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Supporting Information

Table S1: Inter Ionic Contacts[a)] [Å] in $[M(CO)_4][Sb_2F_{11}]_2$, M = Pd, Pt

A) Reference contacts:	**Pt -- F**	**Pd -- F**	**C -- F**	**O -- F**	**F -- F**
Sum of $r_{v.d.Waals}$[167]	3.19	3.10	3.17	2.99	2.94
Significance limit	2.87	2.79	2.85	2.69	2.64

B) Observed Contacts for $[Pt(CO)_4][Sb_2F_{11}]_2$

Contacts to:	Pt:	F(17)	3.091(5)	F(21)	3.203(4)			
Contacts to:	C(1):	F(4)	2.788(10)	F(17)	2.791(9)	F(18)	2.889(9)	F(6) 3.087(9)
		F(14)	3.141(9)		$d(C\text{--}F)_{avg.}$ = 2.939			
	C(2):	F(9)	2.686(10)	F(21)	2.771(10)	F(16)	2.971(9)	F(14) 3.076(9)
		F(2)	3.256(9)		$d(C\text{--}F)_{avg.}$ = 2.876			
	C(3):	F(8)	2.592(10)	F(21)	2.697(9)	F(15)	2.858(9)	F(5) 2.969(9)
		F(2)	3.286(9)		$d(C\text{--}F)_{avg.}$ = 2.779			
	C(4):	F(16)	2.727(10)	F(3)	2.769(10)	F(18)	2.848(9)	F(15) 2.991(9)
		F(5)	2.992(10)		$d(C\text{--}F)_{avg.}$ = 2.865			

C) Observed Contacts for $[Pd(CO)_4][Sb_2F_{11}]_2$

Contacts to:	Pd:	F(3)	3.000(4)	F(4)	3.155(6)			
Contacts to:	C(1):	F(4)	2.695(7)	F(14)	2.763(7)	F(7)	2.868(7)	F(16) 3.003(7)
		F(5)	3.041(6)		$d(C\text{--}F)_{avg.}$ = 2.874			
	C(2):	F(3)	2.784(7)	F(15)	2.800(7)	F(7)	2.897(6)	F(17) 3.078(6)
		F(6)	3.157(6)		$d(C\text{--}F)_{avg.}$ = 2.936			
	C(3):	F(20)	2.681(8)	F(8)	2.776(7)	F(17)	2.997(6)	F(6) 3.056(6)
		F(3)	3.239(8)		$d(C\text{--}F)_{avg.}$ = 2.878			
	C(4):	F(19)	2.613(7)	F(8)	2.669(7)	F(5)	2.820(6)	F(16) 3.005(6)
		F(13)	3.286(7)		$d(C\text{--}F)_{avg.}$ = 2.776			

Table S2: Calculated and Experimental ^{13}C Isotope Shifts (cm^{-1}) for the D_{4h} Cations $[M(CO)_4]^{n+}$, M = Rh, Pd, Pt

Cations:			$[Rh(CO)_4]^+$		$[Pd(CO)_4]^{2+}$		$[Pt(CO)_4]^{2+}$	
Vibrational Modes			exp.[a]	BP86 ECP2	exp.[b]	BP86 ECP2	exp.[b]	BP86 ECP2
ν_1	A_{1g}	ν(CO)	52	52.4	52	53.1	54	54.0
ν_2	A_{1g}	ν(MC)		6.7	6	6.0	7	6.7
ν_3	A_{2g}	δ(MCO)		9.6		9.1		9.7
ν_4	A_{2u}	δ(MCO)		13.2	13	13.0	16	15.1
ν_5	A_{2u}	δ(CMC)		0.0		0.0		0.0
ν_6	B_{1g}	ν(CO)	50	50.2	52	51.7	53	52.5
ν_7	B_{1g}	ν(MC)		6.6		5.8		6.5
ν_8	B_{2g}	δ(MCO)		17.2		15.5		16.5
ν_9	B_{2g}	δ(CMC)		0.4		0.4		0.3
ν_{10}	B_{2u}	δ(MCO)		14.2		13.9		15.2
ν_{11}	B_{2u}	δ(CMC)		0.2		0.3		0.3
ν_{12}	E_g	δ(MCO)		9.5		8.9		9.5
ν_{13}	E_u	ν(CO)	47	47.6	50	50.5	52	50.4
ν_{14}	E_u	δ(MCO)		16.0	13	14.2	15	17.2
ν_{15}	E_u	ν(MC)		5.5	3	5.1	3	4.8
ν_{16}	E_u	δ(CMC)		0.2		0.2		0.2

[a] in HSO_3F; [b] $[M(CO)_4][Sb_2F_{11}]_2$

Table S3: Calculated and Experimental Vibrational Band Intensities for the D_{4h} Cations $[M(CO)_4]^{n+}$, M = Rh, Ir, Pd, Pt.

			$[Rh(CO)_4]^+$		$[Ir(CO)_4]^+$		$[Pd(CO)_4]^{2+}$		$[Pt(CO)_4]^{2+}$	
			exp.	BP86/ ECP2	exp.	BP86/ ECP2	exp.	BP86/ ECP2	exp.	BP86/ ECP2
IR intensities (km mol^{-1})										
ν_4	A_{2u}	δ[MCO]	m	3.4		7.6	m	18.5	s	27.7
ν_5	A_{2u}	δ[CMC]	-	0.5		0.0	-	0.0	-	0.8
ν_{13}	E_u	ν[CO]	vs	1677.2		1927.1	vs	324.6	vs	504.3
ν_{14}	E_u	δ[MCO]	s	129.5		89.6	m	95.2	s	91.5
ν_{15}	E_u	ν[MC]	s	81.7		129.6	w	6.4	w	48.5
ν_{16}	E_u	δ[CMC]	-	0.5		0.0	-	0.0	-	0.6
Raman intensities (Å^4 amu^{-1})										
ν_1	A_{1g}	ν[CO]	s	200.8		209.0	vs	178.6	vs	202.5
ν_2	A_{1g}	ν[MC]	w	18.7		21.8	w	13.1	w	11.4
ν_6	B_{1g}	ν[CO]	vs	286.8		290.8	s	165.1	s	196.8
ν_7	B_{1g}	ν[MC]	vw	1.3		2.6	vw	0.6	vw	0.6
ν_8	B_{2g}	δ[MCO]	-	0.1		0.0	vw	0.1	-	0.0
ν_9	B_{2g}	δ[CMC]	-	8.1		8.8	m	6.1	m	6.5
ν_{12}	E_g	δ[MCO]	-	0.3		0.5	-	0.5	vw	0.9

For Abbreviations see Table 7

Table S4: **Calculated Vibrational Frequencies (cm^{-1}) and ^{13}CO Shifts (cm^{-1}) for the Square Planar (D_{4h}) Cations $[M(CO)_4]^{n+}$, M = Co, Ir, Ni, Au, Hg**

			$[Co(CO)_4]^+$		$[Ir(CO)_4]^+$		$[Ni(CO)_4]^{2+}$		$[Au(CO)_4]^{3+}$		$[Hg(CO)_4]^{4+}$	
			BP86 ECP2	(^{13}CO shift)	BP86 ECP2	(^{13}CO shift)	BP86 ECP2	(^{13}CO shift)	BP86 ECP2	(^{13}CO shift)	BP86 ECP2	(^{13}CO shift)
ν_1	A_{1g}	ν(CO)	2181	(51.4)	2203	(53.3)	2244	(52.3)	2282	(53.6)	2231	(51.0)
ν_2	A_{1g}	ν(MC)	402	(6.4)	467	(7.3)	352	(5.8)	358	(5.8)	215	(3.6)
ν_3	A_{2g}	δ(MCO)	346	(10.6)	343	(10.3)	322	(9.3)	306	(9.1)	278	(8.2)
ν_4	A_{2u}	δ(MCO)	434	(12.3)	486	(15.4)	437	(12.1)	414	(13.5)	331	(10.6)
ν_5	A_{2u}	δ(CMC)	32	(0.0)	53	(0.0)	94	(0.0)	91	(0.1)	82	(0.1)
ν_6	B_{1g}	ν(CO)	2138	(49.9)	2151	(51.0)	2229	(51.7)	2271	(52.8)	2228	(50.8)
ν_7	B_{1g}	ν(MC)	409	(6.7)	449	(7.2)	351	(5.8)	335	(5.5)	185	(3.1)
ν_8	B_{2g}	δ(MCO)	537	(19.6)	496	(17.7)	478	(17.3)	410	(14.6)	329	(11.3)
ν_9	B_{2g}	δ(CMC)	98	(0.3)	96	(0.4)	97	(0.3)	93	(0.4)	85	(0.4)
ν_{10}	B_{2u}	δ(MCO)	417	(13.6)	465	(15.4)	400	(13.5)	399	(13.8)	327	(10.9)
ν_{11}	B_{2u}	δ(CMC)	9	(0.0)	18	(0.1)	52	(0.3)	64	(0.3)	52	(0.3)
ν_{12}	E_g	δ(MCO)	320	(9.8)	338	(10.2)	305	(9.2)	295	(8.8)	265	(7.8)
ν_{13}	E_u	ν(CO)	2103	(47.3)	2114	(47.8)	2214	(50.3)	2263	(52.1)	2227	(51.0)
ν_{14}	E_u	δ(MCO)	590	(13.7)	560	(18.6)	516	(11.4)	444	(14.9)	345	(11.6)
ν_{15}	E_u	ν(MC)	406	(7.7)	369	(5.4)	370	(7.3)	331	(4.6)	260	(3.4)
ν_{16}	E_u	δ(CMC)	94	(0.3)	88	(0.3)	100	(0.3)	97	(0.2)	85	(0.2)

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Table S5: Calculated Vibrational Band Intensities for the Square Planar (D_{4h}) Cations $[M(CO)_4]^{n+}$ (M = Co, Ni, Au).

			$[Co(CO)_4]^+$		$[Ni(CO)_4]^{2+}$		$[Au(CO)_4]^{3+}$		$[Hg(CO)_4]^{3+}$	
			BP86	ECP2	BP86	ECP2	BP86	ECP2	BP86	ECP2
IR intensities (km mol^{-1})										
ν_4	A_{2u}	δ(MCO)	0.8		14.1		37.2		41.0	
ν_5	A_{2u}	δ(CMC)	3.0		1.4		3.0		8.4	
ν_{13}	E_u	ν(CO)	1736.3		304.4		10.3		79.7	
ν_{14}	E_u	δ(MCO)	169.7		101.4		81.1		61.1	
ν_{15}	E_u	ν(MC)	61.3		0.3		7.2		53.7	
ν_{16}	E_u	δ(CMC)	1.9		0.4		2.4		5.5	
Raman intensities (Å^4 amu^{-1})										
ν_1	A_{1g}	ν(CO)	179.7		192.7		116.2		n.c.	
ν_2	A_{1g}	ν(MC)	19.2		9.5		33.3		n.c.	
ν_6	B_{1g}	ν(CO)	259.9		148.0		87.5		n.c.	
ν_7	B_{1g}	ν(MC)	3.3		1.3		9.9		n.c.	
ν_8	B_{2g}	δ(MCO)	0.2		0.1		0.3		n.c.	
ν_9	B_{2g}	δ(CMC)	7.9		5.6		6.4		n.c.	
ν_{12}	E_g	δ(MCO)	0.6		0.5		0.5		n.c.	

n.c. = not calculated

Table S6: **Calculated Vibrational Frequencies (cm^{-1}) at BP86/ECP1 for the Square Planar (D_{4h}) Cations $[M(CO)_4]^{n+}$, M = Co, Rh, Ir, Ni, Pd, Pt, Au, Hg.**

			$[Co(CO)_4]^+$	$[Rh(CO)_4]^+$	$[Ir(CO)_4]^+$	$[Ni(CO)_4]^{2+}$	$[Pd(CO)_4]^{2+}$	$[Pt(CO)_4]^{2+}$	$[Au(CO)_4]^{3+}$	$[Hg(CO)_4]^{4+}$
ν_1	A_{1g}	ν(CO)	2183	2197	2200	2241	2252	2259	2275	2219
ν_2	A_{1g}	ν(MC)	400	424	467	344	372	422	355	198
ν_3	A_{2g}	δ(MCO)	340	316	341	320	302	326	312	285
ν_4	A_{2u}	δ(MCO)	438	443	491	437	431	477	426	334
ν_5	A_{2u}	δ(CMC)	43	58	56	95	88	86	94	82
ν_6	B_{1g}	ν(CO)	2142	2149	2150	2227	2230	2231	2265	2216
ν_7	B_{1g}	ν(MC)	406	402	448	340	345	396	331	161
ν_8	B_{2g}	δ(MCO)	531	482	500	473	433	467	415	331
ν_9	B_{2g}	δ(CMC)	100	92	98	100	91	99	97	87
ν_{10}	B_{2u}	δ(MCO)	421	434	470	402	413	452	410	332
ν_{11}	B_{2u}	δ(CMC)	2	29	16	51	56	57	65	51
ν_{12}	E_g	δ(MCO)	316	315	340	305	299	325	306	275
ν_{13}	E_u	ν(CO)	2108	2119	2112	2212	2216	2209	2256	2217
ν_{14}	E_u	δ(MCO)	588	544	562	509	481	515	449	345
ν_{15}	E_u	ν(MC)	399	352	365	360	329	334	328	248
ν_{16}	E_u	δ(CMC)	96	89	91	103	95	98	100	86

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Fig. S1: Dimensions and Design of a Monel-Kel-F™ Reactor Used for Solution in $HF-SbF_5$

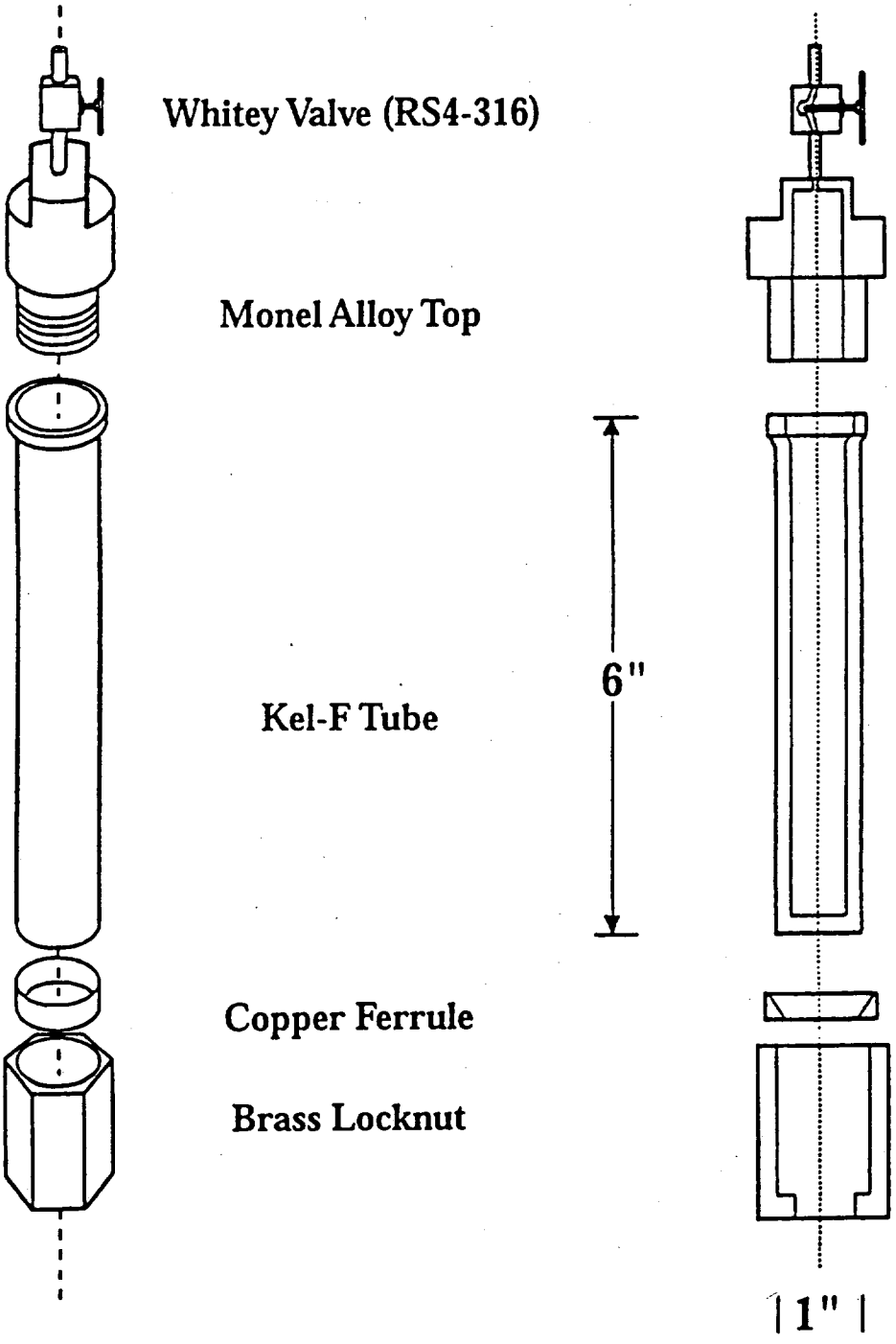

Fig. S2: A Stereoview of the Unit Cells of $[M(CO)_4][Sb_2F_{11}]_2$, M = Pd, Pt.

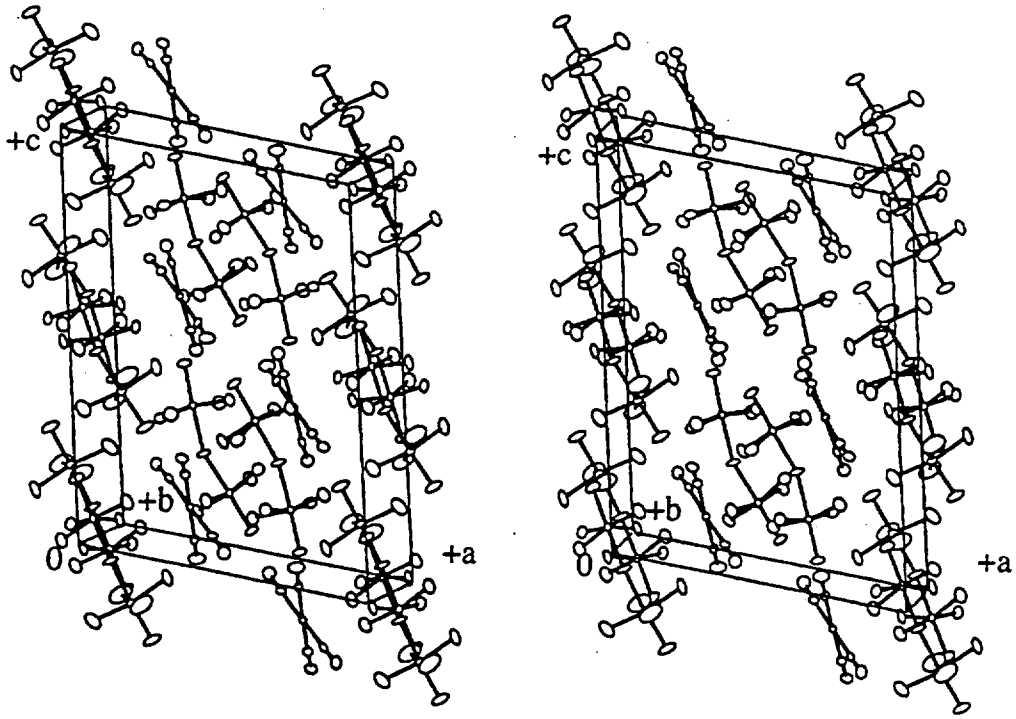

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Fig. S3: The Molecular Structure of $[Pd(CO)_4][Sb_2F_{11}]_2$ Showing One Formula Unit.

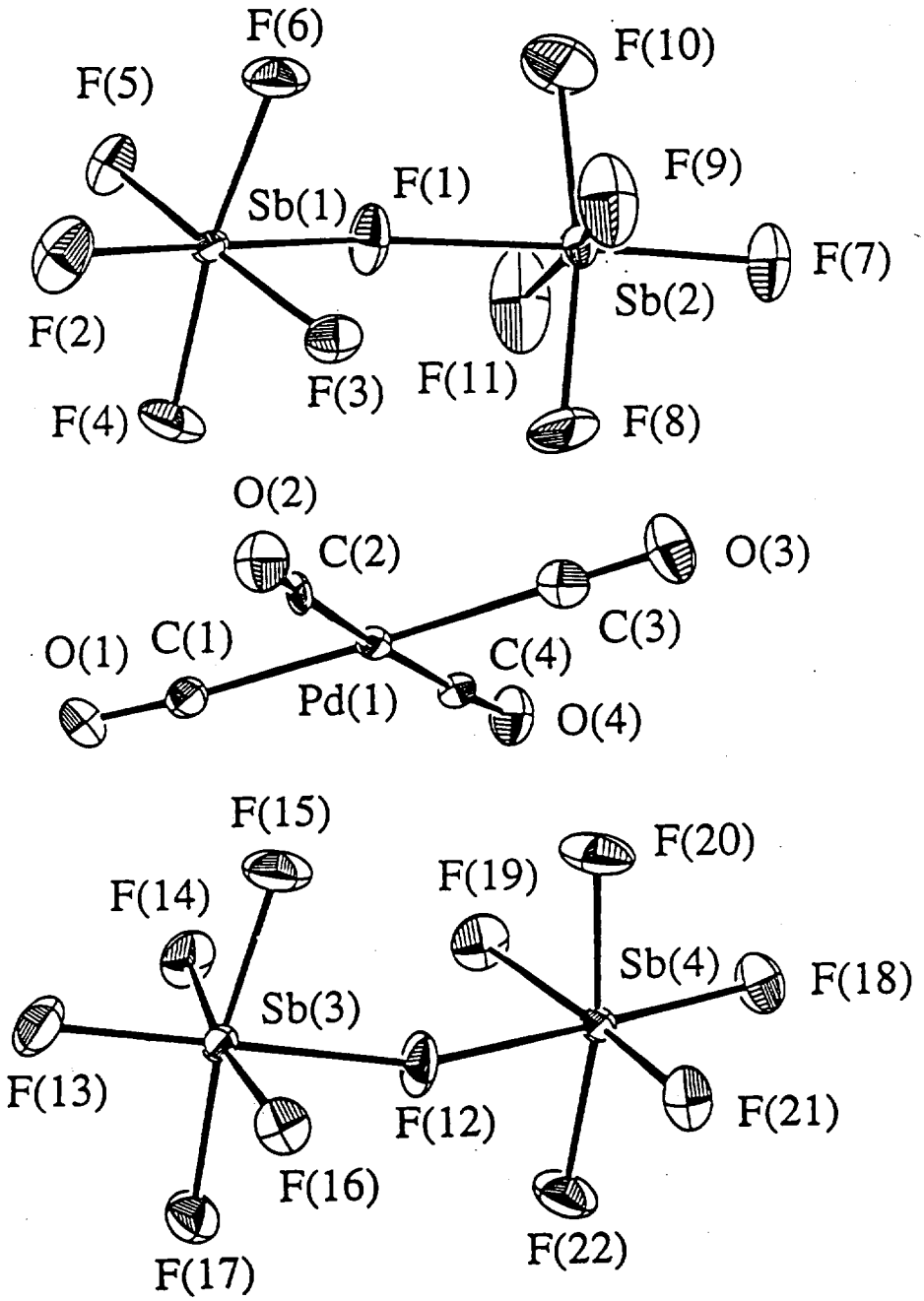
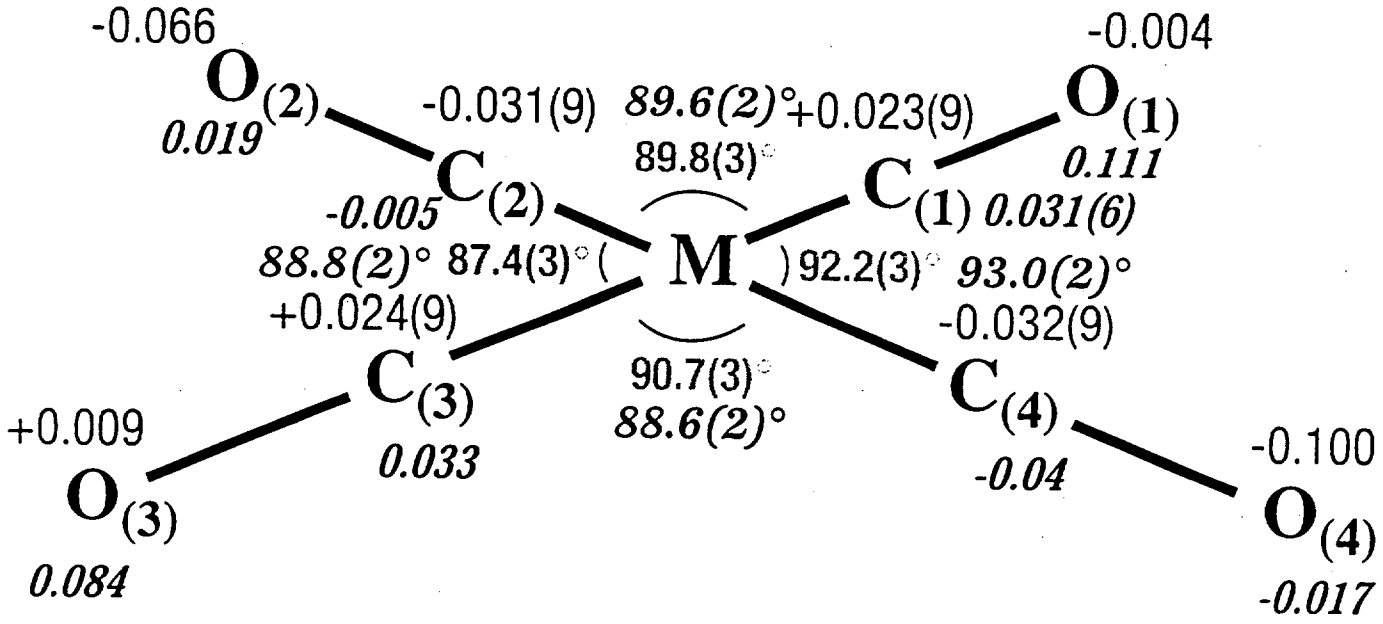


Fig. S4: The $[M(CO)_4]^{2+}$ Cations, M = Pd, Pt - Displacement from Planarity, Bond Parameters and Vibrational Wavenumbers in the CO Stretching Region.



Displacement from plane defined by $M_{(1)}$ and $C_{(1)}$ to $C_{(4)}$ in Å

Data for $[Pt(CO)_4]^{2+}$ are in bold italic

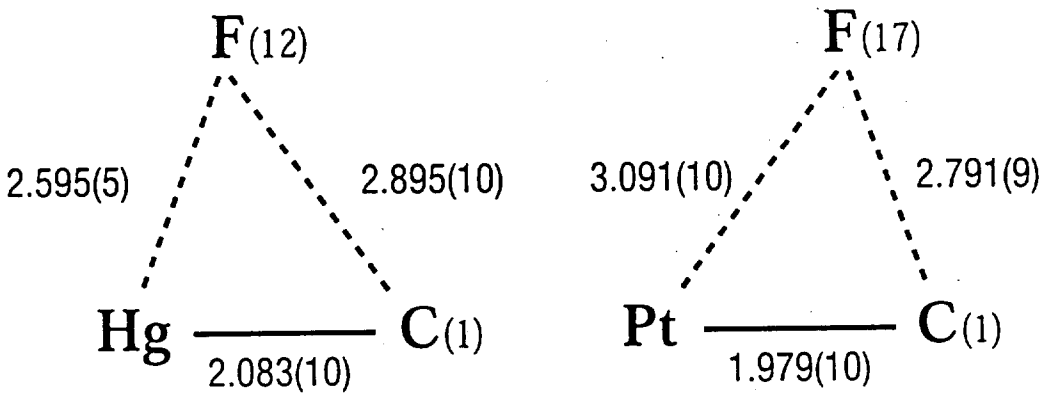
Bond distances in Å

Pt – C	1.979(9) to 1.987(9)	avg 1.982(9)
C – O	1.086(9) to 1.118(9)	avg 1.110(9)
Pd – C	1.984(6) to 2.006(6)	avg 1.992(6)
C – O	1.111(6) to 1.111(7)	avg 1.106(7)

Bond angles in °

Pt – C – O	176.4(7) – 178.1(7)
Pd – C – O	176.1(5) – 177.0(5)

Fig. S5: Selected Bifurcated Inter Ionic Contacts for $[Hg(CO)_2][Sb_2F_{11}]_2$ and $[Pt(CO)_4][Sb_2F_{11}]_2$.



Sum of v.d. Waals radii : Hg--F 3.02 Å; Pt--F 3.19 Å

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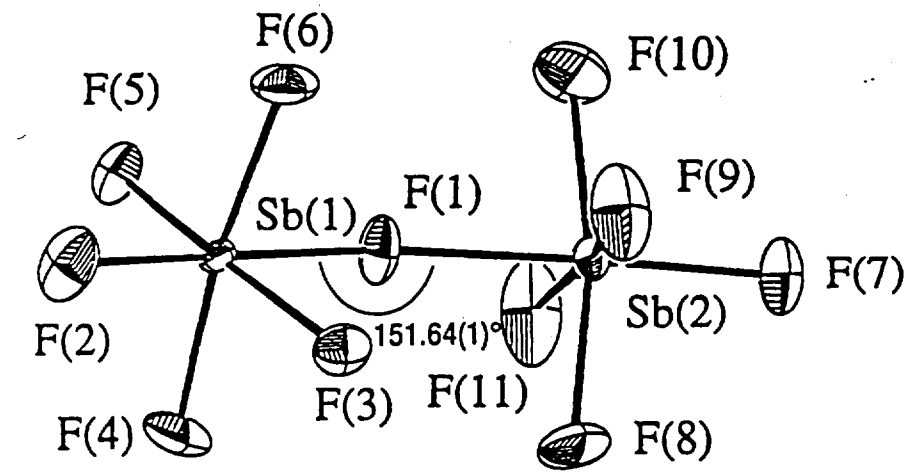
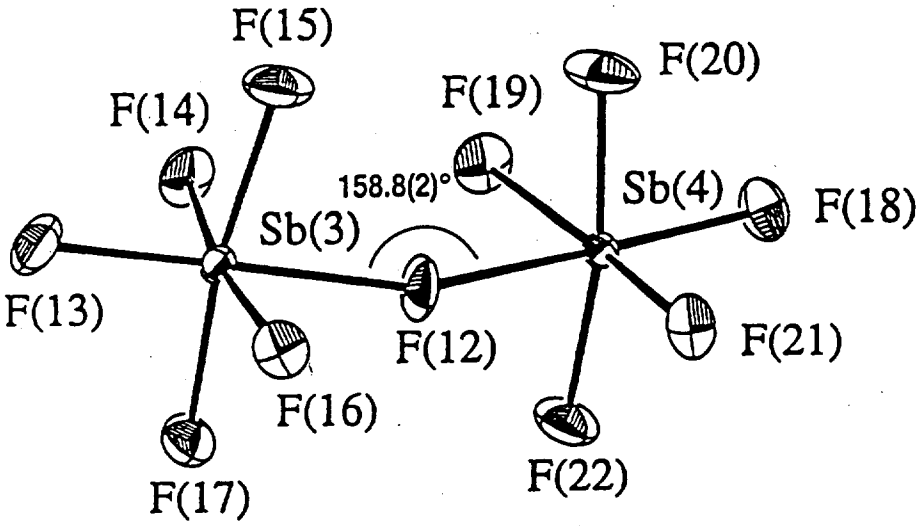
Fig. S6: The $[Sb_2F_{11}]^-$ Anions in $[Pd(CO)_4][Sb_2F_{11}]_2$.



C_1 conformer
dihedral angle: 38°



C_{2v} conformer
dihedral angle: 9°

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Table S1: Calculated Vibrational Frequencies (cm^{-1}) and ^{13}CO Shifts (cm^{-1}) for the square Planar (D_{4h}) Cations $[M(CO)_4]^{n+}$, M = Co, Ni, Au, Hg.

Table S2: Calculated Vibrational Band Intensities for the Square Planar (D_{4h}) Cations $[M(CO)_4]^{n+}$ (M = Co, Ni, Au).

Table S3: Calculated Vibrational Frequencies (cm^{-1}) at BP86/ECP1 for the Square Planar (D_{4h}) Cations $[M(CO)_4]^{n+}$, M = Co, Rh, Ir, Ni, Pd, Pt, Au, Hg.

Figure S1: Dimensions and Design of a Monel™-Kel-F™ Reactor Used for Solution in $HF-SbF_5$.

Figure S2: The Molecular Structure of $[Pd(CO)_4][Sb_2F_{11}]_2$ Showing One Formula Unit.

Attached: X-Ray Crystallographic Structure Report for the Complex Salts $[Pd(CO)_4][Sb_2F_{11}]_2$ and $[Pt(CO)_4][Sb_2F_{11}]_2$.

Table S1: **Calculated Vibrational Frequencies (cm^{-1}) and ^{13}CO Shifts (cm^{-1}) for the Square Planar (D_{4h}) Cations $[M(CO)_4]^{n+}$, M = Co, Ni, Au, Hg**

			$[Co(CO)_4]^+$		$[Ni(CO)_4]^{2+}$		$[Au(CO)_4]^{3+}$		$[Hg(CO)_4]^{4+}$	
			BP86 ECP2	(^{13}CO shift)	BP86 ECP2	(^{13}CO shift)	BP86 ECP2	(^{13}CO shift)	BP86 ECP2	(^{13}CO shift)
ν_1	A_{1g}	ν(CO)	2181	(51.4)	2244	(52.3)	2282	(53.6)	2231	(51.0)
ν_2	A_{1g}	ν(MC)	402	(6.4)	352	(5.8)	358	(5.8)	215	(3.6)
ν_3	A_{2g}	δ(MCO)	346	(10.6)	322	(9.3)	306	(9.1)	278	(8.2)
ν_4	A_{2u}	δ(MCO)	434	(12.3)	437	(12.1)	414	(13.5)	331	(10.6)
ν_5	A_{2u}	δ(CMC)	32	(0.0)	94	(0.0)	91	(0.1)	82	(0.1)
ν_6	B_{1g}	ν(CO)	2138	(49.9)	2229	(51.7)	2271	(52.8)	2228	(50.8)
ν_7	B_{1g}	ν(MC)	409	(6.7)	351	(5.8)	335	(5.5)	185	(3.1)
ν_8	B_{2g}	δ(MCO)	537	(19.6)	478	(17.3)	410	(14.6)	329	(11.3)
ν_9	B_{2g}	δ(CMC)	98	(0.3)	97	(0.3)	93	(0.4)	85	(0.4)
ν_{10}	B_{2u}	δ(MCO)	417	(13.6)	400	(13.5)	399	(13.8)	327	(10.9)
ν_{11}	B_{2u}	δ(CMC)	9	(0.0)	52	(0.3)	64	(0.3)	52	(0.3)
ν_{12}	E_g	δ(MCO)	320	(9.8)	305	(9.2)	295	(8.8)	265	(7.8)
ν_{13}	E_u	ν(CO)	2103	(47.3)	2214	(50.3)	2263	(52.1)	2227	(51.0)
ν_{14}	E_u	δ(MCO)	590	(13.7)	516	(11.4)	444	(14.9)	345	(11.6)
ν_{15}	E_u	ν(MC)	406	(7.7)	370	(7.3)	331	(4.6)	260	(3.4)
ν_{16}	E_u	δ(CMC)	94	(0.3)	100	(0.3)	97	(0.2)	85	(0.2)

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Table S2: Calculated Vibrational Band Intensities for the Square Planar (D_{4h}) Cations $[M(CO)_4]^{n+}$ (M = Co, Ni, Au).

			$[Co(CO)_4]^+$		$[Ni(CO)_4]^{2+}$		$[Au(CO)_4]^{3+}$		$[Hg(CO)_4]^{3+}$	
			BP86	ECP2	BP86	ECP2	BP86	ECP2	BP86	ECP2
IR intensities (km mol^{-1})										
ν_4	A_{2u}	δ(MCO)	0.8		14.1		37.2		41.0	
ν_5	A_{2u}	δ(CMC)	3.0		1.4		3.0		8.4	
ν_{13}	E_u	ν(CO)	1736.3		304.4		10.3		79.7	
ν_{14}	E_u	δ(MCO)	169.7		101.4		81.1		61.1	
ν_{15}	E_u	ν(MC)	61.3		0.3		7.2		53.7	
ν_{16}	E_u	δ(CMC)	1.9		0.4		2.4		5.5	
Raman intensities (Å^4 amu^{-1})										
ν_1	A_{1g}	ν(CO)	179.7		192.7		116.2		n.c.	
ν_2	A_{1g}	ν(MC)	19.2		9.5		33.3		n.c.	
ν_6	B_{1g}	ν(CO)	259.9		148.0		87.5		n.c.	
ν_7	B_{1g}	ν(MC)	3.3		1.3		9.9		n.c.	
ν_8	B_{2g}	δ(MCO)	0.2		0.1		0.3		n.c.	
ν_9	B_{2g}	δ(CMC)	7.9		5.6		6.4		n.c.	
ν_{12}	E_g	δ(MCO)	0.6		0.5		0.5		n.c.	

n.c. = not calculated

Table S3: Calculated Vibrational Frequencies (cm^{-1}) at BP86/ECP1 for the Square Planar (D_{4h}) Cations $[M(CO)_4]^{n+}$, M = Co, Rh, Ir, Ni, Pd, Pt, Au, Hg.

			$[Co(CO)_4]^+$	$[Rh(CO)_4]^+$	$[Ir(CO)_4]^+$	$[Ni(CO)_4]^{2+}$	$[Pd(CO)_4]^{2+}$	$[Pt(CO)_4]^{2+}$	$[Au(CO)_4]^{3+}$	$[Hg(CO)_4]^{4+}$
ν_1	A_{1g}	ν(CO)	2183	2197	2200	2241	2252	2259	2275	2219
ν_2	A_{1g}	ν(MC)	400	424	467	344	372	422	355	198
ν_3	A_{2g}	δ(MCO)	340	316	341	320	302	326	312	285
ν_4	A_{2u}	δ(MCO)	438	443	491	437	431	477	426	334
ν_5	A_{2u}	δ(CMC)	43	58	56	95	88	86	94	82
ν_6	B_{1g}	ν(CO)	2142	2149	2150	2227	2230	2231	2265	2216
ν_7	B_{1g}	ν(MC)	406	402	448	340	345	396	331	161
ν_8	B_{2g}	δ(MCO)	531	482	500	473	433	467	415	331
ν_9	B_{2g}	δ(CMC)	100	92	98	100	91	99	97	87
ν_{10}	B_{2u}	δ(MCO)	421	434	470	402	413	452	410	332
ν_{11}	B_{2u}	δ(CMC)	2	29	16	51	56	57	65	51
ν_{12}	E_g	δ(MCO)	316	315	340	305	299	325	306	275
ν_{13}	E_u	ν(CO)	2108	2119	2112	2212	2216	2209	2256	2217
ν_{14}	E_u	δ(MCO)	588	544	562	509	481	515	449	345
ν_{15}	E_u	ν(MC)	399	352	365	360	329	334	328	248
ν_{16}	E_u	δ(CMC)	96	89	91	103	95	98	100	86

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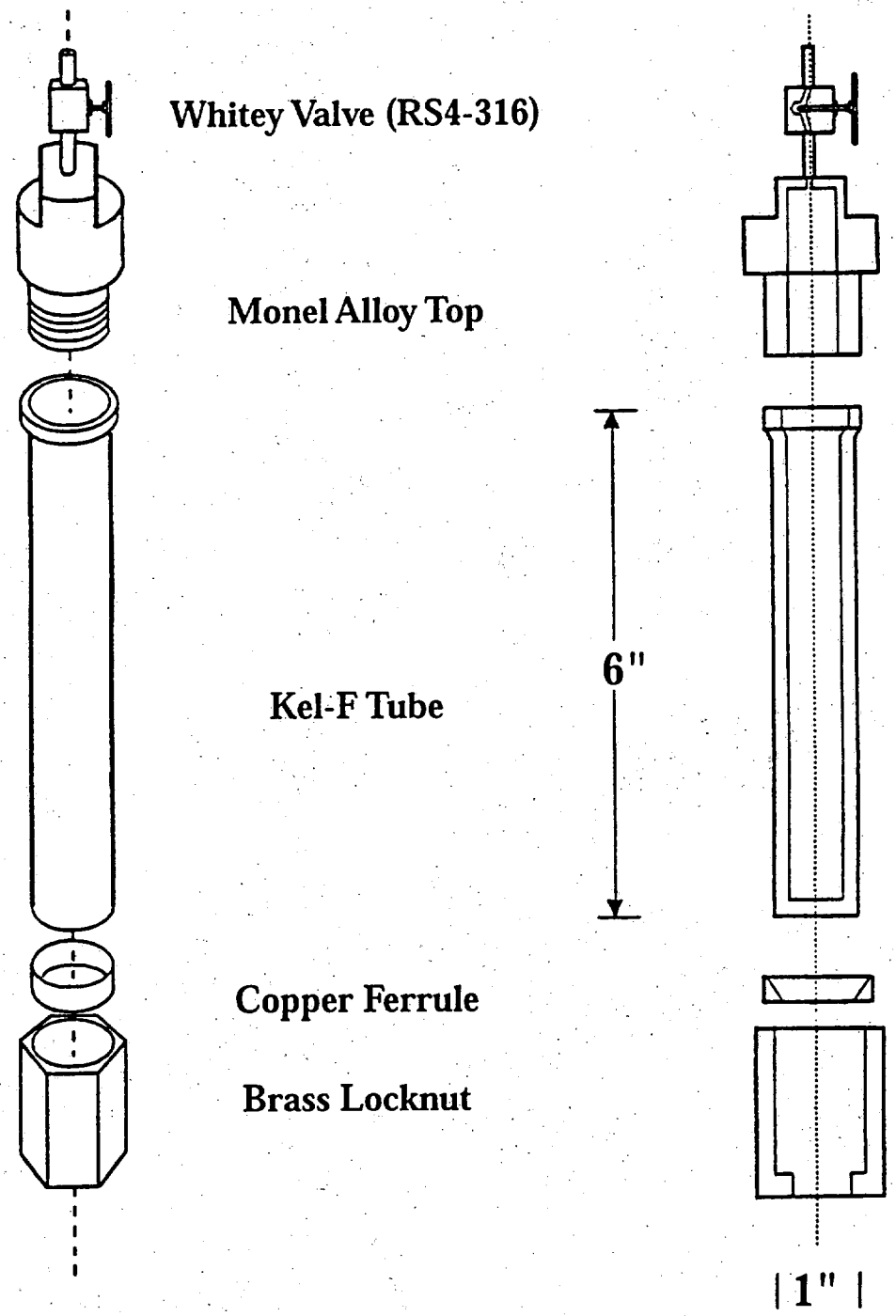
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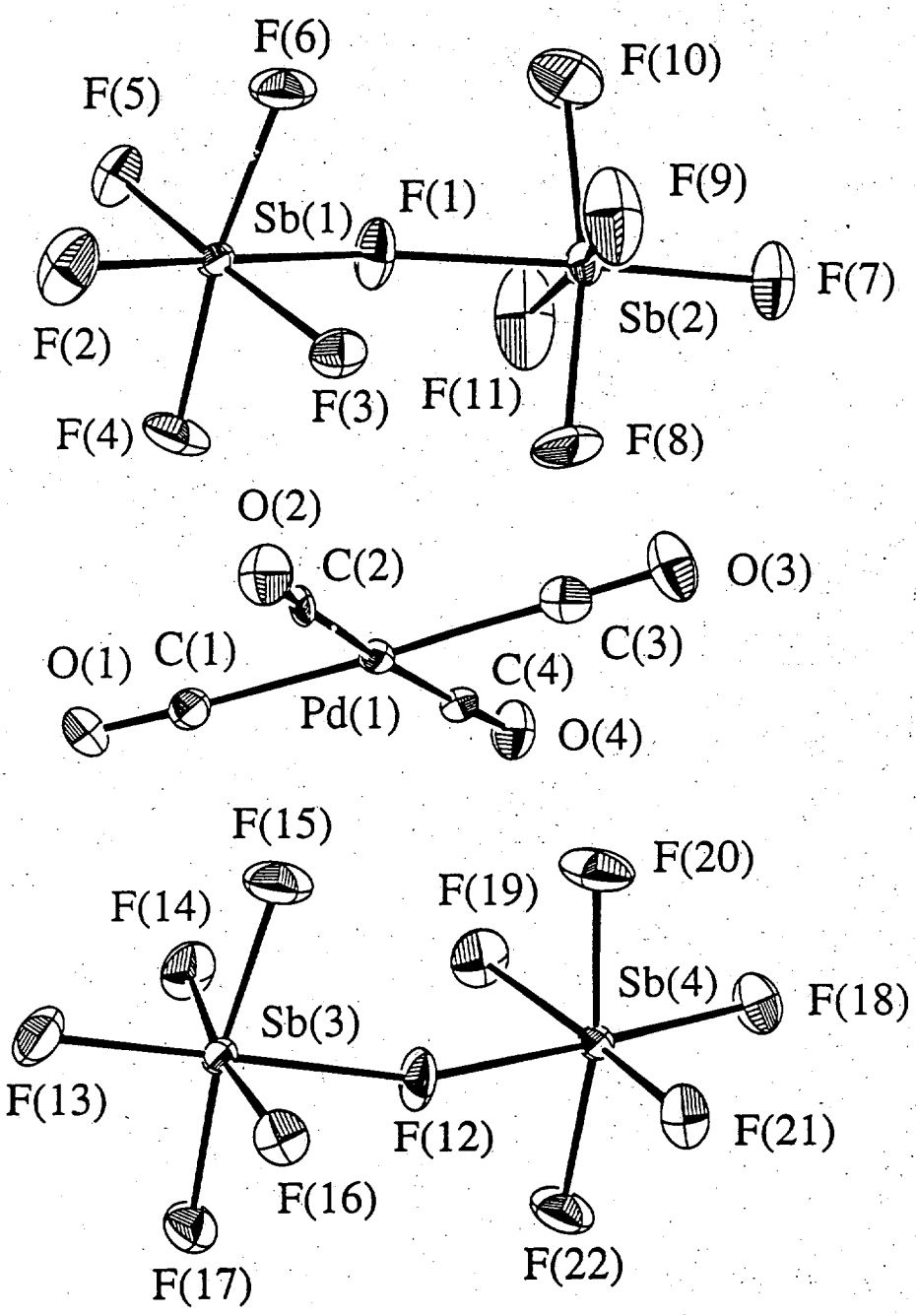
Kel-F Tube
Copper Ferrule
Brass Locknut
1"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Sb(4)
F(18)
Sb(3)
F(13)
F(12)
F(21)
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F(22)
F(17)

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Sample: fa124/[Pt(CO)$_4$][Sb$_2$F$_{11}$]$_2$

P.O. # Charge: $175

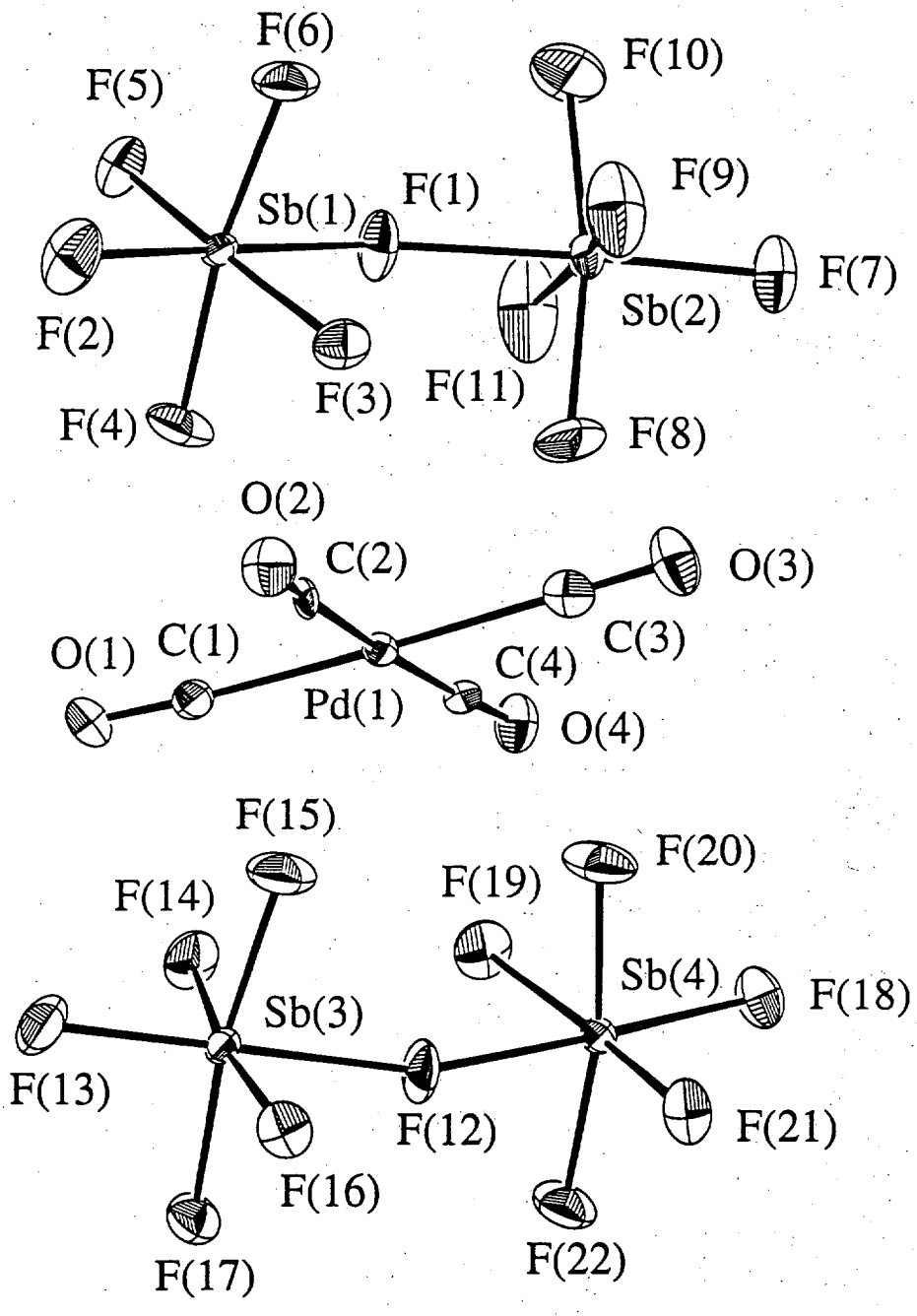
X-ray Structure Report

for

Prof. F. Aubke

UBC Chemistry

Fri Jun 12 1998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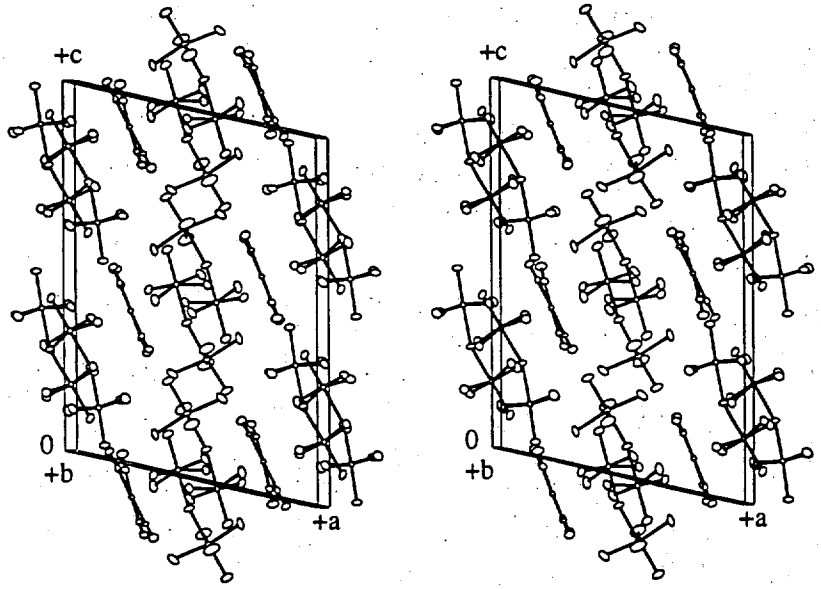
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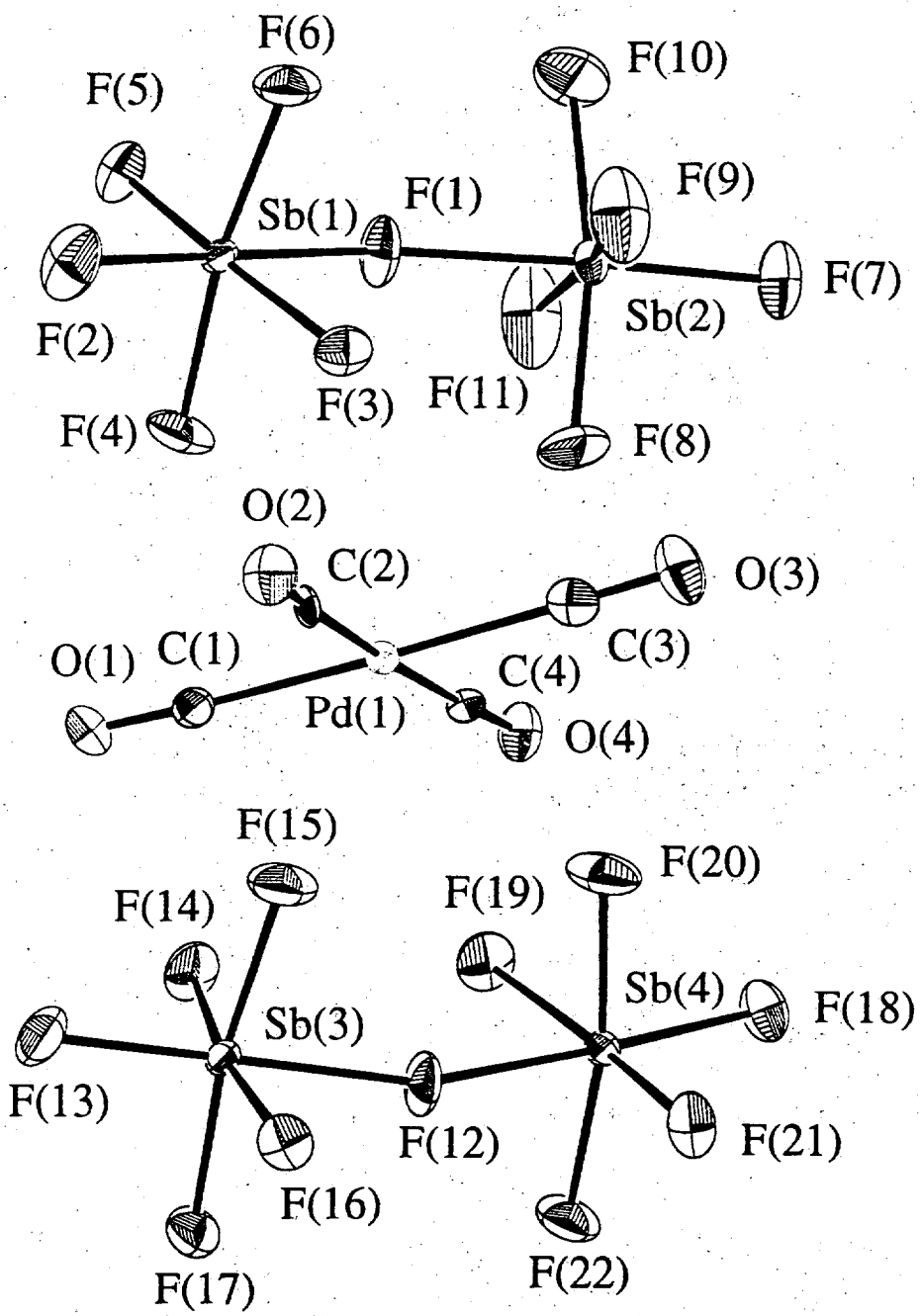
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F(4)
F(8)
O(2)
C(2)
O(3)
O(1)
C(1)
C(4)
C(3)
Pd(1)
O(4)
F(15)
F(14)
F(20)
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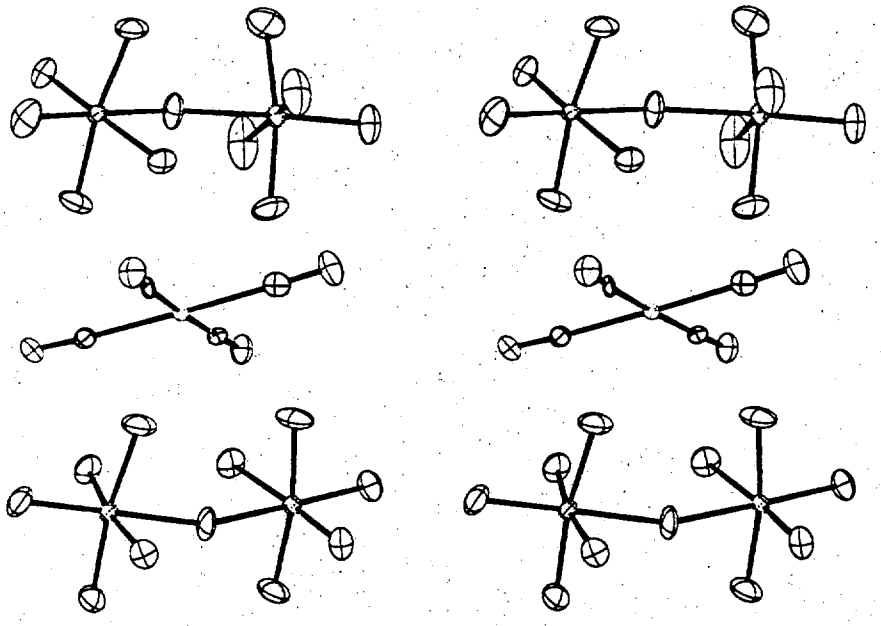
F(22)



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Experimental

Data Collection

A colorless prism crystal of $C_4F_{22}O_4PdSb_4$ having approximate dimensions of 0.30 x 0.30 x 0.40 mm was mounted on a glass fiber. All measurements were made on a Rigaku/ADSC CCD area detector with graphite monochromated Mo-Kα radiation.

Cell constants based on 11367 reflections with 2θ = 4.0-60.0° corresponded to a primitive monoclinic cell with dimensions:

a = 12.583(2) $\AA$
b = 9.8172(9) $\AA$ β = 103.1183(10)°
c = 17.9895(9) $\AA$
V = 2164.2(4) $\AA^3$

For Z = 4 and F.W. = 1123.41, the calculated density is 3.45 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 60.0°. Data were collected in 0.50° oscillations with 14.0 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 39.24(1) mm . The detector swing angle was -10.0°.

Data Reduction

Of the 19815 reflections which were collected, 5593 were unique (R_{int} = 0.033); equivalent reflections were merged.

The linear absorption coefficient, μ, for Mo-Kα radiation is 59.4 cm^{-1}. The data were corrected for Lorentz and polarization effects.

Structure Solution and Refinement

The structure was solved by heavy-atom Patterson methods[1] and expanded using Fourier techniques[2]. All atoms were refined anisotropically. The final cycle of full-matrix least-squares refinement[3] was based on all 5593 unique reflections and 316 variable parameters and converged (largest parameter shift was 0.001 times its esd) with unweighted and weighted agreement factors of:

$$R = \Sigma||Fo^2| - |Fc^2||/\Sigma|Fo^2| = 0.056$$

$$R_w = \sqrt{(\Sigma w(|Fo^2| - |Fc^2|)^2/\Sigma wFo^4)} = 0.047$$

The standard deviation of an observation of unit weight[4] was 1.12. 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, $\sin\theta/\lambda$ and various classes of indices showed no unusual trends. The maximum and minimum peaks on the final difference Fourier map corresponded to 1.58 and -2.07 $e^-/\AA^3$, respectively.

Neutral atom scattering factors were taken from Cromer and Waber[5] . Anomalous dispersion effects were included in Fcalc[6]; the values for $\Delta f'$ and $\Delta f''$ 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) 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: $\Sigma w(|Fo^2| - |Fc^2|)^2$

(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).

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(9) teXsan: Crystal Structure Analysis Package, Molecular Structure Corporation (1985 & 1992).

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EXPERIMENTAL DETAILS

A. Crystal Data

Empirical Formula	$C_4F_{22}O_4PdSb_4$
Formula Weight	1123.41
Crystal Color, Habit	colorless, prism
Crystal Dimensions	0.30 X 0.30 X 0.40 mm
Crystal System	monoclinic
Lattice Type	Primitive
Lattice Parameters	a = 12.583(2)Å b = 9.8172(9) Å c = 17.9895(9) Å β = 103.1183(10)°
	V = 2164.2(4) Å^3
Space Group	$P2_1/c$ (#14)
Z value	4
D_{calc}	3.448 g/cm^3
F_{000}	2016.00
μ(MoKα)	59.35 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 14.0 seconds
ϕ oscillation Range (χ=-90)	0.0 - 190.0°

ω oscillation Range (χ=-90)	-23.0 - 18.0°
Detector Position	39.24(1) mm
Detector Swing Angle	-10.0°
$2\theta_{max}$	60.0°
No. of Reflections Measured	Total: 19815 Unique: 5593 (R_{int} = 0.033)
Corrections	Lorentz-polarization Absorption/decay/scaling (trans. factors: 0.6438 - 1.0000)

C. Structure Solution and Refinement

Structure Solution	Patterson Methods (DIRDIF92 PATTY)
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	5593
No. Variables	316
Reflection/Parameter Ratio	17.70
Residuals (on F^2, all data): R; Rw	0.056 ; 0.047
Goodness of Fit Indicator	1.12
No. Observations (I>3σ(I))	3107
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	1.58 $e^-/\AA^3$ (1.2 $\AA$ from F(7))
Minimum peak in Final Diff. Map	-2.07 $e^-/\AA^3$

Table S2. Atomic coordinates and B_{eq}

atom	x	y	z	B_{eq}
Sb(1)	0.56651(3)	0.24150(3)	0.48533(2)	1.054(6)
Sb(2)	0.44699(3)	0.24417(4)	0.66883(2)	1.455(7)
Sb(3)	-0.01059(3)	0.23994(4)	0.17534(2)	1.156(6)
Sb(4)	-0.12203(3)	0.25510(3)	0.36516(2)	1.033(6)
Pd(1)	0.22813(3)	0.24175(4)	0.41137(2)	0.973(7)
F(1)	0.5244(3)	0.1977(3)	0.5833(2)	2.37(8)
F(2)	0.6042(3)	0.2807(3)	0.3949(2)	3.27(9)
F(3)	0.4497(3)	0.3651(3)	0.4687(2)	2.06(8)
F(4)	0.4632(3)	0.1114(3)	0.4416(2)	2.53(8)
F(5)	0.6690(3)	0.1032(3)	0.5155(2)	2.16(8)
F(6)	0.6576(3)	0.3696(3)	0.5422(2)	2.70(9)
F(7)	0.3723(3)	0.2827(3)	0.7442(2)	3.39(9)
F(8)	0.3205(3)	0.2313(4)	0.5929(2)	3.92(9)
F(9)	0.4567(4)	0.4229(3)	0.6413(2)	4.16(11)
F(10)	0.5858(3)	0.2522(5)	0.7294(2)	4.86(10)
F(11)	0.4427(4)	0.0593(3)	0.6815(2)	4.49(11)
F(12)	-0.0925(3)	0.2613(4)	0.25877(15)	2.49(7)
F(13)	0.0627(3)	0.2230(3)	0.0981(2)	2.81(8)
F(14)	0.0722(3)	0.1087(3)	0.2377(2)	2.42(9)
F(15)	0.0853(3)	0.3682(3)	0.2293(2)	3.01(9)
F(16)	-0.1018(3)	0.3762(3)	0.1274(2)	2.05(8)
F(17)	-0.1150(3)	0.1096(3)	0.1370(2)	2.20(8)
F(18)	-0.1440(3)	0.2495(3)	0.46352(14)	2.17(6)
F(19)	-0.0126(3)	0.1221(3)	0.3854(2)	2.47(9)

Table S2. Atomic coordinates and B_{eq} (continued)

atom	x	y	z	B_{eq}
F(20)	-0.0072(3)	0.3803(3)	0.3914(2)	2.90(10)
F(21)	-0.2164(3)	0.3979(3)	0.3318(2)	2.14(8)
F(22)	-0.2227(3)	0.1219(3)	0.3268(2)	2.71(9)
O(1)	0.2867(4)	-0.0001(3)	0.3174(2)	1.96(9)
O(2)	0.3032(4)	0.4634(4)	0.3113(3)	2.28(10)
O(3)	0.1800(4)	0.4693(3)	0.5178(3)	2.55(11)
O(4)	0.1490(4)	0.0410(3)	0.5199(2)	1.97(10)
C(1)	0.2632(5)	0.0879(5)	0.3489(3)	1.42(12)
C(2)	0.2760(5)	0.3826(5)	0.3450(3)	1.23(12)
C(3)	0.1964(5)	0.3908(5)	0.4779(4)	1.61(13)
C(4)	0.1787(5)	0.1092(5)	0.4796(4)	1.36(12)

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

Table S3. Bond Lengths(Å)

atom	atom	distance	atom	atom	distance
Sb(1)	F(1)	2.000(3)	Sb(1)	F(2)	1.835(3)
Sb(1)	F(3)	1.877(3)	Sb(1)	F(4)	1.864(3)
Sb(1)	F(5)	1.866(3)	Sb(1)	F(6)	1.846(3)
Sb(2)	F(1)	2.049(3)	Sb(2)	F(7)	1.855(3)
Sb(2)	F(8)	1.851(3)	Sb(2)	F(9)	1.835(3)
Sb(2)	F(10)	1.839(4)	Sb(2)	F(11)	1.831(3)
Sb(3)	F(12)	2.015(3)	Sb(3)	F(13)	1.841(3)
Sb(3)	F(14)	1.864(3)	Sb(3)	F(15)	1.858(3)
Sb(3)	F(16)	1.844(3)	Sb(3)	F(17)	1.851(3)
Sb(4)	F(12)	2.032(3)	Sb(4)	F(18)	1.853(3)
Sb(4)	F(19)	1.873(3)	Sb(4)	F(20)	1.874(3)
Sb(4)	F(21)	1.847(3)	Sb(4)	F(22)	1.843(3)
Pd(1)	C(1)	1.991(6)	Pd(1)	C(2)	2.006(6)
Pd(1)	C(3)	1.987(6)	Pd(1)	C(4)	1.984(6)
O(1)	C(1)	1.110(6)	O(2)	C(2)	1.100(6)
O(3)	C(3)	1.105(6)	O(4)	C(4)	1.111(7)

Table S4. Bond Angles(°)

atom	atom	atom	angle	atom	atom	atom	angle
F(1)	Sb(1)	F(2)	179.49(15)	F(1)	Sb(1)	F(3)	85.69(14)
F(1)	Sb(1)	F(4)	85.74(15)	F(1)	Sb(1)	F(5)	83.76(13)
F(1)	Sb(1)	F(6)	85.05(15)	F(2)	Sb(1)	F(3)	94.22(15)
F(2)	Sb(1)	F(4)	93.8(2)	F(2)	Sb(1)	F(5)	96.30(15)
F(2)	Sb(1)	F(6)	95.4(2)	F(3)	Sb(1)	F(4)	85.98(14)
F(3)	Sb(1)	F(5)	168.86(14)	F(3)	Sb(1)	F(6)	90.75(15)
F(4)	Sb(1)	F(5)	89.66(14)	F(4)	Sb(1)	F(6)	170.4(2)
F(5)	Sb(1)	F(6)	91.91(14)	F(1)	Sb(2)	F(7)	177.8(2)
F(1)	Sb(2)	F(8)	84.66(15)	F(1)	Sb(2)	F(9)	86.42(14)
F(1)	Sb(2)	F(10)	84.53(15)	F(1)	Sb(2)	F(11)	84.57(15)
F(7)	Sb(2)	F(8)	93.4(2)	F(7)	Sb(2)	F(9)	94.5(2)
F(7)	Sb(2)	F(10)	97.4(2)	F(7)	Sb(2)	F(11)	94.4(2)
F(8)	Sb(2)	F(9)	88.0(2)	F(8)	Sb(2)	F(10)	169.1(2)
F(8)	Sb(2)	F(11)	88.8(2)	F(9)	Sb(2)	F(10)	90.3(2)
F(9)	Sb(2)	F(11)	170.7(2)	F(10)	Sb(2)	F(11)	91.1(2)
F(12)	Sb(3)	F(13)	178.92(14)	F(12)	Sb(3)	F(14)	86.23(14)
F(12)	Sb(3)	F(15)	85.5(2)	F(12)	Sb(3)	F(16)	84.49(14)
F(12)	Sb(3)	F(17)	84.83(15)	F(13)	Sb(3)	F(14)	94.85(15)
F(13)	Sb(3)	F(15)	94.5(2)	F(13)	Sb(3)	F(16)	94.43(15)
F(13)	Sb(3)	F(17)	95.23(15)	F(14)	Sb(3)	F(15)	86.89(14)
F(14)	Sb(3)	F(16)	170.58(15)	F(14)	Sb(3)	F(17)	90.0(2)
F(15)	Sb(3)	F(16)	90.8(2)	F(15)	Sb(3)	F(17)	170.0(2)
F(16)	Sb(3)	F(17)	90.79(13)	F(12)	Sb(4)	F(18)	178.10(13)
F(12)	Sb(4)	F(19)	85.43(14)	F(12)	Sb(4)	F(20)	85.53(15)

Table S4. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
F(12)	Sb(4)	F(21)	85.00(14)	F(12)	Sb(4)	F(22)	85.7(2)
F(18)	Sb(4)	F(19)	93.22(15)	F(18)	Sb(4)	F(20)	93.03(15)
F(18)	Sb(4)	F(21)	96.22(15)	F(18)	Sb(4)	F(22)	95.6(2)
F(19)	Sb(4)	F(20)	85.26(14)	F(19)	Sb(4)	F(21)	169.3(2)
F(19)	Sb(4)	F(22)	89.5(2)	F(20)	Sb(4)	F(21)	89.2(2)
F(20)	Sb(4)	F(22)	170.1(2)	F(21)	Sb(4)	F(22)	94.61(14)
C(1)	Pd(1)	C(2)	93.0(2)	C(1)	Pd(1)	C(3)	177.4(2)
C(1)	Pd(1)	C(4)	89.6(2)	C(2)	Pd(1)	C(3)	88.8(2)
C(2)	Pd(1)	C(4)	177.4(2)	C(3)	Pd(1)	C(4)	88.6(2)
Sb(1)	F(1)	Sb(2)	151.64(15)	Sb(3)	F(12)	Sb(4)	158.8(2)
Pd(1)	C(1)	O(1)	176.3(5)	Pd(1)	C(2)	O(2)	177.0(5)
Pd(1)	C(3)	O(3)	176.6(5)	Pd(1)	C(4)	O(4)	176.1(5)

Table S5. Anisotropic Displacement Parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Sb(1)	0.0096(2)	0.01807(14)	0.0122(2)	-0.0006(2)	0.00232(13)	0.0009(2)
Sb(2)	0.0186(2)	0.0254(2)	0.0128(2)	-0.0001(2)	0.00659(14)	-0.0003(2)
Sb(3)	0.0104(2)	0.02186(15)	0.0118(2)	0.0013(2)	0.00280(13)	-0.0002(2)
Sb(4)	0.0125(2)	0.01675(13)	0.00962(15)	0.0002(2)	0.00169(12)	0.0002(2)
Pd(1)	0.0108(2)	0.01557(15)	0.0101(2)	-0.0005(2)	0.00142(13)	-0.0004(2)
F(1)	0.038(2)	0.035(2)	0.022(2)	0.0123(15)	0.018(2)	0.0076(13)
F(2)	0.041(2)	0.057(2)	0.032(2)	0.009(2)	0.020(2)	0.018(2)
F(3)	0.022(2)	0.0262(15)	0.027(2)	0.0051(14)	0.000(2)	0.0045(14)
F(4)	0.032(2)	0.0232(15)	0.033(2)	-0.0039(14)	-0.009(2)	-0.0093(14)
F(5)	0.025(2)	0.0274(15)	0.033(2)	0.0076(14)	0.013(2)	0.0063(14)
F(6)	0.023(2)	0.030(2)	0.046(3)	-0.0088(15)	-0.002(2)	-0.010(2)
F(7)	0.050(3)	0.054(2)	0.033(2)	0.004(2)	0.027(2)	-0.006(2)
F(8)	0.017(2)	0.086(3)	0.040(2)	0.001(2)	-0.007(2)	-0.007(2)
F(9)	0.086(4)	0.026(2)	0.059(3)	-0.002(2)	0.043(3)	-0.001(2)
F(10)	0.042(2)	0.109(3)	0.025(2)	0.002(3)	-0.009(2)	-0.009(3)
F(11)	0.098(4)	0.027(2)	0.062(3)	0.007(2)	0.052(3)	0.009(2)
F(12)	0.030(2)	0.054(2)	0.0134(15)	0.015(2)	0.0108(14)	0.002(2)
F(13)	0.021(2)	0.055(2)	0.034(2)	0.005(2)	0.013(2)	0.001(2)
F(14)	0.024(2)	0.039(2)	0.027(2)	0.0158(15)	0.002(2)	0.0060(15)
F(15)	0.029(3)	0.043(2)	0.038(3)	-0.016(2)	-0.001(2)	-0.010(2)
F(16)	0.032(2)	0.0234(14)	0.022(2)	0.0042(14)	0.004(2)	0.0066(14)
F(17)	0.030(2)	0.0244(14)	0.029(2)	-0.0040(15)	0.006(2)	-0.0055(14)
F(18)	0.039(2)	0.0293(14)	0.0161(15)	0.000(2)	0.0100(13)	0.003(2)
F(19)	0.027(3)	0.036(2)	0.027(3)	0.018(2)	-0.002(2)	0.0064(15)

Table S5. Anisotropic Displacement Parameters (continued)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
F(20)	0.033(3)	0.040(2)	0.032(3)	-0.022(2)	-0.002(2)	-0.001(2)
F(21)	0.037(3)	0.0259(14)	0.019(2)	0.014(2)	0.007(2)	0.0075(15)
F(22)	0.035(3)	0.032(2)	0.032(2)	-0.015(2)	0.002(2)	-0.011(2)
O(1)	0.027(3)	0.029(2)	0.018(3)	-0.002(2)	0.004(2)	-0.007(2)
O(2)	0.034(3)	0.028(2)	0.027(3)	-0.001(2)	0.011(2)	0.005(2)
O(3)	0.051(4)	0.021(2)	0.028(3)	-0.002(2)	0.016(3)	-0.005(2)
O(4)	0.030(3)	0.026(2)	0.023(3)	0.001(2)	0.013(2)	0.002(2)
C(1)	0.015(3)	0.026(3)	0.013(3)	0.001(2)	0.003(3)	0.001(2)
C(2)	0.016(3)	0.025(2)	0.007(3)	0.002(2)	0.005(3)	-0.003(2)
C(3)	0.024(4)	0.022(2)	0.015(4)	-0.002(2)	0.003(3)	0.008(2)
C(4)	0.010(3)	0.024(2)	0.017(4)	0.002(2)	0.001(3)	-0.005(2)

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 S6. Torsion Angles(°)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
Sb(1)	F(1)	Sb(2)	F(7)	92.4(34)	Sb(1)	F(1)	Sb(2)	F(8)	65.3(4)
Sb(1)	F(1)	Sb(2)	F(9)	-23.0(4)	Sb(1)	F(1)	Sb(2)	F(10)	-113.7(4)
Sb(1)	F(1)	Sb(2)	F(11)	154.6(4)	Sb(2)	F(1)	Sb(1)	F(2)	-99(15)
Sb(2)	F(1)	Sb(1)	F(3)	-19.6(4)	Sb(2)	F(1)	Sb(1)	F(4)	-105.9(4)
Sb(2)	F(1)	Sb(1)	F(5)	164.0(4)	Sb(2)	F(1)	Sb(1)	F(6)	71.5(4)
Sb(3)	F(12)	Sb(4)	F(18)	21.9(46)	Sb(3)	F(12)	Sb(4)	F(19)	-23.1(5)
Sb(3)	F(12)	Sb(4)	F(20)	62.5(6)	Sb(3)	F(12)	Sb(4)	F(21)	152.0(6)
Sb(3)	F(12)	Sb(4)	F(22)	-112.9(6)	Sb(4)	F(12)	Sb(3)	F(13)	-152.8(73)
Sb(4)	F(12)	Sb(3)	F(14)	24.0(5)	Sb(4)	F(12)	Sb(3)	F(15)	-63.2(6)
Sb(4)	F(12)	Sb(3)	F(16)	-154.4(6)	Sb(4)	F(12)	Sb(3)	F(17)	114.3(6)
O(1)	C(1)	Pd(1)	C(2)	116.4(83)	O(1)	C(1)	Pd(1)	C(3)	-18(13)
O(1)	C(1)	Pd(1)	C(4)	-63.8(83)	O(2)	C(2)	Pd(1)	C(1)	-153(11)
O(2)	C(2)	Pd(1)	C(3)	25(11)	O(2)	C(2)	Pd(1)	C(4)	32(15)
O(3)	C(3)	Pd(1)	C(1)	-15(14)	O(3)	C(3)	Pd(1)	C(2)	-149.7(98)
O(3)	C(3)	Pd(1)	C(4)	30.6(97)	O(4)	C(4)	Pd(1)	C(1)	-173.2(81)
O(4)	C(4)	Pd(1)	C(2)	2(13)	O(4)	C(4)	Pd(1)	C(3)	8.6(80)

Table S7. Non-bonded Contacts out to 3.60 Å

atom	atom	distance	ADC	atom	atom	distance	ADC
Pd(1)	F(3)	3.000(4)	1	Pd(1)	F(4)	3.155(4)	1
Pd(1)	F(19)	3.183(4)	1	Pd(1)	F(20)	3.204(4)	1
Pd(1)	F(8)	3.211(3)	1	Pd(1)	F(14)	3.540(4)	1
Pd(1)	F(15)	3.581(4)	1	F(1)	F(4)	3.077(4)	65603
F(1)	O(1)	3.268(5)	65603	F(2)	F(10)	2.952(5)	55404
F(2)	F(21)	2.979(5)	65501	F(2)	F(9)	3.042(5)	66603
F(2)	F(18)	3.143(5)	65501	F(2)	F(22)	3.145(5)	65501
F(2)	F(7)	3.559(5)	55404	F(3)	C(2)	2.748(7)	1
F(3)	F(6)	2.920(4)	66603	F(3)	F(3)	3.040(6)	66603
F(3)	O(2)	3.159(6)	1	F(3)	C(3)	3.239(8)	1
F(3)	F(9)	3.269(5)	66603	F(4)	C(1)	2.695(7)	1
F(4)	F(5)	2.896(5)	65603	F(4)	O(1)	2.979(5)	1
F(4)	F(4)	3.029(6)	65603	F(4)	F(11)	3.210(5)	65603
F(5)	C(4)	2.820(6)	65603	F(5)	O(4)	2.884(5)	65603
F(5)	C(1)	3.041(6)	65603	F(5)	F(18)	3.077(5)	65501
F(5)	O(1)	3.101(5)	65603	F(5)	F(16)	3.126(5)	65504
F(6)	O(3)	2.973(6)	66603	F(6)	F(17)	2.988(5)	65504
F(6)	O(2)	3.048(5)	66603	F(6)	C(3)	3.056(6)	66603
F(6)	C(2)	3.157(6)	66603	F(6)	F(18)	3.351(5)	65501
F(7)	O(1)	2.845(5)	4	F(7)	C(1)	2.868(7)	4
F(7)	C(2)	2.897(6)	4	F(7)	O(2)	2.920(5)	4
F(8)	C(4)	2.669(7)	1	F(8)	C(3)	2.776(7)	1
F(8)	O(4)	2.930(6)	1	F(8)	O(3)	3.055(6)	1
F(8)	F(13)	3.297(5)	4	F(9)	O(2)	3.151(7)	66603

Table S7. Non-bonded Contacts out to 3.60 Å (continued)

atom	atom	distance	ADC	atom	atom	distance	ADC
F(9)	F(11)	3.425(6)	65602	F(10)	F(22)	2.912(6)	65504
F(10)	F(21)	3.112(5)	65504	F(10)	O(1)	3.165(6)	65603
F(10)	O(2)	3.277(6)	66603	F(10)	F(11)	3.471(6)	65602
F(11)	O(2)	3.231(6)	4	F(11)	F(22)	3.265(6)	55603
F(11)	O(1)	3.449(7)	65603	F(12)	F(14)	3.419(5)	2
F(12)	O(1)	3.437(5)	2	F(13)	O(3)	2.966(5)	55404
F(13)	O(4)	3.037(5)	55404	F(13)	F(18)	3.137(4)	55404
F(13)	C(3)	3.226(7)	55404	F(13)	C(4)	3.286(7)	55404
F(13)	F(20)	3.450(5)	54502	F(14)	C(1)	2.763(7)	1
F(14)	O(1)	2.953(6)	1	F(14)	F(21)	3.189(5)	54502
F(14)	F(20)	3.198(5)	54502	F(14)	F(15)	3.223(5)	54502
F(14)	F(16)	3.290(5)	54502	F(15)	C(2)	2.800(7)	1
F(15)	O(2)	2.955(6)	1	F(15)	F(19)	3.233(5)	2
F(15)	F(22)	3.318(5)	2	F(15)	F(17)	3.336(5)	2
F(16)	F(19)	2.846(4)	2	F(16)	O(1)	2.988(6)	2
F(16)	C(1)	3.003(7)	2	F(16)	C(4)	3.005(6)	2
F(16)	O(4)	3.045(5)	2	F(16)	F(18)	3.128(4)	55404
F(17)	F(20)	2.837(5)	54502	F(17)	C(3)	2.997(6)	54502
F(17)	O(3)	3.048(6)	54502	F(17)	C(2)	3.078(6)	54502
F(17)	O(2)	3.088(6)	54502	F(17)	F(18)	3.357(4)	55404
F(18)	O(3)	2.830(5)	56603	F(18)	O(4)	2.869(5)	55603
F(19)	C(4)	2.613(7)	1	F(19)	O(4)	2.896(6)	1
F(19)	O(4)	3.121(6)	55603	F(20)	C(3)	2.681(8)	1
F(20)	O(3)	3.008(6)	1	F(20)	O(3)	3.345(6)	56603

Table S7. Non-bonded Contacts out to 3.60 $\AA$ (continued)

atom	atom	distance	ADC	atom	atom	distance	ADC
F(21)	O(1)	2.812(5)	2	F(21)	O(3)	2.943(6)	56603
F(22)	O(2)	2.911(5)	54502	F(22)	O(4)	3.141(6)	55603