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Complexation of Diphenyl(phenylacetylenyl)phosphine to Rhodium(III) Tetraphenyl Porphyrins

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_audit_creation_method 'SHELXL-97 plus manual editing'

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denoted 2 in text

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data_2

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    HKL Denzo and Scalepack (Otwinowski & Minor 1997)
;
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_atom_sites_solution_hydrogens    geom
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_refine_ls_extinction_coef         ?
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N2 N 0.2321(8) 0.2530(7) 0.2498(3) 0.0275(16) Uani 1 1 d . A .
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C2 C -0.0125(13) 0.6460(10) 0.3575(5) 0.047(3) Uani 1 1 d . . .
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C5 C 0.1700(12) 0.2930(9) 0.3574(4) 0.041(2) Uani 1 1 d . . .
C6 C 0.2312(10) 0.2100(8) 0.3132(4) 0.032(2) Uani 1 1 d . A .
C7 C 0.3033(11) 0.0659(8) 0.3270(4) 0.036(2) Uani 1 1 d . . .
H7A H 0.3176 0.0113 0.3672 0.044 Uiso 1 1 calc R A .
C8 C 0.3465(10) 0.0229(9) 0.2730(4) 0.034(2) Uani 1 1 d . A .
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C9 C 0.3038(9) 0.1380(8) 0.2243(4) 0.0268(18) Uani 1 1 d . . .
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C11 C 0.2985(9) 0.2469(8) 0.1148(4) 0.0278(19) Uani 1 1 d . . .
C12 C 0.3287(10) 0.2429(8) 0.0499(4) 0.0301(19) Uani 1 1 d . A .
H12A H 0.3741 0.1649 0.0317 0.036 Uiso 1 1 calc R . .
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H13A H 0.2845 0.4020 -0.0238 0.038 Uiso 1 1 calc R A .
C14 C 0.2189(9) 0.4568(8) 0.0656(4) 0.0277(19) Uani 1 1 d . A .
C15 C 0.1577(9) 0.5969(8) 0.0529(4) 0.0268(18) Uani 1 1 d . . .
C16 C 0.0906(9) 0.6803(8) 0.0959(4) 0.0264(18) Uani 1 1 d . A .
C17 C 0.0259(9) 0.8235(8) 0.0819(4) 0.0288(19) Uani 1 1 d . . .
H17A H 0.0191 0.8774 0.0421 0.035 Uiso 1 1 calc R A .
C18 C -0.0241(10) 0.8681(8) 0.1359(4) 0.033(2) Uani 1 1 d . A .
H18A H -0.0734 0.9590 0.1408 0.039 Uiso 1 1 calc R . .
C19 C 0.0113(9) 0.7522(8) 0.1845(4) 0.0285(19) Uani 1 1 d . . .
C20 C -0.0176(10) 0.7541(9) 0.2469(4) 0.032(2) Uani 1 1 d . A .
C21 C 0.1488(19) 0.2296(17) 0.4227(6) 0.070(2) Uiso 0.50 1 d PG A 1
C22 C 0.0089(16) 0.2355(17) 0.4406(7) 0.070(2) Uiso 0.50 1 d PG A 1
H22 H -0.0789 0.2841 0.4125 0.083 Uiso 0.50 1 calc PR A 1
C23 C -0.0026(16) 0.1704(18) 0.4997(8) 0.070(2) Uiso 0.50 1 d PG A 1
H23 H -0.0982 0.1744 0.5119 0.083 Uiso 0.50 1 calc PR A 1
C24 C 0.126(2) 0.0993(17) 0.5408(6) 0.070(2) Uiso 0.50 1 d PG A 1
H24 H 0.1180 0.0548 0.5811 0.083 Uiso 0.50 1 calc PR A 1
C25 C 0.2658(16) 0.0934(17) 0.5228(7) 0.070(2) Uiso 0.50 1 d PG A 1
H25 H 0.3536 0.0448 0.5510 0.083 Uiso 0.50 1 calc PR A 1
C26 C 0.2773(15) 0.1585(18) 0.4638(8) 0.070(2) Uiso 0.50 1 d PG A 1
H26 H 0.3729 0.1544 0.4515 0.083 Uiso 0.50 1 calc PR A 1
C21' C 0.2032(14) 0.2297(9) 0.4247(4) 0.070(2) Uiso 0.50 1 d PG A 2
C22' C 0.0880(12) 0.1889(12) 0.4398(4) 0.070(2) Uiso 0.50 1 d PG A 2
H22' H 0.0086 0.2079 0.4091 0.083 Uiso 0.50 1 calc PR A 2
C23' C 0.0891(16) 0.1203(14) 0.4997(4) 0.070(2) Uiso 0.50 1 d PG A 2
H23' H 0.0104 0.0924 0.5099 0.083 Uiso 0.50 1 calc PR A 2
C24' C 0.2053(17) 0.0924(12) 0.5446(3) 0.070(2) Uiso 0.50 1 d PG A 2
H24' H 0.2060 0.0455 0.5855 0.083 Uiso 0.50 1 calc PR A 2
C25' C 0.3205(15) 0.1332(14) 0.5295(3) 0.070(2) Uiso 0.50 1 d PG A 2
H25' H 0.3999 0.1141 0.5602 0.083 Uiso 0.50 1 calc PR A 2
C26' C 0.3194(15) 0.2018(13) 0.4696(4) 0.070(2) Uiso 0.50 1 d PG A 2
H26' H 0.3981 0.2297 0.4594 0.083 Uiso 0.50 1 calc PR A 2
C27 C 0.4065(8) -0.0006(7) 0.1438(3) 0.0295(19) Uani 1 1 d G . .
C28 C 0.3293(9) -0.0822(7) 0.1456(3) 0.039(2) Uani 1 1 d G A .
H28A H 0.2263 -0.0484 0.1555 0.047 Uiso 1 1 calc R . .

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C29 C 0.3983(11) -0.2104(9) 0.1334(5) 0.041(2) Uani 1 1 d . . .
 H29A H 0.3421 -0.2628 0.1334 0.049 Uiso 1 1 calc R A .
 C30 C 0.5489(11) -0.2625(9) 0.1211(5) 0.040(2) Uani 1 1 d . A .
 H30A H 0.5968 -0.3518 0.1137 0.048 Uiso 1 1 calc R . .
 C31 C 0.6306(11) -0.1876(10) 0.1194(5) 0.044(2) Uani 1 1 d . . .
 H31A H 0.7344 -0.2247 0.1107 0.052 Uiso 1 1 calc R A .
 C32 C 0.5612(10) -0.0564(9) 0.1304(5) 0.037(2) Uani 1 1 d . A .
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 C34 C 0.3150(10) 0.6548(9) -0.0280(4) 0.036(2) Uani 1 1 d . . .
 H34A H 0.3985 0.6140 0.0027 0.043 Uiso 1 1 calc R A .
 C35 C 0.3356(11) 0.7069(10) -0.0878(5) 0.041(2) Uani 1 1 d . A .
 H35A H 0.4334 0.7002 -0.0982 0.049 Uiso 1 1 calc R . .
 C36 C 0.2164(11) 0.7680(9) -0.1324(4) 0.036(2) Uani 1 1 d . . .
 H36A H 0.2311 0.8035 -0.1737 0.044 Uiso 1 1 calc R A .
 C37 C 0.0744(11) 0.7776(9) -0.1169(4) 0.036(2) Uani 1 1 d . A .
 H37A H -0.0093 0.8222 -0.1473 0.043 Uiso 1 1 calc R . .
 C38 C 0.0535(10) 0.7227(9) -0.0573(4) 0.033(2) Uani 1 1 d . . .
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 C39 C -0.0897(10) 0.8885(8) 0.2667(4) 0.0292(19) Uani 1 1 d . . .
 C40 C -0.0001(10) 0.9527(9) 0.2796(5) 0.040(2) Uani 1 1 d . A .
 H40A H 0.1057 0.9129 0.2745 0.048 Uiso 1 1 calc R . .
 C41 C -0.0657(11) 1.0770(9) 0.3002(5) 0.041(2) Uani 1 1 d . . .
 H41A H -0.0036 1.1197 0.3096 0.049 Uiso 1 1 calc R A .
 C42 C -0.2191(11) 1.1363(9) 0.3067(4) 0.037(2) Uani 1 1 d . A .
 H42A H -0.2629 1.2200 0.3204 0.044 Uiso 1 1 calc R . .
 C43 C -0.3101(11) 1.0737(9) 0.2934(4) 0.040(2) Uani 1 1 d . . .
 H43A H -0.4161 1.1149 0.2978 0.048 Uiso 1 1 calc R A .
 C44 C -0.2461(11) 0.9511(9) 0.2736(4) 0.037(2) Uani 1 1 d . A .
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 O1 O -0.0691(7) 0.4577(6) 0.1817(3) 0.0359(15) Uani 1 1 d D . .
 H1O H -0.058(11) 0.404(8) 0.157(4) 0.043 Uiso 1 1 d D . .
 C45 C -0.1713(14) 0.4561(13) 0.2272(6) 0.064(3) Uani 1 1 d . . .
 H45A H -0.2545 0.4423 0.2088 0.095 Uiso 1 1 calc R . .
 H45B H -0.2121 0.5417 0.2421 0.095 Uiso 1 1 calc R . .
 H45C H -0.1188 0.3830 0.2625 0.095 Uiso 1 1 calc R . .
 C46 C 0.4575(12) 0.5833(10) 0.3694(6) 0.186(2) Uiso 0.50 1 d PD B 1
 H46 H 0.4197 0.5817 0.3268 0.223 Uiso 0.50 1 calc PR B 1
 Cl1 Cl 0.3302(18) 0.7242(12) 0.3971(9) 0.186(2) Uiso 0.50 1 d PD B 1
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 Cl2 Cl 0.6348(14) 0.5815(15) 0.3665(8) 0.186(2) Uiso 0.50 1 d PD B 1
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 C17 0.032(5) 0.028(5) 0.024(5) 0.003(4) 0.002(4) -0.013(4)
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 C29 0.048(6) 0.025(5) 0.055(6) -0.007(4) 0.000(5) -0.020(5)
 C30 0.046(6) 0.021(5) 0.046(6) -0.010(4) 0.006(5) -0.006(4)
 C31 0.037(5) 0.034(5) 0.058(7) -0.019(5) 0.011(5) -0.008(4)
 C32 0.035(5) 0.035(5) 0.044(6) -0.014(4) 0.008(4) -0.016(4)
 C33 0.031(5) 0.018(4) 0.039(5) -0.001(4) 0.003(4) -0.010(4)
 C34 0.031(5) 0.037(5) 0.033(5) 0.004(4) -0.002(4) -0.011(4)
 C35 0.034(5) 0.047(6) 0.041(6) -0.001(5) 0.004(4) -0.020(5)
 C36 0.050(6) 0.025(5) 0.033(5) -0.001(4) 0.009(4) -0.016(4)
 C37 0.041(5) 0.024(5) 0.037(5) 0.001(4) -0.009(4) -0.009(4)
 C38 0.034(5) 0.033(5) 0.034(5) -0.003(4) 0.002(4) -0.018(4)
 C39 0.033(5) 0.024(5) 0.026(5) -0.001(4) 0.001(4) -0.008(4)
 C40 0.029(5) 0.036(5) 0.052(6) -0.014(5) 0.006(4) -0.009(4)
 C41 0.039(6) 0.029(5) 0.055(6) -0.012(5) -0.004(5) -0.012(4)
 C42 0.052(6) 0.021(5) 0.032(5) -0.005(4) -0.002(4) -0.009(4)
 C43 0.040(6) 0.029(5) 0.040(6) -0.003(4) 0.010(4) -0.006(4)
 C44 0.041(5) 0.027(5) 0.042(6) -0.006(4) 0.005(4) -0.014(4)
 O1 0.026(3) 0.029(4) 0.055(4) -0.014(3) 0.007(3) -0.012(3)
 C45 0.061(8) 0.081(9) 0.059(8) -0.022(7) 0.022(6) -0.037(7)

_geom_special_details

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All esds (except the esd in the dihedral angle between two l.s. planes)
 are estimated using the full covariance matrix. The cell esds are taken
 into account individually in the estimation of esds in distances, angles
 and torsion angles; correlations between esds in cell parameters are only
 used when they are defined by crystal symmetry. An approximate (isotropic)
 treatment of cell esds is used for estimating esds involving l.s. planes.

Least-squares planes (x,y,z in crystal coordinates) and deviations from them
 (* indicates atom used to define plane)

9.5245 (0.0017) x + 4.8361 (0.0074) y + 4.2985 (0.0175) z = 4.5496 (0.0050)

* -0.0310 (0.0070) N1
 * -0.0417 (0.0065) N2
 * -0.0284 (0.0063) N3
 * -0.0305 (0.0064) N4
 * -0.0183 (0.0087) C1
 * -0.0080 (0.0099) C2

*	0.0050	(0.0109)	C3
*	-0.0012	(0.0096)	C4
*	0.0232	(0.0097)	C5
*	0.0146	(0.0083)	C6
*	0.0640	(0.0085)	C7
*	0.0355	(0.0078)	C8
*	-0.0249	(0.0074)	C9
*	-0.0333	(0.0072)	C10
*	-0.0187	(0.0074)	C11
*	-0.0298	(0.0076)	C12
*	-0.0005	(0.0077)	C13
*	0.0268	(0.0075)	C14
*	0.0670	(0.0072)	C15
*	0.0153	(0.0075)	C16
*	0.0312	(0.0073)	C17
*	0.0031	(0.0076)	C18
*	-0.0108	(0.0076)	C19
*	-0.0084	(0.0080)	C20
	-0.2053	(0.0174)	C21_a
	0.3222	(0.0130)	C21'_b
	-0.0625	(0.0196)	C27
	0.2588	(0.0090)	C33
	0.0394	(0.0094)	C39
	-0.0058	(0.0018)	Rh1

Rms deviation of fitted atoms = 0.0293

Phenyl substituent at C5 (first orientation):

1.9044 (0.0996) x + 10.1052 (0.0495) y + 11.5173 (0.1953) z = 7.4714 (0.0880)
 Angle to porphyrin plane (with approximate esd) = 73.02 (0.61)

*	0.0000	(0.0001)	C21_a
*	0.0000	(0.0001)	C22_a
*	0.0000	(0.0001)	C23_a
*	0.0000	(0.0001)	C24_a
*	0.0000	(0.0000)	C25_a
*	0.0000	(0.0000)	C26_a

Rms deviation of fitted atoms = 0.0000

Phenyl ring at C5 (second orientation):

-1.7713 (0.0475) x + 8.6718 (0.0324) y + 9.9672 (0.0307) z = 5.8652 (0.0193)
 Angle to porphyrin plane (with approximate esd) = 84.66 (0.28)

*	0.0000	(0.0000)	C21'_b
*	0.0000	(0.0000)	C22'_b
*	0.0000	(0.0000)	C23'_b
*	0.0000	(0.0000)	C24'_b
*	0.0000	(0.0000)	C25'_b
*	0.0000	(0.0000)	C26'_b

Rms deviation of fitted atoms = 0.0000

Phenyl ring at C10:

1.3729 (0.0375) x - 1.0285 (0.0424) y + 20.1455 (0.0307) z = 3.4596 (0.0142)

Angle to porphyrin plane (with approximate esd) = 71.23 (0.23)

```
*   -0.0033 (0.0044)  C27
*    0.0100 (0.0047)  C28
*   -0.0098 (0.0067)  C29
*    0.0029 (0.0072)  C30
*    0.0036 (0.0072)  C31
*   -0.0034 (0.0067)  C32
```

Rms deviation of fitted atoms = 0.0063

Phenyl ring at C15:

1.6546 (0.0365) x + 10.3557 (0.0155) y + 9.7893 (0.0716) z = 7.0202 (0.0202)
Angle to porphyrin plane (with approximate esd) = 75.46 (0.23)

```
*   -0.0019 (0.0061)  C33
*    0.0081 (0.0067)  C34
*   -0.0045 (0.0069)  C35
*   -0.0054 (0.0064)  C36
*    0.0115 (0.0063)  C37
*   -0.0079 (0.0062)  C38
```

Rms deviation of fitted atoms = 0.0072

Phenyl ring at C20:

-0.4631 (0.0385) x - 3.3326 (0.0404) y + 19.0388 (0.0389) z = 2.1534 (0.0497)
Angle to porphyrin plane (with approximate esd) = 82.69 (0.23)

```
*    0.0046 (0.0064)  C39
*   -0.0060 (0.0069)  C40
*    0.0030 (0.0071)  C41
*    0.0013 (0.0066)  C42
*   -0.0026 (0.0066)  C43
*   -0.0004 (0.0066)  C44
```

Rms deviation of fitted atoms = 0.0035

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Rh1 N3 2.026(7) . ?

Rh1 N2 2.028(7) . ?

Rh1 N4 2.028(7) . ?

Rh1 O1 2.210(6) . ?

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N1 C4 1.380(11) . ?

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N2 C9 1.388(11) . ?

N3 C11 1.382(10) . ?

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I1 Rh1 N2 C9 -88.5(6) . . . . ?
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N3 Rh1 N4 C19 -179.1(7) . . . . ?
O1 Rh1 N4 C19 91.6(6) . . . . ?
I1 Rh1 N4 C19 -88.3(6) . . . . ?
C4 N1 C1 C2 -1.2(11) . . . . ?
Rh1 N1 C1 C2 -178.4(7) . . . . ?
C4 N1 C1 C20 178.4(9) . . . . ?
Rh1 N1 C1 C20 1.2(13) . . . . ?
N1 C1 C2 C3 0.8(12) . . . . ?
C20 C1 C2 C3 -178.8(10) . . . . ?
C1 C2 C3 C4 -0.2(13) . . . . ?
C1 N1 C4 C5 -178.8(10) . . . . ?
Rh1 N1 C4 C5 -1.5(14) . . . . ?
C1 N1 C4 C3 1.1(11) . . . . ?
Rh1 N1 C4 C3 178.4(7) . . . . ?
C2 C3 C4 N1 -0.6(13) . . . . ?
C2 C3 C4 C5 179.3(10) . . . . ?
N1 C4 C5 C6 -0.3(17) . . . . ?
C3 C4 C5 C6 179.9(10) . . . . ?
N1 C4 C5 C21' 168.3(10) . . . . ?
C3 C4 C5 C21' -11.5(16) . . . . ?
N1 C4 C5 C21 -169.1(11) . . . . ?
C3 C4 C5 C21 11.1(17) . . . . ?
C9 N2 C6 C5 179.9(9) . . . . ?

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Rh1 N2 C6 C5 4.3(13) ?
 C9 N2 C6 C7 -0.1(9) ?
 Rh1 N2 C6 C7 -175.7(6) ?
 C4 C5 C6 N2 -1.2(16) ?
 C21' C5 C6 N2 -169.7(9) ?
 C21 C5 C6 N2 167.4(10) ?
 C4 C5 C6 C7 178.8(10) ?
 C21' C5 C6 C7 10.3(15) ?
 C21 C5 C6 C7 -12.6(16) ?
 N2 C6 C7 C8 -0.1(10) ?
 C5 C6 C7 C8 179.9(9) ?
 C6 C7 C8 C9 0.3(10) ?
 C6 N2 C9 C10 -178.3(8) ?
 Rh1 N2 C9 C10 -2.7(12) ?
 C6 N2 C9 C8 0.3(9) ?
 Rh1 N2 C9 C8 175.9(5) ?
 C7 C8 C9 N2 -0.4(10) ?
 C7 C8 C9 C10 178.2(8) ?
 N2 C9 C10 C11 2.1(13) ?
 C8 C9 C10 C11 -176.3(8) ?
 N2 C9 C10 C27 -177.8(7) ?
 C8 C9 C10 C27 3.8(12) ?
 C14 N3 C11 C10 178.5(8) ?
 Rh1 N3 C11 C10 2.1(11) ?
 C14 N3 C11 C12 -3.1(9) ?
 Rh1 N3 C11 C12 -179.5(5) ?
 C9 C10 C11 N3 -1.8(13) ?
 C27 C10 C11 N3 178.1(7) ?
 C9 C10 C11 C12 -179.9(8) ?
 C27 C10 C11 C12 0.0(12) ?
 N3 C11 C12 C13 2.0(9) ?
 C10 C11 C12 C13 -179.6(8) ?
 C11 C12 C13 C14 -0.1(9) ?
 C11 N3 C14 C15 -178.5(8) ?
 Rh1 N3 C14 C15 -2.1(11) ?
 C11 N3 C14 C13 3.1(9) ?
 Rh1 N3 C14 C13 179.5(5) ?
 C12 C13 C14 N3 -1.9(9) ?
 C12 C13 C14 C15 179.7(8) ?
 N3 C14 C15 C16 -2.2(13) ?
 C13 C14 C15 C16 176.0(8) ?
 N3 C14 C15 C33 174.3(7) ?
 C13 C14 C15 C33 -7.5(12) ?
 C19 N4 C16 C15 177.3(8) ?
 Rh1 N4 C16 C15 1.1(12) ?
 C19 N4 C16 C17 -1.4(9) ?
 Rh1 N4 C16 C17 -177.7(5) ?
 C14 C15 C16 N4 2.7(13) ?
 C33 C15 C16 N4 -173.7(7) ?
 C14 C15 C16 C17 -178.7(8) ?
 C33 C15 C16 C17 4.9(12) ?
 N4 C16 C17 C18 0.4(9) ?
 C15 C16 C17 C18 -178.4(8) ?
 C16 C17 C18 C19 0.8(9) ?
 C16 N4 C19 C20 -178.2(8) ?
 Rh1 N4 C19 C20 -1.9(12) ?
 C16 N4 C19 C18 1.9(9) ?
 Rh1 N4 C19 C18 178.2(5) ?
 C17 C18 C19 C20 178.4(8) ?
 C17 C18 C19 N4 -1.7(9) ?
 N4 C19 C20 C1 0.3(14) ?

C18 C19 C20 C1 -179.8(8) ?
N4 C19 C20 C39 178.9(7) ?
C18 C19 C20 C39 -1.2(13) ?
N1 C1 C20 C19 0.1(15) ?
C2 C1 C20 C19 179.6(9) ?
N1 C1 C20 C39 -178.5(8) ?
C2 C1 C20 C39 1.0(14) ?
C4 C5 C21 C22 68.7(14) ?
C6 C5 C21 C22 -100.8(13) ?
C21' C5 C21 C22 166(3) ?
C4 C5 C21 C26 -114.3(12) ?
C6 C5 C21 C26 76.1(13) ?
C21' C5 C21 C26 -16.6(17) ?
C26 C21 C22 C23 0.0 ?
C5 C21 C22 C23 176.9(15) ?
C21 C22 C23 C24 0.0 ?
C22 C23 C24 C25 0.0 ?
C23 C24 C25 C26 0.0 ?
C24 C25 C26 C21 0.0 ?
C22 C21 C26 C25 0.0 ?
C5 C21 C26 C25 -177.0(14) ?
C4 C5 C21' C22' 101.4(8) ?
C6 C5 C21' C22' -89.1(10) ?
C21 C5 C21' C22' 9(2) ?
C4 C5 C21' C26' -81.6(10) ?
C6 C5 C21' C26' 87.8(10) ?
C21 C5 C21' C26' -174(2) ?
C26' C21' C22' C23' 0.0 ?
C5 C21' C22' C23' 177.5(5) ?
C21' C22' C23' C24' 0.0 ?
C22' C23' C24' C25' 0.0 ?
C23' C24' C25' C26' 0.0 ?
C24' C25' C26' C21' 0.0 ?
C22' C21' C26' C25' 0.0 ?
C5 C21' C26' C25' -176.6(6) ?
C11 C10 C27 C28 -112.0(7) ?
C9 C10 C27 C28 67.9(8) ?
C11 C10 C27 C32 73.8(10) ?
C9 C10 C27 C32 -106.3(9) ?
C32 C27 C28 C29 -1.6(9) ?
C10 C27 C28 C29 -176.0(9) ?
C27 C28 C29 C30 2.2(12) ?
C28 C29 C30 C31 -1.5(15) ?
C29 C30 C31 C32 0.3(16) ?
C30 C31 C32 C27 0.4(15) ?
C28 C27 C32 C31 0.3(11) ?
C10 C27 C32 C31 174.6(9) ?
C16 C15 C33 C34 103.7(10) ?
C14 C15 C33 C34 -73.0(10) ?
C16 C15 C33 C38 -78.7(10) ?
C14 C15 C33 C38 104.6(10) ?
C38 C33 C34 C35 -0.8(14) ?
C15 C33 C34 C35 176.9(9) ?
C33 C34 C35 C36 1.1(15) ?
C34 C35 C36 C37 0.2(14) ?
C35 C36 C37 C38 -1.8(14) ?
C36 C37 C38 C33 2.0(13) ?
C34 C33 C38 C37 -0.7(13) ?
C15 C33 C38 C37 -178.3(8) ?
C19 C20 C39 C40 -82.1(11) ?
C1 C20 C39 C40 96.6(10) ?

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C19 C20 C39 C44 98.9(10) . . . . ?
C1 C20 C39 C44 -82.4(11) . . . . ?
C44 C39 C40 C41 1.1(14) . . . . ?
C20 C39 C40 C41 -177.9(9) . . . . ?
C39 C40 C41 C42 -1.0(15) . . . . ?
C40 C41 C42 C43 0.3(15) . . . . ?
C41 C42 C43 C44 0.2(14) . . . . ?
C42 C43 C44 C39 -0.1(14) . . . . ?
C40 C39 C44 C43 -0.6(14) . . . . ?
C20 C39 C44 C43 178.4(9) . . . . ?
N1 Rh1 O1 C45 -21.8(8) . . . . ?
N3 Rh1 O1 C45 157.7(8) . . . . ?
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N4 Rh1 O1 C45 -111.8(8) . . . . ?

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data_3

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_chemical_name_systematic      ?
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_chemical_melting_point        ?
_chemical_formula_moiety       'C45 H31 N4 Rh'
_chemical_formula_sum          'C45 H31 N4 Rh'
_chemical_formula_weight       730.65

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loop_

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_atom_type_scatter_dispersion_imag
_atom_type_scatter_source
'C' 'C' 0.0033 0.0016
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
'H' 'H' 0.0000 0.0000
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
'N' 'N' 0.0061 0.0033
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
'Rh' 'Rh' -1.1178 0.9187
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

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_symmetry_cell_setting         tetragonal
_symmetry_space_group_name_H-M I4/m

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loop_

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_symmetry_equiv_pos_as_xyz
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'-x, -y, z'
'-y, x, z'
'y, -x, z'
'x+1/2, y+1/2, z+1/2'
'-x+1/2, -y+1/2, z+1/2'
'-y+1/2, x+1/2, z+1/2'
'y+1/2, -x+1/2, z+1/2'
'-x, -y, -z'
'x, y, -z'
'y, -x, -z'
'-y, x, -z'
'-x+1/2, -y+1/2, -z+1/2'
'x+1/2, y+1/2, -z+1/2'
'y+1/2, -x+1/2, -z+1/2'

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'-y+1/2, x+1/2, -z+1/2'

_cell_length_a	13.4741 (5)
_cell_length_b	13.4741 (5)
_cell_length_c	9.6462 (5)
_cell_angle_alpha	90.00
_cell_angle_beta	90.00
_cell_angle_gamma	90.00
_cell_volume	1751.28 (13)
_cell_formula_units_Z	2
_cell_measurement_temperature	180 (2)
_cell_measurement_reflns_used	2739
_cell_measurement_theta_min	1.00
_cell_measurement_theta_max	27.48

_exptl_crystal_description	block
_exptl_crystal_colour	red
_exptl_crystal_size_max	0.10
_exptl_crystal_size_mid	0.10
_exptl_crystal_size_min	0.05
_exptl_crystal_density_meas	?
_exptl_crystal_density_diffn	1.386
_exptl_crystal_density_method	'not measured'
_exptl_crystal_F_000	748
_exptl_absorpt_coefficient_mu	0.526
_exptl_absorpt_correction_type	multi-scan
_exptl_absorpt_correction_T_min	0.893
_exptl_absorpt_correction_T_max	0.974
_exptl_absorpt_process_details	'Sortav Blessing (1995)'

_exptl_special_details

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Molecule on site of 4/m symmetry. Rh is 5-coordinate with the methyl group disordered above and below the plane of the porphyrin - the half occupancy of the methyl group (relative to Rh) is clear from the displacement parameter of C10. A very common phenomenon in 5-coordinate tetraphenylporphyrin complexes!

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_diffn_ambient_temperature	180 (2)
_diffn_radiation_wavelength	0.7107
_diffn_radiation_type	MoK\alpha
_diffn_radiation_source	'fine-focus sealed tube'
_diffn_radiation_monochromator	graphite
_diffn_measurement_device_type	'Nonius KappaCCD'
_diffn_measurement_method	'Thin slice \w and \f scans'
_diffn_standards_number	0
_diffn_reflns_number	3796
_diffn_reflns_av_R_equivalents	0.0739
_diffn_reflns_av_sigmaI/netI	0.0752
_diffn_reflns_limit_h_min	-14
_diffn_reflns_limit_h_max	15
_diffn_reflns_limit_k_min	-14
_diffn_reflns_limit_k_max	15
_diffn_reflns_limit_l_min	-11
_diffn_reflns_limit_l_max	11
_diffn_reflns_theta_min	3.99
_diffn_reflns_theta_max	24.68
_diffn_measured_fraction_theta_max	0.996
_diffn_reflns_theta_full	24.68
_diffn_measured_fraction_theta_full	0.996

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_reflns_number_total      802
_reflns_number_gt         767
_reflns_threshold_expression >2sigma(I)

_computing_data_collection 'Collect (Nonius B.V. 1998)'
_computing_cell_refinement 'HKL Scalepack (Otwinowski & Minor 1997)'
_computing_data_reduction
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    HKL Denzo and Scalepack (Otwinowski & Minor 1997)
;
_computing_structure_solution 'SIR-92 (Altomare et al. 1994)'
_computing_structure_refinement 'SHELXL-97 (Sheldrick 1997)'
_computing_publication_material 'SHELXL-97 (Sheldrick 1997)'

_refine_special_details
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    Refinement of F2 against ALL reflections. The weighted R-factor wR and
    goodness of fit S are based on F2, conventional R-factors R are based
    on F, with F set to zero for negative F2. The threshold expression of
    F2 > 2sigma(F2) is used only for calculating R-factors(gt) etc. and is
    not relevant to the choice of reflections for refinement. R-factors based
    on F2 are statistically about twice as large as those based on F, and R-
    factors based on ALL data will be even larger.
;

_refine_ls_structure_factor_coef Fsqd
_refine_ls_matrix_type full
_refine_ls_weighting_scheme calc
_refine_ls_weighting_details
    'calc w=1/[\s2(Fo2)+(0.0000P)2+4.2911P] where P=(Fo2+2Fc2)/3'
_atom_sites_solution_primary direct
_atom_sites_solution_secondary difmap
_atom_sites_solution_hydrogens geom
_refine_ls_hydrogen_treatment constr
_refine_ls_extinction_method none
_refine_ls_extinction_coef ?
_refine_ls_number_reflns 802
_refine_ls_number_parameters 72
_refine_ls_number_restraints 0
_refine_ls_R_factor_all 0.0434
_refine_ls_R_factor_gt 0.0408
_refine_ls_wR_factor_ref 0.0753
_refine_ls_wR_factor_gt 0.0746
_refine_ls_goodness_of_fit_ref 1.150
_refine_ls_restrained_S_all 1.150
_refine_ls_shift/su_max 0.000
_refine_ls_shift/su_mean 0.000
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_refine_diff_density_rms 0.102

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    _atom_site_fract_y
    _atom_site_fract_z
    _atom_site_U_iso_or_equiv
    _atom_site_adp_type
    _atom_site_occupancy
    _atom_site_symmetry_multiplicity

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    _atom_site_refinement_flags
    _atom_site_disorder_assembly
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Rh1 Rh 0.5000 0.5000 0.0000 0.0259(2) Uani 1 8 d S . .
N1 N 0.4637(2) 0.6453(2) 0.0000 0.0306(8) Uani 1 2 d S . .
C1 C 0.3689(3) 0.6856(3) 0.0000 0.0290(10) Uani 1 2 d S . .
C2 C 0.3753(3) 0.7920(3) 0.0000 0.0355(11) Uani 1 2 d S . .
H2A H 0.3211 0.8370 0.0000 0.043 Uiso 1 2 calc SR . .
C3 C 0.4721(3) 0.8162(3) 0.0000 0.0337(10) Uani 1 2 d S . .
H3A H 0.4987 0.8815 0.0000 0.040 Uiso 1 2 calc SR . .
C4 C 0.5283(3) 0.7250(3) 0.0000 0.0309(10) Uani 1 2 d S . .
C5 C 0.6306(3) 0.7192(3) 0.0000 0.0296(10) Uani 1 2 d S . .
C6 C 0.6884(3) 0.8147(3) 0.0000 0.0294(10) Uani 1 2 d S . .
C7 C 0.7140(3) 0.8602(3) -0.1214(4) 0.0570(11) Uani 1 1 d . . .
H7A H 0.6952 0.8310 -0.2071 0.068 Uiso 1 1 calc R . .
C8 C 0.7670(3) 0.9485(3) -0.1213(4) 0.0636(12) Uani 1 1 d . . .
H8A H 0.7843 0.9791 -0.2068 0.076 Uiso 1 1 calc R . .
C9 C 0.7944(3) 0.9916(3) 0.0000 0.0449(13) Uani 1 2 d S . .
H9A H 0.8322 1.0511 0.0000 0.054 Uiso 1 2 calc SR . .
C10 C 0.5000 0.5000 0.2041(13) 0.042(3) Uani 0.50 4 d SP . .
H10A H 0.5166 0.4335 0.2379 0.063 Uiso 0.13 1 calc PR . .
H10B H 0.4341 0.5189 0.2379 0.063 Uiso 0.13 1 calc PR . .
H10C H 0.5493 0.5476 0.2379 0.063 Uiso 0.13 1 calc PR . .

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Rh1 0.0212(3) 0.0212(3) 0.0355(4) 0.000 0.000 0.000
N1 0.0249(18) 0.0224(17) 0.044(2) 0.000 0.000 0.0007(13)
C1 0.028(2) 0.025(2) 0.035(3) 0.000 0.000 0.0026(16)
C2 0.033(2) 0.026(2) 0.048(3) 0.000 0.000 0.0041(17)
C3 0.035(2) 0.024(2) 0.043(3) 0.000 0.000 -0.0035(17)
C4 0.028(2) 0.026(2) 0.039(3) 0.000 0.000 0.0008(17)
C5 0.030(2) 0.026(2) 0.033(2) 0.000 0.000 -0.0028(17)
C6 0.024(2) 0.026(2) 0.038(3) 0.000 0.000 -0.0010(16)
C7 0.086(3) 0.047(2) 0.038(2) -0.0067(18) 0.015(2) -0.0287(19)
C8 0.089(3) 0.047(2) 0.055(3) 0.002(2) 0.022(2) -0.030(2)
C9 0.027(2) 0.024(2) 0.084(4) 0.000 0.000 -0.0043(17)
C10 0.049(5) 0.049(5) 0.028(7) 0.000 0.000 0.000

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_geom_special_details
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All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

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    _geom_bond_distance
    _geom_bond_site_symmetry_2

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Rh1 C10 1.968(12) 9_665 ?
Rh1 N1 2.018(3) 3_655 ?
Rh1 N1 2.018(3) . ?
Rh1 N1 2.018(3) 9_665 ?
Rh1 N1 2.018(3) 11_565 ?
N1 C4 1.382(5) . ?
N1 C1 1.387(5) . ?
C1 C5 1.400(5) 3_655 ?
C1 C2 1.436(5) . ?
C2 C3 1.344(6) . ?
C2 H2A 0.9500 . ?
C3 C4 1.444(5) . ?
C3 H3A 0.9500 . ?
C4 C5 1.380(5) . ?
C5 C1 1.400(5) 11_565 ?
C5 C6 1.504(5) . ?
C6 C7 1.367(4) 10 ?
C6 C7 1.367(4) . ?
C7 C8 1.388(4) . ?
C7 H7A 0.9500 . ?
C8 C9 1.357(4) . ?
C8 H8A 0.9500 . ?
C9 C8 1.357(4) 10 ?
C9 H9A 0.9500 . ?
C10 H10A 0.9800 . ?
C10 H10B 0.9800 . ?
C10 H10C 0.9800 . ?

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    _geom_angle_site_symmetry_3
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C10 Rh1 N1 90.000(1) . 3_655 ?
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C10 Rh1 N1 90.0 9_665 . ?
N1 Rh1 N1 90.0 3_655 . ?
C10 Rh1 N1 90.0 . 9_665 ?
C10 Rh1 N1 90.0 9_665 9_665 ?
N1 Rh1 N1 90.0 3_655 9_665 ?
N1 Rh1 N1 180.0 . 9_665 ?
C10 Rh1 N1 90.000(1) . 11_565 ?
C10 Rh1 N1 90.000(1) 9_665 11_565 ?
N1 Rh1 N1 180.00(17) 3_655 11_565 ?
N1 Rh1 N1 90.0 . 11_565 ?
N1 Rh1 N1 90.0 9_665 11_565 ?
C4 N1 C1 106.0(3) . . ?
C4 N1 Rh1 126.9(3) . . ?
C1 N1 Rh1 127.1(3) . . ?
N1 C1 C5 125.0(4) . 3_655 ?
N1 C1 C2 109.6(3) . . ?
C5 C1 C2 125.4(4) 3_655 . ?
C3 C2 C1 107.5(4) . . ?
C3 C2 H2A 126.3 . . ?

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C1 C2 H2A 126.3 . . ?
 C2 C3 C4 107.6(4) . . ?
 C2 C3 H3A 126.2 . . ?
 C4 C3 H3A 126.2 . . ?
 C5 C4 N1 125.9(4) . . ?
 C5 C4 C3 124.9(4) . . ?
 N1 C4 C3 109.3(3) . . ?
 C4 C5 C1 125.2(4) . 11_565 ?
 C4 C5 C6 118.0(3) . . ?
 C1 C5 C6 116.9(3) 11_565 . ?
 C7 C6 C7 118.0(4) 10 . ?
 C7 C6 C5 121.0(2) 10 . ?
 C7 C6 C5 121.0(2) . . ?
 C6 C7 C8 121.0(3) . . ?
 C6 C7 H7A 119.5 . . ?
 C8 C7 H7A 119.5 . . ?
 C9 C8 C7 120.4(4) . . ?
 C9 C8 H8A 119.8 . . ?
 C7 C8 H8A 119.8 . . ?
 C8 C9 C8 119.2(4) 10 . ?
 C8 C9 H9A 120.4 10 . ?
 C8 C9 H9A 120.4 . . ?
 Rh1 C10 H10A 109.5 . . ?
 Rh1 C10 H10B 109.5 . . ?
 H10A C10 H10B 109.5 . . ?
 Rh1 C10 H10C 109.5 . . ?
 H10A C10 H10C 109.5 . . ?
 H10B C10 H10C 109.5 . . ?

loop_

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 N1 Rh1 N1 C4 0.0 11_565 ?
 C10 Rh1 N1 C1 -90.0 ?
 C10 Rh1 N1 C1 90.0 9_665 ?
 N1 Rh1 N1 C1 0.0 3_655 ?
 N1 Rh1 N1 C1 180.0 11_565 ?
 C4 N1 C1 C5 180.0 . . . 3_655 ?
 Rh1 N1 C1 C5 0.0 . . . 3_655 ?
 C4 N1 C1 C2 0.0 ?
 Rh1 N1 C1 C2 180.0 ?
 N1 C1 C2 C3 0.0 ?
 C5 C1 C2 C3 180.0 3_655 ?
 C1 C2 C3 C4 0.0 ?
 C1 N1 C4 C5 180.0 ?
 Rh1 N1 C4 C5 0.0 ?
 C1 N1 C4 C3 0.0 ?
 Rh1 N1 C4 C3 180.0 ?
 C2 C3 C4 C5 180.0 ?
 C2 C3 C4 N1 0.0 ?

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N1 C4 C5 C1 0.0 . . . 11_565 ?
C3 C4 C5 C1 180.0 . . . 11_565 ?
N1 C4 C5 C6 180.0 . . . ?
C3 C4 C5 C6 0.0 . . . ?
C4 C5 C6 C7 88.9(4) . . . 10 ?
C1 C5 C6 C7 -91.1(4) 11_565 . . 10 ?
C4 C5 C6 C7 -88.9(4) . . . ?
C1 C5 C6 C7 91.1(4) 11_565 . . . ?
C7 C6 C7 C8 1.9(7) 10 . . . ?
C5 C6 C7 C8 179.8(4) . . . ?
C6 C7 C8 C9 -0.1(7) . . . ?
C7 C8 C9 C8 -1.7(8) . . . 10 ?

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data_4

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'N' 'N' 0.0061 0.0033
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_symmetry_equiv_pos_as_xyz
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'-x+1/2, y+1/2, -z+1/2'
'-x, -y, -z'
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_computing_data_collection	'Collect (Nonius B.V. 1998)'
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_computing_data_reduction	

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;
  HKL Denzo and Scalepack (Otwinowski & Minor 1997)
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_computing_structure_solution      'SHELXS-97 (Sheldrick 1997)'
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_refine_special_details
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  Refinement of F2 against ALL reflections. The weighted R-factor wR and
  goodness of fit S are based on F2, conventional R-factors R are based
  on F, with F set to zero for negative F2. The threshold expression of
  F2 > 2sigma(F2) is used only for calculating R-factors(gt) etc. and is
  not relevant to the choice of reflections for refinement. R-factors based
  on F2 are statistically about twice as large as those based on F, and R-
  factors based on ALL data will be even larger.
;

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_atom_sites_solution_secondary    difmap
_atom_sites_solution_hydrogens    geom
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_refine_ls_extinction_method      none
_refine_ls_extinction_coef        ?
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Rh1 Rh 0.2500 0.2500 0.0000 0.01728(9) Uani 1 2 d S . .
P1 P 0.21426(3) 0.06437(6) 0.01339(3) 0.02073(16) Uani 1 1 d . . .

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N1 N 0.23203(8) 0.29214(18) 0.08038(8) 0.0204(5) Uani 1 1 d . . .
 N2 N 0.18033(8) 0.31305(18) -0.02700(8) 0.0200(5) Uani 1 1 d . . .
 C1 C 0.16131(10) 0.3111(2) -0.08149(10) 0.0211(6) Uani 1 1 d . . .
 C2 C 0.11094(10) 0.3605(2) -0.08270(11) 0.0255(6) Uani 1 1 d . . .
 H2A H 0.0898 0.3721 -0.1152 0.031 Uiso 1 1 calc R . .
 C3 C 0.09872(11) 0.3878(2) -0.02983(11) 0.0268(6) Uani 1 1 d . . .
 H3A H 0.0673 0.4214 -0.0181 0.032 Uiso 1 1 calc R . .
 C4 C 0.14185(10) 0.3568(2) 0.00575(11) 0.0221(6) Uani 1 1 d . . .
 C5 C 0.14374(10) 0.3676(2) 0.06425(11) 0.0221(6) Uani 1 1 d . . .
 C6 C 0.18640(10) 0.3389(2) 0.09810(11) 0.0216(6) Uani 1 1 d . . .
 C7 C 0.19022(11) 0.3578(2) 0.15776(11) 0.0276(6) Uani 1 1 d . . .
 H7A H 0.1642 0.3893 0.1807 0.033 Uiso 1 1 calc R . .
 C8 C 0.23714(11) 0.3228(2) 0.17515(11) 0.0287(6) Uani 1 1 d . . .
 H8A H 0.2504 0.3258 0.2125 0.034 Uiso 1 1 calc R . .
 C9 C 0.26380(10) 0.2801(2) 0.12718(11) 0.0232(6) Uani 1 1 d . . .
 C10 C 0.31337(10) 0.2344(2) 0.12793(11) 0.0220(6) Uani 1 1 d . . .
 C11 C 0.09669(10) 0.4112(2) 0.09301(11) 0.0243(6) Uani 1 1 d . . .
 C12 C 0.07223(11) 0.3427(3) 0.13236(12) 0.0322(7) Uani 1 1 d . . .
 H12A H 0.0849 0.2674 0.1399 0.039 Uiso 1 1 calc R . .
 C13 C 0.02958(12) 0.3832(3) 0.16064(14) 0.0401(8) Uani 1 1 d . . .
 H13A H 0.0136 0.3362 0.1879 0.048 Uiso 1 1 calc R . .
 C14 C 0.01037(12) 0.4915(3) 0.14912(14) 0.0424(8) Uani 1 1 d . . .
 H14A H -0.0188 0.5193 0.1685 0.051 Uiso 1 1 calc R . .
 C15 C 0.03348(12) 0.5594(3) 0.10959(13) 0.0354(7) Uani 1 1 d . . .
 H15A H 0.0199 0.6335 0.1012 0.042 Uiso 1 1 calc R . .
 C16 C 0.07655(11) 0.5200(2) 0.08188(12) 0.0288(6) Uani 1 1 d . . .
 H16A H 0.0925 0.5679 0.0550 0.035 Uiso 1 1 calc R . .
 C17 C 0.34361(11) 0.2349(2) 0.18262(11) 0.0240(6) Uani 1 1 d . . .
 C18 C 0.38647(12) 0.3049(3) 0.18796(12) 0.0355(7) Uani 1 1 d . . .
 H18A H 0.3953 0.3544 0.1579 0.043 Uiso 1 1 calc R . .
 C19 C 0.41704(13) 0.3042(3) 0.23665(14) 0.0443(8) Uani 1 1 d . . .
 H19A H 0.4465 0.3527 0.2398 0.053 Uiso 1 1 calc R . .
 C20 C 0.40403(14) 0.2324(3) 0.28007(14) 0.0460(9) Uani 1 1 d . . .
 H20A H 0.4251 0.2300 0.3131 0.055 Uiso 1 1 calc R . .
 C21 C 0.36095(15) 0.1642(3) 0.27610(13) 0.0445(9) Uani 1 1 d . . .
 H21A H 0.3520 0.1161 0.3066 0.053 Uiso 1 1 calc R . .
 C22 C 0.33034(13) 0.1654(3) 0.22756(12) 0.0335(7) Uani 1 1 d . . .
 H22A H 0.3003 0.1187 0.2251 0.040 Uiso 1 1 calc R . .
 C23 C 0.24803(11) -0.0499(2) -0.02338(12) 0.0242(6) Uani 1 1 d . . .
 C24 C 0.28907(13) -0.1107(3) -0.00024(13) 0.0402(8) Uani 1 1 d . . .
 H24A H 0.2996 -0.0963 0.0375 0.048 Uiso 1 1 calc R . .
 C25 C 0.31504(13) -0.1923(3) -0.03137(14) 0.0397(8) Uani 1 1 d . . .
 H25A H 0.3425 -0.2347 -0.0145 0.048 Uiso 1 1 calc R . .
 C26 C 0.30154(12) -0.2123(3) -0.08581(13) 0.0366(7) Uani 1 1 d . . .
 H26A H 0.3198 -0.2672 -0.1072 0.044 Uiso 1 1 calc R . .
 C27 C 0.26121(14) -0.1520(3) -0.10945(15) 0.0498(9) Uani 1 1 d . . .
 H27A H 0.2515 -0.1658 -0.1475 0.060 Uiso 1 1 calc R . .
 C28 C 0.23440(13) -0.0713(3) -0.07866(13) 0.0417(8) Uani 1 1 d . . .
 H28A H 0.2065 -0.0305 -0.0957 0.050 Uiso 1 1 calc R . .
 C29 C 0.20578(10) 0.0244(2) 0.08682(11) 0.0222(6) Uani 1 1 d . . .
 C30 C 0.24645(11) -0.0139(2) 0.12083(12) 0.0301(7) Uani 1 1 d . . .
 H30A H 0.2802 -0.0177 0.1064 0.036 Uiso 1 1 calc R . .
 C31 C 0.23783(12) -0.0466(2) 0.17580(12) 0.0308(7) Uani 1 1 d . . .
 H31A H 0.2655 -0.0762 0.1981 0.037 Uiso 1 1 calc R . .
 C32 C 0.18985(12) -0.0366(3) 0.19817(12) 0.0323(7) Uani 1 1 d . . .
 H32A H 0.1842 -0.0600 0.2357 0.039 Uiso 1 1 calc R . .
 C33 C 0.14982(12) 0.0075(3) 0.16613(12) 0.0366(7) Uani 1 1 d . . .
 H33A H 0.1169 0.0177 0.1820 0.044 Uiso 1 1 calc R . .
 C34 C 0.15766(11) 0.0371(3) 0.11046(12) 0.0309(7) Uani 1 1 d . . .
 H34A H 0.1298 0.0665 0.0884 0.037 Uiso 1 1 calc R . .
 C35 C 0.15120(11) 0.0583(2) -0.01381(11) 0.0258(6) Uani 1 1 d . . .

C36 C 0.10684(12) 0.0693(2) -0.02780(11) 0.0279(6) Uani 1 1 d . . .
 C37 C 0.05338(11) 0.0887(2) -0.04155(12) 0.0281(6) Uani 1 1 d . . .
 C38 C 0.03090(12) 0.0455(3) -0.09091(12) 0.0330(7) Uani 1 1 d . . .
 H38A H 0.0506 -0.0006 -0.1155 0.040 Uiso 1 1 calc R . .
 C39 C -0.02016(12) 0.0700(3) -0.10389(14) 0.0401(8) Uani 1 1 d . . .
 H39A H -0.0353 0.0416 -0.1377 0.048 Uiso 1 1 calc R . .
 C40 C -0.04901(13) 0.1354(3) -0.06808(15) 0.0425(8) Uani 1 1 d . . .
 H40A H -0.0840 0.1519 -0.0773 0.051 Uiso 1 1 calc R . .
 C41 C -0.02745(12) 0.1773(3) -0.01891(14) 0.0389(8) Uani 1 1 d . . .
 H41A H -0.0477 0.2218 0.0057 0.047 Uiso 1 1 calc R . .
 C42 C 0.02361(12) 0.1545(3) -0.00534(13) 0.0341(7) Uani 1 1 d . . .
 H42A H 0.0384 0.1836 0.0285 0.041 Uiso 1 1 calc R . .
 C43 C 0.39183(14) 0.2375(3) 0.68028(15) 0.0489(9) Uani 1 1 d . . .
 H43A H 0.4271 0.2640 0.6921 0.059 Uiso 1 1 calc R . .
 Cl1 Cl 0.38343(4) 0.09520(9) 0.70289(5) 0.0667(3) Uani 1 1 d . . .
 Cl2 Cl 0.34600(4) 0.32559(11) 0.71241(5) 0.0778(3) Uani 1 1 d . . .
 Cl3 Cl 0.38646(6) 0.24545(14) 0.60755(5) 0.0989(5) Uani 1 1 d . . .

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 P1 0.0215(4) 0.0216(4) 0.0190(3) 0.0009(3) -0.0016(3) -0.0018(3)
 N1 0.0213(12) 0.0231(11) 0.0166(11) -0.0001(9) -0.0028(9) 0.0000(9)
 N2 0.0208(12) 0.0217(12) 0.0174(11) -0.0011(9) -0.0017(9) -0.0015(9)
 C1 0.0243(14) 0.0210(14) 0.0178(13) 0.0025(10) -0.0033(11) -0.0014(11)
 C2 0.0224(15) 0.0307(15) 0.0232(15) 0.0015(12) -0.0067(11) 0.0016(12)
 C3 0.0240(15) 0.0325(16) 0.0237(15) 0.0018(12) -0.0040(12) 0.0059(12)
 C4 0.0215(14) 0.0213(14) 0.0235(14) 0.0012(11) 0.0006(11) -0.0017(11)
 C5 0.0239(15) 0.0219(14) 0.0206(14) -0.0004(11) 0.0012(11) -0.0018(11)
 C6 0.0219(14) 0.0239(14) 0.0192(13) -0.0003(11) 0.0032(11) -0.0005(11)
 C7 0.0298(16) 0.0363(16) 0.0167(14) -0.0038(12) 0.0020(12) 0.0024(13)
 C8 0.0329(17) 0.0371(16) 0.0159(13) -0.0044(12) -0.0013(12) 0.0000(13)
 C9 0.0266(15) 0.0257(14) 0.0171(13) 0.0001(11) -0.0032(11) -0.0011(12)
 C10 0.0257(15) 0.0228(14) 0.0173(13) 0.0019(10) -0.0035(11) -0.0044(11)
 C11 0.0223(15) 0.0297(15) 0.0208(14) -0.0029(11) 0.0005(11) -0.0004(12)
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 C18 0.0359(18) 0.0446(19) 0.0260(16) -0.0001(13) -0.0034(13) -0.0075(15)
 C19 0.0345(19) 0.059(2) 0.0394(19) -0.0106(17) -0.0127(15) -0.0051(16)
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 C21 0.077(3) 0.0339(18) 0.0220(16) 0.0026(13) -0.0118(16) 0.0053(18)
 C22 0.0466(19) 0.0324(16) 0.0214(15) -0.0003(12) -0.0071(13) -0.0056(14)
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 C25 0.0409(19) 0.0379(18) 0.0406(19) 0.0024(14) 0.0045(15) 0.0103(15)
 C26 0.0378(19) 0.0275(16) 0.0449(19) -0.0072(14) 0.0088(15) -0.0029(14)
 C27 0.053(2) 0.060(2) 0.0364(19) -0.0220(17) -0.0062(16) 0.0106(19)
 C28 0.043(2) 0.047(2) 0.0346(18) -0.0109(15) -0.0083(15) 0.0118(16)
 C29 0.0268(15) 0.0199(14) 0.0199(14) -0.0006(10) -0.0010(11) -0.0039(11)
 C30 0.0282(16) 0.0350(16) 0.0270(16) 0.0024(12) -0.0003(12) 0.0002(13)

C31 0.0353(18) 0.0303(16) 0.0265(15) 0.0033(12) -0.0064(13) 0.0013(13)
 C32 0.0417(19) 0.0351(17) 0.0200(15) 0.0030(12) -0.0005(13) -0.0061(14)
 C33 0.0315(17) 0.050(2) 0.0280(16) 0.0022(14) 0.0034(13) -0.0035(15)
 C34 0.0277(16) 0.0394(17) 0.0253(15) 0.0038(12) -0.0027(12) -0.0003(13)
 C35 0.0280(17) 0.0267(15) 0.0224(14) 0.0010(11) -0.0026(12) -0.0041(12)
 C36 0.0325(18) 0.0280(15) 0.0232(15) 0.0022(12) -0.0026(13) -0.0055(13)
 C37 0.0269(16) 0.0299(16) 0.0273(15) 0.0091(12) -0.0024(12) -0.0062(12)
 C38 0.0320(17) 0.0380(17) 0.0289(16) 0.0034(13) -0.0026(13) -0.0058(14)
 C39 0.0363(19) 0.049(2) 0.0345(18) 0.0082(15) -0.0123(15) -0.0069(15)
 C40 0.0276(17) 0.048(2) 0.052(2) 0.0164(17) -0.0044(15) 0.0004(15)
 C41 0.0329(18) 0.0388(18) 0.0452(19) 0.0052(15) 0.0086(15) 0.0021(14)
 C42 0.0335(18) 0.0366(17) 0.0321(17) 0.0029(13) 0.0005(13) -0.0052(14)
 C43 0.043(2) 0.056(2) 0.048(2) -0.0074(17) -0.0022(16) -0.0047(17)
 C11 0.0598(7) 0.0609(6) 0.0801(7) 0.0040(5) 0.0228(5) 0.0025(5)
 C12 0.0669(7) 0.0790(8) 0.0869(8) -0.0305(6) -0.0097(6) 0.0189(6)
 C13 0.1012(10) 0.1530(14) 0.0427(6) 0.0131(7) 0.0050(6) -0.0079(9)

_geom_special_details

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All esds (except the esd in the dihedral angle between two l.s. planes)
 are estimated using the full covariance matrix. The cell esds are taken
 into account individually in the estimation of esds in distances, angles
 and torsion angles; correlations between esds in cell parameters are only
 used when they are defined by crystal symmetry. An approximate (isotropic)
 treatment of cell esds is used for estimating esds involving l.s. planes.

Least-squares planes (x,y,z in crystal coordinates) and deviations from them
 (* indicates atom used to define plane)

10.1957 (0.0074) x + 10.5623 (0.0016) y - 3.4080 (0.0077) z = 5.1895 (0.0015)

* -0.0121 (0.0021) N1
 * 0.0476 (0.0021) N2
 * 0.0187 (0.0024) C1
 * 0.0316 (0.0023) C2
 * 0.0151 (0.0024) C3
 * 0.0062 (0.0024) C4
 * -0.0600 (0.0024) C5
 * -0.0434 (0.0024) C6
 * -0.0085 (0.0024) C7
 * 0.0413 (0.0024) C8
 * 0.0252 (0.0025) C9
 * 0.0450 (0.0023) C10
 * 0.0121 (0.0021) N1_\$1
 * -0.0476 (0.0021) N2_\$1
 * -0.0187 (0.0024) C1_\$1
 * -0.0316 (0.0023) C2_\$1
 * -0.0151 (0.0024) C3_\$1
 * -0.0062 (0.0024) C4_\$1
 * 0.0600 (0.0024) C5_\$1
 * 0.0434 (0.0024) C6_\$1
 * 0.0085 (0.0024) C7_\$1
 * -0.0413 (0.0024) C8_\$1
 * -0.0252 (0.0025) C9_\$1
 * -0.0450 (0.0023) C10_\$1
 -0.1770 (0.0031) C11
 0.1724 (0.0031) C17
 0.0000 (0.0000) Rh1

Rms deviation of fitted atoms = 0.0341

Phenyl ring at C5:

15.1055 (0.0264) x + 4.4753 (0.0138) y + 16.8039 (0.0216) z = 4.8577 (0.0049)
Angle to porphyrin plane (with approximate esd) = 61.16 (0.08)

*	0.0063	(0.0020)	C11
*	-0.0088	(0.0022)	C12
*	0.0033	(0.0023)	C13
*	0.0047	(0.0024)	C14
*	-0.0071	(0.0022)	C15
*	0.0016	(0.0021)	C16

Rms deviation of fitted atoms = 0.0058

Phenyl ring at C10:

14.6374 (0.0282) x - 8.5139 (0.0107) y - 9.3210 (0.0284) z = 1.3146 (0.0145)
Angle to porphyrin plane (with approximate esd) = 66.80 (0.06)

*	0.0130	(0.0021)	C17
*	-0.0056	(0.0023)	C18
*	-0.0062	(0.0024)	C19
*	0.0106	(0.0024)	C20
*	-0.0030	(0.0024)	C21
*	-0.0087	(0.0022)	C22

Rms deviation of fitted atoms = 0.0085

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Rh1	N1	2.041(2)	7	?
Rh1	N2	2.043(2)	7	?
Rh1	N2	2.043(2)	.	?
Rh1	P1	2.3707(7)	.	?
Rh1	P1	2.3707(7)	7	?
P1	C35	1.750(3)	.	?
P1	C23	1.825(3)	.	?
P1	C29	1.829(3)	.	?
N1	C6	1.377(3)	.	?
N1	C9	1.382(3)	.	?
N2	C4	1.377(3)	.	?
N2	C1	1.381(3)	.	?
C1	C10	1.402(4)	7	?
C1	C2	1.428(4)	.	?
C2	C3	1.344(4)	.	?
C2	H2A	0.9500	.	?
C3	C4	1.437(4)	.	?
C3	H3A	0.9500	.	?
C4	C5	1.401(4)	.	?
C5	C6	1.398(4)	.	?
C5	C11	1.500(4)	.	?
C6	C7	1.441(4)	.	?
C7	C8	1.342(4)	.	?

C7 H7A 0.9500 . ?
C8 C9 1.437(4) . ?
C8 H8A 0.9500 . ?
C9 C10 1.392(4) . ?
C10 C1 1.402(4) 7 ?
C10 C17 1.509(4) . ?
C11 C16 1.390(4) . ?
C11 C12 1.393(4) . ?
C12 C13 1.389(4) . ?
C12 H12A 0.9500 . ?
C13 C14 1.379(5) . ?
C13 H13A 0.9500 . ?
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C14 H14A 0.9500 . ?
C15 C16 1.387(4) . ?
C15 H15A 0.9500 . ?
C16 H16A 0.9500 . ?
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C18 C19 1.394(4) . ?
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C30 H30A 0.9500 . ?
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C31 H31A 0.9500 . ?
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C33 H33A 0.9500 . ?
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C38 C39 1.385(4) . ?
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N1 Rh1 P1 90.33(6) 7 . ?
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N2 Rh1 P1 91.26(6) . . ?
N1 Rh1 P1 90.33(6) . 7 ?
N1 Rh1 P1 89.67(6) 7 7 ?
N2 Rh1 P1 91.26(6) 7 7 ?
N2 Rh1 P1 88.74(6) . 7 ?
P1 Rh1 P1 180.00(5) . 7 ?
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C29 P1 Rh1 114.49(8) . . ?
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C6 N1 Rh1 126.63(17) . . ?
C9 N1 Rh1 126.20(18) . . ?
C4 N2 C1 106.8(2) . . ?
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N2 C1 C10 125.8(2) . 7 ?
N2 C1 C2 108.8(2) . . ?
C10 C1 C2 125.3(2) 7 . ?
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C2 C3 C4 107.4(2) . . ?
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N2 C4 C3 108.8(2) . . ?
C5 C4 C3 125.3(2) . . ?
C6 C5 C4 124.5(2) . . ?
C6 C5 C11 117.3(2) . . ?
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N1 C6 C5 126.4(2) . . ?
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N1 C9 C10 125.9(2) . . ?
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 C34 C29 C30 118.4(2) . . ?
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 C30 C29 P1 122.4(2) . . ?
 C31 C30 C29 120.3(3) . . ?
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 C38 C37 C42 119.4(3) . . ?
 C38 C37 C36 121.4(3) . . ?
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 C39 C38 C37 119.8(3) . . ?
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 C41 C40 H40A 119.8 . . ?
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 C41 C42 H42A 120.1 . . ?
 C37 C42 H42A 120.1 . . ?
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 C13 C43 C12 111.3(2) . . ?
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 N1 Rh1 P1 C23 35.07(12) 7 . . . ?
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 N2 Rh1 N1 C6 -177.3(2) 7 . . . ?
 N2 Rh1 N1 C6 2.7(2) . . . ?
 P1 Rh1 N1 C6 -88.6(2) . . . ?
 P1 Rh1 N1 C6 91.4(2) 7 . . . ?
 N2 Rh1 N1 C9 3.5(2) 7 . . . ?
 N2 Rh1 N1 C9 -176.5(2) . . . ?
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 N1 Rh1 N2 C4 -2.8(2) . . . ?
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 P1 Rh1 N2 C4 86.9(2) . . . ?
 P1 Rh1 N2 C4 -93.1(2) 7 . . . ?
 N1 Rh1 N2 C1 -177.2(2) . . . ?
 N1 Rh1 N2 C1 2.8(2) 7 . . . ?
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 P1 Rh1 N2 C1 92.5(2) 7 . . . ?
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 Rh1 N2 C1 C10 -0.2(4) . . . 7 ?
 C4 N2 C1 C2 3.1(3) . . . ?
 Rh1 N2 C1 C2 178.43(17) . . . ?
 N2 C1 C2 C3 -2.4(3) . . . ?
 C10 C1 C2 C3 176.3(3) 7 . . . ?
 C1 C2 C3 C4 0.6(3) . . . ?
 C1 N2 C4 C5 176.1(3) . . . ?
 Rh1 N2 C4 C5 0.9(4) . . . ?
 C1 N2 C4 C3 -2.7(3) . . . ?
 Rh1 N2 C4 C3 -177.99(17) . . . ?
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 N2 C4 C5 C6 2.5(4) . . . ?
 C3 C4 C5 C6 -178.8(3) . . . ?
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 C3 C4 C5 C11 2.1(4) . . . ?
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 C11 C5 C6 C7 -5.9(4) . . . ?
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 C5 C6 C7 C8 -178.1(3) . . . ?
 C6 C7 C8 C9 -0.6(3) . . . ?
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 Rh1 N1 C9 C10 -1.7(4) . . . ?
 C6 N1 C9 C8 -1.0(3) . . . ?
 Rh1 N1 C9 C8 178.29(18) . . . ?
 C7 C8 C9 N1 1.0(3) . . . ?
 C7 C8 C9 C10 -179.0(3) . . . ?

N1 C9 C10 C1 -2.5(4) . . . 7 ?
 C8 C9 C10 C1 177.6(3) . . . 7 ?
 N1 C9 C10 C17 176.3(2) ?
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 C16 C11 C12 C13 -1.5(4) ?
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 P1 C23 C24 C25 -176.4(3) ?
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 Rh1 P1 C35 C36 -50.0(15) ?
 C42 C37 C38 C39 1.2(4) ?
 C36 C37 C38 C39 -177.3(3) ?

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C39 C40 C41 C42 0.5(5) . . . . ?
C40 C41 C42 C37 -0.1(5) . . . . ?
C38 C37 C42 C41 -0.7(4) . . . . ?
C36 C37 C42 C41 177.8(3) . . . . ?

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_chemical_name_common          '(Me) (dpap) Rh (III) TPP'
_chemical_melting_point        ?
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  'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
  'H'  'H'    0.0000  0.0000
  'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
  'N'  'N'    0.0061  0.0033
  'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
  'P'  'P'    0.1023  0.0942
  'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
  'Rh'  'Rh'  -1.1178  0.9187
  'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

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loop_
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  'x, y, z'
  '-x, -y, -z'

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_cell_length_c                  14.1945(9)
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_cell_angle_beta                86.237(3)
_cell_angle_gamma               89.875(4)
_cell_volume                    2527.7(3)
_cell_formula_units_Z           2
_cell_measurement_temperature    180(2)
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_exptl_crystal_density_meas      ?
_exptl_crystal_density_diffn    1.336
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_exptl_crystal_F_000            1048
_exptl_absorpt_coefficient_mu    0.416
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_exptl_absorpt_correction_T_min  0.849
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_exptl_absorpt_process_details   'Sortav Blessing (1995)'

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_exptl_special_details
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;
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Relatively weakly diffracting - data observed only to $2\theta = 22^\circ$. DPAP moiety disordered over 2 orientations, refined as equal occupancy with all phenyl rings constrained to be hexagons (AFIX 66) and with a single isotropic displacement parameter common to all C atoms in both orientations. The C atoms of the porphyrin were refined with anisotropic displacement parameters, but with all ADPs restrained by SIMU. Large difference peaks are largely concentrated around C1 and C11, perhaps suggesting some disorder around these positions - this was not modelled. Although no alternative metric symmetry could be found, the a and b lattice parameters are very similar, and β is close to 90° - possibility of twinning?? No twinning could be interpreted, however...

```
;
```

```

_diffn_ambient_temperature      180(2)
_diffn_radiation_wavelength     0.7107
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_diffn_radiation_monochromator   graphite
_diffn_measurement_device_type   'Nonius KappaCCD'
_diffn_measurement_method       'Thin slice \w and \f scans'
_diffn_standards_number         0
_diffn_reflns_number            15705
_diffn_reflns_av_R_equivalents  0.0815
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_diffn_reflns_theta_min         3.52
_diffn_reflns_theta_max         21.97
_diffn_measured_fraction_theta_max 0.993
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_reflns_number_total            6127
_reflns_number_gt               4980
_reflns_threshold_expression     >2sigma(I)

_computing_data_collection       'Collect (Nonius, 1998)'
_computing_cell_refinement       'HKL Scalepack (Otwinowski & Minor, 1997)'
_computing_data_reduction

;
    HKL Denzo and Scalepack (Otwinowski & Minor, 1997)
;
_computing_structure_solution    'SIR-92 (Altomare et al., 1994)'
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_computing_publication_material 'SHELXTL v6.12 (Bruker AXS, 2001)'

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_refine_special_details

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Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2 , conventional R-factors R are based on F, with F set to zero for negative F^2 . The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

;

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_refine_ls_matrix_type full
_refine_ls_weighting_scheme calc
_refine_ls_weighting_details
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_atom_sites_solution_primary direct
_atom_sites_solution_secondary difmap
_atom_sites_solution_hydrogens geom
_refine_ls_hydrogen_treatment constr
_refine_ls_extinction_method none
_refine_ls_extinction_coef ?
_refine_ls_number_reflns 6127
_refine_ls_number_parameters 385
_refine_ls_number_restraints 178
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P1 P -0.2734(3) 0.2181(3) 0.3722(2) 0.0517(9) Uani 1 1 d . . .
N1 N -0.2978(6) 0.0815(5) 0.1921(6) 0.032(2) Uani 1 1 d D . .
N2 N -0.1156(5) 0.1968(7) 0.1907(6) 0.031(2) Uani 1 1 d D . .
N3 N -0.2292(6) 0.3762(5) 0.1884(6) 0.031(2) Uani 1 1 d D . .
N4 N -0.4120(5) 0.2614(7) 0.1889(6) 0.032(2) Uani 1 1 d D . .
C1 C -0.3917(8) 0.0324(6) 0.1887(8) 0.0338(9) Uani 1 1 d DU A .
C2 C -0.3840(8) -0.0674(6) 0.1839(8) 0.0346(9) Uani 1 1 d DU . .
H2 H -0.4372 -0.1134 0.1801 0.042 Uiso 1 1 calc R A .

C3 C -0.2834(8) -0.0892(9) 0.1855(8) 0.0350(9) Uani 1 1 d U A .
H3 H -0.2543 -0.1538 0.1842 0.042 Uiso 1 1 calc R . .
C4 C -0.2302(8) 0.0038(9) 0.1897(8) 0.0350(9) Uani 1 1 d U A .
C5 C -0.1247(8) 0.0121(9) 0.1866(8) 0.0351(9) Uani 1 1 d U . .
C6 C -0.0744(8) 0.1017(9) 0.1904(8) 0.0352(9) Uani 1 1 d U A .
C7 C 0.0347(8) 0.1112(9) 0.1871(8) 0.0353(9) Uani 1 1 d U . .
H7 H 0.0815 0.0579 0.1866 0.042 Uiso 1 1 calc R A .
C8 C 0.0560(8) 0.2078(8) 0.1849(8) 0.0349(9) Uani 1 1 d U A .
H8 H 0.1210 0.2367 0.1814 0.042 Uiso 1 1 calc R . .
C9 C -0.0428(8) 0.2643(8) 0.1892(8) 0.0342(9) Uani 1 1 d U A .
C10 C -0.0452(8) 0.3670(8) 0.1821(8) 0.0336(9) Uani 1 1 d U . .
C11 C -0.1302(8) 0.4312(6) 0.1895(8) 0.0329(9) Uani 1 1 d DU A .
C12 C -0.1452(8) 0.5313(6) 0.1783(8) 0.0341(9) Uani 1 1 d DU . .
H12 H -0.0942 0.5812 0.1711 0.041 Uiso 1 1 calc R A .
C13 C -0.2434(8) 0.5486(9) 0.1789(8) 0.0346(9) Uani 1 1 d U A .
H13 H -0.2739 0.6128 0.1757 0.042 Uiso 1 1 calc R . .
C14 C -0.2970(8) 0.4510(8) 0.1856(8) 0.0346(9) Uani 1 1 d U A .
C15 C -0.4010(8) 0.4464(8) 0.1832(8) 0.0347(9) Uani 1 1 d U . .
C16 C -0.4514(8) 0.3566(9) 0.1873(8) 0.0348(9) Uani 1 1 d U A .
C17 C -0.5612(8) 0.3474(9) 0.1861(8) 0.0350(9) Uani 1 1 d U . .
H17 H -0.6080 0.4008 0.1862 0.042 Uiso 1 1 calc R A .
C18 C -0.5829(8) 0.2497(8) 0.1846(8) 0.0349(9) Uani 1 1 d U A .
H18 H -0.6475 0.2214 0.1820 0.042 Uiso 1 1 calc R . .
C19 C -0.4870(8) 0.1942(8) 0.1880(8) 0.0345(9) Uani 1 1 d U A .
C20 C -0.4809(8) 0.0922(8) 0.1839(8) 0.0341(9) Uani 1 1 d U . .
C21 C -0.0667(9) -0.0816(9) 0.1753(8) 0.038(3) Uiso 1 1 d . A .
C22 C -0.0251(10) -0.1352(11) 0.2501(10) 0.056(4) Uiso 1 1 d . . .
H22 H -0.0329 -0.1129 0.3116 0.068 Uiso 1 1 calc R A .
C23 C 0.0295(12) -0.2236(13) 0.2365(12) 0.073(4) Uiso 1 1 d . A .
H23 H 0.0595 -0.2600 0.2883 0.088 Uiso 1 1 calc R . .
C24 C 0.0385(11) -0.2557(12) 0.1502(11) 0.067(4) Uiso 1 1 d . . .
H24 H 0.0714 -0.3174 0.1420 0.080 Uiso 1 1 calc R A .
C25 C 0.0014(11) -0.2015(11) 0.0741(11) 0.062(4) Uiso 1 1 d . A .
H25 H 0.0119 -0.2231 0.0126 0.074 Uiso 1 1 calc R . .
C26 C -0.0527(10) -0.1131(11) 0.0867(10) 0.057(4) Uiso 1 1 d . . .
H26 H -0.0794 -0.0753 0.0338 0.068 Uiso 1 1 calc R A .
C27 C 0.0482(8) 0.4269(8) 0.1731(8) 0.034(3) Uiso 1 1 d . A .
C28 C 0.0882(10) 0.4683(11) 0.2490(10) 0.055(3) Uiso 1 1 d . . .
H28 H 0.0527 0.4603 0.3095 0.066 Uiso 1 1 calc R A .
C29 C 0.1767(11) 0.5197(12) 0.2384(11) 0.067(4) Uiso 1 1 d . A .
H29 H 0.2027 0.5460 0.2915 0.080 Uiso 1 1 calc R . .
C30 C 0.2289(11) 0.5338(11) 0.1499(10) 0.059(4) Uiso 1 1 d . . .
H30 H 0.2902 0.5702 0.1427 0.071 Uiso 1 1 calc R A .
C31 C 0.1928(11) 0.4957(11) 0.0737(11) 0.061(4) Uiso 1 1 d . A .
H31 H 0.2282 0.5053 0.0132 0.073 Uiso 1 1 calc R . .
C32 C 0.1023(10) 0.4421(10) 0.0862(9) 0.051(3) Uiso 1 1 d . . .
H32 H 0.0771 0.4151 0.0332 0.061 Uiso 1 1 calc R A .
C33 C -0.4580(8) 0.5429(9) 0.1712(8) 0.036(3) Uiso 1 1 d . A .
C34 C -0.5111(10) 0.5796(10) 0.2473(10) 0.051(3) Uiso 1 1 d . . .
H34 H -0.5132 0.5428 0.3084 0.061 Uiso 1 1 calc R A .
C35 C -0.5620(11) 0.6715(11) 0.2337(10) 0.059(4) Uiso 1 1 d . A .
H35 H -0.5985 0.6974 0.2854 0.071 Uiso 1 1 calc R . .
C36 C -0.5583(10) 0.7226(11) 0.1461(9) 0.051(3) Uiso 1 1 d . . .
H36 H -0.5913 0.7854 0.1372 0.062 Uiso 1 1 calc R A .
C37 C -0.5089(9) 0.6869(10) 0.0711(9) 0.047(3) Uiso 1 1 d . A .
H37 H -0.5081 0.7238 0.0101 0.057 Uiso 1 1 calc R . .
C38 C -0.4593(9) 0.5960(10) 0.0834(9) 0.048(3) Uiso 1 1 d . . .
H38 H -0.4257 0.5702 0.0302 0.057 Uiso 1 1 calc R A .
C39 C -0.5731(8) 0.0346(8) 0.1721(8) 0.034(3) Uiso 1 1 d . A .
C40 C -0.6219(10) -0.0246(10) 0.2485(9) 0.049(3) Uiso 1 1 d . . .
H40 H -0.5951 -0.0302 0.3091 0.059 Uiso 1 1 calc R A .

C41 C -0.7103(10) -0.0756(11) 0.2352(10) 0.057(4) Uiso 1 1 d . A .
H41 H -0.7429 -0.1166 0.2868 0.069 Uiso 1 1 calc R . .
C42 C -0.7499(10) -0.0668(10) 0.1489(9) 0.051(3) Uiso 1 1 d . . .
H42 H -0.8104 -0.1007 0.1407 0.061 Uiso 1 1 calc R A .
C43 C -0.7026(10) -0.0089(11) 0.0737(10) 0.056(4) Uiso 1 1 d . A .
H43 H -0.7301 -0.0037 0.0134 0.067 Uiso 1 1 calc R . .
C44 C -0.6146(10) 0.0423(10) 0.0850(9) 0.050(3) Uiso 1 1 d . . .
H44 H -0.5829 0.0827 0.0326 0.060 Uiso 1 1 calc R A .
C45 C -0.2531(9) 0.2445(9) 0.0479(8) 0.043(3) Uiso 1 1 d . . .
H45A H -0.2670 0.1798 0.0248 0.064 Uiso 1 1 calc R A .
H45B H -0.1854 0.2668 0.0249 0.064 Uiso 1 1 calc R . .
H45C H -0.3017 0.2943 0.0243 0.064 Uiso 1 1 calc R . .
C46 C -0.3589(13) 0.2963(14) 0.4283(16) 0.077(2) Uiso 0.50 1 d PGD A 1
C47 C -0.4597(15) 0.2777(14) 0.4195(15) 0.077(2) Uiso 0.50 1 d PGD A 1
H47A H -0.4795 0.2209 0.3902 0.093 Uiso 0.50 1 calc PR A 1
C48 C -0.5317(11) 0.3421(16) 0.4535(16) 0.077(2) Uiso 0.50 1 d PGD A 1
H48A H -0.6006 0.3295 0.4475 0.093 Uiso 0.50 1 calc PR A 1
C49 C -0.5029(14) 0.4252(15) 0.4964(15) 0.077(2) Uiso 0.50 1 d PGD . 1
H49A H -0.5521 0.4692 0.5196 0.093 Uiso 0.50 1 calc PR A 1
C50 C -0.4020(15) 0.4437(13) 0.5052(15) 0.077(2) Uiso 0.50 1 d PGD A 1
H50A H -0.3823 0.5005 0.5345 0.093 Uiso 0.50 1 calc PR A 1
C51 C -0.3300(11) 0.3793(16) 0.4711(16) 0.077(2) Uiso 0.50 1 d PGD A 1
H51A H -0.2611 0.3920 0.4772 0.093 Uiso 0.50 1 calc PR A 1
C52 C -0.2848(16) 0.0922(12) 0.4421(15) 0.077(2) Uiso 0.50 1 d PGD A 1
C53 C -0.3628(15) 0.0319(15) 0.4207(13) 0.077(2) Uiso 0.50 1 d PGD A 1
H53A H -0.4048 0.0549 0.3716 0.093 Uiso 0.50 1 calc PR A 1
C54 C -0.3792(14) -0.0619(14) 0.4710(15) 0.077(2) Uiso 0.50 1 d PGD A 1
H54A H -0.4325 -0.1031 0.4564 0.093 Uiso 0.50 1 calc PR A 1
C55 C -0.3177(16) -0.0955(12) 0.5428(14) 0.077(2) Uiso 0.50 1 d PGD A 1
H55A H -0.3289 -0.1597 0.5773 0.093 Uiso 0.50 1 calc PR A 1
C56 C -0.2397(15) -0.0352(16) 0.5643(13) 0.077(2) Uiso 0.50 1 d PGD A 1
H56A H -0.1977 -0.0582 0.6133 0.093 Uiso 0.50 1 calc PR A 1
C57 C -0.2233(14) 0.0586(14) 0.5139(15) 0.077(2) Uiso 0.50 1 d PGD A 1
H57A H -0.1700 0.0998 0.5286 0.093 Uiso 0.50 1 calc PR A 1
C58 C -0.150(2) 0.263(2) 0.406(2) 0.077(2) Uiso 0.50 1 d PD A 1
C59 C -0.077(2) 0.286(3) 0.435(2) 0.077(2) Uiso 0.50 1 d PD A 1
C60 C 0.0193(12) 0.3096(17) 0.4712(15) 0.077(2) Uiso 0.50 1 d PGD A 1
C61 C 0.1075(15) 0.2776(16) 0.4269(13) 0.077(2) Uiso 0.50 1 d PGD A 1
H61A H 0.1050 0.2359 0.3769 0.093 Uiso 0.50 1 calc PR A 1
C62 C 0.1993(12) 0.3064(17) 0.4557(15) 0.077(2) Uiso 0.50 1 d PGD A 1
H62A H 0.2596 0.2846 0.4254 0.093 Uiso 0.50 1 calc PR A 1
C63 C 0.2030(12) 0.3673(17) 0.5289(15) 0.077(2) Uiso 0.50 1 d PGD A 1
H63A H 0.2657 0.3871 0.5486 0.093 Uiso 0.50 1 calc PR A 1
C64 C 0.1148(15) 0.3993(16) 0.5732(13) 0.077(2) Uiso 0.50 1 d PGD A 1
H64A H 0.1173 0.4409 0.6232 0.093 Uiso 0.50 1 calc PR A 1
C65 C 0.0230(12) 0.3704(17) 0.5444(14) 0.077(2) Uiso 0.50 1 d PGD A 1
H65A H -0.0373 0.3923 0.5747 0.093 Uiso 0.50 1 calc PR A 1
C46' C -0.4012(14) 0.210(2) 0.4422(19) 0.106(3) Uiso 0.50 1 d PGD A 2
C47' C -0.4601(19) 0.1301(19) 0.4235(17) 0.106(3) Uiso 0.50 1 d PGD A 2
H47B H -0.4381 0.0889 0.3758 0.128 Uiso 0.50 1 calc PR A 2
C48' C -0.5513(18) 0.1105(18) 0.475(2) 0.106(3) Uiso 0.50 1 d PGD A 2
H48B H -0.5916 0.0558 0.4618 0.128 Uiso 0.50 1 calc PR A 2
C49' C -0.5835(16) 0.171(2) 0.5444(18) 0.106(3) Uiso 0.50 1 d PGD A 2
H49B H -0.6459 0.1574 0.5793 0.128 Uiso 0.50 1 calc PR A 2
C50' C -0.525(2) 0.251(2) 0.5631(17) 0.106(3) Uiso 0.50 1 d PGD A 2
H50B H -0.5466 0.2919 0.6108 0.128 Uiso 0.50 1 calc PR A 2
C51' C -0.4334(18) 0.2703(17) 0.512(2) 0.106(3) Uiso 0.50 1 d PGD A 2
H51B H -0.3931 0.3249 0.5247 0.128 Uiso 0.50 1 calc PR A 2
C52' C -0.1972(18) 0.1370(17) 0.4303(19) 0.106(3) Uiso 0.50 1 d PGD A 2
C53' C -0.2320(15) 0.039(2) 0.451(2) 0.106(3) Uiso 0.50 1 d PGD A 2
H53B H -0.2974 0.0219 0.4359 0.128 Uiso 0.50 1 calc PR A 2

C54' C -0.171(2) -0.0340(15) 0.494(2) 0.106(3) Uiso 0.50 1 d PGD A 2
 H54B H -0.1948 -0.1011 0.5082 0.128 Uiso 0.50 1 calc PR A 2
 C55' C -0.0753(19) -0.0090(18) 0.5163(18) 0.106(3) Uiso 0.50 1 d PGD . 2
 H55B H -0.0337 -0.0590 0.5457 0.128 Uiso 0.50 1 calc PR A 2
 C56' C -0.0406(15) 0.089(2) 0.4955(19) 0.106(3) Uiso 0.50 1 d PGD . 2
 H56B H 0.0248 0.1061 0.5107 0.128 Uiso 0.50 1 calc PR A 2
 C57' C -0.1015(19) 0.1620(15) 0.453(2) 0.106(3) Uiso 0.50 1 d PGD A 2
 H57B H -0.0777 0.2290 0.4383 0.128 Uiso 0.50 1 calc PR A 2
 C58' C -0.242(3) 0.351(2) 0.403(3) 0.106(3) Uiso 0.50 1 d PD A 2
 C59' C -0.213(3) 0.427(2) 0.418(3) 0.106(3) Uiso 0.50 1 d PD A 2
 C60' C -0.190(2) 0.5307(14) 0.4343(19) 0.106(3) Uiso 0.50 1 d PGD A 2
 C61' C -0.2461(17) 0.6086(19) 0.3922(18) 0.106(3) Uiso 0.50 1 d PGD A 2
 H61B H -0.2997 0.5943 0.3550 0.128 Uiso 0.50 1 calc PR A 2
 C62' C -0.224(2) 0.7074(16) 0.4047(19) 0.106(3) Uiso 0.50 1 d PGD A 2
 H62B H -0.2620 0.7606 0.3759 0.128 Uiso 0.50 1 calc PR A 2
 C63' C -0.145(2) 0.7283(15) 0.459(2) 0.106(3) Uiso 0.50 1 d PGD A 2
 H63B H -0.1301 0.7959 0.4676 0.128 Uiso 0.50 1 calc PR A 2
 C64' C -0.0894(18) 0.650(2) 0.5012(18) 0.106(3) Uiso 0.50 1 d PGD A 2
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 C65' C -0.1118(19) 0.5516(17) 0.4888(19) 0.106(3) Uiso 0.50 1 d PGD A 2
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Rh1 0.0239(5) 0.0187(5) 0.0377(6) -0.0051(3) -0.0015(3) -0.0027(3)
 P1 0.051(2) 0.065(2) 0.0396(19) -0.0057(17) -0.0001(16) -0.0069(18)
 N1 0.024(5) 0.038(6) 0.034(5) -0.015(4) -0.002(4) 0.001(4)
 N2 0.030(5) 0.029(5) 0.035(5) -0.006(4) -0.010(4) 0.005(4)
 N3 0.030(5) 0.027(5) 0.035(5) 0.002(4) -0.003(4) 0.009(4)
 N4 0.023(5) 0.042(6) 0.030(5) -0.004(4) 0.001(4) 0.008(4)
 C1 0.0295(17) 0.0336(17) 0.0382(18) -0.0046(16) -0.0009(16) -0.0013(16)
 C2 0.0303(17) 0.0341(17) 0.0394(18) -0.0042(16) -0.0010(16) -0.0016(16)
 C3 0.0309(17) 0.0342(17) 0.0400(18) -0.0042(16) -0.0011(16) -0.0013(16)
 C4 0.0311(16) 0.0339(17) 0.0398(18) -0.0042(16) -0.0011(16) -0.0009(15)
 C5 0.0316(16) 0.0338(17) 0.0399(18) -0.0041(16) -0.0012(16) -0.0009(15)
 C6 0.0321(16) 0.0337(17) 0.0399(17) -0.0040(16) -0.0012(15) -0.0010(15)
 C7 0.0325(16) 0.0337(16) 0.0395(17) -0.0037(15) -0.0015(15) -0.0010(15)
 C8 0.0327(15) 0.0334(16) 0.0386(16) -0.0035(14) -0.0017(14) -0.0014(14)
 C9 0.0327(15) 0.0328(15) 0.0370(15) -0.0032(13) -0.0020(13) -0.0015(13)
 C10 0.0322(13) 0.0327(14) 0.0358(14) -0.0030(12) -0.0020(12) -0.0008(12)
 C11 0.0316(12) 0.0328(12) 0.0343(12) -0.0028(9) -0.0019(9) -0.0001(9)
 C12 0.0322(13) 0.0336(14) 0.0364(14) -0.0032(12) -0.0016(12) -0.0007(12)
 C13 0.0323(14) 0.0337(15) 0.0377(15) -0.0035(13) -0.0012(13) -0.0008(13)
 C14 0.0319(15) 0.0337(16) 0.0380(16) -0.0039(14) -0.0009(14) -0.0006(14)
 C15 0.0318(16) 0.0335(16) 0.0386(17) -0.0039(15) -0.0007(15) -0.0008(15)
 C16 0.0316(16) 0.0335(17) 0.0392(17) -0.0041(16) -0.0006(15) -0.0009(15)
 C17 0.0315(16) 0.0336(17) 0.0396(18) -0.0040(16) -0.0003(16) -0.0010(15)
 C18 0.0314(17) 0.0337(17) 0.0395(18) -0.0040(16) -0.0002(16) -0.0013(16)
 C19 0.0309(17) 0.0335(17) 0.0390(18) -0.0042(16) -0.0003(16) -0.0017(16)
 C20 0.0302(17) 0.0336(17) 0.0386(18) -0.0044(16) -0.0005(16) -0.0016(16)

_geom_special_details

;

All esds (except the esd in the dihedral angle between two l.s. planes)
 are estimated using the full covariance matrix. The cell esds are taken

into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Least-squares planes (x,y,z in crystal coordinates) and deviations from them (* indicates atom used to define plane)

$-0.0176 \text{ (0.0127)} x + 0.1166 \text{ (0.0126)} y + 14.0959 \text{ (0.0019)} z = 2.6588 \text{ (0.0050)}$

*	0.0641	(0.0083)	N1
*	0.0536	(0.0083)	N2
*	0.0444	(0.0084)	N3
*	0.0415	(0.0082)	N4
*	0.0120	(0.0102)	C1
*	-0.0677	(0.0098)	C2
*	-0.0489	(0.0099)	C3
*	0.0199	(0.0105)	C4
*	-0.0247	(0.0104)	C5
*	0.0386	(0.0105)	C6
*	-0.0094	(0.0098)	C7
*	-0.0291	(0.0098)	C8
*	0.0390	(0.0103)	C9
*	-0.0479	(0.0100)	C10
*	0.0645	(0.0099)	C11
*	-0.0813	(0.0096)	C12
*	-0.0681	(0.0098)	C13
*	0.0151	(0.0104)	C14
*	-0.0179	(0.0102)	C15
*	0.0308	(0.0104)	C16
*	0.0143	(0.0098)	C17
*	-0.0169	(0.0099)	C18
*	0.0221	(0.0103)	C19
*	-0.0481	(0.0101)	C20
	-0.1962	(0.0123)	C21
	-0.1698	(0.0118)	C27
	-0.1746	(0.0119)	C33
	-0.2184	(0.0118)	C39
	0.1084	(0.0024)	Rh1

Rms deviation of fitted atoms = 0.0434

Phenyl ring at C5:

$-11.2091 \text{ (0.0435)} x - 6.9560 \text{ (0.0664)} y + 0.9691 \text{ (0.0847)} z = 1.4692 \text{ (0.0165)}$
 Angle to porphyrin plane (with approximate esd) = 79.88 (0.36)

*	0.0161	(0.0091)	C21
*	-0.0050	(0.0100)	C22
*	-0.0149	(0.0111)	C23
*	0.0235	(0.0110)	C24
*	-0.0117	(0.0104)	C25
*	-0.0080	(0.0098)	C26

Rms deviation of fitted atoms = 0.0145

Phenyl ring at C10:

$-6.8555 \text{ (0.0622)} x + 11.1108 \text{ (0.0416)} y - 2.3359 \text{ (0.0811)} z = 4.0110 \text{ (0.0345)}$

Angle to porphyrin plane (with approximate esd) = 77.74 (0.34)

```
* -0.0024 (0.0087) C27
*  0.0057 (0.0099) C28
* -0.0046 (0.0105) C29
*  0.0002 (0.0103) C30
*  0.0029 (0.0102) C31
* -0.0019 (0.0095) C32
```

Rms deviation of fitted atoms = 0.0035

Phenyl ring at C15:

-11.2359 (0.0388) x - 6.8382 (0.0605) y - 4.2785 (0.0727) z = 0.7159 (0.0590)
Angle to porphyrin plane (with approximate esd) = 78.60 (0.31)

```
* -0.0148 (0.0085) C33
*  0.0057 (0.0091) C34
*  0.0066 (0.0097) C35
* -0.0100 (0.0094) C36
*  0.0006 (0.0090) C37
*  0.0119 (0.0088) C38
```

Rms deviation of fitted atoms = 0.0095

Phenyl ring at C20:

-6.8901 (0.0596) x + 10.9957 (0.0406) y + 4.2003 (0.0733) z = 5.0549 (0.0388)
Angle to porphyrin plane (with approximate esd) = 75.36 (0.31)

```
* -0.0023 (0.0085) C39
*  0.0033 (0.0091) C40
* -0.0038 (0.0097) C41
*  0.0032 (0.0096) C42
* -0.0021 (0.0097) C43
*  0.0017 (0.0092) C44
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Rms deviation of fitted atoms = 0.0028

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Rh1 N1 2.028(7) . ?
Rh1 N2 2.032(6) . ?
Rh1 N4 2.033(6) . ?
Rh1 C45 2.059(11) . ?
Rh1 P1 2.512(3) . ?
P1 C52' 1.678(18) . ?
P1 C46 1.759(15) . ?
P1 C52 1.866(15) . ?
P1 C58 1.87(3) . ?
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P1 C58' 1.93(3) . ?
N1 C4 1.380(14) . ?
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N2 C6 1.387(14) . ?
N3 C14 1.350(13) . ?
N3 C11 1.520(13) . ?
N4 C19 1.351(14) . ?
N4 C16 1.378(14) . ?
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C3 H3 0.9500 . ?
C4 C5 1.414(15) . ?
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C5 C21 1.493(16) . ?
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C7 C8 1.323(16) . ?
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C8 H8 0.9500 . ?
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C32 H32 0.9500 . ?

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C64 H64A 0.9500 . ?
C65 H65A 0.9500 . ?

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 C48' H48B 0.9500 . ?
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 C49' H49B 0.9500 . ?
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 C50' H50B 0.9500 . ?
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 C54' H54B 0.9500 . ?
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 C55' H55B 0.9500 . ?
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 C57' H57B 0.9500 . ?
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 C60' C65' 1.3900 . ?
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 C62' H62B 0.9500 . ?
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 C64' H64B 0.9500 . ?
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loop_

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 N3 Rh1 N2 88.9(3) . . ?
 N1 Rh1 N2 90.7(3) . . ?
 N3 Rh1 N4 91.0(4) . . ?
 N1 Rh1 N4 89.1(4) . . ?
 N2 Rh1 N4 176.6(3) . . ?
 N3 Rh1 C45 87.9(4) . . ?
 N1 Rh1 C45 89.1(4) . . ?
 N2 Rh1 C45 88.3(4) . . ?
 N4 Rh1 C45 88.3(4) . . ?
 N3 Rh1 P1 89.3(3) . . ?
 N1 Rh1 P1 93.7(3) . . ?
 N2 Rh1 P1 91.1(3) . . ?
 N4 Rh1 P1 92.4(3) . . ?
 C45 Rh1 P1 177.1(4) . . ?

C52' P1 C46 124.0(12) . . ?
C52' P1 C52 43.1(11) . . ?
C46 P1 C52 106.1(10) . . ?
C52' P1 C58 60.6(15) . . ?
C46 P1 C58 102.6(12) . . ?
C52 P1 C58 101.9(11) . . ?
C52' P1 C46' 107.2(12) . . ?
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C52 P1 C46' 71.6(11) . . ?
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C52' P1 C58' 107.7(14) . . ?
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C58 P1 C58' 53.1(11) . . ?
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C46 P1 Rh1 118.1(8) . . ?
C52 P1 Rh1 119.0(7) . . ?
C58 P1 Rh1 106.7(10) . . ?
C46' P1 Rh1 119.9(9) . . ?
C58' P1 Rh1 105.9(12) . . ?
C4 N1 C1 103.0(7) . . ?
C4 N1 Rh1 126.2(7) . . ?
C1 N1 Rh1 130.8(6) . . ?
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C14 N3 Rh1 124.4(7) . . ?
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C16 N4 Rh1 124.7(7) . . ?
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N1 C1 C20 118.8(8) . . ?
C1 C2 C3 106.1(10) . . ?
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C4 C3 H3 126.1 . . ?
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N1 C4 C3 109.4(9) . . ?
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C4 C5 C21 116.7(10) . . ?
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N2 C9 C8 107.2(9) . . ?
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C9 C10 C11 128.5(10) . . ?

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 C12 C11 N3 109.9(9) . . ?
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 C14 C13 H13 125.6 . . ?
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 N3 C14 C13 108.9(9) . . ?
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 C14 C15 C33 118.5(10) . . ?
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 N4 C16 C17 107.6(9) . . ?
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H45A C45 H45C 109.5 . . ?
H45B C45 H45C 109.5 . . ?
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C51 C46 P1 123.2(12) . . ?
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C48 C49 C49 152(2) . 2_466 ?

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 C49 C49 H49A 49.8 2_466 . ?
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 C50 C51 H51A 120.0 . . ?
 C46 C51 H51A 120.0 . . ?
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 C57 C52 P1 124.2(12) . . ?
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 C53 C54 H54A 120.0 . . ?
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 C54 C55 H55A 120.0 . . ?
 C56 C55 H55A 120.0 . . ?
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 C55 C56 H56A 120.0 . . ?
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 C58 C59 C60 176(4) . . ?
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 C60 C65 H65A 120.0 . . ?
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 C51' C46' P1 126.0(16) . . ?
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 C54' C55' C56' 126(3) . 2_556 ?
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 C55' C56' H56B 120.0 . . ?
 C55' C56' H56B 53.8 2_556 . ?
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 C58' C59' C60' 171(4) . . ?
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 C65' C60' C59' 120.5(17) . . ?
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 C62' C61' H61B 120.0 . . ?
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 N4 Rh1 P1 C52' 147.9(11) ?
 N3 Rh1 P1 C46 58.7(8) ?
 N1 Rh1 P1 C46 -121.6(8) ?
 N2 Rh1 P1 C46 147.6(8) ?
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 N2 Rh1 P1 C52 -81.5(8) ?
 N4 Rh1 P1 C52 98.5(8) ?
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 N1 Rh1 P1 C58 123.7(10) ?
 N2 Rh1 P1 C58 32.9(11) ?
 N4 Rh1 P1 C58 -147.0(11) ?
 N3 Rh1 P1 C46' 105.1(10) ?
 N1 Rh1 P1 C46' -75.2(10) ?
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 N2 Rh1 P1 C58' 88.4(12) ?
 N4 Rh1 P1 C58' -91.5(12) ?
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 N4 Rh1 N1 C4 176.8(9) ?
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 P1 Rh1 N1 C4 -90.9(8) ?
 N2 Rh1 N1 C1 -176.8(9) ?
 N4 Rh1 N1 C1 -0.2(9) ?
 C45 Rh1 N1 C1 -88.5(9) ?
 P1 Rh1 N1 C1 92.1(9) ?
 N3 Rh1 N2 C9 2.1(9) ?
 N1 Rh1 N2 C9 179.0(9) ?
 C45 Rh1 N2 C9 90.0(9) ?
 P1 Rh1 N2 C9 -87.2(9) ?
 N3 Rh1 N2 C6 -178.6(9) ?
 N1 Rh1 N2 C6 -1.6(9) ?
 C45 Rh1 N2 C6 -90.7(9) ?
 P1 Rh1 N2 C6 92.1(8) ?
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 N4 Rh1 N3 C14 1.7(9) ?
 C45 Rh1 N3 C14 89.9(9) ?
 P1 Rh1 N3 C14 -90.7(8) ?
 N2 Rh1 N3 C11 -4.2(9) ?
 N4 Rh1 N3 C11 179.2(9) ?
 C45 Rh1 N3 C11 -92.5(9) ?
 P1 Rh1 N3 C11 86.9(9) ?
 N3 Rh1 N4 C19 178.5(9) ?
 N1 Rh1 N4 C19 1.6(9) ?
 C45 Rh1 N4 C19 90.7(9) ?
 P1 Rh1 N4 C19 -92.1(9) ?
 N3 Rh1 N4 C16 -2.6(8) ?
 N1 Rh1 N4 C16 -179.5(8) ?
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 Rh1 N1 C1 C20 1.4(15) ?
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 C20 C1 C2 C3 176.2(11) ?

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Rh1 N1 C4 C5 -1.1(16) ?
C1 N1 C4 C3 -0.3(11) ?
Rh1 N1 C4 C3 -178.0(7) ?
C2 C3 C4 N1 0.9(13) ?
C2 C3 C4 C5 -176.0(11) ?
N1 C4 C5 C6 3.4(19) ?
C3 C4 C5 C6 179.8(11) ?
N1 C4 C5 C21 -174.5(10) ?
C3 C4 C5 C21 2.0(17) ?
C4 C5 C6 N2 -5.1(19) ?
C21 C5 C6 N2 172.7(10) ?
C4 C5 C6 C7 -179.9(11) ?
C21 C5 C6 C7 -2.1(17) ?
C9 N2 C6 C5 -176.3(11) ?
Rh1 N2 C6 C5 4.3(16) ?
C9 N2 C6 C7 -0.9(12) ?
Rh1 N2 C6 C7 179.7(7) ?
C5 C6 C7 C8 175.3(11) ?
N2 C6 C7 C8 -0.3(12) ?
C6 C7 C8 C9 1.3(12) ?
C6 N2 C9 C10 174.8(12) ?
Rh1 N2 C9 C10 -5.7(17) ?
C6 N2 C9 C8 1.6(12) ?
Rh1 N2 C9 C8 -179.0(7) ?
C7 C8 C9 N2 -1.8(12) ?
C7 C8 C9 C10 -175.9(10) ?
N2 C9 C10 C11 11(2) ?
C8 C9 C10 C11 -176.5(10) ?
N2 C9 C10 C27 -174.3(11) ?
C8 C9 C10 C27 -1.9(16) ?
C9 C10 C11 C12 -174.7(12) ?
C27 C10 C11 C12 10.2(18) ?
C9 C10 C11 N3 -11.1(16) ?
C27 C10 C11 N3 173.9(8) ?
C14 N3 C11 C12 -5.8(12) ?
Rh1 N3 C11 C12 176.3(7) ?
C14 N3 C11 C10 -173.7(9) ?
Rh1 N3 C11 C10 8.4(14) ?
C10 C11 C12 C13 169.9(12) ?
N3 C11 C12 C13 5.8(12) ?
C11 C12 C13 C14 -3.5(13) ?
C11 N3 C14 C15 179.8(11) ?
Rh1 N3 C14 C15 -2.1(17) ?
C11 N3 C14 C13 3.5(11) ?
Rh1 N3 C14 C13 -178.4(7) ?
C12 C13 C14 N3 -0.3(13) ?
C12 C13 C14 C15 -176.9(10) ?
N3 C14 C15 C16 2.7(19) ?
C13 C14 C15 C16 178.6(10) ?
N3 C14 C15 C33 -174.4(10) ?
C13 C14 C15 C33 1.5(16) ?
C14 C15 C16 N4 -3.9(19) ?
C33 C15 C16 N4 173.2(10) ?
C14 C15 C16 C17 179.3(10) ?
C33 C15 C16 C17 -3.6(17) ?
C19 N4 C16 C15 -176.7(11) ?
Rh1 N4 C16 C15 4.2(16) ?
C19 N4 C16 C17 0.5(12) ?
Rh1 N4 C16 C17 -178.5(7) ?

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 N4 C16 C17 C18 -1.5(12) ?
 C16 C17 C18 C19 1.7(12) ?
 C16 N4 C19 C20 176.2(11) ?
 Rh1 N4 C19 C20 -4.8(17) ?
 C16 N4 C19 C18 0.6(12) ?
 Rh1 N4 C19 C18 179.6(7) ?
 C17 C18 C19 N4 -1.5(12) ?
 C17 C18 C19 C20 -177.4(11) ?
 N4 C19 C20 C1 6.4(19) ?
 C18 C19 C20 C1 -178.5(10) ?
 N4 C19 C20 C39 -172.8(11) ?
 C18 C19 C20 C39 2.2(16) ?
 C2 C1 C20 C19 -179.3(11) ?
 N1 C1 C20 C19 -4.3(17) ?
 C2 C1 C20 C39 -0.1(17) ?
 N1 C1 C20 C39 174.9(9) ?
 C6 C5 C21 C22 79.8(15) ?
 C4 C5 C21 C22 -102.3(14) ?
 C6 C5 C21 C26 -98.5(14) ?
 C4 C5 C21 C26 79.5(15) ?
 C26 C21 C22 C23 -2(2) ?
 C5 C21 C22 C23 -179.9(13) ?
 C21 C22 C23 C24 -1(2) ?
 C22 C23 C24 C25 4(2) ?
 C23 C24 C25 C26 -4(2) ?
 C22 C21 C26 C25 2(2) ?
 C5 C21 C26 C25 -179.7(12) ?
 C24 C25 C26 C21 1(2) ?
 C9 C10 C27 C32 78.2(15) ?
 C11 C10 C27 C32 -106.2(12) ?
 C9 C10 C27 C28 -99.9(14) ?
 C11 C10 C27 C28 75.6(14) ?
 C32 C27 C28 C29 -1(2) ?
 C10 C27 C28 C29 177.3(13) ?
 C27 C28 C29 C30 1(2) ?
 C28 C29 C30 C31 -1(2) ?
 C29 C30 C31 C32 0(2) ?
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 C30 C31 C32 C27 0(2) ?
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 C14 C15 C33 C38 77.5(14) ?
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 C15 C33 C34 C35 178.7(12) ?
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 C35 C36 C37 C38 -1(2) ?
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 C36 C37 C38 C33 -1.3(19) ?
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 C40 C41 C42 C43 1(2) ?

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Rh1 P1 C46 C47 65.8(12) ?
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C58' P1 C52 C53 140.2(18) ?
Rh1 P1 C52 C53 -53.3(12) ?
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Rh1 P1 C46' C47' 56.4(14) ?
C52' P1 C46' C51' 92.9(18) ?

C46 P1 C46' C51' -29.7(16) ?
 C52 P1 C46' C51' 117.5(17) ?
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