Supporting Information

Table 1: Crystallographic data of *fac*-[Re(CO)$_3$(Quin)(PPh$_3$)] (11), *fac*-[Re(CO)$_3$(diCl-Quin)(PPh$_3$)] (12), *fac*-[Re(CO)$_3$(QuinH)(H$_2$O)].H$_2$O (5) and [Re(CO)$_2$(Trop)(PPh$_3$)$_2$].2C$_7$H$_8$ (20).

Crystallographic data	11	12	5	20
Empirical formula	$C_{30}H_{21}N_1O_4P_1Re_1$	$C_{30}H_{22}N_1O_4Cl_2P_1Re_1$	$C_{14}H_8N_1O_8Re_1$	$C_{45}H_{35}O_4P_2Re_1.2C_7H_8$
Formula weight (g/mol)	676.67	745.53	504.42	1072.14
Temperature (K)	100	100	100	100
Crystal system	Monoclinic	Triclinic	Monoclinic	Triclinic
Space group	*C*2/*c*	$P\bar{1}$	*C*2/*c*	$P\bar{1}$
a (Å)	24.970(2)	8.6218(12)	27.848(2)	11.144 (2)
b (Å)	9.7015(8)	11.8120(17)	11.667(6)	14.985(3)
c (Å)	22.139(2)	14.112(2)	19.101(3)	16.723(2)
α (°)	90	75.594(8)	90	66.491(3)
β (°)	93.355(3)	77.006(2)	100.373(5)	72.612(6)
γ (°)	90	82.534(6)	90	75.940(6)
Volume (Å^3)	5354(1)	1352.2(3)	6105(3)	2419.3(8)
Z	8	2	16	2
ρ_{calc} (g/cm^3)	1.679	1.831	2.195	1.472
Crystal colour	Yellow	Red	Yellow	Orange
Crystal morphology	Cuboid	Needle	Cuboid	Cuboid
Crystal size (mm)	0.54 x 0.263 x 0.121	0.364 × 0.102 × 0.098	0.526 × 0.237 × 0.069	0.45 × 0.246 × 0.124
μ (mm^{-1})	4.635	4.788	8.006	2.626
F(000)	2640.0	724.0	3808.0	1084.0
2Θ range for data (°)	7.208 to 55.998	8.958 to 55.998	4.336 to 55.994	2.994 to 56
Index ranges	$-32 \le h \le 32$	$-8 \le h \le 11$	$-36 \le h \le 36$	$-14 \le h \le 14$
	$-9 \le k \le 12$	$-15 \le k \le 15$	$-15 \le k \le 15$	$-18 \le k \le 19$
	$-29 \le l \le 29$	$-17 \le l \le 18$	$-25 \le l \le 18$	$-22 \le l \le 20$
Reflections collected	58230	38718	55931	72929
Unique reflections	6436	6500	7370	11633
Reflections with I > 2σ(I)	5851	5887	6596	10674
R_{int}	0.0501	0.0371	0.0471	0.0547
Completeness to theta (%)	100	100	100	99.5
Data/restraints/parameters	6436/0/343	6500/0/352	7370/0/461	11633/107/660
GooF	1.136	1.076	1.231	1.101
R[I>2σ (I)]	$R_1 = 0.0188$	$R_1 = 0.0224$	$R_1 = 0.0241$	$R_1 = 0.0254$
	$wR_2 = 0.0548$	$wR_2 = 0.0472$	$wR_2 = 0.0676$	$wR_2 = 0.0568$
R (all data)	$R_1 = 0.0222$	$R_1 = 0.0281$	$R_1 = 0.0317$	$R_1 = 0.0301$
	$wR_2 = 0.0564$	$wR_2 = 0.0492$	$wR_2 = 0.0989$	$wR_2 = 0.0591$
ρ_{min} and ρ_{max} (e Å^{-3})	0.91 and -0.81	1.42 and -1.16	1.90 and -2.50	1.10 and -0.81

Table 2: Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for *fac*-[$Re(CO)_3$(Quin)(PPh_3)]. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Re(1)	1210.3(2)	859.9(2)	2978.8(2)	13.40(3)
P(1)	1280.9(2)	-906.5(6)	3798.8(3)	14.80(11)
N(1)	2068.4(7)	666.5(18)	2842.4(9)	15.5(4)
O(02)	808.5(7)	-1310.2(18)	2054.7(8)	25.3(4)
C(35)	113.8(11)	-3666(3)	3275.1(13)	30.9(6)
O(03)	994.4(7)	3063.0(19)	1983.0(9)	30.2(4)
C(9)	2385.9(9)	1406(2)	3255.6(10)	15.7(4)
C(8)	2110.2(9)	2187(2)	3685.8(10)	17.8(4)
O(04)	1581.2(6)	2183.4(16)	3646.1(7)	19.7(3)
C(12)	2266.5(9)	-2105(2)	3606.7(11)	20.6(5)
C(14)	3076.3(10)	-1722(3)	4223.3(13)	32.2(6)
C(13)	2813.8(10)	-2306(3)	3720.5(12)	26.7(5)
C(32)	1167.5(10)	-3829(2)	3738.6(12)	23.8(5)
C(36)	408.7(9)	-2469(2)	3385.4(11)	21.5(5)
C(22)	900.5(10)	963(3)	4642.1(12)	25.3(5)
C(16)	2241.7(10)	-777(3)	4522.8(11)	25.0(5)
C(31)	939.2(9)	-2535(2)	3621.6(10)	17.9(4)
C(5)	3247.6(9)	2169(3)	3708.7(12)	25.1(5)
C(11)	1976.0(9)	-1337(2)	4011.2(10)	17.2(4)
C(21)	992.9(9)	-413(3)	4506.3(10)	19.3(5)
C(7)	2414.7(10)	2927(3)	4118.0(11)	24.4(5)
C(34)	348.6(11)	-4943(3)	3388.0(14)	35.3(7)
C(1)	2306.8(9)	-57(2)	2423.2(10)	18.7(5)
C(33)	872.2(11)	-5019(3)	3617.3(14)	33.0(6)
C(25)	649.9(12)	-1066(3)	5463.3(13)	36.6(7)
C(23)	682.2(10)	1314(3)	5188.9(12)	32.7(6)
C(15)	2791.3(11)	-965(3)	4628.0(13)	33.0(6)
C(24)	559.8(10)	298(3)	5593.4(12)	34.5(7)
C(26)	860.7(10)	-1427(3)	4919.3(11)	29.5(6)
C(02)	955.6(9)	-485(2)	2400.2(10)	16.9(4)
C(03)	1103.9(8)	2271(2)	2354.6(11)	19.1(5)
C(6)	2977.8(10)	2900(3)	4125.5(12)	29.2(6)
C(01)	481.2(9)	1191(2)	3167(1)	17.1(4)
C(3)	3187.3(9)	627(2)	2800.8(11)	21.5(5)
C(4)	2954.6(9)	1402(2)	3258.6(11)	19.4(5)
C(2)	2866.2(9)	-92(2)	2388.4(11)	21.0(5)
O(01)	41.7(6)	1395.7(18)	3271.6(8)	24.6(4)
O(2)	602(9)	5141(16)	5454(11)	359(13)
O(1)	133(6)	5230(30)	5081(16)	205(13)

Table 3: Anisotropic displacement parameters ($Å^2$ x 10^3) for *fac*-[$Re(CO)_3(Quin)(PPh_3)$].

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Re(1)	12.11(5)	12.66(5)	15.08(5)	-0.19(3)	-2.17(3)	1.15(3)
P(1)	14.7(3)	16.2(3)	13.4(3)	-0.3(2)	-0.2(2)	5.0(2)
N(1)	16.2(9)	13.3(9)	16.8(9)	0.9(7)	-1.2(7)	-0.3(7)
O(02)	26.3(9)	28.3(9)	20.8(9)	-7.3(7)	-2.7(7)	-5.8(7)
C(35)	25.6(13)	22.1(12)	44.3(17)	2.4(12)	-2.9(12)	-2.1(10)
O(03)	24.8(9)	29.3(10)	35.7(11)	16.0(8)	-5.0(8)	-6.2(7)
C(9)	16.5(10)	13(1)	17.1(11)	0.9(8)	-3.4(8)	-0.2(8)
C(8)	16.9(10)	15.6(11)	20.2(11)	-0.9(9)	-2.8(9)	1.5(8)
O(04)	14.7(7)	19.3(8)	24.8(9)	-8.7(7)	-1.7(6)	2.5(6)
C(12)	21.2(11)	20.1(11)	20.6(12)	-0.8(9)	2.1(9)	3.5(9)
C(14)	17.9(12)	41.5(16)	37.0(16)	5.6(13)	-1.8(11)	9.1(11)
C(13)	21.0(12)	27.1(13)	32.5(14)	-0.2(11)	5.4(10)	8.6(10)
C(32)	20.5(11)	21.6(12)	29.4(14)	5.7(10)	2.7(10)	6.6(9)
C(36)	21.0(11)	16.7(11)	26.7(13)	2.1(10)	0.7(9)	3.8(9)
C(22)	23.5(12)	30.9(14)	21.3(12)	-7.3(10)	-0.3(10)	5.4(10)
C(16)	24.1(12)	30.2(13)	20.4(12)	-3.5(10)	-2.6(10)	6.9(10)
C(31)	21.8(11)	15.8(10)	16.8(11)	1.2(9)	4.9(9)	3.4(9)
C(5)	14.6(11)	28.2(13)	31.9(14)	0.6(11)	-3.9(10)	-1.6(9)
C(11)	15.5(10)	16.9(11)	19.1(11)	4.0(9)	0.2(9)	5.5(8)
C(21)	14.5(10)	31.0(13)	12.0(11)	-2.1(9)	-2.0(8)	8.7(9)
C(7)	23.7(12)	24.2(12)	24.8(13)	-9.3(10)	-2.9(10)	1.7(10)
C(34)	34.8(15)	19.7(13)	51.1(19)	2.4(12)	1.3(13)	-4.9(11)
C(1)	22.7(11)	15.8(10)	17.5(11)	-0.5(9)	1.1(9)	0.2(9)
C(33)	36.1(15)	14.7(12)	48.6(18)	5.0(11)	6.5(13)	5.7(10)
C(25)	34.9(15)	55.5(19)	20.2(13)	6.1(13)	7.3(11)	11.1(13)
C(23)	26.3(13)	43.5(16)	28.0(15)	-18.0(12)	-0.6(11)	7.4(12)
C(15)	25.2(13)	46.3(17)	26.3(14)	-3.3(12)	-9.7(11)	6.3(12)
C(24)	22.5(13)	67(2)	14.7(12)	-9.7(13)	1.5(10)	8.1(13)
C(26)	30.7(14)	38.5(15)	19.9(13)	4.1(11)	5.3(10)	13.8(12)
C(02)	14.6(10)	20.8(11)	15.3(11)	3.4(9)	-0.2(8)	-0.1(8)
C(03)	12.6(10)	19.2(11)	25.4(12)	0(1)	-0.6(9)	-4.0(8)
C(6)	25.8(13)	30.4(14)	30.2(14)	-8.7(11)	-8.3(11)	-3.8(10)
C(01)	19.8(11)	12.8(10)	18.1(11)	1.5(8)	-3.2(9)	0.6(8)
C(3)	15.7(11)	20.9(12)	28.3(13)	3.9(10)	3.6(9)	0.5(9)
C(4)	17.9(11)	16.9(11)	23.2(12)	3.6(9)	0.2(9)	0.3(9)
C(2)	22.7(12)	18.6(11)	22.5(12)	-1.0(9)	6.8(10)	0.6(9)
O(01)	15.9(8)	28.6(9)	29.4(10)	0.7(8)	1.5(7)	5.4(7)
O(2)	250(20)	226(15)	600(40)	71(18)	-60(20)	-49(13)
O(1)	48(15)	280(30)	280(30)	20(20)	-6(17)	-12(16)

Table 4: Bond lengths (Å) for *fac*-[$Re(CO)_3(Quin)(PPh_3)$].

Bond	Distance (Å)	Bond	Distance (Å)
Re(1)-P(1)	2.4953(6)	C(12)-C(11)	1.400(3)
Re(1)-N(1)	2.1894(18)	C(14)-C(13)	1.380(4)
Re(1)-O(04)	2.1281(15)	C(14)-C(15)	1.387(4)
Re(1)-O(04)[1]	2.1281(15)	C(32)-C(31)	1.397(3)
Re(1)-C(02)	1.911(2)	C(32)-C(33)	1.388(4)
Re(1)-C(03)	1.952(2)	C(36)-C(31)	1.397(3)
Re(1)-C(01)	1.918(2)	C(22)-C(21)	1.391(3)
P(1)-C(31)	1.827(2)	C(22)-C(23)	1.399(3)
P(1)-C(11)	1.820(2)	C(16)-C(11)	1.389(3)
P(1)-C(21)	1.825(2)	C(16)-C(15)	1.391(4)
N(1)-C(9)	1.376(3)	C(5)-C(6)	1.372(4)
N(1)-C(1)	1.331(3)	C(5)-C(4)	1.413(3)
N(1)-C(02)	1.152(3)	C(21)-C(26)	1.396(4)
C(35)-C(36)	1.389(3)	C(7)-C(6)	1.405(3)
C(35)-C(34)	1.387(4)	C(34)-C(33)	1.377(4)
O(03)-C(03)	1.147(3)	C(1)-C(2)	1.404(3)
C(9)-C(8)	1.425(3)	C(25)-C(24)	1.375(4)
C(9)-C(4)	1.420(3)	C(25)-C(26)	1.387(4)
C(8)-O(04)	1.319(3)	C(23)-C(24)	1.378(4)
C(8)-O(04)[1]	1.319(3)	C(01)-O(01)	1.152(3)
C(8)-C(7)	1.387(3)	C(3)-C(4)	1.414(3)
O(04)-O(04)[1]	0.000(3)	C(3)-C(2)	1.370(3)
C(12)-C(13)	1.389(3)	O(1)-O(1)[2]	0.86(5)

[1]+x,+y,+z [2]-x,1-y,1-z

Table 5: Bond angles (°) for *fac*-[Re(CO)$_3$(Quin)(PPh$_3$)].

Bond angle	Angle (˚)	Bond angle	Angle (˚)
N(1)-Re(1)-P(1)	90.77(5)	C(7)-C(8)-C(9)	118.0(2)
O(04)-Re(1)-P(1)	84.25(5)	C(8)-O(04)-Re(1)	116.18(13)
O(04^1)-Re(1)-P(1)	84.25(5)	O(04^1)-O(04)-Re(1)	0(5)
O(04)-Re(1)-N(1)	75.98(6)	O(04^1)-O(04)-C(8)	0(10)
O(04^1)-Re(1)-N(1)	75.98(6)	C(13)-C(12)-C(11)	120.0(2)
O(04^1)-Re(1)-O(04)	0.00(7)	C(13)-C(14)-C(15)	120.1(2)
C(02)-Re(1)-P(1)	91.45(7)	C(14)-C(13)-C(12)	120.3(2)
C(02)-Re(1)-N(1)	97.99(8)	C(33)-C(32)-C(31)	120.4(2)
C(02)-Re(1)-O(04)	172.51(8)	C(35)-C(36)-C(31)	120.6(2)
C(02)-Re(1)-O(04^1)	172.51(8)	C(21)-C(22)-C(23)	119.9(3)
C(02)-Re(1)-C(03)	88.74(10)	C(11)-C(16)-C(15)	120.3(2)
C(02)-Re(1)-C(01)	88.69(9)	C(32)-C(31)-P(1)	123.83(18)
C(03)-Re(1)-P(1)	175.94(6)	C(32)-C(31)-C(36)	118.6(2)
C(03)-Re(1)-N(1)	93.22(8)	C(36)-C(31)-P(1)	117.49(17)
C(03)-Re(1)-O(04)	95.98(8)	C(6)-C(5)-C(4)	119.5(2)
C0(3)-Re(1)-O(04^1)	95.98(8)	C(12)-C(11)-P(1)	118.61(18)
C(01)-Re(1)-P(1)	89.11(7)	C(16)-C(11)-P(1)	121.57(17)
C(01)-Re(1)-N(1)	173.31(8)	C(16-C(11-C(12	119.3(2)
C(01)-Re(1)-O(04)	97.35(8)	C(22)-C(21)-P(1)	121.05(19)
C(01)-Re(1)-O(04^1)	97.35(8)	C(22)-C(21)-C(26)	119.1(2)
C(01)-Re(1)-C(03)	86.84(9)	C(26)-C(21)-P(1)	119.85(19)
C(31)-P(1)-Re(1)	115.17(7)	C(8)-C(7)-C(6)	120.4(2)
C(11)-P(1)-Re(1)	111.79(7)	C(33)-C(34)-C(35)	119.8(2)
C(11)-P(1)-C(31)	106.47(10)	N(1)-C(1)-C(2)	122.5(2)
C(11)-P(1)-C(21)	104.84(10)	C(34)-C(33)-C(32)	120.6(2)
C(21)-P(1)-Re(1)	115.45(8)	C(24)-C(25)-C(26)	120.0(3)
C(21)-P(1)-C(31)	102.02(11)	C(24)-C(23)-C(22)	120.0(3)
C(9)-N(1)-Re(1)	113.20(14)	C(14)-C(15)-C(16)	120.0(3)
C(1)-N(1)-Re(1)	128.49(16)	C(25)-C(24)-C(23)	120.5(2)
C(1)-N(1)-C(9)	118.31(19)	C(25)-C(26)-C(21)	120.5(3)
C(34)-C(35)-C(36)	120.1(2)	O(02)-C(02)-Re(1)	178.9(2)
N(1)-C(9)-C(8)	116.06(19)	O(03)-C(03)-Re(1)	173.88(19)
N(1)-C(9)-C(4)	122.6(2)	C(5)-C(6)-C(7)	122.1(2)

C(4)-C(9)-C(8)	121.3(2)	O(01)-C(01)-Re(1)	179.0(2)
O(04[1])-C(8)-C(9)	118.4(2)	C(2)-C(3)-C(4)	120.0(2)
O(04)-C(8)-C(9)	118.4(2)	C(5)-C(4)-C(9)	118.6(2)
O(04[1])-C(8)-O(04)	0.00(19)	C(5)-C(4)-C(3)	124.6(2)
O(04[1])-C(8)-C(7)	123.6(2)	C(3)-C(4)-C(9)	116.8(2)
O(04)-C(8)- C(7)	123.6(2)	C(3)-C(2)-C(1)	119.8(2)

[1]+x,+y,+z

Table 6: Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for *fac*-[Re(CO)$_3$(Quin)(PPh$_3$)].

	x	y	z	U(eq)
H(35)	-241	-3611	3125	37
H(12)	2093	-2480	3262	25
H(14)	3445	-1836	4291	39
H(13)	3004	-2837	3457	32
H(32)	1519	-3893	3899	29
H(36)	252	-1616	3301	26
H(22)	984	1649	4370	30
H(16)	2051	-274	4796	30
H(5)	3621	2177	3722	30
H(7)	2245	3444	4405	29
H(34)	153	-5745	3309	42
H(1)	2095	-558	2143	22
H(33)	1030	-5876	3692	40
H(25)	570	-1746	5740	44
H(23)	620	2234	5280	39
H(15)	2968	-584	4970	40
H(24)	415	536	5957	41
H(26)	914	-2352	4829	35
H(6)	3174	3395	4423	35
H(3)	3558	605	2780	26
H(2)	3018	-601	2086	25

Table 7: Hydrogen bonds for *fac*-[Re(CO)$_3$(Quin)(PPh$_3$)] (Å and °).

D-H…A	d(D-H)	d(H…A)	d(D…A)	<(DHA)
C(22)-H(22)…O(04[1])	0.93	2.31	3.097(3)	142.0
C(33)-H(33)...O(04[2])	0.93	2.34	3.241(4)	162.9

[1]+x,+y,+z [2] +x,1+y,+z

Table 8: Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for *fac*-[$Re(CO)_3$(diCl-Quin)(PPh_3)]. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Re(1)	2308.8(2)	1050.6(2)	3268.4(2)	14.71(4)
Cl(1)	8296.9(10)	631.3(8)	-939.1(6)	32.48(18)
Cl(2)	2579.5(9)	3047.3(7)	-446.5(6)	29.76(18)
P(1)	3550.3(8)	2891.3(6)	3126.1(5)	15.15(14)
O(04)	2324(2)	1781.8(17)	1712.2(14)	17.5(4)
O(02)	2892(3)	27(2)	5385.4(16)	30.9(5)
O(01)	-881(3)	2208(2)	4204.7(16)	28.4(5)
C(34)	4009(5)	3593(3)	6121(3)	36.7(9)
O(03)	571(3)	-1157(2)	3469.1(17)	32.3(5)
C(13)	8217(4)	2244(3)	1831(2)	24.5(7)
N(1)	4555(3)	319(2)	2496.8(17)	16.6(5)
C(21)	2364(3)	4232(2)	2651(2)	17.7(6)
C(23)	284(4)	5230(3)	1789(2)	27.7(7)
C(22)	1166(4)	4201(3)	2147(2)	21.2(6)
C(7)	3970(3)	2036(2)	78(2)	18.1(6)
C(16)	5647(4)	3790(3)	1338(2)	23.8(7)
C(6)	5398(4)	1753(3)	-552(2)	22.8(6)
C(11)	5480(3)	3016(3)	2276(2)	17.2(6)
C(12)	6782(3)	2235(3)	2515(2)	20.1(6)
C(26)	2665(4)	5306(3)	2794(2)	24.6(7)
C(1)	5626(4)	-443(3)	2907(2)	22.7(6)
C(24)	596(4)	6286(3)	1927(2)	27.9(7)
C(14)	8366(4)	3005(3)	899(3)	30.3(8)
C(15)	7087(4)	3774(3)	654(3)	31.6(8)
C(35)	5384(4)	3423(3)	5434(3)	34.7(8)
C(8)	3644(3)	1554(2)	1099(2)	15.9(6)
C(2)	7081(4)	-799(3)	2345(2)	25.5(7)
C(36)	5289(4)	3217(3)	4522(2)	26.0(7)
C(3)	7440(4)	-359(3)	1336(2)	24.8(7)
C(4)	6335(3)	442(2)	871(2)	18.5(6)
C(32)	2448(4)	3299(3)	5013(2)	31.5(8)
C(9)	4873(3)	756(2)	1481(2)	16.1(6)
C(25)	1791(4)	6321(3)	2433(3)	29.1(7)
C(5)	6561(3)	973(3)	-164(2)	21.1(6)
C(01)	307(4)	1779(3)	3839(2)	19.2(6)
C(33)	2548(5)	3530(3)	5904(3)	37.2(9)
C(02)	2646(3)	416(3)	4594(2)	20.3(6)
C(31)	3825(4)	3148(3)	4302(2)	19.6(6)
C(03)	1234(4)	-341(3)	3361(2)	21.0(6)

Table 9: Observed π-π interactions and distances in the structure of *fac*-[Re(CO)$_3$(diCl-Quin)(PPh$_3$)].

π-π interaction	Distance (Å)
Ring 1 – Ring 4	3.770(3)
Ring 1 – Ring 2	3.585(3)
Ring 1 – Ring 3	3.738(3)
Ring 5 – Ring 5[1]	3.860(3)

[1]1-x,1-y,1-z

Table 10: Anisotropic displacement parameters (Å^2 x 10^3) for *fac*-[Re(CO)$_3$(diCl-Quin)(PPh$_3$)].

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Re(1)	14.31(6)	16.59(6)	13.15(6)	-1.15(4)	-3.53(4)	-3.89(4)
Cl(1)	23.9(4)	40.3(5)	32.3(4)	-12.3(4)	2.3(3)	-4.8(3)
Cl(2)	24.1(4)	35.8(4)	21.5(4)	3.8(3)	-4.6(3)	5.7(3)
P(1)	12.8(3)	18.4(4)	14.1(3)	-2.8(3)	-2.0(3)	-3.3(3)
O(04)	16.8(10)	20.6(10)	14.1(10)	-1.3(8)	-4.5(8)	0.0(8)
O(02)	39.8(14)	35.1(13)	17.5(11)	2.5(10)	-11.6(10)	-8.8(11)
O(01)	17.8(11)	38.3(13)	27.1(12)	-8.2(10)	-0.6(9)	-0.2(10)
C(34)	52(2)	44(2)	19.3(16)	-9.2(15)	-6.2(16)	-21.3(18)
O(03)	37.3(14)	30.6(13)	30.6(13)	-7.2(10)	-1.1(11)	-17.4(11)
C(13)	14.6(14)	31.5(17)	32.0(17)	-14.5(14)	-6.5(13)	-0.8(12)
N(1)	16.8(12)	15.7(12)	18.4(12)	-4.6(9)	-4.5(10)	-1.8(9)
C(21)	14.9(13)	18.6(14)	16.6(14)	-2.5(11)	1.6(11)	-1.8(11)
C(23)	27.8(17)	30.3(18)	23.0(16)	-1.7(13)	-8.8(13)	2.7(13)
C(22)	22.3(15)	19.5(15)	21.2(15)	-4.3(12)	-4.6(12)	-0.3(12)
C(7)	16.5(14)	19.7(15)	18.2(14)	-2.1(11)	-6.5(11)	-0.9(11)
C(16)	20.4(15)	27.4(17)	21.3(15)	-1.9(13)	-2.6(12)	-3.0(12)
C(6)	20.0(15)	26.8(16)	21.8(15)	-4.5(13)	-1.9(12)	-8.9(12)
C(11)	14.4(13)	22.9(15)	15.8(14)	-6.5(11)	-1.2(11)	-6.0(11)
C(12)	19.0(14)	23.5(15)	21.1(15)	-8.4(12)	-6.3(12)	-3.3(12)
C(26)	21.2(15)	24.7(16)	28.5(17)	-7.5(13)	-2.7(13)	-5.0(12)
C(1)	26.7(16)	20.2(15)	22.8(16)	-2.5(12)	-10.9(13)	-2.2(12)
C(24)	32.7(18)	19.5(16)	22.4(16)	0.7(13)	2.5(14)	6.4(13)
C(14)	17.4(15)	43(2)	29.6(18)	-12.2(15)	5.8(13)	-8.9(14)
C(15)	27.7(18)	36.7(19)	24.2(17)	-1.4(14)	4.9(14)	-8.0(14)
C(35)	38(2)	44(2)	29.6(18)	-13.2(16)	-13.7(16)	-9.8(16)
C(8)	15.2(13)	15.6(14)	18.6(14)	-5.1(11)	-4.0(11)	-3.5(11)
C(2)	21.1(16)	24.1(16)	32.3(18)	-6.3(13)	-11.0(13)	4.8(12)
C(36)	24.5(16)	32.1(18)	25.6(16)	-11.1(14)	-8.3(13)	-2.7(13)
C(3)	20.8(15)	23.1(16)	31.7(17)	-8.7(13)	-6.2(13)	0.5(12)
C(4)	18.4(14)	16.5(14)	22.5(15)	-6.7(11)	-4.6(12)	-2.9(11)
C(32)	24.5(17)	47(2)	25.1(17)	-11.8(15)	0.8(14)	-14.5(15)
C(9)	17.4(14)	14.3(13)	17.8(14)	-5.0(11)	-3.9(11)	-2.5(11)
C(25)	31.4(18)	20.1(16)	32.2(18)	-6.9(14)	2.3(14)	-3.1(13)
C(5)	19.2(15)	22.6(15)	23.6(15)	-9.0(12)	-2.3(12)	-5.8(12)
C(01)	21.3(15)	22.2(15)	15.3(14)	-1.8(12)	-6.8(12)	-5.9(12)
C(33)	40(2)	50(2)	23.3(17)	-16.2(16)	9.1(15)	-18.4(17)
C(02)	20.0(15)	19.4(15)	22.6(16)	-3.6(12)	-5.7(12)	-5.6(12)
C(31)	22.8(15)	21.0(15)	15.9(14)	-3.5(11)	-3.3(12)	-7.5(12)
C(03)	22.9(15)	25.4(16)	15.1(14)	-3.3(12)	-4.7(12)	-3.9(12)

Table 11: Bond lengths (Å) for *fac*-[Re(CO)$_3$(diCl-Quin)(PPh$_3$)].

Bond	Distance (Å)	Bond	Distance (Å)
Re(1)-P(1)	2.4908(8)	C(21)-C(26)	1.399(4)
Re(1)-O(04)	2.1483(19)	C(23)-C(22)	1.392(4)
Re(1)-N(1)	2.184(2)	C(23)-C(24)	1.377(5)
Re(1)-C(01)	1.924(3)	C(7)-C(6)	1.403(4)
Re(1)-C(02)	1.907(3)	C(7)-C(8)	1.389(4)
Re(1)-C(03)	1.952(3)	C(16)-C(11)	1.397(4)
Cl(1)-C(5)	1.710(3)	C(16)-C(15)	1.392(4)
Cl(2)-C(7)	1.732(3)	C(6)-C(5)	1.381(4)
P(1)-C(21)	1.834(3)	C(11)-C(12)	1.404(4)
P(1)-C(11)	1.819(3)	C(26)-C(25)	1.378(5)
P(1)-C(31)	1.830(3)	C(1)-C(2)	1.400(4)
O(04)-C(8)	1.308(3)	C(24)-C(25)	1.389(5)
O(02)-C(02)	1.153(4)	C(14)-C(15)	1.384(5)
O(01)-C(01)	1.153(4)	C(35)-C(36)	1.390(4)
C(34)-C(35)	1.379(5)	C(8)-C(9)	1.431(4)
C(34)-C(33)	1.377(5)	C(2)-C(3)	1.367(5)
O(03)-C(03)	1.145(4)	C(36)-C(31)	1.383(4)
C(13)-C(12)	1.387(4)	C(3)-C(4)	1.403(4)
C(13)-C(14)	1.387(5)	C(4)-C(9)	1.421(4)
N(1)-C(1)	1.328(4)	C(4)-C(5)	1.420(4)
N(1)-C(9)	1.374(4)	C(32)-C(33)	1.375(5)
C(21)-C(22)	1.387(4)	C(32)-C(31)	1.394(4)

Table 12: Bond angles (°) for *fac*-[Re(CO)$_3$(diCl-Quin)(PPh$_3$)].

Bond angle	Angle (°)	Bond angle	Angle (°)
O(04)-Re(1)-P(1)	82.53(5)	C(5)-C(6)-C(7)	120.2(3)
O(04)-Re(1)-N(1)	75.63(8)	C(16)-C(11)-P(1)	121.0(2)
N(1)-Re(1)-P(1)	90.59(6)	C(16)-C(11)-C(12)	119.1(3)
C(01)-Re(1)-P(1)	88.11(9)	C(12)-C(11)-P(1)	119.5(2)
C(01)-Re(1)-O(04)	99.50(10)	C(13)-C(12)-C(11)	120.2(3)
C(01)-Re(1)-N(1)	175.09(10)	C(25)-C(26)-C(21)	120.4(3)
C(01)-Re(1)-C(03)	89.44(12)	N(1)-C(1)-C(2)	122.4(3)
C(02)-Re(1)-P(1)	92.75(9)	C(23)-C(24)-C(25)	119.7(3)
C(02)-Re(1)-O(04)	171.08(10)	C(15)-C(14)-C(13)	120.0(3)
C(02)-Re(1)-N(1)	96.94(11)	C(14)-C(15)-C(16)	120.5(3)
C(02)-Re(1)-C(01)	87.85(12)	C(34)-C(35)-C(36)	120.1(3)
C(02)-Re(1)-C(03)	89.03(12)	O(04)-C(8)-C(7)	124.9(3)
C03)-Re(1)-P(1)	176.92(9)	O(04)-C(8)-C(9)	119.3(2)
C(03)-Re(1)-O(04)	96.03(10)	C(7)-C(8)-C(9)	115.9(3)
C(03)-Re(1)-N(1)	91.69(11)	C(3)-C(2)-C(1)	120.0(3)
C(21)-P(1)-Re(1)	113.99(9)	C(31)-C(36)-C(35)	120.6(3)
C(11)-P(1)-Re(1)	113.58(10)	C(2)-C(3)-C(4)	119.5(3)
C(11)-P(1)-C(21)	104.09(13)	C(3)-C(4)-C(9)	117.8(3)
C(11)-P(1)-C(31)	106.71(13)	C(3)-C(4)-C(5)	125.3(3)
C(31)-P(1)-Re(1)	115.45(9)	C(5)-C(4)-C(9)	116.9(3)
C(31)-P(1)-C(21)	101.72(14)	C(33)-C(32)-C(31)	120.6(3)
C(8)-O(04)-Re(1)	115.46(17)	N(1)-C(9)-C(8)	115.1(2)
C(33)-C(34)-C(35)	119.5(3)	N(1)-C(9)-C(4)	121.6(3)
C(14)-C(13)-C(12)	120.3(3)	C(4)-C(9)-C(8)	123.3(3)
C(1)-N(1)-Re(1)	127.1(2)	C(26)-C(25)-C(24)	120.3(3)
C(1)-N(1)-C(9)	118.8(3)	C(6)-C(5)-Cl(1)	119.9(2)
C(9)-N(1)-Re(1)	114.02(18)	C(6)-C(5)-C(4)	121.0(3)
C(22)-C(21)-P(1)	121.1(2)	C(4)-C(5)-Cl(1)	119.2(2)
C(22)-C(21)-C(26)	119.1(3)	O(01)-C(01)-Re(1)	178.2(2)
C(26)-C(21)-P(1)	119.8(2)	C(32)-C(33)-C(34)	120.7(3)
C(24)-C(23)-C(22)	120.4(3)	O(02)-C(02)-Re(1)	178.2(3)
C(21)-C(22)-C(23)	120.1(3)	C(36)-C(31)-P(1)	124.5(2)
C(6)-C(7)-Cl(2)	118.1(2)	C(36)-C(31)-C(32)	118.5(3)
C(8)-C(7)-Cl(2)	119.2(2)	C(32)-C(31)-P(1)	116.9(2)
C(8)-C(7)-C(6)	122.7(3)	O(03)-C(03)-Re(1)	176.3(3)
C(15)-C(16)-C(11)	120.0(3)		

Table 13: Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for *fac*-[Re(CO)$_3$(diCl-Quin)(PPh$_3$)].

	x	y	z	U(eq)
H(34)	4069	3749	6726	44
H(13)	9083	1737	1999	29
H(23)	-521	5205	1455	33
H(22)	952	3492	2049	25
H(16)	4797	4316	1172	29
H(6)	5563	2091	-1232	27
H(12)	6682	1711	3134	24
H(26)	3460	5336	3135	30
H(1)	5402	-751	3593	27
H(24)	10	6972	1683	34
H(14)	9325	3000	438	36
H(15)	7190	4283	27	38
H(35)	6376	3447	5582	42
H(2)	7802	-1335	2658	31
H(36)	6219	3125	4055	31
H(3)	8408	-589	961	30
H(32)	1454	3242	4883	38
H(25)	2002	7033	2529	35
H(33)	1619	3645	6365	45

Table 14: Hydrogen bonds for *fac*-[Re(CO)$_3$(diCl-Quin)(PPh$_3$)] (Å and °).

D-H…A	d(D-H)	d(H…A)	d(D…A)	<(DHA)
C(3)-H(3)…Cl(1[1])	0.93	2.83	3.575(3)	138.2
C(3)-H(3)…Cl(1[2])	0.93	2.73	3.084(3)	103.9
C(12)-H(12)...O(02[3])	0.93	2.59	3.497(8)	164.5
C(14)-H(14)...Cl(2[4])	0.93	2.81	3.703(7)	162.3
C(22)-H(22)...O(04[2])	0.93	2.29	3.054(9)	139

[1]2-x,-y,-z [2]x,y,z [3]1-x,-y,1-z [4]1+x,+y,+z

Table 15: Observed π-π interactions and distances in the structure of *fac*-[Re(CO)$_3$(diCl-Quin)(PPh$_3$)].

π-π interaction	Distance (Å)
Ring 1 – Ring 3	3.551(4)
Ring 1 – Ring 2	3.646(4)
Ring 1 – Ring 4	3.767(4)
Ring 5 – Ring 5[1]	4.367(5)

[1]1-x,1-y,1-z

Table 16: Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for *fac*-[$Re(CO)_3(QuinH)(H_2O)$].H_2O. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1A)	4084(2)	8008(4)	42(2)	14(1)
C(01A)	3088(2)	9822(4)	-1677(3)	23(1)
C(01B)	6410(2)	1034(5)	3415(3)	23(1)
C(1B)	5868(2)	4448(4)	2236(2)	13(1)
C(02A)	3583(2)	11528(4)	-1075(3)	18(1)
C(2A)	4275(2)	6934(4)	276(2)	15(1)
C(2B)	5627(2)	5455(4)	1977(2)	16(1)
C(02B)	6578(2)	2854(4)	4192(3)	20(1)
C(3A)	4067(2)	5955(4)	-30(2)	14(1)
C(03A)	3058(2)	10275(4)	-301(3)	21(1)
C(3B)	5766(2)	6470(4)	2319(3)	15(1)
C(03B)	7035(2)	2585(4)	3113(3)	20(1)
C(04A)	4313(2)	9101(4)	372(3)	16(1)
C(4A)	3641(2)	6035(4)	-555(2)	13(1)
C(4B)	6158(2)	6484(4)	2913(2)	14(1)
C(04B)	5740(2)	3318(4)	1851(2)	14(1)
C(5A)	3380(2)	5066(4)	-878(3)	22(1)
C(5B)	6330(2)	7503(5)	3294(3)	21(1)
C(6A)	2951(2)	5188(5)	-1345(3)	23(1)
C(6B)	6703(2)	7444(4)	3867(3)	20(1)
C(7A)	2754(2)	6283(5)	-1509(3)	23(1)
C(7B)	6922(2)	6392(4)	4086(3)	19(1)
C(8A)	2995(2)	7245(4)	-1218(3)	19(1)
C(8B)	6765(2)	5404(4)	3733(3)	15(1)
C(9A)	3447(2)	7148(4)	-747(3)	14(1)
C(9B)	6377(2)	5430(4)	3149(2)	14(1)
C(10A)	4297(2)	4841(4)	239(3)	18(1)
C(10B)	5506(2)	7551(4)	2025(3)	20(1)
N(1A)	3690(2)	8132(3)	-462(2)	13(1)
N(1B)	6219(2)	4416(3)	2815(2)	12(1)
O(1)	5264(2)	2162(3)	4780(2)	27(1)
O(1A)	4154(1)	10030(3)	70(2)	16(1)
O(01A)	2805(2)	9774(4)	-2195(2)	38(1)
O(1B)	6016(1)	2457(3)	2109(2)	16(1)
O(01B)	6440(2)	90(3)	3551(3)	40(1)
O(2)	5128(2)	902(4)	3237(3)	38(1)
O(2A)	4627(1)	9049(3)	917(2)	22(1)
O(02A)	3587(2)	12474(3)	-1239(2)	27(1)
O(2B)	5416(1)	3267(3)	1328(2)	19(1)
O(02B)	6703(2)	2961(4)	4799(2)	32(1)
O(3A)	4407(2)	4669(3)	874(2)	22(1)
O(03A)	2752(2)	10470(4)	-1(2)	32(1)
O(3B)	5678(2)	8518(3)	2104(2)	25(1)
O(03B)	7448(2)	2557(4)	3096(3)	31(1)
O(4A)	4363(2)	4118(3)	-259(2)	26(1)
O(4B)	5066(2)	7331(3)	1664(3)	35(1)
O(5A)	4175(2)	9461(3)	-1372(2)	21(1)
O(5B)	5592(1)	2843(3)	3246(2)	19(1)
Re(1A)	3568(1)	9937(1)	-830(1)	12(1)
Re(1B)	6365(1)	2641(1)	3197(1)	13(1)

Table 17: Anisotropic displacement parameters ($Å^2$ x 10^3) for *fac*-[$Re(CO)_3(QuinH)(H_2O)$].H_2O.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1A)	18(2)	10(2)	12(2)	-3(2)	0(2)	-1(2)
C(01A)	34(3)	7(2)	24(3)	0(2)	-2(2)	1(2)
C(01B)	30(3)	14(3)	20(2)	-1(2)	-3(2)	-2(2)
C(1B)	19(2)	6(2)	14(2)	0(2)	3(2)	-1(2)
C(02A)	25(3)	14(2)	14(2)	-4(2)	1(2)	2(2)
C(2A)	21(3)	11(2)	12(2)	0(2)	-2(2)	-1(2)
C(2B)	20(3)	12(2)	13(2)	2(2)	-1(2)	2(2)
C(02B)	30(3)	9(2)	19(2)	1(2)	4(2)	3(2)
C(3A)	22(3)	8(2)	12(2)	2(2)	3(2)	1(2)
C(03A)	24(3)	12(2)	22(3)	-3(2)	-4(2)	-4(2)
C(3B)	19(3)	9(2)	17(2)	2(2)	4(2)	0(2)
C(03B)	25(3)	14(2)	17(2)	-1(2)	-4(2)	4(2)
C(04A)	23(3)	8(2)	16(2)	-2(2)	1(2)	0(2)
C(4A)	22(3)	6(2)	10(2)	1(2)	4(2)	-2(2)
C(4B)	17(2)	9(2)	17(2)	1(2)	3(2)	0(2)
C(04B)	20(3)	9(2)	13(2)	-1(2)	7(2)	-1(2)
C(5A)	36(4)	8(2)	21(3)	0(2)	3(2)	-5(2)
C(5B)	24(3)	11(2)	26(3)	-1(2)	3(2)	2(2)
C(6A)	32(3)	13(2)	22(3)	-3(2)	-2(2)	-6(2)
C(6B)	22(3)	13(2)	23(3)	-2(2)	-2(2)	-2(2)
C(7A)	27(3)	18(3)	21(3)	-1(2)	-4(2)	-5(2)
C(7B)	18(3)	18(2)	18(2)	-2(2)	-2(2)	-3(2)
C(8A)	24(3)	11(2)	18(2)	0(2)	-2(2)	-1(2)
C(8B)	16(2)	9(2)	20(2)	-1(2)	0(2)	0(2)
C(9A)	20(3)	9(2)	14(2)	0(2)	4(2)	-2(2)
C(9B)	17(2)	8(2)	16(2)	-1(2)	2(2)	-4(2)
C(10A)	25(3)	9(2)	19(2)	1(2)	3(2)	-2(2)
C(10B)	26(3)	13(2)	19(3)	1(2)	3(2)	4(2)
N(1A)	16(2)	7(2)	13(2)	0(1)	0(2)	-1(2)
N(1B)	18(2)	6(2)	13(2)	0(1)	4(2)	-2(2)
O(1)	32(2)	16(2)	32(2)	1(2)	-1(2)	-2(2)
O(1A)	21(2)	7(2)	16(2)	-2(1)	-5(2)	1(1)
O(01A)	56(3)	22(2)	24(2)	2(2)	-23(2)	2(2)
O(1B)	24(2)	10(2)	14(2)	-3(1)	2(2)	2(1)
O(01B)	69(4)	8(2)	37(3)	2(2)	-6(2)	1(2)
O(2)	34(3)	18(2)	55(3)	7(2)	-7(2)	-4(2)
O(2A)	28(2)	11(2)	22(2)	-3(1)	-10(2)	2(2)
O(02A)	42(3)	9(2)	34(2)	2(2)	12(2)	2(2)
O(2B)	21(2)	17(2)	18(2)	-4(1)	-1(1)	-1(2)
O(02B)	52(3)	24(2)	16(2)	0(2)	0(2)	-2(2)
O(3A)	33(2)	13(2)	19(2)	4(1)	2(2)	4(2)
O(03A)	24(2)	34(2)	41(2)	-10(2)	12(2)	-1(2)
O(3B)	31(2)	10(2)	32(2)	5(2)	0(2)	0(2)
O(03B)	23(2)	32(2)	36(2)	3(2)	2(2)	8(2)
O(4A)	43(3)	12(2)	22(2)	0(1)	5(2)	9(2)
O(4B)	40(3)	16(2)	38(3)	3(2)	-23(2)	2(2)
O(5A)	32(2)	10(2)	25(2)	1(1)	11(2)	-2(2)
O(5B)	28(2)	12(2)	19(2)	-2(1)	8(2)	-3(2)
Re(1A)	19(1)	5(1)	11(1)	0(1)	-1(1)	1(1)
Re(1B)	21(1)	6(1)	13(1)	0(1)	1(1)	1(1)

Table 18: Bond lengths (Å) for *fac*-[Re(CO)$_3$(QuinH)(H$_2$O)].H$_2$O.

Bond	Distance (Å)	Bond	Distance (Å)
C(1A)-N(1A)	1.330(6)	C(5B)-C(6B)	1.366(8)
C(1A)-C(2A)	1.403(7)	C(5B)-H(5B)	0.93

C(1A)-C(04A)	1.511(7)	C(6A)-C(7A)	1.403(8)
C(01A)-O(01A)	1.150(7)	C(6A)-H(6A)	0.93
C(01A)-Re(1A)	1.909(6)	C(6B)-C(7B)	1.401(7)
C(01B)-O(01B)	1.130(7)	C(6B)-H(6B)	0.93
C(01B)-Re(1B)	1.920(6)	C(7A)-C(8A)	1.373(7)
C(1B)-N(1B)	1.338(6)	C(7A)-H(7A)	0.93
C(1B)-C(2B)	1.398(7)	C(7B)-C(8B)	1.366(7)
C(1B)-C(04B)	1.521(6)	C(7B)-H(7B)	0.93
C(02A)-O(02A)	1.148(6)	C(8A)-C(9A)	1.412(7)
C(02A)-Re(1A)	1.917(5)	C(8A)-H(8A)	0.93
C(2A)-C(3A)	1.363(7)	C(8B)-C(9B)	1.406(7)
C(2A)-H(2A)	0.93	C(8B)-H(8B)	0.93
C(2B)-C(3B)	1.374(7)	C(9A)-N(1A)	1.393(6)
C(2B)-H(2B)	0.93	C(9B)-N(1B)	1.378(6)
C(02B)-O(02B)	1.156(6)	C(10A)-O(3A)	1.212(7)
C(02B)-Re(1B)	1.902(5)	C(10A)-O(4A)	1.310(6)
C(3A)-C(4A)	1.412(7)	C(10B)-O(3B)	1.224(6)
C(3A)-C(10A)	1.499(7)	C(10B)-O(4B)	1.318(7)
C(03A)-O(03A)	1.132(7)	N(1A)-Re(1A)	2.228(4)
C(03A)-Re(1A)	1.926(6)	N(1B)-Re(1B)	2.209(4)
C(3B)-C(4B)	1.425(7)	O(1)-H(1C)	0.85
C(3B)-C(10B)	1.511(7)	O(1)-H(1D)	0.8499
C(03B)-O(03B)	1.158(7)	O(1A)-Re(1A)	2.149(4)
C(03B)-Re(1B)	1.903(6)	O(1B)-Re(1B)	2.142(4)
C(04A)-O(2A)	1.234(6)	O(2)-H(2C)	0.8497
C(04A)-O(1A)	1.270(6)	O(2)-H(2D)	0.8499
C(4A)-C(5A)	1.424(7)	O(4A)-H(4A)	0.82
C(4A)-C(9A)	1.428(6)	O(4B)-H(4B)	0.82
C(4B)-C(9B)	1.411(7)	O(5A)-Re(1A)	2.207(4)
C(4B)-C(5B)	1.431(7)	O(5A)-H(51A)	0.8654
C(04B)-O(2B)	1.221(6)	O(5A)-H(52A)	0.8652
C(04B)-O(1B)	1.306(6)	O(5B)-Re(1B)	2.183(4)
C(5A)-C(6A)	1.364(9)	O(5B)-H(51B)	0.865
C(5A)-H(5A)	0.93	O(5B)-H(52B)	0.8651

Table 19: Bond angles (°) for *fac*-[Re(CO)$_3$(QuinH)(H$_2$O)].H$_2$O.

Bond angle	Angle (°)	Bond angle	Angle (°)
N(1A)-C(1A)-C(2A)	122.9(4)	N(1A)-C(9A)-C(8A)	119.8(4)
N(1A)-C(1A)-C(04A)	116.2(4)	N(1A)-C(9A)-C(4A)	120.9(4)
C(2A)-C(1A)-C(04A)	120.9(4)	C(8A)-C(9A)-C(4A)	119.3(4)
O(01A)-C(01A)-Re(1A)	178.3(6)	N(1B)-C(9B)-C(8B)	119.0(4)
O(01B)-C(01B)-Re(1B)	179.2(6)	N(1B)-C(9B)-C(4B)	121.1(5)
N(1B)-C(1B)-C(2B)	123.3(4)	C(8B)-C(9B)-C(4B)	119.9(4)
N(1B)-C(1B)-C(04B)	116.6(4)	O(3A)-C(10A)-O(4A)	125.3(5)
C(2B)-C(1B)-C(04B)	120.1(4)	O(3A)-C(10A)-C(3A)	120.1(5)
O(02A)-C(02A)-Re(1A)	178.3(5)	O(4A)-C(10A)-C(3A)	114.6(5)
C(3A)-C(2A)-C(1A)	120.3(5)	O(3B)-C(10B)-O(4B)	123.4(5)
C(3A)-C(2A)-H(2A)	119.9	O(3B)-C(10B)-C(3B)	124.9(5)
C(1A)-C(2A)-H(2A)	119.9	O(4B)-C(10B)-C(3B)	111.7(4)
C(3B)-C(2B)-C(1B)	118.7(5)	C(1A)-N(1A)-C(9A)	118.2(4)
C(3B)-C(2B)-H(2B)	120.7	C(1A)-N(1A)-Re(1A)	113.0(3)
C(1B)-C(2B)-H(2B)	120.7	C(9A)-N(1A)-Re(1A)	128.3(3)
O(02B)-C(02B)-Re(1B)	178.6(5)	C(1B)-N(1B)-C(9B)	118.9(4)
C(2A)-C(3A)-C(4A)	119.1(4)	C(1B)-N(1B)-Re(1B)	111.3(3)
C(2A)-C(3A)-C(10A)	117.2(5)	C(9B)-N(1B)-Re(1B)	128.9(3)
C(4A)-C(3A)-C(10A)	123.6(4)	H(1C)-O(1)-H(1D)	109.5
O(03A)-C(03A)-Re(1A)	178.8(5)	C(04A)-O(1A)-Re(1A)	118.2(3)
C(2B)-C(3B)-C(4B)	119.9(4)	C(04B)-O(1B)-Re(1B)	115.0(3)
C(2B)-C(3B)-C(10B)	117.9(5)	H(2C)-O(2)-H(2D)	109.5
C(4B)-C(3B)-C(10B)	122.2(4)	C(10A)-O(4A)-H(4A)	109.5
O(03B)-C(03B)-Re(1B)	176.8(5)	C(10B)-O(4B)-H(4B)	109.5
O(2A)-C(04A)-O(1A)	124.1(5)	Re(1A)-O(5A)-H(51A)	110.4
O(2A)-C(04A)-C(1A)	119.5(4)	Re(1A)-O(5A)-H(52A)	110.1
O(1A)-C(04A)-C(1A)	116.4(4)	H(51A)-O(5A)-H(52A)	108.6
C(3A)-C(4A)-C(5A)	123.6(5)	Re(1B)-O(5B)-H(51B)	110.2
C(3A)-C(4A)-C(9A)	118.3(4)	Re(1B)-O(5B)-H(52B)	110.4
C(5A)-C(4A)-C(9A)	118.1(5)	H(51B)-O(5B)-H(52B)	108.6
C(9B)-C(4B)-C(3B)	118.0(4)	C(01A)-Re(1A)-C(02A)	84.5(2)
C(9B)-C(4B)-C(5B)	118.4(5)	C(01A)-Re(1A)-C(03A)	89.4(2)
C(3B)-C(4B)-C(5B)	123.6(5)	C(02A)-Re(1A)-C(03A)	88.9(2)
O(2B)-C(04B)-O(1B)	124.7(4)	C(01A)-Re(1A)-O(1A)	175.1(2)
O(2B)-C(04B)-C(1B)	120.9(4)	C(02A)-Re(1A)-O(1A)	95.71(18)
O(1B)-C(04B)-C(1B)	114.4(4)	C(03A)-Re(1A)-O(1A)	95.50(19)
C(6A)-C(5A)-C(4A)	121.3(5)	C(01A)-Re(1A)-O(5A)	93.6(2)
C(6A)-C(5A)-H(5A)	119.4	C(02A)-Re(1A)-O(5A)	94.37(18)
C(4A)-C(5A)-H(5A)	119.4	C(03A)-Re(1A)-O(5A)	175.74(19)

C(6B)-C(5B)-C(4B)	120.1(5)	O(1A)-Re(1A)-O(5A)	81.51(15)
C(6B)-C(5B)-H(5B)	120	C(01A)-Re(1A)-N(1A)	104.19(18)
C(4B)-C(5B)-H(5B)	120	C(02A)-Re(1A)-N(1A)	169.73(19)
C(5A)-C(6A)-C(7A)	120.2(5)	C(03A)-Re(1A)-N(1A)	96.55(19)
C(5A)-C(6A)-H(6A)	119.9	O(1A)-Re(1A)-N(1A)	75.17(13)
C(7A)-C(6A)-H(6A)	119.9	O(5A)-Re(1A)-N(1A)	79.78(14)
C(5B)-C(6B)-C(7B)	120.7(5)	C(02B)-Re(1B)-C(03B)	87.5(2)
C(5B)-C(6B)-H(6B)	119.6	C(02B)-Re(1B)-C(01B)	85.1(2)
C(7B)-C(6B)-H(6B)	119.6	C(03B)-Re(1B)-C(01B)	87.6(2)
C(8A)-C(7A)-C(6A)	120.7(5)	C(02B)-Re(1B)-O(1B)	171.2(2)
C(8A)-C(7A)-H(7A)	119.7	C(03B)-Re(1B)-O(1B)	101.26(19)
C(6A)-C(7A)-H(7A)	119.7	C(01B)-Re(1B)-O(1B)	96.46(18)
C(8B)-C(7B)-C(6B)	120.5(5)	C(02B)-Re(1B)-O(5B)	94.3(2)
C(8B)-C(7B)-H(7B)	119.8	C(03B)-Re(1B)-O(5B)	175.16(18)
C(6B)-C(7B)-H(7B)	119.8	C(01B)-Re(1B)-O(5B)	97.0(2)
C(7A)-C(8A)-C(9A)	120.5(5)	O(1B)-Re(1B)-O(5B)	76.88(14)
C(7A)-C(8A)-H(8A)	119.8	C(02B)-Re(1B)-N(1B)	102.35(18)
C(9A)-C(8A)-H(8A)	119.8	C(03B)-Re(1B)-N(1B)	97.43(19)
C(7B)-C(8B)-C(9B)	120.4(5)	C(01B)-Re(1B)-N(1B)	171.16(19)
C(7B)-C(8B)-H(8B)	119.8	O(1B)-Re(1B)-N(1B)	75.46(13)
C(9B)-C(8B)-H(8B)	119.8	O(5B)-Re(1B)-N(1B)	77.80(14)

Table 20: Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for *fac*-[$Re(CO)_3(QuinH)(H_2O)$].H_2O.

	x	y	z	U(eq)
H(2A)	4544	6889	642	18
H(2B)	5378	5438	1581	19
H(5A)	3505	4335	-769	26
H(5B)	6189	8207	3152	25
H(6A)	2789	4544	-1555	28
H(6B)	6811	8108	4114	24
H(7A)	2457	6358	-1817	28
H(7B)	7177	6365	4474	22
H(8A)	2861	7965	-1331	22
H(8B)	6914	4711	3881	18
H(1C)	5385	1495	4856	41
H(1D)	5068	2170	4384	41
H(2C)	5370	559	3118	56
H(2D)	5085	659	3640	56
H(4A)	4523	3569	-78	39
H(4B)	5002	7784	1332	53
H(51A)	4197	9944	-1708	32
H(52A)	4447	9463	-1072	32
H(51B)	5472	2199	3358	29
H(52B)	5555	3350	3562	29

Table 21: Hydrogen bonds for *fac*-[Re(CO)$_3$(QuinH)(H$_2$O)].H$_2$O (Å and °).

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1)-H(1C)...O(1A)[1]	0.85	2.13	2.955(5)	164.5
O(1)-H(1D)...O(2B)[2]	0.85	2.15	2.878(6)	142.8
O(2)-H(2D)...O(5A)[3]	0.85	2.53	2.915(6)	108.3
O(2)-H(2D)...O(2A)[1]	0.85	2.16	2.713(6)	122.9
O(4A)-H(4A)...O(1)[2]	0.82	1.80	2.604(5)	165.3
O(4B)-H(4B)...O(2A)	0.82	1.90	2.632(5)	148.5
O(5A)-H(51A)...O(3B)[4]	0.87	2.00	2.809(5)	154.8
O(5B)-H(51B)...O(2)	0.87	1.78	2.606(6)	158.0
O(5A)-H(52A)...O(2)[5]	0.87	2.53	2.915(6)	107.6
O(5B)-H(52B)...O(3A)[2]	0.87	1.87	2.714(5)	164.3
C(2A)-H(2A)...O(4B)	0.93	2.27	3.162(6)	159.6
C(5A)-H(5A)...O(02A)[6]	0.93	2.38	3.176(6)	144.1
C(5A)-H(5A)...O(02B)[2]	0.93	2.59	3.241(7)	127.2
C(5B)-H(5B)...O(01B)[7]	0.93	2.39	3.064(7)	129.4

[1]-x+1,y-1,-z+1/2 [2] -x+1,y,-z+1/2 [3]x,-y+1,z+1/2 [4] -x+1,-y+2,-z [5]x,-y+1,z-1/2 [6]x,y-1,z [7]x,y+1,z

Table 22: Observed π-π interaction and distance in the structure of *fac*-[Re(CO)$_3$(QuinH)(H$_2$O)].H$_2$O.

π-π interaction	Distance (Å)
Ring 1 – Ring 2[1]	3.766(3)

[1]1/2-x,3/2-y,-z

Table 23: Atomic coordinates (×10⁴) and equivalent isotropic displacement parameters (Å²×10³) for [Re(CO)₂(Trop)(PPh₃)₂]. 2C₇H₈. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(01)	2965(3)	6507(2)	3003.3(18)	16.9(6)
C(1)	6633(3)	6898(2)	2986.7(18)	16.6(6)
C(2)	7707(3)	6275(2)	3289(2)	23.4(6)
C(02)	2664(3)	8382(2)	2209.2(17)	16.2(5)
C(3)	8922(3)	6468(3)	3142(2)	28.6(7)
C(4)	9433(3)	7337(3)	2657(2)	30.7(8)
C(5)	8810(3)	8244(3)	2224(2)	28.7(7)
C(6)	7545(3)	8517(2)	2177(2)	25.4(7)
C(7)	6547(3)	7959(2)	2495.2(18)	17.0(6)
C(11)	6350(3)	7886.5(19)	601.3(17)	14.5(5)
C(12)	6172(3)	8904(2)	407.9(18)	18.8(6)
C(13)	7171(3)	9441(2)	-59.8(19)	23.1(6)
C(14)	8367(3)	8973(2)	-344(2)	25.3(7)
C(15)	8559(3)	7971(2)	-148(2)	23.1(6)
C(16)	7554(3)	7427(2)	323.5(19)	18.2(6)
C(21)	5558(2)	5973.9(19)	1268.7(18)	15.0(5)
C(22)	5753(3)	5235(2)	2070.6(19)	20.3(6)
C(23)	6234(3)	4280(2)	2102(2)	25.8(7)
C(24)	6522(3)	4048(2)	1343(2)	23.4(6)
C(25)	6316(3)	4771(2)	542(2)	22.9(6)
C(26)	5825(3)	5725(2)	508.2(19)	20.4(6)
C(31)	3962(3)	7702.5(19)	424.1(17)	15.4(5)
C(32)	4414(3)	8204(2)	-486.0(18)	20.8(6)
C(33)	3612(3)	8537(2)	-1075(2)	25.8(7)
C(34)	2355(3)	8380(2)	-768(2)	28.4(7)
C(35)	1900(3)	7888(2)	132(2)	28.7(7)
C(36)	2699(3)	7545(2)	723.1(19)	21.8(6)
C(41)	1791(3)	7285(2)	4786.4(18)	16.2(5)
C(42)	770(3)	7384(2)	4418(2)	25.1(7)
C(43)	-326(3)	6986(3)	4956(2)	33.4(8)
C(44)	-414(3)	6480(3)	5869(2)	31.6(8)
C(45)	574(3)	6400(3)	6237(2)	30.0(7)
C(46)	1671(3)	6800(2)	5702.3(19)	23.7(6)
C(51)	2803(3)	9102(2)	3918.0(19)	16.9(6)
C(52)	1965(3)	9413(2)	4599(2)	24.6(6)
C(53)	1660(3)	10406(2)	4485(2)	29.5(7)
C(54)	2183(3)	11097(2)	3699(2)	29.3(7)
C(55)	3021(3)	10801(2)	3021(2)	31.0(8)
C(56)	3324(3)	9812(2)	3125(2)	24.0(6)
C(61)	4360(3)	7315(2)	4756.8(17)	16.4(5)
C(62)	4941(3)	7902(2)	4945(2)	27.7(7)
C(63)	5883(3)	7481(3)	5439(2)	38.0(8)
C(64)	6233(3)	6473(3)	5737(2)	35.3(8)
C(65)	5652(3)	5880(2)	5560(2)	28.8(7)
C(66)	4730(3)	6300(2)	5068.3(19)	22.8(6)
O(01)	2323.8(19)	5902.8(15)	3203.6(14)	23.2(4)
O(02)	1797.6(19)	8922.9(15)	1954.5(14)	23.3(4)
O(03)	5437.2(17)	8387.4(13)	2345.7(12)	15.9(4)
O(04)	5623.0(17)	6520.2(13)	3160.5(12)	15.7(4)

P(1)	4974.7(6)	7237.2(5)	1234.9(4)	12.51(13)
P(2)	3220.2(6)	7801.5(5)	4045.5(4)	13.11(13)
Re(1)	4015.7(2)	7470.9(2)	2659.9(2)	11.29(3)
C(1R)	-1490(3)	12044(2)	2691(2)	29.5(7)
C(6R)	-2583(3)	11617(2)	3054(2)	27.2(7)
C(5R)	-2553(3)	10612(3)	3322(2)	31.1(7)
C(2R)	-328(3)	11472(3)	2593(2)	37.4(8)
C(4R)	-1357(4)	10046(3)	3211(2)	39.0(9)
C(3R)	-256(4)	10478(3)	2851(3)	42.1(9)
C(7R)	-3737(5)	10146(4)	3745(3)	57.4(12)
C(4S)	1487(9)	3659(9)	1455(6)	22(2)
C(6S)	1266(12)	5130(14)	1712(11)	39(4)
C(3S)	345(7)	4002(4)	1175(3)	29.3(15)
C(7S)	3199(10)	3850(9)	2012(7)	51(3)
C(5S)	1964(6)	4231(5)	1718(3)	33.5(17)
C(1S)	145(10)	5483(5)	1438(5)	42(2)
C(2S)	-333(7)	4908(6)	1160(4)	35.5(17)
C(1T)	2754(9)	4451(7)	1972(6)	30(2)
C(3T)	2268(9)	3257(6)	1551(5)	25.0(19)
C(5T)	845(7)	4762(6)	1438(4)	24(2)
C(2T)	3068(11)	3543(8)	1868(7)	29(3)
C(7T)	-339(13)	5391(10)	1215(8)	43(3)
C(4T)	1154(12)	3841(13)	1330(8)	19(3)
C(6T)	1656(16)	5065(15)	1756(14)	22(3)

Table 24: Anisotropic Displacement Parameters ($Å^2×10^3$) for $[Re(CO)_2(Trop)(PPh_3)_2]$ $.2C_7H_8$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(01)	17.9(14)	15.5(13)	13.5(13)	-3.8(10)	-5.1(11)	3.9(11)
C(1)	15.6(13)	22.7(14)	14.8(13)	-11.6(11)	-2.6(10)	-1.0(11)
C(2)	21.8(15)	25.5(15)	24.2(15)	-10.7(13)	-10.4(12)	4.1(12)
C(02)	18.2(14)	17.3(13)	12.1(12)	-6.1(10)	1.5(10)	-5.2(11)
C(3)	18.1(15)	40.2(19)	33.3(18)	-21.1(15)	-11.6(13)	6.9(14)
C(4)	14.0(14)	49(2)	38.4(19)	-26.8(17)	-8.5(13)	1.3(14)
C(5)	22.2(16)	40.5(19)	30.5(17)	-19.2(15)	-1.5(13)	-10.8(14)
C(6)	24.3(16)	30.8(17)	24.2(15)	-12.4(13)	-5.2(13)	-5.2(13)
C(7)	13.2(13)	24.1(14)	16.4(13)	-11.7(11)	-1.9(10)	-1.5(11)
C(11)	17.8(13)	14.5(13)	10.3(12)	-2.8(10)	-3.4(10)	-3(1)
C(12)	19.8(14)	16.1(13)	15.8(13)	-4.1(11)	-1.7(11)	-0.3(11)
C(13)	27.7(16)	15.9(14)	20.4(14)	-2.1(11)	-2.3(12)	-5.3(12)
C(14)	22.9(15)	25.8(16)	25.5(16)	-6.2(13)	-0.3(12)	-11.6(13)
C(15)	12.5(13)	27.8(16)	29.6(16)	-14.9(13)	-0.1(12)	-1.1(12)
C(16)	17.2(14)	18.1(14)	20.4(14)	-8.7(11)	-4.1(11)	-0.9(11)
C(21)	13.6(13)	13.5(12)	16.6(13)	-5.1(10)	-3(1)	-0.8(10)
C(22)	28.8(16)	16.3(13)	15.2(13)	-6.9(11)	-8.2(12)	4.1(12)
C(23)	36.9(18)	15.0(14)	23.2(15)	-5.6(12)	-13.3(13)	6.9(13)
C(24)	25.6(16)	16.9(14)	27.6(16)	-10.6(12)	-6.2(13)	2.0(12)
C(25)	27.1(16)	22.8(15)	20.0(14)	-12.7(12)	-1.1(12)	-2.2(12)
C(26)	26.1(15)	16.7(14)	16.2(13)	-5.4(11)	-2.1(12)	-3.4(12)
C(31)	20.6(14)	12.3(12)	14.5(13)	-6.6(10)	-7.2(11)	2.7(10)
C(32)	22.6(15)	23.9(15)	14.0(13)	-6.7(11)	-4.4(11)	0.5(12)
C(33)	34.9(18)	24.2(15)	15.5(14)	-5.2(12)	-8.9(13)	1.5(13)
C(34)	34.2(18)	31.5(17)	26.1(16)	-13.2(14)	-18.5(14)	4.1(14)

C(35)	23.2(16)	38.0(18)	29.7(17)	-12.8(14)	-10.3(13)	-5.7(14)
C(36)	23.6(15)	25.9(15)	17.1(14)	-6.9(12)	-5.5(12)	-6.0(12)
C(41)	14.2(13)	19.4(13)	13.9(13)	-8.4(11)	1.8(10)	-2.4(11)
C(42)	17.3(14)	39.9(18)	16.5(14)	-10.6(13)	-1.5(11)	-3.1(13)
C(43)	16.6(15)	63(2)	25.1(17)	-20.2(16)	-0.6(13)	-11.1(15)
C(44)	21.4(16)	48(2)	22.9(16)	-12.6(15)	6.1(13)	-14.8(15)
C(45)	25.0(16)	41.8(19)	16.7(15)	-4.6(14)	2.6(12)	-12.6(14)
C(46)	21.5(15)	34.1(17)	15.7(14)	-8.2(12)	-3.0(12)	-6.6(13)
C(51)	14.4(13)	18.6(13)	20.4(14)	-9.9(11)	-6.1(11)	1.1(11)
C(52)	28.0(16)	23.4(15)	20.2(15)	-9.1(12)	-5.5(12)	2.2(13)
C(53)	32.4(18)	28.6(17)	29.7(17)	-18.2(14)	-6.8(14)	5.6(14)
C(54)	32.0(18)	19.4(15)	40.4(19)	-16.2(14)	-11.5(15)	3.7(13)
C(55)	30.5(18)	18.8(15)	36.6(18)	-8.6(14)	3.6(14)	-6.7(13)
C(56)	19.4(15)	22.2(15)	26.6(16)	-11.9(13)	5.7(12)	-4.0(12)
C(61)	14.2(13)	23.3(14)	10.3(12)	-5.2(11)	-2.6(10)	-2.0(11)
C(62)	24.5(16)	29.8(17)	29.4(17)	-5.2(14)	-10.6(13)	-8.6(13)
C(63)	32.4(19)	47(2)	41(2)	-9.4(17)	-19.0(16)	-14.2(17)
C(64)	24.1(17)	51(2)	26.1(17)	-4.9(16)	-12.7(14)	-2.4(15)
C(65)	28.2(17)	30.8(17)	19.5(15)	-4.1(13)	-7.5(13)	4.3(14)
C(66)	23.6(15)	25.4(15)	19.8(14)	-9.1(12)	-7.4(12)	1.1(12)
O(01)	22.6(11)	18.9(10)	27.5(11)	-4.2(9)	-7.7(9)	-6.2(9)
O(02)	17.8(10)	21.9(10)	24.6(11)	-5.2(9)	-7.4(9)	5.4(8)
O(03)	13.5(9)	17.0(9)	17.2(9)	-7.4(8)	-1.6(7)	-2.3(7)
O(04)	14.8(9)	15.6(9)	17.1(9)	-6.4(8)	-6.2(8)	1.6(7)
P(1)	13.3(3)	12.1(3)	10.3(3)	-3.2(2)	-2.5(2)	0.0(3)
P(2)	12.3(3)	14.9(3)	11.5(3)	-4.8(3)	-2.0(3)	-1.2(3)
Re(1)	11.04(5)	11.58(5)	9.36(5)	-2.84(4)	-1.85(4)	-0.29(4)
C(1R)	35.1(18)	25.7(16)	28.0(17)	-9.2(13)	-8.8(14)	-3.5(14)
C(6R)	29.5(17)	26.1(16)	24.9(16)	-10.6(13)	-7.6(13)	2.5(13)
C(5R)	43(2)	36.8(19)	17.3(15)	-6.9(13)	-5.7(14)	-17.3(16)
C(2R)	27.9(18)	47(2)	34.6(19)	-14.3(17)	-3.4(15)	-6.0(16)
C(4R)	64(3)	21.9(17)	30.2(18)	-9.6(14)	-14.2(18)	0.7(17)
C(3R)	38(2)	42(2)	40(2)	-20.5(18)	-8.1(17)	14.6(17)
C(7R)	69(3)	66(3)	43(2)	-14(2)	-3(2)	-41(3)
C(4S)	20(6)	29(6)	19(4)	-8(3)	-6(3)	-6(5)
C(6S)	54(9)	46(6)	23(4)	-14(4)	6(6)	-34(7)
C(3S)	41(4)	26(3)	23(3)	-10(2)	-6(3)	-8(3)
C(7S)	44(5)	81(10)	33(5)	-23(6)	5(4)	-29(6)
C(5S)	38(3)	48(4)	14(3)	-7(2)	5(2)	-23(3)
C(1S)	82(7)	21(3)	20(3)	-10(3)	-1(4)	-9(4)
C(2S)	50(4)	34(4)	16(3)	-8(3)	-3(3)	-3(4)
C(1T)	33(5)	37(5)	18(4)	-3(4)	-1(4)	-19(4)
C(3T)	32(5)	23(4)	22(4)	-9(3)	-4(3)	-10(4)
C(5T)	27(4)	25(4)	13(3)	-1(3)	1(3)	-6(3)
C(2T)	25(5)	32(6)	19(5)	-4(4)	4(4)	-4(4)
C(7T)	55(7)	38(7)	40(7)	-21(6)	-16(5)	6(6)
C(4T)	12(6)	27(7)	17(5)	-5(4)	-9(4)	1(5)
C(6T)	34(8)	18(5)	17(5)	-8(4)	6(5)	-19(6)

Table 25: Bond Lengths (Å) for $[Re(CO)_2(Trop)(PPh_3)_2].2C_7H_8$.

Bond	Distance (Å)	Bond	Distance (Å)
C(01)-O(01)	1.171(3)	C(45)-C(46)	1.389(4)
C(01)-Re(1)	1.883(3)	C(51)-C(52)	1.401(4)
C(1)-C(2)	1.415(4)	C(51)-C(56)	1.394(4)
C(1)-C(7)	1.463(4)	C(51)-P(2)	1.830(3)
C(1)-O(04)	1.287(3)	C(52)-C(53)	1.389(4)
C(2)-C(3)	1.383(4)	C(53)-C(54)	1.374(5)
C(02)-O(02)	1.166(3)	C(54)-C(55)	1.387(4)
C(02)-Re(1)	1.887(3)	C(55)-C(56)	1.389(4)
C(3)-C(4)	1.385(5)	C(61)-C(62)	1.382(4)
C(4)-C(5)	1.381(5)	C(61)-C(66)	1.395(4)
C(5)-C(6)	1.386(4)	C(61)-P(2)	1.823(3)
C(6)-C(7)	1.401(4)	C(62)-C(63)	1.402(5)
C(7)-O(03)	1.295(3)	C(63)-C(64)	1.382(5)
C(11)-C(12)	1.402(4)	C(64)-C(65)	1.378(5)
C(11)-C(16)	1.387(4)	C(65)-C(66)	1.381(4)
C(11)-P(1)	1.830(3)	O(03)-Re(1)	2.1578(19)
C(12)-C(13)	1.383(4)	O(04)-Re(1)	2.1548(18)
C(13)-C(14)	1.389(4)	P(1)-Re(1)	2.4302(8)
C(14)-C(15)	1.378(4)	P(2)-Re(1)	2.4239(8)
C(15)-C(16)	1.394(4)	C(1R)-C(6R)	1.373(5)
C(21)-C(22)	1.395(4)	C(1R)-C(2R)	1.373(5)
C(21)-C(26)	1.394(4)	C(6R)-C(5R)	1.383(5)
C(2)-P(1)	1.830(3)	C(5R)-C(4R)	1.400(5)
C(22)-C(23)	1.386(4)	C(5R)-C(7R)	1.492(5)
C(23)-C(24)	1.376(4)	C(2R)-C(3R)	1.364(5)
C(24)-C(25)	1.388(4)	C(4R)-C(3R)	1.386(6)
C(25)-C(26)	1.386(4)	C(4S)-C(3S)	1.396(9)
C(31)-C(32)	1.396(4)	C(4S)-C(5S)	1.369(15)
C(31)-C(36)	1.390(4)	C(6S)-C(5S)	1.381(19)
C(31)-P(1)	1.837(3)	C(6S)-C(1S)	1.371(17)
C(32)-C(33)	1.391(4)	C(3S)-C(2S)	1.378(10)
C(33)-C(34)	1.383(5)	C(7S)-C(5S)	1.503(11)
C(34)-C(35)	1.380(5)	C(1S)-C(2S)	1.390(11)
C(35)-C(36)	1.391(4)	C(1T)-C(2T)	1.388(14)
C(41)-C(42)	1.400(4)	C(1T)-C(6T)	1.39(2)
C(41)-C(46)	1.389(4)	C(3T)-C(2T)	1.381(14)
C(41)-P(2)	1.824(3)	C(3T)-C(7T)	1.391(12)
C(42)-C(43)	1.387(4)	C(5T)-C(7T)	1.476(15)
C(43)-C(44)	1.392(5)	C(5T)-C(4T)	1.41(2)
C(44)-C(45)	1.373(5)	C(5T)-C(6T)	1.41(2)

Table 26: Bond Angles for $[Re(CO)_2(Trop)(PPh_3)_2].2C_7H_8$.

Bond angle	Angle (°)	Bond angle	Angle (°)
O(01)-C(01)-Re(1)	178.8(2)	C(64)-C(63)-C(62)	119.6(3)
C(2)-C(1)-C(7)	125.8(3)	C(65)-C(64)-C(63)	120.4(3)
O(04)-C(1)-C(2)	118.5(3)	C(64)-C(65)-C(66)	119.7(3)
O(04)-C(1)-C(7)	115.6(2)	C(65)-C(66)-C(61)	121.1(3)
C(3)-C(2)-C(1)	130.5(3)	C(7)-O(03)-Re(1)	117.92(17)
O(02)-C(02)-Re(1)	177.5(2)	C(1)-O(04)-Re(1)	118.03(17)
C(2)-C(3)-C(4)	129.7(3)	C(11)-P(1)-C(31)	102.13(12)
C(5)-C(4)-C(3)	127.3(3)	C(11)-P(1)-Re(1)	112.99(9)
C(4)-C(5)-C(6)	129.4(3)	C(21)-P(1)-C(11)	104.07(12)
C(5)-C(6)-C(7)	131.0(3)	C(21)-P(1)-C(31)	102.79(12)
C(6)-C(7)-C(1)	125.8(3)	C(21)-P(1)-Re(1)	117.06(9)
O(03)-C(7)-C(1)	114.8(2)	C(31)-P(1)-Re(1)	115.97(9)
O(03)-C(7)-C(6)	119.4(3)	C(41)-P(2)-C(51)	102.84(12)
C(12)-C(11)-P(1)	117.5(2)	C(41)-P(2)-Re(1)	116.50(9)
C(16)-C(11)-C(12)	118.7(3)	C(51)-P(2)-Re(1)	115.40(9)
C(16)-C(11)-P(1)	123.8(2)	C(61)-P(2)-C(41)	103.32(13)
C(13)-C(12)-C(11)	120.8(3)	C(61)-P(2)-C(51)	104.59(13)
C(12)-C(13)-C(14)	119.9(3)	C(61)-P(2)-Re(1)	112.69(9)
C(15)-C(14)-C(13)	119.9(3)	C(01)-Re(1)-C(02)	85.97(12)
C(14)-C(15)-C(16)	120.4(3)	C(01)-Re(1)-O(03)	171.09(9)
C(11)-C(16)-C(15)	120.4(3)	C(01)-Re(1)-O(04)	98.15(9)
C(22)-C(21)-P(1)	119.7(2)	C(01)-Re(1)-P(1)	90.99(8)
C(26)-C(21)-C(22)	118.5(2)	C(01)-Re(1)-P(2)	94.55(8)
C(26)-C(21)-P(1)	121.7(2)	C(02)-Re(1)-O(03)	102.93(10)
C(23)-C(22)-C(21)	120.5(3)	C(02)-Re(1)-O(04)	175.80(10)
C(24)-C(23)-C(22)	120.4(3)	C(02)-Re(1)-P(1)	92.13(8)
C(23)-C(24)-C(25)	119.8(3)	C(02)-Re(1)-P(2)	89.25(8)
C(26)-C(25)-C(24)	120.0(3)	O(03)-Re(1)-P(1)	88.27(5)
C(25)-C(26)-C(21)	120.7(3)	O(03)-Re(1)-P(2)	86.10(5)
C(32)-C(31)-P(1)	122.5(2)	O(04)-Re(1)-O(03)	72.96(7)
C(36)-C(31)-C(32)	118.5(3)	O(04)-Re(1)-P(1)	88.63(5)
C(36)-C(31)-P(1)	119.0(2)	O(04)-Re(1)-P(2)	89.61(5)
C(33)-C(32)-C(31)	120.3(3)	P(2)-Re(1)-P(1)	174.38(2)
C(34)-C(33)-C(32)	120.6(3)	C(2R)-C(1R)-C(6R)	120.1(3)
C(35)-C(34)-C(33)	119.4(3)	C(1R)-C(6R)-C(5R)	121.7(3)
C(34)-C(35)-C(36)	120.3(3)	C(6R)-C(5R)-C(4R)	117.0(3)
C(31)-C(36)-C(35)	120.9(3)	C(6R)-C(5R)-C(7R)	121.7(4)
C(42)-C(41)-P(2)	118.7(2)	C(4R)-C(5R)-C(7R)	121.2(4)
C(46)-C(41)-C(42)	118.6(3)	C(3R)-C(2R)-C(1R)	120.1(4)
C(46)-C(41)-P(2)	122.7(2)	C(3R)-C(4R)-C(5R)	121.1(3)
C(43)-C(42)-C(41)	120.5(3)	C(2R)-C(3R)-C(4R)	119.9(3)
C(42)-C(43)-C(44)	120.0(3)	C(5S)-C(4S)-C(3S)	119.9(10)
C(45)-C(44)-C(43)	119.7(3)	C(1S)-C(6S)-C(5S)	123.4(14)
C(44)-C(45)-C(46)	120.5(3)	C(2S)-C(3S)-C(4S)	121.8(8)
C(41)-C(46)-C(45)	120.6(3)	C(4S)-C(5S)-C(6S)	117.7(9)
C(52)-C(51)-P(2)	121.8(2)	C(4S)-C(5S)-C(7S)	119.0(8)
C(56)-C(51)-C(52)	118.4(3)	C(6S)-C(5S)-C(7S)	123.3(9)
C(56)-C(51)-P(2)	119.8(2)	C(6S)-C(1S)-C(2S)	118.9(10)
C(53)-C(52)-C(51)	120.7(3)	C(3S)-C(2S)-C(1S)	118.2(7)
C(54)-C(53)-C(52)	120.2(3)	C(6T)-C(1T)-C(2T)	120.4(12)

C(53)-C(54)-C(55)	119.8(3)	C(2T)-C(3T)-C(7T)	122.8(12)
C(54)-C(55)-C(56)	120.5(3)	C(4T)-C(5T)-C(7T)	118.6(10)
C(55)-C(56)-C(51)	120.4(3)	C(4T)-C(5T)-C(6T)	120.1(12)
C(62)-C(61)-C(66)	118.8(3)	C(6T)-C(5T)-C(7T)	121.3(11)
C(62)-C(61)-P(2)	123.4(2)	C(3T)-C(2T)-C(1T)	119.0(10)
C(66)-C(61)-P(2)	117.6(2)	C(3T)-C(4T)-C(5T)	117.6(14)
C(61)-C(62)-C(63)	120.4(3)	C(1T)-C(6T)-C(5T)	119.9(17)

Table 27: Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for [Re(CO)$_2$(Trop)(PPh$_3$)$_2$].2C$_7$H$_8$.

	x	y	z	U(eq)
H(2)	7574.67	5631.26	3643.43	28
H(3)	9480.13	5935.17	3410.09	34
H(4)	10291.21	7306.32	2617	37
H(5)	9313.68	8744.17	1920.58	34
H(6)	7320.64	9184.88	1884.84	30
H(12)	5372.06	9220.42	596.41	23
H(13)	7041.37	10115.83	-183.7	28
H(14)	9037.4	9333.97	-666.2	30
H(15)	9362.66	7656.8	-332.1	28
H(16)	7691.76	6751.03	452.85	22
H(22)	5559.09	5383.47	2588.31	24
H(23)	6361.77	3793.22	2640.42	31
H(24)	6854.03	3407.73	1365.64	28
H(25)	6507.39	4615.95	27.55	27
H(26)	5672.69	6204.38	-27.15	24
H(32)	5256.31	8316.56	-699.95	25
H(33)	3922.73	8868.61	-1680.13	31
H(34)	1822.3	8604.25	-1163.65	34
H(35)	1054.9	7783.89	343.38	34
H(36)	2384.56	7207.28	1326.53	26
H(42)	826.12	7718.7	3808.11	30
H(43)	-1002.24	7058.08	4707.52	40
H(44)	-1138.46	6197.93	6228.56	38
H(45)	507.46	6074.61	6849.27	36
H(46)	2332.13	6741.98	5960.06	28
H(52)	1609.58	8950.05	5133.93	29
H(53)	1100.09	10602.56	4941.1	35
H(54)	1974.54	11761.41	3622.77	35
H(55)	3382.06	11269.14	2492.06	37
H(56)	3878.8	9622.06	2662.64	29
H(62)	4704.7	8579.83	4742.37	33
H(63)	6270.73	7877.45	5565.99	46
H(64)	6864.86	6192.78	6059.3	42
H(65)	5879.38	5201.79	5770.83	35
H(66)	4348.08	5898.63	4942.43	27
H(1R)	-1538.09	12721.61	2512.7	35
H(6R)	-3362.59	12013.36	3119.79	33
H(2R)	410.2	11761.93	2350.15	45
H(4R)	-1300.08	9368.33	3381.1	47
H(3R)	531.65	10090.53	2784.75	51
H(7RA)	-4460.64	10640.67	3639.31	86

H(7RB)	-3800.44	9827.36	4377.54	86
H(7RC)	-3711.56	9668.72	3488.81	86
H(4S)	1921.7	3042.22	1463.6	26
H(6S)	1572.16	5516.63	1904.24	47
H(3S)	32.86	3608.75	994.35	35
H(7SA)	3410.16	4328.53	2175.32	77
H(7SB)	3115.3	3249.22	2519.42	77
H(7SC)	3858.54	3727.23	1530.76	77
H(1S)	-289.81	6096.87	1438.09	51
H(2S)	-1089.67	5128.43	968.17	43
H(1T)	3283.65	4649.51	2187.94	36
H(3T)	2483.64	2647.31	1483.54	30
H(2T)	3806.3	3132.48	2009	35
H(7TA)	-425.47	5990.5	1320.53	65
H(7TB)	-311.61	5539.3	596.76	65
H(7TC)	-1050.95	5051.52	1584.52	65
H(4T)	630.65	3631.97	1117.83	22
H(6T)	1455.92	5675.42	1821.76	27

Table 28: Atomic Occupancy for $[Re(CO)_2(Trop)(PPh_3)_2].2C_7H_8$.

Atom	Occupancy	Atom	Occupancy	Atom	Occupancy
C(4S)	0.586(7)	H(4S)	0.586(7)	C(6S)	0.586(7)
H(6S)	0.586(7)	C(3S)	0.586(7)	H(3S)	0.586(7)
C(7S)	0.586(7)	H(7SA)	0.586(7)	H(7SB)	0.586(7)
H(7SC)	0.586(7)	C(5S)	0.586(7)	C(1S)	0.586(7)
H(1S)	0.586(7)	C(2S)	0.586(7)	H(2S)	0.586(7)
C(1T)	0.414(7)	H(1T)	0.414(7)	C(3T)	0.414(7)
H(3T)	0.414(7)	C(5T)	0.414(7)	C(2T)	0.414(7)
H(2T)	0.414(7)	C(7T)	0.414(7)	H(7TA)	0.414(7)
H(7TB)	0.414(7)	H(7TC)	0.414(7)	C(4T)	0.414(7)
H(4T)	0.414(7)	C(6T)	0.414(7)	H(6T)	0.414(7)

Table 29: Observed π-π interactions and distances in the structure of $[Re(CO)_2(Trop)(PPh_3)_2].2C_7H_8$.

π-π interaction	Distance (Å)
Ring 1 – Ring 2	3.8726(18)

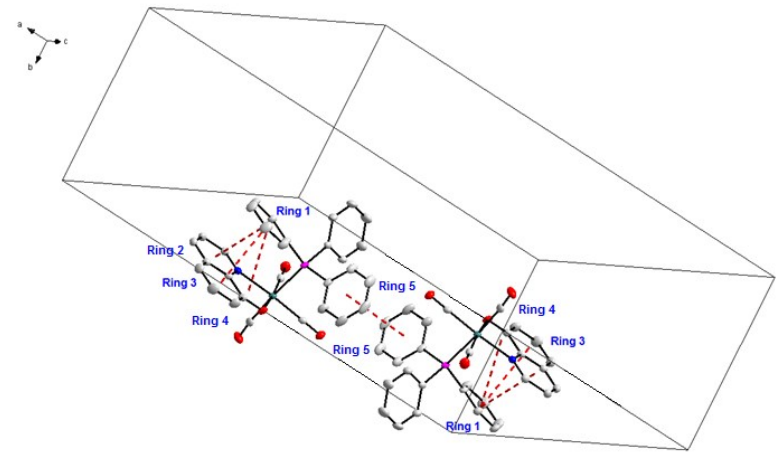

Figure 1: Observed π-π interactions in the structure of *fac*-[Re(CO)$_3$(Quin)(PPh$_3$)].

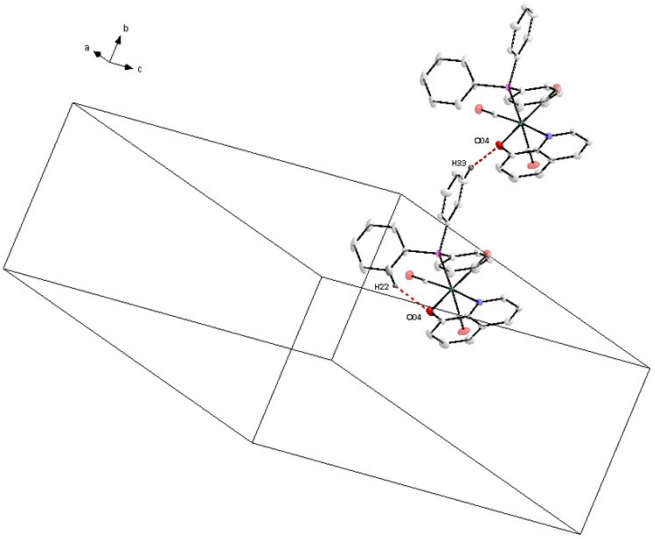

Figure 2: Intermolecular hydrogen interactions in the structure of *fac*-[Re(CO)$_3$(Quin)(PPh$_3$)].

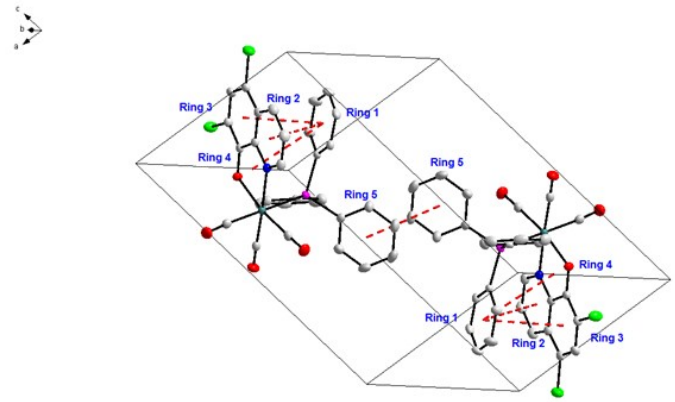

Figure 3: Observed π-π interactions in the structure of *fac*-[Re(CO)$_3$(diCl-Quin)(PPh$_3$)].

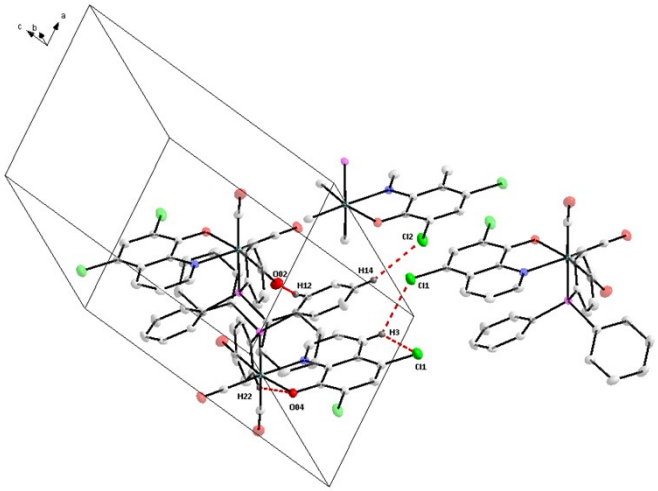

Figure 4: Hydrogen interactions observed in the crystal structure of *fac*-[Re(CO)$_3$(diCl-Quin)(PPh$_3$)].

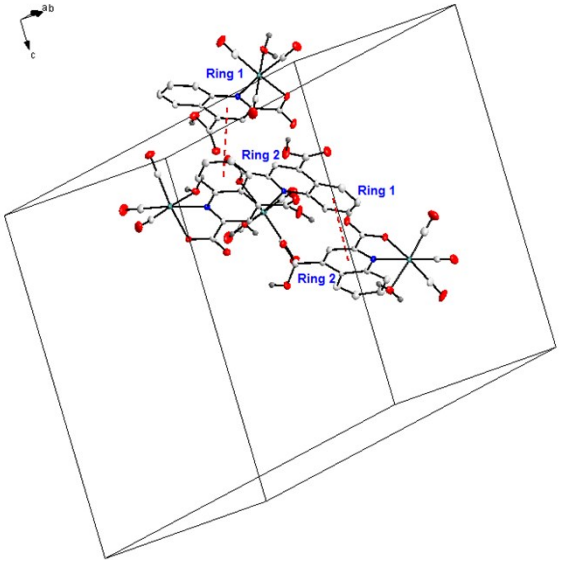

Figure 5: Observed π-π interactions in the structure of *fac*-[Re(CO)$_3$(QuinH)(H$_2$O)].H$_2$O.

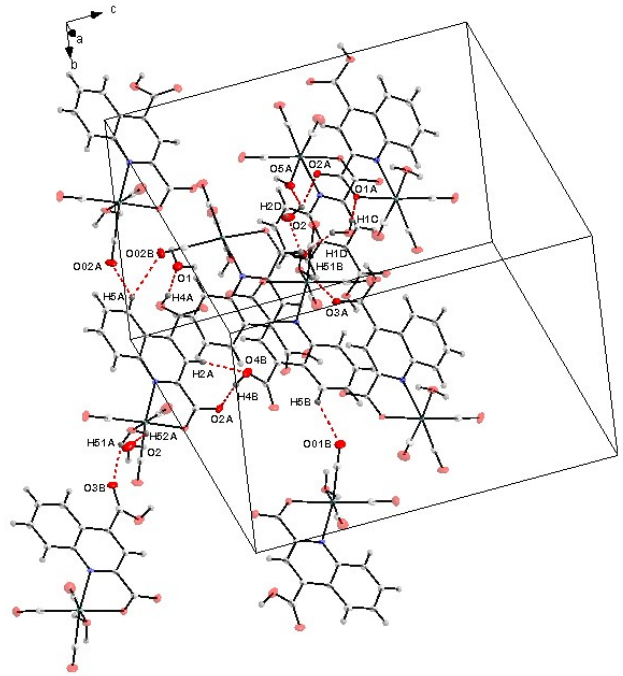

Figure 6: Hydrogen interactions observed in the structure of *fac*-[Re(CO)$_3$(QuinH)(H$_2$O)].H$_2$O.

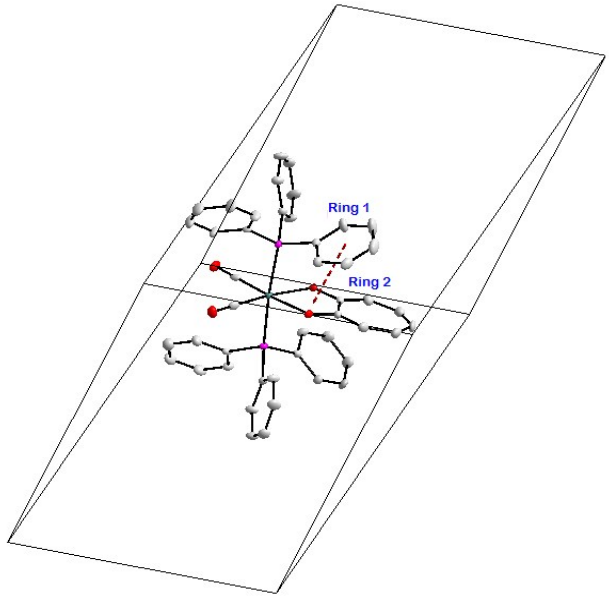

Figure 7: Observed π-π interactions in the structure of [Re(CO)$_2$(Trop)(PPh$_3$)$_2$].2C$_7$H$_8$.