1)	C(135)-C(136)-C(131)	120(1)
C(212)-C(211)-P(2)	119(1)	C(216)-C(211)-P(2)	120(1)
C(216)-C(211)-C(212)	120(1)	C(213)-C(212)-C(211)	120(1)
C(214)-C(213)-C(212)	120(1)	C(215)-C(214)-C(213)	120(1)
C(216)-C(215)-C(214)	120(1)	C(215)-C(216)-C(211)	120(1)
C(222)-C(221)-P(2)	125(1)	C(226)-C(221)-P(2)	115(1)
C(226)-C(221)-C(222)	120(1)	C(223)-C(222)-C(221)	120(1)
C(224)-C(223)-C(222)	120(1)	C(225)-C(224)-C(223)	120(1)
C(226)-C(225)-C(224)	120(1)	C(225)-C(226)-C(221)	120(1)
C(232)-C(231)-P(2)	119(1)	C(236)-C(231)-P(2)	121(1)
C(236)-C(231)-C(232)	120(1)	C(233)-C(232)-C(231)	120(1)
C(234)-C(233)-C(232)	120(1)	C(235)-C(234)-C(233)	120(1)
C(236)-C(235)-C(234)	120(1)	C(235)-C(236)-C(231)	120(1)

TABLE 6 Intermolecular distances (Å) for $[Ru_4(\mu\text{-}H)_3(CO)_{12}][PPN]$

atom1	atom2	dist	S	a	b	c
O(33)	...Ru(3)	3.05	-2	0.0	1.0	1.0
H(215)	...Ru(4)	3.70	-2	0.0	1.0	0.0
H(115)	...O(11)	2.85	2	1.0	0.0	0.0
C(212)	...O(11)	3.34	2	0.0	0.0	0.0
H(212)	...O(11)	2.95	2	0.0	0.0	0.0
H(214)	...O(11)	2.72	-2	0.0	1.0	0.0
H(234)	...O(12)	2.98	2	0.0	0.0	0.0
H(225)	...O(12)	2.89	-2	1.0	1.0	1.0
H(123)	...C(13)	2.99	1	1.0	0.0	0.0
H(123)	...O(13)	2.66	1	1.0	0.0	0.0
O(23)	...O(13)	3.21	-2	0.0	1.0	0.0
H(136)	...O(13)	2.88	-2	1.0	1.0	0.0
H(113)	...C(22)	3.03	1	1.0	0.0	0.0
H(113)	...O(22)	2.87	1	1.0	0.0	0.0
H(225)	...O(23)	2.86	-2	1.0	1.0	1.0
H(115)	...O(31)	2.57	2	1.0	0.0	0.0
H(122)	...O(32)	2.86	-2	1.0	1.0	1.0
H(226)	...O(32)	2.46	-2	1.0	1.0	1.0
O(33)	...C(33)	1.13	-2	0.0	1.0	1.0
H(215)	...C(41)	2.97	-2	0.0	1.0	0.0
H(126)	...O(41)	2.58	-2	0.0	1.0	0.0
C(115)	...O(42)	3.34	2	1.0	0.0	0.0
C(116)	...O(42)	3.26	2	1.0	0.0	0.0
H(115)	...O(42)	2.74	2	1.0	0.0	0.0
H(116)	...O(42)	2.58	2	1.0	0.0	0.0

table 6 continued

H(232)...O(42)	2.90	2	1.0	0.0	0.0
H(133)...O(42)	2.85	-2	0.0	1.0	0.0
C(224)...O(43)	3.41	-2	0.0	1.0	1.0
H(222)...C(114)	2.93	1	-1.0	0.0	0.0
C(211)...H(114)	2.90	1	-1.0	0.0	0.0
C(212)...H(114)	3.07	1	-1.0	0.0	0.0
C(216)...H(114)	3.02	1	-1.0	0.0	0.0
H(135)...C(124)	3.00	-2	0.0	1.0	0.0
C(135)...H(124)	2.95	-2	0.0	1.0	0.0
H(212)...C(133)	2.93	-1	1.0	1.0	0.0
H(212)...C(134)	2.99	-1	1.0	1.0	0.0
C(232)...H(133)	3.06	-1	1.0	1.0	0.0
C(232)...H(134)	2.93	-1	1.0	1.0	0.0
C(233)...H(134)	2.60	-1	1.0	1.0	0.0
C(234)...H(134)	2.81	-1	1.0	1.0	0.0
C(235)...C(233)	3.46	-1	1.0	1.0	1.0
C(234)...C(234)	3.40	-1	1.0	1.0	1.0

Symmetry Transformations:

The second atom is related to the first atom, at (x,y,z), by the symmetry operation S with (a,b,c) added to the (x',y',z') of S.

Where S =

1	x, y, z
2	-x, 0.5+y, 0.5-z

TABLE 7 Intramolecular distances (Å) for $[Ru_4(\mu\text{-}H)_3(CO)_{12}][PPN]$

O(11) ...Ru(1)	3.00	O(12) ...Ru(1)	3.01
O(13) ...Ru(1)	3.04	C(21) ...Ru(1)	3.16
O(21) ...Ru(1)	3.85	C(23) ...Ru(1)	3.45
O(23) ...Ru(1)	4.26	C(31) ...Ru(1)	3.11
O(31) ...Ru(1)	3.96	C(32) ...Ru(1)	3.61
C(41) ...Ru(1)	4.11	C(42) ...Ru(1)	3.59
C(12) ...Ru(2)	3.45	O(12) ...Ru(2)	4.24
C(13) ...Ru(2)	3.72	O(21) ...Ru(2)	3.00
O(22) ...Ru(2)	3.03	O(23) ...Ru(2)	3.07
C(31) ...Ru(2)	4.35	C(32) ...Ru(2)	3.68
C(33) ...Ru(2)	4.13	C(41) ...Ru(2)	4.07
C(43) ...Ru(2)	3.72	C(11) ...Ru(3)	3.58
C(12) ...Ru(3)	3.26	O(12) ...Ru(3)	4.03
C(22) ...Ru(3)	4.20	C(23) ...Ru(3)	3.60
O(31) ...Ru(3)	2.93	O(32) ...Ru(3)	3.00
C(42) ...Ru(3)	3.28	O(42) ...Ru(3)	3.97
C(43) ...Ru(3)	3.32	O(43) ...Ru(3)	4.12
C(11) ...Ru(4)	3.76	C(13) ...Ru(4)	4.06
C(21) ...Ru(4)	3.76	C(22) ...Ru(4)	3.98
C(31) ...Ru(4)	3.40	C(33) ...Ru(4)	3.60
O(41) ...Ru(4)	3.08	O(42) ...Ru(4)	2.98
O(43) ...Ru(4)	3.02	C(12) ...C(11)	2.74
C(13) ...C(11)	2.68	C(31) ...C(11)	2.98
O(31) ...C(11)	3.19	C(42) ...C(11)	3.47
O(31) ...O(11)	3.15	C(13) ...C(12)	2.83

table 7 continued

C(23) ...C(12)	3.00	O(23) ...C(12)	3.31
C(32) ...C(12)	3.01	C(23) ...O(12)	3.30
O(23) ...O(12)	3.20	C(32) ...O(12)	3.25
C(21) ...C(13)	3.03	O(21) ...C(13)	3.10
O(21) ...O(13)	3.16	C(22) ...C(21)	2.83
C(23) ...C(21)	2.70	H(223)...C(21)	2.96
H(223)...O(21)	2.65	C(23) ...C(22)	2.84
C(32) ...C(23)	3.33	C(32) ...C(31)	2.58
C(33) ...C(31)	2.66	C(42) ...C(31)	2.96
O(42) ...C(31)	3.22	O(42) ...O(31)	3.29
C(33) ...C(32)	2.65	C(43) ...C(33)	3.04
O(43) ...C(33)	3.30	C(222)...O(33)	3.36
H(236)...O(33)	2.93	C(42) ...C(41)	2.88
C(43) ...C(41)	2.63	H(224)...O(41)	2.65
C(43) ...C(42)	2.74	H(124)...O(43)	2.95
H(125)...O(43)	2.78	C(111)...N	2.70
C(116)...N	2.98	H(116)...N	2.51
C(121)...N	2.80	C(131)...N	2.81
C(132)...N	3.09	H(132)...N	2.61
C(211)...N	2.82	C(221)...N	2.82
C(226)...N	3.19	H(226)...N	2.88
C(231)...N	2.75	C(232)...N	2.98
H(232)...N	2.50	P(2) ...P(1)	2.98
C(112)...P(1)	2.74	C(116)...P(1)	2.74
H(112)...P(1)	2.88	H(116)...P(1)	2.87
C(122)...P(1)	2.77	C(126)...P(1)	2.73
H(122)...P(1)	2.92	H(126)...P(1)	2.85
C(132)...P(1)	2.74	C(136)...P(1)	2.78

table 7 continued

H(132)...P(1)	2.85	H(136)...P(1)	2.94
C(221)...P(1)	3.75	C(121)...P(2)	3.67
H(132)...P(2)	3.19	C(212)...P(2)	2.77
C(216)...P(2)	2.78	H(212)...P(2)	2.89
H(216)...P(2)	2.92	C(222)...P(2)	2.81
C(226)...P(2)	2.68	H(222)...P(2)	2.98
H(226)...P(2)	2.79	C(232)...P(2)	2.74
C(236)...P(2)	2.78	H(232)...P(2)	2.86
H(236)...P(2)	2.93	C(113)...C(111)	2.42
C(114)...C(111)	2.79	C(115)...C(111)	2.42
H(112)...C(111)	2.15	H(116)...C(111)	2.15
C(121)...C(111)	2.86	C(122)...C(111)	3.20
H(122)...C(111)	2.77	C(131)...C(111)	2.83
C(136)...C(111)	3.41	C(114)...C(112)	2.42
C(115)...C(112)	2.79	C(116)...C(112)	2.42
H(113)...C(112)	2.15	C(121)...C(112)	3.28
C(122)...C(112)	3.40	H(122)...C(112)	2.98
C(131)...C(112)	3.36	C(136)...C(112)	3.36
H(136)...C(112)	2.90	C(115)...C(113)	2.42
C(116)...C(113)	2.79	H(112)...C(113)	2.15
H(114)...C(113)	2.15	C(116)...C(114)	2.42
H(113)...C(114)	2.14	H(115)...C(114)	2.15
H(114)...C(115)	2.14	H(116)...C(115)	2.16
H(115)...C(116)	2.14	H(232)...C(116)	3.05
C(121)...H(112)	2.95	C(136)...H(112)	2.89
C(232)...H(116)	3.06	C(123)...C(121)	2.42
C(124)...C(121)	2.79	C(125)...C(121)	2.42
H(122)...C(121)	2.15	H(126)...C(121)	2.15

table 7 continued

C(131)...C(121)	2.88	C(136)...C(121)	3.31
H(136)...C(121)	3.01	C(226)...C(121)	3.50
C(124)...C(122)	2.42	C(125)...C(122)	2.79
C(126)...C(122)	2.42	H(123)...C(122)	2.15
C(226)...C(122)	3.38	C(125)...C(123)	2.42
C(126)...C(123)	2.79	H(122)...C(123)	2.15
H(124)...C(123)	2.15	C(126)...C(124)	2.42
H(123)...C(124)	2.15	H(125)...C(124)	2.15
H(124)...C(125)	2.15	H(126)...C(125)	2.15
H(125)...C(126)	2.15	C(131)...C(126)	3.17
C(136)...C(126)	3.41	H(216)...C(126)	2.93
C(131)...H(126)	2.74	C(136)...H(126)	3.02
C(133)...C(131)	2.42	C(134)...C(131)	2.79
C(135)...C(131)	2.42	H(132)...C(131)	2.15
H(136)...C(131)	2.15	C(134)...C(132)	2.42
C(135)...C(132)	2.79	C(136)...C(132)	2.42
H(133)...C(132)	2.15	C(211)...C(132)	3.48
C(216)...C(132)	3.47	C(135)...C(133)	2.42
C(136)...C(133)	2.79	H(132)...C(133)	2.15
H(134)...C(133)	2.15	C(136)...C(134)	2.42
H(133)...C(134)	2.15	H(135)...C(134)	2.14
H(134)...C(135)	2.16	H(136)...C(135)	2.14
H(135)...C(136)	2.15	C(211)...H(132)	2.72
C(212)...H(132)	2.94	C(213)...C(211)	2.42
C(214)...C(211)	2.79	C(215)...C(211)	2.42
H(212)...C(211)	2.15	H(216)...C(211)	2.15
C(221)...C(211)	2.90	C(222)...C(211)	3.20
H(222)...C(211)	2.72	C(231)...C(211)	2.93

table 7 continued

C(236)...C(211)	3.35	H(236)...C(211)	3.05
C(214)...C(212)	2.42	C(215)...C(212)	2.79
C(216)...C(212)	2.42	H(213)...C(212)	2.15
C(231)...C(212)	3.16	C(236)...C(212)	3.26
H(236)...C(212)	2.99	C(215)...C(213)	2.42
C(216)...C(213)	2.79	H(212)...C(213)	2.15
H(214)...C(213)	2.15	C(216)...C(214)	2.42
H(213)...C(214)	2.15	H(215)...C(214)	2.15
H(214)...C(215)	2.15	H(216)...C(215)	2.15
H(215)...C(216)	2.15	C(221)...C(216)	3.34
C(222)...C(216)	3.22	H(222)...C(216)	2.56
C(231)...H(212)	2.65	C(236)...H(212)	2.64
C(221)...H(216)	3.00	C(222)...H(216)	2.78
C(223)...C(221)	2.42	C(224)...C(221)	2.79
C(225)...C(221)	2.42	H(222)...C(221)	2.14
H(226)...C(221)	2.16	C(231)...C(221)	2.82
C(236)...C(221)	3.42	C(224)...C(222)	2.42
C(225)...C(222)	2.79	C(226)...C(222)	2.42
H(223)...C(222)	2.15	C(225)...C(223)	2.42
C(226)...C(223)	2.79	H(222)...C(223)	2.15
H(224)...C(223)	2.14	C(226)...C(224)	2.42
H(223)...C(224)	2.16	H(225)...C(224)	2.13
H(224)...C(225)	2.17	H(226)...C(225)	2.13
H(225)...C(226)	2.17	C(231)...C(226)	3.35
C(233)...C(231)	2.42	C(234)...C(231)	2.79
C(235)...C(231)	2.42	H(232)...C(231)	2.15
H(236)...C(231)	2.15	C(234)...C(232)	2.42
C(235)...C(232)	2.79	C(236)...C(232)	2.42

table 7 continued

H(233)...C(232)	2.15	C(235)...C(233)	2.42
C(236)...C(233)	2.79	H(232)...C(233)	2.15
H(234)...C(233)	2.15	C(236)...C(234)	2.42
H(233)...C(234)	2.15	H(235)...C(234)	2.14
H(234)...C(235)	2.16	H(236)...C(235)	2.14
H(235)...C(236)	2.16		

Crystallographic Tables for $[Os_6H_2(CO)_{17}P(OMe)_3]$, {X-ray study presented in section 3.4, Vol.1}.

TABLE 1 Fractional atomic coordinates and thermal parameters ($Å^2$) for $[Os_6H_2(CO)_{17}P(OME)_3]$

Atom	x	y	z	U_{iso} or U_{eq}
Os(1)	0.1062(1)	-0.2924(2)	0.1314(2)	0.028(1)
Os(2)	0.02189(8)	-0.22006(20)	0.00000	0.0265(10)
Os(3)	0.1392(1)	-0.3279(2)	-0.0478(2)	0.029(1)
Os(4)	0.1967(1)	-0.1014(2)	0.0611(2)	0.029(1)
Os(5)	0.0778(1)	-0.0039(2)	0.1083(2)	0.024(1)
Os(6)	-0.0110(1)	-0.1834(2)	0.1755(2)	0.031(1)
P(4)	0.2468(7)	0.0413(17)	-0.0355(11)	0.057(10)
C(11)	0.1766(24)	-0.4038(57)	0.1309(40)	0.044(13)
O(11)	0.2182(18)	-0.4827(44)	0.1427(30)	0.065(12)
C(12)	0.0605(27)	-0.4664(65)	0.1558(42)	0.054(17)
O(12)	0.0397(18)	-0.5710(46)	0.1776(29)	0.062(11)
C(13)	0.1242(28)	-0.2358(67)	0.2484(48)	0.071(17)
O(13)	0.1377(21)	-0.2067(52)	0.3205(36)	0.080(15)
C(21)	-0.0523(19)	-0.1054(45)	-0.0076(31)	0.022(10)
O(21)	-0.0969(17)	-0.0560(40)	-0.0150(26)	0.048(10)
C(22)	-0.0216(25)	-0.3808(63)	-0.0070(43)	0.052(15)
O(22)	-0.0483(20)	-0.4987(50)	-0.0098(34)	0.075(13)
C(23)	0.0319(26)	-0.2097(68)	-0.1304(44)	0.052(16)
O(23)	0.0281(23)	-0.1867(56)	-0.2023(39)	0.092(16)
C(31)	0.2132(26)	-0.4097(64)	-0.0477(43)	0.052(16)
O(31)	0.2591(21)	-0.4806(47)	-0.0507(33)	0.074(13)
C(32)	0.1484(26)	-0.2864(64)	-0.1696(43)	0.053(16)
O(32)	0.1567(19)	-0.2618(45)	-0.2455(32)	0.066(12)
C(33)	0.0930(24)	-0.4920(61)	-0.0609(39)	0.052(14)
O(33)	0.0702(19)	-0.5959(47)	-0.0810(30)	0.063(12)

table 1 continued

C(41)	0.2669(24)	-0.1968(56)	0.0647(39)	0.043(13)
O(41)	0.3115(21)	-0.2626(41)	0.0721(34)	0.067(11)
C(42)	0.2201(25)	-0.0015(63)	0.1657(41)	0.051(15)
O(42)	0.2382(22)	0.0484(51)	0.2305(35)	0.083(15)
C(51)	0.0129(27)	0.1016(65)	0.1085(47)	0.062(16)
O(51)	-0.0312(20)	0.1936(49)	0.0859(33)	0.075(14)
C(52)	0.1278(23)	0.1404(55)	0.0667(38)	0.042(13)
O(52)	0.1481(16)	0.2561(38)	0.0467(27)	0.050(10)
C(53)	0.0953(19)	0.0600(48)	0.2201(31)	0.027(11)
O(53)	0.1036(16)	0.1045(41)	0.2910(28)	0.052(10)
C(61)	-0.0584(23)	-0.3408(57)	0.1887(38)	0.041(13)
O(61)	-0.0924(20)	-0.4339(50)	0.1978(32)	0.072(13)
C(62)	-0.0803(20)	-0.0700(46)	0.1798(31)	0.024(10)
O(62)	-0.1241(17)	0.0010(42)	0.1805(28)	0.058(11)
C(63)	-0.0004(25)	-0.1444(63)	0.3001(42)	0.052(15)
O(63)	0.0042(23)	-0.1199(54)	0.3743(38)	0.086(16)
O(1)	0.1988(20)	0.1003(49)	-0.1108(33)	0.074(13)
O(2)	0.3056(40)	0.0007(38)	-0.0712(72)	0.150(38)
O(3)	0.2706(26)	0.1883(62)	-0.0110(43)	0.126(19)
C(1)	0.2056(27)	0.2107(68)	-0.1798(46)	0.071(18)
C(2)	0.3032(50)	-0.1193(40)	-0.1475(86)	0.137(44)
C(3)	0.3246(34)	0.2176(77)	0.0425(54)	0.081(23)

TABLE 2 Anisotropic thermal parameters (Å ^{2}) for $[Os_6H_2(CO)_{17}P(OME)_3]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Os(1)	0.042(1)	0.024(1)	0.018(1)	0.003(1)	-0.005(1)	0.001(1)
Os(2)	0.032(1)	0.028(1)	0.019(1)	-0.001(1)	-0.004(1)	-0.003(1)
Os(3)	0.043(1)	0.025(1)	0.020(1)	-0.004(1)	0.000(1)	0.003(1)
Os(4)	0.031(1)	0.031(1)	0.025(1)	-0.004(1)	-0.002(1)	-0.001(1)
Os(5)	0.031(1)	0.022(1)	0.017(1)	-0.001(1)	0.000(1)	-0.001(1)
Os(6)	0.039(1)	0.030(1)	0.023(1)	-0.001(1)	0.004(1)	-0.007(1)
P(4)	0.057(9)	0.063(9)	0.052(10)	-0.020(8)	0.017(8)	-0.033(8)

TABLE 3 Bond lengths (Å) for $[Os_6H_2(CO)_{17}P(OME)_3]$

Os(1) -Os(2)	2.815(3)	Os(1) -Os(3)	2.850(4)
Os(1) -Os(4)	2.695(3)	Os(1) -Os(5)	2.829(3)
Os(1) -Os(6)	2.854(3)	Os(1) -C(11)	1.87(5)
Os(1) -C(12)	1.97(6)	Os(1) -C(13)	1.91(7)
Os(2) -Os(3)	2.865(3)	Os(2) -Os(5)	2.907(3)
Os(2) -Os(6)	2.798(3)	Os(2) -C(21)	1.96(4)
Os(2) -C(22)	1.80(6)	Os(2) -C(23)	2.01(7)
Os(3) -Os(4)	2.996(3)	Os(3) -C(31)	1.80(6)
Os(3) -C(32)	1.91(7)	Os(3) -C(33)	1.87(6)
Os(4) -Os(5)	2.862(3)	Os(4) -C(41)	1.79(5)
Os(4) -C(42)	1.93(6)	Os(4) -C(52)	2.75(5)
Os(4) -P(4)	2.284(17)	Os(5) -Os(6)	2.784(3)
Os(5) -C(51)	1.74(6)	Os(5) -C(52)	1.87(5)
Os(5) -C(53)	1.85(5)	Os(6) -C(61)	1.83(5)
Os(6) -C(62)	1.87(4)	Os(6) -C(63)	1.95(6)
C(11) -O(11)	1.19(7)	C(12) -O(12)	1.14(7)
C(13) -O(13)	1.17(9)	C(21) -O(21)	1.09(5)
C(22) -O(22)	1.26(7)	C(23) -O(23)	1.12(9)
C(31) -O(31)	1.21(7)	C(32) -O(32)	1.20(8)
C(33) -O(33)	1.15(7)	C(41) -O(41)	1.17(7)
C(42) -O(42)	1.17(8)	C(51) -O(51)	1.35(8)
C(52) -O(52)	1.22(6)	C(53) -O(53)	1.18(6)
C(61) -O(61)	1.16(7)	C(62) -O(62)	1.17(6)
C(63) -O(63)	1.16(9)	P(4) -O(1)	1.66(5)
P(4) -O(2)	1.45(9)	P(4) -O(3)	1.54(6)
O(1) -C(1)	1.49(8)	O(2) -C(2)	1.63(9)
O(3) -C(3)	1.47(9)		

TABLE 4 Bond angles (°) for $[Os_6H_2(CO)_{17}P(OME)_3]$

Os(3) -Os(1) -Os(2)	60.8(1)	Os(4) -Os(1) -Os(2)	92.0(1)
Os(4) -Os(1) -Os(3)	62.9(1)	Os(5) -Os(1) -Os(2)	62.0(1)
Os(5) -Os(1) -Os(3)	92.9(1)	Os(5) -Os(1) -Os(4)	60.0(1)
Os(6) -Os(1) -Os(2)	59.1(1)	Os(6) -Os(1) -Os(3)	119.9(1)
Os(6) -Os(1) -Os(4)	118.6(1)	Os(6) -Os(1) -Os(5)	58.7(1)
C(11) -Os(1) -Os(2)	133(2)	C(11) -Os(1) -Os(3)	74(2)
C(11) -Os(1) -Os(4)	78(2)	C(11) -Os(1) -Os(5)	137(2)
C(11) -Os(1) -Os(6)	162(2)	C(12) -Os(1) -Os(2)	90(2)
C(12) -Os(1) -Os(3)	102(2)	C(12) -Os(1) -Os(4)	161(2)
C(12) -Os(1) -Os(5)	136(2)	C(12) -Os(1) -Os(6)	78(2)
C(12) -Os(1) -C(11)	87(2)	C(13) -Os(1) -Os(2)	137(2)
C(13) -Os(1) -Os(3)	152(2)	C(13) -Os(1) -Os(4)	92(2)
C(13) -Os(1) -Os(5)	84(2)	C(13) -Os(1) -Os(6)	82(2)
C(13) -Os(1) -C(11)	90(3)	C(13) -Os(1) -C(12)	99(3)
Os(3) -Os(2) -Os(1)	60.2(1)	Os(5) -Os(2) -Os(1)	59.2(1)
Os(5) -Os(2) -Os(3)	91.0(1)	Os(6) -Os(2) -Os(1)	61.1(1)
Os(6) -Os(2) -Os(3)	121.3(1)	Os(6) -Os(2) -Os(5)	58.4(1)
C(21) -Os(2) -Os(1)	136(1)	C(21) -Os(2) -Os(3)	158(1)
C(21) -Os(2) -Os(5)	90(1)	C(21) -Os(2) -Os(6)	77(1)
C(22) -Os(2) -Os(1)	101(2)	C(22) -Os(2) -Os(3)	99(2)
C(22) -Os(2) -Os(5)	149(2)	C(22) -Os(2) -Os(6)	91(2)
C(22) -Os(2) -C(21)	91(2)	C(23) -Os(2) -Os(1)	130(2)
C(23) -Os(2) -Os(3)	70(2)	C(23) -Os(2) -Os(5)	119(2)
C(23) -Os(2) -Os(6)	167(2)	C(23) -Os(2) -C(21)	90(2)
C(23) -Os(2) -C(22)	92(3)	Os(2) -Os(3) -Os(1)	59.0(1)

Os(4) -Os(3) -Os(1)	59.3(1)	Os(4) -Os(3) -Os(2)	88.9(1)
C(31) -Os(3) -Os(1)	106(2)	C(31) -Os(3) -Os(2)	165(2)
C(31) -Os(3) -Os(4)	86(2)	C(32) -Os(3) -Os(1)	159(2)
C(32) -Os(3) -Os(2)	106(2)	C(32) -Os(3) -Os(4)	110(2)
C(32) -Os(3) -C(31)	90(3)	C(33) -Os(3) -Os(1)	94(2)
C(33) -Os(3) -Os(2)	81(2)	C(33) -Os(3) -Os(4)	152(2)
C(33) -Os(3) -C(31)	97(2)	C(33) -Os(3) -C(32)	97(3)
Os(3) -Os(4) -Os(1)	57.8(1)	Os(5) -Os(4) -Os(1)	58.9(1)
Os(5) -Os(4) -Os(3)	89.3(1)	C(41) -Os(4) -Os(1)	105(2)
C(41) -Os(4) -Os(3)	91(2)	C(41) -Os(4) -Os(5)	160(2)
C(42) -Os(4) -Os(1)	101(2)	C(42) -Os(4) -Os(3)	158(2)
C(42) -Os(4) -Os(5)	83(2)	C(42) -Os(4) -C(41)	90(2)
C(52) -Os(4) -Os(1)	98(1)	C(52) -Os(4) -Os(3)	113(1)
C(52) -Os(4) -Os(5)	39(1)	C(52) -Os(4) -C(41)	154(2)
C(52) -Os(4) -C(42)	73(2)	P(4) -Os(4) -Os(1)	160.2(4)
P(4) -Os(4) -Os(3)	105.7(4)	P(4) -Os(4) -Os(5)	114.2(4)
P(4) -Os(4) -C(41)	84(2)	P(4) -Os(4) -C(42)	97(2)
P(4) -Os(4) -C(52)	78(1)	Os(2) -Os(5) -Os(1)	58.8(1)
Os(4) -Os(5) -Os(1)	61.1(1)	Os(4) -Os(5) -Os(2)	90.8(1)
Os(6) -Os(5) -Os(1)	61.1(1)	Os(6) -Os(5) -Os(2)	58.8(1)
Os(6) -Os(5) -Os(4)	122.2(1)	C(51) -Os(5) -Os(1)	137(2)
C(51) -Os(5) -Os(2)	93(2)	C(51) -Os(5) -Os(4)	159(2)
C(51) -Os(5) -Os(6)	77(2)	C(52) -Os(5) -Os(1)	128(2)
C(52) -Os(5) -Os(2)	125(2)	C(52) -Os(5) -Os(4)	67(2)
C(52) -Os(5) -Os(6)	170(2)	C(52) -Os(5) -C(51)	93(3)
C(53) -Os(5) -Os(1)	99(1)	C(53) -Os(5) -Os(2)	147(1)
C(53) -Os(5) -Os(4)	98(1)	C(53) -Os(5) -Os(6)	90(1)
C(53) -Os(5) -C(51)	89(3)	C(53) -Os(5) -C(52)	87(2)

Os(2) -Os(6) -Os(1)	59.7(1)	Os(5) -Os(6) -Os(1)	60.2(1)
Os(5) -Os(6) -Os(2)	62.8(1)	C(61) -Os(6) -Os(1)	104(2)
C(61) -Os(6) -Os(2)	99(2)	C(61) -Os(6) -Os(5)	160(2)
C(62) -Os(6) -Os(1)	162(1)	C(62) -Os(6) -Os(2)	108(1)
C(62) -Os(6) -Os(5)	103(1)	C(62) -Os(6) -C(61)	90(2)
C(63) -Os(6) -Os(1)	101(2)	C(63) -Os(6) -Os(2)	158(2)
C(63) -Os(6) -Os(5)	99(2)	C(63) -Os(6) -C(61)	97(2)
C(63) -Os(6) -C(62)	87(2)	O(11) -C(11) -Os(1)	170(5)
O(12) -C(12) -Os(1)	171(5)	O(13) -C(13) -Os(1)	176(5)
O(21) -C(21) -Os(2)	171(4)	O(22) -C(22) -Os(2)	175(5)
O(23) -C(23) -Os(2)	166(5)	O(31) -C(31) -Os(3)	171(5)
O(32) -C(32) -Os(3)	177(5)	O(33) -C(33) -Os(3)	169(5)
O(41) -C(41) -Os(4)	176(5)	O(42) -C(42) -Os(4)	173(5)
O(51) -C(51) -Os(5)	164(6)	Os(5) -C(52) -Os(4)	74(2)
O(52) -C(52) -Os(4)	123(3)	O(52) -C(52) -Os(5)	163(4)
O(53) -C(53) -Os(5)	176(4)	O(61) -C(61) -Os(6)	175(5)
O(62) -C(62) -Os(6)	178(4)	O(63) -C(63) -Os(6)	178(5)
O(1) -P(4) -Os(4)	110(2)	O(2) -P(4) -Os(4)	121(4)
O(2) -P(4) -O(1)	113(5)	O(3) -P(4) -Os(4)	123(3)
O(3) -P(4) -O(1)	94(3)	O(3) -P(4) -O(2)	92(4)
C(1) -O(1) -P(4)	131(4)	C(2) -O(2) -P(4)	115(7)
C(3) -O(3) -P(4)	126(5)		

TABLE 5 Intermolecular distances (Å) for $[Os_6H_2(CO)_{17}P(OME)_3]$

atom1	atom2	dist	S	a	b	c
O(63)	...Os(2)	3.80	2	0.0	0.0	0.0
O(23)	...Os(5)	4.13	2	0.0	0.0	-1.0
O(23)	...Os(6)	3.99	2	0.0	0.0	-1.0
O(52)	...O(11)	3.27	1	0.0	1.0	0.0
C(51)	...O(12)	3.33	1	0.0	1.0	0.0
O(51)	...O(12)	3.06	1	0.0	1.0	0.0
O(23)	...O(12)	3.30	2	0.0	-1.0	-1.0
O(53)	...C(21)	3.28	2	0.0	0.0	0.0
O(63)	...C(21)	2.99	2	0.0	0.0	0.0
O(53)	...O(21)	3.00	2	0.0	0.0	0.0
O(63)	...O(21)	3.13	2	0.0	0.0	0.0
O(31)	...O(21)	3.23	3	0.0	-1.0	0.0
O(41)	...O(21)	2.96	3	0.0	-1.0	0.0
O(51)	...O(22)	3.29	1	0.0	1.0	0.0
O(53)	...C(23)	3.36	2	0.0	0.0	0.0
O(63)	...C(23)	3.23	2	0.0	0.0	0.0
C(51)	...O(23)	3.13	2	0.0	0.0	0.0
O(51)	...O(23)	3.24	2	0.0	0.0	0.0
C(53)	...O(23)	3.19	2	0.0	0.0	0.0
O(53)	...O(23)	3.00	2	0.0	0.0	0.0
C(62)	...O(23)	3.24	2	0.0	0.0	0.0
O(62)	...O(23)	3.28	2	0.0	0.0	0.0
C(63)	...O(23)	3.20	2	0.0	0.0	0.0
O(63)	...O(23)	3.21	2	0.0	0.0	0.0
O(3)	...O(31)	3.21	1	0.0	1.0	0.0

O(42) ...C(32)	3.32	4	0.0	0.0	0.0
O(61) ...O(32)	3.33	2	0.0	-1.0	0.0
O(62) ...O(32)	2.81	2	0.0	0.0	0.0
O(42) ...O(32)	2.95	4	0.0	0.0	0.0
C(3) ...O(32)	3.27	4	0.0	0.0	0.0
O(52) ...C(33)	3.14	1	0.0	1.0	0.0
O(52) ...O(33)	2.95	1	0.0	1.0	0.0
O(63) ...O(33)	3.23	2	0.0	-1.0	0.0
C(62) ...O(41)	3.30	3	-1.0	-1.0	0.0
O(62) ...O(41)	3.14	3	-1.0	-1.0	0.0
C(3) ...O(51)	3.34	3	0.0	0.0	0.0

Symmetry Transformations:

The second atom is related to the first atom, at (x,y,z), by the symmetry operation S with (a,b,c) added to the (x',y',z') of S.

Where S =

1	x, y, z
2	-x,-y,0.5+z
3	0.5+x,0.5-y,z
4	0.5-x,0.5+y,0.5+z

TABLE 6 Intramolecular distances (Å) for $[Os_6H_2(CO)_{17}P(OME)_3]$

O(11) ...Os(1)	3.06	O(12) ...Os(1)	3.10
O(13) ...Os(1)	3.08	C(22) ...Os(1)	3.61
C(31) ...Os(1)	3.77	C(33) ...Os(1)	3.51
C(41) ...Os(1)	3.78	C(42) ...Os(1)	3.76
C(52) ...Os(1)	4.25	C(53) ...Os(1)	3.62
C(61) ...Os(1)	3.75	C(63) ...Os(1)	3.75
Os(4) ...Os(2)	4.11	C(12) ...Os(2)	3.44
O(21) ...Os(2)	3.05	O(22) ...Os(2)	3.06
O(23) ...Os(2)	3.11	C(32) ...Os(2)	3.85
C(33) ...Os(2)	3.15	O(33) ...Os(2)	3.92
C(51) ...Os(2)	3.48	C(61) ...Os(2)	3.57
C(62) ...Os(2)	3.82	Os(5) ...Os(3)	4.12
Os(6) ...Os(3)	4.94	C(11) ...Os(3)	2.94
O(11) ...Os(3)	3.69	C(12) ...Os(3)	3.79
C(22) ...Os(3)	3.62	C(23) ...Os(3)	2.90
O(23) ...Os(3)	3.65	O(31) ...Os(3)	3.01
O(32) ...Os(3)	3.11	O(33) ...Os(3)	3.00
C(41) ...Os(3)	3.52	P(4) ...Os(3)	4.23
Os(6) ...Os(4)	4.94	C(11) ...Os(4)	3.09
O(11) ...Os(4)	3.86	C(13) ...Os(4)	3.51
C(31) ...Os(4)	3.38	C(32) ...Os(4)	4.08
O(41) ...Os(4)	2.95	O(42) ...Os(4)	3.09
O(52) ...Os(4)	3.56	C(53) ...Os(4)	3.63
O(1) ...Os(4)	3.25	O(2) ...Os(4)	3.28
O(3) ...Os(4)	3.38	C(2) ...Os(4)	3.95

C(3) ...Os(4)	4.14	C(13) ...Os(5)	3.23
O(13) ...Os(5)	3.99	C(21) ...Os(5)	3.50
C(42) ...Os(5)	3.24	O(42) ...Os(5)	4.02
O(51) ...Os(5)	3.06	O(52) ...Os(5)	3.06
O(53) ...Os(5)	3.03	C(62) ...Os(5)	3.69
C(63) ...Os(5)	3.65	P(4) ...Os(5)	4.33
C(12) ...Os(6)	3.12	O(12) ...Os(6)	3.84
C(13) ...Os(6)	3.21	O(13) ...Os(6)	3.95
C(21) ...Os(6)	3.03	O(21) ...Os(6)	3.67
C(22) ...Os(6)	3.37	C(51) ...Os(6)	2.94
O(51) ...Os(6)	3.86	C(53) ...Os(6)	3.35
O(53) ...Os(6)	4.11	O(61) ...Os(6)	2.99
O(62) ...Os(6)	3.04	O(63) ...Os(6)	3.11
C(12) ...C(11)	2.65	C(13) ...C(11)	2.66
C(31) ...C(11)	2.84	O(31) ...C(11)	3.39
C(41) ...C(11)	2.97	O(41) ...C(11)	3.37
C(31) ...O(11)	2.99	O(31) ...O(11)	3.09
C(41) ...O(11)	3.15	O(41) ...O(11)	3.12
C(13) ...C(12)	2.96	C(22) ...C(12)	3.18
C(33) ...C(12)	3.39	C(61) ...C(12)	2.91
C(61) ...O(12)	3.07	O(61) ...O(12)	3.19
C(42) ...C(13)	3.31	C(53) ...C(13)	2.91
O(53) ...C(13)	3.32	C(63) ...C(13)	2.98
C(53) ...O(13)	3.10	O(53) ...O(13)	3.08
C(63) ...O(13)	3.11	O(63) ...O(13)	3.15
C(22) ...C(21)	2.70	C(23) ...C(21)	2.81
C(51) ...C(21)	3.01	O(51) ...C(21)	3.21
C(62) ...C(21)	2.95	C(51) ...O(21)	3.41

O(51) ...O(21)	3.17	C(62) ...O(21)	3.00
O(62) ...O(21)	3.09	C(23) ...C(22)	2.75
C(33) ...C(22)	2.85	O(33) ...C(22)	3.08
C(61) ...C(22)	3.12	C(33) ...O(22)	3.20
O(33) ...O(22)	2.97	C(61) ...O(22)	3.39
C(32) ...C(23)	2.73	O(32) ...C(23)	3.29
C(33) ...C(23)	3.18	C(32) ...O(23)	2.85
O(32) ...O(23)	2.99	C(32) ...C(31)	2.62
C(33) ...C(31)	2.76	C(41) ...C(31)	2.90
O(41) ...C(31)	3.15	C(41) ...O(31)	3.22
O(41) ...O(31)	3.02	C(33) ...C(32)	2.84
C(42) ...C(41)	2.62	P(4) ...C(41)	2.76
O(2) ...C(41)	2.92	C(2) ...C(41)	3.42
P(4) ...O(41)	3.61	O(2) ...O(41)	3.32
C(52) ...C(42)	2.86	C(53) ...C(42)	2.92
O(53) ...C(42)	3.35	P(4) ...C(42)	3.15
C(53) ...O(42)	3.14	O(53) ...O(42)	3.14
C(52) ...C(51)	2.63	C(53) ...C(51)	2.52
C(62) ...C(51)	2.83	O(62) ...C(51)	3.34
C(62) ...O(51)	3.08	O(62) ...O(51)	3.10
C(53) ...C(52)	2.56	P(4) ...C(52)	3.18
O(1) ...C(52)	3.15	O(3) ...C(52)	3.38
P(4) ...O(52)	3.23	O(1) ...O(52)	3.03
O(3) ...O(52)	2.90	C(63) ...C(53)	3.11
C(63) ...O(53)	3.29	O(63) ...O(53)	3.30
C(62) ...C(61)	2.62	C(63) ...C(61)	2.83
C(63) ...C(62)	2.64	C(1) ...P(4)	2.87
C(2) ...P(4)	2.60	C(3) ...P(4)	2.67

O(2)	...O(1)	2.60	O(3)	...O(1)	2.35
C(2)	...O(1)	3.15	O(3)	...O(2)	2.14
C(1)	...O(2)	3.40	C(3)	...O(2)	2.72
C(1)	...O(3)	2.95			

Crystallographic Tables for $[Os_7(\mu\text{-}H)_2(CO)_{22}]$, {X-ray study presented in section 3.5, Vol.1}.

TABLE 1 Fractional atomic coordinates and thermal parameters ($Å^2$) for $[Os_7(\mu\text{-}H)_2(CO)_{22}]$

Atom	x	y	z	U_{iso} or U_{eq}
Os(1)	0.27704(4)	-0.02733(9)	0.18763(4)	0.0218(4)
Os(2)	0.15429(5)	-0.15021(10)	0.23733(5)	0.0280(5)
Os(3)	0.18694(5)	0.13433(10)	0.26543(5)	0.0270(5)
Os(4)	0.27017(5)	-0.07256(10)	0.34057(5)	0.0280(5)
Os(5)	0.11796(5)	0.05239(10)	0.12935(5)	0.0295(5)
Os(6)	0.36011(5)	0.24136(10)	0.16192(5)	0.0280(5)
Os(7)	0.36842(5)	-0.01186(10)	0.08045(5)	0.0292(5)
C(11)	0.3604(11)	-0.1079(23)	0.2436(11)	0.029(5)
O(11)	0.4164(8)	-0.1637(17)	0.2680(8)	0.037(4)
C(12)	0.2531(12)	-0.2072(25)	0.1461(12)	0.032(5)
O(12)	0.2430(9)	-0.3136(19)	0.1146(9)	0.046(4)
C(21)	0.1631(13)	-0.3177(28)	0.2902(13)	0.041(6)
O(21)	0.1963(9)	-0.4315(20)	0.3134(9)	0.050(4)
C(22)	0.0727(13)	-0.1367(28)	0.2813(13)	0.045(6)
O(22)	0.0256(10)	-0.1207(21)	0.3116(10)	0.060(5)
C(23)	0.1034(13)	-0.2621(30)	0.1605(14)	0.047(7)
O(23)	0.0739(10)	-0.3397(22)	0.1184(11)	0.066(6)
C(31)	0.1674(13)	0.2937(29)	0.2060(14)	0.046(7)
O(31)	0.1657(10)	0.4049(22)	0.1797(10)	0.063(5)
C(32)	0.2526(13)	0.2362(29)	0.3350(14)	0.044(6)
O(32)	0.2936(10)	0.3128(22)	0.3683(11)	0.063(5)
C(33)	0.1117(15)	0.1732(30)	0.3125(15)	0.054(7)
O(33)	0.0661(13)	0.2060(27)	0.3471(13)	0.092(7)
C(41)	0.3203(11)	-0.2431(25)	0.3675(11)	0.030(5)
O(41)	0.3516(10)	-0.3442(22)	0.3859(10)	0.062(5)

table 1 continued

C(42)	0.2154(12)	-0.0864(25)	0.4109(12)	0.034(5)
O(42)	0.1823(11)	-0.0881(23)	0.4583(11)	0.072(6)
C(43)	0.3487(13)	0.0289(27)	0.3963(13)	0.041(6)
O(43)	0.3952(11)	0.0829(22)	0.4343(11)	0.065(5)
C(51)	0.0905(15)	-0.0629(32)	0.0491(16)	0.057(8)
O(51)	0.0753(11)	-0.1287(23)	-0.0016(11)	0.069(6)
C(52)	0.0990(12)	0.2106(26)	0.0643(12)	0.035(6)
O(52)	0.0874(12)	0.3083(25)	0.0281(12)	0.079(7)
C(53)	0.0245(17)	0.0568(35)	0.1501(17)	0.067(8)
O(53)	-0.0351(10)	0.0624(22)	0.1656(10)	0.065(5)
C(61)	0.3416(12)	0.4110(27)	0.2081(13)	0.038(6)
O(61)	0.3295(10)	0.5134(21)	0.2356(10)	0.059(5)
C(62)	0.4305(13)	0.1786(26)	0.2436(13)	0.038(6)
O(62)	0.4711(9)	0.1514(19)	0.2943(9)	0.050(5)
C(63)	0.2691(13)	0.2887(27)	0.0787(14)	0.042(6)
O(63)	0.2480(11)	0.3205(22)	0.0292(11)	0.066(6)
C(64)	0.4342(12)	0.3263(26)	0.1171(13)	0.037(6)
O(64)	0.4778(9)	0.3727(20)	0.0910(9)	0.053(5)
C(71)	0.4609(11)	-0.0255(24)	0.1461(11)	0.029(5)
O(71)	0.5162(10)	-0.0337(20)	0.1787(10)	0.055(5)
C(72)	0.3761(13)	-0.2021(28)	0.0572(13)	0.039(6)
O(72)	0.3810(12)	-0.3218(25)	0.0464(12)	0.078(6)
C(73)	0.4167(12)	0.0678(25)	0.0109(12)	0.035(6)
O(73)	0.4444(9)	0.1139(20)	-0.0328(9)	0.054(5)
C(74)	0.2749(14)	0.0101(29)	0.0142(14)	0.048(7)
O(74)	0.2213(10)	0.0055(20)	-0.0246(10)	0.055(5)

TABLE 2 Anisotropic thermal parameters ($Å^2$) for $[Os_7(\mu\text{-}H)_2(CO)_{22}]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Os(1)	0.0221(4)	0.0227(5)	0.0206(4)	0.0013(4)	0.0029(3)	0.0018(4)
Os(2)	0.0253(4)	0.0260(5)	0.0326(5)	0.0012(4)	0.0066(4)	-0.0016(4)
Os(3)	0.0288(5)	0.0234(5)	0.0289(5)	-0.0005(4)	0.0074(4)	0.0041(4)
Os(4)	0.033(1)	0.028(1)	0.023(1)	0.002(1)	0.005(1)	0.002(1)
Os(5)	0.024(1)	0.033(1)	0.032(1)	0.002(1)	0.000(1)	0.002(1)
Os(6)	0.0281(5)	0.0[illegible](5)	0.0300(5)	0.0016(4)	0.0044(4)	-0.0014(4)
Os(7)	0.030(1)	0.033(1)	0.025(1)	0.000(1)	0.008(1)	0.003(1)

TABLE 3 Bond lengths (Å) for $[Os_7(\mu\text{-}H)_2(CO)_{22}]$

Os(1) -Os(2)	2.876(1)	Os(1) -Os(3)	2.868(1)
Os(1) -Os(4)	2.964(1)	Os(1) -Os(5)	3.078(1)
Os(1) -Os(6)	3.052(1)	Os(1) -Os(7)	2.887(1)
Os(1) -C(11)	1.884(21)	Os(1) -C(12)	1.887(24)
Os(2) -Os(3)	2.776(1)	Os(2) -Os(4)	2.752(1)
Os(2) -Os(5)	2.795(1)	Os(2) -C(21)	1.89(3)
Os(2) -C(22)	1.870(25)	Os(2) -C(23)	1.91(3)
Os(3) -Os(4)	2.732(1)	Os(3) -Os(5)	2.787(1)
Os(3) -C(31)	1.87(3)	Os(3) -C(32)	1.90(3)
Os(3) -C(33)	1.83(3)	Os(4) -C(11)	2.733(21)
Os(4) -C(41)	1.883(23)	Os(4) -C(42)	1.828(23)
Os(4) -C(43)	1.907(25)	Os(5) -C(51)	1.87(3)
Os(5) -C(52)	1.927(24)	Os(5) -C(53)	1.86(3)
Os(6) -Os(7)	2.861(1)	Os(6) -C(61)	1.883(25)
Os(6) -C(62)	1.941(24)	Os(6) -C(63)	1.929(25)
Os(6) -C(64)	1.925(24)	Os(7) -C(71)	1.949(21)
Os(7) -C(72)	1.86(3)	Os(7) -C(73)	1.884(23)
Os(7) -C(74)	1.98(3)	C(11) -O(11)	1.189(23)
C(12) -O(12)	1.164(25)	C(21) -O(21)	1.17(3)
C(22) -O(22)	1.15(3)	C(23) -O(23)	1.15(3)
C(31) -O(31)	1.16(3)	C(32) -O(32)	1.16(3)
C(33) -O(33)	1.21(3)	C(41) -O(41)	1.14(3)
C(42) -O(42)	1.18(3)	C(43) -O(43)	1.15(3)
C(51) -O(51)	1.14(3)	C(52) -O(52)	1.15(3)
C(53) -O(53)	1.20(3)	C(61) -O(61)	1.14(3)

C(62) -O(62)	1.145(25)	C(63) -O(63)	1.14(3)
C(64) -O(64)	1.12(3)	C(71) -O(71)	1.110(23)
C(72) -O(72)	1.15(3)	C(73) -O(73)	1.14(3)
C(74) -O(74)	1.13(3)		

TABLE 4 Bond angles (°) for $[Os_7(\mu\text{-}H)_2(CO)_{22}]$

Os(3) -Os(1) -Os(2)	57.8(1)	Os(4) -Os(1) -Os(2)	56.2(1)
Os(4) -Os(1) -Os(3)	55.8(1)	Os(5) -Os(1) -Os(2)	55.9(1)
Os(5) -Os(1) -Os(3)	55.8(1)	Os(5) -Os(1) -Os(4)	100.4(1)
Os(6) -Os(1) -Os(2)	147.6(1)	Os(6) -Os(1) -Os(3)	90.3(1)
Os(6) -Os(1) -Os(4)	112.8(1)	Os(6) -Os(1) -Os(5)	103.2(1)
Os(7) -Os(1) -Os(2)	149.3(1)	Os(7) -Os(1) -Os(3)	144.4(1)
Os(7) -Os(1) -Os(4)	146.5(1)	Os(7) -Os(1) -Os(5)	112.9(1)
Os(7) -Os(1) -Os(6)	57.5(1)	C(11) -Os(1) -Os(2)	106.4(6)
C(11) -Os(1) -Os(3)	115.2(6)	C(11) -Os(1) -Os(4)	64.2(6)
C(11) -Os(1) -Os(5)	162.1(6)	C(11) -Os(1) -Os(6)	91.7(7)
C(11) -Os(1) -Os(7)	83.3(6)	C(12) -Os(1) -Os(2)	68.5(7)
C(12) -Os(1) -Os(3)	125.0(7)	C(12) -Os(1) -Os(4)	103.5(7)
C(12) -Os(1) -Os(5)	85.7(7)	C(12) -Os(1) -Os(6)	139.9(7)
C(12) -Os(1) -Os(7)	82.9(7)	C(12) -Os(1) -C(11)	89.2(9)
Os(3) -Os(2) -Os(1)	61.0(1)	Os(4) -Os(2) -Os(1)	63.5(1)
Os(4) -Os(2) -Os(3)	59.2(1)	Os(5) -Os(2) -Os(1)	65.7(1)
Os(5) -Os(2) -Os(3)	60.0(1)	Os(5) -Os(2) -Os(4)	113.6(1)
C(21) -Os(2) -Os(1)	109.9(7)	C(21) -Os(2) -Os(3)	131.9(7)
C(21) -Os(2) -Os(4)	74.3(7)	C(21) -Os(2) -Os(5)	164.9(7)
C(22) -Os(2) -Os(1)	151.9(8)	C(22) -Os(2) -Os(3)	91.0(8)
C(22) -Os(2) -Os(4)	105.4(8)	C(22) -Os(2) -Os(5)	99.8(8)
C(22) -Os(2) -C(21)	90(1)	C(23) -Os(2) -Os(1)	106.8(8)
C(23) -Os(2) -Os(3)	137.8(8)	C(23) -Os(2) -Os(4)	156.0(8)
C(23) -Os(2) -Os(5)	77.9(8)	C(23) -Os(2) -C(21)	90(1)
C(23) -Os(2) -C(22)	92(1)	Os(2) -Os(3) -Os(1)	61.2(1)

Os(4) -Os(3) -Os(1)	63.9(1)	Os(4) -Os(3) -Os(2)	59.9(1)
Os(5) -Os(3) -Os(1)	65.9(1)	Os(5) -Os(3) -Os(2)	60.3(1)
Os(5) -Os(3) -Os(4)	114.5(1)	C(31) -Os(3) -Os(1)	100.6(8)
C(31) -Os(3) -Os(2)	130.0(8)	C(31) -Os(3) -Os(4)	156.6(8)
C(31) -Os(3) -Os(5)	69.7(8)	C(32) -Os(3) -Os(1)	105.1(7)
C(32) -Os(3) -Os(2)	135.6(8)	C(32) -Os(3) -Os(4)	76.0(8)
C(32) -Os(3) -Os(5)	157.3(8)	C(32) -Os(3) -C(31)	93(1)
C(33) -Os(3) -Os(1)	158.4(9)	C(33) -Os(3) -Os(2)	97.2(9)
C(33) -Os(3) -Os(4)	107.6(9)	C(33) -Os(3) -Os(5)	103.9(9)
C(33) -Os(3) -C(31)	93(1)	C(33) -Os(3) -C(32)	91(1)
Os(2) -Os(4) -Os(1)	60.3(1)	Os(3) -Os(4) -Os(1)	60.3(1)
Os(3) -Os(4) -Os(2)	60.8(1)	C(11) -Os(4) -Os(1)	38.4(4)
C(11) -Os(4) -Os(2)	89.4(4)	C(11) -Os(4) -Os(3)	95.6(5)
C(41) -Os(4) -Os(1)	106.4(7)	C(41) -Os(4) -Os(2)	105.0(7)
C(41) -Os(4) -Os(3)	163.6(7)	C(41) -Os(4) -C(11)	75.1(8)
C(42) -Os(4) -Os(1)	148.8(7)	C(42) -Os(4) -Os(2)	91.7(7)
C(42) -Os(4) -Os(3)	95.3(7)	C(42) -Os(4) -C(11)	168.1(9)
C(42) -Os(4) -C(41)	93(1)	C(43) -Os(4) -Os(1)	108.1(7)
C(43) -Os(4) -Os(2)	163.8(7)	C(43) -Os(4) -Os(3)	104.2(7)
C(43) -Os(4) -C(11)	85.9(8)	C(43) -Os(4) -C(41)	89(1)
C(43) -Os(4) -C(42)	96(1)	Os(2) -Os(5) -Os(1)	58.4(1)
Os(3) -Os(5) -Os(1)	58.3(1)	Os(3) -Os(5) -Os(2)	59.7(1)
C(51) -Os(5) -Os(1)	105.1(9)	C(51) -Os(5) -Os(2)	101.5(9)
C(51) -Os(5) -Os(3)	159.0(9)	C(52) -Os(5) -Os(1)	118.4(7)
C(52) -Os(5) -Os(2)	172.2(7)	C(52) -Os(5) -Os(3)	112.6(7)
C(52) -Os(5) -C(51)	86(1)	C(53) -Os(5) -Os(1)	144(1)
C(53) -Os(5) -Os(2)	88(1)	C(53) -Os(5) -Os(3)	95(1)
C(53) -Os(5) -C(51)	93(1)	C(53) -Os(5) -C(52)	93(1)

Os(7) -Os(6) -Os(1)	58.3(1)	C(61) -Os(6) -Os(1)	119.1(7)
C(61) -Os(6) -Os(7)	172.1(7)	C(62) -Os(6) -Os(1)	85.0(7)
C(62) -Os(6) -Os(7)	94.9(7)	C(62) -Os(6) -C(61)	92(1)
C(63) -Os(6) -Os(1)	91.5(8)	C(63) -Os(6) -Os(7)	81.0(8)
C(63) -Os(6) -C(61)	92(1)	C(63) -Os(6) -C(62)	176(1)
C(64) -Os(6) -Os(1)	147.3(7)	C(64) -Os(6) -Os(7)	89.6(7)
C(64) -Os(6) -C(61)	93(1)	C(64) -Os(6) -C(62)	92(1)
C(64) -Os(6) -C(63)	89(1)	Os(6) -Os(7) -Os(1)	64.1(1)
C(71) -Os(7) -Os(1)	96.5(6)	C(71) -Os(7) -Os(6)	80.5(6)
C(72) -Os(7) -Os(1)	101.5(7)	C(72) -Os(7) -Os(6)	161.1(8)
C(72) -Os(7) -C(71)	89(1)	C(73) -Os(7) -Os(1)	159.0(7)
C(73) -Os(7) -Os(6)	97.3(7)	C(73) -Os(7) -C(71)	89.7(9)
C(73) -Os(7) -C(72)	99(1)	C(74) -Os(7) -Os(1)	83.5(7)
C(74) -Os(7) -Os(6)	97.5(8)	C(74) -Os(7) -C(71)	178(1)
C(74) -Os(7) -C(72)	93(1)	C(74) -Os(7) -C(73)	90(1)
Os(4) -C(11) -Os(1)	77.5(7)	O(11) -C(11) -Os(1)	169(2)
O(11) -C(11) -Os(4)	113(1)	O(12) -C(12) -Os(1)	172(2)
O(21) -C(21) -Os(2)	170(2)	O(22) -C(22) -Os(2)	175(2)
O(23) -C(23) -Os(2)	174(2)	O(31) -C(31) -Os(3)	166(2)
O(32) -C(32) -Os(3)	169(2)	O(33) -C(33) -Os(3)	175(3)
O(41) -C(41) -Os(4)	178(2)	O(42) -C(42) -Os(4)	176(2)
O(43) -C(43) -Os(4)	174(2)	O(51) -C(51) -Os(5)	177(3)
O(52) -C(52) -Os(5)	177(2)	O(53) -C(53) -Os(5)	178(3)
O(61) -C(61) -Os(6)	179(2)	O(62) -C(62) -Os(6)	175(2)
O(63) -C(63) -Os(6)	178(2)	O(64) -C(64) -Os(6)	178(2)
O(71) -C(71) -Os(7)	174(2)	O(72) -C(72) -Os(7)	177(2)
O(73) -C(73) -Os(7)	178(2)	O(74) -C(74) -Os(7)	172(2)

TABLE 5 Intermolecular distances (Å) for $[Os_7(\mu\text{-}H)_2(CO)_{22}]$

atom1	atom2	dist	S	a	b	c
O(53)	...Os(2)	4.14	-2	0.0	1.0	1.0
O(51)	...Os(5)	4.05	-1	0.0	0.0	0.0
O(71)	...Os(6)	4.07	-2	1.0	0.0	1.0
O(73)	...Os(7)	3.89	-1	1.0	0.0	0.0
O(41)	...Os(7)	3.90	2	0.0	-1.0	0.0
C(62)	...O(11)	3.27	-2	1.0	1.0	1.0
O(62)	...O(11)	3.12	-2	1.0	1.0	1.0
C(64)	...O(11)	3.23	-2	1.0	1.0	1.0
O(64)	...O(11)	3.06	-2	1.0	1.0	1.0
O(61)	...C(12)	3.32	1	0.0	1.0	0.0
O(61)	...O(12)	3.04	1	0.0	1.0	0.0
O(42)	...O(12)	3.13	2	0.0	-1.0	0.0
O(31)	...C(21)	3.33	1	0.0	1.0	0.0
O(53)	...C(21)	3.24	-2	0.0	1.0	1.0
C(31)	...O(21)	3.28	1	0.0	1.0	0.0
O(31)	...O(21)	2.94	1	0.0	1.0	0.0
C(32)	...O(21)	3.30	1	0.0	1.0	0.0
O(32)	...O(21)	3.09	1	0.0	1.0	0.0
O(61)	...O(21)	3.16	1	0.0	1.0	0.0
O(74)	...O(21)	3.11	2	0.0	-1.0	-1.0
O(53)	...O(21)	3.11	-2	0.0	1.0	1.0
O(53)	...C(22)	3.13	-2	0.0	1.0	1.0
C(53)	...O(22)	3.30	-2	0.0	1.0	1.0
O(53)	...O(22)	3.01	-2	0.0	1.0	1.0
O(31)	...C(23)	3.34	1	0.0	1.0	0.0

O(33) ...C(23)	3.16	-2	0.0	1.0	1.0
O(31) ...O(23)	3.06	1	0.0	1.0	0.0
O(33) ...O(23)	2.84	-2	0.0	1.0	1.0
O(73) ...O(32)	3.18	2	0.0	0.0	-1.0
C(74) ...O(32)	3.31	2	0.0	0.0	-1.0
O(74) ...O(32)	3.14	2	0.0	0.0	-1.0
O(61) ...O(41)	3.12	1	0.0	1.0	0.0
C(72) ...O(41)	3.24	2	0.0	-1.0	-1.0
C(73) ...O(41)	3.24	2	0.0	-1.0	-1.0
O(73) ...O(41)	3.30	2	0.0	-1.0	-1.0
C(74) ...O(41)	3.42	2	0.0	-1.0	-1.0
O(63) ...C(42)	3.35	2	0.0	0.0	-1.0
O(63) ...O(42)	3.01	2	0.0	0.0	-1.0
O(72) ...C(43)	3.42	2	0.0	-1.0	-1.0
O(64) ...O(43)	3.13	2	0.0	0.0	-1.0
O(72) ...O(43)	3.29	2	0.0	-1.0	-1.0
O(73) ...O(43)	3.03	2	0.0	0.0	-1.0
O(64) ...O(43)	3.19	-2	1.0	1.0	1.0
C(52) ...O(51)	3.36	-1	0.0	0.0	0.0
C(53) ...O(51)	3.17	-1	0.0	0.0	0.0
O(53) ...O(51)	3.14	-1	0.0	0.0	0.0
O(71) ...C(61)	3.15	-2	1.0	0.0	1.0
O(71) ...O(61)	3.08	-2	1.0	0.0	1.0
O(71) ...C(62)	3.16	-2	1.0	0.0	1.0
C(71) ...O(62)	3.41	-2	1.0	0.0	1.0
O(71) ...O(62)	3.01	-2	1.0	0.0	1.0
O(73) ...C(71)	3.14	-1	1.0	0.0	0.0
O(73) ...O(71)	3.09	-1	1.0	0.0	0.0

C(73) ...C(73)	3.46	-1	1.0	0.0	0.0
O(73) ...C(73)	3.08	-1	1.0	0.0	0.0
O(73) ...O(73)	3.09	-1	1.0	0.0	0.0

Symmetry Transformations:

The second atom is related to the first atom, at (x,y,z), by the symmetry operation S with (a,b,c) added to the (x',y',z') of S.

Where S =

1	x, y, z
2	x, 0.5-y, 0.5+z

TABLE 6 Intramolecular distances (Å) for $[Os_7(\mu\text{-}H)_2(CO)_{22}]$

O(11) ...Os(1)	3.06	O(12) ...Os(1)	3.05
C(21) ...Os(1)	3.95	C(23) ...Os(1)	3.89
C(31) ...Os(1)	3.70	C(32) ...Os(1)	3.83
C(41) ...Os(1)	3.94	C(43) ...Os(1)	3.99
C(51) ...Os(1)	3.99	C(62) ...Os(1)	3.47
C(63) ...Os(1)	3.65	C(71) ...Os(1)	3.66
C(72) ...Os(1)	3.73	C(74) ...Os(1)	3.31
O(74) ...Os(1)	3.99	C(11) ...Os(2)	3.86
C(12) ...Os(2)	2.80	O(12) ...Os(2)	3.45
O(21) ...Os(2)	3.05	O(22) ...Os(2)	3.01
O(23) ...Os(2)	3.06	C(31) ...Os(2)	4.23
C(33) ...Os(2)	3.51	C(41) ...Os(2)	3.72
C(42) ...Os(2)	3.35	C(51) ...Os(2)	3.66
C(53) ...Os(2)	3.32	O(53) ...Os(2)	4.09
Os(6) ...Os(3)	4.20	C(11) ...Os(3)	4.05
C(12) ...Os(3)	4.24	C(22) ...Os(3)	3.37
O(22) ...Os(3)	4.07	O(31) ...Os(3)	3.01
O(32) ...Os(3)	3.04	O(33) ...Os(3)	3.04
C(42) ...Os(3)	3.42	C(43) ...Os(3)	3.69
C(52) ...Os(3)	3.95	C(53) ...Os(3)	3.49
C(61) ...Os(3)	4.18	Os(5) ...Os(4)	4.64
O(11) ...Os(4)	3.38	C(12) ...Os(4)	3.87
C(21) ...Os(4)	2.89	O(21) ...Os(4)	3.65
C(22) ...Os(4)	3.71	C(32) ...Os(4)	2.92
O(32) ...Os(4)	3.68	C(33) ...Os(4)	3.72

O(41) ...Os(4)	3.02	O(42) ...Os(4)	3.01
O(43) ...Os(4)	3.05	Os(6) ...Os(5)	4.80
Os(7) ...Os(5)	4.97	C(12) ...Os(5)	3.49
C(22) ...Os(5)	3.62	C(23) ...Os(5)	3.04
O(23) ...Os(5)	3.78	C(31) ...Os(5)	2.77
O(31) ...Os(5)	3.52	C(33) ...Os(5)	3.68
O(51) ...Os(5)	3.01	O(52) ...Os(5)	3.07
O(53) ...Os(5)	3.06	C(63) ...Os(5)	4.15
C(74) ...Os(5)	3.98	O(74) ...Os(5)	3.81
C(11) ...Os(6)	3.63	C(31) ...Os(6)	3.88
O(31) ...Os(6)	4.02	C(32) ...Os(6)	4.15
O(61) ...Os(6)	3.02	O(62) ...Os(6)	3.08
O(63) ...Os(6)	3.07	O(64) ...Os(6)	3.04
C(71) ...Os(6)	3.18	O(71) ...Os(6)	3.87
C(73) ...Os(6)	3.62	C(74) ...Os(6)	3.68
C(11) ...Os(7)	3.26	O(11) ...Os(7)	3.80
C(12) ...Os(7)	3.25	O(12) ...Os(7)	3.81
C(62) ...Os(7)	3.59	C(63) ...Os(7)	3.19
O(63) ...Os(7)	3.88	C(64) ...Os(7)	3.44
O(64) ...Os(7)	4.14	O(71) ...Os(7)	3.06
O(72) ...Os(7)	3.01	O(73) ...Os(7)	3.02
O(74) ...Os(7)	3.10	C(12) ...C(11)	2.65
C(41) ...C(11)	2.89	C(43) ...C(11)	3.22
C(62) ...C(11)	3.00	O(62) ...C(11)	3.23
C(71) ...C(11)	2.97	C(41) ...O(11)	2.93
O(41) ...O(11)	3.21	C(62) ...O(11)	3.27
O(62) ...O(11)	3.15	C(71) ...O(11)	2.90
O(71) ...O(11)	3.00	C(21) ...C(12)	3.40

C(23) ...C(12)	2.91	C(72) ...C(12)	3.09
C(74) ...C(12)	3.32	C(23) ...O(12)	2.94
O(23) ...O(12)	3.19	C(72) ...O(12)	3.08
O(72) ...O(12)	3.09	C(22) ...C(21)	2.66
C(23) ...C(21)	2.70	C(41) ...C(21)	2.81
O(41) ...C(21)	3.36	C(42) ...C(21)	3.14
C(41) ...O(21)	2.95	O(41) ...O(21)	3.10
C(23) ...C(22)	2.73	C(33) ...C(22)	3.04
C(42) ...C(22)	3.33	C(53) ...C(22)	3.09
O(53) ...C(22)	3.29	C(33) ...O(22)	3.20
O(33) ...O(22)	3.21	O(53) ...O(22)	3.29
C(51) ...C(23)	2.81	O(51) ...C(23)	3.28
C(53) ...C(23)	3.33	C(51) ...O(23)	2.96
O(51) ...O(23)	3.03	C(32) ...C(31)	2.73
C(33) ...C(31)	2.69	C(52) ...C(31)	2.88
C(53) ...C(31)	3.50	C(61) ...C(31)	3.43
C(52) ...O(31)	2.96	O(52) ...O(31)	3.13
C(61) ...O(31)	3.24	O(61) ...O(31)	3.23
C(33) ...C(32)	2.66	C(42) ...C(32)	3.48
C(43) ...C(32)	2.77	O(43) ...C(32)	3.31
C(43) ...O(32)	2.88	O(43) ...O(32)	3.00
O(61) ...O(32)	3.31	C(42) ...C(33)	3.45
C(53) ...C(33)	3.41	C(42) ...C(41)	2.70
C(43) ...C(41)	2.65	C(43) ...C(42)	2.78
O(62) ...O(43)	3.30	C(52) ...C(51)	2.59
C(53) ...C(51)	2.71	O(74) ...C(51)	3.10
O(74) ...O(51)	3.11	C(53) ...C(52)	2.74
O(63) ...C(52)	3.15	O(63) ...O(52)	3.00

C(62) ...C(61)	2.76	C(63) ...C(61)	2.73
C(64) ...C(61)	2.77	C(64) ...C(62)	2.79
C(71) ...C(62)	2.80	O(71) ...C(62)	2.96
C(71) ...O(62)	3.25	O(71) ...O(62)	3.04
C(64) ...C(63)	2.71	C(74) ...C(63)	2.89
O(74) ...C(63)	3.42	C(74) ...O(63)	2.99
O(74) ...O(63)	3.15	C(71) ...C(64)	3.38
C(73) ...C(64)	3.14	C(73) ...O(64)	3.35
C(72) ...C(71)	2.68	C(73) ...C(71)	2.70
C(73) ...C(72)	2.84	C(74) ...C(72)	2.77
C(74) ...C(73)	2.72		

Crystallographic Tables for $[Os_7H_2(CO)_{19}\{MeC{=}CMe\}]$, {X-ray study presented in section 3.6, Vol.1}.

TABLE 1 Fractional atomic coordinates and thermal parameters ($Å^2$) for $[Os_7(H)_2(CO)_{19}\{MeC{=}CMe\}]$

Atom	x	y	z	U_{iso} or U_{eq}
Os(1)	0.10048(4)	0.35211(16)	0.22377(7)	0.0216(8)
Os(2)	0.14316(4)	0.08494(16)	0.25321(7)	0.0204(7)
Os(3)	0.18267(4)	0.35182(16)	0.30278(7)	0.0202(8)
Os(4)	0.16789(4)	0.14991(16)	0.38825(7)	0.0201(8)
Os(5)	0.08977(4)	0.14713(16)	0.31137(7)	0.0208(8)
Os(6)	0.11358(5)	0.14198(16)	0.44464(7)	0.0239(8)
Os(7)	0.15416(5)	0.30868(17)	0.16952(7)	0.0253(8)
C(11)	0.0690(13)	0.4398(51)	0.2598(22)	0.048(12)
O(11)	0.0508(10)	0.5152(41)	0.2779(17)	0.066(10)
C(12)	0.0588(11)	0.2687(41)	0.1506(18)	0.028(9)
O(12)	0.0354(8)	0.2324(33)	0.1071(14)	0.047(8)
C(13)	0.1029(12)	0.5293(51)	0.1837(21)	0.043(11)
O(13)	0.1041(11)	0.6527(43)	0.1652(18)	0.075(11)
C(21)	0.1903(11)	0.0200(42)	0.2477(18)	0.030(9)
O(21)	0.2177(8)	-0.0190(32)	0.2465(14)	0.043(7)
C(22)	0.1120(11)	0.0256(42)	0.1707(18)	0.028(9)
O(22)	0.0900(9)	-0.0306(35)	0.1224(16)	0.056(9)
C(23)	0.1389(10)	-0.1067(41)	0.2859(18)	0.027(9)
O(23)	0.1385(8)	-0.2273(32)	0.3030(14)	0.044(8)
C(31)	0.1959(13)	0.4402(54)	0.3858(23)	0.051(12)
O(31)	0.2085(10)	0.5090(41)	0.4308(17)	0.067(10)
C(32)	0.2314(12)	0.2726(46)	0.3211(20)	0.038(10)
O(32)	0.2626(8)	0.2336(33)	0.3318(14)	0.046(8)
C(33)	0.1943(11)	0.5345(45)	0.2691(19)	0.034(10)
O(33)	0.1982(8)	0.6473(32)	0.2519(13)	0.041(7)

table 1 continued

C(41)	0.1971(11)	0.2195(42)	0.4704(19)	0.030(9)
O(41)	0.2151(8)	0.2610(33)	0.5225(15)	0.049(8)
C(42)	0.2111(12)	0.0360(45)	0.4002(19)	0.037(10)
O(42)	0.2391(8)	-0.0416(33)	0.4048(14)	0.048(8)
C(51)	0.0484(15)	0.2206(59)	0.3243(25)	0.061(14)
O(51)	0.0203(9)	0.2676(34)	0.3269(15)	0.050(8)
C(52)	0.0560(11)	0.0447(42)	0.2433(18)	0.029(9)
O(52)	0.0353(10)	-0.0373(38)	0.2066(17)	0.064(10)
C(61)	0.1434(10)	0.1019(39)	0.5293(17)	0.023(8)
O(61)	0.1628(9)	0.0728(35)	0.5838(16)	0.056(9)
C(62)	0.0699(12)	0.0764(47)	0.4584(20)	0.040(10)
O(62)	0.0412(9)	0.0378(35)	0.4627(15)	0.055(9)
C(63)	0.1119(16)	0.3446(63)	0.4600(27)	0.065(15)
O(63)	0.1076(12)	0.4655(49)	0.4682(20)	0.089(13)
C(71)	0.1975(13)	0.2312(49)	0.1578(21)	0.045(11)
O(71)	0.2234(9)	0.1971(35)	0.1485(15)	0.055(9)
C(72)	0.1207(11)	0.2460(43)	0.0903(19)	0.033(10)
O(72)	0.0971(9)	0.2051(35)	0.0377(15)	0.054(9)
C(73)	0.1604(15)	0.4834(65)	0.1296(26)	0.067(15)
O(73)	0.1632(10)	0.5980(41)	0.1057(17)	0.067(10)
C(1)	0.1028(10)	-0.0338(39)	0.3715(17)	0.025(8)
C(2)	0.0756(11)	-0.1675(44)	0.3645(19)	0.034(10)
C(3)	0.1424(11)	-0.0410(42)	0.4117(18)	0.031(9)
C(4)	0.1634(11)	-0.1590(44)	0.4543(19)	0.034(10)

TABLE 2 Fractional atomic coordinates for the hydrogen atoms for $[Os_7(H)_2(CO)_{19}\{MeC{=}CMe\}]$

Atom	x	y	z
H(15)	0.1372	0.4433	0.2943
H(45)	0.1277	0.2826	0.3548

TABLE 3 Anisotropic thermal parameters (Å^2) for $[Os_7(H)_2(CO)_{19}\{MeC{=}CMe\}]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Os(1)	0.022(1)	0.019(1)	0.024(1)	0.002(1)	0.007(1)	0.000(1)
Os(2)	0.025(1)	0.015(1)	0.021(1)	-0.003(1)	0.011(1)	-0.002(1)
Os(3)	0.022(1)	0.019(1)	0.021(1)	-0.001(1)	0.008(1)	-0.004(1)
Os(4)	0.020(1)	0.022(1)	0.018(1)	0.000(1)	0.008(1)	0.001(1)
Os(5)	0.020(1)	0.022(1)	0.021(1)	-0.001(1)	0.008(1)	-0.003(1)
Os(6)	0.027(1)	0.022(1)	0.023(1)	0.000(1)	0.014(1)	-0.001(1)
Os(7)	0.029(1)	0.027(1)	0.021(1)	0.001(1)	0.010(1)	-0.006(1)

TABLE 4 Bond lengths (A°) for $[Os_7(H)_2(CO)_{19}\{MeC{=}CMe\}]$

Os(1) -Os(2)	2.845(1)	Os(1) -Os(3)	2.919(1)
Os(1) -Os(5)	2.856(1)	Os(1) -Os(7)	2.770(1)
Os(1) -C(11)	1.86(6)	Os(1) -C(12)	1.94(3)
Os(1) -C(13)	1.87(5)	Os(2) -Os(3)	2.839(1)
Os(2) -Os(4)	2.882(1)	Os(2) -Os(5)	2.854(1)
Os(2) -Os(7)	2.911(1)	Os(2) -C(21)	1.92(4)
Os(2) -C(22)	1.86(3)	Os(2) -C(23)	1.92(4)
Os(3) -Os(4)	2.868(1)	Os(3) -Os(7)	2.802(1)
Os(3) -C(31)	1.92(5)	Os(3) -C(32)	1.87(4)
Os(3) -C(33)	1.94(4)	Os(4) -Os(5)	2.783(1)
Os(4) -Os(6)	2.801(1)	Os(4) -C(41)	1.86(4)
Os(4) -C(42)	1.86(4)	Os(4) -C(3)	2.15(4)
Os(5) -Os(6)	2.786(1)	Os(5) -C(51)	1.82(6)
Os(5) -C(52)	1.83(3)	Os(5) -C(1)	2.07(4)
Os(6) -C(61)	1.84(3)	Os(6) -C(62)	1.89(5)
Os(6) -C(63)	1.88(6)	Os(6) -C(1)	2.22(4)
Os(6) -C(3)	2.26(4)	Os(7) -C(71)	1.89(5)
Os(7) -C(72)	1.84(4)	Os(7) -C(73)	1.88(6)
C(11) -O(11)	1.15(7)	C(12) -O(12)	1.09(4)
C(13) -O(13)	1.20(6)	C(21) -O(21)	1.10(5)
C(22) -O(22)	1.20(4)	C(23) -O(23)	1.16(5)
C(31) -O(31)	1.13(6)	C(32) -O(32)	1.16(5)
C(33) -O(33)	1.13(5)	C(41) -O(41)	1.17(5)
C(42) -O(42)	1.24(5)	C(51) -O(51)	1.17(7)
C(52) -O(52)	1.16(5)	C(61) -O(61)	1.19(4)

table 4 continued

C(62) -O(62)	1.18(6)	C(63) -O(63)	1.14(7)
C(71) -O(71)	1.12(7)	C(72) -O(72)	1.23(4)
C(73) -O(73)	1.20(7)	C(1) -C(2)	1.56(6)
C(1) -C(3)	1.42(5)	C(3) -C(4)	1.45(5)

TABLE 5 Bond angles (°) for $[Os_7(H)_2(CO)_{19}\{MeC{=}CMe\}]$

Os(3) -Os(1) -Os(2)	59.0(1)	Os(5) -Os(1) -Os(2)	60.1(1)
Os(5) -Os(1) -Os(3)	88.7(1)	Os(7) -Os(1) -Os(2)	62.4(1)
Os(7) -Os(1) -Os(3)	58.9(1)	Os(7) -Os(1) -Os(5)	122.4(1)
C(11) -Os(1) -Os(2)	131(1)	C(11) -Os(1) -Os(3)	116(1)
C(11) -Os(1) -Os(5)	72(1)	C(11) -Os(1) -Os(7)	163(1)
C(12) -Os(1) -Os(2)	94(1)	C(12) -Os(1) -Os(3)	147(1)
C(12) -Os(1) -Os(5)	93(1)	C(12) -Os(1) -Os(7)	93(1)
C(12) -Os(1) -C(11)	95(2)	C(13) -Os(1) -Os(2)	136(2)
C(13) -Os(1) -Os(3)	93(1)	C(13) -Os(1) -Os(5)	161(2)
C(13) -Os(1) -Os(7)	74(2)	C(13) -Os(1) -C(11)	90(2)
C(13) -Os(1) -C(12)	96(2)	Os(3) -Os(2) -Os(1)	61.8(1)
Os(4) -Os(2) -Os(1)	89.7(1)	Os(4) -Os(2) -Os(3)	60.2(1)
Os(5) -Os(2) -Os(1)	60.1(1)	Os(5) -Os(2) -Os(3)	90.4(1)
Os(5) -Os(2) -Os(4)	58.1(1)	Os(7) -Os(2) -Os(1)	57.5(1)
Os(7) -Os(2) -Os(3)	58.3(1)	Os(7) -Os(2) -Os(4)	118.3(1)
Os(7) -Os(2) -Os(5)	117.6(1)	C(21) -Os(2) -Os(1)	134(1)
C(21) -Os(2) -Os(3)	86(1)	C(21) -Os(2) -Os(4)	102(1)
C(21) -Os(2) -Os(5)	158(1)	C(21) -Os(2) -Os(7)	79(1)
C(22) -Os(2) -Os(1)	86(1)	C(22) -Os(2) -Os(3)	132(1)
C(22) -Os(2) -Os(4)	160(1)	C(22) -Os(2) -Os(5)	103(1)
C(22) -Os(2) -Os(7)	75(1)	C(22) -Os(2) -C(21)	95(2)
C(23) -Os(2) -Os(1)	138(1)	C(23) -Os(2) -Os(3)	137(1)
C(23) -Os(2) -Os(4)	80(1)	C(23) -Os(2) -Os(5)	80(1)
C(23) -Os(2) -Os(7)	159(1)	C(23) -Os(2) -C(21)	88(2)
C(23) -Os(2) -C(22)	90(2)	Os(2) -Os(3) -Os(1)	59.2(1)

table 5 continued

Os(4) -Os(3) -Os(1)	88.5(1)	Os(4) -Os(3) -Os(2)	60.7(1)
Os(7) -Os(3) -Os(1)	57.9(1)	Os(7) -Os(3) -Os(2)	62.1(1)
Os(7) -Os(3) -Os(4)	122.6(1)	C(31) -Os(3) -Os(1)	114(1)
C(31) -Os(3) -Os(2)	130(2)	C(31) -Os(3) -Os(4)	70(2)
C(31) -Os(3) -Os(7)	162(1)	C(32) -Os(3) -Os(1)	149(1)
C(32) -Os(3) -Os(2)	95(1)	C(32) -Os(3) -Os(4)	92(1)
C(32) -Os(3) -Os(7)	97(1)	C(32) -Os(3) -C(31)	95(2)
C(33) -Os(3) -Os(1)	96(1)	C(33) -Os(3) -Os(2)	138(1)
C(33) -Os(3) -Os(4)	160(1)	C(33) -Os(3) -Os(7)	76(1)
C(33) -Os(3) -C(31)	91(2)	C(33) -Os(3) -C(32)	94(2)
Os(3) -Os(4) -Os(2)	59.2(1)	Os(5) -Os(4) -Os(2)	60.5(1)
Os(5) -Os(4) -Os(3)	91.2(1)	Os(6) -Os(4) -Os(2)	118.7(1)
Os(6) -Os(4) -Os(3)	133.5(1)	Os(6) -Os(4) -Os(5)	59.9(1)
C(41) -Os(4) -Os(2)	161(1)	C(41) -Os(4) -Os(3)	105(1)
C(41) -Os(4) -Os(5)	134(1)	C(41) -Os(4) -Os(6)	79(1)
C(42) -Os(4) -Os(2)	87(1)	C(42) -Os(4) -Os(3)	94(1)
C(42) -Os(4) -Os(5)	138(1)	C(42) -Os(4) -Os(6)	132(1)
C(42) -Os(4) -C(41)	84(2)	C(3) -Os(4) -Os(2)	96(1)
C(3) -Os(4) -Os(3)	155(1)	C(3) -Os(4) -Os(5)	71.2(9)
C(3) -Os(4) -Os(6)	52(1)	C(3) -Os(4) -C(41)	100(2)
C(3) -Os(4) -C(42)	88(2)	Os(2) -Os(5) -Os(1)	59.8(1)
Os(4) -Os(5) -Os(1)	91.5(1)	Os(4) -Os(5) -Os(2)	61.5(1)
Os(6) -Os(5) -Os(1)	133.2(1)	Os(6) -Os(5) -Os(2)	120.2(1)
Os(6) -Os(5) -Os(4)	60.4(1)	C(51) -Os(5) -Os(1)	103(2)
C(51) -Os(5) -Os(2)	161(2)	C(51) -Os(5) -Os(4)	132(1)
C(51) -Os(5) -Os(6)	77(2)	C(52) -Os(5) -Os(1)	89(1)
C(52) -Os(5) -Os(2)	84(1)	C(52) -Os(5) -Os(4)	139(1)
C(52) -Os(5) -Os(6)	137(1)	C(52) -Os(5) -C(51)	88(2)

table 5 continued

C(1) -Os(5) -Os(1)	156(1)	C(1) -Os(5) -Os(2)	96(1)
C(1) -Os(5) -Os(4)	71(1)	C(1) -Os(5) -Os(6)	52(1)
C(1) -Os(5) -C(51)	101(2)	C(1) -Os(5) -C(52)	93(1)
Os(5) -Os(6) -Os(4)	59.8(1)	C(61) -Os(6) -Os(4)	102(1)
C(61) -Os(6) -Os(5)	159(1)	C(62) -Os(6) -Os(4)	157(1)
C(62) -Os(6) -Os(5)	104(1)	C(62) -Os(6) -C(61)	89(2)
C(63) -Os(6) -Os(4)	98(2)	C(63) -Os(6) -Os(5)	99(2)
C(63) -Os(6) -C(61)	93(2)	C(63) -Os(6) -C(62)	101(2)
C(1) -Os(6) -Os(4)	69(1)	C(1) -Os(6) -Os(5)	47.1(9)
C(1) -Os(6) -C(61)	119(1)	C(1) -Os(6) -C(62)	89(2)
C(1) -Os(6) -C(63)	146(2)	C(3) -Os(6) -Os(4)	49(1)
C(3) -Os(6) -Os(5)	69.7(9)	C(3) -Os(6) -C(61)	91(1)
C(3) -Os(6) -C(62)	112(2)	C(3) -Os(6) -C(63)	147(2)
C(3) -Os(6) -C(1)	37(1)	Os(2) -Os(7) -Os(1)	60.0(1)
Os(3) -Os(7) -Os(1)	63.2(1)	Os(3) -Os(7) -Os(2)	59.6(1)
C(71) -Os(7) -Os(1)	159(1)	C(71) -Os(7) -Os(2)	100(1)
C(71) -Os(7) -Os(3)	102(1)	C(72) -Os(7) -Os(1)	97(1)
C(72) -Os(7) -Os(2)	101(1)	C(72) -Os(7) -Os(3)	157(1)
C(72) -Os(7) -C(71)	93(2)	C(73) -Os(7) -Os(1)	110(2)
C(73) -Os(7) -Os(2)	167(2)	C(73) -Os(7) -Os(3)	109(2)
C(73) -Os(7) -C(71)	88(2)	C(73) -Os(7) -C(72)	88(2)
O(11) -C(11) -Os(1)	168(4)	O(12) -C(12) -Os(1)	174(4)
O(13) -C(13) -Os(1)	171(4)	O(21) -C(21) -Os(2)	178(4)
O(22) -C(22) -Os(2)	169(4)	O(23) -C(23) -Os(2)	174(4)
O(31) -C(31) -Os(3)	166(5)	O(32) -C(32) -Os(3)	175(4)
O(33) -C(33) -Os(3)	172(4)	O(41) -C(41) -Os(4)	179(4)
O(42) -C(42) -Os(4)	177(3)	O(51) -C(51) -Os(5)	174(4)
O(52) -C(52) -Os(5)	170(4)	O(61) -C(61) -Os(6)	179(3)

table 5 continued

O(62)	-C(62)	-Os(6)	175(3)	O(63)	-C(63)	-Os(6)	174(5)
O(71)	-C(71)	-Os(7)	174(4)	O(72)	-C(72)	-Os(7)	178(4)
O(73)	-C(73)	-Os(7)	177(6)	Os(6)	-C(1)	-Os(5)	81(1)
C(2)	-C(1)	-Os(5)	125(2)	C(2)	-C(1)	-Os(6)	124(3)
C(3)	-C(1)	-Os(5)	112(3)	C(3)	-C(1)	-Os(6)	73(2)
C(3)	-C(1)	-C(2)	121(3)	Os(6)	-C(3)	-Os(4)	79(1)
C(1)	-C(3)	-Os(4)	105(3)	C(1)	-C(3)	-Os(6)	70(2)
C(4)	-C(3)	-Os(4)	125(3)	C(4)	-C(3)	-Os(6)	122(3)
C(4)	-C(3)	-C(1)	129(4)				

TABLE 6 Intermolecular distances (Å) for $[Os_7(H)_2(CO)_{19}\{MeC{=}CMe\}]$

atom1	atom2	dist	S	a	b	c
C(2)	...O(11)	3.40	1	0.0	-1.0	0.0
O(23)	...C(13)	3.34	1	0.0	-1.0	0.0
C(22)	...O(13)	3.40	1	0.0	-1.0	0.0
O(22)	...O(13)	3.02	1	0.0	-1.0	0.0
C(23)	...O(13)	3.34	1	0.0	-1.0	0.0
O(23)	...O(13)	3.07	1	0.0	-1.0	0.0
O(33)	...C(21)	3.40	1	0.0	1.0	0.0
O(33)	...O(21)	3.13	1	0.0	1.0	0.0
O(32)	...O(21)	3.12	-2	1.0	1.0	1.0
C(33)	...O(23)	3.31	1	0.0	1.0	0.0
O(33)	...O(23)	3.12	1	0.0	1.0	0.0
H(15)	...O(23)	3.00	1	0.0	1.0	0.0
O(33)	...O(32)	2.92	-2	1.0	1.0	1.0
O(73)	...O(32)	2.88	-2	1.0	1.0	1.0
O(71)	...C(33)	3.29	-2	1.0	0.0	1.0
O(71)	...O(33)	2.98	-2	1.0	0.0	1.0
O(71)	...O(42)	3.22	-2	1.0	1.0	1.0

Symmetry Transformations:

The second atom is related to the first atom, at (x,y,z), by the symmetry operation S with (a,b,c) added to the (x',y',z') of S.

Where S =

1	x, y, z
2	0.5+x, 0.5-y, 0.5+z

TABLE 7 Intramolecular distances (Å) for $[Os_7(H)_2(CO)_{19}\{MeC{=}CMe\}]$

Os(4) ...Os(1)	4.04	O(11) ...Os(1)	2.99
O(12) ...Os(1)	3.03	O(13) ...Os(1)	3.06
C(22) ...Os(1)	3.29	O(22) ...Os(1)	4.09
C(31) ...Os(1)	4.10	C(33) ...Os(1)	3.68
C(51) ...Os(1)	3.72	C(52) ...Os(1)	3.37
C(72) ...Os(1)	3.52	C(73) ...Os(1)	3.84
H(45) ...Os(1)	2.80	Os(6) ...Os(2)	4.89
C(12) ...Os(2)	3.55	O(21) ...Os(2)	3.03
O(22) ...Os(2)	3.04	O(23) ...Os(2)	3.08
C(32) ...Os(2)	3.52	C(42) ...Os(2)	3.35
O(42) ...Os(2)	4.07	C(52) ...Os(2)	3.23
O(52) ...Os(2)	3.95	C(71) ...Os(2)	3.74
C(72) ...Os(2)	3.74	C(1) ...Os(2)	3.71
C(3) ...Os(2)	3.77	H(15) ...Os(2)	3.41
H(45) ...Os(2)	3.14	Os(5) ...Os(3)	4.04
C(11) ...Os(3)	4.09	C(13) ...Os(3)	3.55
C(21) ...Os(3)	3.31	O(21) ...Os(3)	4.00
O(31) ...Os(3)	3.03	O(32) ...Os(3)	3.03
O(33) ...Os(3)	3.06	C(41) ...Os(3)	3.80
C(42) ...Os(3)	3.52	C(71) ...Os(3)	3.69
C(73) ...Os(3)	3.86	H(45) ...Os(3)	2.82
Os(7) ...Os(4)	4.97	C(21) ...Os(4)	3.77
C(23) ...Os(4)	3.16	O(23) ...Os(4)	3.88
C(31) ...Os(4)	2.85	O(31) ...Os(4)	3.57
C(32) ...Os(4)	3.48	O(41) ...Os(4)	3.03

table 7 continued

O(42) ...Os(4)	3.10	C(51) ...Os(4)	4.22
C(61) ...Os(4)	3.66	C(63) ...Os(4)	3.59
C(1) ...Os(4)	2.87	C(4) ...Os(4)	3.21
H(15) ...Os(4)	3.32	Os(7) ...Os(5)	4.93
C(11) ...Os(5)	2.88	O(11) ...Os(5)	3.61
C(12) ...Os(5)	3.53	C(22) ...Os(5)	3.75
C(23) ...Os(5)	3.15	O(23) ...Os(5)	3.90
O(51) ...Os(5)	2.99	O(52) ...Os(5)	2.98
C(62) ...Os(5)	3.73	C(63) ...Os(5)	3.61
C(2) ...Os(5)	3.22	C(3) ...Os(5)	2.92
H(15) ...Os(5)	3.33	C(41) ...Os(6)	3.06
O(41) ...Os(6)	3.70	C(51) ...Os(6)	2.96
O(51) ...Os(6)	3.68	O(61) ...Os(6)	3.03
O(62) ...Os(6)	3.06	O(63) ...Os(6)	3.01
C(2) ...Os(6)	3.35	C(4) ...Os(6)	3.28
H(45) ...Os(6)	2.62	C(12) ...Os(7)	3.48
C(13) ...Os(7)	2.89	O(13) ...Os(7)	3.63
C(21) ...Os(7)	3.16	O(21) ...Os(7)	3.80
C(22) ...Os(7)	3.03	O(22) ...Os(7)	3.81
C(32) ...Os(7)	3.55	C(33) ...Os(7)	2.99
O(33) ...Os(7)	3.64	O(71) ...Os(7)	3.01
O(72) ...Os(7)	3.07	O(73) ...Os(7)	3.08
H(15) ...Os(7)	3.35	C(12) ...C(11)	2.81
C(13) ...C(11)	2.64	C(51) ...C(11)	2.75
O(51) ...C(11)	3.20	H(15) ...C(11)	2.38
H(45) ...C(11)	2.81	C(13) ...O(11)	3.41
C(51) ...O(11)	2.89	O(51) ...O(11)	2.93
C(13) ...C(12)	2.82	C(22) ...C(12)	2.90

table 7 continued

O(22) ...C(12)	3.12	C(52) ...C(12)	2.95
O(52) ...C(12)	3.31	C(72) ...C(12)	3.13
C(22) ...O(12)	3.28	O(22) ...O(12)	3.08
C(52) ...O(12)	3.33	O(52) ...O(12)	3.32
C(72) ...O(12)	3.38	O(72) ...O(12)	3.28
C(33) ...C(13)	3.24	C(73) ...C(13)	2.90
H(15) ...C(13)	2.45	O(33) ...O(13)	3.33
C(73) ...O(13)	2.97	O(73) ...O(13)	3.06
C(22) ...C(21)	2.79	C(23) ...C(21)	2.67
C(32) ...C(21)	2.90	O(32) ...C(21)	3.29
C(42) ...C(21)	3.22	O(42) ...C(21)	3.35
C(71) ...C(21)	2.88	O(71) ...C(21)	3.37
C(32) ...O(21)	3.07	O(32) ...O(21)	3.05
C(71) ...O(21)	2.93	O(71) ...O(21)	3.03
C(23) ...C(22)	2.68	C(52) ...C(22)	3.14
O(52) ...C(22)	3.34	C(72) ...C(22)	2.80
O(72) ...C(22)	3.27	O(52) ...O(22)	3.30
C(72) ...O(22)	2.97	O(72) ...O(22)	2.95
C(42) ...C(23)	3.21	C(52) ...C(23)	3.21
C(1) ...C(23)	2.84	C(3) ...C(23)	2.85
C(1) ...O(23)	2.98	C(2) ...O(23)	3.22
C(3) ...O(23)	2.94	C(4) ...O(23)	3.23
C(32) ...C(31)	2.78	C(33) ...C(31)	2.75
C(41) ...C(31)	2.76	O(41) ...C(31)	3.31
H(15) ...C(31)	2.38	H(45) ...C(31)	2.79
C(41) ...O(31)	2.86	O(41) ...O(31)	3.00
C(33) ...C(32)	2.78	C(42) ...C(32)	3.07
O(42) ...C(32)	3.37	C(71) ...C(32)	3.42

table 7 continued

O(42)	...O(32)	3.30	C(73)	...C(33)	2.94
H(15)	...C(33)	2.57	C(73)	...O(33)	2.97
O(73)	...O(33)	3.08	C(42)	...C(41)	2.49
C(61)	...C(41)	3.01	C(63)	...C(41)	3.33
C(3)	...C(41)	3.08	H(45)	...C(41)	2.95
C(42)	...O(41)	3.39	C(61)	...O(41)	3.12
O(61)	...O(41)	3.29	C(3)	...C(42)	2.79
C(4)	...C(42)	3.09	C(52)	...C(51)	2.53
C(62)	...C(51)	3.10	C(63)	...C(51)	3.27
C(1)	...C(51)	3.00	H(45)	...C(51)	2.86
C(52)	...O(51)	3.38	C(62)	...O(51)	3.32
C(1)	...C(52)	2.84	C(2)	...C(52)	3.19
C(62)	...C(61)	2.62	C(63)	...C(61)	2.70
C(3)	...C(61)	2.94	C(4)	...C(61)	3.17
C(63)	...C(62)	2.90	C(1)	...C(62)	2.88
C(2)	...C(62)	3.13	C(3)	...C(62)	3.45
H(45)	...C(63)	2.72	C(72)	...C(71)	2.71
C(73)	...C(71)	2.63	C(73)	...C(72)	2.58
C(4)	...C(1)	2.59	C(3)	...C(2)	2.59
C(4)	...C(2)	3.15			

Crystallographic Tables for $[H_5Os_{10}(CO)_{24}][PPN].(CH_2Cl_2)$, {X-ray study presented in section 3.7, Vol.1}.

TABLE 1 Fractional atomic coordinates and thermal parameters ($Å^2$) for $[H_5Os_{10}(CO)_{24}][PPN].[CH_2Cl_2]$

Atom	x	y	z	U_{iso} or U_{eq}
Os(1)	0.30836(17)	0.00306(12)	0.12931(6)	0.0426(13)
Os(2)	0.10636(15)	0.00535(10)	0.16650(5)	0.0258(11)
Os(3)	0.29472(20)	-0.08325(10)	0.19587(6)	0.0263(13)
Os(4)	0.29198(20)	0.08094(10)	0.20146(6)	0.0279(14)
Os(5)	-0.10461(15)	-0.00163(11)	0.19820(6)	0.0289(11)
Os(6)	0.08183(18)	-0.08779(10)	0.23372(5)	0.0228(12)
Os(7)	0.27978(18)	-0.16502(10)	0.26415(6)	0.0274(13)
Os(8)	0.26484(15)	-0.01014(10)	0.26828(5)	0.0250(11)
Os(9)	0.27949(17)	0.14570(10)	0.27444(6)	0.0283(13)
Os(10)	0.08102(19)	0.07227(10)	0.23735(6)	0.0249(13)
P(1)	0.3520(13)	-0.2650(7)	0.4772(4)	0.043(9)
P(2)	0.1628(11)	-0.1495(7)	0.4952(4)	0.040(8)
Cl(1)	0.2655(14)	0.0192(9)	0.6324(6)	0.101(13)
Cl(2)	0.4258(20)	-0.0949(11)	0.6188(5)	0.112(15)
C(11)	0.2929(74)	0.0684(44)	0.0945(24)	0.110(28)
O(11)	0.2715(46)	0.1214(30)	0.0712(15)	0.119(18)
C(12)	0.2724(51)	-0.0706(29)	0.0979(17)	0.058(17)
O(12)	0.2491(45)	-0.1310(28)	0.0738(15)	0.118(17)
C(13)	0.4402(61)	0.0010(37)	0.1195(20)	0.091(21)
O(13)	0.5447(47)	0.0044(32)	0.1210(17)	0.128(19)
C(21)	0.0479(49)	-0.0576(29)	0.1283(16)	0.055(16)
O(21)	0.0042(35)	-0.0972(23)	0.1061(12)	0.076(12)
C(22)	0.0581(44)	0.0926(27)	0.1387(14)	0.039(13)
O(22)	0.0380(34)	0.1394(21)	0.1180(11)	0.070(11)
C(31)	0.2840(60)	-0.1742(37)	0.1669(20)	0.081(21)

table 1 continued

O(31)	0.2798(46)	-0.2351(29)	0.1499(15)	0.114(17)
C(32)	0.4611(62)	-0.1010(36)	0.1991(18)	0.074(19)
O(32)	0.5554(38)	-0.1049(22)	0.1972(11)	0.069(12)
C(41)	0.4462(48)	0.1147(28)	0.2074(15)	0.049(15)
O(41)	0.5481(33)	0.1153(19)	0.2083(10)	0.055(10)
C(42)	0.2449(38)	0.1827(24)	0.1826(13)	0.026(12)
O(42)	0.2263(33)	0.2396(21)	0.1744(11)	0.064(11)
C(51)	-0.2253(40)	-0.0034(27)	0.2337(14)	0.039(12)
O(51)	-0.2884(31)	-0.0071(21)	0.2567(11)	0.064(11)
C(52)	-0.1691(63)	0.0618(36)	0.1706(20)	0.084(21)
O(52)	-0.2260(41)	0.1244(27)	0.1564(13)	0.099(15)
C(53)	-0.1828(44)	-0.0640(25)	0.1654(14)	0.036(13)
O(53)	-0.2269(35)	-0.1191(23)	0.1457(11)	0.077(13)
C(61)	0.0230(48)	-0.1093(29)	0.2789(16)	0.052(15)
O(61)	-0.0345(40)	-0.1125(25)	0.3079(13)	0.091(14)
C(62)	0.0433(45)	-0.1767(27)	0.2156(15)	0.042(14)
O(62)	0.0127(41)	-0.2387(25)	0.1991(14)	0.096(15)
C(71)	0.4326(42)	-0.1815(24)	0.2740(13)	0.033(13)
O(71)	0.5285(29)	-0.2044(17)	0.2779(9)	0.043(9)
C(72)	0.2495(40)	-0.2622(25)	0.2454(13)	0.030(12)
O(72)	0.2343(35)	-0.3206(21)	0.2385(11)	0.063(11)
C(73)	0.2435(36)	-0.1885(22)	0.3167(13)	0.021(11)
O(73)	0.2210(31)	-0.1961(19)	0.3458(11)	0.052(10)
C(81)	0.2140(39)	-0.0096(27)	0.3138(14)	0.042(13)
O(81)	0.1753(30)	-0.0084(20)	0.3462(11)	0.065(11)
C(82)	0.4104(66)	-0.0243(41)	0.2946(22)	0.102(25)
O(82)	0.5108(35)	-0.0244(21)	0.3051(11)	0.073(12)
C(91)	0.2617(45)	0.1533(27)	0.3224(16)	0.046(14)

table 1 continued

O(91)	0.2501(39)	0.1637(23)	0.3577(13)	0.063(13)
C(92)	0.2585(37)	0.2453(22)	0.2620(12)	0.021(11)
O(92)	0.2313(39)	0.3076(23)	0.2579(12)	0.078(13)
C(93)	0.4294(39)	0.1591(23)	0.2823(12)	0.025(11)
O(93)	0.5264(34)	0.1727(19)	0.2932(11)	0.060(11)
C(101)	-0.0209(49)	0.0673(28)	0.2779(17)	0.046(15)
O(101)	-0.0638(34)	0.0646(19)	0.3043(11)	0.058(11)
C(102)	0.0085(31)	0.1526(19)	0.2166(10)	0.006(9)
O(102)	-0.0289(33)	0.2129(20)	0.2028(11)	0.060(11)
N	0.2453(35)	-0.2134(20)	0.4918(11)	0.047(11)
C(111)	0.3114(26)	-0.3595(13)	0.4665(9)	0.017(9)
C(112)	0.3638(26)	-0.4194(13)	0.4862(9)	0.063(17)
C(113)	0.3310(26)	-0.4937(13)	0.4779(9)	0.108(24)
C(114)	0.2458(26)	-0.5079(13)	0.4499(9)	0.074(17)
C(115)	0.1934(26)	-0.4479(13)	0.4301(9)	0.100(23)
C(116)	0.2262(26)	-0.3737(13)	0.4384(9)	0.097(22)
C(121)	0.4168(31)	-0.2315(18)	0.4358(8)	0.053(15)
C(122)	0.4160(31)	-0.1541(18)	0.4283(8)	0.055(15)
C(123)	0.4640(31)	-0.1265(18)	0.3954(8)	0.056(15)
C(124)	0.5130(31)	-0.1764(18)	0.3700(8)	0.060(16)
C(125)	0.5138(31)	-0.2539(18)	0.3776(8)	0.054(15)
C(126)	0.4658(31)	-0.2814(18)	0.4105(8)	0.087(21)
C(131)	0.4700(21)	-0.2675(15)	0.5131(8)	0.022(10)
C(132)	0.4502(21)	-0.2605(15)	0.5518(8)	0.053(15)
C(133)	0.5404(21)	-0.2675(15)	0.5789(8)	0.049(14)
C(134)	0.6503(21)	-0.2813(15)	0.5671(8)	0.047(13)
C(135)	0.6701(21)	-0.2883(15)	0.5284(8)	0.059(16)
C(136)	0.5800(21)	-0.2814(15)	0.5013(8)	0.052(15)

table 1 continued

C(211)	0.2320(25)	-0.0608(14)	0.4852(9)	0.045(13)
C(212)	0.2101(25)	-0.0172(14)	0.4525(9)	0.048(13)
C(213)	0.2671(25)	0.0512(14)	0.4480(9)	0.082(19)
C(214)	0.3459(25)	0.0761(14)	0.4762(9)	0.077(19)
C(215)	0.3677(25)	0.0326(14)	0.5089(9)	0.063(16)
C(216)	0.3108(25)	-0.0359(14)	0.5134(9)	0.048(14)
C(221)	0.0436(25)	-0.1619(16)	0.4621(8)	0.032(11)
C(222)	-0.0679(25)	-0.1489(16)	0.4726(8)	0.060(15)
C(223)	-0.1581(25)	-0.1554(16)	0.4456(8)	0.094(21)
C(224)	-0.1368(25)	-0.1748(16)	0.4080(8)	0.041(13)
C(225)	-0.0253(25)	-0.1878(16)	0.3975(8)	0.059(16)
C(226)	0.0649(25)	-0.1813(16)	0.4245(8)	0.054(15)
C(231)	0.1100(25)	-0.1425(15)	0.5416(7)	0.020(10)
C(232)	0.0957(25)	-0.2117(15)	0.5599(7)	0.040(13)
C(233)	0.0491(25)	-0.2141(15)	0.5957(7)	0.052(15)
C(234)	0.0169(25)	-0.1472(15)	0.6134(7)	0.063(16)
C(235)	0.0312(25)	-0.0779(15)	0.5952(7)	0.060(16)
C(236)	0.0777(25)	-0.0756(15)	0.5593(7)	0.055(15)
C(1)	0.3189(64)	-0.0544(37)	0.6459(21)	0.104(24)

TABLE 2 Anisotropic thermal parameters ($Å^2$) for $[H_5Os_{10}(CO)_{24}][PPN].[CH_2Cl_2]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Os(1)	0.043(1)	0.053(1)	0.032(1)	0.007(1)	0.010(1)	0.001(1)
Os(2)	0.027(1)	0.029(1)	0.022(1)	0.000(1)	0.000(1)	0.001(1)
Os(3)	0.025(2)	0.028(1)	0.025(1)	0.002(1)	0.003(1)	0.003(1)
Os(4)	0.025(2)	0.033(1)	0.026(1)	0.000(1)	0.002(1)	-0.003(1)
Os(5)	0.023(1)	0.030(1)	0.034(1)	-0.002(1)	-0.003(1)	0.000(1)
Os(6)	0.019(1)	0.025(1)	0.025(1)	0.001(1)	-0.002(1)	0.001(1)
Os(7)	0.026(1)	0.026(1)	0.030(1)	0.004(1)	-0.001(1)	0.002(1)
Os(8)	0.024(1)	0.025(1)	0.026(1)	0.000(1)	-0.001(1)	0.000(1)
Os(9)	0.026(1)	0.028(1)	0.031(1)	-0.005(1)	-0.003(1)	-0.005(1)
Os(10)	0.023(1)	0.024(1)	0.028(1)	-0.001(1)	0.001(1)	0.002(1)
P(1)	0.056(10)	0.031(7)	0.044(9)	-0.006(7)	-0.004(7)	0.014(7)
P(2)	0.045(9)	0.036(7)	0.037(8)	0.006(7)	-0.017(7)	0.012(7)
Cl(1)	0.069(11)	0.071(10)	0.163(18)	0.027(12)	-0.045(12)	-0.016(9)
Cl(2)	0.154(20)	0.106(13)	0.074(12)	0.001(11)	0.002(13)	0.017(14)

TABLE 3 Bond lengths (A°) for $[H_5Os_{10}(CO)_{24}][PPN].[CH_2Cl_2]$

Os(1) -Os(2)	2.759(3)	Os(1) -Os(3)	2.799(3)
Os(1) -Os(4)	2.894(3)	Os(1) -C(11)	1.68(8)
Os(1) -C(12)	1.74(5)	Os(1) -C(13)	1.60(7)
Os(2) -Os(3)	2.865(3)	Os(2) -Os(4)	2.794(3)
Os(2) -Os(5)	2.764(3)	Os(2) -Os(6)	2.900(3)
Os(2) -Os(10)	2.799(3)	Os(2) -C(21)	1.85(5)
Os(2) -C(22)	1.90(5)	Os(3) -Os(4)	2.910(3)
Os(3) -Os(6)	2.885(3)	Os(3) -Os(7)	2.809(3)
Os(3) -Os(8)	2.885(3)	Os(3) -C(31)	1.90(7)
Os(3) -C(32)	1.98(7)	Os(4) -Os(8)	2.873(3)
Os(4) -Os(9)	2.813(3)	Os(4) -Os(10)	2.834(3)
Os(4) -C(41)	1.91(6)	Os(4) -C(42)	1.99(4)
Os(5) -Os(6)	2.903(3)	Os(5) -Os(10)	2.842(3)
Os(5) -C(51)	1.93(5)	Os(5) -C(52)	1.64(7)
Os(5) -C(53)	1.81(5)	Os(6) -Os(7)	2.862(3)
Os(6) -Os(8)	2.783(3)	Os(6) -Os(10)	2.833(3)
Os(6) -C(61)	1.80(6)	Os(6) -C(62)	1.75(5)
Os(7) -Os(8)	2.748(3)	Os(7) -C(71)	1.84(5)
Os(7) -C(72)	1.87(4)	Os(7) -C(73)	1.96(4)
Os(8) -Os(9)	2.769(3)	Os(8) -Os(10)	2.785(3)
Os(8) -C(81)	1.73(5)	Os(8) -C(82)	1.92(8)
Os(9) -Os(10)	2.923(3)	Os(9) -C(91)	1.71(5)
Os(9) -C(92)	1.83(4)	Os(9) -C(93)	1.79(5)
Os(10)-C(101)	1.90(6)	Os(10)-C(102)	1.79(3)
C(11) -O(11)	1.26(9)	C(12) -O(12)	1.38(7)

table 3 continued

C(13) -O(13)	1.23(9)	C(21) -O(21)	1.15(7)
C(22) -O(22)	1.12(6)	C(31) -O(31)	1.23(8)
C(32) -O(32)	1.12(8)	C(41) -O(41)	1.20(7)
C(42) -O(42)	1.07(6)	C(51) -O(51)	1.12(6)
C(52) -O(52)	1.38(8)	C(53) -O(53)	1.29(6)
C(61) -O(61)	1.25(7)	C(62) -O(62)	1.28(7)
C(71) -O(71)	1.20(6)	C(72) -O(72)	1.07(6)
C(73) -O(73)	1.07(6)	C(81) -O(81)	1.24(6)
C(82) -O(82)	1.22(9)	C(91) -O(91)	1.26(7)
C(92) -O(92)	1.15(6)	C(93) -O(93)	1.21(6)
C(101)-O(101)	1.07(7)	C(102)-O(102)	1.24(5)
P(1) -N	1.65(4)	P(1) -C(111)	1.77(3)
P(1) -C(121)	1.77(3)	P(1) -C(131)	1.83(3)
P(2) -N	1.50(4)	P(2) -C(211)	1.81(3)
P(2) -C(221)	1.79(3)	P(2) -C(231)	1.77(3)
C(111)-C(112)	1.39(4)	C(111)-C(116)	1.39(4)
C(112)-C(113)	1.39(3)	C(113)-C(114)	1.39(4)
C(114)-C(115)	1.39(4)	C(115)-C(116)	1.39(3)
C(121)-C(122)	1.39(4)	C(121)-C(126)	1.39(5)
C(122)-C(123)	1.39(4)	C(123)-C(124)	1.39(5)
C(124)-C(125)	1.39(4)	C(125)-C(126)	1.39(4)
C(131)-C(132)	1.39(4)	C(131)-C(136)	1.39(3)
C(132)-C(133)	1.39(3)	C(133)-C(134)	1.39(3)
C(134)-C(135)	1.39(4)	C(135)-C(136)	1.39(3)
C(211)-C(212)	1.39(4)	C(211)-C(216)	1.39(4)
C(212)-C(213)	1.39(4)	C(213)-C(214)	1.39(4)
C(214)-C(215)	1.39(4)	C(215)-C(216)	1.39(4)
C(221)-C(222)	1.39(4)	C(221)-C(226)	1.39(4)

table 3 continued

C(222)-C(223)	1.39(4)	C(223)-C(224)	1.39(4)
C(224)-C(225)	1.39(4)	C(225)-C(226)	1.39(4)
C(231)-C(232)	1.39(4)	C(231)-C(236)	1.39(4)
C(232)-C(233)	1.39(3)	C(233)-C(234)	1.39(4)
C(234)-C(235)	1.39(4)	C(235)-C(236)	1.39(3)
Cl(1) -C(1)	1.51(7)	Cl(2) -C(1)	1.76(8)

TABLE 4 Bond angles (°) for $[H_5Os_{10}(CO)_{24}][PPN].[CH_2Cl_2]$

Os(3) -Os(1) -Os(2)	62.0(1)	Os(4) -Os(1) -Os(2)	59.2(1)
Os(4) -Os(1) -Os(3)	61.5(1)	C(11) -Os(1) -Os(2)	105(3)
C(11) -Os(1) -Os(3)	166(3)	C(11) -Os(1) -Os(4)	107(3)
C(12) -Os(1) -Os(2)	97(2)	C(12) -Os(1) -Os(3)	96(2)
C(12) -Os(1) -Os(4)	152(2)	C(12) -Os(1) -C(11)	92(3)
C(13) -Os(1) -Os(2)	164(2)	C(13) -Os(1) -Os(3)	105(2)
C(13) -Os(1) -Os(4)	107(2)	C(13) -Os(1) -C(11)	86(4)
C(13) -Os(1) -C(12)	93(3)	Os(3) -Os(2) -Os(1)	59.7(1)
Os(4) -Os(2) -Os(1)	62.8(1)	Os(4) -Os(2) -Os(3)	61.9(1)
Os(5) -Os(2) -Os(1)	174.4(1)	Os(5) -Os(2) -Os(3)	121.5(1)
Os(5) -Os(2) -Os(4)	122.8(1)	Os(6) -Os(2) -Os(1)	119.6(1)
Os(6) -Os(2) -Os(3)	60.0(1)	Os(6) -Os(2) -Os(4)	91.1(1)
Os(6) -Os(2) -Os(5)	61.6(1)	Os(10)-Os(2) -Os(1)	123.9(1)
Os(10)-Os(2) -Os(3)	91.4(1)	Os(10)-Os(2) -Os(4)	61.1(1)
Os(10)-Os(2) -Os(5)	61.7(1)	Os(10)-Os(2) -Os(6)	59.8(1)
C(21) -Os(2) -Os(1)	87(2)	C(21) -Os(2) -Os(3)	101(2)
C(21) -Os(2) -Os(4)	150(2)	C(21) -Os(2) -Os(5)	87(2)
C(21) -Os(2) -Os(6)	101(2)	C(21) -Os(2) -Os(10)	148(2)
C(22) -Os(2) -Os(1)	91(2)	C(22) -Os(2) -Os(3)	147(2)
C(22) -Os(2) -Os(4)	93(1)	C(22) -Os(2) -Os(5)	89(2)
C(22) -Os(2) -Os(6)	147(2)	C(22) -Os(2) -Os(10)	94(1)
C(22) -Os(2) -C(21)	91(2)	Os(2) -Os(3) -Os(1)	58.3(1)
Os(4) -Os(3) -Os(1)	60.9(1)	Os(4) -Os(3) -Os(2)	57.9(1)
Os(6) -Os(3) -Os(1)	118.8(1)	Os(6) -Os(3) -Os(2)	60.6(1)
Os(6) -Os(3) -Os(4)	89.1(1)	Os(7) -Os(3) -Os(1)	177.9(1)

table 4 continued

Os(7) -Os(3) -Os(2)	120.7(1)	Os(7) -Os(3) -Os(4)	117.1(1)
Os(7) -Os(3) -Os(6)	60.3(1)	Os(8) -Os(3) -Os(1)	120.2(1)
Os(8) -Os(3) -Os(2)	87.1(1)	Os(8) -Os(3) -Os(4)	59.4(1)
Os(8) -Os(3) -Os(6)	57.7(1)	Os(8) -Os(3) -Os(7)	57.7(1)
C(31) -Os(3) -Os(1)	91(2)	C(31) -Os(3) -Os(2)	104(2)
C(31) -Os(3) -Os(4)	151(2)	C(31) -Os(3) -Os(6)	101(2)
C(31) -Os(3) -Os(7)	91(2)	C(31) -Os(3) -Os(8)	147(2)
C(32) -Os(3) -Os(1)	92(2)	C(32) -Os(3) -Os(2)	149(2)
C(32) -Os(3) -Os(4)	100(2)	C(32) -Os(3) -Os(6)	147(2)
C(32) -Os(3) -Os(7)	88(2)	C(32) -Os(3) -Os(8)	100(2)
C(32) -Os(3) -C(31)	86(3)	Os(2) -Os(4) -Os(1)	58.0(1)
Os(3) -Os(4) -Os(1)	57.7(1)	Os(3) -Os(4) -Os(2)	60.3(1)
Os(8) -Os(4) -Os(1)	117.4(1)	Os(8) -Os(4) -Os(2)	88.7(1)
Os(8) -Os(4) -Os(3)	59.8(1)	Os(9) -Os(4) -Os(1)	175.5(1)
Os(9) -Os(4) -Os(2)	121.5(1)	Os(9) -Os(4) -Os(3)	117.9(1)
Os(9) -Os(4) -Os(8)	58.3(1)	Os(10)-Os(4) -Os(1)	117.1(1)
Os(10)-Os(4) -Os(2)	59.2(1)	Os(10)-Os(4) -Os(3)	89.3(1)
Os(10)-Os(4) -Os(8)	58.4(1)	Os(10)-Os(4) -Os(9)	62.3(1)
C(41) -Os(4) -Os(1)	98(2)	C(41) -Os(4) -Os(2)	156(2)
C(41) -Os(4) -Os(3)	108(1)	C(41) -Os(4) -Os(8)	103(2)
C(41) -Os(4) -Os(9)	82(2)	C(41) -Os(4) -Os(10)	144(2)
C(42) -Os(4) -Os(1)	100(1)	C(42) -Os(4) -Os(2)	95(1)
C(42) -Os(4) -Os(3)	152(1)	C(42) -Os(4) -Os(8)	138(1)
C(42) -Os(4) -Os(9)	85(1)	C(42) -Os(4) -Os(10)	88(1)
C(42) -Os(4) -C(41)	90(2)	Os(6) -Os(5) -Os(2)	61.5(1)
Os(10)-Os(5) -Os(2)	59.4(1)	Os(10)-Os(5) -Os(6)	59.1(1)
C(51) -Os(5) -Os(2)	163(1)	C(51) -Os(5) -Os(6)	106(1)
C(51) -Os(5) -Os(10)	105(1)	C(52) -Os(5) -Os(2)	97(3)

table 4 continued

C(52) -Os(5) -Os(6)	158(3)	C(52) -Os(5) -Os(10)	107(2)
C(52) -Os(5) -C(51)	93(3)	C(53) -Os(5) -Os(2)	102(2)
C(53) -Os(5) -Os(6)	108(1)	C(53) -Os(5) -Os(10)	160(2)
C(53) -Os(5) -C(51)	92(2)	C(53) -Os(5) -C(52)	80(3)
Os(3) -Os(6) -Os(2)	59.4(1)	Os(5) -Os(6) -Os(2)	56.9(1)
Os(5) -Os(6) -Os(3)	116.2(1)	Os(7) -Os(6) -Os(2)	117.7(1)
Os(7) -Os(6) -Os(3)	58.5(1)	Os(7) -Os(6) -Os(5)	174.5(1)
Os(8) -Os(6) -Os(2)	88.3(1)	Os(8) -Os(6) -Os(3)	61.2(1)
Os(8) -Os(6) -Os(5)	118.8(1)	Os(8) -Os(6) -Os(7)	58.3(1)
Os(10)-Os(6) -Os(2)	58.0(1)	Os(10)-Os(6) -Os(3)	89.9(1)
Os(10)-Os(6) -Os(5)	59.4(1)	Os(10)-Os(6) -Os(7)	117.7(1)
Os(10)-Os(6) -Os(8)	59.4(1)	C(61) -Os(6) -Os(2)	153(2)
C(61) -Os(6) -Os(3)	142(2)	C(61) -Os(6) -Os(5)	100(2)
C(61) -Os(6) -Os(7)	85(2)	C(61) -Os(6) -Os(8)	92(2)
C(61) -Os(6) -Os(10)	100(2)	C(62) -Os(6) -Os(2)	104(2)
C(62) -Os(6) -Os(3)	94(2)	C(62) -Os(6) -Os(5)	98(2)
C(62) -Os(6) -Os(7)	84(2)	C(62) -Os(6) -Os(8)	142(2)
C(62) -Os(6) -Os(10)	156(2)	C(62) -Os(6) -C(61)	91(2)
Os(6) -Os(7) -Os(3)	61.1(1)	Os(8) -Os(7) -Os(3)	62.5(1)
Os(8) -Os(7) -Os(6)	59.4(1)	C(71) -Os(7) -Os(3)	98(1)
C(71) -Os(7) -Os(6)	157(1)	C(71) -Os(7) -Os(8)	102(1)
C(72) -Os(7) -Os(3)	101(1)	C(72) -Os(7) -Os(6)	100(1)
C(72) -Os(7) -Os(8)	157(1)	C(72) -Os(7) -C(71)	95(2)
C(73) -Os(7) -Os(3)	160(1)	C(73) -Os(7) -Os(6)	104(1)
C(73) -Os(7) -Os(8)	98(1)	C(73) -Os(7) -C(71)	92(2)
C(73) -Os(7) -C(72)	95(2)	Os(4) -Os(8) -Os(3)	60.7(1)
Os(6) -Os(8) -Os(3)	61.2(1)	Os(6) -Os(8) -Os(4)	91.9(1)
Os(7) -Os(8) -Os(3)	59.8(1)	Os(7) -Os(8) -Os(4)	120.4(1)

table 4 continued

Os(7) -Os(8) -Os(6)	62.3(1)	Os(9) -Os(8) -Os(3)	120.3(1)
Os(9) -Os(8) -Os(4)	59.8(1)	Os(9) -Os(8) -Os(6)	124.7(1)
Os(9) -Os(8) -Os(7)	172.7(1)	Os(10)-Os(8) -Os(3)	90.8(1)
Os(10)-Os(8) -Os(4)	60.1(1)	Os(10)-Os(8) -Os(6)	61.2(1)
Os(10)-Os(8) -Os(7)	123.4(1)	Os(10)-Os(8) -Os(9)	63.5(1)
C(81) -Os(8) -Os(3)	151(2)	C(81) -Os(8) -Os(4)	144(2)
C(81) -Os(8) -Os(6)	96(1)	C(81) -Os(8) -Os(7)	94(2)
C(81) -Os(8) -Os(9)	87(2)	C(81) -Os(8) -Os(10)	94(1)
C(82) -Os(8) -Os(3)	103(2)	C(82) -Os(8) -Os(4)	110(2)
C(82) -Os(8) -Os(6)	143(2)	C(82) -Os(8) -Os(7)	81(2)
C(82) -Os(8) -Os(9)	92(2)	C(82) -Os(8) -Os(10)	156(2)
C(82) -Os(8) -C(81)	84(3)	Os(8) -Os(9) -Os(4)	61.9(1)
Os(10)-Os(9) -Os(4)	59.2(1)	Os(10)-Os(9) -Os(8)	58.5(1)
C(91) -Os(9) -Os(4)	160(2)	C(91) -Os(9) -Os(8)	98(2)
C(91) -Os(9) -Os(10)	110(2)	C(92) -Os(9) -Os(4)	101(1)
C(92) -Os(9) -Os(8)	159(1)	C(92) -Os(9) -Os(10)	103(1)
C(92) -Os(9) -C(91)	98(2)	C(93) -Os(9) -Os(4)	96(1)
C(93) -Os(9) -Os(8)	102(1)	C(93) -Os(9) -Os(10)	153(1)
C(93) -Os(9) -C(91)	90(2)	C(93) -Os(9) -C(92)	92(2)
Os(4) -Os(10)-Os(2)	59.7(1)	Os(5) -Os(10)-Os(2)	58.9(1)
Os(5) -Os(10)-Os(4)	118.5(1)	Os(6) -Os(10)-Os(2)	62.2(1)
Os(6) -Os(10)-Os(4)	91.7(1)	Os(6) -Os(10)-Os(5)	61.5(1)
Os(8) -Os(10)-Os(2)	90.7(1)	Os(8) -Os(10)-Os(4)	61.5(1)
Os(8) -Os(10)-Os(5)	120.8(1)	Os(8) -Os(10)-Os(6)	59.4(1)
Os(9) -Os(10)-Os(2)	118.1(1)	Os(9) -Os(10)-Os(4)	58.5(1)
Os(9) -Os(10)-Os(5)	177.0(1)	Os(9) -Os(10)-Os(6)	117.4(1)
Os(9) -Os(10)-Os(8)	58.0(1)	C(101)-Os(10)-Os(2)	138(2)
C(101)-Os(10)-Os(4)	158(2)	C(101)-Os(10)-Os(5)	81(2)

table 4 continued

C(101)-Os(10)-Os(6)	89(1)	C(101)-Os(10)-Os(8)	101(2)
C(101)-Os(10)-Os(9)	102(2)	C(102)-Os(10)-Os(2)	92(1)
C(102)-Os(10)-Os(4)	101(1)	C(102)-Os(10)-Os(5)	80(1)
C(102)-Os(10)-Os(6)	141(1)	C(102)-Os(10)-Os(8)	157(1)
C(102)-Os(10)-Os(9)	101(1)	C(102)-Os(10)-C(101)	92(2)
O(11) -C(11) -Os(1)	172(7)	O(12) -C(12) -Os(1)	177(5)
O(13) -C(13) -Os(1)	165(6)	O(21) -C(21) -Os(2)	175(5)
O(22) -C(22) -Os(2)	170(5)	O(31) -C(31) -Os(3)	176(6)
O(32) -C(32) -Os(3)	171(5)	O(41) -C(41) -Os(4)	162(4)
O(42) -C(42) -Os(4)	174(4)	O(51) -C(51) -Os(5)	174(4)
O(52) -C(52) -Os(5)	165(6)	O(53) -C(53) -Os(5)	168(4)
O(61) -C(61) -Os(6)	166(5)	O(62) -C(62) -Os(6)	174(4)
O(71) -C(71) -Os(7)	169(4)	O(72) -C(72) -Os(7)	172(4)
O(73) -C(73) -Os(7)	175(4)	O(81) -C(81) -Os(8)	178(4)
O(82) -C(82) -Os(8)	166(6)	O(91) -C(91) -Os(9)	176(4)
O(92) -C(92) -Os(9)	169(4)	O(93) -C(93) -Os(9)	170(4)
O(101)-C(101)-Os(10)	169(5)	O(102)-C(102)-Os(10)	172(3)
C(111)-P(1) -N	113(2)	C(121)-P(1) -N	116(2)
C(121)-P(1) -C(111)	105(2)	C(131)-P(1) -N	111(2)
C(131)-P(1) -C(111)	108(1)	C(131)-P(1) -C(121)	103(2)
C(211)-P(2) -N	110(2)	C(221)-P(2) -N	110(2)
C(221)-P(2) -C(211)	109(1)	C(231)-P(2) -N	112(2)
C(231)-P(2) -C(211)	107(1)	C(231)-P(2) -C(221)	108(1)
P(2) -N -P(1)	161(3)	C(112)-C(111)-P(1)	120(2)
C(116)-C(111)-P(1)	120(2)	C(116)-C(111)-C(112)	120(2)
C(113)-C(112)-C(111)	120(3)	C(114)-C(113)-C(112)	120(2)
C(115)-C(114)-C(113)	120(2)	C(116)-C(115)-C(114)	120(3)
C(115)-C(116)-C(111)	120(2)	C(122)-C(121)-P(1)	119(2)

table 4 continued

C(126)-C(121)-P(1)	121(2)	C(126)-C(121)-C(122)	120(3)
C(123)-C(122)-C(121)	120(3)	C(124)-C(123)-C(122)	120(3)
C(125)-C(124)-C(123)	120(3)	C(126)-C(125)-C(124)	120(3)
C(125)-C(126)-C(121)	120(3)	C(132)-C(131)-P(1)	121(2)
C(136)-C(131)-P(1)	119(2)	C(136)-C(131)-C(132)	120(2)
C(133)-C(132)-C(131)	120(2)	C(134)-C(133)-C(132)	120(2)
C(135)-C(134)-C(133)	120(2)	C(136)-C(135)-C(134)	120(2)
C(135)-C(136)-C(131)	120(2)	C(212)-C(211)-P(2)	125(2)
C(216)-C(211)-P(2)	115(2)	C(216)-C(211)-C(212)	120(2)
C(213)-C(212)-C(211)	120(3)	C(214)-C(213)-C(212)	120(3)
C(215)-C(214)-C(213)	120(2)	C(216)-C(215)-C(214)	120(3)
C(215)-C(216)-C(211)	120(3)	C(222)-C(221)-P(2)	122(2)
C(226)-C(221)-P(2)	118(2)	C(226)-C(221)-C(222)	120(3)
C(223)-C(222)-C(221)	120(3)	C(224)-C(223)-C(222)	120(3)
C(225)-C(224)-C(223)	120(3)	C(226)-C(225)-C(224)	120(3)
C(225)-C(226)-C(221)	120(3)	C(232)-C(231)-P(2)	114(2)
C(236)-C(231)-P(2)	125(2)	C(236)-C(231)-C(232)	120(2)
C(233)-C(232)-C(231)	120(2)	C(234)-C(233)-C(232)	120(2)
C(235)-C(234)-C(233)	120(2)	C(236)-C(235)-C(234)	120(2)
C(235)-C(236)-C(231)	120(2)	Cl(2) -C(1) -Cl(1)	119(4)

TABLE 5 Intermolecular distances (Å) for $[H_5Os_{10}(CO)_{24}][PPN].[CH_2Cl_2]$

atom1	atom2	dist	S	a	b	c
O(92)	...Os(5)	4.02	-2	0.0	1.0	1.0
O(92)	...Os(6)	4.14	-2	0.0	1.0	1.0
O(102)	...Os(7)	3.87	-2	0.0	1.0	1.0
O(62)	...Os(9)	4.14	-2	0.0	0.0	1.0
O(71)	...Os(9)	3.98	-2	1.0	0.0	1.0
C(132)	...O(12)	3.17	2	0.0	-1.0	0.0
C(232)	...O(12)	3.34	2	0.0	-1.0	0.0
C(233)	...O(21)	3.40	2	0.0	-1.0	0.0
C(225)	...O(22)	3.11	-2	0.0	0.0	1.0
C(233)	...O(31)	3.36	2	0.0	-1.0	0.0
Cl(2)	...O(31)	3.65	2	0.0	-1.0	0.0
C(51)	...O(32)	3.35	1	-1.0	0.0	0.0
O(51)	...O(32)	3.22	1	-1.0	0.0	0.0
C(53)	...O(32)	3.40	1	-1.0	0.0	0.0
O(53)	...O(32)	3.21	1	-1.0	0.0	0.0
O(92)	...O(32)	3.29	-2	1.0	1.0	1.0
O(71)	...C(41)	3.25	-2	1.0	0.0	1.0
O(51)	...O(41)	3.31	1	-1.0	0.0	0.0
O(52)	...O(41)	3.29	1	-1.0	0.0	0.0
O(72)	...O(41)	3.30	-2	1.0	0.0	1.0
C(224)	...O(42)	3.39	-2	0.0	0.0	1.0
O(72)	...C(51)	3.38	-2	0.0	0.0	1.0
O(92)	...C(51)	3.36	-2	0.0	1.0	1.0
O(82)	...O(51)	2.98	1	1.0	0.0	0.0
O(73)	...O(52)	3.18	-2	0.0	0.0	1.0

table 5 continued

C(115)...O(52)	3.33	-2	0.0	0.0	1.0
C(116)...O(52)	3.32	-2	0.0	0.0	1.0
O(102)...C(61)	3.21	-2	0.0	1.0	1.0
O(102)...O(61)	3.20	-2	0.0	1.0	1.0
O(92) ...C(62)	3.41	-2	0.0	1.0	1.0
C(92) ...O(71)	3.05	-2	1.0	1.0	1.0
O(92) ...O(71)	3.15	-2	1.0	1.0	1.0
C(93) ...O(71)	3.26	-2	1.0	1.0	1.0
O(93) ...C(72)	3.22	-2	1.0	1.0	1.0
O(102)...C(72)	3.26	-2	0.0	1.0	1.0
O(93) ...O(72)	3.07	-2	1.0	1.0	1.0
C(101)...O(72)	3.23	-2	0.0	1.0	1.0
O(101)...O(72)	3.18	-2	0.0	1.0	1.0
C(102)...O(72)	3.35	-2	0.0	1.0	1.0
O(102)...O(72)	3.30	-2	0.0	1.0	1.0
O(102)...C(73)	3.12	-2	0.0	1.0	1.0
O(102)...O(73)	3.20	-2	0.0	1.0	1.0
Cl(1) ...O(82)	3.35	-1	1.0	0.0	1.0
Cl(2) ...O(82)	3.46	-1	1.0	0.0	1.0
C(1) ...O(82)	2.93	-1	1.0	0.0	1.0
C(234)...O(91)	3.35	-1	0.0	0.0	1.0
Cl(2) ...O(93)	3.40	-1	1.0	0.0	1.0
C(234)...O(101)	3.26	-1	0.0	0.0	1.0
Cl(1) ...O(101)	3.63	-1	0.0	0.0	1.0
Cl(1) ...C(124)	3.81	-1	1.0	0.0	1.0

Symmetry Transformations:

The second atom is related to the first atom, at (x,y,z), by the symmetry operation S with (a,b,c) added to the (x',y',z') of S.

Where S =

1	x, y, z
2	x, 0.5-y, 0.5+z

TABLE 6 Intramolecular distances (Å) for $[H_5Os_{10}(CO)_{24}][PPN].[CH_2Cl_2]$

Os(6) ...Os(1)	4.89	Os(8) ...Os(1)	4.93
Os(10)...Os(1)	4.89	O(11) ...Os(1)	2.94
O(12) ...Os(1)	3.13	O(13) ...Os(1)	2.81
C(21) ...Os(1)	3.24	O(21) ...Os(1)	4.04
C(22) ...Os(1)	3.37	O(22) ...Os(1)	3.99
C(31) ...Os(1)	3.42	C(32) ...Os(1)	3.49
O(32) ...Os(1)	4.14	C(41) ...Os(1)	3.69
C(42) ...Os(1)	3.78	Os(7) ...Os(2)	4.93
Os(8) ...Os(2)	3.96	Os(9) ...Os(2)	4.89
C(11) ...Os(2)	3.59	C(12) ...Os(2)	3.44
O(21) ...Os(2)	3.00	O(22) ...Os(2)	3.01
C(31) ...Os(2)	3.80	C(42) ...Os(2)	3.57
C(52) ...Os(2)	3.40	C(53) ...Os(2)	3.61
C(62) ...Os(2)	3.74	C(102)...Os(2)	3.37
Os(5) ...Os(3)	4.91	Os(9) ...Os(3)	4.90
Os(10)...Os(3)	4.04	C(12) ...Os(3)	3.44
C(13) ...Os(3)	3.57	C(21) ...Os(3)	3.69
O(31) ...Os(3)	3.13	O(32) ...Os(3)	3.08
C(41) ...Os(3)	3.94	C(62) ...Os(3)	3.48
C(71) ...Os(3)	3.57	C(72) ...Os(3)	3.66
C(82) ...Os(3)	3.81	Os(5) ...Os(4)	4.88
Os(6) ...Os(4)	4.07	Os(7) ...Os(4)	4.88
C(11) ...Os(4)	3.76	C(13) ...Os(4)	3.71
C(22) ...Os(4)	3.45	C(32) ...Os(4)	3.79
O(41) ...Os(4)	3.07	O(42) ...Os(4)	3.05

table 6 continued

C(82) ...Os(4)	3.95	C(92) ...Os(4)	3.63
C(93) ...Os(4)	3.48	C(102)...Os(4)	3.63
Os(8) ...Os(5)	4.89	C(21) ...Os(5)	3.25
O(21) ...Os(5)	3.91	C(22) ...Os(5)	3.34
O(22) ...Os(5)	4.17	O(51) ...Os(5)	3.05
O(52) ...Os(5)	2.99	O(53) ...Os(5)	3.09
C(61) ...Os(5)	3.67	C(62) ...Os(5)	3.59
C(101)...Os(5)	3.17	O(101)...Os(5)	3.91
C(102)...Os(5)	3.09	O(102)...Os(5)	3.90
Os(9) ...Os(6)	4.92	C(21) ...Os(6)	3.74
C(31) ...Os(6)	3.74	C(51) ...Os(6)	3.90
C(53) ...Os(6)	3.86	O(61) ...Os(6)	3.02
O(62) ...Os(6)	3.03	C(72) ...Os(6)	3.67
C(73) ...Os(6)	3.84	C(81) ...Os(6)	3.44
C(101)...Os(6)	3.40	O(101)...Os(6)	4.09
Os(10)...Os(7)	4.87	C(31) ...Os(7)	3.41
C(32) ...Os(7)	3.38	C(61) ...Os(7)	3.24
O(61) ...Os(7)	4.17	C(62) ...Os(7)	3.20
O(62) ...Os(7)	4.01	O(71) ...Os(7)	3.02
O(72) ...Os(7)	2.94	O(73) ...Os(7)	3.03
C(81) ...Os(7)	3.36	C(82) ...Os(7)	3.09
O(82) ...Os(7)	3.91	C(32) ...Os(8)	3.78
C(41) ...Os(8)	3.79	C(61) ...Os(8)	3.37
C(71) ...Os(8)	3.62	C(73) ...Os(8)	3.60
O(81) ...Os(8)	2.97	O(82) ...Os(8)	3.12
C(91) ...Os(8)	3.46	C(93) ...Os(8)	3.59
C(101)...Os(8)	3.66	C(41) ...Os(9)	3.17
O(41) ...Os(9)	4.03	C(42) ...Os(9)	3.29

table 6 continued

O(42) ...Os(9)	3.90	C(81) ...Os(9)	3.18
O(81) ...Os(9)	3.94	C(82) ...Os(9)	3.43
O(82) ...Os(9)	4.16	O(91) ...Os(9)	2.97
O(92) ...Os(9)	2.97	O(93) ...Os(9)	2.98
C(101)...Os(9)	3.80	C(102)...Os(9)	3.70
C(22) ...Os(10)	3.47	C(42) ...Os(10)	3.40
O(42) ...Os(10)	4.11	C(51) ...Os(10)	3.84
C(52) ...Os(10)	3.68	C(61) ...Os(10)	3.60
C(51) ...Os(10)	3.37	C(91) ...Os(10)	3.86
C(92) ...Os(10)	3.78	O(101)...Os(10)	2.96
O(102)...Os(10)	3.03	C(12) ...C(11)	2.47
C(13) ...C(11)	2.25	O(13) ...C(11)	3.26
C(22) ...C(11)	3.25	O(22) ...C(11)	3.38
C(13) ...O(11)	3.32	O(22) ...O(11)	3.28
C(13) ...C(12)	2.43	C(21) ...C(12)	2.90
O(21) ...C(12)	3.21	C(31) ...C(12)	3.03
C(21) ...O(12)	3.37	O(21) ...O(12)	3.19
C(31) ...O(12)	3.36	O(31) ...O(12)	3.25
C(32) ...C(13)	3.32	O(32) ...O(13)	3.30
C(22) ...C(21)	2.68	C(53) ...C(21)	3.06
C(53) ...O(21)	3.15	O(53) ...O(21)	3.13
C(42) ...C(22)	3.07	C(52) ...C(22)	2.99
C(102)...C(22)	3.01	O(102)...C(22)	3.29
C(42) ...O(22)	3.34	C(52) ...O(22)	3.41
C(32) ...C(31)	2.66	C(62) ...C(31)	3.37
C(72) ...C(31)	3.20	C(72) ...O(31)	3.42
C(71) ...C(32)	3.02	O(71) ...C(32)	3.38
C(71) ...O(32)	3.39	C(42) ...C(41)	2.76

table 6 continued

C(93) ...C(41)	2.76	O(93) ...C(41)	3.28
C(93) ...O(41)	3.10	O(93) ...O(41)	3.16
C(92) ...C(42)	2.99	C(102)...C(42)	3.12
O(102)...C(42)	3.37	C(92) ...O(42)	3.08
O(92) ...O(42)	3.16	C(102)...O(42)	3.38
O(102)...O(42)	3.24	C(52) ...C(51)	2.61
C(53) ...C(51)	2.69	C(101)...C(51)	3.07
O(101)...C(51)	3.28	O(101)...O(51)	3.31
C(53) ...C(52)	2.24	O(53) ...C(52)	3.38
C(102)...C(52)	3.04	O(102)...C(52)	3.31
C(53) ...O(52)	3.38	O(102)...O(52)	3.18
C(62) ...C(61)	2.54	C(73) ...C(61)	3.18
C(81) ...C(61)	3.07	O(81) ...C(61)	3.40
C(101)...C(61)	3.17	O(101)...C(61)	3.37
O(81) ...O(61)	3.31	C(101)...O(61)	3.35
O(101)...O(61)	3.15	C(225)...O(61)	3.41
C(72) ...C(62)	3.00	C(72) ...O(62)	3.18
O(72) ...O(62)	3.23	C(72) ...C(71)	2.73
C(73) ...C(71)	2.74	C(82) ...C(71)	2.89
O(82) ...C(71)	3.11	C(124)...C(71)	3.45
O(82) ...O(71)	3.33	C(124)...O(71)	3.28
C(73) ...C(72)	2.82	C(81) ...C(73)	3.18
C(226)...O(73)	3.39	C(82) ...C(81)	2.45
C(91) ...C(81)	2.95	C(101)...C(81)	3.28
C(82) ...O(81)	3.38	C(91) ...O(81)	3.16
O(91) ...O(81)	3.19	C(93) ...C(82)	3.28
C(92) ...C(91)	2.67	C(93) ...C(91)	2.47
O(93) ...C(91)	3.34	C(93) ...C(92)	2.59

table 6 continued

C(102)...C(101)	2.66	P(2) ...P(1)	3.10
C(112)...P(1)	2.75	C(116)...P(1)	2.75
C(122)...P(1)	2.73	C(126)...P(1)	2.76
C(132)...P(1)	2.81	C(136)...P(1)	2.79
C(212)...P(2)	2.85	C(216)...P(2)	2.71
C(222)...P(2)	2.79	C(226)...P(2)	2.74
C(232)...P(2)	2.67	C(236)...P(2)	2.82
C(111)...N	2.85	C(116)...N	3.40
C(121)...N	2.89	C(122)...N	3.24
C(131)...N	2.88	C(132)...N	3.23
C(211)...N	2.71	C(216)...N	3.31
C(221)...N	2.70	C(226)...N	3.15
C(231)...N	2.72	C(232)...N	3.03
C(113)...C(111)	2.42	C(114)...C(111)	2.79
C(115)...C(111)	2.42	C(121)...C(111)	2.82
C(126)...C(111)	3.06	C(131)...C(111)	2.92
C(114)...C(112)	2.42	C(115)...C(112)	2.79
C(116)...C(112)	2.42	C(131)...C(112)	3.09
C(115)...C(113)	2.42	C(116)...C(113)	2.79
C(116)...C(114)	2.42	C(121)...C(116)	3.37
C(126)...C(116)	3.43	C(123)...C(121)	2.42
C(124)...C(121)	2.79	C(125)...C(121)	2.42
C(131)...C(121)	2.82	C(136)...C(121)	3.06
C(124)...C(122)	2.42	C(125)...C(122)	2.79
C(126)...C(122)	2.42	C(211)...C(122)	3.43
C(125)...C(123)	2.42	C(126)...C(123)	2.79
C(126)...C(124)	2.42	C(136)...C(126)	3.40
C(133)...C(131)	2.42	C(134)...C(131)	2.79

table 6 continued

C(135)...C(131)	2.42	C(134)...C(132)	2.42
C(135)...C(132)	2.79	C(136)...C(132)	2.42
Cl(2) ...C(132)	3.77	C(135)...C(133)	2.42
C(136)...C(133)	2.79	Cl(2) ...C(133)	3.64
C(136)...C(134)	2.42	C(213)...C(211)	2.42
C(214)...C(211)	2.79	C(215)...C(211)	2.42
C(221)...C(211)	2.93	C(231)...C(211)	2.88
C(236)...C(211)	3.24	C(214)...C(212)	2.42
C(215)...C(212)	2.79	C(216)...C(212)	2.42
C(221)...C(212)	3.25	C(226)...C(212)	3.48
C(215)...C(213)	2.42	C(216)...C(213)	2.79
C(216)...C(214)	2.42	C(231)...C(216)	3.21
C(236)...C(216)	3.31	C(223)...C(221)	2.42
C(224)...C(221)	2.79	C(225)...C(221)	2.42
C(231)...C(221)	2.88	C(224)...C(222)	2.42
C(225)...C(222)	2.79	C(226)...C(222)	2.42
C(231)...C(222)	3.13	C(225)...C(223)	2.42
C(226)...C(223)	2.79	C(226)...C(224)	2.42
C(233)...C(231)	2.42	C(234)...C(231)	2.79
C(235)...C(231)	2.42	C(234)...C(232)	2.42
C(235)...C(232)	2.79	C(236)...C(232)	2.42
C(235)...C(233)	2.42	C(236)...C(233)	2.79
C(236)...C(234)	2.42	Cl(1) ...C(235)	3.45
Cl(1) ...C(236)	3.71	Cl(2) ...Cl(1)	2.82

Crystallographic Tables for $[HOs_{11}C(CO)_{27}][PPh_3Me]$, {X-ray study presented in section 3.8, Vol.1}.

TABLE 1 Fractional atomic coordinates and thermal parameters ($Å^2$) for $[HOs_{11}C(CO)_{27}][PPh_3Me]$

Atom	x	y	z	U_{iso} or U_{eq}
Os(1)	-0.2011(3)	0.0734(3)	0.1061(4)	0.038(3)
Os(2)	-0.2882(3)	0.1023(3)	-0.0958(4)	0.026(3)
Os(3)	-0.2023(2)	0.2390(3)	0.0853(4)	0.023(3)
Os(4)	-0.1170(2)	0.1404(3)	-0.0669(4)	0.024(3)
Os(5)	-0.4261(3)	0.1277(3)	-0.2204(4)	0.040(3)
Os(6)	-0.2898(2)	0.2555(3)	-0.1243(4)	0.025(3)
Os(7)	-0.2045(3)	0.3951(3)	0.0414(5)	0.031(3)
Os(8)	-0.1184(2)	0.2931(3)	-0.0983(4)	0.026(3)
Os(9)	0.0190(3)	0.2274(3)	-0.1464(5)	0.038(3)
Os(10)	-0.1162(3)	0.1665(3)	-0.3112(4)	0.035(3)
Os(11)	-0.2586(3)	0.1319(3)	-0.3399(4)	0.038(3)
P	0.2493(21)	0.2999(22)	0.4504(27)	0.050(14)
C(11)	-0.2684(56)	0.0452(59)	0.2146(84)	0.020(15)
O(11)	-0.3358(50)	0.0371(50)	0.2705(74)	0.077(15)
C(12)	-0.0995(68)	0.0863(72)	0.2344(22)	0.052(16)
O(12)	-0.0740(43)	0.0902(45)	0.3199(67)	0.042(14)
C(13)	-0.2081(57)	-0.0161(70)	0.0413(86)	0.027(15)
O(13)	-0.2004(45)	-0.0900(51)	0.0106(68)	0.058(14)
C(21)	-0.3822(62)	0.0649(63)	-0.0086(91)	0.039(16)
O(21)	-0.4304(45)	0.0811(47)	0.0815(69)	0.054(14)
C(22)	-0.3005(61)	0.0055(72)	-0.1687(93)	0.036(16)
O(22)	-0.3011(47)	-0.0702(52)	-0.2254(73)	0.068(15)
C(31)	-0.3003(71)	0.2661(74)	0.1861(22)	0.058(16)
O(31)	-0.3423(54)	0.2550(55)	0.2231(80)	0.086(16)
C(32)	-0.1318(68)	0.2860(68)	0.2026(96)	0.052(16)

table 1 continued

O(32)	-0.0565(47)	0.3226(47)	0.2649(70)	0.057(15)
C(41)	-0.0140(74)	0.1911(77)	0.0827(40)	0.065(17)
O(41)	0.0158(52)	0.1761(54)	0.1376(78)	0.080(15)
C(42)	-0.1037(69)	0.0388(77)	-0.1373(40)	0.061(16)
O(42)	-0.0927(47)	-0.0211(52)	-0.1793(73)	0.066(15)
C(51)	-0.4972(58)	0.1254(61)	-0.1108(86)	0.027(15)
O(51)	-0.5620(51)	0.1254(50)	-0.0472(76)	0.078(15)
C(52)	-0.4624(61)	0.0291(68)	-0.2791(92)	0.036(16)
O(52)	-0.5018(55)	-0.0320(53)	-0.3597(82)	0.089(16)
C(53)	-0.4884(66)	0.1844(69)	-0.3040(99)	0.048(16)
O(53)	-0.5203(55)	0.2165(56)	-0.3624(84)	0.095(16)
C(61)	-0.3033(57)	0.3323(61)	-0.2350(89)	0.026(15)
O(61)	-0.3123(43)	0.3475(46)	-0.3254(70)	0.048(14)
C(62)	-0.3772(71)	0.2769(72)	-0.0851(40)	0.072(16)
O(62)	-0.4357(50)	0.3201(51)	-0.0044(75)	0.078(15)
C(71)	-0.1181(65)	0.4671(68)	0.1497(96)	0.051(16)
O(71)	-0.0743(54)	0.5100(54)	0.2388(81)	0.096(16)
C(72)	-0.2803(77)	0.4208(77)	0.1231(40)	0.084(17)
O(72)	-0.3302(54)	0.4478(54)	0.1867(80)	0.086(16)
C(73)	-0.2061(59)	0.4816(65)	-0.0570(88)	0.027(15)
O(73)	-0.2062(47)	0.5263(49)	-0.1007(72)	0.067(15)
C(81)	-0.0307(60)	0.3738(63)	-0.0100(88)	0.027(15)
O(81)	0.0262(54)	0.4111(54)	0.0433(79)	0.083(15)
C(82)	-0.1099(67)	0.3513(72)	-0.2334(98)	0.056(16)
O(82)	-0.1144(50)	0.4108(52)	-0.2842(77)	0.081(15)
C(91)	0.0574(70)	0.1658(75)	-0.1528(40)	0.064(16)
O(91)	0.0939(47)	0.0872(49)	-0.2518(71)	0.070(15)
C(92)	0.0903(69)	0.3022(72)	-0.2167(40)	0.061(16)

table 1 continued

O(92)	0.1091(50)	0.3452(51)	-0.2840(76)	0.077(15)
C(93)	0.1151(74)	0.2670(76)	-0.0587(40)	0.073(17)
O(93)	0.1511(59)	0.2820(59)	0.0431(89)	0.112(16)
C(101)	-0.0881(72)	0.0736(80)	-0.3968(40)	0.075(17)
O(101)	-0.1102(55)	0.0020(60)	-0.4367(84)	0.103(16)
C(102)	-0.0429(74)	0.1872(78)	-0.4296(40)	0.070(17)
O(102)	0.0075(55)	0.2544(55)	-0.4603(80)	0.097(16)
C(111)	-0.3500(40)	0.1666(40)	-0.4552(40)	0.050(18)
O(111)	-0.3708(49)	0.1916(50)	-0.5241(75)	0.082(15)
C(112)	-0.3250(67)	0.0369(75)	-0.4285(40)	0.060(16)
O(112)	-0.3316(48)	-0.0379(51)	-0.5099(75)	0.072(15)
C	-0.2100(68)	0.1745(69)	-0.1876(98)	0.060(16)
C(3)	0.1729(66)	0.2246(67)	0.3839(95)	0.052(16)
C(112)	0.2557(31)	0.2008(37)	0.6118(53)	0.073(17)
C(113)	0.2809(31)	0.1883(37)	0.7277(53)	0.057(16)
C(114)	0.3217(31)	0.2555(37)	0.8248(53)	0.097(17)
C(115)	0.3375(31)	0.3352(37)	0.8058(53)	0.085(17)
C(116)	0.3123(31)	0.3477(37)	0.6899(53)	0.092(17)
C(111)	0.2715(31)	0.2805(37)	0.5929(53)	0.023(15)
C(122)	0.1382(34)	0.3901(37)	0.4445(49)	0.079(17)
C(123)	0.1100(34)	0.4633(37)	0.4646(49)	0.138(17)
C(124)	0.1653(34)	0.5396(37)	0.5066(49)	0.098(17)
C(125)	0.2488(34)	0.5427(37)	0.5285(49)	0.060(16)
C(126)	0.2770(34)	0.4696(37)	0.5084(49)	0.026(15)
C(121)	0.2217(34)	0.3933(37)	0.4664(49)	0.023(15)

TABLE 2 Anisotropic thermal parameters (Å ^{2}) for $[HOs_{11}C(CO)_{27}][PPh_3Me]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Os(1)	0.048(3)	0.051(4)	0.015(3)	0.020(3)	0.010(2)	0.013(3)
Os(2)	0.024(2)	0.039(4)	0.014(3)	0.010(3)	0.001(2)	-0.006(2)
Os(3)	0.026(2)	0.030(3)	0.013(2)	0.003(2)	0.001(2)	0.006(2)
Os(4)	0.025(2)	0.031(3)	0.014(2)	0.008(2)	0.005(2)	0.006(2)
Os(5)	0.019(3)	0.068(4)	0.032(3)	0.013(3)	0.001(2)	-0.004(3)
Os(6)	0.024(2)	0.035(4)	0.015(3)	0.010(3)	0.001(2)	0.009(2)
Os(7)	0.031(3)	0.024(3)	0.039(3)	0.005(3)	-0.002(2)	0.004(2)
Os(8)	0.018(2)	0.033(4)	0.027(3)	0.012(3)	0.001(2)	0.003(2)
Os(9)	0.018(2)	0.046(4)	0.051(3)	0.022(3)	0.007(2)	0.008(2)
Os(10)	0.034(3)	0.054(4)	0.018(3)	0.016(3)	0.012(2)	0.006(3)
Os(11)	0.028(3)	0.071(4)	0.014(3)	0.010(3)	-0.001(2)	-0.002(3)
P	0.070(14)	0.070(15)	0.011(12)	0.006(12)	0.013(12)	-0.009(13)

TABLE 3 Bond lengths (Å) for $[HOs_{11}C(CO)_{27}][PPh_3Me]$

Os(1) -Os(2)	2.773(7)	Os(1) -Os(3)	2.883(8)
Os(1) -Os(4)	2.764(7)	Os(1) -C(11)	1.78(9)
Os(1) -O(11)	3.05(8)	Os(1) -C(12)	2.08(9)
Os(1) -O(12)	2.99(7)	Os(1) -C(13)	1.50(9)
Os(1) -O(13)	2.74(8)	Os(1) -C(21)	3.18(9)
Os(1) -C(22)	3.20(9)	Os(1) -C(42)	3.23(9)
Os(2) -Os(3)	2.759(6)	Os(2) -Os(4)	2.796(6)
Os(2) -Os(5)	2.773(7)	Os(2) -Os(6)	2.703(8)
Os(2) -Os(8)	3.875(6)	Os(2) -Os(10)	3.976(7)
Os(2) -Os(11)	2.848(7)	Os(2) -C(13)	3.22(9)
Os(2) -C(21)	1.98(9)	Os(2) -O(21)	3.20(8)
Os(2) -C(22)	1.62(9)	Os(3) -Os(4)	2.767(7)
Os(3) -Os(5)	4.647(6)	Os(3) -Os(6)	2.754(7)
Os(3) -Os(7)	2.814(8)	Os(3) -Os(8)	2.764(7)
Os(3) -Os(9)	4.655(7)	Os(3) -Os(10)	4.651(6)
Os(3) -Os(11)	4.634(6)	Os(3) -C(31)	2.11(9)
Os(3) -O(31)	2.90(9)	Os(4) -Os(6)	3.905(7)
Os(4) -Os(8)	2.703(8)	Os(4) -Os(9)	2.771(7)
Os(4) -Os(10)	2.827(7)	Os(4) -Os(11)	3.982(6)
Os(4) -C(13)	3.31(9)	Os(4) -C(41)	2.20(9)
Os(4) -O(41)	2.93(8)	Os(4) -C(42)	1.79(9)
Os(5) -Os(6)	2.777(6)	Os(5) -Os(11)	2.728(7)
Os(5) -C(21)	2.89(9)	Os(5) -C(22)	3.35(9)
Os(5) -C(51)	1.75(9)	Os(5) -O(51)	3.07(9)
Os(5) -C(52)	1.63(9)	Os(5) -O(52)	2.79(8)

table 3 continued

Os(5) -C(53)	1.89(9)	Os(5) -O(53)	2.99(9)
Os(6) -Os(7)	2.706(6)	Os(6) -Os(8)	2.800(6)
Os(6) -Os(10)	3.990(7)	Os(6) -Os(11)	2.790(6)
Os(6) -C(61)	2.02(9)	Os(6) -O(61)	3.04(9)
Os(6) -C(62)	1.64(9)	Os(6) -O(62)	3.13(9)
Os(7) -Os(8)	2.745(7)	Os(7) -C(31)	3.24(9)
Os(7) -C(32)	3.20(9)	Os(7) -C(61)	3.21(9)
Os(7) -C(62)	3.20(9)	Os(7) -C(71)	1.85(9)
Os(7) -O(71)	3.01(7)	Os(7) -C(72)	1.68(9)
Os(7) -O(72)	2.89(9)	Os(7) -C(73)	2.02(9)
Os(8) -Os(9)	2.788(7)	Os(8) -Os(10)	2.796(6)
Os(8) -Os(11)	3.907(6)	Os(8) -C(81)	1.84(8)
Os(8) -O(81)	2.91(8)	Os(8) -C(82)	1.97(9)
Os(8) -O(82)	3.17(9)	Os(9) -Os(10)	2.703(6)
Os(9) -C(41)	2.80(9)	Os(9) -C(81)	2.90(9)
Os(9) -C(91)	1.33(9)	Os(9) -O(91)	2.96(8)
Os(9) -C(92)	1.90(9)	Os(9) -O(92)	3.02(9)
Os(9) -C(93)	1.75(9)	Os(9) -O(93)	2.80(9)
Os(10)-Os(11)	2.784(6)	Os(10)-C(42)	3.24(9)
Os(10)-C(82)	3.04(9)	Os(10)-C(91)	3.33(9)
Os(10)-C(101)	1.83(9)	Os(10)-O(101)	2.86(9)
Os(11)-C(22)	3.16(9)	Os(11)-C(52)	3.28(9)
Os(11)-C(111)	1.86(9)	Os(11)-O(111)	2.86(9)
Os(11)-C(112)	1.66(9)	C(11) -O(11)	1.32(9)
C(12) -O(12)	0.99(9)	C(13) -O(13)	1.26(9)
C(21) -O(21)	1.34(9)	C(22) -O(22)	1.29(9)
C(31) -O(31)	0.85(9)	C(32) -O(32)	1.35(9)
C(41) -O(41)	0.88(9)	C(42) -O(42)	1.08(9)

table 3 continued

C(51) -O(51)	1.33(9)	C(52) -O(52)	1.24(9)
C(53) -O(53)	1.11(9)	C(61) -O(61)	1.09(9)
C(62) -O(62)	1.55(9)	C(71) -O(71)	1.18(9)
C(72) -O(72)	1.22(9)	C(73) -O(73)	0.99(9)
C(81) -O(81)	1.08(9)	C(82) -O(82)	1.28(9)
C(91) -O(91)	1.76(9)	C(91) -C(93)	1.83(9)
C(92) -O(92)	1.17(9)	C(93) -O(93)	1.19(9)
C(101)-O(101)	1.17(9)	C(102)-O(102)	1.40(9)
C(111)-O(111)	1.03(9)	C(112)-O(112)	1.36(9)
P -C(3)	1.62(9)	P -C(111)	1.71(7)
P -C(121)	1.72(8)	C(112)-C(113)	1.39(9)
C(112)-C(111)	1.39(9)	C(113)-C(114)	1.39(7)
C(114)-C(115)	1.39(9)	C(115)-C(116)	1.39(9)
C(116)-C(111)	1.39(7)	C(122)-C(123)	1.39(9)
C(122)-C(121)	1.39(8)	C(123)-C(124)	1.39(7)
C(124)-C(125)	1.39(8)	C(125)-C(126)	1.39(9)
C(126)-C(121)	1.39(7)		

TABLE 4 Bond angles (°) for $[HOs_{11}C(CO)_{27}][PPh_3Me]$

Os(3) -Os(1) -Os(2)	58.4(2)	Os(4) -Os(1) -Os(2)	60.7(2)
Os(4) -Os(1) -Os(3)	58.6(2)	C(11) -Os(1) -Os(2)	110(3)
C(11) -Os(1) -Os(3)	110(3)	C(11) -Os(1) -Os(4)	168(3)
C(12) -Os(1) -Os(2)	156(3)	C(12) -Os(1) -Os(3)	105(3)
C(12) -Os(1) -Os(4)	97(3)	C(12) -Os(1) -C(11)	91(4)
C(13) -Os(1) -Os(2)	93(4)	C(13) -Os(1) -Os(3)	148(4)
C(13) -Os(1) -Os(4)	97(4)	C(13) -Os(1) -C(11)	91(5)
C(13) -Os(1) -C(12)	97(5)	Os(3) -Os(2) -Os(1)	62.8(2)
Os(4) -Os(2) -Os(1)	59.5(2)	Os(4) -Os(2) -Os(3)	59.7(2)
Os(5) -Os(2) -Os(1)	154.0(2)	Os(5) -Os(2) -Os(3)	114.3(2)
Os(5) -Os(2) -Os(4)	144.0(3)	Os(6) -Os(2) -Os(1)	123.4(2)
Os(6) -Os(2) -Os(3)	60.6(2)	Os(6) -Os(2) -Os(4)	90.5(2)
Os(6) -Os(2) -Os(5)	60.9(2)	Os(11)-Os(2) -Os(1)	147.9(2)
Os(11)-Os(2) -Os(3)	111.5(2)	Os(11)-Os(2) -Os(4)	89.7(2)
Os(11)-Os(2) -Os(5)	58.1(2)	Os(11)-Os(2) -Os(6)	60.3(2)
C(21) -Os(2) -Os(1)	82(3)	C(21) -Os(2) -Os(3)	101(2)
C(21) -Os(2) -Os(4)	141(3)	C(21) -Os(2) -Os(5)	73(3)
C(21) -Os(2) -Os(6)	109(3)	C(21) -Os(2) -Os(11)	129(3)
C(22) -Os(2) -Os(1)	89(4)	C(22) -Os(2) -Os(3)	150(4)
C(22) -Os(2) -Os(4)	97(4)	C(22) -Os(2) -Os(5)	96(4)
C(22) -Os(2) -Os(6)	145(4)	C(22) -Os(2) -Os(11)	85(4)
C(22) -Os(2) -C(21)	86(5)	C -Os(2) -Os(1)	110(3)
C -Os(2) -Os(3)	73(3)	C -Os(2) -Os(4)	52(3)
C -Os(2) -Os(5)	92(3)	C -Os(2) -Os(6)	51(3)
C -Os(2) -Os(11)	43(3)	C -Os(2) -C(21)	160(5)

table 4 continued

C -Os(2) -C(22)	109(5)	Os(2) -Os(3) -Os(1)	58.8(2)
Os(4) -Os(3) -Os(1)	58.5(2)	Os(4) -Os(3) -Os(2)	60.8(2)
Os(6) -Os(3) -Os(1)	117.5(2)	Os(6) -Os(3) -Os(2)	58.7(2)
Os(6) -Os(3) -Os(4)	90.0(2)	Os(7) -Os(3) -Os(1)	174.8(2)
Os(7) -Os(3) -Os(2)	116.8(2)	Os(7) -Os(3) -Os(4)	117.4(2)
Os(7) -Os(3) -Os(6)	58.1(2)	Os(8) -Os(3) -Os(1)	117.0(2)
Os(8) -Os(3) -Os(2)	89.1(2)	Os(8) -Os(3) -Os(4)	58.5(2)
Os(8) -Os(3) -Os(6)	61.0(2)	Os(8) -Os(3) -Os(7)	59.0(2)
C(31) -Os(3) -Os(1)	102(4)	C(31) -Os(3) -Os(2)	98(3)
C(31) -Os(3) -Os(4)	156(3)	C(31) -Os(3) -Os(6)	88(3)
C(31) -Os(3) -Os(7)	81(4)	C(31) -Os(3) -Os(8)	138(4)
C(32) -Os(3) -Os(1)	96(4)	C(32) -Os(3) -Os(2)	154(4)
C(32) -Os(3) -Os(4)	101(4)	C(32) -Os(3) -Os(6)	145(4)
C(32) -Os(3) -Os(7)	88(4)	C(32) -Os(3) -Os(8)	97(4)
C(32) -Os(3) -C(31)	95(5)	Os(2) -Os(4) -Os(1)	59.8(2)
Os(3) -Os(4) -Os(1)	62.8(2)	Os(3) -Os(4) -Os(2)	59.5(2)
Os(8) -Os(4) -Os(1)	123.5(2)	Os(8) -Os(4) -Os(2)	89.6(2)
Os(8) -Os(4) -Os(3)	60.7(2)	Os(9) -Os(4) -Os(1)	154.1(2)
Os(9) -Os(4) -Os(2)	143.6(3)	Os(9) -Os(4) -Os(3)	114.4(2)
Os(9) -Os(4) -Os(8)	61.2(2)	Os(10)-Os(4) -Os(1)	148.2(2)
Os(10)-Os(4) -Os(2)	90.0(2)	Os(10)-Os(4) -Os(3)	112.5(2)
Os(10)-Os(4) -Os(8)	60.7(2)	Os(10)-Os(4) -Os(9)	57.7(2)
C(41) -Os(4) -Os(1)	87(3)	C(41) -Os(4) -Os(2)	140(3)
C(41) -Os(4) -Os(3)	86(3)	C(41) -Os(4) -Os(8)	91(4)
C(41) -Os(4) -Os(9)	67(3)	C(41) -Os(4) -Os(10)	125(3)
C(42) -Os(4) -Os(1)	88(4)	C(42) -Os(4) -Os(2)	97(3)
C(42) -Os(4) -Os(3)	148(4)	C(42) -Os(4) -Os(8)	146(4)
C(42) -Os(4) -Os(9)	97(4)	C(42) -Os(4) -Os(10)	86(4)

table 4 continued

C(42) -Os(4) -C(41)	104(5)	C -Os(4) -Os(1)	106(3)
C -Os(4) -Os(2)	47(3)	C -Os(4) -Os(3)	71(3)
C -Os(4) -Os(5)	53(3)	C -Os(4) -Os(9)	96(3)
C -Os(4) -Os(10)	48(3)	C -Os(4) -C(41)	144(4)
C -Os(4) -C(42)	110(4)	Os(6) -Os(5) -Os(2)	58.3(2)
Os(11)-Os(5) -Os(2)	62.3(2)	Os(11)-Os(5) -Os(6)	60.9(2)
C(51) -Os(5) -Os(2)	103(3)	C(51) -Os(5) -Os(6)	110(3)
C(51) -Os(5) -Os(11)	165(3)	C(52) -Os(5) -Os(2)	93(4)
C(52) -Os(5) -Os(6)	148(4)	C(52) -Os(5) -Os(11)	94(4)
C(52) -Os(5) -C(51)	89(5)	C(53) -Os(5) -Os(2)	157(3)
C(53) -Os(5) -Os(6)	99(3)	C(53) -Os(5) -Os(11)	104(3)
C(53) -Os(5) -C(51)	89(5)	C(53) -Os(5) -C(52)	107(5)
C(62) -Os(5) -Os(2)	84(3)	C(62) -Os(5) -Os(6)	35(3)
C(62) -Os(5) -Os(11)	94(3)	C(62) -Os(5) -C(51)	81(4)
C(62) -Os(5) -C(52)	168(5)	C(62) -Os(5) -C(53)	79(4)
Os(3) -Os(6) -Os(2)	60.7(2)	Os(5) -Os(6) -Os(2)	60.8(2)
Os(5) -Os(6) -Os(3)	114.3(2)	Os(7) -Os(6) -Os(2)	122.7(2)
Os(7) -Os(6) -Os(3)	62.0(2)	Os(7) -Os(6) -Os(5)	154.7(2)
Os(8) -Os(6) -Os(2)	89.5(2)	Os(8) -Os(6) -Os(3)	59.7(2)
Os(8) -Os(6) -Os(5)	142.7(2)	Os(8) -Os(6) -Os(7)	59.8(2)
Os(11)-Os(6) -Os(2)	62.4(2)	Os(11)-Os(6) -Os(3)	113.4(2)
Os(11)-Os(6) -Os(5)	58.7(2)	Os(11)-Os(6) -Os(7)	146.6(2)
Os(11)-Os(6) -Os(8)	88.7(2)	C(61) -Os(6) -Os(2)	150(2)
C(61) -Os(6) -Os(3)	145(2)	C(61) -Os(6) -Os(5)	100(2)
C(61) -Os(6) -Os(7)	84(2)	C(61) -Os(6) -Os(8)	96(3)
C(61) -Os(6) -Os(11)	89(3)	C(62) -Os(6) -Os(2)	108(4)
C(62) -Os(6) -Os(3)	108(4)	C(62) -Os(6) -Os(5)	65(4)
C(62) -Os(6) -Os(7)	91(3)	C(62) -Os(6) -Os(8)	151(3)

table 4 continued

C -Os(8) -Os(7)	106(3)	C -Os(8) -Os(9)	95(3)
C -Os(8) -Os(10)	48(3)	C -Os(8) -C(81)	166(5)
C -Os(8) -C(82)	103(4)	Os(8) -Os(9) -Os(4)	58.2(2)
Os(10)-Os(9) -Os(4)	62.2(2)	Os(10)-Os(9) -Os(8)	61.2(2)
C(91) -Os(9) -Os(4)	92(5)	C(91) -Os(9) -Os(8)	150(5)
C(91) -Os(9) -Os(10)	106(4)	C(92) -Os(9) -Os(4)	164(4)
C(92) -Os(9) -Os(8)	107(4)	C(92) -Os(9) -Os(10)	106(3)
C(92) -Os(9) -C(91)	103(6)	C(93) -Os(9) -Os(4)	125(4)
C(93) -Os(9) -Os(8)	124(4)	C(93) -Os(9) -Os(10)	172(4)
C(93) -Os(9) -C(91)	72(6)	C(93) -Os(9) -C(92)	67(5)
Os(8) -Os(10)-Os(4)	57.5(2)	Os(9) -Os(10)-Os(4)	60.1(2)
Os(9) -Os(10)-Os(8)	60.9(2)	Os(11)-Os(10)-Os(4)	90.4(2)
Os(11)-Os(10)-Os(8)	88.9(2)	Os(11)-Os(10)-Os(9)	145.4(2)
C(1o1)-Os(10)-Os(4)	101(4)	C(1o1)-Os(10)-Os(8)	154(4)
C(1o1)-Os(10)-Os(9)	97(3)	C(1o1)-Os(10)-Os(11)	107(3)
C(1o2)-Os(10)-Os(4)	139(4)	C(1o2)-Os(10)-Os(8)	119(3)
C(1o2)-Os(10)-Os(9)	82(3)	C(1o2)-Os(10)-Os(11)	130(4)
C(1o2)-Os(10)-C(1o1)	66(6)	C -Os(10)-Os(4)	51(3)
C -Os(10)-Os(8)	52(3)	C -Os(10)-Os(9)	101(3)
C -Os(10)-Os(11)	45(3)	C -Os(10)-C(1o1)	128(5)
C -Os(10)-C(1o2)	164(5)	Os(5) -Os(11)-Os(2)	59.6(2)
Os(6) -Os(11)-Os(2)	57.3(2)	Os(6) -Os(11)-Os(5)	60.4(2)
Os(10)-Os(11)-Os(2)	89.8(2)	Os(10)-Os(11)-Os(5)	145.9(2)
Os(10)-Os(11)-Os(6)	91.4(2)	C(111)-Os(11)-Os(2)	142(8)
C(111)-Os(11)-Os(5)	83(8)	C(111)-Os(11)-Os(6)	100(8)
C(111)-Os(11)-Os(10)	123(9)	C(112)-Os(11)-Os(2)	101(4)
C(112)-Os(11)-Os(5)	92(4)	C(112)-Os(11)-Os(6)	150(4)
C(112)-Os(11)-Os(10)	110(4)	C(112)-Os(11)-C(111)	86(9)

table 4 continued

C(62) -Os(6) -Os(11)	120(3)	C(62) -Os(6) -C(61)	81(5)
C -Os(6) -Os(2)	49(3)	C -Os(6) -Os(3)	72(3)
C -Os(6) -Os(5)	91(3)	C -Os(6) -Os(7)	110(2)
C -Os(6) -Os(8)	52(3)	C -Os(6) -Os(11)	44(3)
C -Os(6) -C(61)	114(4)	C -Os(6) -C(62)	155(5)
Os(6) -Os(7) -Os(3)	59.8(2)	Os(8) -Os(7) -Os(3)	59.6(2)
Os(8) -Os(7) -Os(6)	61.5(2)	C(71) -Os(7) -Os(3)	105(4)
C(71) -Os(7) -Os(6)	159(4)	C(71) -Os(7) -Os(8)	99(4)
C(72) -Os(7) -Os(3)	101(5)	C(72) -Os(7) -Os(6)	99(4)
C(72) -Os(7) -Os(8)	157(4)	C(72) -Os(7) -C(71)	98(5)
C(73) -Os(7) -Os(3)	156(3)	C(73) -Os(7) -Os(6)	102(2)
C(73) -Os(7) -Os(8)	102(3)	C(73) -Os(7) -C(71)	89(4)
C(73) -Os(7) -C(72)	93(6)	Os(4) -Os(8) -Os(3)	60.8(2)
Os(6) -Os(8) -Os(3)	59.3(2)	Os(6) -Os(8) -Os(4)	90.4(2)
Os(7) -Os(8) -Os(3)	61.4(2)	Os(7) -Os(8) -Os(4)	122.2(2)
Os(7) -Os(8) -Os(6)	58.4(2)	Os(9) -Os(8) -Os(3)	114.0(2)
Os(9) -Os(8) -Os(4)	60.6(2)	Os(9) -Os(8) -Os(6)	144.2(2)
Os(9) -Os(8) -Os(7)	154.2(2)	Os(10)-Os(8) -Os(3)	113.5(2)
Os(10)-Os(8) -Os(4)	61.8(2)	Os(10)-Os(8) -Os(6)	91.0(2)
Os(10)-Os(8) -Os(7)	147.9(2)	Os(10)-Os(8) -Os(9)	57.9(2)
C(81) -Os(8) -Os(3)	104(3)	C(81) -Os(8) -Os(4)	114(4)
C(81) -Os(8) -Os(6)	140(3)	C(81) -Os(8) -Os(7)	82(3)
C(81) -Os(8) -Os(9)	75(3)	C(81) -Os(8) -Os(10)	128(3)
C(82) -Os(8) -Os(3)	151(3)	C(82) -Os(8) -Os(4)	139(3)
C(82) -Os(8) -Os(6)	95(3)	C(82) -Os(8) -Os(7)	95(3)
C(82) -Os(8) -Os(9)	95(3)	C(82) -Os(8) -Os(10)	77(3)
C(82) -Os(8) -C(81)	87(4)	C -Os(8) -Os(3)	71(3)
C -Os(8) -Os(4)	53(3)	C -Os(8) -Os(6)	49(3)

table 4 continued

C -Os(11)-Os(2)	47(3)	C -Os(11)-Os(5)	96(3)
C -Os(11)-Os(6)	50(3)	C -Os(11)-Os(10)	50(3)
C -Os(11)-C(111)	142(9)	C -Os(11)-C(112)	132(6)
O(11) -C(11) -Os(1)	158(9)	O(12) -C(12) -Os(1)	151.9(6)
O(13) -C(13) -Os(1)	165(9)	O(21) -C(21) -Os(2)	150(7)
O(22) -C(22) -Os(2)	173(9)	O(31) -C(31) -Os(3)	155(3)
O(32) -C(32) -Os(3)	159(9)	O(41) -C(41) -Os(4)	141(2)
O(42) -C(42) -Os(4)	177.3(1)	O(51) -C(51) -Os(5)	168(9)
O(52) -C(52) -Os(5)	154.3(6)	O(53) -C(53) -Os(5)	173.0(5)
O(61) -C(61) -Os(6)	154(5)	Os(6) -C(62) -Os(5)	79(4)
O(62) -C(62) -Os(5)	121(6)	O(62) -C(62) -Os(6)	157(7)
O(71) -C(71) -Os(7)	165( )	O(72) -C(72) -Os(7)	173( )
O(73) -C(73) -Os(7)	177(9)	O(81) -C(81) -Os(8)	169(1)
O(82) -C(82) -Os(8)	155(9)	O(91) -C(91) -Os(9)	146(9)
C(93) -C(91) -Os(9)	65(6)	C(93) -C(91) -O(91)	129(8)
O(92) -C(92) -Os(9)	157(9)	C(91) -C(93) -Os(9)	43(5)
O(93) -C(93) -Os(9)	144.1(8)	O(93) -C(93) -C(91)	127(2)
O(1o1)-C(1o1)-Os(10)	143.9(4)	O(1o2)-C(1o2)-Os(10)	139(9)
O(111)-C(111)-Os(11)	167(5)	O(112)-C(112)-Os(11)	163(9)
Os(4) -C -Os(2)	81(4)	Os(6) -C -Os(2)	79(4)
Os(6) -C -Os(4)	126(5)	Os(8) -C -Os(2)	127(5)
Os(8) -C -Os(4)	74(3)	Os(8) -C -Os(6)	79(4)
Os(10)-C -Os(2)	141(6)	Os(10)-C -Os(4)	81(4)
Os(10)-C -Os(6)	138(6)	Os(10)-C -Os(8)	79(4)
Os(11)-C -Os(2)	89(4)	Os(11)-C -Os(4)	143(6)
Os(11)-C -Os(6)	85(5)	Os(11)-C -Os(8)	136(6)
Os(11)-C -Os(10)	86(4)	C(111)-P -C(3)	103(5)
C(121)-P -C(3)	110(5)	C(121)-P -C(111)	112(3)

table 4 continued

C(111)-C(112)-C(113)	120(5)	C(114)-C(113)-C(112)	120(6)
C(115)-C(114)-C(113)	120(6)	C(116)-C(115)-C(114)	120(5)
C(111)-C(116)-C(115)	120(6)	C(112)-C(111)-P	123(4)
C(116)-C(111)-P	117(5)	C(116)-C(111)-C(112)	120(6)
C(121)-C(122)-C(123)	120(5)	C(124)-C(123)-C(122)	120(5)
C(125)-C(124)-C(123)	120(6)	C(126)-C(125)-C(124)	120(5)
C(121)-C(126)-C(125)	120(5)	C(122)-C(121)-P	116(4)
C(126)-C(121)-P	123(5)	C(126)-C(121)-C(122)	120(6)

TABLE 5 Intermolecular distances (A°) for $[HOs_{11}C(CO)_{27}][PPh_3Me]$

atom1	atom2	dist	S	a	b	c
O(91)	...Os(1)	4.11	-1	0.0	0.0	0.0
O(12)	...Os(10)	4.14	1	0.0	0.0	1.0
C(111)	...O(11)	3.36	1	0.0	0.0	-1.0
O(111)	...O(11)	3.23	1	0.0	0.0	-1.0
C(112)	...O(11)	3.31	1	0.0	0.0	-1.0
O(112)	...O(11)	2.99	1	0.0	0.0	-1.0
O(51)	...O(11)	3.33	-1	-1.0	0.0	0.0
C(52)	...O(11)	3.36	-1	-1.0	0.0	0.0
O(52)	...O(11)	2.95	-1	-1.0	0.0	0.0
O(91)	...C(12)	3.02	-1	0.0	0.0	0.0
C(1o1)	...O(12)	3.22	1	0.0	0.0	-1.0
C(1o2)	...O(12)	2.82	1	0.0	0.0	-1.0
O(1o2)	...O(12)	3.23	1	0.0	0.0	-1.0
O(91)	...O(12)	2.88	-1	0.0	0.0	0.0
C(91)	...O(13)	3.40	-1	0.0	0.0	0.0
O(91)	...O(13)	3.09	-1	0.0	0.0	0.0
O(51)	...C(21)	3.39	-1	-1.0	0.0	0.0
O(21)	...O(21)	3.30	-1	-1.0	0.0	0.0
O(111)	...O(31)	3.24	1	0.0	0.0	-1.0
O(42)	...O(41)	3.27	-1	0.0	0.0	0.0
C(111)	...O(52)	3.24	-1	-1.0	0.0	-1.0
O(111)	...O(52)	3.05	-1	-1.0	0.0	-1.0
C(125)	...O(61)	3.33	-1	0.0	1.0	0.0
O(92)	...C(71)	3.17	-1	0.0	1.0	0.0
O(82)	...O(71)	3.14	-1	0.0	1.0	0.0

table 5 continued

C(92) ...O(71)	3.32	-1	0.0	1.0	0.0
O(92) ...O(71)	2.59	-1	0.0	1.0	0.0
C(123)...O(71)	3.31	-1	0.0	1.0	1.0
C(116)...O(72)	3.38	-1	0.0	1.0	1.0
C(125)...O(72)	3.30	-1	0.0	1.0	1.0
C(126)...O(72)	3.31	-1	0.0	1.0	1.0
O(81) ...C(73)	3.18	-1	0.0	1.0	0.0
O(81) ...O(73)	2.97	-1	0.0	1.0	0.0
O(93) ...O(73)	3.11	-1	0.0	1.0	0.0
C(123)...O(82)	3.24	-1	0.0	1.0	0.0
C(124)...O(82)	2.90	-1	0.0	1.0	0.0
C(113)...O(91)	3.31	1	0.0	0.0	1.0
C(111)...O(92)	3.39	1	0.0	0.0	1.0
C(122)...O(92)	3.30	1	0.0	0.0	1.0
C(122)...O(1o2)	3.26	1	0.0	0.0	1.0
C(112)...O(112)	3.28	-1	0.0	0.0	0.0
C(113)...O(112)	3.37	-1	0.0	0.0	0.0

Symmetry Transformations:

The second atom is related to the first atom, at (x,y,z), by the symmetry operation S with (a,b,c) added to the (x',y',z') of S.

Where S =

1 x, y, z

TABLE 6 Intramolecular distances (A°) for $[HOs_{11}C(CO)_{27}][PPh_3Me]$

Os(6) ...Os(1)	4.82	Os(8) ...Os(1)	4.82
O(11) ...Os(1)	3.05	O(12) ...Os(1)	2.99
O(13) ...Os(1)	2.74	C(21) ...Os(1)	3.18
O(21) ...Os(1)	3.87	C(22) ...Os(1)	3.20
O(22) ...Os(1)	3.95	C(31) ...Os(1)	3.92
C(32) ...Os(1)	3.46	C(41) ...Os(1)	3.43
O(41) ...Os(1)	3.67	C(42) ...Os(1)	3.23
O(42) ...Os(1)	3.92	C ...Os(1)	4.01
Os(7) ...Os(2)	4.75	Os(8) ...Os(2)	3.88
Os(10)...Os(2)	3.98	C(11) ...Os(2)	3.78
C(13) ...Os(2)	3.22	O(21) ...Os(2)	3.20
O(22) ...Os(2)	2.91	C(31) ...Os(2)	3.71
O(31) ...Os(2)	4.13	C(42) ...Os(2)	3.50
C(51) ...Os(2)	3.61	C(52) ...Os(2)	3.29
C(62) ...Os(2)	3.57	C(112)...Os(2)	3.55
Os(5) ...Os(3)	4.65	Os(9) ...Os(3)	4.66
Os(10)...Os(3)	4.65	Os(11)...Os(3)	4.63
C(11) ...Os(3)	3.88	C(12) ...Os(3)	3.98
C(13) ...Os(3)	4.24	C(21) ...Os(3)	3.68
C(22) ...Os(3)	4.24	O(31) ...Os(3)	2.90
O(32) ...Os(3)	2.93	C(41) ...Os(3)	3.42
O(41) ...Os(3)	4.06	C(62) ...Os(3)	3.63
C(71) ...Os(3)	3.74	C(72) ...Os(3)	3.54
C(81) ...Os(3)	3.68	C ...Os(3)	2.94
Os(6) ...Os(4)	3.90	Os(7) ...Os(4)	4.77

table 6 continued

Os(11)...Os(4)	3.98	C(12) ...Os(4)	3.65
C(13) ...Os(4)	3.31	C(22) ...Os(4)	3.40
C(32) ...Os(4)	3.46	O(32) ...Os(4)	4.13
O(41) ...Os(4)	2.93	O(42) ...Os(4)	2.86
C(51) ...Os(4)	3.83	C(91) ...Os(4)	3.12
C(93) ...Os(4)	4.04	C(101)...Os(4)	3.64
C(21) ...Os(5)	2.89	O(21) ...Os(5)	3.60
C(22) ...Os(5)	3.35	O(51) ...Os(5)	3.07
O(52) ...Os(5)	2.79	O(53) ...Os(5)	2.99
C(61) ...Os(5)	3.72	O(62) ...Os(5)	3.62
C(111)...Os(5)	3.11	O(111)...Os(5)	3.86
C(112)...Os(5)	3.23	C ...Os(5)	3.53
Os(10)...Os(6)	3.99	C(21) ...Os(6)	3.84
C(22) ...Os(6)	4.13	C(31) ...Os(6)	3.40
O(31) ...Os(6)	3.99	C(32) ...Os(6)	4.20
C(51) ...Os(6)	3.77	C(52) ...Os(6)	4.24
C(53) ...Os(6)	3.59	O(61) ...Os(6)	3.04
O(62) ...Os(6)	3.13	C(72) ...Os(6)	3.41
C(73) ...Os(6)	3.70	C(82) ...Os(6)	3.56
C(111)...Os(6)	3.60	C(31) ...Os(7)	3.24
O(31) ...Os(7)	3.96	C(32) ...Os(7)	3.20
O(32) ...Os(7)	3.95	C(61) ...Os(7)	3.21
O(61) ...Os(7)	4.15	C(62) ...Os(7)	3.20
O(62) ...Os(7)	3.80	O(71) ...Os(7)	3.01
O(72) ...Os(7)	2.89	O(73) ...Os(7)	3.01
C(81) ...Os(7)	3.08	O(81) ...Os(7)	3.83
C(82) ...Os(7)	3.51	O(82) ...Os(7)	4.03
C ...Os(7)	3.99	Os(11)...Os(8)	3.91

table 6 continued

C(32) ...Os(8)	3.37	O(32) ...Os(8)	3.96
C(41) ...Os(8)	3.52	C(61) ...Os(8)	3.61
C(71) ...Os(8)	3.54	C(73) ...Os(8)	3.74
O(81) ...Os(8)	2.91	O(82) ...Os(8)	3.17
C(91) ...Os(8)	3.99	C(92) ...Os(8)	3.81
C(93) ...Os(8)	4.04	C(1o2)...Os(8)	4.08
C(41) ...Os(9)	2.80	O(41) ...Os(9)	3.44
C(42) ...Os(9)	3.48	C(81) ...Os(9)	2.90
O(81) ...Os(9)	3.31	C(82) ...Os(9)	3.54
O(91) ...Os(9)	2.96	O(92) ...Os(9)	3.02
O(93) ...Os(9)	2.80	C(1o1)...Os(9)	3.44
C(1o2)...Os(9)	3.10	O(1o2)...Os(9)	3.59
C ...Os(9)	3.74	C(42) ...Os(10)	3.24
O(42) ...Os(10)	3.88	C(81) ...Os(10)	4.18
C(82) ...Os(10)	3.04	O(82) ...Os(10)	4.09
C(91) ...Os(10)	3.33	O(91) ...Os(10)	4.12
C(92) ...Os(10)	3.72	O(1o1)...Os(10)	2.86
O(1o2)...Os(10)	3.12	C(111)...Os(10)	4.11
C(112)...Os(10)	3.69	C(22) ...Os(11)	3.16
O(22) ...Os(11)	3.90	C(52) ...Os(11)	3.28
O(52) ...Os(11)	4.03	C(53) ...Os(11)	3.66
C(61) ...Os(11)	3.40	O(61) ...Os(11)	3.74
C(62) ...Os(11)	3.88	C(82) ...Os(11)	4.17
C(1o1)...Os(11)	3.75	O(1o1)...Os(11)	4.12
O(111)...Os(11)	2.86	O(112)...Os(11)	2.98
C(12) ...C(11)	2.76	O(12) ...C(11)	3.27
C(13) ...C(11)	2.35	O(13) ...C(11)	3.26
C(21) ...C(11)	3.13	O(21) ...C(11)	3.24

table 6 continued

C(21) ...O(11)	3.29	O(21) ...O(11)	2.86
C(13) ...C(12)	2.72	C(41) ...C(12)	2.95
O(41) ...C(12)	2.66	O(41) ...O(12)	3.05
C(22) ...C(13)	2.84	O(22) ...C(13)	3.08
C(42) ...C(13)	2.91	O(42) ...C(13)	3.20
C(22) ...O(13)	3.39	O(22) ...O(13)	3.13
C(42) ...O(13)	3.27	O(42) ...O(13)	3.13
C(22) ...C(21)	2.46	C(51) ...C(21)	2.66
O(51) ...C(21)	3.41	C(52) ...C(21)	3.06
C(31) ...O(21)	3.36	O(31) ...O(21)	3.03
C(51) ...O(21)	2.66	O(51) ...O(21)	2.87
C(42) ...C(22)	3.22	C(52) ...C(22)	3.04
C(112)...C(22)	3.05	C ...C(22)	3.03
C(42) ...O(22)	3.41	C(112)...O(22)	3.25
O(112)...O(22)	3.33	C(32) ...C(31)	2.77
C(62) ...C(31)	3.24	O(62) ...C(31)	3.39
C(72) ...C(31)	2.84	O(72) ...C(31)	3.23
C(72) ...O(31)	3.27	C(41) ...C(32)	2.98
O(41) ...C(32)	3.41	C(71) ...C(32)	3.23
C(81) ...C(32)	3.42	C(41) ...O(32)	2.88
O(41) ...O(32)	3.08	C(71) ...O(32)	3.32
O(71) ...O(32)	3.34	C(81) ...O(32)	3.37
C(42) ...C(41)	3.15	C(91) ...C(41)	2.91
C(93) ...C(41)	3.01	O(93) ...C(41)	3.00
C(91) ...O(41)	3.29	C(93) ...O(41)	3.29
O(93) ...O(41)	3.01	C(91) ...C(42)	3.15
C(1o1)...C(42)	3.07	O(1o1)...C(42)	3.20
C ...C(42)	3.31	C(1o1)...O(42)	3.18

table 6 continued

O(1o1)...O(42)	2.95	C(52) ...C(51)	2.36
O(52) ...C(51)	3.35	C(53) ...C(51)	2.56
C(62) ...C(51)	2.88	O(62) ...C(51)	3.18
C(53) ...C(52)	2.83	C(112)...C(52)	2.92
C(112)...O(52)	3.17	C(62) ...C(53)	2.88
C(111)...C(53)	2.97	O(111)...C(53)	3.24
C(111)...O(53)	3.30	O(111)...O(53)	3.21
C(62) ...C(61)	2.38	C(73) ...C(61)	2.93
O(73) ...C(61)	3.32	C(82) ...C(61)	3.20
O(82) ...C(61)	3.32	C(111)...C(61)	3.19
C ...C(61)	3.49	C(62) ...O(61)	3.31
O(82) ...O(61)	3.25	C(111)...O(61)	3.00
O(111)...O(61)	2.96	C(72) ...C(62)	3.04
C(72) ...O(62)	2.89	O(72) ...O(62)	2.86
C(72) ...C(71)	2.65	C(73) ...C(71)	2.72
C(81) ...C(71)	2.78	O(81) ...C(71)	2.99
C(81) ...O(71)	3.38	O(81) ...O(71)	3.20
C(73) ...C(72)	2.70	C(82) ...C(73)	3.34
O(82) ...C(73)	3.15	O(82) ...O(73)	3.18
C(82) ...C(81)	2.63	C(92) ...C(81)	3.33
C(93) ...C(81)	3.33	C(92) ...O(81)	3.40
C(93) ...O(81)	3.15	O(93) ...O(81)	3.33
C ...C(82)	3.31	C(92) ...C(91)	2.55
O(93) ...C(91)	2.72	C(1o1)...C(91)	3.36
C(93) ...O(91)	3.24	C(1o1)...O(91)	3.29
C(93) ...C(92)	2.01	O(93) ...C(92)	3.09
C(1o2)...C(92)	3.13	O(1o2)...C(92)	2.80
C(93) ...O(92)	3.08	C(1o2)...O(92)	3.32

table 6 continued

O(1o2)...O(92)	2.49	C(1o2)...C(1o1)	2.05
O(1o2)...C(1o1)	3.42	C(1o2)...O(1o1)	3.11
C(112)...C(111)	2.41	C(112)...O(111)	3.26
C ...C(112)	3.30	C(112)...P	2.73
C(116)...P	2.65	C(122)...P	2.65
C(126)...P	2.74	C(112)...C(3)	2.94
C(111)...C(3)	2.61	C(122)...C(3)	2.93
C(121)...C(3)	2.74	C(114)...C(112)	2.42
C(115)...C(112)	2.79	C(116)...C(112)	2.42
C(115)...C(113)	2.42	C(116)...C(113)	2.79
C(111)...C(113)	2.42	C(116)...C(114)	2.42
C(111)...C(114)	2.79	C(111)...C(115)	2.42
C(126)...C(116)	3.30	C(121)...C(116)	3.14
C(121)...C(111)	2.84	C(124)...C(122)	2.42
C(125)...C(122)	2.79	C(126)...C(122)	2.42
C(125)...C(123)	2.42	C(126)...C(123)	2.79
C(121)...C(123)	2.42	C(126)...C(124)	2.42
C(121)...C(124)	2.79	C(121)...C(125)	2.42