Crystal data for [(CNN)Pt{C(NH^{t}Bu)(NHMe)}]ClO_4•0.5 H_2O, **2**(ClO_4)•0.5 H_2O

Complex **2**(ClO_4)•0.5 H_2O: kkc 471

Crystal data. {[$Pt N_4 C_{22} H_{25}$]$^+$ ClO_4^- . 0.5 H_2O}; formula weight = 649.01, triclinic, space group $P\bar{1}$ (No. 2), a = 12.474(5) Å, b =12.670(4) Å, c = 8.465(2) Å, α = 97.09(2)°, β = 97.08(3)°, γ = 72.32(3)°, V = 1259.7(7) Å^3, Z = 2, D_c =1.711 g cm^{-3}, μ(Mo-Kα) = 56.89 cm^{-1}, F(000) = 634, T = 301 K. A orange crystal of dimensions 0.15 × 0.15 × 0.25 mm in a glass capillary was used for data collection at 28°C on a Rigaku AFC7R diffractometer with graphite monochromatized Mo-Kα radiation (λ = 0.71073 Å) using ω-2θ scans with ω-scan angle (0.84 + 0.35 tan θ)° at a scan speed of 16.0 deg min^{-1} (up to 6 scans for reflection I < 15 σ(I)). Intensity data (in the range of 2 θ_{max} = 47° ; h: 0 to 13; k: -13 to 13; l: -9 to 9 and 3 standard reflections measured after every 300 reflections showed decay of 2.66%), were corrected for decay and for Lorentz and polarization effects, and empirical absorption corrections based on the ψ-scan of five strong reflections (minimum and maximum transmission factors 0.616 and 1.000). 3920 reflections were measured, of which 3720 were unique (R_{int} = 0.026). 3203 reflections with $I > 3\,\sigma(I)$ were considered observed and used in the structural analysis. The space group was determined based on a statistical analysis of intensity distribution and the successful refinement of the structure solved by Patterson methods and expanded by Fourier methods (*PATTY*[1]) and refinement by full-matrix least-squares using the software package *TeXsan*[2] on a Silicon Graphics Indy computer. One formula unit constitutes a crystallographic asymmetric unit and all 33 non-H atoms were refined anisotropically. The H atoms bonded to N(3) and N(4) were located in difference Fourier synthesis and their positional parameters were refined. The O atom of the water molecule is at special position and the H atoms were not located. The remaining 23 H atoms of the complex cation at calculated positions with thermal parameters equal to 1.3 times that of the attached C atoms were not refined. Convergence for 301 variable parameters by least-squares refinement on F with $w = 4\,F_o^2 / \sigma^2(F_o^2)$, where $\sigma^2(F_o^2) = [\sigma^2(I) + (0.018\,F_o^2)^2]$ for 3203 reflections with $I > 3\,\sigma(I)$ was reached at R = 0.033 and wR = 0.042 with a goodness-of-fit of 1.97. $(\Delta / \sigma)_{max}$ = 0.03 for non-H atoms. The final difference

Crystal data for [(CNN)Pt{C(NH^{t}Bu)(NHMe)}]ClO_4•0.5 H_2O, **2**(ClO_4)•0.5 H_2O

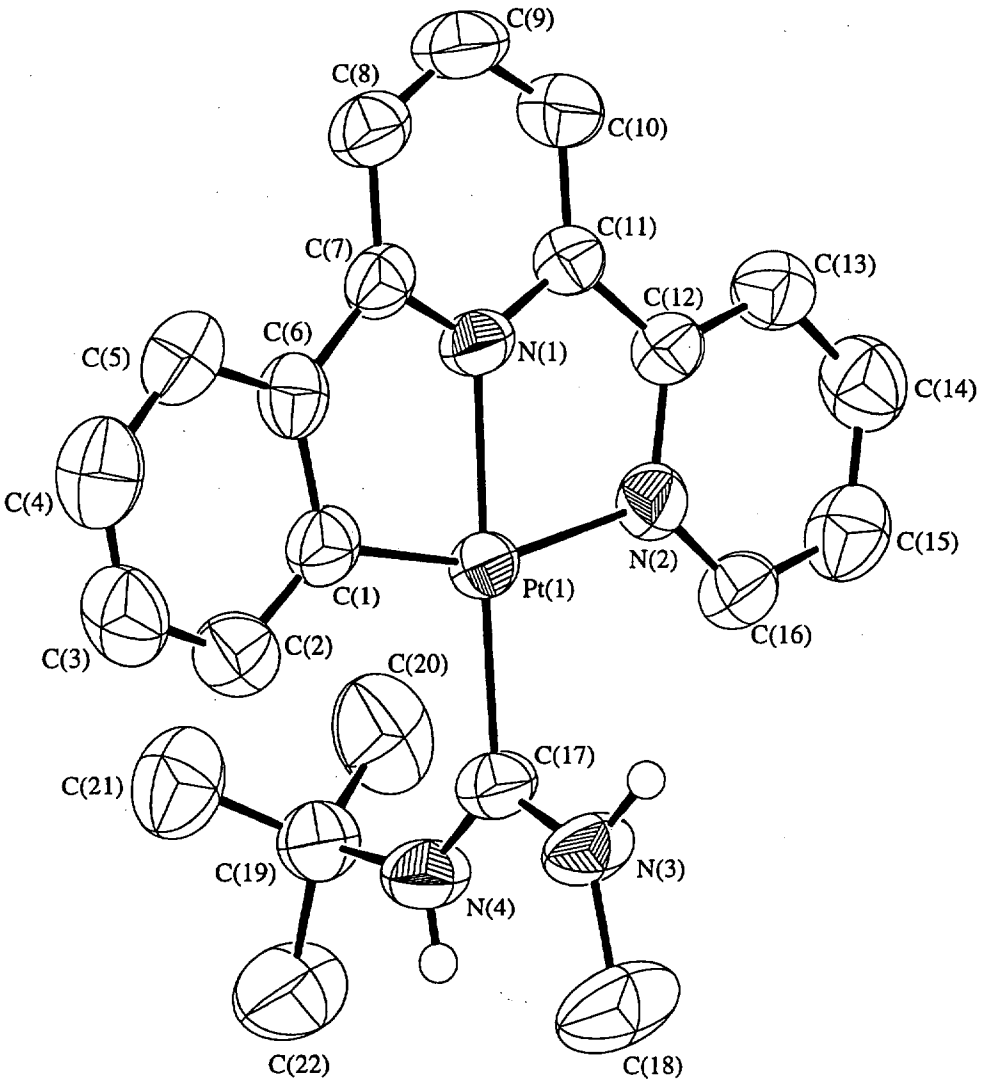
Fourier map was featureless, with maximum positive and negative peaks of 1.11 and 0.98 e $Å^{-3}$ respectively.

Ref:

1. *PATTY*: Beurskens, P.T., Admiraal, G., Beurskens, G., Bosman, W.P., Garcia-Granda, S., Gould, R.O., Smits, J.M.M. and Smykalla, C. (1992). The *DIRDIF* program system, Technical Report of the Crystallography Laboratory, University of Nijmegen, The Netherlands.

2. *TeXsan*: Crystal Structure Analysis Package, Molecular Structure Corporation, (1985 &, 1992), The Woodlands, Texas, U.S.A.

Crystal data for [(CNN)Pt{C(NH^{t}Bu)(NHMe)}]ClO_4•0.5 H_2O, **2**(ClO_4)•0.5 H_2O



Crystal data for [(CNN)Pt{C(NH^{t}Bu)(NHMe)}]ClO_4•0.5 H_2O, **2**(ClO_4)•0.5 H_2O

Table 1. Atomic coordinates and B_{iso}/B_{eq}

atom	x	y	z	B_{eq}
Pt(1)	0.11690(2)	0.20890(2)	0.42143(3)	3.447(6)
Cl(1)	0.5746(2)	0.1744(2)	0.8279(3)	6.28(6)
O(1)	0.6672(6)	0.0851(5)	0.7838(10)	9.0(2)
O(2)	0.6006(9)	0.2205(9)	0.983(1)	15.4(4)
O(3)	0.558(1)	0.2584(9)	0.747(1)	25.5(5)
O(4)	0.4886(8)	0.144(1)	0.831(2)	25.5(6)
O(5)	0.5000	0.5000	1.0000	34.9(8)
N(1)	-0.0308(5)	0.1825(4)	0.4390(7)	3.8(1)
N(2)	0.1491(5)	0.1369(4)	0.6417(7)	3.9(1)
N(3)	0.3420(5)	0.1432(5)	0.3265(8)	5.1(2)
N(4)	0.3009(5)	0.3179(5)	0.4504(9)	5.1(2)
C(1)	0.0341(6)	0.2663(6)	0.2170(9)	4.3(2)
C(2)	0.0684(7)	0.3134(6)	0.0974(9)	4.8(2)
C(3)	-0.0053(8)	0.3490(7)	-0.0348(10)	5.9(2)
C(4)	-0.1098(8)	0.3369(7)	-0.0562(10)	5.9(2)
C(5)	-0.1482(7)	0.2912(6)	0.0578(10)	5.2(2)
C(6)	-0.0767(6)	0.2564(5)	0.1938(8)	3.9(2)
C(7)	-0.1130(6)	0.2109(5)	0.3221(9)	3.8(2)
C(8)	-0.2170(6)	0.1968(6)	0.3344(10)	4.7(2)
C(9)	-0.2326(7)	0.1546(7)	0.469(1)	5.7(2)
C(10)	-0.1460(7)	0.1260(6)	0.5892(10)	4.9(2)
C(11)	-0.0440(6)	0.1393(5)	0.5724(9)	3.8(2)
C(12)	0.0573(6)	0.1123(6)	0.6853(9)	4.0(2)
C(13)	0.0649(7)	0.0650(6)	0.8253(9)	4.7(2)

Table 1. Atomic coordinates and B_{iso}/B_{eq} (continued)

atom	x	y	z	B_{eq}
C(14)	0.1632(8)	0.0429(7)	0.9228(10)	5.5(2)
C(15)	0.2540(7)	0.0658(7)	0.8787(10)	5.4(2)
C(16)	0.2452(6)	0.1139(6)	0.7360(10)	4.7(2)
C(17)	0.2668(6)	0.2295(6)	0.4005(9)	4.2(2)
C(18)	0.4577(8)	0.1388(8)	0.302(1)	8.3(3)
C(19)	0.2419(7)	0.4253(6)	0.534(1)	4.9(2)
C(20)	0.2012(10)	0.4050(7)	0.684(1)	7.8(3)
C(21)	0.1452(9)	0.4887(7)	0.427(1)	7.1(3)
C(22)	0.3324(8)	0.4868(8)	0.574(2)	8.7(3)
H(1)	0.318(6)	0.076(6)	0.301(9)	6.3813
H(2)	0.365(6)	0.322(6)	0.448(9)	6.3813
H(3)	0.1424	0.3210	0.1072	5.7736
H(4)	0.0185	0.3829	-0.1127	7.1371
H(5)	-0.1574	0.3600	-0.1501	7.0981
H(6)	-0.2223	0.2833	0.0434	6.1908
H(7)	-0.2763	0.2157	0.2516	5.6293
H(8)	-0.3039	0.1450	0.4792	6.7978
H(9)	-0.1578	0.0974	0.6822	5.9232
H(10)	0.0016	0.0474	0.8548	5.6696
H(11)	0.1682	0.0117	1.0208	6.5549
H(12)	0.3230	0.0491	0.9445	6.4112
H(13)	0.3088	0.1304	0.7060	5.6591
H(14)	0.5094	0.0763	0.3492	9.9571
H(15)	0.4656	0.1319	0.1910	9.9571

Table 1. Atomic coordinates and B_{iso}/B_{eq} (continued)

atom	x	y	z	B_{eq}
H(16)	0.4729	0.2049	0.3509	9.9571
H(17)	0.1625	0.4741	0.7380	9.3754
H(18)	0.1507	0.3608	0.6579	9.3754
H(19)	0.2636	0.3671	0.7526	9.3754
H(20)	0.1075	0.5570	0.4828	8.5604
H(21)	0.1730	0.5027	0.3348	8.5604
H(22)	0.0940	0.4459	0.3963	8.5604
H(23)	0.3932	0.4445	0.6407	10.3475
H(24)	0.3592	0.4962	0.4784	10.3475
H(25)	0.3001	0.5576	0.6288	10.3475

$$B_{eq} = \frac{8}{3}\pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}aa^*bb^*\cos\gamma + 2U_{13}aa^*cc^*\cos\beta + 2U_{23}bb^*cc^*\cos\alpha)$$

Crystal data for [(CNN)Pt{C(NH^{t}Bu)(NHMe)}]ClO_4•0.5 H_2O, **2**(ClO_4)•0.5 H_2O

Table 2. Anisotropic Displacement Parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Pt(1)	0.0378(2)	0.0420(1)	0.0511(2)	-0.0114(1)	0.0057(1)	0.0029(1)
Cl(1)	0.060(1)	0.078(1)	0.092(2)	-0.013(1)	-0.004(1)	0.007(1)
O(1)	0.095(5)	0.078(4)	0.167(7)	-0.005(4)	0.044(5)	0.028(4)
O(2)	0.18(1)	0.196(10)	0.176(9)	-0.050(8)	-0.033(8)	-0.038(8)
O(3)	0.44(2)	0.200(9)	0.222(10)	0.17(1)	0.15(1)	0.145(7)
O(4)	0.084(6)	0.28(1)	0.59(3)	-0.098(7)	0.04(1)	-0.11(2)
O(5)	0.40(3)	0.23(2)	0.40(2)	0.14(2)	-0.24(2)	-0.20(1)
N(1)	0.035(3)	0.045(3)	0.063(4)	-0.013(2)	0.005(3)	0.001(3)
N(2)	0.047(3)	0.048(3)	0.054(4)	-0.014(3)	-0.001(3)	0.008(3)
N(3)	0.044(4)	0.058(4)	0.087(5)	-0.011(3)	0.024(3)	-0.016(3)
N(4)	0.049(4)	0.053(4)	0.094(5)	-0.022(3)	0.018(4)	-0.009(3)
C(1)	0.049(4)	0.041(4)	0.067(5)	-0.009(3)	0.005(4)	-0.001(4)
C(2)	0.066(5)	0.059(5)	0.058(5)	-0.018(4)	0.015(4)	0.001(4)
C(3)	0.093(7)	0.083(6)	0.054(5)	-0.023(5)	0.007(5)	0.027(4)
C(4)	0.090(7)	0.072(6)	0.051(5)	-0.008(5)	0.000(5)	0.006(4)
C(5)	0.055(5)	0.063(5)	0.066(5)	-0.005(4)	-0.003(4)	0.003(4)
C(6)	0.057(5)	0.039(4)	0.050(4)	-0.010(3)	0.001(4)	0.001(3)
C(7)	0.042(4)	0.041(4)	0.056(4)	-0.008(3)	0.003(4)	-0.001(3)
C(8)	0.044(4)	0.059(4)	0.074(5)	-0.016(3)	0.000(4)	0.003(4)
C(9)	0.044(4)	0.079(5)	0.099(7)	-0.027(4)	0.012(5)	0.004(5)
C(10)	0.055(5)	0.065(5)	0.073(5)	-0.022(4)	0.015(4)	0.009(4)
C(11)	0.043(4)	0.045(4)	0.059(4)	-0.011(3)	0.010(3)	0.006(3)
C(12)	0.042(4)	0.047(4)	0.064(5)	-0.010(3)	0.010(4)	0.005(4)
C(13)	0.057(5)	0.064(5)	0.060(5)	-0.017(4)	0.011(4)	0.007(4)

Table 2. Anisotropic Displacement Parameters (continued)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(14)	0.078(6)	0.074(5)	0.058(5)	-0.020(4)	0.006(4)	0.017(4)
C(15)	0.064(5)	0.067(5)	0.065(5)	-0.015(4)	-0.013(4)	0.005(4)
C(16)	0.047(4)	0.058(5)	0.071(5)	-0.014(4)	0.000(4)	0.008(4)
C(17)	0.041(4)	0.059(4)	0.063(5)	-0.018(3)	0.003(4)	0.005(4)
C(18)	0.060(6)	0.100(7)	0.143(9)	-0.016(5)	0.038(6)	-0.043(7)
C(19)	0.057(5)	0.044(4)	0.083(6)	-0.015(4)	0.014(4)	-0.007(4)
C(20)	0.136(9)	0.063(6)	0.092(7)	-0.019(6)	0.039(7)	-0.015(5)
C(21)	0.089(7)	0.067(6)	0.101(7)	-0.008(5)	0.002(6)	-0.001(5)
C(22)	0.079(7)	0.067(6)	0.18(1)	-0.032(5)	0.013(7)	-0.027(6)

The general temperature factor expression:

$$\exp(-2\pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$$

Crystal data for [(CNN)Pt{C(NH^{t}Bu)(NHMe)}]ClO_4•0.5 H_2O, **2**(ClO_4)•0.5 H_2O

Table 3. Bond Lengths(Å)

atom	atom	distance	atom	atom	distance
Pt(1)	N(1)	1.995(6)	Pt(1)	N(2)	2.117(6)
Pt(1)	C(1)	2.001(8)	Pt(1)	C(17)	1.997(7)
Cl(1)	O(1)	1.401(7)	Cl(1)	O(2)	1.411(10)
Cl(1)	O(3)	1.29(1)	Cl(1)	O(4)	1.25(1)
N(1)	C(7)	1.332(8)	N(1)	C(11)	1.363(9)
N(2)	C(12)	1.376(9)	N(2)	C(16)	1.330(9)
N(3)	C(17)	1.349(9)	N(3)	C(18)	1.47(1)
N(4)	C(17)	1.321(9)	N(4)	C(19)	1.476(9)
C(1)	C(2)	1.40(1)	C(1)	C(6)	1.41(1)
C(2)	C(3)	1.39(1)	C(3)	C(4)	1.35(1)
C(4)	C(5)	1.39(1)	C(5)	C(6)	1.396(10)
C(6)	C(7)	1.466(10)	C(7)	C(8)	1.38(1)
C(8)	C(9)	1.37(1)	C(9)	C(10)	1.39(1)
C(10)	C(11)	1.36(1)	C(11)	C(12)	1.466(10)
C(12)	C(13)	1.37(1)	C(13)	C(14)	1.36(1)
C(14)	C(15)	1.35(1)	C(15)	C(16)	1.40(1)
C(19)	C(20)	1.50(1)	C(19)	C(21)	1.50(1)
C(19)	C(22)	1.54(1)			

Table 4. Bond Lengths(Å)

atom	atom	distance	atom	atom	distance
N(3)	H(1)	0.97(7)	N(4)	H(2)	0.82(8)
C(2)	H(3)	0.95	C(3)	H(4)	0.95
C(4)	H(5)	0.95	C(5)	H(6)	0.95
C(8)	H(7)	0.95	C(9)	H(8)	0.95
C(10)	H(9)	0.95	C(13)	H(10)	0.95
C(14)	H(11)	0.95	C(15)	H(12)	0.95
C(16)	H(13)	0.95	C(18)	H(14)	0.95
C(18)	H(15)	0.94	C(18)	H(16)	0.95
C(20)	H(17)	0.95	C(20)	H(18)	0.95
C(20)	H(19)	0.95	C(21)	H(20)	0.95
C(21)	H(21)	0.95	C(21)	H(22)	0.95
C(22)	H(23)	0.95	C(22)	H(24)	0.95
C(22)	H(25)	0.95			

Table 5. Bond Angles(°)

atom	atom	atom	angle	atom	atom	atom	angle
N(1)	Pt(1)	N(2)	78.8(2)	N(1)	Pt(1)	C(1)	80.8(3)
N(1)	Pt(1)	C(17)	177.9(3)	N(2)	Pt(1)	C(1)	159.6(3)
N(2)	Pt(1)	C(17)	101.0(3)	C(1)	Pt(1)	C(17)	99.4(3)
O(1)	Cl(1)	O(2)	109.0(5)	O(1)	Cl(1)	O(3)	113.1(7)
O(1)	Cl(1)	O(4)	111.9(7)	O(2)	Cl(1)	O(3)	100.8(8)
O(2)	Cl(1)	O(4)	107.7(10)	O(3)	Cl(1)	O(4)	113(1)
Pt(1)	N(1)	C(7)	118.6(5)	Pt(1)	N(1)	C(11)	118.5(5)
C(7)	N(1)	C(11)	122.9(6)	Pt(1)	N(2)	C(12)	113.2(5)
Pt(1)	N(2)	C(16)	127.4(5)	C(12)	N(2)	C(16)	119.4(6)
C(17)	N(3)	C(18)	125.7(7)	C(17)	N(4)	C(19)	130.6(7)
Pt(1)	C(1)	C(2)	130.7(6)	Pt(1)	C(1)	C(6)	112.4(5)
C(2)	C(1)	C(6)	116.8(7)	C(1)	C(2)	C(3)	120.4(8)
C(2)	C(3)	C(4)	121.8(8)	C(3)	C(4)	C(5)	120.3(8)
C(4)	C(5)	C(6)	119.1(8)	C(1)	C(6)	C(5)	121.4(7)
C(1)	C(6)	C(7)	116.4(6)	C(5)	C(6)	C(7)	122.1(7)
N(1)	C(7)	C(6)	111.7(6)	N(1)	C(7)	C(8)	119.5(7)
C(6)	C(7)	C(8)	128.8(7)	C(7)	C(8)	C(9)	118.6(7)
C(8)	C(9)	C(10)	121.0(7)	C(9)	C(10)	C(11)	119.0(8)
N(1)	C(11)	C(10)	119.0(7)	N(1)	C(11)	C(12)	114.2(6)
C(10)	C(11)	C(12)	126.8(7)	N(2)	C(12)	C(11)	115.2(6)
N(2)	C(12)	C(13)	120.2(7)	C(11)	C(12)	C(13)	124.6(7)
C(12)	C(13)	C(14)	120.2(8)	C(13)	C(14)	C(15)	119.5(8)
C(14)	C(15)	C(16)	119.8(8)	N(2)	C(16)	C(15)	120.9(7)
Pt(1)	C(17)	N(3)	116.3(5)	Pt(1)	C(17)	N(4)	127.5(5)

Table 5. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
N(3)	C(17)	N(4)	116.1(7)	N(4)	C(19)	C(20)	109.6(7)
N(4)	C(19)	C(21)	110.2(7)	N(4)	C(19)	C(22)	104.4(7)
C(20)	C(19)	C(21)	110.8(8)	C(20)	C(19)	C(22)	110.7(8)
C(21)	C(19)	C(22)	110.9(7)				

Complex $3(ClO_4) \cdot 0.5\ H_2O$: afc 627

Crystal data. $\{[Pt N_5 C_{21} H_{24}]^+ ClO_4^- . 0.5\ H_2O\}$; formula weight = 650.00, triclinic, space group $P\bar{1}$ (No. 2), a = 11.866(4) Å, b =13.102(5) Å, c = 8.392(2) Å, α = 100.30(3)°, β = 97.50(4)°, γ = 72.88(3)°, V = 1222.6(8) Å^3, Z = 2, D_c = 1.766 g cm^{-3}, μ(Mo-Kα) = 58.63 cm^{-1}, F(000) = 634, T = 301 K. A yellow crystal of dimensions 0.25 × 0.10 × 0.30 mm in a glass capillary was used for data collection at 28°C on a Nonius-Enraf CAD4 diffractometer with graphite monochromatized Mo-Kα radiation (λ = 0.71073 Å) using ω-2θ scans with ω-scan angle (0.73 + 0.344 tan θ)° at a scan speed of 1.03 to 5.49 deg min^{-1}. Intensity data (in the range of $2\theta_{max}$ = 50° ; h: 0 to 14; k: -15 to 15; l: -10 to 10 and 3 standard reflections measured after every 2 hours showed decay of 1.09 %) were corrected for decay and for Lorentz and polarization effects, and empirical absorption corrections based on the ψ-scan of five strong reflections (minimum and maximum transmission factors 0.604 and 1.000). 4496 reflections were measured, of which 4272 were unique (R_{int} = 0.014). 3852 reflections with $I > 3\ \sigma(I)$ were considered observed and used in the structural analysis. The space group was determined based on a statistical analysis of intensity distribution and the successful refinement of the structure solved by Patterson and Fourier methods (*PATTY* [1]) and refinement by full-matrix least-squares using the software package *TeXsan* [2] on a Silicon Graphics Indy computer. A crystallographic asymmetric unit consists of one formula unit and all 33 non-H atoms were refined anisotropically. The 4 H atoms bonded to N(3), N(4), and N(5) were located in difference Fourier synthesis and their positional parameter were refined. The O atom of the water molecule is at special position and the H atoms bonded to it were not located. 20 H atoms at calculated positions with thermal parameters equal to 1.3 times that of the attached C atoms were not refined. Convergence for 307 variable parameters by least-squares refinement on F with $w = 4\ F_o^2 / \sigma^2(F_o^2)$, where $\sigma^2(F_o^2) = [\sigma^2(I) + (0.017\ F_o^2)^2]$ for 3852 reflections with $I > 3\ \sigma(I)$ was reached at R = 0.022 and wR = 0.028 with a goodness-of-fit of 1.73. $(\Delta / \sigma)_{max}$ = 0.01 for non-H atoms. The final difference Fourier map was featureless, with maximum positive and negative peaks of 0.85 and 0.59 e Å^{-3} respectively.

Crystal data for [(CNN)Pt{C(NH^{t}Bu)(NHNH$_2$)}]ClO$_4$•0.5 H$_2$O, **3**(ClO$_4$)•0.5 H$_2$O

Table 1. Atomic coordinates and B_{iso}/B_{eq}

atom	x	y	z	B_{eq}
Pt(1)	0.09696(2)	0.21497(1)	0.39199(2)	3.401(5)
Cl(1)	0.4348(1)	-0.1494(1)	0.1817(2)	5.66(4)
O(1)	0.3173(4)	-0.0864(4)	0.1477(6)	7.6(1)
O(2)	0.4754(5)	-0.1105(5)	0.3387(6)	9.7(2)
O(3)	0.4331(6)	-0.2542(4)	0.179(1)	15.9(3)
O(4)	0.5084(7)	-0.1353(8)	0.0822(8)	16.3(3)
O(5)	0.5000	0.5000	0.0000	34.5(5)
N(1)	-0.0634(3)	0.1983(3)	0.4055(5)	3.62(9)
N(2)	0.1250(3)	0.1428(3)	0.6044(5)	3.98(9)
N(3)	0.3283(4)	0.1434(4)	0.2865(5)	4.7(1)
N(4)	0.4488(4)	0.1383(4)	0.2759(7)	5.7(1)
N(5)	0.3060(4)	0.3062(3)	0.4338(6)	4.5(1)
C(1)	0.0157(4)	0.2747(4)	0.1892(6)	3.9(1)
C(2)	0.0565(5)	0.3173(4)	0.0746(7)	4.9(1)
C(3)	-0.0158(6)	0.3552(5)	-0.0572(7)	5.8(2)
C(4)	-0.1312(6)	0.3492(5)	-0.0818(7)	5.9(2)
C(5)	-0.1750(5)	0.3076(5)	0.0275(7)	5.3(1)
C(6)	-0.1045(4)	0.2721(4)	0.1633(6)	4.1(1)
C(7)	-0.1478(4)	0.2312(4)	0.2877(6)	4.0(1)
C(8)	-0.2616(5)	0.2244(5)	0.2990(7)	5.2(1)
C(9)	-0.2826(5)	0.1851(5)	0.4312(8)	5.5(2)
C(10)	-0.1943(5)	0.1501(5)	0.5467(7)	5.1(1)
C(11)	-0.0822(4)	0.1570(4)	0.5329(6)	4.0(1)
C(12)	0.0259(4)	0.1231(4)	0.6430(6)	4.0(1)

Table 1. Atomic coordinates and B_{iso}/B_{eq} (continued)

atom	x	y	z	B_{eq}
C(13)	0.0287(5)	0.0739(4)	0.7779(7)	5.0(1)
C(14)	0.1309(6)	0.0455(5)	0.8731(7)	5.6(2)
C(15)	0.2314(5)	0.0656(5)	0.8362(7)	5.3(1)
C(16)	0.2263(5)	0.1136(4)	0.7009(7)	4.5(1)
C(17)	0.2578(4)	0.2268(4)	0.3713(6)	3.6(1)
C(18)	0.2551(5)	0.4118(4)	0.5324(8)	5.0(1)
C(19)	0.1565(7)	0.4801(5)	0.4333(9)	7.2(2)
C(20)	0.2125(7)	0.3972(5)	0.6845(8)	7.8(2)
C(21)	0.3567(7)	0.4632(6)	0.575(1)	8.6(2)
H(1)	0.312(5)	0.087(4)	0.280(6)	5.8457
H(2)	0.492(5)	0.080(4)	0.322(7)	5.8457
H(3)	0.466(5)	0.132(4)	0.196(7)	5.8457
H(4)	0.380(5)	0.281(4)	0.416(6)	5.8457
H(5)	0.1362	0.3207	0.0880	5.8262
H(6)	0.0139	0.3856	-0.1316	6.9992
H(7)	-0.1804	0.3740	-0.1739	7.0649
H(8)	-0.2541	0.3027	0.0103	6.4412
H(9)	-0.3234	0.2465	0.2175	6.1783
H(10)	-0.3606	0.1823	0.4405	6.5712
H(11)	-0.2098	0.1219	0.6357	6.1247
H(12)	-0.0410	0.0603	0.8027	5.9849
H(13)	0.1338	0.0116	0.9655	6.8054
H(14)	0.3033	0.0468	0.9028	6.3294
H(15)	0.2956	0.1270	0.6753	5.4284

Table 1. Atomic coordinates and B_{iso}/B_{eq} (continued)

atom	x	y	z	B_{eq}
H(16)	0.1241	0.5479	0.4961	8.6347
H(17)	0.1860	0.4911	0.3393	8.6347
H(18)	0.0961	0.4444	0.3997	8.6347
H(19)	0.1809	0.4656	0.7459	9.2628
H(20)	0.1532	0.3602	0.6569	9.2628
H(21)	0.2770	0.3557	0.7468	9.2628
H(22)	0.4198	0.4179	0.6343	10.2287
H(23)	0.3840	0.4720	0.4784	10.2287
H(24)	0.3304	0.5316	0.6399	10.2287

$$B_{eq} = \frac{8}{3}\pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}aa^*bb^*\cos\gamma + 2U_{13}aa^*cc^*\cos\beta + 2U_{23}bb^*cc^*\cos\alpha)$$

Table 2. Anisotropic Displacement Parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Pt(1)	0.0367(1)	0.0402(1)	0.0545(1)	-0.01197(8)	0.00764(8)	0.00753(8)
Cl(1)	0.0632(9)	0.0679(9)	0.087(1)	-0.0230(8)	0.0054(8)	0.0128(8)
O(1)	0.088(3)	0.082(3)	0.117(4)	-0.019(3)	-0.022(3)	0.035(3)
O(2)	0.120(4)	0.158(5)	0.090(4)	-0.047(4)	-0.024(3)	0.029(3)
O(3)	0.108(5)	0.062(3)	0.41(1)	-0.019(3)	-0.044(6)	0.031(5)
O(4)	0.163(7)	0.38(1)	0.121(5)	-0.120(8)	0.068(5)	0.022(7)
O(5)	0.34(1)	0.212(10)	0.41(1)	0.168(9)	-0.28(1)	-0.212(9)
N(1)	0.040(2)	0.042(2)	0.056(2)	-0.014(2)	0.007(2)	0.003(2)
N(2)	0.048(2)	0.047(2)	0.059(3)	-0.014(2)	0.005(2)	0.013(2)
N(3)	0.044(2)	0.053(3)	0.081(3)	-0.018(2)	0.016(2)	-0.005(2)
N(4)	0.047(3)	0.086(4)	0.085(4)	-0.019(2)	0.021(3)	0.003(3)
N(5)	0.041(2)	0.052(3)	0.082(3)	-0.018(2)	0.015(2)	0.000(2)
C(1)	0.052(3)	0.041(3)	0.057(3)	-0.013(2)	0.012(2)	0.005(2)
C(2)	0.064(4)	0.060(3)	0.065(3)	-0.019(3)	0.014(3)	0.011(3)
C(3)	0.091(5)	0.069(4)	0.063(4)	-0.018(4)	0.015(3)	0.018(3)
C(4)	0.080(4)	0.075(4)	0.060(4)	-0.008(3)	-0.003(3)	0.020(3)
C(5)	0.059(4)	0.059(3)	0.076(4)	-0.011(3)	-0.004(3)	0.003(3)
C(6)	0.052(3)	0.042(3)	0.059(3)	-0.012(2)	0.003(2)	0.003(2)
C(7)	0.042(3)	0.043(3)	0.066(3)	-0.011(2)	0.005(2)	0.001(2)
C(8)	0.048(3)	0.067(4)	0.080(4)	-0.023(3)	-0.001(3)	0.002(3)
C(9)	0.046(3)	0.077(4)	0.094(5)	-0.028(3)	0.009(3)	0.010(3)
C(10)	0.055(3)	0.080(4)	0.071(4)	-0.032(3)	0.013(3)	0.014(3)
C(11)	0.046(3)	0.048(3)	0.062(3)	-0.018(2)	0.015(2)	0.004(2)
C(12)	0.051(3)	0.044(3)	0.061(3)	-0.014(2)	0.011(2)	0.009(2)

Table 2. Anisotropic Displacement Parameters (continued)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(13)	0.067(4)	0.063(3)	0.069(4)	-0.023(3)	0.014(3)	0.019(3)
C(14)	0.089(5)	0.063(4)	0.067(4)	-0.019(3)	0.007(3)	0.025(3)
C(15)	0.068(4)	0.062(3)	0.066(4)	-0.010(3)	-0.002(3)	0.015(3)
C(16)	0.049(3)	0.055(3)	0.068(3)	-0.012(3)	0.002(3)	0.014(3)
C(17)	0.042(3)	0.043(3)	0.052(3)	-0.009(2)	0.006(2)	0.011(2)
C(18)	0.060(3)	0.044(3)	0.087(4)	-0.019(3)	0.011(3)	0.000(3)
C(19)	0.099(5)	0.055(4)	0.108(6)	-0.006(4)	0.006(4)	0.006(4)
C(20)	0.142(7)	0.070(4)	0.084(5)	-0.033(4)	0.039(5)	-0.013(4)
C(21)	0.086(5)	0.077(5)	0.164(8)	-0.043(4)	0.016(5)	-0.024(5)

The general temperature factor expression:

$$\exp(-2\pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$$

Crystal data for [(CNN)Pt{C(NH^{t}Bu)(NHNH$_2$)}]ClO$_4$•0.5 H$_2$O, **3**(ClO$_4$)•0.5 H$_2$O

Table 3. Bond Lengths($\AA$)

atom	atom	distance	atom	atom	distance
Pt(1)	N(1)	1.998(4)	Pt(1)	N(2)	2.109(4)
Pt(1)	C(1)	2.010(5)	Pt(1)	C(17)	1.992(4)
Cl(1)	O(1)	1.418(5)	Cl(1)	O(2)	1.403(5)
Cl(1)	O(3)	1.375(6)	Cl(1)	O(4)	1.355(6)
N(1)	C(7)	1.344(6)	N(1)	C(11)	1.351(6)
N(2)	C(12)	1.365(6)	N(2)	C(16)	1.353(6)
N(3)	N(4)	1.425(6)	N(3)	C(17)	1.319(6)
N(5)	C(17)	1.327(6)	N(5)	C(18)	1.481(6)
C(1)	C(2)	1.394(7)	C(1)	C(6)	1.424(7)
C(2)	C(3)	1.380(8)	C(3)	C(4)	1.381(9)
C(4)	C(5)	1.371(8)	C(5)	C(6)	1.388(7)
C(6)	C(7)	1.464(7)	C(7)	C(8)	1.396(7)
C(8)	C(9)	1.382(8)	C(9)	C(10)	1.364(8)
C(10)	C(11)	1.381(7)	C(11)	C(12)	1.482(7)
C(12)	C(13)	1.391(7)	C(13)	C(14)	1.355(8)
C(14)	C(15)	1.377(8)	C(15)	C(16)	1.381(7)
C(18)	C(19)	1.502(9)	C(18)	C(20)	1.495(8)
C(18)	C(21)	1.521(8)			

Table 4. Bond Lengths(Å)

atom	atom	distance	atom	atom	distance
N(3)	H(1)	0.81(5)	N(4)	H(2)	0.91(5)
N(4)	H(3)	0.71(5)	N(5)	H(4)	0.86(5)
C(2)	H(5)	0.95	C(3)	H(6)	0.95
C(4)	H(7)	0.95	C(5)	H(8)	0.95
C(8)	H(9)	0.95	C(9)	H(10)	0.95
C(10)	H(11)	0.95	C(13)	H(12)	0.95
C(14)	H(13)	0.95	C(15)	H(14)	0.95
C(16)	H(15)	0.95	C(19)	H(16)	0.95
C(19)	H(17)	0.95	C(19)	H(18)	0.95
C(20)	H(19)	0.95	C(20)	H(20)	0.95
C(20)	H(21)	0.95	C(21)	H(22)	0.95
C(21)	H(23)	0.95	C(21)	H(24)	0.95

Table 5. Bond Angles(°)

atom	atom	atom	angle	atom	atom	atom	angle
N(1)	Pt(1)	N(2)	78.9(2)	N(1)	Pt(1)	C(1)	81.4(2)
N(1)	Pt(1)	C(17)	177.8(2)	N(2)	Pt(1)	C(1)	160.2(2)
N(2)	Pt(1)	C(17)	101.7(2)	C(1)	Pt(1)	C(17)	98.0(2)
O(1)	Cl(1)	O(2)	108.4(3)	O(1)	Cl(1)	O(3)	108.3(3)
O(1)	Cl(1)	O(4)	110.6(4)	O(2)	Cl(1)	O(3)	108.4(5)
O(2)	Cl(1)	O(4)	105.0(4)	O(3)	Cl(1)	O(4)	115.8(6)
Pt(1)	N(1)	C(7)	117.6(3)	Pt(1)	N(1)	C(11)	118.8(3)
C(7)	N(1)	C(11)	123.5(4)	Pt(1)	N(2)	C(12)	113.1(3)
Pt(1)	N(2)	C(16)	128.5(3)	C(12)	N(2)	C(16)	118.5(4)
N(4)	N(3)	C(17)	121.2(4)	C(17)	N(5)	C(18)	130.4(4)
Pt(1)	C(1)	C(2)	131.3(4)	Pt(1)	C(1)	C(6)	112.0(3)
C(2)	C(1)	C(6)	116.6(5)	C(1)	C(2)	C(3)	121.8(5)
C(2)	C(3)	C(4)	120.5(5)	C(3)	C(4)	C(5)	119.8(5)
C(4)	C(5)	C(6)	120.5(5)	C(1)	C(6)	C(5)	120.8(5)
C(1)	C(6)	C(7)	116.2(4)	C(5)	C(6)	C(7)	123.0(5)
N(1)	C(7)	C(6)	112.7(4)	N(1)	C(7)	C(8)	118.3(5)
C(6)	C(7)	C(8)	128.9(5)	C(7)	C(8)	C(9)	118.6(5)
C(8)	C(9)	C(10)	121.5(5)	C(9)	C(10)	C(11)	118.9(5)
N(1)	C(11)	C(10)	119.0(5)	N(1)	C(11)	C(12)	113.2(4)
C(10)	C(11)	C(12)	127.8(5)	N(2)	C(12)	C(11)	115.9(4)
N(2)	C(12)	C(13)	120.9(5)	C(11)	C(12)	C(13)	123.2(4)
C(12)	C(13)	C(14)	119.7(5)	C(13)	C(14)	C(15)	120.0(5)
C(14)	C(15)	C(16)	119.1(5)	N(2)	C(16)	C(15)	121.9(5)
Pt(1)	C(17)	N(3)	116.2(3)	Pt(1)	C(17)	N(5)	129.2(4)

Table 5. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
N(3)	C(17)	N(5)	114.6(4)	N(5)	C(18)	C(19)	109.8(5)
N(5)	C(18)	C(20)	111.0(5)	N(5)	C(18)	C(21)	104.9(5)
C(19)	C(18)	C(20)	110.9(6)	C(19)	C(18)	C(21)	110.2(5)
C(20)	C(18)	C(21)	109.9(6)				

Complex 4(ClO$_4$): afc 842

Crystal data. [($C_{28}H_{29}N_4Pt$)$^+$ ClO_4^-]; F_w =716.10, triclinic, space group $P\bar{1}$ (No. 2), a = 11.070(2) Å, b = 11.216(2) Å, c = 13.065(3) Å, α = 111.29(1)°, β = 106.97(1)°, γ = 101.67(1)°, V = 1356(1) Å^3, Z = 2, D_c = 1.753 g cm^{-3}, μ(Mo-Kα) = 52.91 cm^{-1}, F(000) = 704, T = 301K. A orange crystal of dimensions 0.30 × 0.10 × 0.07 mm in a glass capillary was used for data collection at 28°C on a Rigaku AFC7R diffractometer with graphite monochromatized Mo-Kα radiation (λ = 0.71073 Å) using ω-2θ scans with ω-scan angle (0.79 + 0.35 tan θ)° at a scan speed of 8.0 deg min^{-1} (up to 6 scans for reflection with $I < 15\ \sigma(I)$). Unit cell dimensions were determined based on 25 reflections in the 2θ range of 25.0 to 31.9°. Intensity data (in the range of $2\theta_{max}$ = 50° ; h: -13 to 12; k: 0 to 13; l: -15 to 14 and 3 standard reflections measured after every 300 reflections showed no decay) were corrected for Lorentz and polarization effects, and empirical absorption corrections based on the ψ-scan of five strong reflections (minimum and maximum transmission factors 0.640 and 1.000). 5051 reflections were measured, of which 4786 were unique and R_{int} = 0.033. 3957 reflections with $I > 3\ \sigma(I)$ were considered observed and used in the structural analysis. The space group was determined based on a statistical analysis of intensity distribution and the successful refinement of the structure solved by Patterson methods and expanded by Fourier methods (*PATTY*[1]) and refinement by full-matrix least-squares using the software package *TeXsan*[2] on a Silicon Graphics Indy computer. One crystallographic asymmetric unit consists of one formula unit. The 6-phenyl-2,2'-bipyridyl ligand has two alternative positions relative to the diamino-carbene ligand and C(1') and N(2') were placed at the same positions as N(2) and C(1) respectively with all four having occupation number of 0.5. The O atoms of the perchlorate anion were disordered and were placed at 9 positions with O(1), O(1'), O(2), O(2'), O(3), O(3'), O(3"), O(4) and O(4') having occupation numbers of 0.7, 0.3, 0.58, 0.49, 0.56, 0.38, 0.28, 0.4 and 0.31 respectively. In the least-squares refinement, 32 non-H atoms were refined anisotropically, N(2) and C(1) were refined isotropically, C(1') and N(2') constraint to N(2) and C(1) respectively were not refined, the positional parameters of H(1) to H(4) located in the difference Fourier synthesis were refined, and 25 other H atoms at calculated positions with thermal parameters equal to 1.3 times that of the attached C atoms were not refined. Convergence for 345 variable parameters by least-squares refinement on F with $w = 4F_o^2 / \sigma^2(F_o^2)$, where $\sigma^2(F_o^2) = [\sigma^2(I) + (0.030\ F_o^2)^2]$ for 3957 reflections with $I > 3\ \sigma(I)$ was reached at R = 0.029 and wR = 0.037 with a goodness-of-fit of 1.30. $(\Delta/\sigma)_{max}$ = 0.03 except for the disordered O atoms. The final difference Fourier map was featureless, with maximum positive and negative peaks of 0.90 and 0.71 e Å^{-3} respectively.

Crystal data for [(CNN)Pt{C(NH^{t}Bu)(NHCH$_2$Ph)}]ClO$_4$, 4(ClO$_4$)

Table 1. Atomic coordinates and B_{iso}/B_{eq}

atom	x	y	z	B_{eq}
Pt(1)	0.20045(2)	0.35971(2)	0.15448(2)	3.239(5)
Cl(1)	0.5707(2)	0.1386(2)	0.3162(2)	6.30(5)
O(1)	0.690(1)	0.249(1)	0.386(1)	8.8(2)
O(1')	0.709(2)	0.163(3)	0.392(2)	9.0(6)
O(2)	0.513(1)	0.149(1)	0.398(1)	8.8(3)
O(2')	0.447(2)	0.132(2)	0.328(1)	8.8(4)
O(3)	0.543(1)	0.072(2)	0.198(1)	9.0(3)
O(3')	0.507(2)	0.167(2)	0.211(2)	9.0(5)
O(3")	0.611(3)	0.288(3)	0.335(3)	8.9(6)
O(4')	0.608(3)	0.019(3)	0.329(2)	9.0(6)
O(4)	0.563(2)	0.012(2)	0.247(2)	8.9(5)
N(1)	0.1431(5)	0.2047(5)	-0.0074(4)	3.9(1)
N(2')	0.0007	0.2698	0.1189	4.4271
N(2)	0.3807(6)	0.3902(6)	0.1307(5)	4.1(1)
N(3)	0.3012(6)	0.4954(5)	0.4153(4)	3.8(1)
N(4)	0.2576(6)	0.6399(5)	0.3408(5)	3.9(1)
C(1)	0.0007(6)	0.2698(6)	0.1189(5)	4.4(1)
C(1')	0.3807	0.3902	0.1307	4.0851
C(2)	-0.0688(8)	0.3101(8)	0.1894(7)	4.8(2)
C(3)	-0.2030(8)	0.2340(10)	0.1505(9)	6.1(2)
C(4)	-0.2682(8)	0.1202(10)	0.0412(10)	6.8(2)
C(5)	-0.1997(8)	0.0805(8)	-0.0299(8)	6.0(2)
C(6)	-0.0655(7)	0.1562(7)	0.0099(6)	4.5(2)
C(7)	0.0143(7)	0.1190(6)	-0.0620(6)	4.4(1)

Crystal data for [(CNN)Pt{C(NH^{t}Bu)(NHCH$_2$Ph)}]ClO$_4$, 4(ClO$_4$)

Table 1. Atomic coordinates and B_{iso}/B_{eq} (continued)

atom	x	y	z	B_{eq}
C(8)	-0.0253(9)	0.0104(7)	-0.1749(7)	5.9(2)
C(9)	0.066(1)	-0.0035(7)	-0.2267(6)	6.2(2)
C(10)	0.1956(9)	0.0851(8)	-0.1688(6)	5.6(2)
C(11)	0.2344(7)	0.1933(6)	-0.0547(6)	4.4(2)
C(12)	0.3685(7)	0.2974(6)	0.0228(6)	4.2(1)
C(13)	0.4788(9)	0.3052(8)	-0.0077(7)	5.6(2)
C(14)	0.6001(9)	0.4067(10)	0.0700(8)	6.5(2)
C(15)	0.6124(8)	0.4974(9)	0.1798(8)	6.0(2)
C(16)	0.5029(7)	0.4900(8)	0.2094(7)	4.7(2)
C(17)	0.2571(5)	0.5126(5)	0.3162(5)	3.2(1)
C(18)	0.3159(6)	0.3708(6)	0.4170(5)	3.7(1)
C(19)	0.2345(6)	0.3114(6)	0.4735(5)	3.5(1)
C(20)	0.1290(7)	0.3507(7)	0.4939(6)	4.3(1)
C(21)	0.0552(7)	0.2889(8)	0.5418(7)	5.2(2)
C(22)	0.0875(8)	0.1913(7)	0.5729(7)	5.4(2)
C(23)	0.1925(8)	0.1535(7)	0.5542(7)	5.2(2)
C(24)	0.2656(6)	0.2114(6)	0.5042(6)	4.1(1)
C(25)	0.2162(8)	0.6993(7)	0.2576(6)	4.6(2)
C(26)	0.300(1)	0.691(1)	0.184(1)	9.0(4)
C(27)	0.2450(9)	0.8485(7)	0.3374(8)	5.9(2)
C(28)	0.0673(9)	0.6289(8)	0.1788(8)	6.6(2)
H(1)	0.325(7)	0.556(8)	0.484(7)	5.5780
H(2)	0.294(7)	0.699(7)	0.414(7)	5.5780
H(3)	-0.028(7)	0.383(7)	0.263(7)	5.5780

Crystal data for [(CNN)Pt{C(NH^{t}Bu)(NHCH$_2$Ph)}]ClO$_4$, **4**(ClO$_4$)

Table 1. Atomic coordinates and B_{iso}/B_{eq} (continued)

atom	x	y	z	B_{eq}
H(4)	0.508(7)	0.551(8)	0.282(7)	5.5780
H(5)	-0.2504	0.2608	0.1999	7.3313
H(6)	-0.3603	0.0691	0.0150	8.1307
H(7)	-0.2438	0.0020	-0.1055	7.2011
H(8)	-0.1147	-0.0532	-0.2157	7.0199
H(9)	0.0387	-0.0761	-0.3041	7.4848
H(10)	0.2584	0.0740	-0.2047	6.6815
H(11)	0.4702	0.2399	-0.0828	6.6983
H(12)	0.6749	0.4143	0.0480	7.7540
H(13)	0.6971	0.5656	0.2357	7.1800
H(14)	0.2885	0.3046	0.3366	4.3901
H(15)	0.4083	0.3891	0.4608	4.3901
H(16)	0.1074	0.4200	0.4749	5.1954
H(17)	-0.0184	0.3144	0.5532	6.2220
H(18)	0.0378	0.1504	0.6071	6.4706
H(19)	0.2152	0.0863	0.5758	6.2392
H(20)	0.3372	0.1831	0.4908	4.9072
H(21)	0.2880	0.5985	0.1384	10.6927
H(22)	0.2712	0.7295	0.1308	10.6927
H(23)	0.3918	0.7405	0.2353	10.6927
H(24)	0.3383	0.8915	0.3874	7.0817
H(25)	0.2200	0.8926	0.2889	7.0817
H(26)	0.1946	0.8547	0.3856	7.0817
H(27)	0.0174	0.6405	0.2276	7.9556

Table 1. Atomic coordinates and B_{iso}/B_{eq} (continued)

atom	x	y	z	B_{eq}
H(28)	0.0420	0.6677	0.1259	7.9556
H(29)	0.0493	0.5345	0.1337	7.9556

$$B_{eq} = \frac{8}{3}\pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}aa^*bb^*\cos\gamma + 2U_{13}aa^*cc^*\cos\beta + 2U_{23}bb^*cc^*\cos\alpha)$$

Table 2. Anisotropic Displacement Parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Pt(1)	0.0539(1)	0.0312(1)	0.0350(1)	0.01666(9)	0.01532(10)	0.01293(9)
Cl(1)	0.082(1)	0.071(1)	0.066(1)	0.0145(10)	0.044(1)	0.0070(10)
N(1)	0.073(3)	0.033(3)	0.034(3)	0.023(2)	0.011(2)	0.013(2)
N(3)	0.073(3)	0.031(3)	0.036(3)	0.015(2)	0.022(3)	0.015(2)
N(4)	0.073(3)	0.036(3)	0.042(3)	0.023(2)	0.026(3)	0.016(2)
C(2)	0.073(5)	0.062(4)	0.064(4)	0.033(4)	0.029(4)	0.039(4)
C(3)	0.071(5)	0.090(6)	0.103(7)	0.037(5)	0.040(5)	0.068(6)
C(4)	0.067(5)	0.088(6)	0.108(7)	0.015(5)	0.022(5)	0.067(6)
C(5)	0.079(5)	0.059(5)	0.076(5)	0.009(4)	0.007(4)	0.043(4)
C(6)	0.063(4)	0.048(4)	0.054(4)	0.016(3)	0.005(3)	0.032(3)
C(7)	0.074(4)	0.033(3)	0.041(3)	0.014(3)	-0.001(3)	0.017(3)
C(8)	0.108(6)	0.036(4)	0.046(4)	0.019(4)	-0.002(4)	0.014(3)
C(9)	0.136(8)	0.043(4)	0.035(4)	0.035(5)	0.018(4)	0.005(3)
C(10)	0.113(6)	0.057(4)	0.040(4)	0.042(4)	0.026(4)	0.017(3)
C(11)	0.087(5)	0.043(3)	0.040(3)	0.036(3)	0.022(3)	0.016(3)
C(12)	0.076(4)	0.047(4)	0.043(3)	0.035(3)	0.023(3)	0.019(3)
C(13)	0.099(6)	0.073(5)	0.055(4)	0.050(5)	0.039(4)	0.027(4)
C(14)	0.089(6)	0.101(7)	0.083(6)	0.049(5)	0.053(5)	0.046(5)
C(15)	0.063(4)	0.085(6)	0.074(5)	0.024(4)	0.024(4)	0.034(5)
C(16)	0.066(4)	0.059(4)	0.052(4)	0.025(3)	0.021(3)	0.022(3)
C(17)	0.043(3)	0.036(3)	0.038(3)	0.010(2)	0.018(2)	0.015(2)
C(18)	0.061(4)	0.044(3)	0.046(3)	0.025(3)	0.023(3)	0.028(3)
C(19)	0.052(3)	0.034(3)	0.032(3)	0.008(2)	0.011(2)	0.009(2)
C(20)	0.060(4)	0.057(4)	0.045(4)	0.021(3)	0.020(3)	0.022(3)

Table 2. Anisotropic Displacement Parameters (continued)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(21)	0.064(4)	0.065(5)	0.063(4)	0.019(3)	0.036(4)	0.018(4)
C(22)	0.079(5)	0.055(4)	0.071(5)	0.011(4)	0.045(4)	0.024(4)
C(23)	0.090(5)	0.048(4)	0.065(5)	0.019(4)	0.035(4)	0.030(4)
C(24)	0.064(4)	0.045(3)	0.047(4)	0.021(3)	0.024(3)	0.019(3)
C(25)	0.091(5)	0.044(4)	0.058(4)	0.035(3)	0.042(4)	0.029(3)
C(26)	0.20(1)	0.117(8)	0.149(10)	0.108(8)	0.136(9)	0.107(8)
C(27)	0.103(6)	0.044(4)	0.089(6)	0.033(4)	0.043(5)	0.034(4)
C(28)	0.111(7)	0.064(5)	0.069(5)	0.035(5)	0.015(5)	0.036(4)

The general temperature factor expression:

$$\exp(-2\pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$$

Table 3. Bond Lengths(Å)

atom	atom	distance	atom	atom	distance
Pt(1)	N(1)	1.999(5)	Pt(1)	N(2')	2.0683(5)
Pt(1)	N(2)	2.087(6)	Pt(1)	C(17)	1.989(6)
Cl(1)	O(1)	1.39(1)	Cl(1)	O(1')	1.47(2)
Cl(1)	O(2)	1.38(1)	Cl(1)	O(2')	1.42(2)
Cl(1)	O(3)	1.36(1)	Cl(1)	O(3')	1.53(2)
Cl(1)	O(3")	1.55(3)	Cl(1)	O(4')	1.53(3)
Cl(1)	O(4)	1.35(2)	O(1)	O(1')	1.05(2)
O(1)	O(3")	1.19(3)	O(1')	O(4')	1.52(3)
O(2)	O(2')	0.92(2)	O(3)	O(3')	1.18(2)
O(3)	O(4)	1.11(2)	O(3')	O(3")	1.59(3)
O(4')	O(4)	0.99(3)	N(1)	C(7)	1.349(8)
N(1)	C(11)	1.334(8)	N(2')	C(2)	1.377(8)
N(2')	C(6)	1.373(7)	N(2)	C(12)	1.362(8)
N(2)	C(16)	1.371(9)	N(3)	C(17)	1.343(7)
N(3)	C(18)	1.447(7)	N(4)	C(17)	1.344(7)
N(4)	C(25)	1.482(8)	C(1)	C(2)	1.377(9)
C(1)	C(6)	1.373(9)	C(1')	C(12)	1.362(6)
C(1')	C(16)	1.371(7)	C(2)	C(3)	1.39(1)
C(3)	C(4)	1.38(1)	C(4)	C(5)	1.37(1)
C(5)	C(6)	1.38(1)	C(6)	C(7)	1.48(1)
C(7)	C(8)	1.398(9)	C(8)	C(9)	1.38(1)
C(9)	C(10)	1.36(1)	C(10)	C(11)	1.407(9)
C(11)	C(12)	1.468(9)	C(12)	C(13)	1.39(1)
C(13)	C(14)	1.37(1)	C(14)	C(15)	1.37(1)

Table 3. Bond Lengths($\AA$) (continued)

atom	atom	distance	atom	atom	distance
C(15)	C(16)	1.37(1)	C(18)	C(19)	1.518(8)
C(19)	C(20)	1.390(8)	C(19)	C(24)	1.393(8)
C(20)	C(21)	1.387(9)	C(21)	C(22)	1.37(1)
C(22)	C(23)	1.37(1)	C(23)	C(24)	1.381(9)
C(25)	C(26)	1.51(1)	C(25)	C(27)	1.521(9)
C(25)	C(28)	1.51(1)			

Table 4. Bond Lengths(Å)

atom	atom	distance	atom	atom	distance
N(3)	H(1)	0.82(7)	N(4)	H(2)	0.85(7)
C(2)	H(3)	0.91(7)	C(3)	H(5)	0.95
C(4)	H(6)	0.95	C(5)	H(7)	0.95
C(8)	H(8)	0.95	C(9)	H(9)	0.95
C(10)	H(10)	0.95	C(13)	H(11)	0.95
C(14)	H(12)	0.95	C(15)	H(13)	0.95
C(16)	H(4)	0.92(7)	C(18)	H(14)	0.95
C(18)	H(15)	0.95	C(20)	H(16)	0.95
C(21)	H(17)	0.95	C(22)	H(18)	0.95
C(23)	H(19)	0.95	C(24)	H(20)	0.95
C(26)	H(21)	0.95	C(26)	H(22)	0.95
C(26)	H(23)	0.95	C(27)	H(24)	0.95
C(27)	H(25)	0.95	C(27)	H(26)	0.95
C(28)	H(27)	0.95	C(28)	H(28)	0.95
C(28)	H(29)	0.95			

Hydrogen Bonds

A	H	B	A-H	H...B	A...B	A-H...B
N(3)	H(1)	O(3")	0.82(7)	2.16(8)	2.98(3)	179(7)
N(4)	H(2)	O(1)	0.85(7)	2.41(7)	3.15(1)	146(6)
N(3)	H(1)	O(1)	0.82(7)	2.31(7)	3.05(1)	151(7)
N(4)	H(2)	O(2)	0.85(7)	2.43(7)	3.21(1)	153(6)
N(4)	H(2)	O(1')	0.85(7)	2.46(8)	3.25(3)	154(6)

Crystal data for [(CNN)Pt{C(NH^{t}Bu)(NHCH$_2$Ph)}]ClO$_4$, 4(ClO$_4$)

Table 5. Bond Angles(°)

atom	atom	atom	angle	atom	atom	atom	angle
N(1)	Pt(1)	N(2')	80.1(2)	N(1)	Pt(1)	N(2)	79.2(2)
N(1)	Pt(1)	C(17)	179.4(2)	N(2')	Pt(1)	N(2)	159.2(2)
N(2')	Pt(1)	C(17)	99.7(1)	N(2)	Pt(1)	C(17)	101.1(2)
O(1)	Cl(1)	O(1')	43.2(10)	O(1)	Cl(1)	O(2)	101.0(7)
O(1)	Cl(1)	O(2')	125.7(8)	O(1)	Cl(1)	O(3)	116.3(7)
O(1)	Cl(1)	O(3')	102.8(9)	O(1)	Cl(1)	O(3")	47.3(10)
O(1)	Cl(1)	O(4')	104(1)	O(1)	Cl(1)	O(4)	124.1(10)
O(1')	Cl(1)	O(2)	99(1)	O(1')	Cl(1)	O(2')	137(1)
O(1')	Cl(1)	O(3)	112(1)	O(1')	Cl(1)	O(3')	134(1)
O(1')	Cl(1)	O(3")	90(1)	O(1')	Cl(1)	O(4')	61(1)
O(1')	Cl(1)	O(4)	88(1)	O(2)	Cl(1)	O(2')	38.3(7)
O(2)	Cl(1)	O(3)	141.9(8)	O(2)	Cl(1)	O(3')	119.2(9)
O(2)	Cl(1)	O(3")	100(1)	O(2)	Cl(1)	O(4')	90(1)
O(2)	Cl(1)	O(4)	115(1)	O(2')	Cl(1)	O(3)	107.4(9)
O(2')	Cl(1)	O(3')	83.6(10)	O(2')	Cl(1)	O(3")	96(1)
O(2')	Cl(1)	O(4')	108(1)	O(2')	Cl(1)	O(4)	108(1)
O(3)	Cl(1)	O(3')	47.7(8)	O(3)	Cl(1)	O(3")	99(1)
O(3)	Cl(1)	O(4')	87(1)	O(3)	Cl(1)	O(4)	48.5(9)
O(3')	Cl(1)	O(3")	61(1)	O(3')	Cl(1)	O(4')	134(1)
O(3')	Cl(1)	O(4)	94(1)	O(3")	Cl(1)	O(4')	150(1)
O(3")	Cl(1)	O(4)	144(1)	O(4')	Cl(1)	O(4)	39(1)
Cl(1)	O(1)	O(1')	72(1)	Cl(1)	O(1)	O(3")	73(1)
O(1')	O(1)	O(3")	145(2)	Cl(1)	O(1')	O(1)	64(1)
Cl(1)	O(1')	O(4')	61(1)	O(1)	O(1')	O(4')	125(2)

Crystal data for $[(CNN)Pt\{C(NH^tBu)(NHCH_2Ph)\}]ClO_4$, $4(ClO_4)$

Table 5. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
Cl(1)	O(2)	O(2')	72(1)	Cl(1)	O(2')	O(2)	68(1)
Cl(1)	O(3)	O(3')	73(1)	Cl(1)	O(3)	O(4)	65(1)
O(3')	O(3)	O(4)	136(2)	Cl(1)	O(3')	O(3)	58(1)
Cl(1)	O(3')	O(3")	59(1)	O(3)	O(3')	O(3")	106(1)
Cl(1)	O(3")	O(1)	59(1)	Cl(1)	O(3")	O(3')	58(1)
O(1)	O(3")	O(3')	109(2)	Cl(1)	O(4')	O(1')	57(1)
Cl(1)	O(4')	O(4)	60(1)	O(1')	O(4')	O(4)	100(2)
Cl(1)	O(4)	O(3)	66(1)	Cl(1)	O(4)	O(4')	79(2)
O(3)	O(4)	O(4')	143(3)	Pt(1)	N(1)	C(7)	117.8(5)
Pt(1)	N(1)	C(11)	117.9(4)	C(7)	N(1)	C(11)	124.3(6)
Pt(1)	N(2')	C(2)	128.3(3)	Pt(1)	N(2')	C(6)	112.6(3)
C(2)	N(2')	C(6)	119.1(5)	Pt(1)	N(2)	C(12)	112.9(5)
Pt(1)	N(2)	C(16)	127.4(5)	C(12)	N(2)	C(16)	119.6(6)
C(17)	N(3)	C(18)	125.1(5)	C(17)	N(4)	C(25)	129.3(5)
Pt(1)	C(1)	C(2)	128.3(5)	Pt(1)	C(1)	C(6)	112.6(5)
C(2)	C(1)	C(6)	119.1(6)	Pt(1)	C(1')	C(12)	112.9(3)
Pt(1)	C(1')	C(16)	127.4(3)	C(12)	C(1')	C(16)	119.6(4)
N(2')	C(2)	C(3)	119.7(7)	C(2)	C(3)	C(4)	120.7(8)
C(3)	C(4)	C(5)	119.8(8)	C(4)	C(5)	C(6)	119.2(8)
N(2')	C(6)	C(5)	121.5(7)	N(2')	C(6)	C(7)	116.5(5)
C(5)	C(6)	C(7)	122.0(7)	N(1)	C(7)	C(6)	113.0(5)
N(1)	C(7)	C(8)	117.7(7)	C(6)	C(7)	C(8)	129.3(7)
C(7)	C(8)	C(9)	119.5(7)	C(8)	C(9)	C(10)	121.2(7)
C(9)	C(10)	C(11)	118.8(8)	N(1)	C(11)	C(10)	118.6(7)

Crystal data for [(CNN)Pt{C(NH^{t}Bu)(NHCH$_2$Ph)}]ClO$_4$, 4(ClO$_4$)

Table 5. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
N(1)	C(11)	C(12)	114.2(5)	C(10)	C(11)	C(12)	127.1(7)
N(2)	C(12)	C(11)	115.7(6)	N(2)	C(12)	C(13)	120.1(6)
C(11)	C(12)	C(13)	124.2(6)	C(12)	C(13)	C(14)	120.2(7)
C(13)	C(14)	C(15)	119.2(7)	C(14)	C(15)	C(16)	120.3(8)
N(2)	C(16)	C(15)	120.5(7)	Pt(1)	C(17)	N(3)	120.9(4)
Pt(1)	C(17)	N(4)	126.5(4)	N(3)	C(17)	N(4)	112.6(5)
N(3)	C(18)	C(19)	114.7(5)	C(18)	C(19)	C(20)	122.9(5)
C(18)	C(19)	C(24)	118.3(5)	C(20)	C(19)	C(24)	118.8(6)
C(19)	C(20)	C(21)	120.1(6)	C(20)	C(21)	C(22)	120.7(6)
C(21)	C(22)	C(23)	119.3(6)	C(22)	C(23)	C(24)	121.1(7)
C(19)	C(24)	C(23)	120.0(6)	N(4)	C(25)	C(26)	110.8(6)
N(4)	C(25)	C(27)	105.4(6)	N(4)	C(25)	C(28)	110.2(6)
C(26)	C(25)	C(27)	108.8(7)	C(26)	C(25)	C(28)	111.4(8)
C(27)	C(25)	C(28)	110.1(6)				

Complex **6**(ClO_4): ip 072

Crystal data. [(Pt N_4 C_{26} H_{25})$^+$ Cl O_4^-] ; formula weight = 688.05, orthorhombic, space group *Pbca* (No. 61), a = 8.758(2) Å, b = 21.560(3) Å, c = 26.533(3) Å, V = 5010(1) Å^3, Z = 8, D_c = 1.824 g cm^{-3}, μ(Mo-Kα) = 57.26 cm^{-1}, F(000) = 2688, T = 301 K. A yellow crystal of dimensions 0.25 × 0.20 × 0.40 mm in a glass capillary was used for data collection at 28°C on a MAR diffractometer with a 300 mm image plate detector using graphite monochromatized Mo-Kα radiation (λ = 0.71073 Å). Data collection were made with 2.5° oscillation (64 images) at 120 mm distance and 3 minute exposure. The images were interpreted and intensities integrated using program *DENZO*.[3] 4799 unique reflections were obtained from a total of 32599 measured reflections. 2876 reflections with $I > 3\,\sigma(I)$ were considered observed and used in the structural analysis. These reflections were in the range h : 0 to 9; k : 0 to 26; and l : -32 to 32 with a $2\theta_{max}$ = 51.2°. The space group was determined from systematic absences and the structure was solved by direct methods (*SIR92* [4]) and expanded by Fourier methods and refinement by full-matrix least-squares using the software package *TeXsan* on a Silicon Graphics Indy computer. One formula unit constitutes a crystallographic asymmetric unit. All 36 non-H atoms were refined anisotropically. The H atoms bonded to N(3) and N(4) were located from the differenced Fourier synthesis and their positional parameters were refined. The other 23 H atoms at calculated positions with thermal parameters equal to 1.3 times that of the attached C atoms were not refined. Convergence for 331 variable parameters by least-squares refinement on F with $w = 4\,F_o^2 / \sigma^2(F_o^2)$, where $\sigma^2(F_o^2) = [\,\sigma^2(I) + (0.022\,F_o^2)^2]$ for 2944 reflections with $I > 3\,\sigma(I)$ was reached at R = 0.037 and wR = 0.046 with a goodness-of-fit of 2.14. $(\Delta / \sigma)_{max}$ = 0.03 for non-H atoms. The final difference Fourier map was featureless, with maximum positive and negative peaks of 0.86 and 1.47 e Å^{-3} respectively.

Ref:

3. *DENZO* : In "The HKL Manual - A description of programs *DENZO*, *XDISPLAYF*, and *SCALEPACK* " written by Gewirth, D. with the cooperation of the program authors Otwinowski, Z. and Minor, W. (1995).
4. *SIR92* : Altomare, A., Cascarano, M., Giacovazzo, C., Guagliardi, A., Burla, M.C., Polidori, G., Camalli, M., J. Appl. Crystallogr., (1994), *27*, 435.

Crystal data for [(CNN)Pt{C(NH(2,6-$Me_2C_6H_3$))(NHMe)}]ClO_4, **6**(ClO_4)

Table 1. Atomic coordinates and B_{iso}/B_{eq}

atom	x	y	z	B_{eq}
Pt(1)	0.12550(3)	-0.04683(1)	-0.10579(1)	4.128(8)
Cl(1)	0.3005(3)	0.2134(1)	0.0967(1)	6.00(7)
O(1)	0.2353(8)	0.1565(3)	0.1113(3)	7.8(2)
O(2)	0.410(1)	0.2322(5)	0.1279(5)	14.2(4)
O(3)	0.401(1)	0.2010(6)	0.0563(7)	17.4(6)
O(4)	0.202(1)	0.2526(4)	0.0846(6)	21.1(6)
N(1)	0.0696(8)	0.0326(3)	-0.0710(3)	4.7(2)
N(2)	0.2602(7)	-0.0520(3)	-0.0400(3)	4.8(2)
N(3)	0.3262(7)	-0.1353(3)	-0.1560(3)	4.6(2)
N(4)	0.0884(7)	-0.1732(3)	-0.1421(3)	4.5(2)
C(1)	-0.0359(9)	-0.0156(4)	-0.1547(3)	4.5(2)
C(2)	-0.0958(10)	-0.0431(4)	-0.1970(4)	5.8(3)
C(3)	-0.215(1)	-0.0167(5)	-0.2237(4)	6.6(3)
C(4)	-0.271(1)	0.0390(6)	-0.2108(5)	7.8(4)
C(5)	-0.214(1)	0.0695(4)	-0.1689(5)	6.8(3)
C(6)	-0.094(1)	0.0418(4)	-0.1411(4)	5.5(2)
C(7)	-0.0324(10)	0.0691(4)	-0.0945(4)	5.5(2)
C(8)	-0.067(1)	0.1249(4)	-0.0731(5)	6.7(3)
C(9)	-0.002(1)	0.1400(4)	-0.0279(6)	7.8(3)
C(10)	0.102(1)	0.1018(5)	-0.0036(4)	6.9(3)
C(11)	0.1363(10)	0.0460(4)	-0.0265(4)	5.2(2)
C(12)	0.2420(10)	-0.0026(4)	-0.0089(4)	4.9(2)
C(13)	0.315(1)	0.0025(5)	0.0366(4)	6.3(3)
C(14)	0.410(1)	-0.0457(5)	0.0515(4)	6.6(3)

Table 1. Atomic coordinates and B_{iso}/B_{eq} (continued)

atom	x	y	z	B_{eq}
C(15)	0.430(1)	-0.0958(5)	0.0211(4)	6.6(3)
C(16)	0.3541(9)	-0.0976(4)	-0.0253(4)	5.3(2)
C(17)	0.1854(9)	-0.1260(3)	-0.1394(3)	4.2(2)
C(18)	0.4477(9)	-0.0887(4)	-0.1562(4)	5.9(3)
C(19)	0.1266(9)	-0.2357(4)	-0.1572(4)	4.6(2)
C(20)	0.102(1)	-0.2536(5)	-0.2063(4)	7.2(3)
C(21)	0.130(1)	-0.3149(6)	-0.2202(5)	9.0(4)
C(22)	0.177(1)	-0.3561(5)	-0.1845(6)	9.3(4)
C(23)	0.198(1)	-0.3388(4)	-0.1353(5)	6.5(3)
C(24)	0.173(1)	-0.2778(4)	-0.1205(4)	5.0(2)
C(25)	0.047(2)	-0.2083(6)	-0.2448(5)	12.2(5)
C(26)	0.192(1)	-0.2594(4)	-0.0665(4)	6.4(3)
H(1)	0.369(8)	-0.173(4)	-0.157(4)	7.0109
H(2)	0.00(1)	-0.164(4)	-0.129(4)	7.0109
H(3)	-0.0551	-0.0818	-0.2082	6.9745
H(4)	-0.2583	-0.0382	-0.2518	7.9420
H(5)	-0.3486	0.0581	-0.2302	9.4967
H(6)	-0.2558	0.1084	-0.1588	8.0974
H(7)	-0.1358	0.1526	-0.0892	8.0202
H(8)	-0.0286	0.1781	-0.0124	9.2216
H(9)	0.1473	0.1139	0.0274	8.3957
H(10)	0.3008	0.0382	0.0572	7.4442
H(11)	0.4614	-0.0435	0.0830	7.9204
H(12)	0.4948	-0.1288	0.0310	8.0544

Table 1. Atomic coordinates and B_{iso}/B_{eq} (continued)

atom	x	y	z	B_{eq}
H(13)	0.3696	-0.1320	-0.0470	6.3911
H(14)	0.5207	-0.0984	-0.1311	7.2272
H(15)	0.4979	-0.0899	-0.1887	7.2272
H(16)	0.4058	-0.0495	-0.1511	7.2272
H(17)	0.1189	-0.3281	-0.2537	10.6973
H(18)	0.1941	-0.3979	-0.1940	10.9230
H(19)	0.2291	-0.3688	-0.1109	7.6840
H(20)	0.1173	-0.1752	-0.2479	14.7860
H(21)	0.0357	-0.2285	-0.2765	14.7860
H(22)	-0.0502	-0.1922	-0.2347	14.7860
H(23)	0.2938	-0.2675	-0.0559	7.6386
H(24)	0.1718	-0.2161	-0.0632	7.6386
H(25)	0.1229	-0.2820	-0.0461	7.6386

$$B_{eq} = \frac{8}{3}\pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}aa^*bb^*\cos\gamma + 2U_{13}aa^*cc^*\cos\beta + 2U_{23}bb^*cc^*\cos\alpha)$$