

ORGANOMETALLICS

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Supporting material

Complex $[\text{Os}\{\overline{\text{C}[\text{C}(\text{O})\text{OCH}_3]=\text{CH}_2}\}(\text{C}=\text{C}=\text{CPh}_2)(\text{CO})(\text{P}^i\text{Pr}_3)_2]\text{BF}_4 \cdot 1/4(\text{CH}_3\text{CH}_2)_2\text{O}$ (4)

Atomic coordinates for the non-hydrogen atoms **Table 1**

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Bond distances and angles (SHELXL93) **Table 5**

Complex $\text{Os}\{\overline{\text{C}[\text{C}(=\text{CH}_2)\text{C}(\text{O})\text{OCH}_3]=\text{C}=\text{CPh}_2}\}\text{Cl}(\text{CO})(\text{P}^i\text{Pr}_3)_2$ (9).

Atomic coordinates for the non-hydrogen atoms **Table 6**

Anisotropic displacement coefficients **Table 7**

Atomic coordinates for hydrogen atoms **Table 8**

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Bond distances and angles (SHELXL93) **Table 10**

Table to be deposited

Table 1. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement coefficients ($\text{\AA}^2 \times 10^3$) for the compound $[\text{Os}\{\overline{\text{C}[\text{C}(\text{O})\text{OCH}_3]=\text{CH}_2}\}(\text{C}=\text{C}=\text{CPh}_2)(\text{CO})(\text{P}^i\text{Pr}_3)_2]\text{BF}_4 \cdot 1/4(\text{CH}_3\text{CH}_2)_2\text{O}$ (4).

Atom	X/a	Y/b	Z/c	U_{eq}^a
Os	2020 (1)	2538 (1)	2838 (1)	17 (1)
P (1)	1969 (1)	4437 (1)	2800 (1)	22 (1)
P (2)	1974 (1)	649 (1)	2874 (1)	21 (1)
C (101)	2138 (3)	2488 (6)	1858 (3)	21 (1)
O (101)	2202 (2)	2449 (5)	1231 (2)	32 (1)
O (1)	1648 (2)	2587 (4)	3904 (2)	23 (1)
O (2)	438 (2)	2581 (4)	3750 (2)	26 (1)
C (1)	181 (3)	2535 (8)	2048 (4)	28 (1)
C (2)	855 (3)	2549 (6)	2595 (3)	23 (1)
C (3)	979 (3)	2563 (6)	3461 (3)	21 (1)
C (4)	639 (4)	2621 (7)	4624 (4)	37 (2)
C (5)	3071 (3)	2578 (6)	3455 (3)	23 (1)
C (6)	3731 (4)	2690 (5)	3891 (4)	28 (2)
C (7)	4418 (4)	2908 (5)	4444 (4)	28 (2)
C (8)	1166 (5)	4952 (5)	1990 (5)	23 (2)
C (9)	1112 (6)	6123 (6)	1930 (6)	46 (3)
C (10)	1026 (6)	4476 (7)	1149 (5)	37 (2)
C (11)	2843 (5)	5010 (5)	2751 (5)	26 (2)
C (12)	2974 (6)	6162 (6)	2946 (7)	54 (3)
C (13)	2954 (6)	4781 (7)	1960 (6)	47 (3)
C (14)	1908 (5)	5088 (5)	3726 (5)	25 (2)
C (15)	2520 (6)	4716 (6)	4487 (5)	39 (2)
C (16)	1142 (6)	5066 (6)	3787 (6)	35 (2)
C (17)	2833 (5)	73 (6)	2807 (6)	36 (3)
C (18)	3038 (6)	-1004 (6)	3193 (6)	49 (3)
C (19)	2835 (6)	36 (6)	1953 (6)	45 (3)
C (20)	1933 (6)	75 (6)	3813 (6)	34 (2)
C (21)	1165 (6)	82 (7)	3894 (6)	42 (3)
C (22)	2505 (6)	513 (6)	4562 (5)	40 (2)
C (23)	1158 (6)	73 (6)	2082 (6)	34 (2)
C (24)	984 (6)	514 (6)	1249 (5)	37 (2)
C (25)	1183 (6)	-1127 (6)	2053 (6)	43 (3)
C (31)	4472 (4)	3213 (5)	5266 (4)	29 (2)
C (32)	3959 (4)	2820 (6)	5590 (4)	37 (2)
C (33)	3993 (5)	3134 (7)	6345 (5)	51 (2)
C (34)	4505 (5)	3849 (7)	6769 (5)	54 (2)
C (35)	4985 (4)	4265 (6)	6433 (5)	41 (2)
C (36)	4977 (4)	3936 (6)	5698 (5)	37 (2)
C (41)	5067 (4)	2857 (5)	4206 (5)	30 (2)
C (42)	5765 (4)	2683 (6)	4785 (4)	34 (2)
C (43)	6385 (4)	2607 (7)	4566 (5)	43 (2)

^a Equivalent isotropic U defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table to be deposited

Table 1 (cont.). Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement coefficients ($\text{\AA}^2 \times 10^3$) for the compound $[\text{Os}\{\text{C}[\text{C}(\text{O})\text{OCH}_3]=\text{CH}_2\}(\text{C}=\text{C}=\text{CPh}_2)(\text{CO})(\text{P}^i\text{Pr}_3)_2]\text{BF}_4 \cdot 1/4(\text{CH}_3\text{CH}_2)_2\text{O}$ (4).

Atom	X/a	Y/b	Z/c	U_{eq}^a
C (44)	6313 (4)	2712 (6)	3761 (5)	48 (2)
C (45)	5628 (5)	2877 (6)	3187 (5)	44 (2)
C (46)	5017 (4)	2947 (6)	3416 (5)	36 (2)
B	1587 (4)	-2588 (8)	29 (5)	34 (2)
F (1)	1833 (4)	-1678 (4)	447 (4)	63 (2)
F (2)	1698 (2)	-2547 (4)	-700 (2)	45 (1)
F (3)	1991 (3)	-3413 (4)	476 (4)	55 (2)
F (4)	854 (2)	-2754 (5)	-98 (3)	70 (2)
O (200) #	5194 (8)	0	4916 (9)	89 (3)
C (200) #	5029 (13)	-160 (17)	4176 (14)	67 (6)
C (201) #	5276 (15)	-176 (19)	3851 (16)	80 (7)

^a Equivalent isotropic U defined as one third of the trace of the orthogonalized U_{ij} tensor. # Atoms refined isotropically.

Table to be deposited

Table 2. Anisotropic displacement coefficients U_{ij}^* ($\text{\AA}^2 \times 10^3$) for the non-hydrogen atoms for the compound $[\text{Os}\{\text{C}[\text{C}(\text{O})\text{OCH}_3]=\text{CH}_2\}(\text{C}=\text{C}=\text{CPh}_2)(\text{CO})(\text{P}^i\text{Pr}_3)_2]\text{BF}_4 \cdot 1/4(\text{CH}_3\text{CH}_2)_2\text{O}$ (4).

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Os	14 (1)	16 (1)	18 (1)	-1 (1)	4 (1)	0 (1)
P(1)	22 (1)	16 (1)	26 (1)	0 (1)	8 (1)	1 (1)
P(2)	20 (1)	18 (1)	25 (1)	-1 (1)	8 (1)	-2 (1)
C(101)	20 (3)	19 (3)	24 (3)	4 (4)	7 (2)	3 (4)
O(101)	35 (2)	38 (2)	26 (2)	-4 (3)	15 (2)	2 (3)
O(1)	22 (2)	26 (2)	22 (2)	-3 (2)	8 (2)	0 (3)
O(2)	19 (2)	37 (3)	24 (2)	-4 (3)	8 (2)	-7 (3)
C(1)	18 (3)	41 (4)	25 (3)	-1 (5)	6 (2)	-2 (5)
C(2)	25 (3)	18 (3)	27 (3)	-4 (4)	11 (2)	-2 (4)
C(3)	21 (3)	19 (3)	22 (3)	0 (4)	6 (2)	0 (4)
C(4)	38 (4)	51 (5)	26 (3)	3 (4)	18 (3)	-6 (5)
C(5)	23 (3)	22 (3)	23 (3)	-1 (4)	9 (2)	-1 (4)
C(6)	26 (3)	27 (5)	32 (3)	1 (3)	11 (3)	-2 (3)
C(7)	22 (4)	27 (3)	32 (4)	3 (3)	5 (3)	-1 (3)
C(8)	16 (5)	29 (4)	24 (4)	5 (3)	4 (4)	10 (3)
C(9)	51 (7)	24 (4)	57 (6)	5 (4)	12 (5)	12 (4)
C(10)	35 (6)	51 (5)	15 (4)	1 (4)	-5 (4)	5 (4)
C(11)	21 (6)	23 (4)	33 (5)	3 (3)	9 (4)	-2 (3)
C(12)	54 (7)	21 (4)	95 (8)	-11 (5)	36 (6)	-18 (4)
C(13)	43 (6)	59 (6)	52 (6)	-8 (5)	33 (5)	-22 (5)
C(14)	27 (5)	20 (4)	25 (4)	-8 (3)	6 (4)	-1 (3)
C(15)	42 (6)	40 (5)	32 (5)	-5 (4)	8 (5)	-3 (4)
C(16)	38 (6)	29 (4)	45 (6)	-8 (4)	24 (5)	-2 (4)
C(17)	20 (6)	21 (4)	66 (7)	-4 (4)	16 (5)	3 (3)
C(18)	41 (6)	33 (5)	75 (7)	0 (4)	22 (5)	11 (4)
C(19)	51 (7)	23 (4)	73 (8)	-6 (4)	38 (6)	-1 (4)
C(20)	40 (6)	20 (4)	44 (6)	4 (3)	17 (5)	2 (4)
C(21)	58 (8)	38 (5)	38 (6)	6 (4)	27 (5)	-7 (5)
C(22)	49 (7)	33 (4)	30 (5)	8 (4)	3 (5)	8 (4)
C(23)	35 (6)	23 (4)	46 (6)	-2 (4)	18 (5)	-6 (4)
C(24)	43 (7)	38 (5)	33 (5)	-16 (4)	17 (5)	-20 (4)
C(25)	38 (6)	31 (5)	62 (7)	-10 (4)	19 (5)	-21 (4)
C(31)	23 (4)	28 (4)	31 (4)	8 (3)	5 (3)	7 (3)
C(32)	30 (4)	40 (5)	36 (4)	-3 (3)	7 (3)	3 (3)
C(33)	38 (5)	67 (6)	52 (6)	2 (5)	21 (4)	11 (5)
C(34)	40 (5)	77 (7)	34 (5)	-19 (5)	1 (4)	16 (5)
C(35)	30 (4)	43 (5)	39 (5)	-7 (4)	-2 (4)	9 (4)
C(36)	27 (4)	36 (4)	41 (5)	-2 (4)	4 (4)	2 (3)
C(41)	15 (3)	28 (4)	45 (4)	-1 (3)	9 (3)	-3 (3)
C(42)	26 (3)	41 (5)	31 (3)	2 (3)	6 (3)	-5 (4)
C(43)	25 (3)	47 (5)	56 (4)	2 (5)	12 (3)	-6 (5)

* The anisotropic displacement exponent takes the form: $-2\pi^2(h^2a^{*2}U_{11} + \dots + 2hka^*b^*U_{12})$.

Table to be deposited

Table 2 (cont.). Anisotropic displacement coefficients U_{ij}^* ($\text{\AA}^2 \times 10^3$) for the non-hydrogen atoms for the compound $[\text{Os}\{\overline{\text{C}[\text{C}(\text{O})\text{OCH}_3]=\text{CH}_2}\}(\text{C}=\text{C}=\text{CPh}_2)(\text{CO})(\text{P}^i\text{Pr}_3)_2]\text{BF}_4 \cdot 1/4(\text{CH}_3\text{CH}_2)_2\text{O}$ (4).

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(44)	29(4)	53(6)	69(6)	-4(5)	24(4)	-7(4)
C(45)	39(5)	50(5)	45(5)	-1(4)	18(4)	-9(4)
C(46)	31(4)	41(4)	34(4)	6(3)	9(3)	0(3)
B	29(4)	33(5)	33(4)	-2(5)	3(3)	-1(5)
F(1)	96(6)	40(3)	52(4)	-9(3)	25(4)	-4(3)
F(2)	55(2)	46(2)	40(2)	-8(3)	25(2)	-2(3)
F(3)	47(3)	47(3)	63(4)	20(3)	9(3)	9(2)
F(4)	29(2)	134(6)	46(3)	0(3)	13(2)	4(3)

* The anisotropic displacement exponent takes the form: $-2\pi^2(h^2a^{*2}U_{11} + \dots + 2hka^{*b}U_{12})$.

Table to be deposited

Table 3. Hydrogen atom coordinates* ($\times 10^4$) and isotropic displacement coefficients ($\text{\AA}^2 \times 10^3$) for the compound $[\text{Os}\{\text{C}[\text{C}(\text{O})\text{OCH}_3]=\text{CH}_2\}(\text{C}=\text{C}=\text{CPh}_2)(\text{CO})(\text{P}^i\text{Pr}_3)_2]\text{BF}_4 \cdot 1/4(\text{CH}_3\text{CH}_2)_2\text{O}$ (4).

Atom	X/a	Y/b	Z/c	U
H(1)**	71 (27)	2531 (55)	1483 (32)	10 (12)
H(2)**	-230 (41)	2426 (74)	2261 (43)	58 (22)
H(4A)	913 (27)	1995 (22)	4864 (5)	44
H(4B)	192 (4)	2666 (42)	4761 (4)	44
H(4C)	948 (26)	3230 (26)	4835 (5)	44
H(8)	734 (5)	4734 (5)	2136 (5)	28
H(9A)	1485 (22)	6389 (7)	1723 (34)	55
H(9B)	1194 (33)	6416 (6)	2467 (9)	55
H(9C)	621 (12)	6320 (6)	1563 (28)	55
H(10A)	1035 (30)	3720 (7)	1191 (7)	44
H(10B)	1411 (16)	4705 (32)	946 (14)	44
H(10C)	544 (12)	4701 (33)	777 (9)	44
H(11)	3252 (5)	4643 (5)	3176 (5)	31
H(12A)	2955 (32)	6298 (10)	3483 (16)	64
H(12B)	2591 (19)	6567 (6)	2543 (21)	64
H(12C)	3458 (14)	6359 (11)	2935 (35)	64
H(13A)	2570 (17)	5128 (32)	1517 (7)	56
H(13B)	2926 (29)	4033 (8)	1864 (16)	56
H(13C)	3439 (12)	5034 (36)	1986 (12)	56
H(14)	2016 (5)	5834 (5)	3670 (5)	30
H(15A)	2533 (19)	5152 (25)	4945 (8)	47
H(15B)	2995 (7)	4759 (36)	4407 (12)	47
H(15C)	2426 (15)	3997 (14)	4598 (18)	47
H(16A)	964 (12)	4351 (7)	3742 (29)	41
H(16B)	803 (8)	5481 (29)	3350 (17)	41
H(16C)	1165 (7)	5353 (33)	4309 (12)	41
H(17)	3243 (5)	547 (6)	3113 (6)	43
H(18A)	2635 (14)	-1489 (12)	2938 (23)	58
H(18B)	3123 (30)	-960 (10)	3772 (9)	58
H(18C)	3487 (18)	-1248 (19)	3116 (30)	58
H(19A)	2701 (29)	716 (12)	1700 (12)	54
H(19B)	2477 (20)	-480 (29)	1642 (10)	54
H(19C)	3327 (9)	-155 (39)	1962 (6)	54
H(20)	2064 (6)	-671 (6)	3797 (6)	41
H(21A)	1195 (8)	-244 (34)	4406 (14)	50
H(21B)	817 (9)	-302 (33)	3444 (17)	50
H(21C)	995 (14)	797 (7)	3885 (31)	50

* Hydrogen atoms were included in calculated positions and refined riding on their respective carbon atoms, with displacement coefficients related to those of the carbon atoms to which they are bonded (1.2 times).

** These hydrogens were refined as free isotropic atoms.

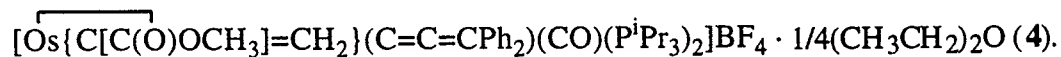
Table 3 (cont.). Hydrogen atom coordinates* ($\times 10^4$) and isotropic displacement coefficients ($\text{\AA}^2 \times 10^3$) for the compound $[\text{Os}\{\text{C}[\text{C}(\text{O})\text{OCH}_3]=\text{CH}_2\}(\text{C}=\text{C}=\text{CPh}_2)(\text{CO})(\text{P}^i\text{Pr}_3)_2]\text{BF}_4 \cdot 1/4(\text{CH}_3\text{CH}_2)_2\text{O}$ (**4**).

Atom	X/a	Y/b	Z/c	U
H(22A)	2990 (7)	484 (36)	4505 (13)	48
H(22B)	2514 (20)	106 (25)	5033 (6)	48
H(22C)	2383 (16)	1233 (14)	4633 (18)	48
H(23)	727 (6)	246 (6)	2244 (6)	40
H(24A)	930 (30)	1266 (8)	1268 (8)	44
H(24B)	523 (15)	213 (31)	886 (9)	44
H(24C)	1384 (13)	351 (34)	1051 (13)	44
H(25A)	690 (9)	-1393 (6)	1750 (30)	52
H(25B)	1349 (31)	-1403 (6)	2604 (6)	52
H(25C)	1525 (25)	-1342 (6)	1785 (32)	52
H(32)	3592 (4)	2343 (6)	5290 (4)	44
H(33)	3659 (5)	2852 (7)	6576 (5)	61
H(34)	4527 (5)	4057 (7)	7293 (5)	64
H(35)	5324 (4)	4784 (6)	6716 (5)	49
H(36)	5323 (4)	4209 (6)	5481 (5)	44
H(42)	5816 (4)	2615 (6)	5337 (4)	40
H(43)	6854 (4)	2484 (7)	4965 (5)	52
H(44)	6734 (4)	2670 (6)	3606 (5)	58
H(45)	5575 (5)	2943 (6)	2634 (5)	53
H(46)	4548 (4)	3060 (6)	3013 (5)	43

* Hydrogen atoms were included in calculated positions and refined riding on their respective carbon atoms, with displacement coefficients related to those of the carbon atoms to which they are bonded.

Table to be deposited

Table 4. Full experimental details for the X-ray analysis of the compound



Crystal data:

Formula	$\text{C}_{38}\text{H}_{57}\text{BF}_4\text{O}_3\text{OsP}_2 \cdot 1/4\text{C}_4\text{H}_{10}\text{O}$
Molecular weight	919.32
Color and habit	violet, irregular prism
Size (mm)	0.34 x 0.30 x 0.30
Symmetry	Monoclinic, $P2_1/c$ (no. 14)
Unit cell determination	Least-squares fit to 24 reflections. ($18 \leq 2\theta \leq 25^\circ$)
Unit cell dimensions	19.385(2), 12.931(2), 17.677(2) 90, 110.48(1), 90
Packing: V ($\text{\AA}^3$), Z	4151.0(9), 4
D calc (g cm^{-3}), F (000)	1.471, 2026

Experimental data:

Diffractometer	Four-circle Siemens-STOE AED
Radiation and technique	Mo- $K\alpha$ ($\lambda = 0.71073 \text{ \AA}$) Bisecting geometry
Monochromator	Graphite oriented
Collection mode/range	$\omega/2\theta$ scan ($5 \leq 2\theta \leq 50^\circ$)
Number of reflections:	
measured	7908
unique	7291 (merging R factor 0.0150)
Standard reflections	3 standards measured every 55 min; no decay observed
Absorption correction	Semiempirical method (ψ -scan)*
Max. and min. trans. fact.	0.251, 0.173
μ (mm^{-1}) and $\mu \cdot R$	3.20, 0.75
Temperature (K)	173.0(2)

Table to be deposited

Table 4 (cont.). Full experimental details for the X-ray analysis of the compound

$[\text{Os}\{\text{C}[\text{C}(\text{O})\text{OCH}_3]=\text{CH}_2\}(\text{C}=\text{C}=\text{CPh}_2)(\text{CO})(\text{P}^i\text{Pr}_3)_2]\text{BF}_4 \cdot 1/4(\text{CH}_3\text{CH}_2)_2\text{O}$ (**4**).

<i>Solution and refinement:</i>	SHELXTL-PLUS v. 5.0, system ALPHA AXP
Solution mode	Patterson
Refinement	Full-matrix least-squares on F^2 's All reflections
Hydrogen atoms	From observed and calculated positions. Refined riding on C atoms, except H1 and H2.
No. parameters	474
Weighting scheme	$w^{-1} = \sigma^2(F_o^2) + (0.0372P)^2 + 3.37P$, where $P = [\max(F_o^2, 0) + 2F_c^2]/3$
ΔF final (max.)	1.44 e/Å ³ (to 0.55 Å from O(1))
ΔF final (min.)	-0.84 e/Å ³
Max. thermal values (Å ²)	$U_{22}(F_4) = 0.13(6)$
Max. shift/esd	1.280
R_1^a [$F^2 > 2\sigma(F^2)$]	0.0350
wR_2^b [all data]	0.0935
S^c [all data]	1.132
Data-to-Parameter Ratio	15.4:1

Atomic scattering factors from the International Tables for X-Ray Crystallography; Vol. C (1992). Anomalous dispersion applied for Os and P atoms.

^a $R_1(F) = \sum ||F_o| - |F_c|| / \sum |F_o|$. ^b $wR_2(F^2) = [\sum [w(F_o^2 - F_c^2)^2] / \sum [w(F_o^2)^2]]^{1/2}$; $w^{-1} = [\sigma^2(F_o^2) + (aP)^2 + bP]$, where $P = [\max(F_o^2, 0) + 2F_c^2]/3$ ($a = 0.0372$, $b = 3.37$).
^c $S = [\sum [w(F_o^2 - F_c^2)^2] / (n-p)]^{1/2}$, where n is the number of reflections and p the number of parameters.

Table to be deposited

Table 5. Bond lengths (Å) and angles (deg.) of the compound

$[\text{Os}\{\text{C}[\text{C}(\text{O})\text{OCH}_3]=\text{CH}_2\}(\text{C}=\text{C}=\text{CPh}_2)(\text{CO})(\text{P}^i\text{Pr}_3)_2]\text{BF}_4 \cdot 1/4(\text{CH}_3\text{CH}_2)_2\text{O}$ (4).

Os-C(101)	1.826(5)
Os-C(5)	1.947(6)
Os-C(2)	2.146(6)
Os-O(1)	2.242(4)
Os-P(2)	2.446(2)
Os-P(1)	2.457(2)
P(1)-C(8)	1.833(8)
P(1)-C(11)	1.878(9)
P(1)-C(14)	1.880(8)
P(2)-C(20)	1.846(9)
P(2)-C(23)	1.862(10)
P(2)-C(17)	1.865(9)
C(101)-O(101)	1.158(6)
O(1)-C(3)	1.259(7)
O(2)-C(3)	1.317(6)
O(2)-C(4)	1.456(7)
C(1)-C(2)	1.325(8)
C(2)-C(3)	1.464(7)
C(5)-C(6)	1.250(8)
C(6)-C(7)	1.376(9)
C(7)-C(41)	1.462(9)
C(7)-C(31)	1.472(10)
C(8)-C(9)	1.519(9)
C(8)-C(10)	1.543(11)
C(11)-C(13)	1.518(12)
C(11)-C(12)	1.530(10)
C(14)-C(15)	1.528(12)
C(14)-C(16)	1.528(12)
C(17)-C(19)	1.512(13)
C(17)-C(18)	1.541(11)
C(20)-C(22)	1.508(13)
C(20)-C(21)	1.546(14)
C(23)-C(24)	1.502(12)
C(23)-C(25)	1.554(10)
C(31)-C(36)	1.375(10)
C(31)-C(32)	1.406(10)
C(32)-C(33)	1.375(11)
C(33)-C(34)	1.372(12)
C(34)-C(35)	1.377(12)
C(35)-C(36)	1.363(11)
C(41)-C(46)	1.371(10)
C(41)-C(42)	1.400(9)
C(42)-C(43)	1.388(9)
C(43)-C(44)	1.388(11)
C(44)-C(45)	1.377(11)
C(45)-C(46)	1.382(10)

Table to be deposited

Table 5 (cont.). Bond lengths (Å) and angles (deg.) of the compound
 $[\text{Os}\{\text{C}[\text{C}(\text{O})\text{OCH}_3]=\text{CH}_2\}(\text{C}=\text{C}=\text{CPh}_2)(\text{CO})(\text{P}^i\text{Pr}_3)_2]\text{BF}_4 \cdot 1/4(\text{CH}_3\text{CH}_2)_2\text{O}$ (**4**).

B-F(4)	1.375(9)
B-F(2)	1.379(8)
B-F(3)	1.394(10)
B-F(1)	1.383(11)
O(200)-C(200)	1.25(3)
O(200)-C(200)#1	1.81(3)
C(200)-C(201)	0.87(3)
C(101)-Os-C(5)	94.5(2)
C(101)-Os-C(2)	106.5(2)
C(5)-Os-C(2)	159.0(2)
C(101)-Os-O(1)	169.2(2)
C(5)-Os-O(1)	96.3(2)
C(2)-Os-O(1)	62.8(2)
C(101)-Os-P(2)	90.4(3)
C(5)-Os-P(2)	93.0(2)
C(2)-Os-P(2)	88.1(2)
O(1)-Os-P(2)	88.9(2)
C(101)-Os-P(1)	91.5(3)
C(5)-Os-P(1)	90.7(2)
C(2)-Os-P(1)	87.6(2)
O(1)-Os-P(1)	88.4(2)
P(2)-Os-P(1)	175.67(5)
C(8)-P(1)-C(11)	110.7(4)
C(8)-P(1)-C(14)	102.8(4)
C(11)-P(1)-C(14)	101.3(4)
C(8)-P(1)-Os	113.5(3)
C(11)-P(1)-Os	111.6(3)
C(14)-P(1)-Os	116.0(3)
C(20)-P(2)-C(23)	102.9(4)
C(20)-P(2)-C(17)	102.5(4)
C(23)-P(2)-C(17)	109.5(4)
C(20)-P(2)-Os	116.0(3)
C(23)-P(2)-Os	114.1(3)
C(17)-P(2)-Os	110.8(3)
O(101)-C(101)-Os	178.9(6)
C(3)-O(1)-Os	92.3(3)
C(3)-O(2)-C(4)	117.3(5)
C(1)-C(2)-C(3)	121.5(5)
C(1)-C(2)-Os	147.6(4)
C(3)-C(2)-Os	90.8(3)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y,-z+1

Table to be deposited

Table 5 (cont.). Bond lengths (Å) and angles (deg.) of the compound

$[\text{Os}\{\text{C}[\text{C}(\text{O})\text{OCH}_3]=\text{CH}_2\}(\text{C}=\text{C}=\text{CPh}_2)(\text{CO})(\text{P}^i\text{Pr}_3)_2]\text{BF}_4 \cdot 1/4(\text{CH}_3\text{CH}_2)_2\text{O}$ (4).

O(1)-C(3)-O(2)	122.9(5)
O(1)-C(3)-C(2)	114.1(5)
O(2)-C(3)-C(2)	123.0(5)
C(6)-C(5)-Os	173.5(6)
C(5)-C(6)-C(7)	171.2(7)
C(6)-C(7)-C(41)	120.2(6)
C(6)-C(7)-C(31)	118.2(6)
C(41)-C(7)-C(31)	121.6(6)
C(9)-C(8)-C(10)	110.3(7)
C(9)-C(8)-P(1)	115.9(6)
C(10)-C(8)-P(1)	115.0(6)
C(13)-C(11)-C(12)	109.3(7)
C(13)-C(11)-P(1)	112.8(6)
C(12)-C(11)-P(1)	117.1(6)
C(15)-C(14)-C(16)	114.0(7)
C(15)-C(14)-P(1)	111.1(6)
C(16)-C(14)-P(1)	114.4(6)
C(19)-C(17)-C(18)	108.8(7)
C(19)-C(17)-P(2)	113.0(7)
C(18)-C(17)-P(2)	115.5(7)
C(22)-C(20)-C(21)	110.7(8)
C(22)-C(20)-P(2)	112.9(6)
C(21)-C(20)-P(2)	115.3(7)
C(24)-C(23)-C(25)	110.2(7)
C(24)-C(23)-P(2)	115.2(6)
C(25)-C(23)-P(2)	113.4(7)
C(36)-C(31)-C(32)	119.1(7)
C(36)-C(31)-C(7)	121.4(7)
C(32)-C(31)-C(7)	119.2(6)
C(33)-C(32)-C(31)	119.3(7)
C(34)-C(33)-C(32)	120.6(9)
C(35)-C(34)-C(33)	119.8(8)
C(34)-C(35)-C(36)	120.3(8)
C(31)-C(36)-C(35)	120.7(8)
C(46)-C(41)-C(42)	117.6(7)
C(46)-C(41)-C(7)	121.9(7)
C(42)-C(41)-C(7)	120.5(7)
C(43)-C(42)-C(41)	121.2(7)
C(42)-C(43)-C(44)	119.5(7)
C(45)-C(44)-C(43)	119.7(7)
C(44)-C(45)-C(46)	119.9(8)
C(45)-C(46)-C(41)	122.0(7)
F(4)-B-F(2)	110.1(6)
F(4)-B-F(3)	108.4(8)
F(2)-B-F(3)	108.6(7)
F(4)-B-F(1)	111.3(7)
F(2)-B-F(1)	109.3(8)
F(3)-B-F(1)	109.1(6)

Table to be deposited

Table 5 (cont.). Bond lengths (Å) and angles (deg.) of the compound
 $[\text{Os}\{\text{C}[\text{C}(\text{O})\text{OCH}_3]=\text{CH}_2\}(\text{C}=\text{C}=\text{CPh}_2)(\text{CO})(\text{P}^i\text{Pr}_3)_2]\text{BF}_4 \cdot 1/4(\text{CH}_3\text{CH}_2)_2\text{O}$ (4).

C (201) - C (200) - O (200)	134 (3)
C (200) - O (200) - O (200) #1	114 (3)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y,-z+1

Table to be deposited

Table 6. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement coefficients ($\text{\AA}^2 \times 10^3$) for the compound $\text{Os}\{\text{C}[\text{C}(=\text{CH}_2)\text{C}(\text{O})\text{OCH}_3]=\text{C}=\text{CPh}_2\}\text{Cl}(\text{CO})(\text{P}^i\text{Pr}_3)_2$ (**9**).

Atom	X/a	Y/b	Z/c	U_{eq}^a
Os (1)	3646 (1)	2408 (1)	1176 (1)	25 (1)
P (1)	2481 (1)	2989 (1)	254 (1)	30 (1)
P (2)	4986 (1)	1943 (1)	2059 (1)	33 (1)
Cl	5110 (1)	2847 (1)	630 (1)	40 (1)
O (1)	3263 (3)	4150 (2)	1888 (1)	58 (1)
O (2)	3828 (2)	1005 (2)	745 (1)	31 (1)
O (3)	3338 (2)	-516 (2)	744 (1)	45 (1)
C (1)	2198 (4)	2138 (3)	-410 (2)	39 (1)
C (2)	3181 (4)	1843 (3)	-659 (2)	48 (1)
C (3)	1548 (4)	1281 (3)	-279 (2)	53 (1)
C (4)	3052 (4)	4010 (3)	-117 (2)	39 (1)
C (5)	3425 (4)	4839 (3)	323 (2)	65 (2)
C (6)	2413 (4)	4394 (3)	-732 (2)	63 (2)
C (7)	1137 (3)	3298 (3)	375 (2)	38 (1)
C (8)	1098 (4)	4111 (4)	830 (2)	64 (2)
C (9)	298 (4)	3446 (4)	-201 (2)	65 (2)
C (10)	5550 (4)	736 (3)	1954 (2)	44 (1)
C (11)	6229 (4)	749 (4)	1451 (2)	59 (1)
C (12)	6128 (4)	202 (4)	2530 (2)	69 (2)
C (13)	4672 (4)	1845 (3)	2858 (2)	44 (1)
C (14)	4337 (4)	2789 (3)	3107 (2)	55 (1)
C (15)	3837 (4)	1081 (4)	2897 (2)	58 (1)
C (16)	6148 (3)	2739 (3)	2148 (2)	45 (1)
C (17)	6983 (4)	2559 (4)	2727 (2)	69 (2)
C (18)	5880 (4)	3808 (3)	2100 (2)	60 (2)
C (19)	3431 (3)	3487 (3)	1598 (2)	36 (1)
C (20)	3279 (3)	379 (3)	927 (2)	33 (1)
C (21)	4104 (4)	-732 (3)	347 (2)	61 (2)
C (22)	2566 (3)	584 (3)	1359 (2)	33 (1)
C (23)	2157 (4)	-122 (3)	1642 (2)	60 (1)
C (24)	2427 (3)	1637 (3)	1454 (2)	27 (1)
C (25)	1573 (3)	1846 (3)	1664 (2)	36 (1)
C (26)	663 (3)	1969 (3)	1849 (2)	37 (1)
C (27)	597 (3)	1965 (3)	2534 (2)	40 (1)
C (28)	1349 (4)	2402 (4)	2964 (2)	61 (1)
C (29)	1335 (4)	2321 (4)	3603 (2)	74 (2)
C (30)	538 (5)	1840 (4)	3807 (2)	66 (2)
C (31)	-215 (5)	1422 (4)	3380 (2)	64 (2)
C (32)	-191 (4)	1473 (4)	2747 (2)	57 (1)
C (33)	-322 (4)	2074 (3)	1387 (2)	43 (1)
C (34)	-1063 (4)	2768 (3)	1465 (2)	52 (1)
C (35)	-1942 (4)	2911 (4)	1017 (3)	69 (2)
C (36)	-2121 (4)	2365 (5)	490 (3)	82 (2)
C (37)	-1423 (5)	1661 (5)	413 (3)	79 (2)
C (38)	-531 (4)	1524 (4)	854 (2)	59 (1)

^a Equivalent isotropic U defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table to be deposited

Table 7. Anisotropic displacement coefficients U_{ij}^* ($\text{\AA}^2 \times 10^3$) for the non-hydrogen atoms for the compound $\text{Os}\{\text{C}[\text{C}(\text{=CH}_2)\text{C}(\text{O})\text{OCH}_3]\text{=C=CPh}_2\}\text{Cl}(\text{CO})(\text{P}^i\text{Pr}_3)_2$ (**9**).

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Os (1)	28 (1)	28 (1)	20 (1)	1 (1)	4 (1)	3 (1)
P (1)	34 (1)	31 (1)	24 (1)	1 (1)	1 (1)	4 (1)
P (2)	37 (1)	38 (1)	23 (1)	0 (1)	1 (1)	8 (1)
Cl	36 (1)	50 (1)	35 (1)	6 (1)	8 (1)	-2 (1)
O (1)	79 (3)	49 (2)	42 (2)	-19 (2)	-2 (2)	16 (2)
O (2)	36 (2)	30 (2)	26 (1)	-3 (1)	9 (1)	-2 (1)
O (3)	59 (2)	29 (2)	54 (2)	-8 (1)	29 (2)	-4 (2)
C (1)	53 (3)	36 (2)	23 (2)	-1 (2)	-4 (2)	7 (2)
C (2)	62 (3)	52 (3)	29 (2)	-2 (2)	6 (2)	13 (3)
C (3)	56 (3)	50 (3)	49 (3)	-12 (2)	-2 (3)	1 (3)
C (4)	45 (3)	38 (2)	33 (2)	10 (2)	7 (2)	1 (2)
C (5)	95 (5)	43 (3)	55 (3)	4 (2)	6 (3)	-19 (3)
C (6)	88 (4)	56 (3)	41 (3)	23 (2)	-2 (3)	6 (3)
C (7)	34 (2)	42 (3)	38 (2)	3 (2)	4 (2)	10 (2)
C (8)	49 (3)	69 (4)	73 (4)	-19 (3)	7 (3)	18 (3)
C (9)	39 (3)	95 (4)	55 (3)	2 (3)	-5 (3)	18 (3)
C (10)	56 (3)	38 (3)	36 (2)	3 (2)	5 (2)	20 (2)
C (11)	66 (4)	62 (3)	50 (3)	-9 (2)	15 (3)	27 (3)
C (12)	84 (4)	64 (3)	54 (3)	14 (3)	0 (3)	44 (3)
C (13)	56 (3)	51 (3)	25 (2)	3 (2)	5 (2)	14 (3)
C (14)	62 (3)	71 (4)	33 (2)	-7 (2)	9 (2)	14 (3)
C (15)	74 (4)	70 (4)	30 (2)	17 (2)	11 (3)	11 (3)
C (16)	38 (2)	55 (3)	38 (2)	-4 (2)	-1 (2)	2 (2)
C (17)	48 (3)	97 (4)	53 (3)	7 (3)	-15 (2)	-10 (4)
C (18)	62 (4)	51 (3)	61 (3)	-10 (3)	-2 (3)	-14 (3)
C (19)	52 (3)	37 (2)	18 (2)	-2 (2)	5 (2)	9 (2)
C (20)	35 (2)	30 (2)	34 (2)	-1 (2)	7 (2)	3 (2)
C (21)	79 (4)	41 (3)	76 (4)	-14 (3)	46 (3)	0 (3)
C (22)	35 (2)	32 (2)	35 (2)	1 (2)	11 (2)	-3 (2)
C (23)	70 (4)	43 (3)	78 (4)	0 (3)	44 (3)	-7 (3)
C (24)	28 (2)	34 (2)	22 (2)	-1 (2)	9 (2)	2 (2)
C (25)	44 (3)	32 (2)	30 (2)	0 (2)	4 (2)	-3 (2)
C (26)	39 (3)	32 (2)	44 (2)	-2 (2)	19 (2)	2 (2)
C (27)	35 (2)	41 (2)	48 (2)	-6 (2)	21 (2)	2 (2)
C (28)	70 (3)	68 (3)	53 (3)	-15 (3)	27 (2)	-12 (3)
C (29)	88 (4)	89 (5)	48 (3)	-29 (3)	22 (3)	-12 (4)
C (30)	88 (4)	65 (4)	55 (3)	1 (3)	38 (3)	13 (3)
C (31)	71 (4)	67 (4)	65 (3)	10 (3)	40 (3)	-10 (3)
C (32)	55 (3)	64 (3)	56 (3)	0 (3)	23 (3)	-8 (3)
C (33)	33 (2)	44 (3)	53 (3)	5 (2)	15 (2)	-3 (2)
C (34)	46 (3)	53 (3)	61 (3)	6 (2)	21 (3)	6 (3)
C (35)	44 (3)	66 (4)	99 (4)	20 (3)	17 (3)	11 (3)
C (36)	44 (3)	102 (5)	95 (4)	24 (4)	-2 (3)	-12 (4)
C (37)	63 (4)	103 (5)	65 (4)	-14 (4)	-2 (3)	-21 (4)
C (38)	49 (3)	61 (3)	66 (3)	-16 (3)	12 (3)	-7 (3)

* The anisotropic displacement exponent takes the form: $-2\pi^2(h^2a^{*2}U_{11} + \dots + 2hka^*b^*U_{12})$.

Table to be deposited

Table 8. Hydrogen atom coordinates* ($\times 10^4$) and isotropic displacement coefficients ($\text{\AA}^2 \times 10^3$) for the compound $\text{Os}\{\text{C}[\text{C}(\text{=CH}_2)\text{C}(\text{O})\text{OCH}_3]\text{=C=CPh}_2\}\text{Cl}(\text{CO})(\text{P}^i\text{Pr}_3)_2$ (9).

Atom	X/a	Y/b	Z/c	U
H(1A)	1763 (4)	2486 (3)	-752 (2)	74 (2)
H(2A)	3000 (5)	1379 (15)	-984 (9)	74 (2)
H(2B)	3680 (10)	1574 (19)	-325 (4)	74 (2)
H(2C)	3482 (13)	2391 (5)	-824 (12)	74 (2)
H(3A)	1372 (20)	905 (12)	-652 (4)	74 (2)
H(3B)	917 (12)	1497 (3)	-150 (13)	74 (2)
H(3C)	1945 (10)	903 (12)	48 (10)	74 (2)
H(4A)	3693 (4)	3756 (3)	-235 (2)	74 (2)
H(5A)	3801 (21)	5286 (11)	112 (5)	74 (2)
H(5B)	3878 (19)	4603 (4)	689 (7)	74 (2)
H(5C)	2831 (5)	5147 (13)	443 (11)	74 (2)
H(6A)	2843 (8)	4813 (17)	-927 (7)	74 (2)
H(6B)	1814 (14)	4735 (19)	-644 (3)	74 (2)
H(6C)	2184 (21)	3872 (4)	-1008 (6)	74 (2)
H(7A)	902 (3)	2740 (3)	583 (2)	74 (2)
H(8A)	389 (6)	4203 (14)	890 (11)	74 (2)
H(8B)	1348 (22)	4682 (6)	664 (7)	74 (2)
H(8C)	1532 (19)	3962 (10)	1224 (5)	74 (2)
H(9A)	-377 (4)	3480 (23)	-78 (3)	74 (2)
H(9B)	308 (17)	2924 (12)	-484 (7)	74 (2)
H(9C)	432 (15)	4028 (12)	-404 (9)	74 (2)
H(10A)	4948 (4)	334 (3)	1785 (2)	74 (2)
H(11A)	6387 (19)	108 (4)	1347 (10)	74 (2)
H(11B)	6869 (11)	1083 (18)	1604 (5)	74 (2)
H(11C)	5860 (10)	1063 (18)	1085 (5)	74 (2)
H(12A)	6265 (22)	-439 (7)	2415 (4)	74 (2)
H(12B)	5702 (11)	194 (19)	2849 (6)	74 (2)
H(12C)	6779 (12)	517 (13)	2686 (9)	74 (2)
H(13A)	5314 (4)	1645 (3)	3137 (2)	74 (2)
H(14A)	4142 (22)	2690 (5)	3509 (7)	74 (2)
H(14B)	3749 (15)	3039 (11)	2821 (7)	74 (2)
H(14C)	4908 (8)	3231 (7)	3148 (13)	74 (2)
H(15A)	3750 (17)	1007 (15)	3325 (3)	74 (2)
H(15B)	4057 (11)	488 (6)	2744 (13)	74 (2)
H(15C)	3184 (7)	1272 (10)	2647 (11)	74 (2)
H(16A)	6488 (3)	2601 (3)	1789 (2)	74 (2)
H(17A)	7590 (10)	2940 (17)	2705 (7)	74 (2)
H(17B)	7174 (17)	1899 (6)	2745 (8)	74 (2)
H(17C)	6709 (9)	2726 (20)	3096 (2)	74 (2)
H(18A)	6511 (5)	4170 (4)	2114 (14)	74 (2)
H(18B)	5547 (21)	3989 (6)	2444 (8)	74 (2)
H(18C)	5414 (19)	3931 (5)	1713 (7)	74 (2)
H(21A)	4129 (17)	-1407 (4)	284 (11)	74 (2)
H(21B)	4782 (6)	-510 (18)	546 (6)	74 (2)
H(21C)	3906 (13)	-420 (17)	-50 (5)	74 (2)
H(23A)	2325 (4)	-749 (3)	1565 (2)	74 (2)
H(23B)	1702 (4)	10 (3)	1918 (2)	74 (2)
H(28A)	1873 (4)	2756 (4)	2829 (2)	74 (2)

Table 8. Hydrogen atom coordinates* ($\times 10^4$) and isotropic displacement coefficients ($\text{\AA}^2 \times 10^3$) for the compound $\text{Os}\{\text{C}[\text{C}(=\text{CH}_2)\text{C}(\text{O})\text{OCH}_3]=\text{C}=\text{CPh}_2\}\text{Cl}(\text{CO})(\text{P}^i\text{Pr}_3)_2$ (**9**).

<i>Atom</i>	<i>X/a</i>	<i>Y/b</i>	<i>Z/c</i>	<i>U</i>
H(29A)	1868(4)	2594(4)	3892(2)	74(2)
H(30A)	516(5)	1801(4)	4232(2)	74(2)
H(31A)	-757(5)	1096(4)	3516(2)	74(2)
H(32A)	-711(4)	1174(4)	2462(2)	74(2)
H(34A)	-959(4)	3139(3)	1826(2)	74(2)
H(35A)	-2418(4)	3384(4)	1074(3)	74(2)
H(36A)	-2711(4)	2469(5)	186(3)	74(2)
H(37A)	-1553(5)	1273(5)	60(3)	74(2)
H(38A)	-60(4)	1051(4)	791(2)	74(2)

* Hydrogen atoms were included in calculated positions and refined riding on their respective carbon atoms with a fixed common thermal parameter.

Table to be deposited

Table 9. Full experimental details for the X-ray analysis of the compound

$\text{Os}\{\text{C}[\text{C}(=\text{CH}_2)\text{C}(\text{O})\text{OCH}_3]=\text{C}=\text{CPh}_2\}\text{Cl}(\text{CO})(\text{P}^i\text{Pr}_3)_2$ (**9**).

Crystal data:

Formula	$\text{C}_{38}\text{H}_{57}\text{ClO}_3\text{OsP}_2$
Molecular weight	849.43
Color and habit	Orange, irregular prism
Size (mm)	0.34 x 0.44 x 0.20
Symmetry	Monoclinic, $P2_1/n$ (no. 14)
Unit cell determination	Least-squares fit to 49 reflections. ($29 \leq 2\theta \leq 39^\circ$)
Unit cell dimensions	12.968(1), 14.058(1), 21.703(2) 90, 110.188(7), 90
Packing: V ($\text{\AA}^3$), Z	3894.2(5), 4
D calc (g cm^{-3}), F (000)	1.449, 1728

Experimental data:

Diffractometer	Four-circle Siemens-P4
Radiation and technique	Mo- $K\alpha$ ($\lambda = 0.71073 \text{ \AA}$) Bisecting geometry
Monochromator	Graphite oriented
Collection mode/range	$\omega/2\theta$ scan ($2 \leq 2\theta \leq 51^\circ$)
Number of reflections:	
measured	9253
unique	7179 (merging R factor 0.0242)
Standard reflections	3 standards measured every 100 refl.; no decay observed
Absorption correction	Semiempirical method (ψ -scan)*
Max. and min. trans. fact.	0.227, 0.158
μ (mm^{-1}) and $\mu \cdot R$	3.46, 0.57
Temperature (K)	193.0(2)

* North, A. C. T.; Phillips, D. C.; Mathews, F. S. *Acta Crystallogr., Sect. A* **1968**, *24*, 351.

Table to be deposited

Table 9. Full experimental details for the X-ray analysis of the compound

$\text{Os}\{\text{C}[\text{C}(=\text{CH}_2)\text{C}(\text{O})\text{OCH}_3]=\text{C}=\text{CPh}_2\}\text{Cl}(\text{CO})(\text{P}^i\text{Pr}_3)_2$ (**9**). (cont.)

<i>Solution and refinement:</i>	SHELXS-86 and SHELXL-93, system ALPHA AXP
Solution mode	Patterson
Refinement	Full-matrix least-squares on F^2 's All reflections
Hydrogen atoms	From calculated positions. Refined riding on C atoms.
No. parameters	420
Weighting scheme	$w^{-1} = \sigma^2(F_o^2) + (0.0242P)^2$, where $P = [\max(F_o^2, 0) + 2F_c^2] / 3$
ΔF final (max.)	1.11 e/Å ³ (at 0.97 Å from Os)
ΔF final (min.)	-0.86 e/Å ³
Max. thermal values (Å ²)	$U_{22}(\text{C}(37)) = 0.103(5)$
Max. shift/esd	-0.024
R_1^a [$F^2 > 2\sigma(F^2)$]	0.0262
wR_2^b [all data]	0.0522
S^c [all data]	0.856
Data-to-Parameter Ratio	17.1:1

Atomic scattering factors from the International Tables for X-Ray Crystallography; Vol. C (1992). Anomalous dispersion applied for Os and P atoms.

^a $R_1(F) = \sum \|F_o| - |F_c\| / \sum |F_o|$. ^b $wR_2(F^2) = [\sum [w(F_o^2 - F_c^2)^2] / \sum [w(F_o^2)^2]]^{1/2}$; $w^{-1} = [\sigma^2(F_o^2) + (aP)^2 + bP]$, where $P = [\max(F_o^2, 0) + 2F_c^2] / 3$ ($a = 0.0326$, $b = 2.70$). ^c $\text{GooF} = S = [\sum [w(F_o^2 - F_c^2)^2] / (n-p)]^{1/2}$, where n is the number of reflections and p the number of parameters.

Table to be deposited

Table 10. Bond lengths (Å) and angles (deg.) for the compound
 $\text{Os}\{\text{C}[\text{C}(=\text{CH}_2)\text{C}(\text{O})\text{OCH}_3]=\text{C}=\text{CPh}_2\}\text{Cl}(\text{CO})(\text{P}^i\text{Pr}_3)_2$ (**9**).

Os (1) -C (19)	1.818 (4)
Os (1) -C (24)	2.091 (4)
Os (1) -O (2)	2.214 (2)
Os (1) -P (1)	2.4257 (10)
Os (1) -P (2)	2.4375 (10)
Os (1) -Cl	2.4875 (10)
P (1) -C (1)	1.860 (4)
P (1) -C (7)	1.859 (4)
P (1) -C (4)	1.862 (4)
P (2) -C (13)	1.855 (4)
P (2) -C (16)	1.860 (5)
P (2) -C (10)	1.878 (4)
O (1) -C (19)	1.166 (4)
O (2) -C (20)	1.241 (4)
O (3) -C (20)	1.326 (5)
O (3) -C (21)	1.457 (5)
C (1) -C (3)	1.525 (6)
C (1) -C (2)	1.527 (6)
C (4) -C (5)	1.529 (6)
C (4) -C (6)	1.538 (5)
C (7) -C (9)	1.519 (5)
C (7) -C (8)	1.517 (6)
C (10) -C (11)	1.519 (6)
C (10) -C (12)	1.536 (5)
C (13) -C (14)	1.524 (6)
C (13) -C (15)	1.537 (6)
C (16) -C (17)	1.529 (5)
C (16) -C (18)	1.541 (6)
C (20) -C (22)	1.457 (5)
C (22) -C (23)	1.327 (6)
C (22) -C (24)	1.510 (5)
C (24) -C (25)	1.304 (5)
C (25) -C (26)	1.322 (6)
C (26) -C (33)	1.485 (6)
C (26) -C (27)	1.505 (5)
C (27) -C (28)	1.371 (6)
C (27) -C (32)	1.379 (6)
C (28) -C (29)	1.393 (6)
C (29) -C (30)	1.373 (7)
C (30) -C (31)	1.355 (7)
C (31) -C (32)	1.381 (6)
C (33) -C (38)	1.377 (6)
C (33) -C (34)	1.401 (6)
C (34) -C (35)	1.376 (7)
C (35) -C (36)	1.363 (8)
C (36) -C (37)	1.372 (8)
C (37) -C (38)	1.379 (7)
C (19) -Os (1) -C (24)	95.5 (2)
C (19) -Os (1) -O (2)	173.45 (14)
C (24) -Os (1) -O (2)	78.66 (12)

Table to be deposited

Table 10 (cont.). Bond lengths (Å) and angles (deg.) of the compound

$$\text{Os}\{\text{C}[\text{C}(=\text{CH}_2)\text{C}(\text{O})\text{OCH}_3]=\text{C}=\text{CPh}_2\}\text{Cl}(\text{CO})(\text{P}^i\text{Pr}_3)_2 \text{ (9)}.$$

C(19)-Os(1)-P(1)	90.32(12)
C(24)-Os(1)-P(1)	91.19(10)
O(2)-Os(1)-P(1)	92.77(7)
C(19)-Os(1)-P(2)	88.83(12)
C(24)-Os(1)-P(2)	95.96(10)
O(2)-Os(1)-P(2)	88.81(7)
P(1)-Os(1)-P(2)	172.85(4)
C(19)-Os(1)-Cl	103.33(14)
C(24)-Os(1)-Cl	161.02(10)
O(2)-Os(1)-Cl	82.63(7)
P(1)-Os(1)-Cl	86.55(4)
P(2)-Os(1)-Cl	86.74(4)
C(1)-P(1)-C(7)	101.5(2)
C(1)-P(1)-C(4)	101.5(2)
C(7)-P(1)-C(4)	109.6(2)
C(1)-P(1)-Os(1)	115.58(13)
C(7)-P(1)-Os(1)	115.13(13)
C(4)-P(1)-Os(1)	112.28(13)
C(13)-P(2)-C(16)	104.8(2)
C(13)-P(2)-C(10)	101.6(2)
C(16)-P(2)-C(10)	103.3(2)
C(13)-P(2)-Os(1)	120.7(2)
C(16)-P(2)-Os(1)	111.82(14)
C(10)-P(2)-Os(1)	112.66(14)
C(20)-O(2)-Os(1)	112.7(2)
C(20)-O(3)-C(21)	117.1(3)
C(3)-C(1)-C(2)	112.1(4)
C(3)-C(1)-P(1)	113.7(3)
C(2)-C(1)-P(1)	112.7(3)
C(3)-C(1)-H(1A)	105.8(2)
C(2)-C(1)-H(1A)	105.8(2)
P(1)-C(1)-H(1A)	105.85(13)
C(1)-C(2)-H(2A)	109.5(2)
C(1)-C(2)-H(2B)	109.5(2)
C(1)-C(2)-H(2C)	109.5(2)
C(1)-C(3)-H(3A)	109.5(2)
C(1)-C(3)-H(3B)	109.5(2)
C(1)-C(3)-H(3C)	109.5(2)
C(5)-C(4)-C(6)	109.7(4)
C(5)-C(4)-P(1)	115.1(3)
C(6)-C(4)-P(1)	116.8(3)
C(5)-C(4)-H(4A)	104.6(3)
C(6)-C(4)-H(4A)	104.6(3)
P(1)-C(4)-H(4A)	104.60(14)
C(4)-C(5)-H(5A)	109.5(2)
C(4)-C(5)-H(5B)	109.5(2)
C(4)-C(5)-H(5C)	109.5(3)
C(4)-C(6)-H(6A)	109.5(3)
C(4)-C(6)-H(6B)	109.5(3)
C(4)-C(6)-H(6C)	109.5(2)
C(9)-C(7)-C(8)	109.3(4)

Table to be deposited

Table 10 (cont.). Bond lengths (Å) and angles (deg.) of the compound
$$\text{Os}\{\text{C}[\text{C}(=\text{CH}_2)\text{C}(\text{O})\text{OCH}_3]=\text{C}=\text{CPh}_2\}\text{Cl}(\text{CO})(\text{P}^i\text{Pr}_3)_2$$
 (**9**).

C(9)-C(7)-P(1)	118.0(3)
C(8)-C(7)-P(1)	114.1(3)
C(9)-C(7)-H(7A)	104.7(3)
C(8)-C(7)-H(7A)	104.7(3)
P(1)-C(7)-H(7A)	104.67(14)
C(7)-C(8)-H(8A)	109.5(3)
C(7)-C(8)-H(8B)	109.5(3)
C(7)-C(8)-H(8C)	109.5(2)
C(7)-C(9)-H(9A)	109.5(2)
C(7)-C(9)-H(9B)	109.5(3)
C(7)-C(9)-H(9C)	109.5(3)
C(11)-C(10)-C(12)	109.2(4)
C(11)-C(10)-P(2)	111.4(3)
C(12)-C(10)-P(2)	119.1(3)
C(11)-C(10)-H(10A)	105.3(3)
C(12)-C(10)-H(10A)	105.3(3)
P(2)-C(10)-H(10A)	105.3(2)
C(10)-C(11)-H(11A)	109.5(2)
C(10)-C(11)-H(11B)	109.5(3)
C(10)-C(11)-H(11C)	109.5(2)
C(10)-C(12)-H(12A)	109.5(2)
C(10)-C(12)-H(12B)	109.5(3)
C(10)-C(12)-H(12C)	109.5(3)
C(14)-C(13)-C(15)	109.9(4)
C(14)-C(13)-P(2)	113.0(3)
C(15)-C(13)-P(2)	112.1(3)
C(14)-C(13)-H(13A)	107.2(2)
C(15)-C(13)-H(13A)	107.2(2)
P(2)-C(13)-H(13A)	107.2(2)
C(13)-C(14)-H(14A)	109.5(2)
C(13)-C(14)-H(14B)	109.5(2)
C(13)-C(14)-H(14C)	109.5(3)
C(13)-C(15)-H(15A)	109.5(2)
C(13)-C(15)-H(15B)	109.5(3)
C(13)-C(15)-H(15C)	109.5(2)
C(17)-C(16)-C(18)	109.6(4)
C(17)-C(16)-P(2)	115.4(3)
C(18)-C(16)-P(2)	114.2(3)
C(17)-C(16)-H(16A)	105.6(3)
C(18)-C(16)-H(16A)	105.6(3)
P(2)-C(16)-H(16A)	105.58(14)
C(16)-C(17)-H(17A)	109.5(3)
C(16)-C(17)-H(17B)	109.5(3)
C(16)-C(17)-H(17C)	109.5(3)
C(16)-C(18)-H(18A)	109.5(3)
C(16)-C(18)-H(18B)	109.5(3)
C(16)-C(18)-H(18C)	109.5(2)
O(1)-C(19)-Os(1)	176.3(4)
O(2)-C(20)-O(3)	120.7(4)
O(2)-C(20)-C(22)	122.0(4)
O(3)-C(20)-C(22)	117.2(4)

Table to be deposited

Table 10 (cont.). Bond lengths (Å) and angles (deg.) of the compound
$$\overline{\text{Os}\{\text{C}[\text{C}(=\text{CH}_2)\text{C}(\text{O})\text{OCH}_3]=\text{C}=\text{CPh}_2\}\text{Cl}(\text{CO})(\text{P}^i\text{Pr}_3)_2\text{(9)}}.$$

O(3)-C(21)-H(21A)	109.5(2)
O(3)-C(21)-H(21B)	109.5(2)
O(3)-C(21)-H(21C)	109.5(2)
C(23)-C(22)-C(20)	120.1(4)
C(23)-C(22)-C(24)	127.1(4)
C(20)-C(22)-C(24)	112.8(3)
C(22)-C(23)-H(23A)	120.0(3)
C(22)-C(23)-H(23B)	120.0(3)
C(25)-C(24)-C(22)	113.5(4)
C(25)-C(24)-Os(1)	135.8(3)
C(22)-C(24)-Os(1)	110.7(3)
C(24)-C(25)-C(26)	173.7(4)
C(25)-C(26)-C(33)	121.1(4)
C(25)-C(26)-C(27)	120.6(4)
C(33)-C(26)-C(27)	118.3(4)
C(28)-C(27)-C(32)	118.5(4)
C(28)-C(27)-C(26)	120.9(4)
C(32)-C(27)-C(26)	120.6(4)
C(27)-C(28)-C(29)	120.5(5)
C(27)-C(28)-H(28A)	119.7(3)
C(29)-C(28)-H(28A)	119.7(3)
C(30)-C(29)-C(28)	120.2(5)
C(30)-C(29)-H(29A)	119.9(3)
C(28)-C(29)-H(29A)	119.9(3)
C(31)-C(30)-C(29)	119.1(5)
C(31)-C(30)-H(30A)	120.5(3)
C(29)-C(30)-H(30A)	120.5(3)
C(30)-C(31)-C(32)	121.1(5)
C(30)-C(31)-H(31A)	119.4(3)
C(32)-C(31)-H(31A)	119.4(3)
C(31)-C(32)-C(27)	120.5(5)
C(31)-C(32)-H(32A)	119.7(3)
C(27)-C(32)-H(32A)	119.7(3)
C(38)-C(33)-C(34)	117.1(4)
C(38)-C(33)-C(26)	121.9(4)
C(34)-C(33)-C(26)	121.0(4)
C(35)-C(34)-C(33)	121.1(5)
C(35)-C(34)-H(34A)	119.4(3)
C(33)-C(34)-H(34A)	119.4(3)
C(36)-C(35)-C(34)	120.5(5)
C(36)-C(35)-H(35A)	119.8(4)
C(34)-C(35)-H(35A)	119.8(3)
C(35)-C(36)-C(37)	119.5(5)
C(35)-C(36)-H(36A)	120.3(4)
C(37)-C(36)-H(36A)	120.3(4)
C(36)-C(37)-C(38)	120.4(6)
C(36)-C(37)-H(37A)	119.8(4)
C(38)-C(37)-H(37A)	119.8(4)
C(33)-C(38)-C(37)	121.5(5)
C(33)-C(38)-H(38A)	119.3(3)
C(37)-C(38)-H(38A)	119.3(4)