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Experimental

Data Collection

A yellow prismatic crystal of $C_{26}H_{36}O_4N_4PtI_2Cl_6$ having approximate dimensions of $0.45 \times 0.18 \times 0.13$ mm was mounted on a glass fiber. All measurements were made on a Rigaku AFC5R diffractometer with graphite monochromated Mo-K α radiation and a rotating anode generator.

Cell constants and an orientation matrix for data collection, obtained from a least-squares refinement using the setting angles of 23 carefully centered reflections in the range $25.27 < 2\theta < 29.61^\circ$ corresponded to a primitive triclinic cell with dimensions:

$$\begin{array}{ll} a = 12.494(2) \text{ \AA} & \alpha = 97.69(2)^\circ \\ b = 13.917(3) \text{ \AA} & \beta = 99.25(2)^\circ \\ c = 12.251(3) \text{ \AA} & \gamma = 115.49(1) \\ V = 1847.9(7) \text{ \AA}^3 & \end{array}$$

For $Z = 2$ and F.W. = 1130.21, the calculated density is 2.03 g/cm^3 . Based on a statistical analysis of intensity distribution, and the successful solution and refinement of the structure, the space group was determined to be:

P $\bar{1}$ (#2)

The data were collected at a temperature of $-78 \pm 1^\circ\text{C}$ using the ω - 2θ scan technique to a maximum 2θ value of 55.0° . Omega scans of several intense reflections, made prior to data collection, had an average width at half-height of 0.27° with a take-off angle of 6.0° . Scans of $(0.89 + 0.30 \tan \theta)^\circ$ were made at a speed of $16.0^\circ/\text{min}$ (in omega). The weak reflections ($I < 5.0\sigma(I)$) were rescanned (maximum of 10 scans) and the counts were accumulated to ensure good counting statistics. Stationary background counts were recorded on each side of the reflection. The ratio of peak counting time to background counting time was 2:1. The diameter of the incident beam collimator was 1.0 mm, the crystal to detector distance was 258 mm, and the detector aperture was 9.0×13.0 mm (horizontal x vertical).

Data Reduction

Of the 8870 reflections which were collected, 8482 were unique ($R_{\text{int}} = 0.020$). The intensities of three representative reflection were measured after every 150 reflections. No decay correction was applied.

The linear absorption coefficient, μ , for Mo-K α radiation is 59.2 cm^{-1} . An empirical absorption correction based on azimuthal scans of several reflections was applied which resulted in transmission factors ranging from 0.72 to 1.00. The data were corrected for Lorentz and polarization effects.

Structure Solution and Refinement

The structure was solved by heavy-atom Patterson methods¹ and expanded using Fourier techniques². The non-hydrogen atoms were refined anisotropically. Hydrogen atoms were refined isotropically. The final

cycle of full-matrix least-squares refinement³ was based on 6825 observed reflections ($I > 3.00\sigma(I)$) and 429 variable parameters and converged (largest parameter shift was 0.19 times its esd) with unweighted and weighted agreement factors of:

$$R = \Sigma ||Fo| - |Fc|| / \Sigma |Fo| = 0.041$$

$$R_w = \sqrt{\Sigma w(|Fo| - |Fc|)^2} / \sqrt{\Sigma w|Fo|^2} = 0.042$$

The standard deviation of an observation of unit weight⁴ was 1.61. The weighting scheme was based on counting statistics and included a factor ($p = 0.020$) to downweight the intense reflections. Plots of $\Sigma w(|Fo| - |Fc|)^2$ versus $|Fo|$, reflection order in data collection, $\sin \theta/\lambda$ and various classes of indices showed no unusual trends. The maximum and minimum peaks on the final difference Fourier map corresponded to 1.56 and -1.49 $e^-/\text{\AA}^3$, respectively.

Neutral atom scattering factors were taken from Cromer and Waber⁵. Anomalous dispersion effects were included in F_{calc} ⁶; the values for $\Delta f'$ and $\Delta f''$ were those of Creagh and McAuley⁷. The values for the mass attenuation coefficients are those of Creagh and Hubbel⁸. All calculations were performed using the teXsan⁹ crystallographic software package of Molecular Structure Corporation.

References

(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) DIRDIF94: Beurskens, P.T., Admiraal, G., Beurskens, G., Bosman, W.P., de Gelder, R., Israel, R. and Smits, J.M.M. (1994). The DIRDIF-94 program system, Technical Report of the Crystallography Laboratory, University of Nijmegen, The Netherlands.

(3) Least-Squares:

Function minimized: $\Sigma w(|Fo| - |Fc|)^2$

where $w = \frac{1}{\sigma^2(Fo)} = [\sigma_c^2(Fo) + \frac{p^2}{4} Fo^2]^{-1}$

$\sigma_c(Fo)$ = e.s.d. based on counting statistics

p = p-factor

(4) Standard deviation of an observation of unit weight:

$$\sqrt{\Sigma w(|Fo| - |Fc|)^2} / (No - Nv)$$

where: No = number of observations

Nv = number of variables

(5) Cromer, D. T. & Waber, J. T.; "International Tables for X-ray Crystallography", Vol. IV, The Kynoch Press, Birmingham, England, Table 2.2 A (1974).

- (6) Ibers, J. A. & Hamilton, W. C.; *Acta Crystallogr.*, 17, 781 (1964).
- (7) Creagh, D. C. & McAuley, W.J.; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.6.8, pages 219-222 (1992).
- (8) Creagh, D. C. & Hubbell, J.H.; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.4.3, pages 200-206 (1992).
- (9) teXsan: Crystal Structure Analysis Package, Molecular Structure Corporation (1985 & 1992).

EXPERIMENTAL DETAILS**A. Crystal Data**

Empirical Formula	C ₂₆ H ₃₆ O ₄ N ₄ PtI ₂ Cl ₆
Formula Weight	1130.21
Crystal Color, Habit	yellow, prismatic
Crystal Dimensions	0.45 X 0.18 X 0.13 mm
Crystal System	triclinic
Lattice Type	Primitive
No. of Reflections Used for Unit Cell Determination (2θ range)	23 (25.3 - 29.6°)
Omega Scan Peak Width at Half-height	0.27°
Lattice Parameters	a = 12.494(2) Å b = 13.917(3) Å c = 12.251(3) Å α = 97.69(2)° β = 99.25(2)° γ = 115.49(1)°
	V = 1847.9(7) Å ³
Space Group	P $\bar{1}$ (#2)
Z value	2
D _{calc}	2.031 g/cm ³
F ₀₀₀	1076.00
μ(MoKα)	59.22 cm ⁻¹

B. Intensity Measurements

Diffractometer	Rigaku AFC5R
Radiation	MoKα ($λ = 0.71069$ Å)

	graphite monochromated
Attenuator	Zr foil (factors = 1.00, 3.40, 11.34, 38.03)
Take-off Angle	6.0°
Detector Aperture	9.0 mm horizontal 13.0 mm vertical
Crystal to Detector Distance	258 mm
Temperature	-78.0°C
Scan Type	ω -2θ
Scan Rate	16.0°/min (in ω) (up to 10 scans)
Scan Width	(0.89 + 0.30 tan θ)°
$2\theta_{max}$	55.0°
No. of Reflections Measured	Total: 8870 Unique: 8482 ($R_{int} = 0.020$)
Corrections	Lorentz-polarization Absorption (trans. factors: 0.7219 - 1.0000)

C. Structure Solution and Refinement

Structure Solution	Patterson Methods (DIRDIF92 PATTY)
Refinement	Full-matrix least-squares
Function Minimized	$\Sigma w(Fo - Fc)^2$
Least Squares Weights	$w = \frac{1}{\sigma^2(Fo)} = [\sigma_c^2(Fo) + \frac{p^2}{4}Fo^2]^{-1}$
p-factor	0.0200
Anomalous Dispersion	All non-hydrogen atoms
No. Observations ($I > 3.00\sigma(I)$)	6825
No. Variables	429
Reflection/Parameter Ratio	15.91
Residuals: R; R _w	0.041 ; 0.042
Residuals: R1	0.041

No. of Reflections to calc R1	6825
Goodness of Fit Indicator	1.61
Max Shift/Error in Final Cycle	0.19
Maximum peak in Final Diff. Map	$1.56 \text{ e}^-/\text{\AA}^3$
Minimum peak in Final Diff. Map	$-1.49 \text{ e}^-/\text{\AA}^3$

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

atom	x	y	z	B_{eq}	occ
Pt(1)	0.03115(2)	0.19995(2)	0.24739(2)	2.142(5)	1.0000
I(1)	0.07286(4)	0.40175(4)	0.21057(5)	3.30(1)	1.0000
I(2)	-0.18795(4)	0.09984(4)	0.08644(4)	2.828(10)	1.0000
Cl(1)	0.5962(3)	0.2345(2)	0.0277(4)	10.1(1)	1.0000
Cl(2)	0.7348(3)	0.4408(2)	0.1790(2)	7.07(8)	1.0000
Cl(3)	0.7860(3)	0.4080(3)	-0.0366(3)	8.66(9)	1.0000
Cl(4)	0.5412(4)	0.0035(4)	0.1994(3)	16.7(1)	1.0000
Cl(5)	0.3800(4)	0.0198(4)	0.3280(5)	15.1(2)	1.0000
Cl(6)	0.4328(5)	-0.1471(5)	0.3289(5)	16.1(2)	1.0000
O(1)	-0.0039(5)	-0.2554(4)	0.2707(4)	3.2(1)	1.0000
O(2)	0.4531(6)	0.4262(5)	0.6832(6)	6.3(2)	1.0000
O(3)	-0.1114(4)	0.0208(3)	0.3966(4)	2.9(1)	1.0000
O(4)	0.3283(4)	0.2633(5)	0.2811(5)	4.2(1)	1.0000
N(1)	0.1168(5)	0.0718(5)	0.1185(5)	2.5(1)	1.0000
N(2)	0.0378(5)	0.2779(5)	0.4776(5)	2.7(1)	1.0000
N(3)	0.1628(5)	0.2299(5)	0.0579(5)	2.9(1)	1.0000
N(4)	-0.1577(5)	0.2074(5)	0.3712(5)	2.8(1)	1.0000
C(1)	0.1149(6)	0.1677(5)	0.1268(6)	2.4(1)	1.0000
C(2)	-0.0430(6)	0.2288(5)	0.3786(6)	2.4(1)	1.0000
C(3)	0.0099(6)	0.0495(5)	0.2648(6)	2.2(1)	1.0000
C(4)	0.1831(6)	0.2704(5)	0.3787(6)	2.2(1)	1.0000
C(5)	0.0633(6)	0.0073(5)	0.1942(6)	2.3(1)	1.0000
C(6)	0.1591(6)	0.3014(5)	0.4804(6)	2.7(1)	1.0000
C(7)	0.0637(6)	-0.0936(6)	0.1907(6)	2.6(1)	1.0000

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

atom	x	y	z	B_{eq}	occ
C(8)	0.2493(7)	0.3544(6)	0.5841(7)	3.2(2)	1.0000
C(9)	0.0021(6)	-0.1551(5)	0.2626(6)	2.4(1)	1.0000
C(10)	0.3674(7)	0.3735(6)	0.5815(7)	4.0(2)	1.0000
C(11)	-0.0566(6)	-0.1181(5)	0.3304(6)	2.5(1)	1.0000
C(12)	0.3963(7)	0.3437(6)	0.4806(8)	3.6(2)	1.0000
C(13)	-0.0544(6)	-0.0179(5)	0.3313(5)	2.3(1)	1.0000
C(14)	0.3037(6)	0.2924(5)	0.3812(6)	2.9(1)	1.0000
C(15)	0.2335(7)	0.2095(6)	-0.0194(6)	3.5(2)	1.0000
C(16)	-0.2138(7)	0.2187(6)	0.4671(7)	4.0(2)	1.0000
C(17)	0.2936(8)	0.3111(7)	-0.0702(8)	4.7(2)	1.0000
C(18)	-0.214(2)	0.3251(10)	0.492(2)	16.1(5)	1.0000
C(19A)	0.387(1)	0.401(1)	0.000(2)	4.2(4)	0.5000
C(19B)	0.375(2)	0.303(1)	-0.133(1)	4.5(4)	0.5000
C(20)	-0.175(2)	0.408(1)	0.465(1)	15.1(6)	1.0000
C(21)	0.0468(8)	-0.3016(6)	0.1919(7)	3.9(2)	1.0000
C(22)	0.5750(8)	0.4400(8)	0.6898(9)	6.1(3)	1.0000
C(23)	-0.2003(7)	-0.0560(6)	0.4456(6)	3.3(2)	1.0000
C(24)	0.4541(7)	0.2943(9)	0.2801(9)	5.8(3)	1.0000
C(25)	0.413(1)	-0.0650(9)	0.241(1)	7.3(3)	1.0000
C(26)	0.7406(8)	0.3460(6)	0.0748(7)	4.1(2)	1.0000
H(1)	0.144(6)	0.048(5)	0.069(6)	3(1)	1.0000
H(2)	0.013(5)	0.288(5)	0.526(5)	1(1)	1.0000
H(3)	0.162(5)	0.288(5)	0.067(5)	0(1)	1.0000
H(4)	-0.199(6)	0.174(5)	0.314(6)	2(1)	1.0000

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

atom	x	y	z	B_{eq}	occ
H(5)	0.105(6)	-0.119(6)	0.143(6)	4(1)	1.0000
H(6)	0.231(7)	0.376(6)	0.670(7)	5(1)	1.0000
H(7)	-0.097(6)	-0.158(5)	0.369(6)	2(1)	1.0000
H(8)	0.491(6)	0.364(6)	0.483(6)	3(1)	1.0000

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

Table 2. Anisotropic Displacement Parameters

atom	U ₁₁	U ₂₂	U ₃₃	U ₁₂	U ₁₃	U ₂₃
Pt(1)	0.0238(1)	0.0258(1)	0.0360(1)	0.01194(9)	0.01116(10)	0.01317(10)
I(1)	0.0388(2)	0.0314(2)	0.0635(3)	0.0177(2)	0.0183(2)	0.0237(2)
I(2)	0.0294(2)	0.0413(2)	0.0398(3)	0.0173(2)	0.0100(2)	0.0123(2)
Cl(1)	0.057(2)	0.062(2)	0.247(5)	0.023(1)	0.037(2)	-0.010(2)
Cl(2)	0.111(2)	0.080(2)	0.083(2)	0.047(2)	0.041(2)	0.003(1)
Cl(3)	0.141(2)	0.187(3)	0.088(2)	0.122(2)	0.075(2)	0.081(2)
Cl(4)	0.122(3)	0.204(5)	0.117(3)	-0.090(3)	0.072(2)	-0.039(3)
Cl(5)	0.109(3)	0.191(5)	0.284(7)	0.076(3)	0.072(4)	0.023(5)
Cl(6)	0.218(6)	0.177(5)	0.244(6)	0.092(4)	0.076(5)	0.105(4)
O(1)	0.059(3)	0.031(2)	0.046(3)	0.029(2)	0.024(2)	0.016(2)
O(2)	0.057(4)	0.076(4)	0.079(5)	0.029(3)	-0.024(4)	-0.022(4)
O(3)	0.049(3)	0.026(2)	0.045(3)	0.018(2)	0.028(2)	0.013(2)
O(4)	0.030(3)	0.072(4)	0.058(4)	0.021(3)	0.014(2)	0.015(3)
N(1)	0.031(3)	0.034(3)	0.037(3)	0.017(2)	0.019(2)	0.014(2)
N(2)	0.039(3)	0.029(3)	0.038(4)	0.019(2)	0.014(3)	0.006(3)
N(3)	0.034(3)	0.035(3)	0.048(4)	0.017(3)	0.017(3)	0.020(3)
N(4)	0.032(3)	0.035(3)	0.044(4)	0.017(2)	0.015(3)	0.012(3)
C(1)	0.025(3)	0.037(4)	0.035(4)	0.013(3)	0.012(3)	0.018(3)
C(2)	0.037(4)	0.025(3)	0.036(4)	0.018(3)	0.011(3)	0.012(3)
C(3)	0.027(3)	0.025(3)	0.036(4)	0.014(2)	0.010(3)	0.011(3)
C(4)	0.025(3)	0.021(3)	0.035(4)	0.009(2)	0.005(3)	0.011(3)
C(5)	0.027(3)	0.030(3)	0.036(4)	0.013(3)	0.014(3)	0.014(3)
C(6)	0.031(3)	0.018(3)	0.051(4)	0.011(3)	0.006(3)	0.007(3)
C(7)	0.029(3)	0.036(4)	0.041(4)	0.018(3)	0.014(3)	0.012(3)

Table 2. Anisotropic Displacement Parameters (continued)

atom	U ₁₁	U ₂₂	U ₃₃	U ₁₂	U ₁₃	U ₂₃
C(8)	0.039(4)	0.027(4)	0.048(5)	0.013(3)	-0.001(3)	0.002(3)
C(9)	0.035(3)	0.026(3)	0.031(4)	0.015(3)	0.009(3)	0.009(3)
C(10)	0.046(5)	0.029(4)	0.057(5)	0.013(3)	-0.012(4)	-0.005(4)
C(11)	0.038(4)	0.032(3)	0.031(4)	0.016(3)	0.016(3)	0.013(3)
C(12)	0.027(4)	0.030(4)	0.068(6)	0.010(3)	-0.002(4)	0.008(4)
C(13)	0.033(3)	0.029(3)	0.029(3)	0.015(3)	0.011(3)	0.009(3)
C(14)	0.030(3)	0.030(3)	0.051(4)	0.012(3)	0.008(3)	0.015(3)
C(15)	0.042(4)	0.055(4)	0.054(4)	0.026(3)	0.032(3)	0.036(4)
C(16)	0.059(5)	0.046(4)	0.067(5)	0.032(4)	0.043(4)	0.013(4)
C(17)	0.054(5)	0.057(5)	0.090(6)	0.025(4)	0.044(4)	0.052(4)
C(18)	0.32(1)	0.072(7)	0.36(2)	0.121(7)	0.30(1)	0.103(8)
C(19A)	0.043(9)	0.039(9)	0.06(1)	0.008(7)	0.009(8)	0.006(8)
C(19B)	0.07(1)	0.09(1)	0.044(9)	0.042(9)	0.045(7)	0.036(8)
C(20)	0.42(2)	0.109(9)	0.12(1)	0.17(1)	0.09(1)	0.037(9)
C(21)	0.073(5)	0.043(4)	0.056(5)	0.041(4)	0.032(4)	0.014(4)
C(22)	0.035(5)	0.075(7)	0.100(8)	0.024(4)	-0.022(5)	-0.003(6)
C(23)	0.047(4)	0.035(4)	0.050(4)	0.015(3)	0.035(3)	0.017(3)
C(24)	0.027(4)	0.105(8)	0.089(7)	0.028(5)	0.023(4)	0.020(6)
C(25)	0.075(7)	0.085(8)	0.103(9)	0.015(6)	0.043(6)	0.030(7)
C(26)	0.057(5)	0.046(5)	0.061(5)	0.026(4)	0.028(4)	0.012(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)	I(1)	2.7417(5)	Pt(1)	I(2)	2.7514(6)
Pt(1)	C(1)	2.050(7)	Pt(1)	C(2)	2.057(7)
Pt(1)	C(3)	2.039(6)	Pt(1)	C(4)	2.037(6)
Cl(1)	C(26)	1.736(8)	Cl(2)	C(26)	1.743(8)
Cl(3)	C(26)	1.753(9)	Cl(4)	C(25)	1.67(1)
Cl(5)	C(25)	1.71(1)	Cl(6)	C(25)	1.73(1)
O(1)	C(9)	1.384(8)	O(1)	C(21)	1.458(9)
O(2)	C(10)	1.373(9)	O(2)	C(22)	1.44(1)
O(3)	C(13)	1.355(8)	O(3)	C(23)	1.450(7)
O(4)	C(14)	1.364(9)	O(4)	C(24)	1.442(9)
N(1)	C(1)	1.336(9)	N(1)	C(5)	1.420(8)
N(1)	H(1)	0.83(7)	N(2)	C(2)	1.322(9)
N(2)	C(6)	1.400(9)	N(2)	H(2)	0.74(6)
N(3)	C(1)	1.315(8)	N(3)	C(15)	1.474(9)
N(3)	H(3)	0.81(6)	N(4)	C(2)	1.317(9)
N(4)	C(16)	1.485(9)	N(4)	H(4)	0.75(6)
C(3)	C(5)	1.387(9)	C(3)	C(13)	1.398(8)
C(4)	C(6)	1.385(10)	C(4)	C(14)	1.396(9)
C(5)	C(7)	1.401(9)	C(6)	C(8)	1.415(10)
C(7)	C(9)	1.398(9)	C(7)	H(5)	0.96(7)
C(8)	C(10)	1.39(1)	C(8)	H(6)	1.14(8)
C(9)	C(11)	1.378(9)	C(10)	C(12)	1.40(1)
C(11)	C(13)	1.381(9)	C(11)	H(7)	0.83(6)
C(12)	C(14)	1.39(1)	C(12)	H(8)	1.09(7)

Table 3. Bond Lengths(Å) (continued)

atom	atom	distance	atom	atom	distance
C(15)	C(17)	1.556(10)	C(16)	C(18)	1.47(1)
C(17)	C(19A)	1.34(2)	C(17)	C(19B)	1.41(2)
C(18)	C(20)	1.16(2)			

Table 4. Bond Angles(°)

atom	atom	atom	angle	atom	atom	atom	angle
I(1)	Pt(1)	I(2)	91.56(2)	I(1)	Pt(1)	C(1)	94.9(2)
I(1)	Pt(1)	C(2)	88.3(2)	I(1)	Pt(1)	C(3)	174.7(2)
I(1)	Pt(1)	C(4)	90.4(2)	I(2)	Pt(1)	C(1)	89.4(2)
I(2)	Pt(1)	C(2)	94.6(2)	I(2)	Pt(1)	C(3)	89.0(2)
I(2)	Pt(1)	C(4)	174.1(2)	C(1)	Pt(1)	C(2)	174.8(3)
C(1)	Pt(1)	C(3)	79.8(3)	C(1)	Pt(1)	C(4)	96.0(3)
C(2)	Pt(1)	C(3)	96.9(3)	C(2)	Pt(1)	C(4)	79.9(3)
C(3)	Pt(1)	C(4)	89.5(2)	C(9)	O(1)	C(21)	117.2(5)
C(10)	O(2)	C(22)	118.5(8)	C(13)	O(3)	C(23)	117.5(5)
C(14)	O(4)	C(24)	118.0(6)	C(1)	N(1)	C(5)	116.8(6)
C(1)	N(1)	H(1)	123(4)	C(5)	N(1)	H(1)	120(4)
C(2)	N(2)	C(6)	117.3(6)	C(2)	N(2)	H(2)	115(4)
C(6)	N(2)	H(2)	126(4)	C(1)	N(3)	C(15)	125.1(6)
C(1)	N(3)	H(3)	115(4)	C(15)	N(3)	H(3)	118(4)
C(2)	N(4)	C(16)	126.6(7)	C(2)	N(4)	H(4)	112(5)
C(16)	N(4)	H(4)	118(5)	Pt(1)	C(1)	N(1)	114.4(4)
Pt(1)	C(1)	N(3)	126.8(5)	N(1)	C(1)	N(3)	118.8(6)
Pt(1)	C(2)	N(2)	113.7(5)	Pt(1)	C(2)	N(4)	126.7(5)
N(2)	C(2)	N(4)	119.5(7)	Pt(1)	C(3)	C(5)	113.3(4)
Pt(1)	C(3)	C(13)	130.1(5)	C(5)	C(3)	C(13)	116.6(6)
Pt(1)	C(4)	C(6)	112.3(5)	Pt(1)	C(4)	C(14)	130.8(5)
C(6)	C(4)	C(14)	116.9(6)	N(1)	C(5)	C(3)	115.7(6)
N(1)	C(5)	C(7)	119.5(6)	C(3)	C(5)	C(7)	124.8(6)
N(2)	C(6)	C(4)	116.6(6)	N(2)	C(6)	C(8)	119.6(7)

Table 4. Bond Angles($^{\circ}$) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C(4)	C(6)	C(8)	123.8(7)	C(5)	C(7)	C(9)	115.8(6)
C(5)	C(7)	H(5)	122(4)	C(9)	C(7)	H(5)	121(4)
C(6)	C(8)	C(10)	116.7(7)	C(6)	C(8)	H(6)	125(3)
C(10)	C(8)	H(6)	117(4)	O(1)	C(9)	C(7)	122.9(6)
O(1)	C(9)	C(11)	116.0(6)	C(7)	C(9)	C(11)	121.2(6)
O(2)	C(10)	C(8)	115.3(8)	O(2)	C(10)	C(12)	123.0(8)
C(8)	C(10)	C(12)	121.6(7)	C(9)	C(11)	C(13)	121.1(6)
C(9)	C(11)	H(7)	119(4)	C(13)	C(11)	H(7)	119(4)
C(10)	C(12)	C(14)	118.9(7)	C(10)	C(12)	H(8)	118(3)
C(14)	C(12)	H(8)	122(3)	O(3)	C(13)	C(3)	116.9(6)
O(3)	C(13)	C(11)	122.6(6)	C(3)	C(13)	C(11)	120.5(6)
O(4)	C(14)	C(4)	117.2(6)	O(4)	C(14)	C(12)	120.7(7)
C(4)	C(14)	C(12)	122.1(7)	N(3)	C(15)	C(17)	109.4(6)
N(4)	C(16)	C(18)	112.7(8)	C(15)	C(17)	C(19A)	117(1)
C(15)	C(17)	C(19B)	112.5(10)	C(19A)	C(17)	C(19B)	88(1)
C(16)	C(18)	C(20)	138(1)	Cl(4)	C(25)	Cl(5)	112.3(7)
Cl(4)	C(25)	Cl(6)	110.9(8)	Cl(5)	C(25)	Cl(6)	101.8(7)
Cl(1)	C(26)	Cl(2)	108.2(5)	Cl(1)	C(26)	Cl(3)	110.9(5)
Cl(2)	C(26)	Cl(3)	108.7(5)				

Table 5. Torsion Angles(°)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
Pt(1)	C(1)	N(1)	C(5)	-0.9(7)	Pt(1)	C(1)	N(3)	C(15)	173.2(5)
Pt(1)	C(2)	N(2)	C(6)	-1.0(8)	Pt(1)	C(2)	N(4)	C(16)	173.9(5)
Pt(1)	C(3)	C(5)	N(1)	-3.4(7)	Pt(1)	C(3)	C(5)	C(7)	178.9(5)
Pt(1)	C(3)	C(13)	O(3)	-0.9(9)	Pt(1)	C(3)	C(13)	C(11)	-179.9(5)
Pt(1)	C(4)	C(6)	N(2)	1.4(7)	Pt(1)	C(4)	C(6)	C(8)	-178.5(5)
Pt(1)	C(4)	C(14)	O(4)	0.0(9)	Pt(1)	C(4)	C(14)	C(12)	178.8(5)
I(1)	Pt(1)	C(1)	N(1)	178.7(5)	I(1)	Pt(1)	C(1)	N(3)	-2.7(6)
I(1)	Pt(1)	C(2)	N(2)	-89.4(5)	I(1)	Pt(1)	C(2)	N(4)	87.8(6)
I(1)	Pt(1)	C(3)	C(5)	-4(2)	I(1)	Pt(1)	C(3)	C(13)	178(1)
I(1)	Pt(1)	C(4)	C(6)	86.7(4)	I(1)	Pt(1)	C(4)	C(14)	-92.5(6)
I(2)	Pt(1)	C(1)	N(1)	-89.8(5)	I(2)	Pt(1)	C(1)	N(3)	88.8(6)
I(2)	Pt(1)	C(2)	N(2)	179.2(5)	I(2)	Pt(1)	C(2)	N(4)	-3.6(6)
I(2)	Pt(1)	C(3)	C(5)	91.7(5)	I(2)	Pt(1)	C(3)	C(13)	-84.6(6)
I(2)	Pt(1)	C(4)	C(6)	-22(2)	I(2)	Pt(1)	C(4)	C(14)	157(1)
O(1)	C(9)	C(7)	C(5)	-178.8(6)	O(1)	C(9)	C(11)	C(13)	178.5(6)
O(2)	C(10)	C(8)	C(6)	179.3(7)	O(2)	C(10)	C(12)	C(14)	-178.8(7)
O(3)	C(13)	C(3)	C(5)	-177.1(6)	O(3)	C(13)	C(11)	C(9)	179.7(6)
O(4)	C(14)	C(4)	C(6)	-179.3(6)	O(4)	C(14)	C(12)	C(10)	179.3(7)
N(1)	C(1)	Pt(1)	C(2)	50(2)	N(1)	C(1)	Pt(1)	C(3)	-0.7(5)
N(1)	C(1)	Pt(1)	C(4)	87.8(5)	N(1)	C(1)	N(3)	C(15)	-8(1)
N(1)	C(5)	C(3)	C(13)	173.5(6)	N(1)	C(5)	C(7)	C(9)	-175.9(6)
N(2)	C(2)	Pt(1)	C(1)	38(2)	N(2)	C(2)	Pt(1)	C(3)	89.6(5)
N(2)	C(2)	Pt(1)	C(4)	1.3(5)	N(2)	C(2)	N(4)	C(16)	-9(1)
N(2)	C(6)	C(4)	C(14)	-179.2(6)	N(2)	C(6)	C(8)	C(10)	178.8(6)

Table 5. Torsion Angles(°) (continued)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
N(3)	C(1)	Pt(1)	C(2)	-130(2)	N(3)	C(1)	Pt(1)	C(3)	177.9(6)
N(3)	C(1)	Pt(1)	C(4)	-93.7(6)	N(3)	C(1)	N(1)	C(5)	-179.6(6)
N(3)	C(15)	C(17)	C(19A)	71(1)	N(3)	C(15)	C(17)	C(19B)	172.3(10)
N(4)	C(2)	Pt(1)	C(1)	-143(2)	N(4)	C(2)	Pt(1)	C(3)	-93.2(6)
N(4)	C(2)	Pt(1)	C(4)	178.5(6)	N(4)	C(2)	N(2)	C(6)	-178.4(6)
N(4)	C(16)	C(18)	C(20)	-7(3)	C(1)	Pt(1)	C(3)	C(5)	2.2(5)
C(1)	Pt(1)	C(3)	C(13)	-174.1(7)	C(1)	Pt(1)	C(4)	C(6)	-178.3(5)
C(1)	Pt(1)	C(4)	C(14)	2.5(6)	C(1)	N(1)	C(5)	C(3)	2.9(9)
C(1)	N(1)	C(5)	C(7)	-179.2(6)	C(1)	N(3)	C(15)	C(17)	-170.0(7)
C(2)	Pt(1)	C(3)	C(5)	-173.7(5)	C(2)	Pt(1)	C(3)	C(13)	9.9(6)
C(2)	Pt(1)	C(4)	C(6)	-1.4(5)	C(2)	Pt(1)	C(4)	C(14)	179.3(6)
C(2)	N(2)	C(6)	C(4)	-0.3(9)	C(2)	N(2)	C(6)	C(8)	179.6(6)
C(2)	N(4)	C(16)	C(18)	94(1)	C(3)	Pt(1)	C(4)	C(6)	-98.5(5)
C(3)	Pt(1)	C(4)	C(14)	82.2(6)	C(3)	C(5)	C(7)	C(9)	1(1)
C(3)	C(13)	O(3)	C(23)	166.3(6)	C(3)	C(13)	C(11)	C(9)	-1(1)
C(4)	Pt(1)	C(3)	C(5)	-94.0(5)	C(4)	Pt(1)	C(3)	C(13)	89.7(6)
C(4)	C(6)	C(8)	C(10)	-1(1)	C(4)	C(14)	O(4)	C(24)	174.4(7)
C(4)	C(14)	C(12)	C(10)	0(1)	C(5)	C(3)	C(13)	C(11)	3.9(10)
C(5)	C(7)	C(9)	C(11)	1.1(10)	C(6)	C(4)	C(14)	C(12)	-0.5(10)
C(6)	C(8)	C(10)	C(12)	1(1)	C(7)	C(5)	C(3)	C(13)	-4.2(10)
C(7)	C(9)	O(1)	C(21)	-6.0(9)	C(7)	C(9)	C(11)	C(13)	-1(1)
C(8)	C(6)	C(4)	C(14)	0.9(10)	C(8)	C(10)	O(2)	C(22)	174.4(8)
C(8)	C(10)	C(12)	C(14)	0(1)	C(11)	C(9)	O(1)	C(21)	174.1(6)
C(11)	C(13)	O(3)	C(23)	-14.7(9)	C(12)	C(10)	O(2)	C(22)	-7(1)

Table 5. Torsion Angles($^{\circ}$) (continued)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
C(12)	C(14)	O(4)	C(24)	-4(1)					

Table 6. Non-bonded Contacts out to 3.27 Å

atom	atom	distance	ADC	atom	atom	distance	ADC
I(2)	H(1)	2.91(7)	2	I(2)	H(5)	3.16(7)	2
Cl(2)	H(6)	2.77(8)	66602	Cl(4)	H(4)	3.03(6)	65501
O(1)	H(2)	2.60(6)	55602	O(1)	H(6)	2.88(8)	55602
O(1)	N(2)	3.217(8)	55602	O(2)	C(19B)	3.04(2)	55601
O(3)	H(7)	3.24(6)	55602	N(1)	H(1)	3.25(7)	2
N(2)	H(7)	2.88(7)	55602	C(6)	H(7)	2.84(7)	55602
C(8)	H(7)	2.78(6)	55602	C(19A)	C(19A)	2.98(3)	66502
H(2)	H(7)	2.79(9)	55602	H(6)	H(7)	2.68(10)	55602

The ADC (atom designator code) specifies the position of an atom in a crystal. The 5-digit number shown in the table is a composite of three one-digit numbers and one two-digit number: TA (first digit) + TB (second digit) + TC (third digit) + SN (last two digits). TA, TB and TC are the crystal lattice translation digits along cell edges a, b and c. A translation digit of 5 indicates the origin unit cell. If TA = 4, this indicates a translation of one unit cell length along the a-axis in the negative direction. Each translation digit can range in value from 1 to 9 and thus ± 4 lattice translations from the origin (TA=5, TB=5, TC=5) can be represented.

The SN, or symmetry operator number, refers to the number of the symmetry operator used to generate the coordinates of the target atom. A list of symmetry operators relevant to this structure are given below.

For a given intermolecular contact, the first atom (origin atom) is located in the origin unit cell and its position can be generated using the identity operator (SN=1). Thus, the ADC for an origin atom is always 55501. The position of the second atom (target atom) can be generated using the ADC and the coordinates of the atom in the parameter table. For example, an ADC of 47502 refers to the target atom moved through symmetry operator two, then translated -1 cell translations along the a axis, +2 cell translations along the b axis, and 0 cell translations along the c axis.

An ADC of 1 indicates an intermolecular contact between two fragments (eg. cation and anion) that reside in the same asymmetric unit.

Symmetry Operators:

(1)	X,	Y,	Z	(2)	-X,	-Y,	-Z
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Table 7. Least Squares Planes**Plane number 1**

Atoms defining plane	Distance
Pt(1)	0.0000(3)
C(1)	-0.005(7)
N(1)	-0.006(6)
C(5)	0.023(7)
C(3)	-0.021(7)

Plane number 2

Atoms defining plane	Distance
Pt(1)	0.0000(3)
C(2)	-0.015(7)
N(2)	0.007(6)
C(6)	0.009(7)
C(4)	-0.014(7)

Plane number 3

Atoms defining plane	Distance
C(3)	0.022(7)
C(5)	-0.016(7)
C(7)	-0.002(8)
C(9)	0.012(7)
C(11)	-0.006(8)
C(13)	-0.013(7)

Plane number 4

Atoms defining plane	Distance
C(4)	0.000(7)
C(6)	-0.003(7)
C(8)	0.007(8)
C(10)	-0.008(9)
C(12)	0.003(8)
C(14)	0.001(7)

