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,	1/2+y,	1/2-z
(3)	-x,	-y,	-z	(4)	x,	1/2-y,	1/2+z

Table S8. Least Squares Planes

Plane number 1

Atoms defining plane	Distance
Pd(1)	-0.0002(4)
C(1)	0.031(6)
C(2)	-0.005(6)
C(3)	0.033(6)
C(4)	-0.004(6)

Additional Atoms	Distance
O(1)	0.111
O(2)	0.019
O(3)	0.084
O(4)	-0.017

Plane number 2

Atoms defining plane	Distance
Sb(1)	0.0016(3)
F(1)	0.002(3)
F(2)	-0.014(4)
F(3)	-0.054(3)
F(5)	-0.060(3)

Plane number 3

Atoms defining plane	Distance
Sb(1)	0.0008(3)
F(1)	0.003(3)
F(2)	-0.004(3)
F(4)	-0.040(3)
F(6)	-0.042(3)

Plane number 4

Atoms defining plane	Distance
Sb(1)	0.0038(3)
F(3)	-0.169(3)
F(4)	-0.143(4)
F(5)	-0.168(3)
F(6)	-0.149(4)

Plane number 5

Atoms defining plane	Distance
Sb(2)	0.0003(4)
F(1)	-0.013(3)
F(7)	-0.019(3)
F(8)	0.012(4)
F(10)	0.017(5)

Plane number 6

Atoms defining plane	Distance
Sb(2)	0.0006(3)
F(1)	-0.026(4)
F(7)	-0.038(4)
F(9)	-0.038(5)
F(11)	-0.040(5)

Plane number 7

Atoms defining plane	Distance
Sb(2)	-0.0043(3)
F(8)	0.157(4)
F(9)	0.137(4)
F(10)	0.182(4)
F(11)	0.142(4)

Plane number 8

Atoms defining plane	Distance
Sb(3)	-0.0325(4)
F(12)	-0.308(4)
F(13)	0.191(3)
F(14)	1.504(3)
F(15)	1.010(3)

Plane number 9

Atoms defining plane	Distance
Sb(3)	-0.0005(3)
F(12)	-0.019(3)
F(13)	-0.018(3)
F(15)	0.045(4)
F(17)	0.033(3)

Plane number 10

Atoms defining plane	Distance
Sb(3)	0.0048(3)
F(14)	-0.146(4)
F(15)	-0.172(4)
F(16)	-0.146(4)
F(17)	-0.133(4)

Plane number 11

Atoms defining plane	Distance
Sb(4)	-0.0019(3)
F(12)	0.018(4)
F(18)	0.025(3)
F(19)	0.078(4)
F(21)	0.077(4)

Plane number 12

Atoms defining plane	Distance
Sb(4)	-0.0019(3)
F(12)	0.015(3)
F(18)	0.024(3)
F(20)	0.076(4)
F(22)	0.072(4)

Plane number 13

Atoms defining plane	Distance
Sb(4)	-0.0052(3)
F(19)	0.163(4)
F(20)	0.129(4)
F(21)	0.136(4)
F(22)	0.146(4)

Summary

plane	mean deviation	χ^2
1	0.0145	48.6
2	0.0263	650.5
3	0.0179	307.3
4	0.1264	7484.9
5	0.0125	77.9
6	0.0286	284.8
7	0.1245	6691.3
8	0.6090	317672.2
9	0.0231	315.7
10	0.1202	8753.3
11	0.0401	1030.5
12	0.0377	879.5
13	0.1157	9515.4

Dihedral angles between planes (°)

plane	1	2	3	4	5	6	7	8	9	10	11	12
2	47.3											
3	44.2	90.8										
4	95.6	89.8	89.1									
5	94.4	50.2	130.4	65.2								
6	9.4	40.7	52.5	101.1	89.9							
7	82.2	97.6	63.5	26.9	89.5	90.4						
8	10.2	57.0	35.7	99.5	104.6	16.9	82.3					
9	44.8	90.2	22.8	111.9	139.2	49.7	86.1	34.6				
10	82.2	93.4	67.5	21.9	83.6	89.9	6.0	83.4	90.3			
11	46.7	12.0	87.3	78.3	47.8	42.4	85.8	56.9	91.4	81.4		
12	45.4	92.4	4.1	92.9	133.9	53.3	67.0	36.3	19.1	71.2	89.7	
13	100.9	101.6	85.5	12.3	76.1	107.8	22.3	102.9	108.0	19.7	89.9	88.9

Sample: fa122/$[Pt(CO)_4][Sb_2F_{11}]_2$

P.O. # Charge: $175

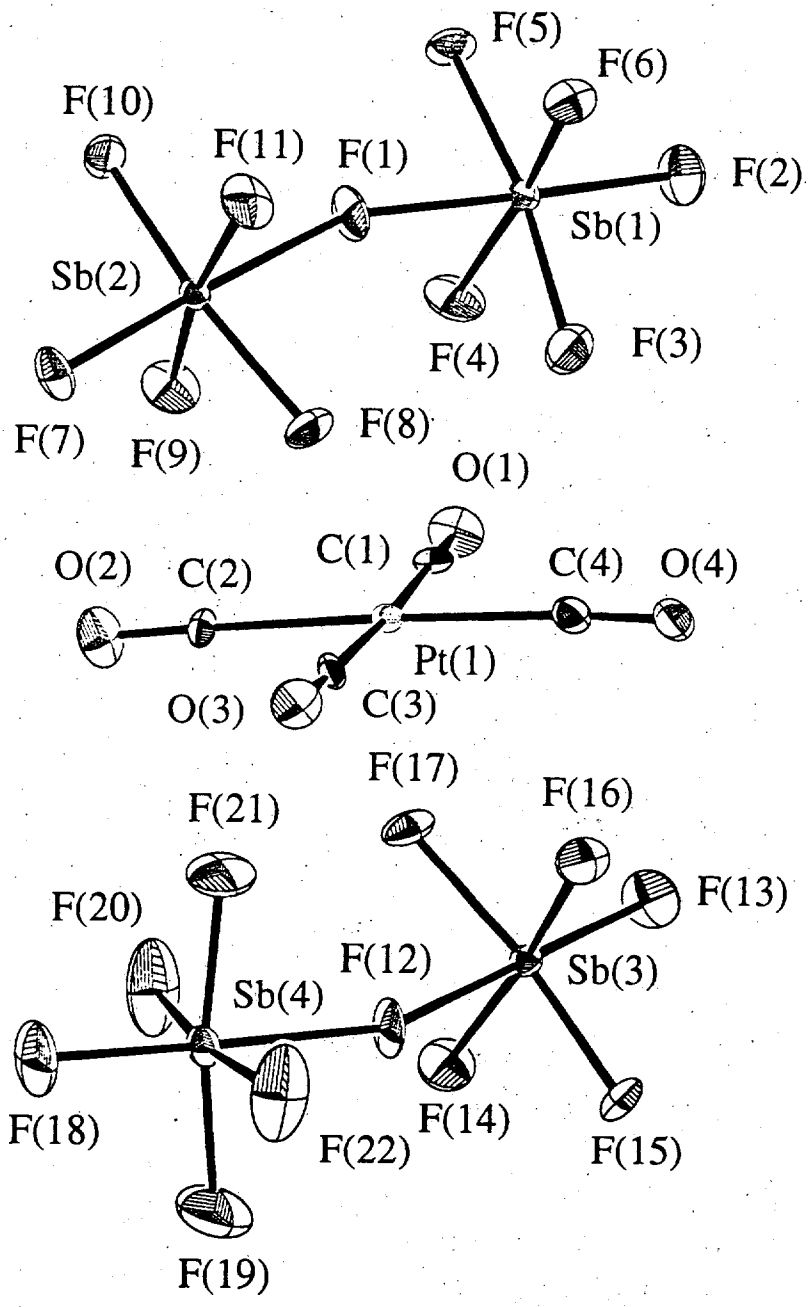
X-ray Structure Report

for

Prof. F. Aubke

UBC Chemistry

Wed Feb 25 1998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F(9)
F(8)
O(1)
O(2)
C(2)
C(1)
C(4)
O(4)
Pt(1)
O(3)
C(3)
F(17)
F(16)
F(21)
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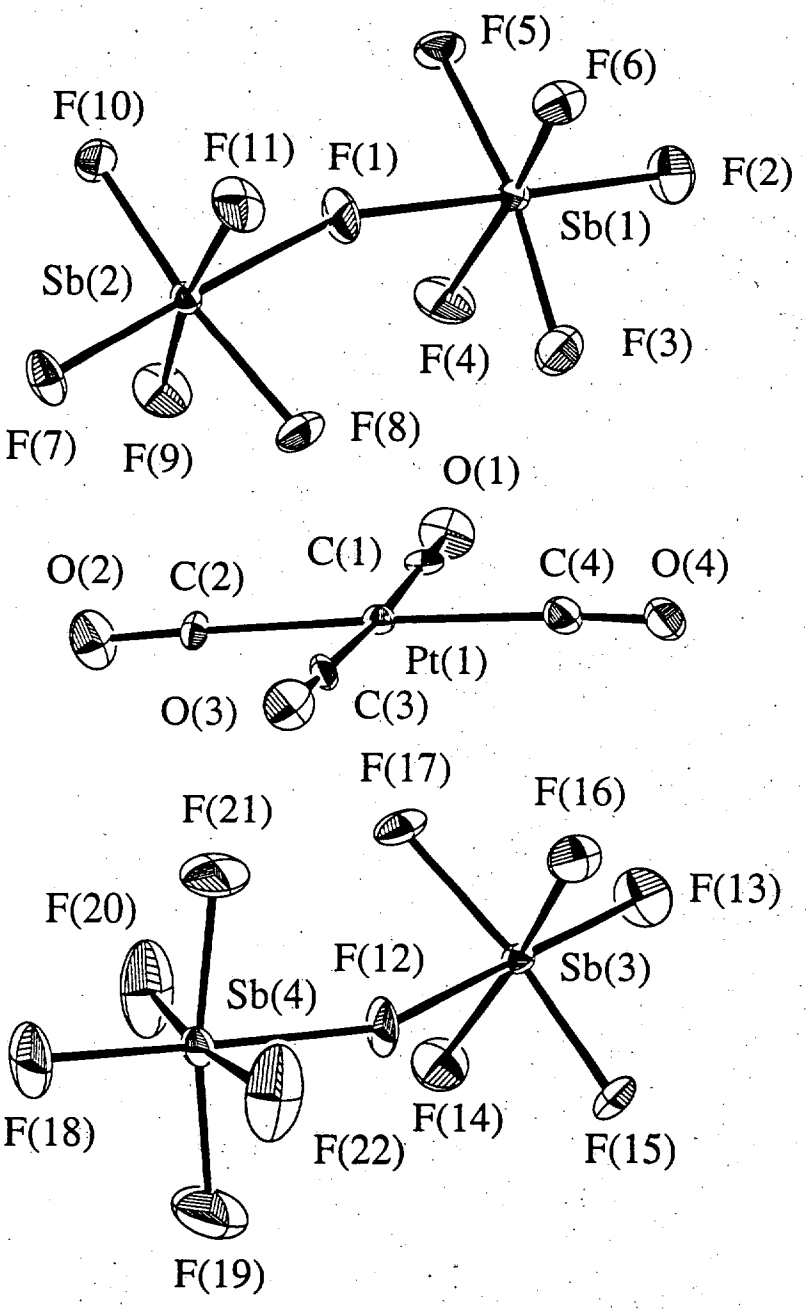
F(12)
Sb(3)
Sb(4)
F(18)
F(14)
F(15)
F(22)
F(19)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F(9)
F(8)
O(1)
O(2)
C(2)
C(1)
C(4)
O(4)
Pt(1)
O(3)
C(3)
F(17)
F(16)
F(21)
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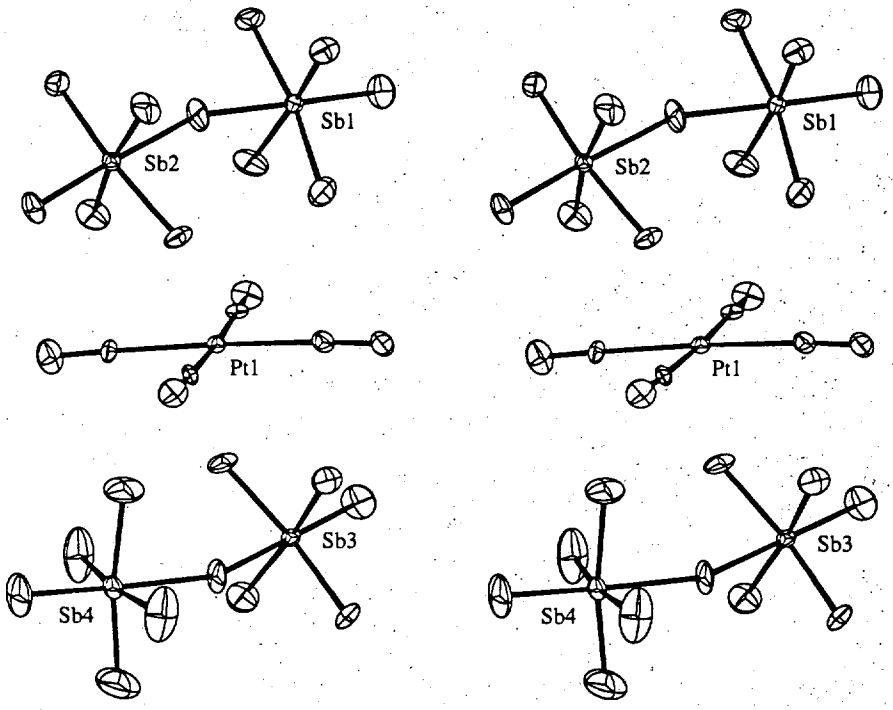
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Pt1
Sb3
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Sb1
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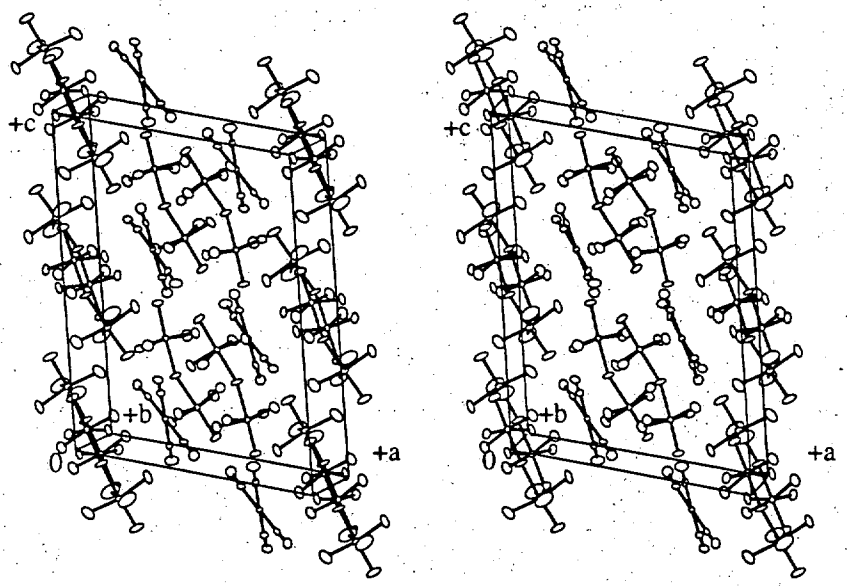
Sb3
Sb4


+c
+b
+a
+c
+b
+a

Experimental

Data Collection

A colorless irregular crystal of $C_4F_{22}O_4PtSb_4$ having approximate dimensions of 0.40 x 0.25 x 0.18 mm was mounted in a glass capillary. All measurements were made on a Rigaku/ADSC CCD area detector with graphite monochromated Mo-Kα radiation.

Cell constants and an orientation matrix for data collection based on 11597 reflections with 2θ = 4.0-60.1° corresponded to a primitive monoclinic cell with dimensions:

a = 12.757(2) $\AA$
b = 9.726(2) $\AA$ β = 103.3576(7)°
c = 17.8576(7) $\AA$
V = 2155.7(5) $\AA^3$

For Z = 4 and F.W. = 1212.10, the calculated density is 3.73 g/cm^3. The systematic absences of:

h0l: l $\neq$ 2n
0k0: k $\neq$ 2n

uniquely determine the space group to be:

$P2_1/c$ (#14)

The data were collected at a temperature of -93 $\pm$ 1°C to a maximum 2θ value of 60.1°. Data were collected in 0.50° oscillations with 25.0 second exposures. A sweep of data was done using ϕ oscillations from 0.0 to 190.0° at χ=-90° and a second sweep was performed using ω oscillations between -23.0 and 18.0° at χ=-90°. The crystal-to-detector distance was 39.18(1) mm . The detector swing angle was -10.0°.

Data Reduction

Of the 19985 reflections which were collected, 5596 were unique (R_{int} = 0.038); equivalent reflections were merged.

The linear absorption coefficient, μ, for Mo-Kα radiation is 115.8 cm^{-1}. The data were corrected for Lorentz and polarization effects.

Structure Solution and Refinement

The structure was solved by direct methods[1] and expanded using Fourier techniques[2]. The non-hydrogen atoms were refined anisotropically. The final cycle of full-matrix least-squares refinement[3] was based on all 5596 unique reflections and 316 variable parameters and converged (largest parameter shift was 0.001 times its esd) with unweighted and weighted agreement factors of:

$$R = \Sigma||Fo^2| - |Fc^2||/\Sigma|Fo^2| = 0.053$$

$$R_w = \sqrt{(\Sigma w(|Fo^2| - |Fc^2|)^2/\Sigma wFo^4)}] = 0.048$$

The standard deviation of an observation of unit weight[4] was 1.16. The weighting scheme was based on counting statistics. Plots of $\Sigma w(|Fo^2| - |Fc^2|)^2$ versus $|Fo^2|$, reflection order in data collection, sin θ/λ and various classes of indices showed no unusual trends. The maximum and minimum peaks on the final difference Fourier map corresponded to 2.27 and -4.22 $e^-/\mathring{A}^3$, respectively (both near Pt).

Neutral atom scattering factors were taken from Cromer and Waber[5] . Anomalous dispersion effects were included in Fcalc[6]; the values for Δf' and Δf" were those of Creagh and McAuley[7]. The values for the mass attenuation coefficients are those of Creagh and Hubbell[8]. All calculations were performed using the teXsan[9] crystallographic software package of Molecular Structure Corporation.

References

(1) SIR92: Altomare, A., Cascarano, M., Giacovazzo, C., Guagliardi, A. (1993). J. Appl. Cryst., 26, 343.

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

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

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

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	$C_4F_{22}O_4PtSb_4$
Formula Weight	1212.10
Crystal Color, Habit	colorless, irregular
Crystal Dimensions	0.40 X 0.25 X 0.18 mm
Crystal System	monoclinic
Lattice Type	Primitive
Lattice Parameters	a = 12.757(2)Å b = 9.726(2) Å c = 17.8576(7) Å β = 103.3576(7)°
	V = 2155.7(5) Å^3
Space Group	$P2_1/c$ (#14)
Z value	4
D_{calc}	3.734 g/cm^3
F_{000}	2144.00
μ(MoKα)	115.80 cm^{-1}

B. Intensity Measurements

Diffractometer	Rigaku/ADSC CCD
Radiation	MoKα (λ = 0.71069 Å) graphite monochromated
Detector Aperture	94 mm x 94 mm
Data Images	462 exposures of 25.0 seconds
ϕ oscillation Range (χ=-90)	0.0 - 190.0°

ω oscillation Range (χ=-90)	-23.0 - 18.0°
Detector Position	39.18(1) mm
Detector Swing Angle	-10.0°
$2\theta_{max}$	60.1°
No. of Reflections Measured	Total: 19985 Unique: 5596 (R_{int} = 0.038)
Corrections	Lorentz-polarization Absorption/scaling (trans. factors: 0.3496 - 1.0000)

C. Structure Solution and Refinement

Structure Solution	Direct Methods (SIR92)
Refinement	Full-matrix least-squares
Function Minimized	$\Sigma w(\|Fo^2\| - \|Fc^2\|)^2$
Least Squares Weights	$w = \frac{1}{\sigma^2(Fo^2)}$
p-factor	0.0000
Anomalous Dispersion	All non-hydrogen atoms
No. Observations	5596
No. Variables	316
Reflection/Parameter Ratio	17.71
Residuals (on F^2, all data): R; Rw	0.053 ; 0.048
Goodness of Fit Indicator	1.16
No. Observations (I>3σ(I))	3158
Residuals (on F, I>3σ(I)): R; Rw	0.025 ; 0.022
Max Shift/Error in Final Cycle	0.001
Maximum peak in Final Diff. Map	2.27 $e^-/\AA^3$ (near Pt)
Minimum peak in Final Diff. Map	-4.22 $e^-/\AA^3$ (near Pt)

Table 2. Atomic coordinates and B_{eq}

atom	x	y	z	B_{eq}
Pt(1)	0.27127(2)	0.25811(4)	0.589614(11)	0.882(4)
Sb(1)	0.51094(3)	0.25891(7)	0.82403(2)	1.019(8)
Sb(2)	0.62244(3)	0.24515(6)	0.63288(2)	0.911(8)
Sb(3)	-0.06862(3)	0.25847(6)	0.51511(2)	0.932(8)
Sb(4)	0.05277(3)	0.25522(7)	0.33117(2)	1.318(8)
F(1)	0.5896(3)	0.2394(6)	0.7390(2)	2.35(9)
F(2)	0.4413(3)	0.2744(6)	0.9030(2)	2.82(11)
F(3)	0.4269(5)	0.3894(6)	0.7620(3)	2.63(13)
F(4)	0.4154(4)	0.1297(6)	0.7701(3)	2.55(12)
F(5)	0.6037(4)	0.1216(5)	0.8710(3)	1.95(11)
F(6)	0.6140(4)	0.3911(5)	0.8623(3)	1.92(11)
F(7)	0.6468(3)	0.2514(6)	0.5349(2)	1.84(8)
F(8)	0.5143(4)	0.3792(5)	0.6106(3)	2.13(12)
F(9)	0.5099(5)	0.1197(5)	0.6039(3)	2.41(13)
F(10)	0.7152(4)	0.1032(5)	0.6689(3)	1.93(11)
F(11)	0.7210(5)	0.3770(5)	0.6740(3)	2.35(12)
F(12)	-0.0212(4)	0.3004(5)	0.4177(2)	2.24(10)
F(13)	-0.1116(4)	0.2218(6)	0.6037(2)	2.97(11)
F(14)	-0.1586(4)	0.1320(5)	0.4558(3)	2.55(12)
F(15)	-0.1677(4)	0.3969(5)	0.4815(2)	1.83(10)
F(16)	0.0323(4)	0.3886(5)	0.5613(2)	2.28(11)
F(17)	0.0440(4)	0.1326(5)	0.5338(2)	1.85(10)
F(18)	0.1244(4)	0.2172(6)	0.2547(2)	3.45(13)
F(19)	-0.0831(4)	0.2460(10)	0.2704(2)	5.68(15)

Table 2. Atomic coordinates and B_{eq} (continued)

atom	x	y	z	B_{eq}
F(20)	0.0456(5)	0.0746(5)	0.3596(3)	4.6(2)
F(21)	0.1781(3)	0.2669(8)	0.4070(2)	4.15(13)
F(22)	0.0566(5)	0.4413(6)	0.3184(3)	4.6(2)
O(1)	0.1968(5)	0.0372(6)	0.6909(3)	2.03(14)
O(2)	0.3222(6)	0.0304(6)	0.4844(3)	2.44(15)
O(3)	0.3501(5)	0.4596(6)	0.4810(3)	2.09(14)
O(4)	0.2121(5)	0.5014(6)	0.6838(3)	1.72(13)
C(1)	0.2251(7)	0.1187(9)	0.6561(4)	1.3(2)
C(2)	0.3046(7)	0.1095(8)	0.5227(4)	1.0(2)
C(3)	0.3227(7)	0.3898(8)	0.5215(4)	1.1(2)
C(4)	0.2349(7)	0.4120(9)	0.6522(4)	1.3(2)

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

Table 3. Bond Lengths($\AA$)

atom	atom	distance	atom	atom	distance
Pt(1)	C(1)	1.979(9)	Pt(1)	C(2)	1.984(8)
Pt(1)	C(3)	1.980(8)	Pt(1)	C(4)	1.987(8)
Sb(1)	F(1)	2.013(3)	Sb(1)	F(2)	1.839(3)
Sb(1)	F(3)	1.854(5)	Sb(1)	F(4)	1.857(5)
Sb(1)	F(5)	1.852(5)	Sb(1)	F(6)	1.853(5)
Sb(2)	F(1)	2.034(3)	Sb(2)	F(7)	1.847(3)
Sb(2)	F(8)	1.873(5)	Sb(2)	F(9)	1.865(5)
Sb(2)	F(10)	1.835(5)	Sb(2)	F(11)	1.827(5)
Sb(3)	F(12)	2.011(3)	Sb(3)	F(13)	1.825(3)
Sb(3)	F(14)	1.842(5)	Sb(3)	F(15)	1.849(4)
Sb(3)	F(16)	1.857(5)	Sb(3)	F(17)	1.859(5)
Sb(4)	F(12)	2.036(3)	Sb(4)	F(18)	1.847(4)
Sb(4)	F(19)	1.822(4)	Sb(4)	F(20)	1.836(5)
Sb(4)	F(21)	1.844(4)	Sb(4)	F(22)	1.826(5)
O(1)	C(1)	1.118(9)	O(2)	C(2)	1.086(9)
O(3)	C(3)	1.106(9)	O(4)	C(4)	1.110(9)

Table 4. Bond Angles(°)

atom	atom	atom	angle	atom	atom	atom	angle
C(1)	Pt(1)	C(2)	89.8(3)	C(1)	Pt(1)	C(3)	176.8(3)
C(1)	Pt(1)	C(4)	92.2(3)	C(2)	Pt(1)	C(3)	87.4(3)
C(2)	Pt(1)	C(4)	177.3(3)	C(3)	Pt(1)	C(4)	90.7(3)
F(1)	Sb(1)	F(2)	178.8(2)	F(1)	Sb(1)	F(3)	86.2(2)
F(1)	Sb(1)	F(4)	85.8(2)	F(1)	Sb(1)	F(5)	84.0(2)
F(1)	Sb(1)	F(6)	84.7(2)	F(2)	Sb(1)	F(3)	95.0(2)
F(2)	Sb(1)	F(4)	94.4(2)	F(2)	Sb(1)	F(5)	94.8(2)
F(2)	Sb(1)	F(6)	95.1(2)	F(3)	Sb(1)	F(4)	86.2(2)
F(3)	Sb(1)	F(5)	170.1(2)	F(3)	Sb(1)	F(6)	90.5(2)
F(4)	Sb(1)	F(5)	91.2(2)	F(4)	Sb(1)	F(6)	170.2(2)
F(5)	Sb(1)	F(6)	90.5(2)	F(1)	Sb(2)	F(7)	177.8(2)
F(1)	Sb(2)	F(8)	85.3(2)	F(1)	Sb(2)	F(9)	86.0(2)
F(1)	Sb(2)	F(10)	84.7(2)	F(1)	Sb(2)	F(11)	85.2(2)
F(7)	Sb(2)	F(8)	93.0(2)	F(7)	Sb(2)	F(9)	92.6(2)
F(7)	Sb(2)	F(10)	96.9(2)	F(7)	Sb(2)	F(11)	96.1(2)
F(8)	Sb(2)	F(9)	85.1(2)	F(8)	Sb(2)	F(10)	169.1(2)
F(8)	Sb(2)	F(11)	90.1(2)	F(9)	Sb(2)	F(10)	89.9(2)
F(9)	Sb(2)	F(11)	170.2(2)	F(10)	Sb(2)	F(11)	93.4(2)
F(12)	Sb(3)	F(13)	179.5(2)	F(12)	Sb(3)	F(14)	84.8(2)
F(12)	Sb(3)	F(15)	83.8(2)	F(12)	Sb(3)	F(16)	86.0(2)
F(12)	Sb(3)	F(17)	85.1(2)	F(13)	Sb(3)	F(14)	95.5(2)
F(13)	Sb(3)	F(15)	96.0(2)	F(13)	Sb(3)	F(16)	93.7(2)
F(13)	Sb(3)	F(17)	95.2(2)	F(14)	Sb(3)	F(15)	90.7(2)
F(14)	Sb(3)	F(16)	170.7(2)	F(14)	Sb(3)	F(17)	90.9(2)

Table 4. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
F(15)	Sb(3)	F(16)	90.0(2)	F(15)	Sb(3)	F(17)	168.6(2)
F(16)	Sb(3)	F(17)	86.6(2)	F(12)	Sb(4)	F(18)	177.9(2)
F(12)	Sb(4)	F(19)	85.3(2)	F(12)	Sb(4)	F(20)	86.3(2)
F(12)	Sb(4)	F(21)	84.5(2)	F(12)	Sb(4)	F(22)	84.9(2)
F(18)	Sb(4)	F(19)	96.6(2)	F(18)	Sb(4)	F(20)	94.4(2)
F(18)	Sb(4)	F(21)	93.6(2)	F(18)	Sb(4)	F(22)	94.2(2)
F(19)	Sb(4)	F(20)	90.9(4)	F(19)	Sb(4)	F(21)	169.7(2)
F(19)	Sb(4)	F(22)	91.3(4)	F(20)	Sb(4)	F(21)	86.9(3)
F(20)	Sb(4)	F(22)	170.7(2)	F(21)	Sb(4)	F(22)	89.3(3)
Sb(1)	F(1)	Sb(2)	161.1(2)	Sb(3)	F(12)	Sb(4)	153.8(2)
Pt(1)	C(1)	O(1)	177.1(7)	Pt(1)	C(2)	O(2)	178.1(7)
Pt(1)	C(3)	O(3)	177.0(7)	Pt(1)	C(4)	O(4)	176.4(7)

Table 5. Anisotropic Displacement Parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Pt(1)	0.00984(11)	0.01255(13)	0.01071(9)	-0.0004(2)	0.00153(8)	0.00019(14)
Sb(1)	0.0103(2)	0.0178(3)	0.01083(15)	0.0009(3)	0.00286(14)	-0.0003(2)
Sb(2)	0.0119(2)	0.0132(2)	0.00970(15)	-0.0003(3)	0.00290(14)	0.0000(2)
Sb(3)	0.0089(2)	0.0143(2)	0.01229(15)	-0.0002(3)	0.00268(14)	0.0008(2)
Sb(4)	0.0182(2)	0.0214(3)	0.0122(2)	0.0001(3)	0.00693(15)	-0.0001(3)
F(1)	0.038(2)	0.042(3)	0.0149(15)	0.006(3)	0.017(2)	0.002(3)
F(2)	0.032(3)	0.057(4)	0.025(2)	0.003(3)	0.021(2)	0.004(3)
F(3)	0.032(4)	0.041(4)	0.028(3)	0.016(3)	0.011(3)	0.007(2)
F(4)	0.025(3)	0.038(3)	0.029(3)	-0.012(3)	-0.005(2)	-0.007(2)
F(5)	0.027(3)	0.017(3)	0.025(3)	0.009(2)	-0.004(2)	0.004(2)
F(6)	0.020(3)	0.017(3)	0.032(3)	-0.004(2)	0.000(2)	-0.003(2)
F(7)	0.039(2)	0.021(2)	0.0136(14)	-0.002(3)	0.0131(15)	0.001(2)
F(8)	0.022(4)	0.030(3)	0.028(3)	0.014(2)	0.003(3)	0.006(2)
F(9)	0.028(4)	0.030(3)	0.032(3)	-0.013(3)	0.004(3)	-0.004(2)
F(10)	0.030(4)	0.027(3)	0.018(2)	0.012(3)	0.008(2)	0.007(2)
F(11)	0.032(4)	0.024(3)	0.031(3)	-0.011(3)	0.002(3)	-0.012(2)
F(12)	0.043(3)	0.031(3)	0.019(2)	0.011(2)	0.023(2)	0.005(2)
F(13)	0.040(3)	0.055(4)	0.023(2)	0.003(3)	0.019(2)	0.017(2)
F(14)	0.027(3)	0.030(3)	0.037(3)	-0.008(2)	0.001(2)	-0.008(2)
F(15)	0.017(3)	0.023(3)	0.031(3)	0.010(2)	0.006(2)	0.002(2)
F(16)	0.028(3)	0.019(3)	0.036(3)	0.000(2)	-0.002(2)	-0.005(2)
F(17)	0.011(3)	0.020(3)	0.035(3)	0.001(2)	-0.005(2)	-0.003(2)
F(18)	0.057(3)	0.051(4)	0.034(2)	0.004(3)	0.034(2)	-0.002(2)
F(19)	0.037(3)	0.131(6)	0.038(2)	0.005(6)	-0.010(2)	-0.016(5)

Table 5. Anisotropic Displacement Parameters (continued)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
F(20)	0.100(5)	0.020(3)	0.069(4)	0.001(3)	0.051(4)	-0.003(3)
F(21)	0.015(2)	0.094(5)	0.041(2)	-0.001(4)	-0.008(2)	-0.012(4)
F(22)	0.092(5)	0.025(3)	0.075(4)	0.007(3)	0.055(4)	0.010(3)
O(1)	0.024(4)	0.023(4)	0.030(3)	-0.010(3)	0.006(3)	0.002(3)
O(2)	0.053(5)	0.015(3)	0.026(3)	0.005(3)	0.013(3)	0.001(3)
O(3)	0.032(4)	0.018(3)	0.029(3)	0.000(3)	0.007(3)	0.003(3)
O(4)	0.028(4)	0.021(3)	0.016(3)	0.002(3)	0.003(3)	-0.002(2)
C(1)	0.011(5)	0.023(5)	0.014(4)	0.004(4)	-0.004(3)	-0.002(3)
C(2)	0.012(5)	0.011(4)	0.017(4)	0.000(3)	0.006(3)	-0.004(3)
C(3)	0.020(5)	0.013(4)	0.009(4)	0.004(3)	0.002(3)	-0.003(3)
C(4)	0.018(5)	0.021(5)	0.013(4)	0.000(4)	0.003(4)	0.000(3)

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 6. Selected Torsion Angles(°)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
Sb(1)	F(1)	Sb(2)	F(8)	22.8(10)	Sb(1)	F(1)	Sb(2)	F(9)	-62.6(10)
Sb(1)	F(1)	Sb(2)	F(10)	-152.9(10)	Sb(1)	F(1)	Sb(2)	F(11)	113.2(10)
Sb(2)	F(1)	Sb(1)	F(3)	-22.9(10)	Sb(2)	F(1)	Sb(1)	F(4)	63.6(10)
Sb(2)	F(1)	Sb(1)	F(5)	155.2(10)	Sb(2)	F(1)	Sb(1)	F(6)	-113.7(10)
Sb(3)	F(12)	Sb(4)	F(19)	109.0(7)	Sb(3)	F(12)	Sb(4)	F(20)	17.8(6)
Sb(3)	F(12)	Sb(4)	F(21)	-69.5(6)	Sb(3)	F(12)	Sb(4)	F(22)	-159.2(6)
Sb(4)	F(12)	Sb(3)	F(14)	-68.1(6)	Sb(4)	F(12)	Sb(3)	F(15)	-159.4(6)
Sb(4)	F(12)	Sb(3)	F(16)	110.2(6)	Sb(4)	F(12)	Sb(3)	F(17)	23.3(6)

Table 7. Non-bonded Contacts out to 3.60 Å

atom	atom	distance	ADC	atom	atom	distance	ADC
Pt(1)	F(17)	3.091(5)	1	Pt(1)	F(21)	3.203(4)	1
Pt(1)	F(16)	3.233(5)	1	Pt(1)	F(8)	3.257(6)	1
Pt(1)	F(9)	3.284(6)	1	Pt(1)	F(3)	3.496(5)	1
Pt(1)	F(4)	3.549(5)	1	Sb(2)	F(13)	3.557(4)	65501
Sb(2)	O(2)	3.571(6)	65603	Sb(2)	O(3)	3.583(6)	66603
F(1)	F(3)	3.411(8)	64602	F(1)	O(4)	3.471(8)	64602
F(2)	O(2)	3.008(8)	4	F(2)	O(3)	3.037(8)	4
F(2)	F(7)	3.104(5)	4	F(2)	C(2)	3.256(9)	4
F(2)	C(3)	3.286(9)	4	F(2)	F(21)	3.399(6)	4
F(2)	F(9)	3.423(8)	65602	F(3)	C(4)	2.769(10)	1
F(3)	O(4)	2.979(8)	1	F(3)	F(10)	3.188(7)	65602
F(3)	F(4)	3.220(7)	65602	F(3)	F(5)	3.234(7)	65602
F(3)	F(9)	3.242(7)	65602	F(4)	C(1)	2.788(10)	1
F(4)	O(1)	2.961(8)	1	F(4)	F(8)	3.224(7)	64602
F(4)	F(6)	3.272(7)	64602	F(4)	F(11)	3.297(7)	64602
F(5)	F(8)	2.857(7)	64602	F(5)	C(3)	2.969(9)	64602
F(5)	O(4)	2.984(8)	64602	F(5)	C(4)	2.992(10)	64602
F(5)	O(3)	3.016(7)	64602	F(5)	F(7)	3.107(6)	4
F(5)	F(15)	3.126(7)	65504	F(6)	F(9)	2.871(7)	65602
F(6)	C(2)	2.971(9)	65602	F(6)	O(2)	2.994(7)	65602
F(6)	F(14)	3.003(7)	65504	F(6)	C(1)	3.087(9)	65602
F(6)	O(1)	3.131(8)	65602	F(6)	F(7)	3.318(6)	4
F(7)	O(2)	2.802(8)	65603	F(7)	O(3)	2.826(8)	66603
F(7)	F(13)	3.056(6)	65501	F(7)	F(15)	3.091(6)	65501

Table 7. Non-bonded Contacts out to 3.60 Å (continued)

atom	atom	distance	ADC	atom	atom	distance	ADC
F(7)	F(14)	3.336(6)	65501	F(8)	C(3)	2.592(10)	1
F(8)	O(3)	2.848(8)	1	F(8)	O(3)	3.071(8)	66603
F(9)	C(2)	2.686(10)	1	F(9)	O(2)	2.945(9)	1
F(9)	O(2)	3.281(8)	65603	F(10)	O(4)	2.764(7)	64602
F(10)	F(13)	2.960(6)	65501	F(10)	O(2)	2.968(8)	65603
F(10)	F(19)	3.147(8)	65504	F(11)	O(1)	2.861(7)	65602
F(11)	F(19)	2.943(8)	65504	F(11)	F(13)	3.107(7)	65501
F(11)	O(3)	3.138(8)	66603	F(11)	F(22)	3.319(8)	66603
F(12)	F(16)	3.055(6)	56603	F(12)	O(4)	3.300(7)	56603
F(13)	F(19)	2.931(6)	4	F(13)	F(20)	3.033(8)	55603
F(13)	F(22)	3.565(8)	56603	F(13)	F(18)	3.596(7)	4
F(14)	F(17)	2.944(7)	55603	F(14)	O(2)	3.003(8)	55603
F(14)	O(1)	3.035(7)	55603	F(14)	C(2)	3.076(9)	55603
F(14)	C(1)	3.141(9)	55603	F(15)	C(3)	2.858(9)	56603
F(15)	F(16)	2.921(7)	56603	F(15)	O(3)	2.921(7)	56603
F(15)	C(4)	2.991(9)	56603	F(15)	O(4)	3.040(7)	56603
F(16)	C(4)	2.727(10)	1	F(16)	O(4)	2.989(8)	1
F(16)	F(16)	3.055(9)	56603	F(16)	F(22)	3.125(7)	56603
F(16)	F(18)	3.535(6)	4	F(17)	C(1)	2.791(9)	1
F(17)	F(17)	2.957(9)	55603	F(17)	O(1)	3.162(8)	1
F(17)	F(20)	3.162(7)	55603	F(17)	C(2)	3.383(10)	1
F(18)	O(4)	2.834(7)	55404	F(18)	C(4)	2.848(9)	55404
F(18)	O(1)	2.889(8)	55404	F(18)	C(1)	2.889(9)	55404
F(18)	F(22)	3.583(8)	54502	F(19)	O(4)	3.168(10)	56603

Table 7. Non-bonded Contacts out to 3.60 $\AA$ (continued)

atom	atom	distance	ADC	atom	atom	distance	ADC
F(19)	O(1)	3.261(11)	55603	F(19)	F(22)	3.415(10)	54502
F(20)	O(1)	3.204(9)	55603	F(20)	F(22)	3.401(8)	54502
F(21)	C(3)	2.697(9)	1	F(21)	C(2)	2.771(10)	1
F(21)	O(3)	2.955(9)	1	F(21)	O(2)	3.068(9)	1
F(22)	O(1)	3.211(7)	55404	F(22)	O(4)	3.464(9)	56603

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,	1/2+y,	1/2-z
(3)	-x,	-y,	-z	(4)	x,	1/2-y,	1/2+z

Table 8. Least Squares Plane

Plane number 1

Atoms defining plane	Distance
Pt(1)	0.0000(2)
C(1)	0.023(9)
C(2)	-0.031(9)
C(3)	0.024(9)
C(4)	-0.032(9)

Additional Atoms	Distance
O(1)	-0.004
O(2)	-0.066
O(3)	0.009
O(4)	-0.100

Summary

plane	mean deviation	χ^2
1	0.0219	29.0