# Crystal structure of 1,3-bis(diphenylphosphino)-propane rhodium(I)-norborna-2,5-diene tetrafluoroborate, $C_{34}H_{34}BF_4P_2Rh$, and of 1,3-bis(diphenylphosphino)-propane rhodium(I)-(Z,Z)-cycloocta-1,5-diene tetrafluoroborate, $C_{35}H_{38}BF_4P_2Rh$

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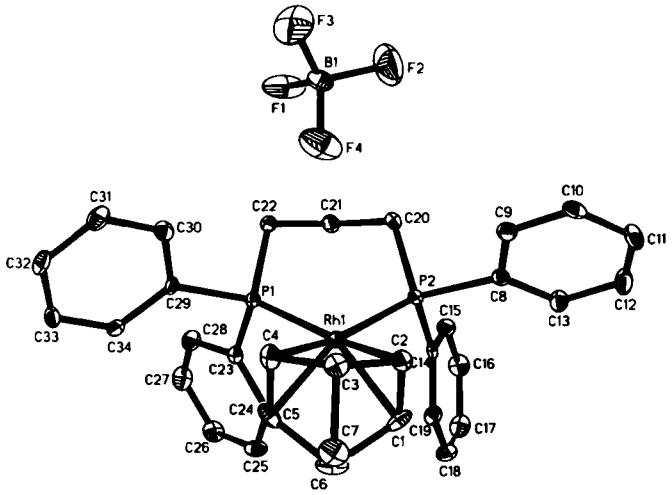


**Abstract**

$C_{34}H_{34}BF_4P_2Rh$, monoclinic, $P12_1/c1$ (No. 14), $a = 15.193(3)$ Å, $b = 12.835(3)$ Å, $c = 17.096(3)$ Å, $\beta = 114.29(3)°$, $V = 3038.7$ Å$^3$, $Z = 4$, $R_{gt}(F) = 0.033$, $wR_{all}(F^2) = 0.058$, $T = 200$ K.

$C_{35}H_{38}BF_4P_2Rh$, monoclinic, $P12_1/n1$ (No. 14), $a = 10.343(2)$ Å, $b = 15.150(2)$ Å, $c = 20.432(3)$ Å, $\beta = 99.76(2)°$, $V = 3155.3$ Å$^3$, $Z = 4$, $R_{gt}(F) = 0.035$, $wR_{all}(F^2) = 0.067$, $T = 200$ K.

**Source of material**

Standard procedure according to [1] – the bisphosphine ligand is commercially available.

**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 [2]) motivated us to determine the crystal structures. The ratio of the rate constants for the hydrogenation of the diolefine complexes is 65 [3]. Also for six-membered ring chelates [4], 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 10.6°, for the nbd-complex 2.5°.

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## 1. 1,3-bis(diphenylphosphino)-propane rhodium(I)-norborna-2,5-diene tetrafluoroborate, $C_{34}H_{34}BF_4P_2Rh$

**Table 1.** Data collection and handling.

| | |
|---|---|
| Crystal: | orange prism, size 0.2 × 0.3 × 0.3 mm |
| Wavelength: | Mo $K_\alpha$ radiation (0.71073 Å) |
| $\mu$: | 7.15 cm$^{-1}$ |
| Diffractometer, scan mode: | STOE IPDS, 100 exposures, $\Delta\varphi = 2°$ |
| $2\theta_{max}$: | 48.54° |
| $N(hkl)_{measured}$, $N(hkl)_{unique}$: | 8831, 4825 |
| Criterion for $I_{obs}$, $N(hkl)_{gt}$: | $I_{obs} > 2\,\sigma(I_{obs})$, 3197 |
| $N(param)_{refined}$: | 379 |
| Programs: | SHELXS-86 [4], SHELXL-93 [5] |

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

| Atom | Site | x | y | z | $U_{iso}$ |
|---|---|---|---|---|---|
| H(1) | 4e | 0.4192(3) | –0.1301(3) | 0.4264(3) | 0.034 |
| H(2) | 4e | 0.2665(3) | –0.1688(3) | 0.4433(2) | 0.028 |
| H(3) | 4e | 0.2052(3) | –0.3489(3) | 0.3792(3) | 0.032 |
| H(4) | 4e | 0.1584(3) | –0.2751(3) | 0.2278(3) | 0.032 |
| H(5) | 4e | 0.3082(3) | –0.2339(3) | 0.2079(3) | 0.035 |
| H(6) | 4e | 0.4551(3) | –0.2832(3) | 0.3461(3) | 0.044 |
| H(7A) | 4e | 0.3392(3) | –0.4311(3) | 0.3445(3) | 0.046 |
| H(7B) | 4e | 0.3882(3) | –0.3832(3) | 0.4410(3) | 0.046 |
| H(9) | 4e | 0.1577(3) | –0.0315(3) | 0.4386(3) | 0.029 |
| H(10) | 4e | 0.1607(3) | –0.0236(3) | 0.5766(3) | 0.033 |
| H(11) | 4e | 0.2811(3) | 0.0708(3) | 0.6836(3) | 0.044 |
| H(12) | 4e | 0.3940(3) | 0.1649(4) | 0.6513(3) | 0.045 |
| H(13) | 4e | 0.3929(3) | 0.1542(3) | 0.5150(2) | 0.033 |
| H(15) | 4e | 0.2987(3) | 0.2755(3) | 0.3334(3) | 0.030 |
| H(16) | 4e | 0.4303(3) | 0.3722(3) | 0.3392(3) | 0.040 |
| H(17) | 4e | 0.5776(3) | 0.2914(3) | 0.3673(3) | 0.042 |
| H(18) | 4e | 0.5903(3) | 0.1111(3) | 0.3829(3) | 0.037 |
| H(19) | 4e | 0.4586(3) | 0.0128(3) | 0.3759(2) | 0.029 |
| H(20A) | 4e | 0.1001(2) | 0.0989(3) | 0.3017(2) | 0.027 |
| H(20B) | 4e | 0.1649(2) | 0.2019(3) | 0.3252(2) | 0.027 |
| H(21A) | 4e | 0.0828(3) | 0.2097(3) | 0.1802(2) | 0.031 |
| H(21B) | 4e | 0.1890(3) | 0.1743(3) | 0.1941(2) | 0.031 |
| H(22A) | 4e | 0.0619(3) | 0.0797(3) | 0.0826(2) | 0.026 |
| H(22B) | 4e | 0.0335(3) | 0.0297(3) | 0.1547(2) | 0.026 |
| H(24) | 4e | 0.3809(3) | –0.0286(3) | 0.2142(3) | 0.027 |
| H(25) | 4e | 0.4826(3) | 0.0420(3) | 0.1572(3) | 0.036 |
| H(26) | 4e | 0.4197(3) | 0.1097(3) | 0.0185(3) | 0.039 |
| H(27) | 4e | 0.2525(3) | 0.1101(3) | –0.0623(3) | 0.042 |
| H(28) | 4e | 0.1501(3) | 0.0440(3) | –0.0052(3) | 0.036 |
| H(30) | 4e | 0.0052(3) | –0.1599(3) | 0.1376(2) | 0.029 |
| H(31) | 4e | –0.0860(3) | –0.2927(3) | 0.0483(3) | 0.038 |
| H(32) | 4e | –0.0426(3) | –0.3628(3) | –0.0565(3) | 0.035 |
| H(33) | 4e | 0.0913(3) | –0.2976(3) | –0.0738(3) | 0.031 |
| H(34) | 4e | 0.1848(3) | –0.1668(3) | 0.0160(2) | 0.025 |

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

| Atom | Site | x | y | z | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{12}$ | $U_{13}$ | $U_{23}$ |
|---|---|---|---|---|---|---|---|---|---|---|
| C(1) | 4e | 0.3772(3) | -0.1876(3) | 0.4027(3) | 0.016(2) | 0.024(2) | 0.031(3) | 0.000(2) | -0.003(2) | 0.010(2) |
| C(2) | 4e | 0.2939(3) | -0.2092(3) | 0.4124(2) | 0.028(2) | 0.021(2) | 0.021(2) | 0.002(2) | 0.010(2) | 0.004(2) |
| C(3) | 4e | 0.2535(3) | -0.3104(3) | 0.3644(3) | 0.032(2) | 0.020(2) | 0.030(3) | -0.005(2) | 0.016(2) | 0.006(2) |
| C(4) | 4e | 0.2227(3) | -0.2786(3) | 0.2705(3) | 0.038(3) | 0.010(2) | 0.028(3) | -0.004(2) | 0.010(2) | -0.003(2) |
| C(5) | 4e | 0.3046(3) | -0.2564(3) | 0.2595(3) | 0.049(3) | 0.014(2) | 0.032(3) | 0.006(2) | 0.026(2) | 0.001(2) |
| C(6) | 4e | 0.3897(3) | -0.2745(3) | 0.3461(3) | 0.028(3) | 0.033(3) | 0.057(3) | 0.008(2) | 0.026(2) | 0.013(2) |
| C(7) | 4e | 0.3490(3) | -0.3674(3) | 0.3798(3) | 0.047(3) | 0.024(3) | 0.044(3) | 0.007(2) | 0.020(2) | 0.010(2) |
| C(8) | 4e | 0.2748(3) | 0.0613(3) | 0.4629(2) | 0.021(2) | 0.018(2) | 0.019(2) | 0.004(2) | 0.008(2) | 0.001(2) |
| C(9) | 4e | 0.2062(3) | 0.0081(3) | 0.4820(3) | 0.022(2) | 0.024(2) | 0.029(3) | -0.003(2) | 0.011(2) | -0.007(2) |
| C(10) | 4e | 0.2081(3) | 0.0124(3) | 0.5642(3) | 0.026(2) | 0.034(3) | 0.033(3) | 0.001(2) | 0.021(2) | 0.002(2) |
| C(11) | 4e | 0.2787(3) | 0.0690(3) | 0.6272(3) | 0.046(3) | 0.050(3) | 0.021(3) | 0.003(2) | 0.020(2) | 0.001(2) |
| C(12) | 4e | 0.3466(3) | 0.1238(4) | 0.6083(3) | 0.041(3) | 0.048(3) | 0.021(2) | -0.009(2) | 0.009(2) | -0.010(2) |
| C(13) | 4e | 0.3451(3) | 0.1184(3) | 0.5270(2) | 0.027(2) | 0.035(2) | 0.022(2) | -0.012(2) | 0.011(2) | -0.005(2) |
| C(14) | 4e | 0.3646(3) | 0.1338(3) | 0.3537(2) | 0.024(2) | 0.019(2) | 0.009(2) | -0.002(2) | 0.006(2) | -0.003(2) |
| C(15) | 4e | 0.3578(3) | 0.2413(3) | 0.3434(3) | 0.024(2) | 0.024(2) | 0.027(3) | 0.001(2) | 0.011(2) | -0.001(2) |
| C(16) | 4e | 0.4363(3) | 0.2989(3) | 0.3474(3) | 0.041(3) | 0.023(2) | 0.039(3) | -0.008(2) | 0.018(2) | 0.001(2) |
| C(17) | 4e | 0.5234(3) | 0.2511(3) | 0.3632(3) | 0.031(3) | 0.039(3) | 0.034(3) | -0.016(2) | 0.015(2) | -0.001(2) |
| C(18) | 4e | 0.5310(3) | 0.1447(3) | 0.3730(3) | 0.019(2) | 0.036(3) | 0.034(3) | -0.002(2) | 0.009(2) | -0.003(2) |
| C(19) | 4e | 0.4524(3) | 0.0862(3) | 0.3686(2) | 0.023(2) | 0.023(2) | 0.023(2) | -0.003(2) | 0.006(2) | -0.002(2) |
| C(20) | 4e | 0.1556(2) | 0.1334(3) | 0.2961(2) | 0.023(2) | 0.023(2) | 0.021(2) | 0.002(2) | 0.010(2) | -0.004(2) |
| C(21) | 4e | 0.1300(3) | 0.1519(3) | 0.2005(2) | 0.029(2) | 0.025(2) | 0.020(2) | 0.011(2) | 0.007(2) | 0.001(2) |
| C(22) | 4e | 0.0880(3) | 0.0573(3) | 0.1434(2) | 0.019(2) | 0.028(2) | 0.016(2) | 0.004(2) | 0.005(2) | 0.000(2) |
| C(23) | 4e | 0.2543(3) | 0.0028(3) | 0.1117(2) | 0.022(2) | 0.014(2) | 0.016(2) | -0.001(2) | 0.007(2) | 0.001(2) |
| C(24) | 4e | 0.3542(3) | 0.0010(3) | 0.1583(3) | 0.020(2) | 0.025(2) | 0.022(2) | 0.001(2) | 0.008(2) | -0.001(2) |
| C(25) | 4e | 0.4148(3) | 0.0418(3) | 0.1240(3) | 0.020(2) | 0.023(2) | 0.048(3) | -0.003(2) | 0.016(2) | -0.003(2) |
| C(26) | 4e | 0.3777(3) | 0.0823(3) | 0.0421(3) | 0.036(3) | 0.036(3) | 0.036(3) | -0.010(2) | 0.025(2) | 0.001(2) |
| C(27) | 4e | 0.2785(3) | 0.0826(3) | -0.0057(3) | 0.047(3) | 0.034(3) | 0.025(3) | -0.008(2) | 0.016(2) | 0.007(2) |
| C(28) | 4e | 0.2178(3) | 0.0435(3) | 0.0283(3) | 0.029(2) | 0.030(2) | 0.028(3) | -0.005(2) | 0.010(2) | -0.001(2) |
| C(29) | 4e | 0.1037(2) | -0.1481(3) | 0.0853(2) | 0.017(2) | 0.019(2) | 0.012(2) | 0.001(2) | 0.000(2) | -0.002(2) |
| C(30) | 4e | 0.0231(3) | -0.1875(3) | 0.0947(2) | 0.027(2) | 0.029(2) | 0.022(2) | -0.004(2) | 0.015(2) | 0.000(2) |
| C(31) | 4e | -0.0309(3) | -0.2667(3) | 0.0417(3) | 0.026(2) | 0.035(3) | 0.030(3) | -0.012(2) | 0.008(2) | 0.002(2) |
| C(32) | 4e | -0.0055(3) | -0.3082(3) | -0.0206(3) | 0.028(2) | 0.022(2) | 0.026(3) | -0.006(2) | -0.001(2) | -0.005(2) |
| C(33) | 4e | 0.0742(3) | -0.2699(3) | -0.0304(3) | 0.029(2) | 0.023(2) | 0.022(3) | 0.003(2) | 0.006(2) | -0.008(2) |
| C(34) | 4e | 0.1292(3) | -0.1915(3) | 0.0224(2) | 0.015(2) | 0.023(2) | 0.021(2) | -0.001(2) | 0.005(2) | -0.001(2) |
| B(1) | 4e | -0.0852(4) | -0.0460(4) | 0.2555(4) | 0.035(3) | 0.028(3) | 0.040(3) | 0.002(2) | 0.025(3) | 0.004(3) |
| F(1) | 4e | -0.0947(2) | 0.0118(2) | 0.1853(2) | 0.052(2) | 0.101(2) | 0.077(2) | 0.033(2) | 0.042(2) | 0.060(2) |
| F(2) | 4e | -0.0685(3) | 0.0183(3) | 0.3233(2) | 0.117(3) | 0.084(2) | 0.082(3) | -0.016(2) | 0.048(2) | -0.040(2) |
| F(3) | 4e | -0.1682(2) | -0.0993(3) | 0.2401(2) | 0.082(2) | 0.089(2) | 0.098(3) | -0.047(2) | 0.043(2) | -0.001(2) |
| F(4) | 4e | -0.0068(2) | -0.1111(3) | 0.2776(2) | 0.091(2) | 0.090(2) | 0.078(2) | 0.054(2) | 0.052(2) | 0.042(2) |
| P(1) | 4e | 0.17531(7) | -0.04764(8) | 0.15924(6) | 0.0157(5) | 0.0202(6) | 0.0146(6) | -0.0001(4) | 0.0060(4) | -0.0016(5) |
| P(2) | 4e | 0.26352(7) | 0.05453(8) | 0.35189(6) | 0.0165(5) | 0.0169(5) | 0.0160(6) | 0.0004(4) | 0.0074(5) | -0.0025(5) |
| Rh(1) | 4e | 0.25760(2) | -0.10993(2) | 0.29652(2) | 0.0170(2) | 0.0157(1) | 0.0143(2) | 0.0007(2) | 0.0052(1) | -0.0005(2) |

## 2. 1,3-bis(diphenylphosphino)-propane rhodium(I)-(*Z*,*Z*)-cycloocta-1,5-diene tetrafluoroborate, $C_{35}H_{38}BF_4P_2Rh$

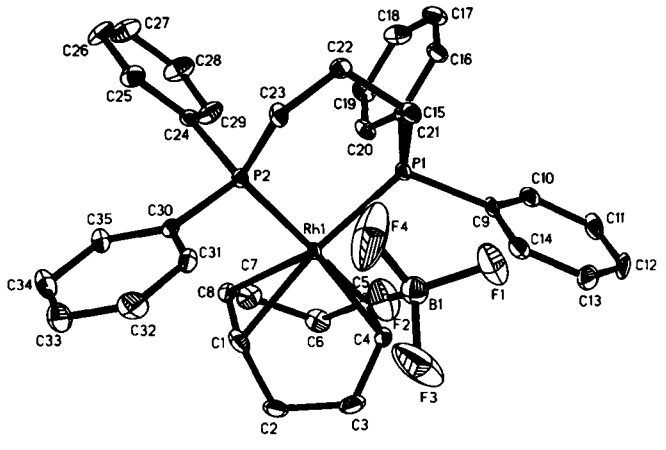


**Table 4.** Data collection and handling.

| | |
|---|---|
| Crystal: | Orange prism, size 0.2 × 0.2 × 0.3 mm |
| Wavelength: | Mo $K_\alpha$ radiation (0.71069 Å) |
| μ: | 6.91 $cm^{-1}$ |
| Diffractometer, scan mode: | STOE IPDS, 100 exposures, $\Delta\varphi = 2°$ |
| $2\theta_{max}$: | 48.38° |
| $N(hkl)_{measured}$, $N(hkl)_{unique}$: | 9157, 4718 |
| Criterion for $I_{obs}$, $N(hkl)_{gt}$: | $I_{obs} > 2\ \sigma(I_{obs})$, 2537 |
| $N(param)_{refined}$: | 388 |
| Programs: | SHELXS-86 [4], SHELXL-93 [5] |

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

| Atom | Site | $x$ | $y$ | $z$ | $U_{iso}$ |
|---|---|---|---|---|---|
| H(1) | 4*e* | 0.0795(7) | 0.1096(4) | 0.3511(3) | 0.040 |
| H(2A) | 4*e* | –0.1581(6) | 0.1959(3) | 0.2950(3) | 0.041 |
| H(2B) | 4*e* | –0.0640(6) | 0.1436(3) | 0.2539(3) | 0.041 |
| H(3A) | 4*e* | 0.0690(6) | 0.2597(3) | 0.2503(2) | 0.046 |
| H(3B) | 4*e* | –0.0715(6) | 0.3060(3) | 0.2428(2) | 0.046 |
| H(4) | 4*e* | 0.1248(6) | 0.3600(3) | 0.3322(3) | 0.036 |
| H(5) | 4*e* | 0.0270(6) | 0.3819(3) | 0.4194(3) | 0.035 |
| H(6A) | 4*e* | –0.2058(6) | 0.3012(4) | 0.3545(3) | 0.046 |
| H(6B) | 4*e* | –0.1867(6) | 0.3485(4) | 0.4254(3) | 0.046 |
| H(7A) | 4*e* | –0.1202(6) | 0.2251(4) | 0.4806(3) | 0.048 |
| H(7B) | 4*e* | –0.2182(6) | 0.1840(4) | 0.4195(3) | 0.048 |
| H(8) | 4*e* | 0.0237(6) | 0.1267(3) | 0.4521(3) | 0.032 |
| H(10) | 4*e* | 0.2150(6) | 0.5406(3) | 0.4685(3) | 0.036 |
| H(11) | 4*e* | 0.2117(6) | 0.6638(4) | 0.3991(4) | 0.046 |
| H(12) | 4*e* | 0.2926(7) | 0.6534(4) | 0.3004(4) | 0.055 |
| H(13) | 4*e* | 0.3764(6) | 0.5205(4) | 0.2698(3) | 0.049 |
| H(14) | 4*e* | 0.3719(6) | 0.3950(3) | 0.3358(3) | 0.035 |
| H(16) | 4*e* | 0.4317(7) | 0.4564(3) | 0.5706(3) | 0.036 |
| H(17) | 4*e* | 0.3769(7) | 0.5139(4) | 0.6679(3) | 0.045 |

**Table 5.** Continued.

| Atom | Site | $x$ | $y$ | $z$ | $U_{iso}$ |
|---|---|---|---|---|---|
| H(18) | 4*e* | 0.1763(7) | 0.4815(4) | 0.6986(3) | 0.046 |
| H(19) | 4*e* | 0.0197(6) | 0.4001(3) | 0.6265(3) | 0.040 |
| H(20) | 4*e* | 0.0697(6) | 0.3487(3) | 0.5268(3) | 0.034 |
| H(21A) | 4*e* | 0.4949(6) | 0.3162(3) | 0.4327(3) | 0.030 |
| H(21B) | 4*e* | 0.5136(6) | 0.3785(3) | 0.4967(3) | 0.030 |
| H(22A) | 4*e* | 0.4511(4) | 0.2506(4) | 0.5585(2) | 0.034 |
| H(22B) | 4*e* | 0.5934(4) | 0.2462(4) | 0.5377(2) | 0.034 |
| H(23A) | 4*e* | 0.5056(6) | 0.1099(3) | 0.5105(3) | 0.029 |
| H(23B) | 4*e* | 0.4938(6) | 0.1599(3) | 0.4409(3) | 0.029 |
| H(25) | 4*e* | 0.3692(6) | –0.0032(3) | 0.5643(3) | 0.036 |
| H(26) | 4*e* | 0.3246(7) | –0.0363(4) | 0.6700(3) | 0.050 |
| H(27) | 4*e* | 0.1882(7) | 0.0542(4) | 0.7197(3) | 0.056 |
| H(28) | 4*e* | 0.0921(6) | 0.1779(4) | 0.6634(3) | 0.055 |
| H(29) | 4*e* | 0.1260(6) | 0.2071(3) | 0.5557(3) | 0.038 |
| H(31) | 4*e* | 0.4008(6) | 0.0734(3) | 0.3587(3) | 0.033 |
| H(32) | 4*e* | 0.3926(7) | –0.0558(4) | 0.2970(3) | 0.047 |
| H(33) | 4*e* | 0.2629(7) | –0.1734(4) | 0.3196(3) | 0.050 |
| H(34) | 4*e* | 0.1408(7) | –0.1617(4) | 0.4049(3) | 0.045 |
| H(35) | 4*e* | 0.1520(6) | –0.0343(3) | 0.4695(3) | 0.030 |

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

| Atom | Site | $x$ | $y$ | $z$ | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{12}$ | $U_{13}$ | $U_{23}$ |
|---|---|---|---|---|---|---|---|---|---|---|
| C(1) | 4*e* | 0.0060(7) | 0.1460(4) | 0.3541(3) | 0.024(4) | 0.024(3) | 0.048(5) | –0.005(3) | –0.004(3) | –0.006(3) |
| C(2) | 4*e* | –0.0654(6) | 0.1858(3) | 0.2907(3) | 0.036(4) | 0.035(3) | 0.026(3) | 0.000(3) | –0.008(3) | –0.008(2) |
| C(3) | 4*e* | –0.0050(6) | 0.2727(3) | 0.2738(2) | 0.036(4) | 0.052(4) | 0.023(3) | –0.001(3) | –0.005(2) | 0.009(3) |
| C(4) | 4*e* | 0.0439(6) | 0.3303(3) | 0.3322(3) | 0.018(4) | 0.025(3) | 0.041(4) | –0.003(2) | –0.016(3) | 0.015(3) |
| C(5) | 4*e* | –0.0171(6) | 0.3442(3) | 0.3857(3) | 0.030(4) | 0.015(3) | 0.037(4) | 0.005(2) | –0.013(3) | 0.000(3) |
| C(6) | 4*e* | –0.1462(6) | 0.3066(4) | 0.3976(3) | 0.027(4) | 0.039(4) | 0.047(4) | 0.010(3) | 0.003(3) | –0.008(3) |
| C(7) | 4*e* | –0.1340(6) | 0.2157(4) | 0.4320(3) | 0.024(4) | 0.055(4) | 0.042(4) | 0.000(3) | 0.008(3) | 0.010(3) |
| C(8) | 4*e* | –0.0266(6) | 0.1580(3) | 0.4162(3) | 0.012(4) | 0.026(3) | 0.037(4) | –0.004(2) | –0.009(3) | 0.012(3) |
| C(9) | 4*e* | 0.2925(6) | 0.4554(3) | 0.4085(3) | 0.021(4) | 0.009(3) | 0.032(4) | –0.002(2) | –0.003(3) | 0.001(2) |
| C(10) | 4*e* | 0.2462(6) | 0.5357(3) | 0.4275(3) | 0.020(4) | 0.027(3) | 0.038(4) | –0.005(2) | –0.006(3) | 0.001(3) |
| C(11) | 4*e* | 0.2454(6) | 0.6092(4) | 0.3865(4) | 0.026(5) | 0.018(3) | 0.066(5) | –0.001(3) | –0.006(4) | 0.010(3) |
| C(12) | 4*e* | 0.2931(7) | 0.6031(4) | 0.3282(4) | 0.040(5) | 0.030(4) | 0.061(5) | –0.011(3) | –0.013(4) | 0.032(3) |
| C(13) | 4*e* | 0.3416(6) | 0.5242(4) | 0.3098(3) | 0.031(4) | 0.049(4) | 0.041(4) | –0.016(3) | –0.001(3) | 0.017(3) |
| C(14) | 4*e* | 0.3402(6) | 0.4497(3) | 0.3494(3) | 0.025(4) | 0.030(3) | 0.031(4) | –0.008(3) | 0.004(3) | –0.004(3) |
| C(15) | 4*e* | 0.2543(6) | 0.3956(3) | 0.5372(3) | 0.019(4) | 0.010(3) | 0.018(3) | –0.001(2) | –0.001(3) | 0.002(2) |
| C(16) | 4*e* | 0.3472(7) | 0.4455(3) | 0.5813(3) | 0.028(4) | 0.033(3) | 0.028(3) | –0.010(3) | 0.000(3) | –0.005(3) |
| C(17) | 4*e* | 0.3152(7) | 0.4784(4) | 0.6397(3) | 0.035(5) | 0.047(4) | 0.028(4) | –0.009(3) | –0.001(3) | –0.009(3) |
| C(18) | 4*e* | 0.1956(7) | 0.4606(4) | 0.6575(3) | 0.038(5) | 0.048(4) | 0.027(4) | 0.015(3) | 0.002(3) | –0.009(3) |
| C(19) | 4*e* | 0.1032(6) | 0.4120(3) | 0.6150(3) | 0.023(4) | 0.040(3) | 0.040(4) | –0.002(3) | 0.011(3) | –0.004(3) |
| C(20) | 4*e* | 0.1340(6) | 0.3812(3) | 0.5558(3) | 0.023(4) | 0.024(3) | 0.037(4) | –0.001(2) | 0.002(3) | –0.010(3) |
| C(21) | 4*e* | 0.4646(6) | 0.3270(3) | 0.4755(3) | 0.019(4) | 0.022(3) | 0.033(4) | 0.000(2) | –0.001(3) | –0.004(3) |
| C(22) | 4*e* | 0.4981(4) | 0.2463(4) | 0.5202(2) | 0.022(3) | 0.024(2) | 0.036(3) | 0.004(3) | –0.008(2) | 0.004(3) |
| C(23) | 4*e* | 0.4610(6) | 0.1590(3) | 0.4836(3) | 0.020(4) | 0.013(3) | 0.039(4) | 0.005(2) | 0.003(3) | –0.001(2) |
| C(24) | 4*e* | 0.2498(6) | 0.1061(3) | 0.5502(3) | 0.022(4) | 0.024(3) | 0.015(3) | –0.001(2) | 0.002(3) | 0.000(2) |
| C(25) | 4*e* | 0.3112(6) | 0.0328(3) | 0.5841(3) | 0.030(4) | 0.030(3) | 0.030(4) | 0.012(3) | 0.002(3) | 0.000(3) |
| C(26) | 4*e* | 0.2857(7) | 0.0140(4) | 0.6469(3) | 0.051(6) | 0.043(4) | 0.027(4) | 0.011(3) | 0.000(4) | 0.017(3) |
| C(27) | 4*e* | 0.2044(7) | 0.0674(4) | 0.6763(3) | 0.045(5) | 0.067(5) | 0.027(4) | 0.013(4) | 0.009(3) | 0.014(3) |
| C(28) | 4*e* | 0.1467(6) | 0.1402(4) | 0.6429(3) | 0.053(5) | 0.059(4) | 0.027(4) | 0.023(3) | 0.011(3) | 0.001(3) |
| C(29) | 4*e* | 0.1683(6) | 0.1581(3) | 0.5793(3) | 0.031(4) | 0.036(3) | 0.029(3) | 0.018(3) | 0.008(3) | 0.006(3) |
| C(30) | 4*e* | 0.2789(6) | 0.0330(3) | 0.4211(3) | 0.018(4) | 0.016(3) | 0.018(3) | 0.005(2) | 0.002(2) | 0.003(2) |
| C(31) | 4*e* | 0.3486(6) | 0.0254(3) | 0.3690(3) | 0.036(4) | 0.019(3) | 0.027(3) | –0.002(2) | 0.005(3) | 0.005(2) |
| C(32) | 4*e* | 0.3430(7) | –0.0512(4) | 0.3320(3) | 0.052(5) | 0.040(4) | 0.028(4) | 0.009(3) | 0.011(3) | –0.010(3) |
| C(33) | 4*e* | 0.2664(7) | –0.1209(4) | 0.3452(3) | 0.056(5) | 0.022(3) | 0.045(5) | 0.009(3) | 0.002(4) | –0.009(3) |
| C(34) | 4*e* | 0.1949(7) | –0.1140(4) | 0.3960(3) | 0.036(5) | 0.022(3) | 0.054(4) | –0.006(3) | 0.005(3) | –0.006(3) |
| C(35) | 4*e* | 0.2010(6) | –0.0380(3) | 0.4342(3) | 0.024(4) | 0.019(3) | 0.033(3) | –0.001(2) | 0.008(3) | –0.001(2) |
| B(1) | 4*e* | 0.4921(7) | 0.2365(5) | 0.2848(3) | 0.041(5) | 0.032(4) | 0.034(4) | 0.000(4) | 0.011(3) | –0.005(3) |
| F(1) | 4*e* | 0.5502(4) | 0.3198(2) | 0.2889(2) | 0.069(3) | 0.053(2) | 0.083(3) | –0.026(2) | 0.026(2) | –0.017(2) |
| F(2) | 4*e* | 0.3709(3) | 0.2378(3) | 0.3047(2) | 0.048(2) | 0.055(2) | 0.088(2) | –0.007(2) | 0.035(2) | –0.008(2) |
| F(3) | 4*e* | 0.4715(5) | 0.2160(3) | 0.2201(2) | 0.141(5) | 0.173(5) | 0.074(3) | –0.106(4) | 0.057(3) | –0.071(3) |
| F(4) | 4*e* | 0.5673(5) | 0.1815(4) | 0.3233(4) | 0.048(4) | 0.118(4) | 0.263(8) | 0.015(3) | 0.014(4) | 0.123(5) |
| P(1) | 4*e* | 0.2900(2) | 0.35429(9) | 0.45856(8) | 0.018(1) | 0.0132(7) | 0.0237(9) | –0.0008(6) | 0.0003(7) | –0.0005(6) |
| P(2) | 4*e* | 0.2841(2) | 0.13704(9) | 0.46719(8) | 0.019(1) | 0.0123(7) | 0.0226(9) | 0.0020(6) | 0.0025(7) | –0.0007(6) |
| Rh(1) | 4*e* | 0.14581(4) | 0.24497(3) | 0.41384(2) | 0.0156(2) | 0.0098(2) | 0.0232(2) | –0.0007(3) | –0.0020(1) | 0.0005(3) |

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