Crystal structure of 1,2-bis(diphenylphosphinoxy)-ethane rhodium(I)-norborna-2,5-diene tetrafluoroborate, $C_{33}H_{32}BF_4O_2P_2Rh$, and of 1,2-bis(diphenylphosphinoxy)-ethane rhodium(I)-(Z,Z)-cycloocta-1,5-diene tetrafluoroborate, $C_{34}H_{36}BF_4O_2P_2Rh \cdot C_4H_8O \cdot 1/4CH_2Cl_2$

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Abstract

$C_{33}H_{32}BF_4O_2P_2Rh$, triclinic, $P\bar{1}$ (No. 2), $a = 9.342(2)$ Å, $b = 10.279(3)$ Å, $c = 16.964(3)$ Å, $\alpha = 74.88(2)^\circ$, $\beta = 82.13(2)^\circ$, $\gamma = 83.63(2)^\circ$, $V = 1552.9$ Å³, $Z = 2$, $R_{gt}(F) = 0.042$, $wR_{obs}(F^2) = 0.095$, $T = 200$ K.

$C_{38.25}H_{44.50}BCl_{0.50}F_4O_3P_2Rh$, monoclinic, $P12_1/n1$ (No. 14), $a = 9.629(2)$ Å, $b = 24.925(5)$ Å, $c = 16.639(3)$ Å, $\beta = 92.31(3)^\circ$, $V = 3990.2$ Å³, $Z = 4$, $R_{gt}(F) = 0.060$, $wR_{obs}(F^2) = 0.170$, $T = 200$ K.

Source of material

Attempt to isolate 1,2-bis(diphenylphosphinoxy) ethane (1) following Maier's procedure [1] gave 1,2-bis(diphenylphosphinyl)-ethane – the product of Michaelis-Arbuzov rearrangement. Thus, the diphosphinite prepared from ethylenglycol and Ph_2PCl in presence of pyridine was converted without any further purification in the corresponding Rh(I) complex $[Rh(I)(COD)]BF_4$ by subsequent treatment with $[Rh(COD)(acac)]$ and HBF_4 [2]. The rhodium complex with the ligand (1) was prepared recently in analogous manner [3]. Hydro-

genation of the cod-complex leads to the solvent complex. Addition of excess norborna-2,5-diene and precipitation with Et_2O gives the nbd-complex.

Discussion

Unexpected differences between the title compounds in the catalytic hydrogenation of the diolefines norborna-2,5-diene and (Z,Z)-cycloocta-1,5-diene (compare with [4]) motivated us to determine the crystal structures. 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 cod-complex 20.5° , for the nbd-complex 7.2° .

1. 1,2-bis(diphenylphosphinoxy)-ethane rhodium(I)-norborna-2,5-diene tetrafluoroborate, $C_{33}H_{32}BF_4O_2P_2Rh$

Table 1. Data collection and handling.

Crystal:	orange prism, size $0.2 \times 0.2 \times 0.3$ mm
Wavelength:	Mo K_α radiation (0.71069 Å)
μ :	7.07 cm^{-1}
Diffraction, scan mode:	STOE IPDS, 100 exposures, $\Delta\varphi = 2^\circ$
$2\theta_{max}$:	48.3°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	4526, 4526
Criterion for I_{obs} , $N(hkl)_{gt}$:	$I_{obs} > 2\sigma(I_{obs})$, 3368
$N(param)_{refined}$:	385
Programs:	SHELXS-86 [4], SHELXL-93 [5]

Table 2. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	Occ.	x	y	z	U_{iso}
H(1)	2i		0.2938(6)	0.2615(6)	0.7086(4)	0.040
H(2)	2i		0.3985(6)	0.2625(6)	0.5608(4)	0.041
H(3)	2i		0.2610(7)	0.0546(6)	0.5687(3)	0.041
H(4)	2i		-0.0029(7)	0.1266(6)	0.5696(3)	0.040
H(5)	2i		-0.0392(6)	0.3800(6)	0.5624(4)	0.044
H(6A)	2i		0.2132(7)	0.4679(6)	0.5307(3)	0.041
H(6B)	2i		0.2000(7)	0.3737(6)	0.4689(3)	0.041
H(7)	2i		0.0301(6)	0.3382(5)	0.7086(4)	0.036
H(9)	2i		-0.1080(6)	-0.3309(6)	0.6938(4)	0.041
H(10)	2i		-0.3384(6)	-0.3423(6)	0.6570(4)	0.043

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Table 2. Continued.

Atom	Site	Occ.	x	y	z	U _{iso}
H(11)	2i		-0.4862(6)	-0.1475(7)	0.6170(4)	0.048
H(12)	2i		-0.4196(6)	0.0598(6)	0.6237(4)	0.043
H(13)	2i		-0.1919(6)	0.0741(6)	0.6620(4)	0.038
H(15)	2i		0.2523(6)	-0.3439(6)	0.7743(4)	0.041
H(16)	2i		0.4217(6)	-0.4761(6)	0.7095(4)	0.048
H(17)	2i		0.4462(6)	-0.4371(6)	0.5671(4)	0.044
H(18)	2i		0.3009(6)	-0.2643(6)	0.4893(4)	0.040
H(19)	2i		0.1279(6)	-0.1348(6)	0.5550(3)	0.034
H(21)	2i		0.3536(6)	0.1884(6)	0.8771(4)	0.042
H(22)	2i		0.3693(8)	0.3962(7)	0.9054(4)	0.058
H(23)	2i		0.1650(8)	0.5365(7)	0.9257(4)	0.052
H(24)	2i		-0.0613(8)	0.4785(6)	0.9085(4)	0.052
H(25)	2i		-0.0809(6)	0.2776(6)	0.8722(3)	0.040
H(27)	2i		0.1778(6)	-0.1096(6)	0.9973(4)	0.047

Table 2. Continued.

Atom	Site	Occ.	x	y	z	U _{iso}
H(28)	2i		0.3646(7)	-0.2732(8)	1.0440(4)	0.074
H(29)	2i		0.5604(8)	-0.3168(9)	0.9497(5)	0.088
H(30)	2i		0.5708(8)	-0.199(1)	0.8135(5)	0.100
H(31)	2i		0.3848(6)	-0.0390(8)	0.7678(4)	0.066
H(32A)	2i		-0.0667(6)	-0.2522(6)	0.9276(4)	0.039
H(32B)	2i		-0.1744(6)	-0.2397(6)	0.8600(4)	0.039
H(33A)	2i		-0.1602(6)	-0.0031(6)	0.8212(4)	0.040
H(33B)	2i		-0.2254(6)	-0.0550(6)	0.9152(4)	0.040
F(2A)	2i	0.50	-0.360(1)	0.4116(9)	0.7818(6)	0.071(3)
F(2B)	2i	0.50	-0.418(1)	0.367(1)	0.7951(6)	0.101(4)
F(3A)	2i	0.50	-0.4474(9)	0.2440(9)	0.7461(7)	0.081(3)
F(4A)	2i	0.50	-0.261(1)	0.428(1)	0.6878(8)	0.139(5)
F(3B)	2i	0.50	-0.316(1)	0.381(1)	0.6525(5)	0.093(3)
F(4B)	2i	0.50	-0.405(2)	0.293(2)	0.6770(9)	0.147(5)

Table 3. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	x	y	z	U ₁₁	U ₂₂	U ₃₃	U ₁₂	U ₁₃	U ₂₃
C(1)	2i	0.2381(6)	0.2776(6)	0.6637(4)	0.041(4)	0.027(3)	0.034(4)	-0.016(3)	-0.006(3)	-0.006(3)
C(2)	2i	0.2916(6)	0.2630(6)	0.5776(4)	0.033(3)	0.033(3)	0.029(4)	-0.003(3)	-0.001(3)	0.003(3)
C(3)	2i	0.2160(7)	0.1408(6)	0.5719(3)	0.053(4)	0.023(3)	0.021(3)	0.003(3)	0.002(3)	-0.003(3)
C(4)	2i	0.0719(7)	0.1803(6)	0.5723(3)	0.059(4)	0.024(3)	0.013(3)	-0.017(3)	-0.011(3)	0.009(3)
C(5)	2i	0.0534(6)	0.3267(6)	0.5781(4)	0.031(3)	0.038(3)	0.043(4)	0.000(3)	-0.015(3)	-0.010(3)
C(6)	2i	0.1946(7)	0.3767(6)	0.5271(3)	0.059(4)	0.021(3)	0.017(3)	-0.007(3)	-0.006(3)	0.005(3)
C(7)	2i	0.0936(6)	0.3185(5)	0.6637(4)	0.035(4)	0.022(3)	0.033(4)	-0.006(2)	0.004(3)	-0.009(3)
C(8)	2i	-0.1278(6)	-0.1270(5)	0.6830(3)	0.029(3)	0.021(3)	0.018(3)	-0.005(2)	-0.001(2)	0.001(3)
C(9)	2i	-0.1710(6)	-0.2512(6)	0.6801(4)	0.026(3)	0.037(4)	0.042(4)	-0.006(3)	0.005(3)	-0.019(3)
C(10)	2i	-0.3070(6)	-0.2576(6)	0.6571(4)	0.034(4)	0.039(4)	0.040(4)	-0.014(3)	0.001(3)	-0.015(3)
C(11)	2i	-0.3954(6)	-0.1424(7)	0.6348(4)	0.025(3)	0.063(5)	0.037(4)	-0.013(3)	-0.006(3)	-0.014(4)
C(12)	2i	-0.3555(6)	-0.0191(6)	0.6376(4)	0.020(3)	0.042(4)	0.038(4)	0.000(3)	-0.007(3)	0.006(3)
C(13)	2i	-0.2209(6)	-0.0111(6)	0.6610(4)	0.031(3)	0.026(3)	0.038(4)	-0.006(3)	-0.007(3)	-0.002(3)
C(14)	2i	0.1724(5)	-0.2256(5)	0.6714(3)	0.019(3)	0.020(3)	0.033(3)	-0.001(2)	-0.006(2)	-0.008(3)
C(15)	2i	0.2613(6)	-0.3278(6)	0.7161(4)	0.026(3)	0.038(4)	0.034(4)	-0.004(3)	0.001(3)	-0.004(3)
C(16)	2i	0.3623(6)	-0.4063(6)	0.6779(4)	0.023(3)	0.032(3)	0.064(5)	0.001(3)	-0.004(3)	-0.010(4)
C(17)	2i	0.3768(6)	-0.3831(6)	0.5936(4)	0.035(4)	0.024(3)	0.052(5)	-0.006(3)	0.003(3)	-0.017(3)
C(18)	2i	0.2902(6)	-0.2810(6)	0.5475(4)	0.039(4)	0.035(3)	0.027(4)	-0.013(3)	0.001(3)	-0.008(3)
C(19)	2i	0.1881(6)	-0.2037(6)	0.5866(3)	0.031(3)	0.026(3)	0.027(3)	0.003(2)	-0.009(3)	-0.006(3)
C(20)	2i	0.1336(6)	0.2102(6)	0.8731(3)	0.033(3)	0.035(3)	0.015(3)	-0.005(3)	0.000(2)	-0.005(3)
C(21)	2i	0.2688(6)	0.2469(6)	0.8827(4)	0.039(4)	0.041(4)	0.027(4)	-0.006(3)	-0.009(3)	-0.007(3)
C(22)	2i	0.2772(8)	0.3700(7)	0.9006(4)	0.063(5)	0.052(4)	0.034(4)	-0.026(4)	-0.011(3)	-0.010(4)
C(23)	2i	0.1568(8)	0.4544(7)	0.9114(4)	0.078(5)	0.032(4)	0.020(4)	-0.016(4)	-0.001(3)	-0.001(3)
C(24)	2i	0.0228(8)	0.4198(6)	0.9014(4)	0.071(5)	0.028(3)	0.023(4)	0.002(3)	0.009(3)	-0.001(3)
C(25)	2i	0.0109(6)	0.2995(6)	0.8809(3)	0.037(4)	0.038(4)	0.025(4)	-0.003(3)	0.002(3)	-0.009(3)
C(26)	2i	0.2634(6)	-0.0602(6)	0.8780(3)	0.024(3)	0.035(3)	0.018(3)	0.000(2)	-0.006(2)	-0.005(3)
C(27)	2i	0.2576(6)	-0.1285(6)	0.9598(4)	0.031(3)	0.054(4)	0.018(3)	0.013(3)	0.001(3)	0.007(3)
C(28)	2i	0.3685(7)	-0.2255(8)	0.9877(4)	0.047(4)	0.091(6)	0.031(4)	0.024(4)	-0.001(3)	0.000(4)
C(29)	2i	0.4845(8)	-0.2507(9)	0.9317(5)	0.051(5)	0.109(7)	0.046(5)	0.042(5)	-0.013(4)	-0.010(5)
C(30)	2i	0.4903(8)	-0.182(1)	0.8512(5)	0.033(4)	0.17(1)	0.037(5)	0.046(5)	0.000(3)	-0.027(6)
C(31)	2i	0.3802(6)	-0.0866(8)	0.8241(4)	0.026(4)	0.109(6)	0.020(4)	0.018(4)	-0.004(3)	-0.008(4)
C(32)	2i	-0.0911(6)	-0.1999(6)	0.8726(4)	0.037(4)	0.032(3)	0.022(3)	-0.009(3)	0.006(3)	0.004(3)
C(33)	2i	-0.1367(6)	-0.0566(6)	0.8761(4)	0.021(3)	0.043(4)	0.035(4)	-0.003(3)	0.004(3)	-0.013(3)
B(1)	2i	-0.3317(5)	0.3202(5)	0.7347(3)	0.048(5)	0.061(6)	0.073(7)	0.002(4)	-0.004(5)	-0.034(6)
O(1)	2i	0.0311(4)	-0.2153(4)	0.8129(2)	0.029(2)	0.026(2)	0.026(2)	-0.001(2)	-0.001(2)	0.000(2)
O(2)	2i	-0.0245(4)	0.0052(4)	0.9014(2)	0.020(2)	0.040(2)	0.026(2)	-0.005(2)	0.002(2)	-0.012(2)
F(1)	2i	-0.2165(4)	0.2312(4)	0.7586(3)	0.051(3)	0.059(3)	0.135(5)	0.028(2)	-0.042(3)	-0.025(3)
P(1)	2i	0.0440(2)	-0.1176(1)	0.72028(9)	0.0236(8)	0.0217(7)	0.0240(8)	-0.0012(6)	-0.0048(6)	-0.0055(7)
P(2)	2i	0.1151(1)	0.0600(1)	0.83967(8)	0.0222(8)	0.0278(8)	0.0159(8)	0.0001(6)	-0.0026(6)	-0.0035(7)
Rh(1)	2i	0.11148(5)	0.09363(4)	0.70226(3)	0.0228(2)	0.0218(2)	0.0168(2)	-0.0043(2)	-0.0042(2)	-0.0039(2)

2. 1,2-bis(diphenylphosphinoxy)-ethane rhodium(I)-(Z,Z)-cycloocta-1,5- diene tetrafluoroborate, C₃₄H₃₆BF₄O₂P₂Rh · C₄H₈O · 1/4CH₂Cl₂

Table 4. Data collection and handling.

Crystal:	red, prism, size 0.5 x 0.5 x 0.5 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	5.94 cm ⁻¹
Diffractometer, scan mode:	STOE IPDS, 100 exposures, $\Delta\phi = 2^\circ$
2 θ_{max} :	45°
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$:	8937, 5069
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 4216
$N(\text{param})_{\text{refined}}$:	431
Programs:	SHELXS-86 [4], SHELXL-93 [5]

Table 5. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	Occ.	x	y	z	U_{iso}
H(1A)	4e		-0.2551(6)	0.1979(3)	0.1113(4)	0.041
H(1B)	4e		-0.4048(6)	0.2204(3)	0.0914(4)	0.041
H(2A)	4e		-0.3132(6)	0.3008(3)	0.0532(4)	0.045
H(2B)	4e		-0.2659(6)	0.2876(3)	0.1421(4)	0.045
H(4)	4e		-0.3392(6)	0.0914(2)	-0.0082(4)	0.041
H(5)	4e		-0.4543(6)	0.0255(2)	-0.0843(4)	0.047
H(6)	4e		-0.4199(7)	0.0189(3)	-0.2200(4)	0.057
H(7)	4e		-0.2737(8)	0.0785(3)	-0.2809(4)	0.056
H(8)	4e		-0.1600(6)	0.1451(2)	-0.2059(4)	0.042
H(10)	4e		-0.2592(7)	0.2783(2)	-0.1099(4)	0.045
H(11)	4e		-0.1610(9)	0.3390(3)	-0.2004(4)	0.067
H(12)	4e		0.0520(9)	0.3226(3)	-0.2536(4)	0.072
H(13)	4e		0.1696(8)	0.2464(3)	-0.2186(4)	0.066
H(14)	4e		0.0832(6)	0.1869(3)	-0.1289(4)	0.046
H(16)	4e		0.0232(6)	0.3218(3)	0.2257(4)	0.041
H(17)	4e		-0.0111(6)	0.3214(3)	0.3622(4)	0.052
H(18)	4e		-0.0699(7)	0.2435(3)	0.4260(4)	0.056
H(19)	4e		-0.0894(7)	0.1645(3)	0.3541(4)	0.058
H(20)	4e		-0.0549(6)	0.1640(3)	0.2173(4)	0.043
H(22)	4e		0.2777(6)	0.2647(3)	0.1780(4)	0.042
H(23)	4e		0.4600(7)	0.3195(3)	0.1537(4)	0.052
H(24)	4e		0.4513(8)	0.3766(3)	0.0465(5)	0.061
H(25)	4e		0.2566(9)	0.3791(3)	-0.0397(5)	0.064
H(26)	4e		0.0694(7)	0.3221(3)	-0.0180(4)	0.047
H(27)	4e		-0.1012(7)	0.0765(2)	0.0503(4)	0.043
H(28)	4e		0.0115(7)	0.0885(2)	-0.0599(4)	0.051
H(29A)	4e		0.2459(7)	0.0414(3)	0.0167(5)	0.060
H(29B)	4e		0.2321(7)	0.0557(3)	-0.0749(5)	0.060

Table 5. Continued.

Atom	Site	Occ.	x	y	z	U_{iso}
H(30A)	4e		0.3014(7)	0.1391(3)	-0.0555(5)	0.065
H(30B)	4e		0.3968(7)	0.1072(3)	0.0062(5)	0.065
H(31)	4e		0.2588(6)	0.1900(3)	0.0518(4)	0.047
H(32)	4e		0.1783(7)	0.1637(3)	0.1672(4)	0.048
H(33A)	4e		0.1997(8)	0.0787(3)	0.2172(4)	0.057
H(33B)	4e		0.2659(8)	0.0590(3)	0.1382(4)	0.057
H(34A)	4e		0.0705(8)	0.0140(3)	0.1322(4)	0.057
H(34B)	4e		-0.0124(8)	0.0593(3)	0.1743(4)	0.057
F(2A)	4e	0.50	-0.574(1)	-0.0593(4)	-0.2530(4)	0.067(3)
F(3A)	4e	0.50	-0.7463(8)	-0.1084(3)	-0.1936(6)	0.066(2)
F(4A)	4e	0.50	-0.554(1)	-0.1044(4)	-0.1340(5)	0.071(3)
F(2B)	4e	0.50	-0.5244(8)	-0.0700(4)	-0.2312(5)	0.061(3)
F(3B)	4e	0.50	-0.743(1)	-0.0897(6)	-0.2357(7)	0.107(4)
F(4B)	4e	0.50	-0.638(2)	-0.1197(4)	-0.1392(9)	0.135(5)
O(100)	4e	0.50	0.210(2)	0.0966(9)	0.438(1)	0.139(6)
C(100)	4e	0.50	0.317(3)	0.004(1)	0.426(2)	0.119(8)
C(101)	4e	0.50	0.352(3)	0.064(1)	0.426(1)	0.103(7)
C(102)	4e	0.50	0.181(5)	0.004(2)	0.419(2)	0.19(2)
C(103)	4e	0.50	0.131(1)	0.0597(4)	0.4032(6)	0.17(1)
C(200)	4e	0.50	0.276(1)	0.1195(4)	0.7282(6)	0.29(3)
O(200)	4e	0.50	0.144(1)	0.1013(4)	0.7526(6)	0.055(3)
C(202)	4e	0.50	0.106(1)	0.0560(4)	0.7049(6)	0.27(3)
C(203)	4e	0.50	0.214(1)	0.0462(4)	0.6510(6)	0.17(1)
C(204)	4e	0.50	0.319(1)	0.0855(4)	0.6654(6)	0.098(8)
C(300)	4e	0.25	0.281(2)	0.100(2)	0.741(2)	0.063(9)
Cl(1)	4e	0.25	0.094(2)	0.0769(8)	0.742(1)	0.134(5)
Cl(2)	4e	0.25	0.369(1)	0.0871(5)	0.6433(7)	0.096(3)

Table 6. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Rh	4e	0.02208(4)	0.15901(2)	0.04724(3)	0.0235(3)	0.0177(3)	0.0288(3)	0.0025(2)	0.0015(2)	-0.0025(2)
P(1)	4e	-0.1593(2)	0.17789(6)	-0.03807(9)	0.0252(8)	0.0200(8)	0.0294(8)	0.0001(6)	0.0024(6)	-0.0010(6)
P(2)	4e	0.0089(2)	0.24275(6)	0.09961(9)	0.0254(8)	0.0195(8)	0.0296(8)	0.0002(6)	0.0031(6)	-0.0028(6)
O(1)	4e	-0.2992(4)	0.2046(2)	-0.0059(2)	0.025(2)	0.036(2)	0.036(2)	0.005(2)	0.001(2)	-0.003(2)
O(2)	4e	-0.1130(4)	0.2835(2)	0.0664(2)	0.032(2)	0.018(2)	0.040(2)	0.003(2)	0.000(2)	0.001(2)
C(1)	4e	-0.3087(6)	0.2219(3)	0.0763(4)	0.023(3)	0.041(4)	0.039(4)	0.007(3)	0.005(3)	-0.010(3)
C(2)	4e	-0.2561(6)	0.2769(3)	0.0866(4)	0.029(3)	0.032(4)	0.053(4)	0.008(3)	0.002(3)	-0.011(3)
C(3)	4e	-0.2388(6)	0.1249(2)	-0.0991(3)	0.027(3)	0.018(3)	0.038(4)	-0.001(2)	0.003(3)	0.002(3)
C(4)	4e	-0.3260(6)	0.0891(2)	-0.0631(4)	0.024(3)	0.033(3)	0.045(4)	-0.001(3)	0.004(3)	0.004(3)
C(5)	4e	-0.3949(6)	0.0493(2)	-0.1088(4)	0.031(3)	0.023(3)	0.063(5)	-0.003(3)	-0.002(3)	-0.001(3)
C(6)	4e	-0.3748(7)	0.0455(3)	-0.1897(4)	0.051(4)	0.029(4)	0.061(5)	0.007(3)	-0.019(4)	-0.015(3)

Table 6. Continued.

Atom	Site	x	y	z	U ₁₁	U ₂₂	U ₃₃	U ₁₂	U ₁₃	U ₂₃
C(7)	4e	-0.2872(8)	0.0812(3)	-0.2260(4)	0.060(5)	0.041(4)	0.040(4)	-0.001(4)	-0.002(3)	-0.009(3)
C(8)	4e	-0.2187(6)	0.1211(2)	-0.1811(4)	0.035(3)	0.028(3)	0.042(4)	0.002(3)	0.007(3)	-0.006(3)
C(9)	4e	-0.0985(6)	0.2262(2)	-0.1096(3)	0.026(3)	0.025(3)	0.032(3)	-0.003(3)	-0.002(3)	0.000(3)
C(10)	4e	-0.1728(7)	0.2715(2)	-0.1307(4)	0.047(4)	0.027(3)	0.038(4)	-0.004(3)	-0.004(3)	0.004(3)
C(11)	4e	-0.1127(9)	0.3080(3)	-0.1858(4)	0.094(6)	0.026(4)	0.045(4)	-0.011(4)	-0.023(4)	0.009(3)
C(12)	4e	0.0146(9)	0.2984(3)	-0.2178(4)	0.077(6)	0.060(6)	0.042(4)	-0.035(5)	0.006(4)	0.011(4)
C(13)	4e	0.0842(8)	0.2533(3)	-0.1965(4)	0.055(5)	0.065(5)	0.045(4)	-0.015(4)	0.008(4)	0.007(4)
C(14)	4e	0.0322(6)	0.2174(3)	-0.1432(4)	0.035(4)	0.040(4)	0.040(4)	-0.006(3)	0.005(3)	0.004(3)
C(15)	4e	-0.0111(6)	0.2425(2)	0.2079(3)	0.021(3)	0.028(3)	0.035(3)	-0.003(2)	0.006(2)	-0.002(3)
C(16)	4e	0.0010(6)	0.2900(3)	0.2514(4)	0.029(3)	0.037(4)	0.038(4)	-0.007(3)	0.006(3)	-0.012(3)
C(17)	4e	-0.0203(6)	0.2897(3)	0.3329(4)	0.029(3)	0.057(5)	0.045(4)	-0.003(3)	0.004(3)	-0.023(4)
C(18)	4e	-0.0547(7)	0.2433(3)	0.3712(4)	0.033(4)	0.076(6)	0.031(4)	-0.004(4)	0.010(3)	-0.009(4)
C(19)	4e	-0.0669(7)	0.1961(3)	0.3281(4)	0.049(4)	0.054(5)	0.042(4)	0.001(4)	0.014(3)	0.006(3)
C(20)	4e	-0.0457(6)	0.1958(3)	0.2463(4)	0.034(3)	0.032(4)	0.041(4)	0.001(3)	0.009(3)	-0.004(3)
C(21)	4e	0.1538(6)	0.2870(2)	0.0827(4)	0.036(4)	0.017(3)	0.040(4)	0.001(3)	0.004(3)	-0.004(3)
C(22)	4e	0.2728(6)	0.2874(3)	0.1336(4)	0.035(4)	0.032(3)	0.040(4)	0.004(3)	0.007(3)	-0.006(3)
C(23)	4e	0.3813(7)	0.3203(3)	0.1194(4)	0.032(4)	0.043(4)	0.055(4)	0.001(3)	0.006(3)	-0.016(4)
C(24)	4e	0.3763(8)	0.3542(3)	0.0556(5)	0.043(4)	0.038(4)	0.074(5)	-0.018(3)	0.028(4)	-0.016(4)
C(25)	4e	0.2599(9)	0.3556(3)	0.0038(5)	0.071(5)	0.034(4)	0.057(5)	-0.010(4)	0.031(4)	0.007(3)
C(26)	4e	0.1474(7)	0.3216(3)	0.0168(4)	0.042(4)	0.037(4)	0.038(4)	-0.005(3)	0.008(3)	-0.002(3)
C(27)	4e	-0.0060(7)	0.0700(2)	0.0534(4)	0.033(3)	0.025(3)	0.049(4)	0.003(3)	-0.001(3)	-0.004(3)
C(28)	4e	0.0625(7)	0.0774(2)	-0.0142(4)	0.047(4)	0.028(3)	0.051(4)	0.012(3)	-0.011(3)	-0.016(3)
C(29)	4e	0.2155(7)	0.0689(3)	-0.0213(5)	0.051(4)	0.047(4)	0.052(4)	0.019(4)	0.006(3)	-0.015(3)
C(30)	4e	0.3016(7)	0.1181(3)	-0.0063(5)	0.038(4)	0.062(5)	0.063(5)	0.008(4)	0.011(4)	-0.007(4)
C(31)	4e	0.2541(6)	0.1532(3)	0.0603(4)	0.028(3)	0.029(3)	0.061(5)	0.008(3)	-0.002(3)	-0.006(3)
C(32)	4e	0.2050(7)	0.1370(3)	0.1319(4)	0.039(4)	0.035(4)	0.045(4)	0.015(3)	-0.011(3)	-0.011(3)
C(33)	4e	0.1899(8)	0.0797(3)	0.1590(4)	0.055(4)	0.045(4)	0.042(4)	0.013(4)	-0.008(3)	-0.001(3)
C(34)	4e	0.0550(8)	0.0524(3)	0.1338(4)	0.060(5)	0.029(4)	0.054(4)	0.010(3)	-0.001(4)	0.010(3)
B	4e	-0.6368(5)	-0.0740(2)	-0.1843(3)	0.055(5)	0.032(4)	0.062(5)	-0.023(4)	0.024(4)	0.001(4)
F(1)	4e	-0.6749(6)	-0.0286(2)	-0.1453(4)	0.099(4)	0.040(3)	0.140(5)	-0.006(3)	0.046(3)	-0.044(3)

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