Electronic Supplementary Information for Dalton Transactions

jl80f4b in P c c n : Apr 26 11:18:23 2007

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S U P P L E M E N T A R Y M A T E R I A L
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B E L O N G I N G TO T H E P A P E R

b y

C o n t e n t s
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Table S9 - Hydrogen Bonds (Angstrom, Deg)
for: jl80f4b in P c c n

Table S1 - Crystal Data and Details of the Structure Determination for: jl80f4b in P c c n

Crystal Data

Identification code	jl80f4b
Empirical formula	C11 H17 Cl2 N3 O5 Pt
Formula weight	537.27
Temperature	150(2) K
Wavelength	0.71069 A
Crystal system, space group	Orthorhombic, Pccn
Unit cell dimensions	a = 15.1631(4) A alpha = 90 deg. b = 29.3035(7) A beta = 90 deg. c = 7.5829(2) A gamma = 90 deg.
Volume	3369.32(15) A^3
Z, Calculated density	8, 2.118 Mg/m^3
Absorption coefficient	8.670 mm^-1
F(000)	2048
Crystal size	0.18 x 0.14 x 0.11 mm
Theta range for data collection	2.69 to 25.34 deg.
Limiting indices	-18<=h<=18, -34<=k<=35, -9<=l<=8
Reflections collected / unique	18444 / 3069 [R(int) = 0.0322]
Completeness to theta = 25.34	99.6 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.4489 and 0.3044
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3069 / 0 / 213
Goodness-of-fit on F^2	1.173
Final R indices [I>2sigma(I)]	R1 = 0.0283, wR2 = 0.0684
R indices (all data)	R1 = 0.0345, wR2 = 0.0701
Largest diff. peak and hole	1.449 and -1.452 e.A^-3

Table S2 - Final Coordinates and Equivalent Isotropic Displacement Parameters of the non-Hydrogen atoms for: jl80f4b in P c c n

Atom	x	y	z	U(eq) [Ang^2]
Pt1	-0.04678	0.08930	0.02320	0.0192
Cl1	-0.01760	0.14664	0.22056	0.0283
Cl2	-0.07629	0.03350	-0.18155	0.0256
O1	0.22965	0.08776	-0.03998	0.0269
O121	0.19489	0.18259	0.11609	0.0360
O122	0.11270	0.22085	-0.08336	0.0368
O221	-0.26210	0.18599	0.28454	0.0355
O222	-0.40389	0.19591	0.21334	0.0354
N1	0.08130	0.07464	0.01013	0.0208
N2	-0.17384	0.10379	0.04455	0.0234
N11	0.24220	0.04423	0.04935	0.0256
C10	0.14494	0.09942	-0.04663	0.0254
C11	0.13202	0.14406	-0.13529	0.0253
C12	0.15124	0.18374	-0.01449	0.0282
C13	0.32387	0.03450	0.05660	0.0243
C20	-0.24426	0.11547	0.06053	0.0209
C21	-0.33256	0.13320	0.08771	0.0286
C22	-0.32734	0.17501	0.20528	0.0232
C122	0.12448	0.26384	0.00581	0.0479
C131	0.39926	0.06247	-0.01142	0.0284
C132	0.34374	-0.00968	0.14658	0.0295
C222	-0.40521	0.23469	0.33443	0.0449

U(eq) = 1/3 of the trace of the orthogonalized U Tensor

Table S3 - Hydrogen Atom Positions and Isotropic Displacement Parameters
for: jl80f4b in P c c n

Atom	x	y	z	U(iso) [Ang^2]
H1	0.10154	0.04866	0.04806	0.0103
H11A	0.07036	0.14626	-0.17738	0.0800
H11B	0.17124	0.14583	-0.23943	0.0800
H12A	0.09294	0.28783	-0.05847	0.0800
H12B	0.18743	0.27132	0.01057	0.0800
H12C	0.10107	0.26162	0.12597	0.0800
H13A	0.37640	0.09000	-0.06881	0.0800
H13B	0.43308	0.04451	-0.09693	0.0800
H13C	0.43761	0.07119	0.08699	0.0800
H13D	0.28852	-0.02404	0.18437	0.0800
H13E	0.38108	-0.00398	0.24975	0.0800
H13F	0.37467	-0.02999	0.06464	0.0800
H21A	-0.35668	0.13909	-0.01601	0.0384
H21B	-0.37202	0.11053	0.14520	0.0538
H22A	-0.46385	0.24875	0.33321	0.0800
H22B	-0.36113	0.25719	0.29731	0.0800
H22C	-0.39153	0.22415	0.45399	0.0800

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The Temperature Factor has the Form of Exp(-T) Where
T = 8*(Pi**2)*U*(Sin(Theta)/Lambda)**2 for Isotropic Atoms

Table S4 - (An)isotropic Displacement Parameters
for: jl80f4b in P c c n

Atom	U(1,1) or U	U(2,2)	U(3,3)	U(2,3)	U(1,3)	U(1,2)
Pt1	0.0145	0.0192	0.0241	0.0030	0.0018	0.0013
Cl1	0.0224	0.0284	0.0340	-0.0056	0.0043	-0.0005
Cl2	0.0235	0.0215	0.0317	-0.0014	-0.0010	-0.0010
O1	0.0166	0.0283	0.0357	0.0113	0.0022	0.0022
O121	0.0362	0.0309	0.0410	0.0018	-0.0112	-0.0054
O122	0.0389	0.0254	0.0460	0.0013	-0.0080	0.0062
O221	0.0297	0.0313	0.0456	-0.0034	-0.0071	0.0004
O222	0.0202	0.0315	0.0545	-0.0025	0.0085	0.0042
N1	0.0169	0.0227	0.0229	0.0026	0.0021	0.0049
N2	0.0223	0.0211	0.0269	0.0049	0.0004	-0.0022
N11	0.0204	0.0252	0.0312	0.0043	0.0016	0.0010
C10	0.0240	0.0234	0.0288	-0.0025	0.0001	-0.0005
C11	0.0178	0.0276	0.0303	0.0082	0.0010	-0.0016
C12	0.0213	0.0295	0.0337	0.0071	-0.0022	-0.0019
C13	0.0233	0.0280	0.0215	-0.0070	0.0005	0.0024
C20	0.0185	0.0211	0.0232	0.0018	-0.0003	-0.0019
C21	0.0184	0.0339	0.0335	0.0031	0	0.0026
C22	0.0227	0.0188	0.0282	0.0094	0.0046	0.0005
C122	0.0618	0.0303	0.0516	-0.0055	-0.0119	-0.0050
C131	0.0212	0.0314	0.0326	-0.0006	0	-0.0011
C132	0.0249	0.0281	0.0354	0.0037	-0.0045	0.0027
C222	0.0358	0.0299	0.0690	-0.0100	0.0149	0.0042

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The Temperature Factor has the Form of Exp(-T) Where
T = 8*(Pi**2)*U*(Sin(Theta)/Lambda)**2 for Isotropic Atoms
T = 2*(Pi**2)*Sumij(h(i)*h(j)*U(i,j)*Astar(i)*Astar(j)), for Anisotropic Atoms. Astar(i) are Reciprocal Axial Lengths and h(i) are the Reflection Indices.

Table S5 - Bond Distances (Angstrom)
for: jl80f4b in P c c n

Pt1	-Cl1	2.2932	C13	-C132	1.4941
Pt1	-Cl2	2.2988	C20	-C21	1.4509
Pt1	-N1	1.9915	C21	-C22	1.5173
Pt1	-N2	1.9795	C11	-H11A	0.9900
O1	-N11	1.4568	C11	-H11B	0.9900
O1	-C10	1.3301	C21	-H21A	0.8800
O121	-C12	1.1915	C21	-H21B	0.9900
O122	-C12	1.3404	C122	-H12A	0.9800
O122	-C122	1.4409	C122	-H12B	0.9800
O221	-C22	1.2014	C122	-H12C	0.9800
O222	-C22	1.3138	C131	-H13A	0.9800
O222	-C222	1.4611	C131	-H13B	0.9800
N1	-C10	1.2821	C131	-H13C	0.9800
N2	-C20	1.1278	C132	-H13D	0.9800
N11	-C13	1.2720	C132	-H13E	0.9800
N1	-H1	0.8700	C132	-H13F	0.9800
C10	-C11	1.4838	C222	-H22A	0.9800
C11	-C12	1.5087	C222	-H22B	0.9800
C13	-C131	1.4982	C222	-H22C	0.9800

Table S6 - Bond Angles (Degrees)
for: jl80f4b in P c c n

Cl1	-Pt1	-Cl2	178.21	O221	-C22	-C21	123.58
Cl1	-Pt1	-N1	90.14	C10	-C11	-H11A	109.00
Cl1	-Pt1	-N2	88.70	C10	-C11	-H11B	109.00
Cl2	-Pt1	-N1	90.16	C12	-C11	-H11A	109.00
Cl2	-Pt1	-N2	91.05	C12	-C11	-H11B	109.00
N1	-Pt1	-N2	178.16	H11A	-C11	-H11B	108.00
N11	-O1	-C10	111.64	C20	-C21	-H21A	109.00
C12	-O122	-C122	118.19	C20	-C21	-H21B	112.00
C22	-O222	-C222	113.82	C22	-C21	-H21A	113.00
Pt1	-N1	-C10	128.94	C22	-C21	-H21B	108.00
Pt1	-N2	-C20	174.48	H21A	-C21	-H21B	106.00
O1	-N11	-C13	110.09	O122	-C122	-H12A	109.00
Pt1	-N1	-H1	121.00	O122	-C122	-H12B	109.00
C10	-N1	-H1	110.00	O122	-C122	-H12C	109.00
N1	-C10	-C11	123.51	H12A	-C122	-H12B	109.00
O1	-C10	-C11	111.79	H12A	-C122	-H12C	109.00
O1	-C10	-N1	124.65	H12B	-C122	-H12C	109.00
C10	-C11	-C12	112.26	C13	-C131	-H13A	109.00
O121	-C12	-O122	126.08	C13	-C131	-H13B	109.00
O121	-C12	-C11	126.16	C13	-C131	-H13C	109.00
O122	-C12	-C11	107.73	H13A	-C131	-H13B	109.00
N11	-C13	-C131	127.25	H13A	-C131	-H13C	109.00
C131	-C13	-C132	118.51	H13B	-C131	-H13C	109.00
N11	-C13	-C132	114.22	C13	-C132	-H13D	109.00
N2	-C20	-C21	176.05	C13	-C132	-H13E	109.00
C20	-C21	-C22	108.93	C13	-C132	-H13F	109.00
O222	-C22	-C21	110.96	H13D	-C132	-H13E	109.00
O221	-C22	-O222	125.40	H13D	-C132	-H13F	109.00

Table S6 - Bond Angles (Degrees) (continued)
for: jl80f4b in P c c n

H13E	-C132	-H13F	109.00	H22A	-C222	-H22B	109.00
O222	-C222	-H22A	109.00	H22A	-C222	-H22C	109.00
O222	-C222	-H22B	109.00	H22B	-C222	-H22C	109.00
O222	-C222	-H22C	109.00				

Table S7 - Torsion Angles (Degrees)
for: jl80f4b in P c c n

Cl1	-Pt1	-N1	-C10	-63.86
Cl2	-Pt1	-N1	-C10	114.37
C10	-O1	-N11	-C13	-178.72
N11	-O1	-C10	-N1	-3.29
N11	-O1	-C10	-C11	179.19
C222	-O222	-C22	-C21	175.89
C222	-O222	-C22	-O221	-1.49
Pt1	-N1	-C10	-C11	-7.22
Pt1	-N1	-C10	-O1	175.54
O1	-N11	-C13	-C132	179.87
O1	-N11	-C13	-C131	0.91
N1	-C10	-C11	-C12	102.65
O1	-C10	-C11	-C12	-79.80
C10	-C11	-C12	-O121	20.81
C10	-C11	-C12	-O122	-161.10
C20	-C21	-C22	-O222	171.13
C20	-C21	-C22	-O221	-11.43

Table S8 - Contact Distances(Angstrom)
for: jl80f4b in P c c n

Pt1	.C12	4.0934	O1	.O121	3.0660
Pt1	.Cl2_b	4.2277	O1	.H13A	2.2400
Pt1	.C132_a	3.8039	O121	.O1	3.0660
Pt1	.C21_c	3.9884	O121	.C122_i	3.2658
Pt1	.C22_c	3.9703	O122	.C122_j	3.1525
Pt1	.O222_c	3.9799	O122	.C222_c	3.2329
Pt1	.H13E_a	3.2300	O121	.H12C	2.7200
Pt1	.H11A	2.8700	O121	.H12B_i	2.3800
Pt1	.H13B_d	3.6000	O121	.H11B_d	2.5500
Pt1	.H21B_c	3.1800	O221	.C20_e	2.9427
Cl1	.N1	3.0408	O121	.H12B	2.7200
Cl1	.N2	2.9951	O221	.C21_e	3.1206
Cl1	.C10	3.4776	O221	.N2_e	3.2608
Cl1	.C11	3.5262	O122	.H22A_c	2.4800
Cl1	.C12	3.3035	O122	.H12C_j	2.2700
Cl1	.C21_e	3.6150	O222	.Pt1_e	3.9799
Cl2	.Pt1_b	4.2277	O221	.H22C	2.6000
Cl2	.N1_b	3.4260	O221	.H22B_k	2.5000
Cl2	.N1	3.0456	O221	.H21A_e	2.7200
Cl2	.N2	3.0610	O221	.H22B	2.5700
Cl1	.H12A_f	3.0500	N1	.Cl1	3.0408
Cl1	.H21A_e	2.7700	N1	.Cl2	3.0456
Cl1	.H13A_d	3.1400	N1	.N11	2.6144
Cl2	.H13F_g	3.0000	N1	.Cl2_b	3.4260
Cl2	.H13B_g	2.8400	N2	.Cl1	2.9951
Cl2	.H1_b	2.6400	N2	.Cl2	3.0610
Cl2	.H13C_h	2.9500	N2	.O221_c	3.2608
Cl2	.H21B_c	2.7300	N2	.C22_c	3.3128

Table S8 - Contact Distances(Angstrom) (continued)
for: jl80f4b in P c c n

N11	.N1	2.6144	H12A	.H22A_c	2.4100
N11	.H1	2.1400	H12A	.Cl1_j	3.0500
C10	.C13_h	3.5909	H12B	.O121	2.7200
C11	.Cl1	3.5262	H12B	.O121_i	2.3800
C12	.Pt1	4.0934	H12B	.C12_i	2.7800
C12	.Cl1	3.3035	H12B	.C122_i	3.0300
C13	.C10_d	3.5909	H12B	.H12B_i	2.2700
C20	.C22_c	3.3881	H12C	.O121	2.7200
C20	.O221_c	2.9427	H12C	.O122_f	2.2700
C21	.O221_c	3.1206	H12C	.C122_f	3.0000
C21	.Pt1_e	3.9884	H13A	.O1	2.2400
C21	.Cl1_c	3.6150	H13A	.Cl1_h	3.1400
C22	.Pt1_e	3.9703	H13B	.Cl2_m	2.8400
C22	.N2_e	3.3128	H13B	.Pt1_h	3.6000
C22	.C20_e	3.3881	H13C	.Cl2_d	2.9500
C12	.H12B_i	2.7800	H13E	.Pt1_l	3.2300
C122	.O121_i	3.2658	H13F	.Cl2_m	3.0000
C122	.O122_f	3.1525	H21A	.Cl1_c	2.7700
C132	.Pt1_l	3.8039	H21A	.O221_c	2.7200
C122	.H12B_i	3.0300	H21B	.Pt1_e	3.1800
C122	.H12C_j	3.0000	H21B	.Cl2_e	2.7300
C122	.H22A_c	2.8000	H22A	.O122_e	2.4800
C222	.O122_e	3.2329	H22A	.C122_e	2.8000
H1	.N11	2.1400	H22A	.H12A_e	2.4100
H1	.Cl2_b	2.6400	H22B	.O221	2.5700
H11A	.Pt1	2.8700	H22B	.O221_k	2.5000
H11B	.O121_h	2.5500	H22C	.O221	2.6000

Table S9 - Hydrogen Bonds (Angstrom, Deg)
for: jl80f4b in P c c n

N1	-- H1	.. N11	0.8700	2.1400	2.6144	114.00	.
N1	-- H1	.. Cl2	0.8700	2.6400	3.4260	151.00	5_555
C11	-- H11B	.. O121	0.9900	2.5500	3.4231	148.00	7_554
C122	-- H12B	.. O121	0.9800	2.3800	3.2658	151.00	2_555
C122	-- H12C	.. O122	0.9800	2.2700	3.1525	149.00	8_555
C131	-- H13A	.. O1	0.9800	2.2400	2.6852	107.00	.
C21	-- H21A	.. Cl1	0.8800	2.7700	3.6150	160.00	7_454
C21	-- H21B	.. Cl2	0.9900	2.7300	3.6752	160.00	7_455
C222	-- H22A	.. O122	0.9800	2.4800	3.2329	133.00	7_455
C222	-- H22B	.. O221	0.9800	2.5000	3.4615	165.00	2_455

Translation of Symmetry Code to Equiv.Pos

a =[3455.00] = -1/2+x,-y,1/2-z
b =[5555.00] = -x,-y,-z
c =[7454.00] = -1/2-x,y,-1/2+z
d =[7555.00] = 1/2-x,y,1/2+z
e =[7455.00] = -1/2-x,y,1/2+z
f =[8555.00] = x,1/2-y,1/2+z
g =[3454.00] = -1/2+x,-y,-1/2-z
h =[7554.00] = 1/2-x,y,-1/2+z
i =[2555.00] = 1/2-x,1/2-y,z
j =[8554.00] = x,1/2-y,-1/2+z
k =[2455.00] = -1/2-x,1/2-y,z
l =[3555.00] = 1/2+x,-y,1/2-z
m =[3554.00] = 1/2+x,-y,-1/2-z