Crystal structures of 1-2-(dicyclohexylphosphinophenyl)pyrol-2-dicyclohexylphosphino-rhodium(I) norborna-2,5-diene tetrafluoroborate tetrahydrofuran hemisolvate, $[Rh(C_{34}H_{51}NP_2)(C_7H_8)]\,[BF_4]\cdot 0.5C_4H_8O$, and 1-2-(dicyclohexylphosphinophenyl)-pyrol-2-dicyclohexylphosphino-rhodium(I) (Z,Z)-cycloocta...

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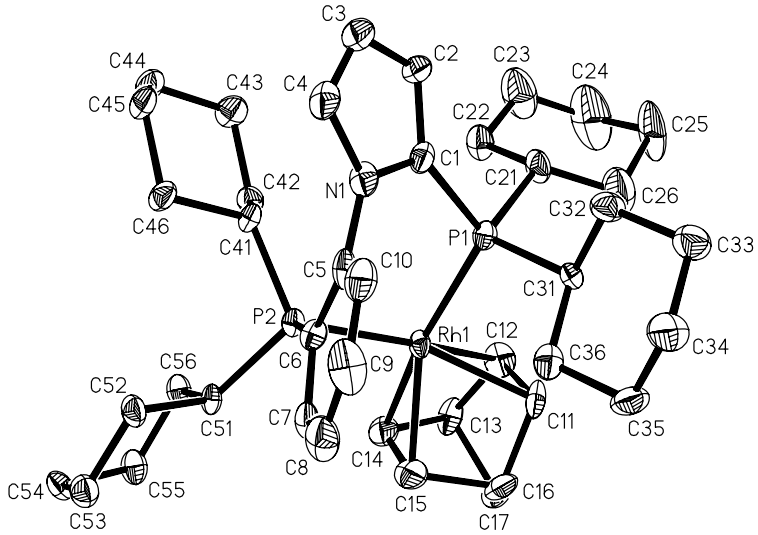

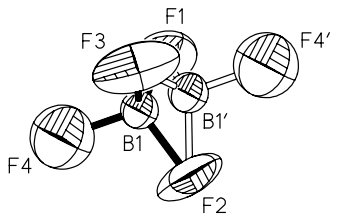

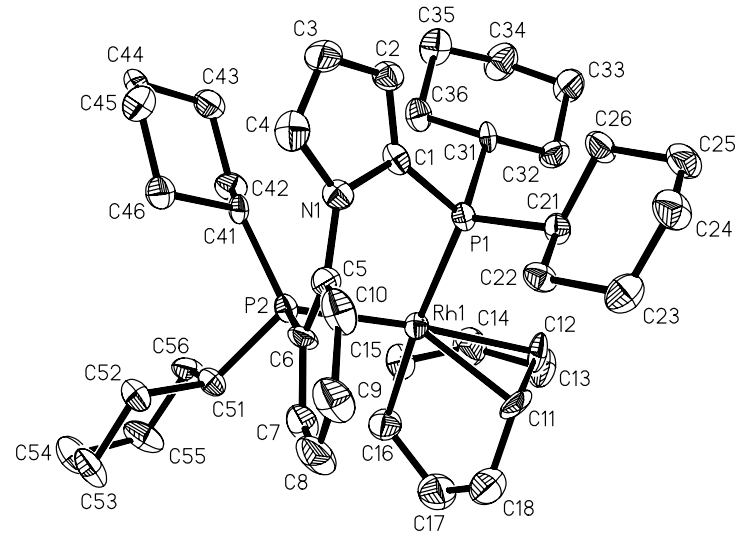

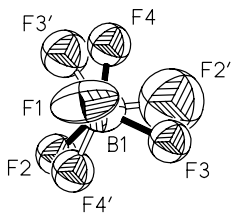

Abstract

$C_{43}H_{63}BF_4NO_{0.50}P_2Rh$, monoclinic, $P12_1/n1$ (no. 14), a = 10.341(2) Å, b = 16.063(3) Å, c = 27.425(5) Å, β = 98.76(3)°, V = 4502.4 Å^3, Z = 4, $R_{gt}(F)$ = 0.060, $wR_{ref}(F^2)$ = 0.143, T = 200 K.

$C_{42}H_{63}BF_4NP_2Rh$, monoclinic, $P12_1/c1$ (no. 14), a = 10.503(2) Å, b = 17.665(4) Å, c = 21.946(4) Å, β = 101.95(3)°, V = 3983.5 Å^3, Z = 4, $R_{gt}(F)$ = 0.045, $wR_{ref}(F^2)$ = 0.073, T = 200 K.

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Source of material
Standard procedures were performed according [1]. The ligand is commercially available.

Experimental details
The small $2\theta_{max}$ values are caused by the limits of the diffractometer system and resulted in small N_{gt}/N_{param} ratios.

Discussion
Unexpected differences between the title compounds in the catalytic hydrogenation of the diolefines norborna-2,5-diene (NBD) and (*Z*,*Z*)-cycloocta-1,5-diene (COD; cp. [2]) motivated us to determine the crystal structures. The ratio of the rate constants for the hydrogenation of the diolefine complexes is approximately 630 [2].
It is well known that the double bonds of the diolefines are not coordinated perpendicular to the P,Rh,P plane. The dihedral angle between the planes P,Rh,P and *X*,Rh,*X* (*X* = centroid of the double bond) is in the case of the NBD-complex 11.8° and for the COD-complex 30.7°.

1. 1-(2-(Dicyclohexylphosphinophenyl)pyrol-2-dicyclohexylphosphino-rhodium(I) norborna-2,5-diene tetrafluoroborate tetrahydrofuran hemisolvate, $[Rh(C_{34}H_{51}NP_2)(C_7H_8)][BF_4] \cdot 0.5\,C_4H_8O$

Table 1. Data collection and handling.

Crystal:	red needle, size 0.1 × 0.1 × 0.4 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	4.97 cm^{-1}
Diffractometer, scan mode:	Stoe IPDS I, φ
$2\theta_{max}$:	42.06°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	11957, 4730
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 2750
$N(param)_{refined}$:	455
Programs:	SHELXS-97 [3], SHELXL-97 [4]

Table 2. Atomic coordinates and displacement parameters (in $Å^2$).

Atom	Site	Occ.	*x*	*y*	*z*	U_{iso}
H(2A)	4*e*		0.3308	0.3208	0.1430	0.08
H(3A)	4*e*		0.0872	0.3108	0.1410	0.08
H(4A)	4*e*		0.0347	0.1713	0.1691	0.08
H(7A)	4*e*		0.3549	–0.1225	0.1890	0.08
H(8A)	4*e*		0.2659	–0.1398	0.2623	0.08
H(9A)	4*e*		0.1529	–0.0310	0.2930	0.08
H(10A)	4*e*		0.1484	0.0997	0.2564	0.08
H(11A)	4*e*		0.8048	0.0904	0.2173	0.08
H(12A)	4*e*		0.8078	0.1360	0.1328	0.08
H(13A)	4*e*		0.8438	0.0155	0.0800	0.08
H(14A)	4*e*		0.6459	–0.0724	0.0804	0.08
H(15A)	4*e*		0.6363	–0.1224	0.1618	0.08
H(16A)	4*e*		0.8311	–0.0676	0.2188	0.08
H(17A)	4*e*		0.9855	–0.0198	0.1618	0.08
H(17B)	4*e*		0.9156	–0.1017	0.1398	0.08
H(21A)	4*e*		0.5374	0.3096	0.1753	0.08
H(22A)	4*e*		0.4853	0.2705	0.0960	0.08
H(22B)	4*e*		0.6159	0.2216	0.0984	0.08
H(23A)	4*e*		0.5914	0.3933	0.0985	0.08
H(23B)	4*e*		0.6454	0.3417	0.0583	0.08
H(24A)	4*e*		0.8001	0.4137	0.1062	0.08
H(24B)	4*e*		0.8238	0.3182	0.1101	0.08
H(25A)	4*e*		0.7228	0.4108	0.1825	0.08
H(25B)	4*e*		0.8641	0.3744	0.1897	0.08
H(26A)	4*e*		0.7758	0.2384	0.1857	0.08
H(26B)	4*e*		0.7197	0.2848	0.2277	0.08
H(31A)	4*e*		0.6470	0.1766	0.2593	0.08
H(32A)	4*e*		0.3941	0.2145	0.2740	0.08
H(32B)	4*e*		0.4971	0.2820	0.2664	0.08
H(33A)	4*e*		0.4888	0.2647	0.3523	0.08
H(33B)	4*e*		0.6265	0.2390	0.3410	0.08
H(34A)	4*e*		0.4286	0.1246	0.3492	0.08
H(34B)	4*e*		0.5485	0.1361	0.3902	0.08
H(35A)	4*e*		0.5796	0.0194	0.3412	0.08

Table 2. Continued.

Atom	Site	Occ.	*x*	*y*	*z*	U_{iso}
H(35B)	4*e*		0.6847	0.0860	0.3342	0.08
H(36A)	4*e*		0.5919	0.0378	0.2556	0.08
H(36B)	4*e*		0.4527	0.0606	0.2663	0.08
H(41A)	4*e*		0.2660	0.1304	0.0963	0.08
H(42A)	4*e*		0.3352	0.0587	0.0117	0.08
H(42B)	4*e*		0.4264	0.1190	0.0455	0.08
H(43A)	4*e*		0.3057	0.1937	–0.0219	0.08
H(43B)	4*e*		0.2712	0.2260	0.0280	0.08
H(44A)	4*e*		0.1133	0.1152	–0.0340	0.08
H(44B)	4*e*		0.0747	0.2069	–0.0256	0.08
H(45A)	4*e*		–0.0359	0.1148	0.0207	0.08
H(45B)	4*e*		0.0519	0.1754	0.0554	0.08
H(46A)	4*e*		0.0842	0.0417	0.0885	0.08
H(46B)	4*e*		0.1206	0.0089	0.0389	0.08
H(51A)	4*e*		0.4087	–0.1333	0.1118	0.08
H(52A)	4*e*		0.1460	–0.1182	0.0697	0.08
H(52B)	4*e*		0.1864	–0.1394	0.1253	0.08
H(53A)	4*e*		0.1421	–0.2643	0.0797	0.08
H(53B)	4*e*		0.2879	–0.2622	0.1041	0.08
H(54A)	4*e*		0.2009	–0.2255	0.0044	0.08
H(54B)	4*e*		0.2802	–0.3047	0.0226	0.08
H(55A)	4*e*		0.4182	–0.2016	–0.0055	0.08
H(55B)	4*e*		0.4638	–0.2211	0.0500	0.08
H(56A)	4*e*		0.4548	–0.0735	0.0377	0.08
H(56B)	4*e*		0.3058	–0.0816	0.0183	0.08
B(1)	4*e*	0.49(6)	0.506(1)	–0.3184(6)	0.1780(4)	0.06(1)
F(4)	4*e*	0.49	0.449(1)	–0.3775(8)	0.1491(5)	0.18
B(1′)	4*e*	0.51	0.540(1)	–0.2811(6)	0.1967(4)	0.07(2)
F(4′)	4*e*	0.51	0.593(2)	–0.2222(8)	0.2266(5)	0.18
O(101)	4*e*	0.50	0.264(6)	0.499(2)	0.078(2)	0.32(2)
C(102)	4*e*	0.50	0.335(4)	0.477(3)	0.036(3)	0.32
C(103)	4*e*	0.50	0.241(8)	0.431(3)	–0.002(2)	0.32
C(104)	4*e*	0.50	0.112(6)	0.425(3)	0.017(3)	0.32
C(105)	4*e*	0.50	0.126(5)	0.467(4)	0.066(2)	0.32

Table 3. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Rh(1)	4*e*	0.58088(7)	0.04899(4)	0.14634(3)	0.0183(4)	0.0345(4)	0.0346(4)	–0.0054(4)	0.0033(3)	–0.0067(5)
P(1)	4*e*	0.5107(2)	0.1689(2)	0.18369(9)	0.023(2)	0.037(2)	0.034(2)	–0.004(1)	0.002(1)	–0.001(1)
P(2)	4*e*	0.3676(2)	0.0060(2)	0.11993(9)	0.026(2)	0.034(1)	0.028(1)	–0.005(1)	0.002(1)	–0.001(1)
N(1)	4*e*	0.2346(8)	0.1482(5)	0.1802(3)	0.020(5)	0.050(6)	0.048(6)	–0.001(5)	0.011(5)	–0.013(5)
C(1)	4*e*	0.337(1)	0.1999(6)	0.1728(3)	0.025(6)	0.048(7)	0.032(6)	0.005(6)	0.000(6)	–0.013(5)
C(2)	4*e*	0.284(1)	0.2744(6)	0.1535(4)	0.038(8)	0.041(7)	0.044(7)	0.010(5)	–0.004(6)	–0.004(6)
C(3)	4*e*	0.150(1)	0.2679(7)	0.1515(4)	0.039(8)	0.053(8)	0.064(8)	0.011(6)	–0.005(7)	–0.010(7)
C(4)	4*e*	0.121(1)	0.1924(7)	0.1673(4)	0.024(7)	0.066(8)	0.053(7)	0.007(6)	0.007(6)	–0.022(7)
C(5)	4*e*	0.2423(9)	0.0626(7)	0.1993(4)	0.024(6)	0.056(8)	0.029(6)	–0.018(6)	0.007(5)	–0.006(6)
C(6)	4*e*	0.2964(9)	–0.0016(6)	0.1767(3)	0.015(6)	0.042(6)	0.033(6)	–0.001(5)	0.009(5)	0.000(6)
C(7)	4*e*	0.310(1)	–0.0772(6)	0.2020(4)	0.038(7)	0.046(7)	0.026(6)	–0.016(5)	0.001(6)	–0.003(5)
C(8)	4*e*	0.257(1)	–0.0873(8)	0.2453(4)	0.063(9)	0.065(8)	0.047(8)	–0.032(7)	0.004(7)	0.011(7)
C(9)	4*e*	0.194(1)	–0.0225(9)	0.2642(4)	0.061(9)	0.09(1)	0.037(7)	–0.026(7)	0.032(7)	–0.018(8)
C(10)	4*e*	0.188(1)	0.0532(8)	0.2424(4)	0.032(6)	0.068(9)	0.051(8)	–0.009(6)	0.006(6)	–0.006(7)
C(11)	4*e*	0.7813(9)	0.0558(7)	0.1888(4)	0.028(6)	0.070(8)	0.034(6)	–0.004(6)	–0.005(5)	–0.022(7)
C(12)	4*e*	0.783(1)	0.0806(7)	0.1408(4)	0.029(7)	0.060(7)	0.058(8)	0.001(5)	0.021(6)	–0.013(7)
C(13)	4*e*	0.8128(9)	0.0057(7)	0.1107(4)	0.015(6)	0.077(8)	0.042(6)	–0.009(6)	0.009(6)	–0.005(7)
C(14)	4*e*	0.686(1)	–0.0435(7)	0.1094(4)	0.034(7)	0.049(7)	0.058(7)	0.011(6)	0.002(6)	–0.009(7)
C(15)	4*e*	0.680(1)	–0.0720(6)	0.1551(4)	0.027(7)	0.046(7)	0.080(9)	0.004(5)	0.007(7)	0.003(7)
C(16)	4*e*	0.8063(9)	–0.0407(6)	0.1876(4)	0.037(7)	0.050(7)	0.051(6)	0.005(6)	–0.004(6)	0.022(6)
C(17)	4*e*	0.9028(9)	–0.0457(7)	0.1504(4)	0.023(6)	0.055(6)	0.056(6)	0.004(6)	0.003(6)	0.002(7)
C(21)	4*e*	0.589(1)	0.2645(6)	0.1660(4)	0.039(7)	0.038(6)	0.051(7)	–0.019(5)	0.003(7)	–0.002(5)
C(22)	4*e*	0.576(1)	0.2703(6)	0.1100(3)	0.055(8)	0.050(7)	0.036(6)	–0.019(6)	0.005(6)	0.004(6)
C(23)	4*e*	0.644(2)	0.3458(8)	0.0932(5)	0.14(2)	0.09(1)	0.068(9)	–0.05(1)	0.01(1)	0.003(8)
C(24)	4*e*	0.768(2)	0.363(1)	0.1180(6)	0.17(2)	0.14(2)	0.10(1)	–0.10(1)	0.04(1)	–0.00(1)
C(25)	4*e*	0.776(2)	0.3655(8)	0.1740(5)	0.13(1)	0.11(1)	0.067(9)	–0.10(1)	0.00(1)	–0.005(9)
C(26)	4*e*	0.720(1)	0.2832(8)	0.1927(5)	0.09(1)	0.08(1)	0.074(9)	–0.037(8)	0.001(9)	–0.004(8)
C(31)	4*e*	0.5556(9)	0.1631(5)	0.2521(3)	0.035(6)	0.024(5)	0.031(6)	0.000(5)	–0.001(5)	–0.008(5)
C(32)	4*e*	0.486(1)	0.2274(6)	0.2794(3)	0.055(7)	0.037(6)	0.038(6)	0.009(5)	0.010(6)	–0.002(5)
C(33)	4*e*	0.535(1)	0.2249(6)	0.3353(4)	0.077(9)	0.042(7)	0.049(7)	0.001(6)	0.006(7)	0.003(6)
C(34)	4*e*	0.520(1)	0.1379(6)	0.3552(4)	0.09(1)	0.058(8)	0.033(6)	0.020(7)	0.015(7)	–0.009(6)
C(35)	4*e*	0.593(1)	0.0737(6)	0.3282(3)	0.075(9)	0.045(7)	0.037(6)	0.022(6)	–0.001(6)	0.007(5)
C(36)	4*e*	0.543(1)	0.0763(6)	0.2725(3)	0.039(7)	0.051(7)	0.044(6)	–0.004(5)	0.001(6)	–0.005(6)
C(41)	4*e*	0.2698(8)	0.0802(5)	0.0776(3)	0.022(6)	0.040(6)	0.025(5)	–0.002(4)	–0.001(5)	0.002(5)
C(42)	4*e*	0.337(1)	0.1049(5)	0.0340(3)	0.040(7)	0.034(6)	0.033(6)	–0.005(5)	0.006(6)	0.002(5)
C(43)	4*e*	0.265(1)	0.1790(6)	0.0062(4)	0.047(8)	0.051(7)	0.049(7)	–0.005(6)	0.006(7)	0.016(6)
C(44)	4*e*	0.119(1)	0.1591(6)	–0.0101(4)	0.048(8)	0.049(7)	0.036(6)	–0.005(6)	–0.008(6)	0.016(6)
C(45)	4*e*	0.053(1)	0.1298(6)	0.0327(4)	0.030(7)	0.055(7)	0.058(7)	0.005(6)	–0.009(6)	–0.008(6)
C(46)	4*e*	0.1244(8)	0.0562(6)	0.0604(3)	0.023(6)	0.045(6)	0.048(6)	–0.002(5)	0.000(5)	0.008(6)
C(51)	4*e*	0.3449(8)	–0.0987(5)	0.0924(3)	0.017(6)	0.039(6)	0.029(6)	–0.009(5)	0.005(5)	–0.003(5)
C(52)	4*e*	0.2117(9)	–0.1442(5)	0.0932(4)	0.029(6)	0.037(6)	0.048(6)	–0.010(5)	0.003(6)	–0.005(5)
C(53)	4*e*	0.224(1)	–0.2364(6)	0.0796(4)	0.040(7)	0.043(7)	0.045(7)	–0.007(5)	0.004(6)	–0.001(6)
C(54)	4*e*	0.268(1)	–0.2468(6)	0.0293(4)	0.046(7)	0.028(6)	0.059(8)	–0.003(5)	–0.001(7)	–0.013(6)
C(55)	4*e*	0.395(1)	–0.1974(6)	0.0269(4)	0.033(7)	0.053(7)	0.048(7)	–0.012(5)	0.011(6)	–0.006(6)
C(56)	4*e*	0.3772(9)	–0.1048(6)	0.0406(3)	0.030(6)	0.043(6)	0.037(6)	–0.009(5)	0.009(6)	–0.007(5)
F(1)	4*e*	0.564(1)	–0.2660(6)	0.1518(3)	0.18(1)	0.18(1)	0.160(9)	–0.028(8)	0.019(8)	0.092(8)
F(2)	4*e*	0.5897(8)	–0.3532(6)	0.2124(3)	0.123(8)	0.19(1)	0.162(9)	0.015(7)	–0.030(7)	0.110(8)
F(3)	4*e*	0.413(1)	–0.2786(7)	0.1966(4)	0.20(1)	0.21(1)	0.18(1)	0.10(1)	0.06(1)	0.072(9)

2. 1-(2-(Dicyclohexylphosphinophenyl)-pyrol-2-dicyclohexylphosphino-rhodium(I) (*Z*,*Z*)-cycloocta-1,5-diene tetrafluoroborate, $[Rh(C_{34}H_{51}NP_2)(C_8H_{12})][BF_4]$

Table 4. Data collection and handling.

Crystal:	red, prism-like, size 0.3 × 0.3 × 0.4 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	5.59 cm^{-1}
Diffractometer, scan mode:	Stoe IPDS I, φ
$2\theta_{max}$:	45°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	9728, 4985
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 2732
$N(param)_{refined}$:	458
Programs:	SHELXS-97 [3], SHELXL-97 [4]

Table 5. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	Occ.	*x*	*y*	*z*	U_{iso}
H(2A)	4*e*		0.5344	0.3481	0.2718	0.08
H(3A)	4*e*		0.7685	0.3636	0.2608	0.08
H(4A)	4*e*		0.9051	0.2775	0.3382	0.08
H(7A)	4*e*		0.7873	0.1361	0.5527	0.08
H(8A)	4*e*		0.8766	0.0285	0.5168	0.08
H(9A)	4*e*		0.9175	0.0245	0.4160	0.08
H(10A)	4*e*		0.8504	0.1254	0.3483	0.08
H(11A)	4*e*		0.4003	0.0849	0.4444	0.08
H(12A)	4*e*		0.2473	0.1659	0.4191	0.08
H(13A)	4*e*		0.1902	0.1570	0.5332	0.08
H(13B)	4*e*		0.1126	0.2041	0.4780	0.08
H(14A)	4*e*		0.2231	0.3099	0.5105	0.08
H(14B)	4*e*		0.2137	0.2740	0.5739	0.08
H(15A)	4*e*		0.4298	0.3192	0.5722	0.08
H(16A)	4*e*		0.5544	0.2271	0.6102	0.08
H(17A)	4*e*		0.3429	0.1368	0.6030	0.08
H(17B)	4*e*		0.4849	0.1143	0.6336	0.08
H(18A)	4*e*		0.5191	0.0626	0.5444	0.08
H(18B)	4*e*		0.3785	0.0361	0.5449	0.08
H(21A)	4*e*		0.3366	0.1344	0.3368	0.08
H(22A)	4*e*		0.5463	0.0840	0.3717	0.08
H(22B)	4*e*		0.5891	0.1191	0.3142	0.08
H(23A)	4*e*		0.3997	0.0041	0.3058	0.08
H(23B)	4*e*		0.5388	–0.0082	0.2936	0.08
H(24A)	4*e*		0.3852	0.0017	0.1994	0.08
H(24B)	4*e*		0.4897	0.0651	0.2047	0.08
H(25A)	4*e*		0.2871	0.1199	0.1721	0.08
H(25B)	4*e*		0.2415	0.0854	0.2292	0.08
H(26A)	4*e*		0.4327	0.1993	0.2387	0.08
H(26B)	4*e*		0.2927	0.2136	0.2492	0.08
H(31A)	4*e*		0.3516	0.3226	0.2981	0.08
H(32A)	4*e*		0.1961	0.3001	0.3858	0.08
H(32B)	4*e*		0.1783	0.2543	0.3240	0.08
H(33A)	4*e*		0.1309	0.3664	0.2680	0.08
H(33B)	4*e*		0.0326	0.3575	0.3116	0.08
H(34A)	4*e*		0.1153	0.4821	0.3146	0.08
H(34B)	4*e*		0.1506	0.4445	0.3801	0.08
H(35A)	4*e*		0.3351	0.5030	0.3602	0.08
H(35B)	4*e*		0.3211	0.4598	0.2975	0.08
H(36A)	4*e*		0.4803	0.4010	0.3717	0.08
H(36B)	4*e*		0.3816	0.3902	0.4149	0.08
H(41A)	4*e*		0.6881	0.3648	0.4250	0.08
H(42A)	4*e*		0.7025	0.4467	0.5341	0.08
H(42B)	4*e*		0.5715	0.4249	0.4902	0.08
H(43A)	4*e*		0.6222	0.4968	0.4108	0.08
H(43B)	4*e*		0.6332	0.5484	0.4690	0.08
H(44A)	4*e*		0.8108	0.5654	0.4209	0.08
H(44B)	4*e*		0.8563	0.5386	0.4894	0.08
H(45A)	4*e*		0.9675	0.4691	0.4284	0.08
H(45B)	4*e*		0.8369	0.4447	0.3857	0.08
H(46A)	4*e*		0.9117	0.3450	0.4541	0.08
H(46B)	4*e*		0.9140	0.3985	0.5107	0.08
H(51A)	4*e*		0.7568	0.2331	0.6052	0.08
H(52A)	4*e*		0.9633	0.3228	0.5863	0.08
H(52B)	4*e*		0.9578	0.2360	0.5737	0.08
H(53A)	4*e*		1.0801	0.2588	0.6750	0.08
H(53B)	4*e*		0.9545	0.2143	0.6793	0.08
H(54A)	4*e*		0.9775	0.3134	0.7509	0.08
H(54B)	4*e*		0.9798	0.3704	0.6971	0.08
H(55A)	4*e*		0.7756	0.3733	0.7188	0.08
H(55B)	4*e*		0.7633	0.2862	0.7089	0.08
H(56A)	4*e*		0.7747	0.3902	0.6134	0.08
H(56B)	4*e*		0.6492	0.3463	0.6189	0.08
F(2)	4*e*	0.52(2)	–0.1058(8)	0.4901(7)	0.2275(3)	0.061(4)
F(3)	4*e*	0.52	–0.2145(8)	0.4119(5)	0.1577(5)	0.065(4)
F(4)	4*e*	0.52	–0.178(1)	0.5267(6)	0.1282(4)	0.067(4)
F(2′)	4*e*	0.48	–0.2374(7)	0.445(1)	0.1341(6)	0.153(7)
F(3′)	4*e*	0.48	–0.123(1)	0.5495(4)	0.1555(7)	0.082(5)
F(4′)	4*e*	0.48	–0.119(1)	0.4657(7)	0.2291(3)	0.065(5)

Table 6. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	*x*	*y*	*z*	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Rh(1)	4*e*	0.48074(6)	0.22665(3)	0.48159(2)	0.0199(3)	0.0214(3)	0.0203(3)	–0.0019(3)	0.0033(2)	–0.0019(3)
P(1)	4*e*	0.4649(2)	0.2396(1)	0.37297(7)	0.017(1)	0.020(1)	0.021(1)	0.0004(8)	0.0005(8)	–0.0030(8)
P(2)	4*e*	0.6905(2)	0.2784(1)	0.50464(7)	0.015(1)	0.023(1)	0.0213(9)	0.001(1)	0.0006(8)	–0.002(1)
N(1)	4*e*	0.7317(6)	0.2481(2)	0.3649(2)	0.022(4)	0.028(4)	0.020(3)	0.002(2)	0.007(3)	0.000(2)
C(1)	4*e*	0.6041(6)	0.2721(4)	0.3423(2)	0.013(4)	0.029(4)	0.019(3)	0.005(4)	0.004(3)	–0.004(4)
C(2)	4*e*	0.6085(7)	0.3226(4)	0.2961(3)	0.025(6)	0.032(4)	0.021(4)	0.000(3)	0.007(3)	0.001(3)
C(3)	4*e*	0.7380(8)	0.3308(4)	0.2897(3)	0.042(6)	0.042(5)	0.021(4)	–0.007(4)	0.014(4)	0.001(4)
C(4)	4*e*	0.8127(7)	0.2843(4)	0.3322(3)	0.029(5)	0.038(5)	0.033(4)	–0.001(4)	0.011(4)	–0.007(4)
C(5)	4*e*	0.7788(7)	0.1905(4)	0.4094(3)	0.021(5)	0.025(4)	0.029(4)	0.000(3)	0.003(3)	0.004(3)
C(6)	4*e*	0.7647(7)	0.1978(3)	0.4726(3)	0.030(5)	0.017(4)	0.021(4)	0.005(3)	–0.007(3)	0.004(3)
C(7)	4*e*	0.7999(7)	0.1345(4)	0.5106(3)	0.031(5)	0.025(4)	0.034(5)	0.007(4)	–0.005(4)	–0.008(4)
C(8)	4*e*	0.8555(8)	0.0713(4)	0.4897(4)	0.037(6)	0.037(5)	0.042(5)	0.016(4)	–0.010(4)	0.000(4)
C(9)	4*e*	0.8760(7)	0.0679(4)	0.4297(4)	0.035(6)	0.036(5)	0.046(5)	0.018(4)	–0.002(4)	–0.008(4)
C(10)	4*e*	0.8366(7)	0.1270(4)	0.3902(3)	0.017(5)	0.042(5)	0.039(5)	0.012(4)	0.002(4)	–0.012(4)
C(11)	4*e*	0.3870(8)	0.1156(3)	0.4786(3)	0.055(6)	0.010(4)	0.037(5)	–0.011(4)	0.011(4)	–0.003(3)
C(12)	4*e*	0.2875(7)	0.1671(4)	0.4626(3)	0.013(5)	0.028(5)	0.049(5)	–0.009(3)	0.005(4)	–0.011(4)
C(13)	4*e*	0.1977(8)	0.1951(4)	0.5030(3)	0.030(6)	0.047(5)	0.048(5)	–0.013(4)	0.011(4)	–0.006(4)
C(14)	4*e*	0.2508(7)	0.2678(5)	0.5377(3)	0.033(6)	0.054(5)	0.051(5)	–0.002(5)	0.010(4)	0.000(5)
C(15)	4*e*	0.3962(7)	0.2704(5)	0.5578(3)	0.029(5)	0.037(4)	0.025(4)	0.001(4)	0.008(3)	–0.012(4)
C(16)	4*e*	0.4758(8)	0.2113(4)	0.5824(3)	0.035(6)	0.036(5)	0.029(4)	–0.002(4)	0.010(4)	0.001(4)
C(17)	4*e*	0.4302(8)	0.1336(4)	0.5963(3)	0.046(6)	0.056(6)	0.039(5)	–0.004(4)	0.010(4)	0.007(4)
C(18)	4*e*	0.4314(8)	0.0797(4)	0.5416(3)	0.045(6)	0.039(5)	0.053(6)	–0.006(4)	0.010(4)	0.005(4)
C(21)	4*e*	0.4084(7)	0.1570(3)	0.3226(3)	0.020(5)	0.019(4)	0.028(4)	0.002(3)	0.000(3)	–0.003(3)
C(22)	4*e*	0.5170(7)	0.0974(3)	0.3287(3)	0.031(5)	0.024(4)	0.017(4)	0.006(3)	0.004(3)	–0.002(3)
C(23)	4*e*	0.4685(7)	0.0274(3)	0.2897(3)	0.042(6)	0.024(4)	0.042(5)	0.001(4)	0.015(4)	–0.005(4)
C(24)	4*e*	0.4191(8)	0.0463(4)	0.2220(3)	0.051(6)	0.035(5)	0.025(4)	0.003(4)	0.004(4)	–0.010(4)
C(25)	4*e*	0.3150(8)	0.1061(4)	0.2152(3)	0.056(6)	0.034(5)	0.022(4)	–0.001(4)	–0.004(4)	–0.004(4)
C(26)	4*e*	0.3617(7)	0.1770(3)	0.2537(3)	0.038(6)	0.021(4)	0.027(4)	0.004(3)	–0.009(4)	–0.001(3)

Table 6. Continued.

Atom	Site	*x*	*y*	*z*	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(31)	4*e*	0.3483(7)	0.3169(3)	0.3412(3)	0.013(5)	0.024(4)	0.022(4)	–0.004(3)	–0.002(3)	–0.005(3)
C(32)	4*e*	0.2057(7)	0.3020(3)	0.3433(3)	0.028(6)	0.023(5)	0.041(5)	–0.001(3)	0.002(4)	0.009(3)
C(33)	4*e*	0.1225(7)	0.3662(4)	0.3108(3)	0.018(5)	0.036(5)	0.066(6)	0.001(4)	–0.006(4)	0.017(4)
C(34)	4*e*	0.1658(8)	0.4428(4)	0.3385(4)	0.030(6)	0.039(5)	0.062(6)	0.000(4)	0.012(4)	0.002(4)
C(35)	4*e*	0.3080(7)	0.4561(3)	0.3394(3)	0.032(6)	0.021(4)	0.047(5)	0.007(3)	0.009(4)	–0.009(3)
C(36)	4*e*	0.3903(7)	0.3922(3)	0.3723(3)	0.028(5)	0.028(4)	0.027(4)	–0.002(3)	0.002(3)	–0.009(3)
C(41)	4*e*	0.7285(6)	0.3693(3)	0.4683(3)	0.009(5)	0.028(4)	0.026(4)	–0.003(3)	0.001(3)	0.001(3)
C(42)	4*e*	0.6613(7)	0.4367(3)	0.4916(3)	0.032(5)	0.023(4)	0.026(4)	0.006(3)	0.005(3)	0.000(3)
C(43)	4*e*	0.6711(7)	0.5057(4)	0.4523(3)	0.034(6)	0.029(4)	0.027(5)	0.003(4)	0.000(4)	0.001(3)
C(44)	4*e*	0.8097(7)	0.5236(4)	0.4488(3)	0.034(6)	0.031(5)	0.024(4)	–0.010(4)	–0.011(4)	0.005(4)
C(45)	4*e*	0.8783(8)	0.4567(4)	0.4278(3)	0.034(6)	0.042(5)	0.042(5)	–0.008(4)	0.009(4)	0.005(4)
C(46)	4*e*	0.8699(7)	0.3876(4)	0.4688(3)	0.022(5)	0.037(5)	0.034(5)	0.000(3)	0.003(4)	0.004(4)
C(51)	4*e*	0.7822(6)	0.2786(4)	0.5870(2)	0.018(5)	0.027(4)	0.021(3)	0.005(4)	0.002(3)	0.000(4)
C(52)	4*e*	0.9308(6)	0.2754(4)	0.5983(3)	0.025(5)	0.036(4)	0.031(4)	0.001(4)	–0.005(3)	0.004(4)
C(53)	4*e*	0.9869(7)	0.2618(4)	0.6676(3)	0.029(5)	0.050(6)	0.035(4)	0.008(4)	–0.012(3)	–0.003(4)
C(54)	4*e*	0.9437(8)	0.3234(4)	0.7075(3)	0.045(7)	0.056(6)	0.023(4)	0.000(4)	–0.006(4)	–0.005(4)
C(55)	4*e*	0.7993(8)	0.3316(4)	0.6954(3)	0.050(7)	0.046(5)	0.022(5)	0.016(4)	–0.001(4)	0.000(4)
C(56)	4*e*	0.7424(7)	0.3433(3)	0.6263(3)	0.035(5)	0.025(4)	0.024(4)	0.006(3)	0.001(4)	0.007(3)
B(1)	4*e*	–0.1261(6)	0.4718(3)	0.1671(2)	0.09(1)	0.063(9)	0.062(9)	0.013(7)	0.031(8)	–0.013(7)
F(1)	4*e*	–0.0199(5)	0.4423(3)	0.1505(2)	0.092(5)	0.088(4)	0.114(5)	0.033(3)	0.059(4)	0.041(3)

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