Experimental data for jonsx1

Crystal Data

C71.25 H75.75 Cl11.75 N2 O2 P2 Pt2, M = 1860.75, Monoclinic, space group P2(1)/c
a = 9.84920(10), b = 25.0091(2), c = 32.0254(4) A ,
alpha = 90 deg., beta = 91.2630(10) deg., gamma = 90 deg.,
U = 7886.57(14) A^3 (by least squares refinement on 8192 reflection positions),
T =180(2)K, lambda = 0.71073 A, Z = 4,
D(cal) = 1.567 Mg/m^3, F(000) = 3676.
mu(MoK-alpha) = 4.025 mm^-1.
Crystal character: weakly diffracting orange needles.
Crystal dimensions 0.6 x 0.06 x 0.04 mm,

Data Collection and Processing.

Siemens SMART (Siemens, 1994) three-circle system with CCD area detector.
The crystal was held at 180(2)
K with the Oxford Cryosystem Cryostream Cooler (Cosier & Glazer, 1986).
Maximum theta was 29.14 deg.
The hkl ranges were -13/ 12, -33/ 32, -32/ 43.
49851 reflections measured, 19139 unique [R(int) = 0.1173].
Absorption correction by Semi-empirical from equivalents;
minimum and maximum transmission factors: 0.74; 0.93.
no crystal decay

Structure Analysis and Refinement.

Systematic absences indicated space group P2(1)/c

The structure was solved by direct methods
using SHELXS (Sheldrick, 1990) (TREF) with additional light atoms found by Fourier methods. The asymmetric unit includes three full occupancy molecules of solvent CHCl3, and one with occupancy estimated at 0.25; the atoms in one of the hydrocarbon chains have very high displacement parameters, probably indicating partial disorder (though it was refined with 100% occupancy); the alternative position lies in the same region as the partial occupancy solvent and it could not be fully modelled.

Hydrogen atoms were added at calculated positions and refined using a riding model with freely rotating methyl groups. Anisotropic displacement parameters were used for all non-H atoms apart from carbon of the partly occupied solvent and the outer atoms of the disordered chain;
H-atoms were given isotropic displacement parameters equal to 1.2 (or 1.5 for methyl hydrogen atoms) times the equivalent isotropic displacement parameter of the atom to which the H-atom is attached.

The weighting scheme was calc w=1/[\s^2^(Fo^2^)+(0.0580P)^2^+17.0000P] where P=(Fo^2^+2Fc^2^)/3.
Goodness-of-fit on F^2 was 1.016,
R1[for 8813 reflections with
I>2sigma(I)] = 0.0771, wR2 = 0.1741.
Data / restraints / parameters 19139/ 9/ 811.
Largest difference Fourier peak and hole 1.103 and -1.308 e.A^-3. All these peaks lie in the solvent region and indicate additional disorder that could not be fully modelled. The relatively high R-value is to be expected in view of the disorder and the weak diffraction

Refinement used SHELXL 96 (Sheldrick, 1996).

We thank EPSRC and Siemens Analytical Instruments for grants in support of the diffractometer.

Additional material available from the Cambridge Crystallographic Data Centre comprises H-atom coordinates, thermal parameters and the remaining bond lengths and angles.

References

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SHELDRICK, G.M. (1990), Acta Cryst. A46, 467-473

SHELDRICK, G.M. (1993), Acta Cryst. D49, 18-23

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SIEMENS (1994), SMART User's manual, Siemens Industrial Automation Inc, Madison, Wis. USA.

Table 1. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for jonsx1. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Pt(1)	2953.8(4)	5285.6(2)	3057.2(1)	28(1)
Pt(2)	5561.8(4)	4705.6(2)	3815.9(1)	27(1)
Cl(1)	4328(3)	4514.6(11)	3189.6(9)	38(1)
P(1)	6742(3)	3938.1(11)	3776.8(9)	29(1)
P(2)	1908(3)	4892.3(11)	2505.7(10)	31(1)

C(1)	14250(20)	3293(8)	7317(6)	105(7)
C(2)	13030(20)	3294(7)	7053(7)	103(7)
C(3)	13233(15)	3494(7)	6627(6)	90(6)
C(4)	11930(20)	3501(8)	6339(10)	207(18)
C(5)	11380(30)	3841(7)	6165(7)	157(12)
C(6)	10100(17)	3896(6)	5881(5)	75(5)
C(7)	10445(14)	4106(6)	5469(5)	68(5)
C(8)	9250(13)	4162(5)	5164(4)	45(3)
O(9)	8478(8)	4607(3)	5316(2)	47(2)
C(10)	7592(12)	4835(4)	5047(4)	36(3)
C(11)	7218(11)	4635(5)	4652(3)	34(3)
C(12)	6302(11)	4909(4)	4388(3)	32(3)
C(13)	5763(11)	5409(4)	4523(3)	28(3)
C(14)	6111(11)	5583(4)	4922(3)	31(3)
C(15)	7007(12)	5314(5)	5184(4)	40(3)
C(16)	4809(11)	5677(4)	4254(3)	28(3)
N(17)	4515(9)	5441(3)	3887(3)	25(2)
N(18)	3698(9)	5657(3)	3604(3)	26(2)
C(19)	3172(11)	6147(4)	3663(4)	30(3)
C(20)	3443(11)	6417(4)	4038(4)	37(3)
C(21)	4244(12)	6190(4)	4332(3)	30(3)
C(22)	2327(10)	6350(4)	3314(3)	24(2)
C(23)	2066(11)	6011(4)	2978(4)	29(3)
C(24)	1366(12)	6204(5)	2639(4)	39(3)
C(25)	836(12)	6727(4)	2627(4)	33(3)
C(26)	1072(12)	7052(4)	2964(4)	38(3)
C(27)	1798(12)	6885(4)	3312(4)	39(3)
O(28)	120(10)	6940(3)	2306(3)	52(3)
C(29)	-310(18)	6590(6)	1979(5)	79(5)
C(30)	-1430(30)	6911(9)	1707(7)	164(12)
C(31)	-2330(30)	6589(11)	1386(9)	184(12)
C(32)	-1260(30)	6032(13)	1157(10)	224(15)
C(33)	-2420(40)	5753(15)	889(12)	290(20)
C(34)	-1660(30)	5324(12)	660(9)	213(14)
C(35)	-2180(30)	4968(12)	290(9)	360(30)
C(36)	-2970(30)	5285(12)	60(9)	320(20)
C(101)	6608(11)	3568(5)	3284(4)	33(3)
C(102)	6355(14)	3022(6)	3262(4)	54(4)
C(103)	6411(18)	2725(6)	2910(5)	78(6)
C(104)	6692(17)	2968(8)	2558(6)	81(6)
C(105)	6979(14)	3518(9)	2542(4)	80(6)
C(106)	6921(12)	3839(6)	2918(4)	46(3)
C(107)	6152(13)	3480(4)	4177(4)	36(3)
C(108)	4748(14)	3376(5)	4168(4)	56(4)
C(109)	4235(17)	3046(6)	4462(6)	83(6)
C(110)	5050(20)	2827(6)	4765(5)	74(5)
C(111)	6389(18)	2925(5)	4780(4)	58(4)
C(112)	6991(15)	3254(5)	4476(4)	50(4)
C(113)	8594(11)	4002(4)	3822(3)	29(3)
C(114)	9187(12)	4496(5)	3845(4)	41(3)
C(115)	10597(12)	4542(6)	3842(3)	44(3)
C(116)	11416(13)	4092(6)	3812(4)	45(3)

C(117)	10843(13)	3608(6)	3791(4)	46(3)
C(118)	9411(13)	3555(5)	3785(4)	43(3)
C(201)	1903(11)	4167(4)	2524(3)	30(3)
C(202)	3057(13)	3887(5)	2395(4)	42(3)
C(203)	3050(14)	3330(5)	2410(4)	52(4)
C(204)	1959(14)	3046(5)	2569(4)	47(3)
C(205)	875(14)	3323(5)	2697(4)	47(4)
C(206)	833(13)	3885(4)	2687(4)	37(3)
C(207)	2704(13)	5050(5)	2016(4)	44(3)
C(208)	2451(14)	4740(5)	1658(4)	51(3)
C(209)	3045(18)	4871(7)	1287(5)	80(5)
C(210)	3941(19)	5290(7)	1275(5)	92(6)
C(211)	4208(17)	5623(7)	1609(5)	81(5)
C(212)	3559(14)	5483(6)	1995(4)	55(4)
C(213)	74(12)	5039(4)	2456(3)	30(3)
C(214)	-625(13)	5167(4)	2813(4)	41(3)
C(215)	-2030(13)	5230(5)	2798(5)	50(3)
C(216)	-2736(15)	5178(5)	2430(5)	54(4)
C(217)	-2049(15)	5065(6)	2062(6)	68(5)
C(218)	-640(14)	4987(5)	2075(4)	53(4)
Cl(2)	1809(4)	7386.1(14)	-653.4(11)	58(1)
C(010)	-86(16)	6527(7)	-1190(5)	80(5)
Cl(11)	638(7)	6413(2)	-1665.0(18)	138(2)
Cl(12)	-1703(7)	6723(3)	-1307(3)	211(4)
Cl(13)	-151(12)	6002(4)	-883(2)	268(6)
C(020)	4319(19)	6653(7)	-1046(5)	89(6)
Cl(21)	5271(7)	6489(3)	-628(2)	164(3)
Cl(22)	4982(8)	7201(4)	-1320(3)	230(5)
Cl(23)	4343(8)	6146(4)	-1414(3)	208(4)
C(030)	-810(20)	7303(11)	-31(6)	147(11)
Cl(31)	-447(6)	7704(4)	375(2)	202(4)
Cl(32)	-2005(8)	7635(3)	-403(2)	167(3)
Cl(33)	-1759(8)	6765(3)	106(2)	167(3)
C(040)	-7080(50)	6551(19)	472(15)	39(12)
Cl(41)	-5616(16)	6459(6)	461(7)	99(7)
Cl(42)	-8336(18)	6137(7)	345(6)	84(5)
Cl(43)	-7500(30)	6890(7)	944(6)	115(8)

Table 2. Selected bond lengths [A] and angles [deg] for jonsx1.

Pt(1)-C(23)	2.027(10)
Pt(1)-N(18)	2.101(8)
Pt(1)-P(2)	2.251(3)
Pt(1)-Cl(1)	2.388(3)
Pt(2)-C(12)	2.023(11)
Pt(2)-N(17)	2.122(8)
Pt(2)-P(1)	2.249(3)
Pt(2)-Cl(1)	2.371(3)

C(23)-Pt(1)-N(18)	81.3(4)
C(23)-Pt(1)-P(2)	96.0(3)
N(18)-Pt(1)-P(2)	173.1(3)
C(23)-Pt(1)-Cl(1)	170.3(3)
N(18)-Pt(1)-Cl(1)	91.3(2)
P(2)-Pt(1)-Cl(1)	91.95(10)
C(12)-Pt(2)-N(17)	81.4(4)
C(12)-Pt(2)-P(1)	95.1(3)
N(17)-Pt(2)-P(1)	176.5(2)
C(12)-Pt(2)-Cl(1)	170.1(3)
N(17)-Pt(2)-Cl(1)	91.4(2)
P(1)-Pt(2)-Cl(1)	92.11(10)

Symmetry transformations used to generate equivalent atoms:

Table 3. Bond lengths [A] and angles [deg] for jonsx1.

Pt(1)-C(23)	2.027(10)
Pt(1)-N(18)	2.101(8)
Pt(1)-P(2)	2.251(3)
Pt(1)-Cl(1)	2.388(3)
Pt(2)-C(12)	2.023(11)
Pt(2)-N(17)	2.122(8)
Pt(2)-P(1)	2.249(3)
Pt(2)-Cl(1)	2.371(3)
P(1)-C(101)	1.832(11)
P(1)-C(107)	1.825(12)
P(1)-C(113)	1.834(11)
P(2)-C(207)	1.813(13)
P(2)-C(201)	1.814(11)
P(2)-C(213)	1.847(12)
C(1)-C(2)	1.45(2)
C(2)-C(3)	1.47(2)
C(3)-C(4)	1.57(2)
C(4)-C(5)	1.14(2)
C(5)-C(6)	1.55(2)
C(6)-C(7)	1.47(2)
C(7)-C(8)	1.519(17)
C(8)-O(9)	1.438(13)
O(9)-C(10)	1.341(13)
C(10)-C(11)	1.400(15)
C(10)-C(15)	1.403(15)
C(11)-C(12)	1.401(15)
C(12)-C(13)	1.429(14)
C(13)-C(14)	1.386(14)
C(13)-C(16)	1.430(14)
C(14)-C(15)	1.379(15)
C(16)-N(17)	1.342(13)

C(16)-C(21)	1.423(14)
N(17)-N(18)	1.314(11)
N(18)-C(19)	1.344(12)
C(19)-C(20)	1.399(15)
C(19)-C(22)	1.468(14)
C(20)-C(21)	1.340(14)
C(22)-C(23)	1.388(14)
C(22)-C(27)	1.436(14)
C(23)-C(24)	1.363(15)
C(24)-C(25)	1.410(15)
C(25)-O(28)	1.344(13)
C(25)-C(26)	1.364(15)
C(26)-C(27)	1.376(15)
O(28)-C(29)	1.421(16)
C(29)-C(30)	1.61(2)
C(30)-C(31)	1.56(3)
C(31)-C(32)	1.90(4)
C(32)-C(33)	1.576(18)
C(33)-C(34)	1.508(18)
C(34)-C(35)	1.560(18)
C(35)-C(36)	1.3212
C(101)-C(102)	1.391(17)
C(101)-C(106)	1.395(17)
C(102)-C(103)	1.353(18)
C(103)-C(104)	1.32(2)
C(104)-C(105)	1.41(2)
C(105)-C(106)	1.448(19)
C(107)-C(112)	1.371(16)
C(107)-C(108)	1.407(17)
C(108)-C(109)	1.359(19)
C(109)-C(110)	1.36(2)
C(110)-C(111)	1.34(2)
C(111)-C(112)	1.415(18)
C(113)-C(114)	1.369(15)
C(113)-C(118)	1.382(15)
C(114)-C(115)	1.393(15)
C(115)-C(116)	1.389(17)
C(116)-C(117)	1.337(17)
C(117)-C(118)	1.416(16)
C(201)-C(206)	1.381(15)
C(201)-C(202)	1.405(15)
C(202)-C(203)	1.395(16)
C(203)-C(204)	1.393(17)
C(204)-C(205)	1.343(17)
C(205)-C(206)	1.406(16)
C(207)-C(212)	1.375(17)
C(207)-C(208)	1.400(16)
C(208)-C(209)	1.377(19)
C(209)-C(210)	1.37(2)
C(210)-C(211)	1.38(2)
C(211)-C(212)	1.448(19)
C(213)-C(214)	1.384(16)

C(213)-C(218)	1.401(16)
C(214)-C(215)	1.393(16)
C(215)-C(216)	1.360(18)
C(216)-C(217)	1.40(2)
C(217)-C(218)	1.401(18)
C(010)-Cl(13)	1.644(18)
C(010)-Cl(12)	1.701(17)
C(010)-Cl(11)	1.719(17)
C(020)-Cl(21)	1.670(18)
C(020)-Cl(23)	1.731(17)
C(020)-Cl(22)	1.761(19)
C(030)-Cl(31)	1.67(2)
C(030)-Cl(33)	1.70(2)
C(030)-Cl(32)	1.86(2)
C(040)-Cl(41)	1.46(5)
C(040)-Cl(42)	1.66(5)
C(040)-Cl(43)	1.79(5)

C(23)-Pt(1)-N(18)	81.3(4)
C(23)-Pt(1)-P(2)	96.0(3)
N(18)-Pt(1)-P(2)	173.1(3)
C(23)-Pt(1)-Cl(1)	170.3(3)
N(18)-Pt(1)-Cl(1)	91.3(2)
P(2)-Pt(1)-Cl(1)	91.95(10)
C(12)-Pt(2)-N(17)	81.4(4)
C(12)-Pt(2)-P(1)	95.1(3)
N(17)-Pt(2)-P(1)	176.5(2)
C(12)-Pt(2)-Cl(1)	170.1(3)
N(17)-Pt(2)-Cl(1)	91.4(2)
P(1)-Pt(2)-Cl(1)	92.11(10)
Pt(2)-Cl(1)-Pt(1)	105.39(11)
C(101)-P(1)-C(107)	105.7(6)
C(101)-P(1)-C(113)	99.5(5)
C(107)-P(1)-C(113)	109.3(5)
C(101)-P(1)-Pt(2)	116.9(4)
C(107)-P(1)-Pt(2)	108.9(4)
C(113)-P(1)-Pt(2)	115.9(4)
C(207)-P(2)-C(201)	104.3(5)
C(207)-P(2)-C(213)	108.8(6)
C(201)-P(2)-C(213)	101.4(5)
C(207)-P(2)-Pt(1)	112.7(4)
C(201)-P(2)-Pt(1)	114.3(4)
C(213)-P(2)-Pt(1)	114.3(3)
C(1)-C(2)-C(3)	114.3(16)
C(2)-C(3)-C(4)	115.2(18)
C(5)-C(4)-C(3)	132(2)
C(4)-C(5)-C(6)	135.9(19)
C(7)-C(6)-C(5)	111.0(16)
C(6)-C(7)-C(8)	114.8(13)
O(9)-C(8)-C(7)	105.1(10)
C(10)-O(9)-C(8)	116.9(9)
O(9)-C(10)-C(11)	125.6(10)

O(9)-C(10)-C(15)	115.3(10)
C(11)-C(10)-C(15)	119.0(11)
C(10)-C(11)-C(12)	121.5(11)
C(11)-C(12)-C(13)	118.9(10)
C(11)-C(12)-Pt(2)	129.6(8)
C(13)-C(12)-Pt(2)	111.4(8)
C(14)-C(13)-C(12)	117.9(10)
C(14)-C(13)-C(16)	123.7(10)
C(12)-C(13)-C(16)	118.2(9)
C(15)-C(14)-C(13)	123.2(10)
C(14)-C(15)-C(10)	119.2(10)
N(17)-C(16)-C(21)	118.3(10)
N(17)-C(16)-C(13)	116.6(9)
C(21)-C(16)-C(13)	124.9(10)
N(18)-N(17)-C(16)	122.5(9)
N(18)-N(17)-Pt(2)	125.1(6)
C(16)-N(17)-Pt(2)	112.3(7)
N(17)-N(18)-C(19)	120.8(9)
N(17)-N(18)-Pt(1)	126.1(6)
C(19)-N(18)-Pt(1)	113.0(7)
N(18)-C(19)-C(20)	119.5(10)
N(18)-C(19)-C(22)	115.0(9)
C(20)-C(19)-C(22)	125.5(10)
C(21)-C(20)-C(19)	119.8(10)
C(20)-C(21)-C(16)	119.0(10)
C(23)-C(22)-C(27)	120.2(10)
C(23)-C(22)-C(19)	118.1(9)
C(27)-C(22)-C(19)	121.7(10)
C(24)-C(23)-C(22)	118.9(10)
C(24)-C(23)-Pt(1)	128.7(9)
C(22)-C(23)-Pt(1)	112.2(8)
C(23)-C(24)-C(25)	122.0(11)
O(28)-C(25)-C(26)	116.6(10)
O(28)-C(25)-C(24)	125.1(11)
C(26)-C(25)-C(24)	118.3(11)
C(25)-C(26)-C(27)	122.4(11)
C(26)-C(27)-C(22)	118.0(11)
C(25)-O(28)-C(29)	117.7(9)
O(28)-C(29)-C(30)	106.5(13)
C(31)-C(30)-C(29)	118.1(19)
C(30)-C(31)-C(32)	109(2)
C(33)-C(32)-C(31)	98(2)
C(34)-C(33)-C(32)	103(3)
C(33)-C(34)-C(35)	128(3)
C(36)-C(35)-C(34)	105.0(19)
C(102)-C(101)-C(106)	118.6(11)
C(102)-C(101)-P(1)	123.3(10)
C(106)-C(101)-P(1)	117.8(9)
C(103)-C(102)-C(101)	124.8(14)
C(104)-C(103)-C(102)	118.4(16)
C(103)-C(104)-C(105)	121.8(15)
C(104)-C(105)-C(106)	120.1(15)

C(101)-C(106)-C(105)	116.3(13)
C(112)-C(107)-C(108)	121.0(12)
C(112)-C(107)-P(1)	123.5(10)
C(108)-C(107)-P(1)	115.4(9)
C(109)-C(108)-C(107)	118.6(14)
C(110)-C(109)-C(108)	121.0(16)
C(111)-C(110)-C(109)	121.1(15)
C(110)-C(111)-C(112)	120.5(14)
C(107)-C(112)-C(111)	117.7(14)
C(114)-C(113)-C(118)	119.0(11)
C(114)-C(113)-P(1)	120.3(9)
C(118)-C(113)-P(1)	120.2(9)
C(113)-C(114)-C(115)	119.9(12)
C(116)-C(115)-C(114)	121.0(12)
C(117)-C(116)-C(115)	119.5(12)
C(116)-C(117)-C(118)	120.2(12)
C(113)-C(118)-C(117)	120.4(12)
C(206)-C(201)-C(202)	119.0(10)
C(206)-C(201)-P(2)	121.8(9)
C(202)-C(201)-P(2)	119.1(9)
C(203)-C(202)-C(201)	118.9(12)
C(204)-C(203)-C(202)	121.7(13)
C(205)-C(204)-C(203)	118.3(12)
C(204)-C(205)-C(206)	122.1(13)
C(201)-C(206)-C(205)	119.9(12)
C(212)-C(207)-C(208)	119.7(12)
C(212)-C(207)-P(2)	119.3(10)
C(208)-C(207)-P(2)	121.0(10)
C(209)-C(208)-C(207)	120.1(14)
C(210)-C(209)-C(208)	119.5(15)
C(209)-C(210)-C(211)	123.6(15)
C(210)-C(211)-C(212)	115.9(15)
C(207)-C(212)-C(211)	120.8(13)
C(214)-C(213)-C(218)	119.5(12)
C(214)-C(213)-P(2)	118.5(9)
C(218)-C(213)-P(2)	121.9(10)
C(213)-C(214)-C(215)	120.6(12)
C(216)-C(215)-C(214)	120.5(13)
C(215)-C(216)-C(217)	120.0(14)
C(218)-C(217)-C(216)	120.0(14)
C(217)-C(218)-C(213)	119.3(14)
Cl(13)-C(010)-Cl(12)	108.3(10)
Cl(13)-C(010)-Cl(11)	114.8(11)
Cl(12)-C(010)-Cl(11)	104.9(10)
Cl(21)-C(020)-Cl(23)	110.5(11)
Cl(21)-C(020)-Cl(22)	112.6(11)
Cl(23)-C(020)-Cl(22)	102.7(10)
Cl(31)-C(030)-Cl(33)	112.5(12)
Cl(31)-C(030)-Cl(32)	110.6(16)
Cl(33)-C(030)-Cl(32)	99.9(11)
Cl(41)-C(040)-Cl(42)	129(3)
Cl(41)-C(040)-Cl(43)	110(3)

Cl(42)-C(040)-Cl(43) 108(3)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for jonsx1.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Pt(1)	26(1)	25(1)	34(1)	-4(1)	0(1)	0(1)
Pt(2)	23(1)	28(1)	30(1)	-4(1)	1(1)	2(1)
Cl(1)	39(2)	34(2)	42(2)	-11(1)	-12(1)	10(1)
P(1)	29(2)	26(2)	31(2)	-4(1)	1(1)	3(1)
P(2)	32(2)	24(2)	35(2)	-7(1)	-1(1)	1(1)
C(1)	121(19)	102(16)	91(15)	12(12)	-27(14)	-3(13)
C(2)	98(17)	71(13)	140(20)	33(13)	56(15)	3(11)
C(3)	44(10)	81(12)	143(18)	50(12)	-25(11)	-13(9)
C(4)	120(20)	103(17)	390(40)	140(20)	-170(30)	-40(15)
C(5)	220(30)	66(13)	180(20)	42(14)	-150(20)	-50(15)
C(6)	85(13)	59(10)	78(12)	3(9)	-28(10)	-10(9)
C(7)	41(9)	60(10)	104(14)	-15(10)	-11(9)	17(8)
C(8)	50(9)	35(7)	50(8)	-4(6)	0(7)	8(6)
O(9)	43(5)	58(6)	40(5)	-3(4)	-13(4)	9(5)
C(10)	29(7)	31(7)	47(8)	-8(6)	-1(6)	4(5)
C(11)	31(7)	37(7)	34(7)	2(6)	1(5)	-6(6)
C(12)	31(7)	31(6)	33(7)	-5(5)	7(5)	-7(5)
C(13)	35(7)	22(6)	27(6)	-8(5)	-1(5)	-2(5)
C(14)	35(7)	27(6)	33(7)	-13(5)	7(5)	1(5)
C(15)	42(7)	46(7)	32(6)	-20(7)	4(5)	-3(7)
C(16)	19(6)	24(6)	41(7)	-2(5)	2(5)	-1(5)
N(17)	23(5)	25(5)	29(5)	-6(4)	2(4)	-3(4)
N(18)	29(5)	22(5)	27(5)	0(4)	-1(4)	2(4)
C(19)	29(7)	24(6)	37(7)	-7(5)	6(5)	-5(5)
C(20)	30(7)	25(6)	58(8)	-7(6)	1(6)	14(5)
C(21)	44(8)	25(6)	23(6)	-7(5)	-4(5)	8(5)
C(22)	20(6)	20(6)	33(6)	-7(5)	1(5)	4(5)
C(23)	26(6)	19(6)	43(7)	-2(5)	5(5)	8(5)
C(24)	39(8)	31(7)	46(8)	9(6)	1(6)	-3(6)
C(25)	35(7)	27(7)	38(7)	0(6)	2(6)	6(5)
C(26)	36(7)	18(6)	61(9)	14(6)	3(6)	3(5)
C(27)	38(8)	24(6)	55(8)	-5(6)	1(6)	9(6)
O(28)	80(7)	28(5)	47(6)	5(4)	-17(5)	11(5)
C(29)	109(15)	59(10)	68(11)	2(9)	-22(10)	35(10)
C(30)	240(30)	108(18)	140(20)	38(16)	-100(20)	-50(19)
C(101)	27(7)	35(7)	37(7)	-23(6)	-9(5)	12(5)

C(102)	60(10)	64(10)	37(8)	2(7)	-8(7)	2(8)
C(103)	123(17)	44(9)	66(12)	-33(9)	-4(11)	19(10)
C(104)	61(12)	99(15)	82(14)	-64(12)	-21(10)	37(11)
C(105)	31(9)	180(20)	29(8)	-13(11)	3(6)	14(11)
C(106)	36(8)	68(9)	34(8)	-18(7)	3(6)	9(7)
C(107)	40(8)	31(7)	39(7)	1(6)	14(6)	7(6)
C(108)	52(10)	49(9)	66(10)	33(8)	23(8)	10(7)
C(109)	55(11)	60(11)	136(17)	31(11)	19(11)	6(9)
C(110)	96(15)	50(10)	77(12)	1(9)	51(11)	-11(10)
C(111)	102(14)	42(8)	29(8)	-14(7)	-7(8)	9(9)
C(112)	60(10)	42(8)	48(9)	2(7)	-3(7)	7(7)
C(113)	29(7)	34(7)	23(6)	-11(5)	0(5)	6(5)
C(114)	28(7)	47(8)	48(8)	-6(6)	1(6)	5(6)
C(115)	33(7)	65(9)	33(7)	-6(6)	2(6)	-7(7)
C(116)	26(7)	73(10)	36(7)	4(7)	3(6)	4(7)
C(117)	34(8)	54(9)	51(9)	-9(7)	5(6)	20(7)
C(118)	45(8)	45(8)	40(8)	-5(6)	2(6)	13(7)
C(201)	28(7)	28(6)	34(7)	1(5)	-1(5)	1(5)
C(202)	40(8)	36(7)	49(8)	-13(6)	-1(6)	-4(6)
C(203)	43(9)	41(8)	72(10)	-18(7)	-1(7)	2(7)
C(204)	52(9)	28(7)	59(9)	-6(6)	-5(7)	11(7)
C(205)	58(10)	41(8)	40(8)	8(6)	-10(7)	0(7)
C(206)	42(8)	27(7)	44(8)	-2(6)	5(6)	1(6)
C(207)	51(9)	36(7)	43(8)	-5(6)	6(7)	-6(7)
C(208)	66(10)	52(8)	36(7)	-10(7)	6(7)	0(8)
C(209)	108(15)	82(13)	51(10)	-10(9)	14(10)	-31(11)
C(210)	123(16)	111(15)	45(9)	-43(11)	45(10)	-30(14)
C(211)	85(13)	91(13)	68(12)	-5(10)	28(10)	-33(10)
C(212)	53(9)	61(9)	50(9)	-19(7)	5(7)	2(8)
C(213)	45(6)	13(5)	32(6)	-14(4)	-6(5)	2(5)
C(214)	48(8)	32(7)	44(8)	-6(6)	-7(6)	-2(6)
C(215)	36(8)	38(8)	75(10)	-12(7)	7(7)	4(6)
C(216)	46(9)	30(8)	86(12)	-1(7)	-6(9)	3(6)
C(217)	49(10)	56(9)	98(14)	7(9)	-42(10)	3(8)
C(218)	48(9)	52(8)	58(9)	3(7)	-19(7)	5(7)
Cl(2)	62(2)	55(2)	59(2)	-13(2)	16(2)	-25(2)
C(010)	58(11)	83(12)	101(14)	-18(11)	8(10)	-28(10)
Cl(11)	181(6)	111(4)	125(5)	-45(4)	78(4)	-40(4)
Cl(12)	102(5)	200(8)	331(12)	-156(8)	-27(6)	15(5)
Cl(13)	421(15)	232(9)	142(6)	89(6)	-149(8)	-214(10)
C(020)	92(14)	93(13)	82(13)	-28(11)	20(11)	2(11)
Cl(21)	150(6)	217(8)	122(5)	-14(5)	-45(5)	53(6)
Cl(22)	146(7)	220(9)	328(12)	116(9)	129(7)	74(6)
Cl(23)	168(7)	278(10)	175(7)	-118(7)	-45(6)	82(7)
C(030)	89(17)	280(30)	73(14)	-22(18)	15(12)	-67(19)
Cl(31)	84(4)	342(11)	181(7)	-191(7)	41(4)	-81(6)
Cl(32)	165(7)	191(7)	147(6)	-27(6)	15(5)	-14(6)
Cl(33)	181(7)	145(6)	175(7)	12(5)	3(6)	-59(5)
Cl(41)	60(11)	37(8)	200(20)	71(11)	39(12)	3(8)
Cl(42)	79(13)	78(11)	94(13)	-28(10)	7(10)	-24(10)
Cl(43)	200(20)	55(11)	92(14)	-18(10)	10(15)	-47(13)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for jonsx1.

	x	y	z	U(eq)
H(1A)	14064	3119	7583	158
H(1B)	14548	3662	7368	158
H(1C)	14976	3098	7176	158
H(2A)	12337	3518	7188	123
H(2B)	12673	2925	7036	123
H(3A)	13927	3269	6493	108
H(3B)	13598	3862	6645	108
H(4A)	12115	3235	6118	248
H(4B)	11215	3338	6511	248
H(5A)	12109	3997	5994	188
H(5B)	11230	4107	6389	188
H(6A)	9662	3542	5848	90
H(6B)	9446	4140	6014	90
H(7A)	11126	3867	5344	82
H(7B)	10873	4462	5506	82
H(8A)	9568	4233	4878	54
H(8B)	8694	3832	5159	54
H(11A)	7595	4307	4561	41
H(14A)	5714	5904	5020	38
H(15A)	7226	5450	5454	48
H(20A)	3060	6760	4085	45
H(21A)	4431	6370	4588	37
H(24A)	1232	5979	2403	47
H(26A)	724	7406	2957	46
H(27A)	1943	7116	3544	47
H(29A)	-704	6260	2095	95
H(29B)	467	6492	1804	95
H(30A)	-2050	7090	1903	197
H(30B)	-963	7195	1551	197
H(31A)	-2665	6829	1160	220
H(31B)	-3125	6435	1527	220
H(32A)	-527	6171	983	269
H(32B)	-879	5792	1376	269
H(33A)	-3122	5596	1069	346
H(33B)	-2859	6008	692	346
H(34A)	-1347	5070	878	255
H(34B)	-836	5502	557	255
H(35A)	-1416	4832	127	433
H(35B)	-2708	4659	395	433
H(36A)	-3132	5122	-215	484
H(36B)	-2518	5631	25	484
H(36C)	-3836	5337	198	484

H(10A)	6125	2844	3513	65
H(10B)	6252	2350	2917	93
H(10C)	6701	2765	2307	97
H(10D)	7212	3679	2285	96
H(10E)	7086	4213	2915	55
H(10F)	4172	3533	3960	67
H(10G)	3291	2966	4456	100
H(11B)	4667	2600	4969	88
H(11C)	6938	2773	4997	69
H(11D)	7942	3317	4478	60
H(11E)	8639	4807	3862	49
H(11F)	11003	4885	3862	52
H(11G)	12375	4128	3806	54
H(11H)	11399	3298	3781	55
H(11I)	9010	3212	3756	52
H(20B)	3829	4074	2299	50
H(20C)	3809	3138	2309	62
H(20D)	1981	2667	2587	56
H(20E)	113	3133	2797	56
H(20F)	70	4069	2792	45
H(20G)	1868	4438	1672	62
H(20H)	2835	4673	1041	96
H(21B)	4403	5353	1023	111
H(21C)	4784	5926	1587	97
H(21E)	3726	5694	2238	66
H(21F)	-141	5213	3070	50
H(21G)	-2500	5310	3046	60
H(21H)	-3695	5218	2423	65
H(21I)	-2538	5042	1803	82
H(21J)	-173	4900	1827	64
H(01A)	409	6824	-1042	96
H(02A)	3365	6729	-963	106
H(03A)	40	7189	-173	177
H(04A)	-7202	6840	259	47