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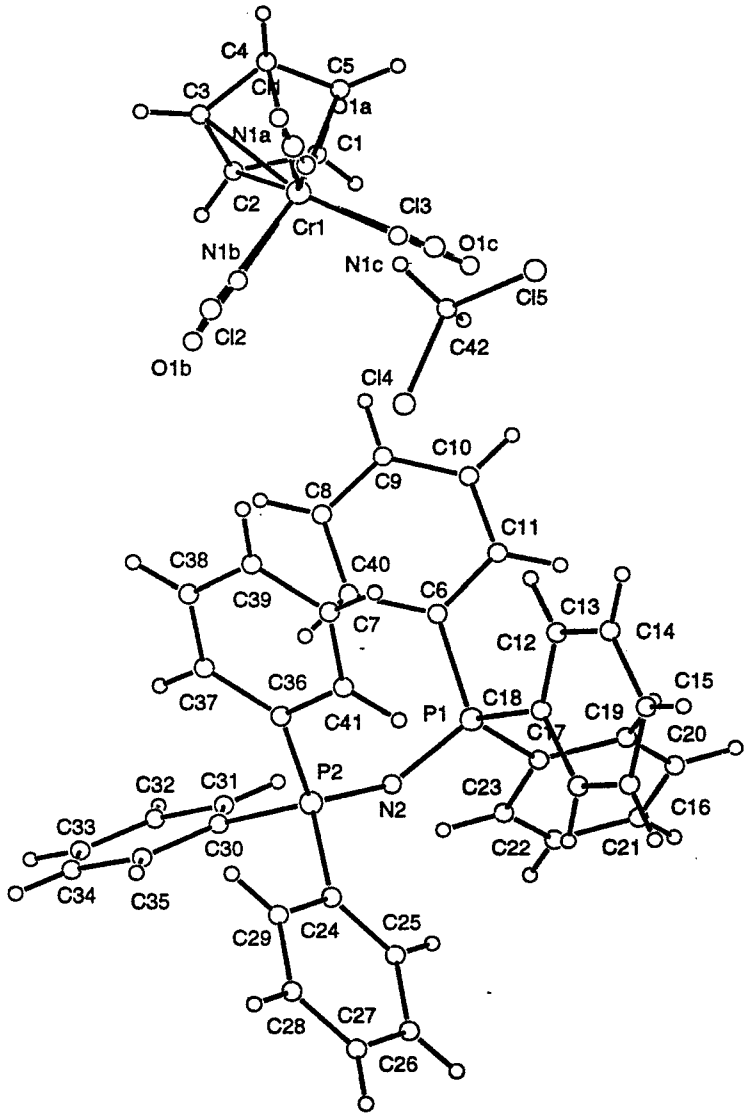
C4
C5
C3
C1
O1a
N1a
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Cl3
Cr1
O1c
N1b
N1c
Cl5
Cl2
C42
O1b
Cl4
C10
C9
C8
C11
C38
C40
C6
C39
C7
C13
C12
C14
C15
C36
C37
C41
P1
C18
C19
C17
C20
P2
C32
C31
N2
C23
C16
C33
C30
C22
C21
C34
C35
C29
C24
C25
C28
C27
C26

EXPERIMENTAL DETAILS

A. Crystal Data

Empirical Formula	$C_{42}H_{37}Cl_4CrN_2P_2O$
Formula Weight	841.52
Crystal Color, Habit	green, prism
Crystal Dimensions	0.25 X 0.30 X 0.45 mm
Crystal System	triclinic
Lattice Type	Primitive
No. of Reflections Used for Unit Cell Determination (2θ range)	25 (18.0 - 25.9°)
Omega Scan Peak Width at Half-height	0.30°
Lattice Parameters	a = 12.729(2) Å b = 15.480(2) Å c = 11.778(2) Å α = 101.25(1)° β = 101.40(1)° γ = 111.129(10)°
	V = 2029.9(6) Å^3
Space Group	$P\bar{1}$ (#2)
Z value	2
D_{calc}	1.377 g/cm^3
F_{000}	866.00
μ(MoKα)	6.59 cm^{-1}

B. Intensity Measurements

Diffractometer	Rigaku AFC6S
Radiation	MoKα (λ = 0.71069 Å) graphite monochromated
Take-off Angle	6.0°
Detector Aperture	6.0 mm horizontal 6.0 mm vertical
Crystal to Detector Distance	285 mm
Voltage, Current	50kV, 30mA
Temperature	21.0°C
Scan Type	ω-2θ
Scan Rate	16.0°/min (in ω) (up to 9 scans)
Scan Width	(1.05 + 0.35 tan θ)°
$2\theta_{max}$	55°
No. of Reflections Measured	Total: 9770 Unique: 9343 (R_{int} = 0.048)
Corrections	Lorentz-polarization Absorption (trans. factors: 0.939 - 1.000)

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	0.0000
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (I>3σ(I))	2823
No. Variables	494
Reflection/Parameter Ratio	5.71

Residuals: R; Rw	0.052 ; 0.044
Goodness of Fit Indicator	1.92
Max Shift/Error in Final Cycle	0.008
Maximum peak in Final Diff. Map	0.35 $e^-/\AA^3$
Minimum peak in Final Diff. Map	-0.44 $e^-/\AA^3$

Table 2. Atomic coordinates and B_{eq}

atom	x	y	z	B_{eq}	occ
Cr(1)	0.60735(8)	0.37101(6)	0.89864(8)	3.98(2)	
Cl(1)	0.6614(3)	0.2648(2)	0.7823(3)	5.07(9)	0.725
Cl(2)	0.4111(3)	0.2654(2)	0.8486(3)	5.03(7)	0.775
Cl(3)	0.6079(9)	0.4657(5)	0.7735(7)	4.8(2)	0.500
Cl(4)	0.3934(2)	0.2039(1)	0.3959(2)	10.05(7)	
Cl(5)	0.6275(2)	0.3202(2)	0.3993(3)	13.8(1)	
P(1)	0.0276(1)	0.30160(10)	0.2718(1)	3.21(4)	
P(2)	-0.1570(1)	0.1039(1)	0.2323(1)	3.25(4)	
O(1a)	0.690(2)	0.245(1)	0.791(2)	4.4(6)	0.275
O(1b)	0.361(1)	0.242(2)	0.832(2)	5.2(7)	0.225
O(1c)	0.603(2)	0.496(1)	0.746(2)	6.3(4)	0.500
N(1a)	0.644(2)	0.299(1)	0.799(1)	5.3(6)	0.275
N(1b)	0.4619(8)	0.298(2)	0.860(2)	3.0(6)	0.225
N(1c)	0.603(3)	0.439(2)	0.803(2)	5.2(4)	0.500
N(2)	-0.0955(3)	0.2160(3)	0.2585(3)	3.36(8)	
C(1)	0.6676(6)	0.4981(5)	1.0608(6)	6.3(2)	
C(2)	0.6017(6)	0.4192(5)	1.0876(5)	6.2(2)	
C(3)	0.6562(7)	0.3560(5)	1.0832(6)	6.7(2)	
C(4)	0.7592(6)	0.3989(6)	1.0527(6)	7.1(2)	
C(5)	0.7637(6)	0.4863(5)	1.0352(5)	7.0(2)	
C(6)	0.1419(4)	0.3218(4)	0.4036(4)	3.2(1)	
C(7)	0.1209(5)	0.2595(4)	0.4767(5)	4.3(1)	
C(8)	0.2068(5)	0.2776(4)	0.5820(5)	5.3(2)	
C(9)	0.3131(5)	0.3583(5)	0.6163(5)	5.3(2)	

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

atom	x	y	z	B_{eq}	occ
C(10)	0.3324(5)	0.4191(4)	0.5453(5)	5.0(2)	
C(11)	0.2497(5)	0.4019(4)	0.4391(5)	4.2(1)	
C(12)	0.0786(4)	0.2846(3)	0.1401(4)	3.3(1)	
C(13)	0.1848(5)	0.2799(4)	0.1444(5)	4.1(1)	
C(14)	0.2161(5)	0.2634(4)	0.0383(6)	5.3(2)	
C(15)	0.1409(6)	0.2503(4)	-0.0709(6)	6.1(2)	
C(16)	0.0345(6)	0.2550(4)	-0.0739(5)	5.7(2)	
C(17)	0.0034(5)	0.2730(4)	0.0302(5)	4.5(1)	
C(18)	0.0076(4)	0.4116(3)	0.2883(4)	3.1(1)	
C(19)	0.0815(4)	0.4898(4)	0.2579(5)	3.9(1)	
C(20)	0.0686(5)	0.5740(4)	0.2760(5)	5.1(2)	
C(21)	-0.0193(5)	0.5835(4)	0.3221(5)	4.8(2)	
C(22)	-0.0925(5)	0.5087(4)	0.3518(5)	4.4(2)	
C(23)	-0.0811(4)	0.4229(4)	0.3355(4)	3.7(1)	
C(24)	-0.2619(4)	0.0502(4)	0.0839(4)	3.4(1)	
C(25)	-0.3038(5)	0.1051(4)	0.0266(5)	4.6(2)	
C(26)	-0.3880(5)	0.0639(5)	-0.0850(6)	5.7(2)	
C(27)	-0.4323(5)	-0.0345(5)	-0.1393(5)	5.5(2)	
C(28)	-0.3914(5)	-0.0900(4)	-0.0827(5)	4.9(2)	
C(29)	-0.3067(4)	-0.0490(4)	0.0287(4)	3.7(1)	
C(30)	-0.2349(4)	0.0791(4)	0.3426(4)	3.3(1)	
C(31)	-0.2137(4)	0.1532(4)	0.4437(5)	4.1(1)	
C(32)	-0.2704(5)	0.1355(5)	0.5304(5)	5.4(2)	
C(33)	-0.3475(5)	0.0436(5)	0.5150(5)	5.7(2)	

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

atom	x	y	z	B_{eq}	occ
C(34)	-0.3711(5)	-0.0304(5)	0.4173(6)	5.8(2)	
C(35)	-0.3156(5)	-0.0139(4)	0.3282(5)	4.7(1)	
C(36)	-0.0602(4)	0.0434(3)	0.2397(4)	3.5(1)	
C(37)	-0.0393(5)	-0.0006(4)	0.3282(5)	4.9(2)	
C(38)	0.0462(6)	-0.0350(5)	0.3388(5)	6.1(2)	
C(39)	0.1174(5)	-0.0235(5)	0.2644(6)	6.1(2)	
C(40)	0.0977(5)	0.0195(4)	0.1744(5)	5.0(2)	
C(41)	0.0102(5)	0.0525(4)	0.1621(4)	4.0(1)	
C(42)	0.5349(8)	0.2875(6)	0.4828(6)	11.1(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(Å)

atom	atom	distance	atom	atom	distance
Cr(1)	Cl(1)	2.315(4)	Cr(1)	Cl(2)	2.314(4)
Cr(1)	Cl(3)	2.271(5)	Cr(1)	N(1a)	1.707(9)
Cr(1)	N(1b)	1.696(9)	Cr(1)	N(1c)	1.685(7)
Cr(1)	C(1)	2.230(8)	Cr(1)	C(2)	2.229(8)
Cr(1)	C(3)	2.221(8)	Cr(1)	C(4)	2.218(8)
Cr(1)	C(5)	2.188(8)	Cr(1)	CP	1.88
Cl(4)	C(42)	1.74(1)	Cl(5)	C(42)	1.68(1)
P(1)	N(2)	1.600(5)	P(1)	C(6)	1.793(7)
P(1)	C(12)	1.806(7)	P(1)	C(18)	1.790(7)
P(2)	N(2)	1.560(5)	P(2)	C(24)	1.800(7)
P(2)	C(30)	1.803(6)	P(2)	C(36)	1.796(7)
O(1a)	N(1a)	1.186(9)*	O(1b)	N(1b)	1.193(9)*
O(1c)	N(1c)	1.214(8)*	C(1)	C(2)	1.35(1)
C(1)	C(5)	1.38(1)	C(2)	C(3)	1.39(1)
C(3)	C(4)	1.39(1)	C(4)	C(5)	1.39(1)
C(6)	C(7)	1.404(8)	C(6)	C(11)	1.393(8)
C(7)	C(8)	1.386(9)	C(8)	C(9)	1.387(10)
C(9)	C(10)	1.366(9)	C(10)	C(11)	1.375(9)
C(12)	C(13)	1.370(9)	C(12)	C(17)	1.386(9)
C(13)	C(14)	1.390(9)	C(14)	C(15)	1.37(1)
C(15)	C(16)	1.38(1)	C(16)	C(17)	1.370(9)
C(18)	C(19)	1.401(8)	C(18)	C(23)	1.403(8)
C(19)	C(20)	1.353(9)	C(20)	C(21)	1.377(10)
C(21)	C(22)	1.356(9)	C(22)	C(23)	1.369(9)

Table 3. Bond Lengths($\AA$) (continued)

atom	atom	distance	atom	atom	distance
C(24)	C(25)	1.366(9)	C(24)	C(29)	1.393(9)
C(25)	C(26)	1.381(10)	C(26)	C(27)	1.38(1)
C(27)	C(28)	1.364(10)	C(28)	C(29)	1.382(9)
C(30)	C(31)	1.387(8)	C(30)	C(35)	1.387(9)
C(31)	C(32)	1.377(9)	C(32)	C(33)	1.36(1)
C(33)	C(34)	1.35(1)	C(34)	C(35)	1.390(9)
C(36)	C(37)	1.386(9)	C(36)	C(41)	1.393(9)
C(37)	C(38)	1.369(10)	C(38)	C(39)	1.37(1)
C(39)	C(40)	1.39(1)	C(40)	C(41)	1.377(9)

* restrained during refinement

CP refers to the unweighted centroid of the C(1-5) ring

Table 4. Bond Angles(°)

atom	atom	atom	angle	atom	atom	atom	angle
Cl(1)	Cr(1)	Cl(2)	95.6(2)	Cl(1)	Cr(1)	Cl(3)	96.8(3)
Cl(1)	Cr(1)	N(1b)	97(1)	Cl(1)	Cr(1)	N(1c)	96(1)
Cl(1)	Cr(1)	CP	120.4	Cl(2)	Cr(1)	Cl(3)	103.7(4)
Cl(2)	Cr(1)	N(1a)	96(1)	Cl(2)	Cr(1)	N(1c)	101(1)
Cl(2)	Cr(1)	CP	117.7	Cl(3)	Cr(1)	N(1a)	90.0(9)
Cl(3)	Cr(1)	N(1b)	101(1)	Cl(3)	Cr(1)	CP	118.3
N(1a)	Cr(1)	N(1b)	97(1)	N(1a)	Cr(1)	N(1c)	89(1)
N(1a)	Cr(1)	CP	125.5	N(1b)	Cr(1)	N(1c)	99(2)
N(1b)	Cr(1)	CP	118.4	N(1c)	Cr(1)	CP	119.8
N(2)	P(1)	C(6)	113.1(3)	N(2)	P(1)	C(12)	113.1(3)
N(2)	P(1)	C(18)	108.2(3)	C(6)	P(1)	C(12)	109.1(3)
C(6)	P(1)	C(18)	106.4(3)	C(12)	P(1)	C(18)	106.5(3)
N(2)	P(2)	C(24)	110.1(3)	N(2)	P(2)	C(30)	108.0(3)
N(2)	P(2)	C(36)	115.4(3)	C(24)	P(2)	C(30)	108.5(3)
C(24)	P(2)	C(36)	107.2(3)	C(30)	P(2)	C(36)	107.4(3)
Cr(1)	N(1a)	O(1a)	144(2)*	Cr(1)	N(1b)	O(1b)	176(4)*
Cr(1)	N(1c)	O(1c)	172(4)*	P(1)	N(2)	P(2)	142.0(4)
C(2)	C(1)	C(5)	109.0(10)	C(1)	C(2)	C(3)	108.8(9)
C(2)	C(3)	C(4)	107.4(9)	C(3)	C(4)	C(5)	107.2(9)
C(1)	C(5)	C(4)	107.7(9)	P(1)	C(6)	C(7)	119.9(5)
P(1)	C(6)	C(11)	121.0(6)	C(7)	C(6)	C(11)	119.0(6)
C(6)	C(7)	C(8)	120.2(7)	C(7)	C(8)	C(9)	119.9(8)
C(8)	C(9)	C(10)	119.6(7)	C(9)	C(10)	C(11)	121.8(7)
C(6)	C(11)	C(10)	119.5(7)	P(1)	C(12)	C(13)	123.1(6)

Table 4. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
P(1)	C(12)	C(17)	117.0(6)	C(13)	C(12)	C(17)	119.9(7)
C(12)	C(13)	C(14)	119.6(7)	C(13)	C(14)	C(15)	120.6(8)
C(14)	C(15)	C(16)	119.1(8)	C(15)	C(16)	C(17)	120.9(8)
C(12)	C(17)	C(16)	119.8(8)	P(1)	C(18)	C(19)	121.4(6)
P(1)	C(18)	C(23)	120.7(6)	C(19)	C(18)	C(23)	117.9(7)
C(18)	C(19)	C(20)	120.7(7)	C(19)	C(20)	C(21)	120.5(7)
C(20)	C(21)	C(22)	120.0(8)	C(21)	C(22)	C(23)	120.9(7)
C(18)	C(23)	C(22)	120.0(7)	P(2)	C(24)	C(25)	120.6(6)
P(2)	C(24)	C(29)	120.3(6)	C(25)	C(24)	C(29)	119.0(7)
C(24)	C(25)	C(26)	121.1(8)	C(25)	C(26)	C(27)	119.7(8)
C(26)	C(27)	C(28)	119.7(8)	C(27)	C(28)	C(29)	120.8(8)
C(24)	C(29)	C(28)	119.7(7)	P(2)	C(30)	C(31)	120.0(5)
P(2)	C(30)	C(35)	120.7(6)	C(31)	C(30)	C(35)	119.4(6)
C(30)	C(31)	C(32)	120.9(7)	C(31)	C(32)	C(33)	118.5(8)
C(32)	C(33)	C(34)	122.3(8)	C(33)	C(34)	C(35)	120.1(8)
C(30)	C(35)	C(34)	118.8(7)	P(2)	C(36)	C(37)	124.0(6)
P(2)	C(36)	C(41)	117.9(6)	C(37)	C(36)	C(41)	117.4(7)
C(36)	C(37)	C(38)	121.7(8)	C(37)	C(38)	C(39)	120.6(8)
C(38)	C(39)	C(40)	118.9(8)	C(39)	C(40)	C(41)	120.5(8)
C(36)	C(41)	C(40)	120.9(7)	Cl(4)	C(42)	Cl(5)	113.1(6)

* restrained during refinement

Table 5. Hydrogen atom coordinates and B_{iso}

atom	x	y	z	B_{iso}
H(1)	0.6506	0.5548	1.0594	7.6
H(2)	0.5275	0.4082	1.1072	7.5
H(3)	0.6282	0.2929	1.0983	8.1
H(4)	0.8183	0.3729	1.0448	8.6
H(5)	0.8245	0.5315	1.0091	8.5
H(6)	0.0454	0.2031	0.4528	5.1
H(7)	0.1927	0.2335	0.6322	6.3
H(8)	0.3744	0.3720	0.6905	6.3
H(9)	0.4074	0.4767	0.5703	6.0
H(10)	0.2667	0.4458	0.3886	5.0
H(11)	0.2382	0.2881	0.2222	4.9
H(12)	0.2924	0.2610	0.0418	6.4
H(13)	0.1623	0.2378	-0.1456	7.3
H(14)	-0.0204	0.2453	-0.1515	6.8
H(15)	-0.0717	0.2779	0.0273	5.3
H(16)	0.1434	0.4836	0.2230	4.7
H(17)	0.1226	0.6285	0.2556	6.1
H(18)	-0.0284	0.6444	0.3330	5.8
H(19)	-0.1541	0.5164	0.3852	5.2
H(20)	-0.1347	0.3693	0.3567	4.5
H(21)	-0.2734	0.1748	0.0652	5.6
H(22)	-0.4157	0.1044	-0.1260	6.8
H(23)	-0.4927	-0.0642	-0.2181	6.5
H(24)	-0.4225	-0.1598	-0.1219	5.9

Table 5. Hydrogen atom coordinates and B_{iso} (continued)

atom	x	y	z	B_{iso}
H(25)	-0.2781	-0.0896	0.0686	4.4
H(26)	-0.1578	0.2192	0.4541	4.9
H(27)	-0.2557	0.1878	0.6020	6.5
H(28)	-0.3876	0.0305	0.5771	6.9
H(29)	-0.4277	-0.0957	0.4100	7.0
H(30)	-0.3337	-0.0672	0.2568	5.7
H(31)	-0.0865	-0.0072	0.3846	5.8
H(32)	0.0576	-0.0680	0.3997	7.3
H(33)	0.1818	-0.0448	0.2739	7.3
H(34)	0.1461	0.0264	0.1185	6.0
H(35)	-0.0023	0.0828	0.0977	4.8
H(36)	0.5292	0.3453	0.5277	13.4
H(37)	0.5665	0.2585	0.5404	13.4

Table 6. Anisotropic Displacement Parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Cr(1)	0.0489(6)	0.0503(7)	0.0447(6)	0.0134(5)	0.0133(5)	0.0118(5)
Cl(1)	0.078(2)	0.057(2)	0.084(2)	0.043(2)	0.052(2)	0.016(1)
Cl(2)	0.045(2)	0.057(2)	0.066(2)	-0.001(2)	0.012(2)	0.017(1)
Cl(3)	0.059(3)	0.071(7)	0.051(5)	0.022(6)	0.006(5)	0.035(2)
Cl(4)	0.125(2)	0.126(2)	0.107(2)	0.035(1)	0.036(1)	0.011(1)
Cl(5)	0.159(2)	0.144(2)	0.244(3)	0.045(2)	0.127(2)	0.070(2)
P(1)	0.0351(9)	0.0415(9)	0.0417(9)	0.0117(7)	0.0123(7)	0.0112(8)
P(2)	0.0397(9)	0.0405(9)	0.0409(9)	0.0114(7)	0.0175(7)	0.0107(7)
O(1c)	0.061(8)	0.08(1)	0.076(8)	-0.005(7)	-0.006(7)	0.073(6)
N(1c)	0.045(9)	0.07(1)	0.06(1)	0.00(1)	-0.021(10)	0.041(6)
N(2)	0.038(2)	0.037(2)	0.048(3)	0.009(2)	0.018(2)	0.011(2)
C(1)	0.089(6)	0.062(4)	0.059(4)	0.023(4)	0.005(4)	-0.014(2)
C(2)	0.076(5)	0.096(6)	0.043(3)	0.019(4)	0.017(4)	0.002(4)
C(3)	0.118(6)	0.081(6)	0.048(3)	0.036(4)	0.010(4)	0.028(4)
C(4)	0.078(5)	0.125(6)	0.061(4)	0.065(5)	-0.019(3)	0.009(5)
C(5)	0.060(4)	0.103(5)	0.047(4)	-0.012(3)	-0.004(3)	0.009(4)
C(6)	0.036(3)	0.044(3)	0.041(3)	0.018(2)	0.011(2)	0.005(2)
C(7)	0.052(4)	0.061(4)	0.051(3)	0.020(3)	0.015(3)	0.029(3)
C(8)	0.059(4)	0.088(5)	0.051(4)	0.025(3)	0.013(3)	0.029(4)
C(9)	0.057(4)	0.086(5)	0.049(4)	0.028(3)	0.000(3)	0.017(3)
C(10)	0.042(4)	0.067(4)	0.060(4)	0.011(3)	0.000(3)	0.011(3)
C(11)	0.038(3)	0.059(4)	0.054(3)	0.010(2)	0.013(2)	0.019(3)
C(12)	0.046(3)	0.034(3)	0.043(2)	0.011(3)	0.023(2)	0.008(3)
C(13)	0.047(3)	0.045(4)	0.058(3)	0.015(3)	0.016(3)	0.014(3)

Table 6. Anisotropic Displacement Parameters (continued)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(14)	0.072(5)	0.061(4)	0.074(3)	0.021(4)	0.052(3)	0.009(4)
C(15)	0.105(5)	0.060(4)	0.062(4)	0.017(4)	0.053(4)	0.007(4)
C(16)	0.100(5)	0.061(4)	0.041(3)	0.018(4)	0.027(4)	0.010(3)
C(17)	0.066(4)	0.059(4)	0.043(3)	0.023(3)	0.018(3)	0.016(3)
C(18)	0.040(3)	0.043(3)	0.028(3)	0.017(2)	0.000(2)	0.005(3)
C(19)	0.049(4)	0.043(3)	0.063(4)	0.019(3)	0.027(3)	0.019(3)
C(20)	0.063(4)	0.039(3)	0.089(5)	0.018(3)	0.022(3)	0.023(4)
C(21)	0.075(5)	0.044(4)	0.063(4)	0.032(3)	0.012(3)	0.009(3)
C(22)	0.068(4)	0.061(4)	0.051(4)	0.040(3)	0.023(3)	0.014(3)
C(23)	0.042(3)	0.053(3)	0.044(3)	0.015(3)	0.016(3)	0.014(3)
C(24)	0.035(3)	0.050(3)	0.040(2)	0.013(3)	0.018(2)	0.005(2)
C(25)	0.057(4)	0.059(4)	0.067(4)	0.025(3)	0.017(3)	0.032(3)
C(26)	0.070(5)	0.089(4)	0.066(4)	0.035(4)	0.013(3)	0.043(3)
C(27)	0.055(4)	0.096(4)	0.045(4)	0.022(4)	0.003(3)	0.024(3)
C(28)	0.050(4)	0.069(5)	0.041(3)	0.009(3)	0.008(2)	-0.004(3)
C(29)	0.050(4)	0.051(3)	0.038(3)	0.021(3)	0.014(2)	0.012(2)
C(30)	0.033(3)	0.050(3)	0.039(3)	0.013(2)	0.014(2)	0.013(2)
C(31)	0.053(4)	0.045(3)	0.048(3)	0.013(3)	0.019(3)	0.008(2)
C(32)	0.074(5)	0.100(5)	0.048(4)	0.046(4)	0.035(3)	0.023(4)
C(33)	0.052(4)	0.115(5)	0.057(4)	0.030(4)	0.029(4)	0.037(3)
C(34)	0.058(4)	0.084(5)	0.073(4)	0.006(4)	0.034(4)	0.037(3)
C(35)	0.054(4)	0.050(3)	0.057(4)	0.005(3)	0.014(3)	0.008(3)
C(36)	0.039(3)	0.036(3)	0.040(3)	0.008(2)	0.005(2)	-0.004(2)
C(37)	0.081(5)	0.080(5)	0.033(3)	0.041(4)	0.017(3)	0.017(3)

Table 6. Anisotropic Displacement Parameters (continued)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(38)	0.100(6)	0.106(6)	0.061(4)	0.082(5)	0.020(4)	0.024(4)
C(39)	0.061(4)	0.089(5)	0.068(5)	0.043(4)	-0.006(3)	-0.003(4)
C(40)	0.048(4)	0.066(5)	0.076(4)	0.025(3)	0.029(4)	0.004(3)
C(41)	0.052(4)	0.051(4)	0.051(4)	0.020(3)	0.022(3)	0.010(3)
C(42)	0.156(5)	0.131(7)	0.083(6)	0.056(4)	-0.033(2)	-0.007(5)

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 7. Bond Lengths($\AA$) Involving Hydrogen

atom	atom	distance	atom	atom	distance
C(1)	H(1)	0.98	C(2)	H(2)	0.98
C(3)	H(3)	0.98	C(4)	H(4)	0.98
C(5)	H(5)	0.99	C(7)	H(6)	0.98
C(8)	H(7)	0.98	C(9)	H(8)	0.98
C(10)	H(9)	0.98	C(11)	H(10)	0.98
C(13)	H(11)	0.98	C(14)	H(12)	0.98
C(15)	H(13)	0.98	C(16)	H(14)	0.98
C(17)	H(15)	0.98	C(19)	H(16)	0.98
C(20)	H(17)	0.98	C(21)	H(18)	0.98
C(22)	H(19)	0.98	C(23)	H(20)	0.98
C(25)	H(21)	0.98	C(26)	H(22)	0.98
C(27)	H(23)	0.98	C(28)	H(24)	0.98
C(29)	H(25)	0.98	C(31)	H(26)	0.98
C(32)	H(27)	0.98	C(33)	H(28)	0.98
C(34)	H(29)	0.98	C(35)	H(30)	0.98
C(37)	H(31)	0.98	C(38)	H(32)	0.98
C(39)	H(33)	0.98	C(40)	H(34)	0.98
C(41)	H(35)	0.98	C(42)	H(36)	0.98
C(42)	H(37)	0.98			

Table 8. Bond Angles(°) Involving Hydrogen

atom	atom	atom	angle	atom	atom	atom	angle
C(2)	C(1)	H(1)	125.9	C(5)	C(1)	H(1)	125.1
C(1)	C(2)	H(2)	125.6	C(3)	C(2)	H(2)	125.6
C(2)	C(3)	H(3)	126.9	C(4)	C(3)	H(3)	125.7
C(3)	C(4)	H(4)	127.0	C(5)	C(4)	H(4)	125.9
C(1)	C(5)	H(5)	126.4	C(4)	C(5)	H(5)	126.0
C(6)	C(7)	H(6)	119.7	C(8)	C(7)	H(6)	120.1
C(7)	C(8)	H(7)	120.2	C(9)	C(8)	H(7)	119.9
C(8)	C(9)	H(8)	120.7	C(10)	C(9)	H(8)	119.8
C(9)	C(10)	H(9)	119.5	C(11)	C(10)	H(9)	118.7
C(6)	C(11)	H(10)	120.3	C(10)	C(11)	H(10)	120.2
C(12)	C(13)	H(11)	120.0	C(14)	C(13)	H(11)	120.4
C(13)	C(14)	H(12)	119.5	C(15)	C(14)	H(12)	119.9
C(14)	C(15)	H(13)	120.7	C(16)	C(15)	H(13)	120.2
C(15)	C(16)	H(14)	120.0	C(17)	C(16)	H(14)	119.1
C(12)	C(17)	H(15)	119.9	C(16)	C(17)	H(15)	120.3
C(18)	C(19)	H(16)	119.7	C(20)	C(19)	H(16)	119.6
C(19)	C(20)	H(17)	119.3	C(21)	C(20)	H(17)	120.2
C(20)	C(21)	H(18)	119.4	C(22)	C(21)	H(18)	120.6
C(21)	C(22)	H(19)	119.4	C(23)	C(22)	H(19)	119.8
C(18)	C(23)	H(20)	119.8	C(22)	C(23)	H(20)	120.2
C(24)	C(25)	H(21)	119.5	C(26)	C(25)	H(21)	119.4
C(25)	C(26)	H(22)	120.2	C(27)	C(26)	H(22)	120.1
C(26)	C(27)	H(23)	120.1	C(28)	C(27)	H(23)	120.2
C(27)	C(28)	H(24)	119.5	C(29)	C(28)	H(24)	119.8

Table 8. Bond Angles(°) Involving Hydrogen (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C(24)	C(29)	H(25)	120.2	C(28)	C(29)	H(25)	120.1
C(30)	C(31)	H(26)	119.9	C(32)	C(31)	H(26)	119.2
C(31)	C(32)	H(27)	121.1	C(33)	C(32)	H(27)	120.3
C(32)	C(33)	H(28)	118.8	C(34)	C(33)	H(28)	118.9
C(33)	C(34)	H(29)	119.3	C(35)	C(34)	H(29)	120.6
C(30)	C(35)	H(30)	121.1	C(34)	C(35)	H(30)	120.1
C(36)	C(37)	H(31)	119.3	C(38)	C(37)	H(31)	119.0
C(37)	C(38)	H(32)	120.5	C(39)	C(38)	H(32)	118.9
C(38)	C(39)	H(33)	121.5	C(40)	C(39)	H(33)	119.7
C(39)	C(40)	H(34)	120.0	C(41)	C(40)	H(34)	119.5
C(36)	C(41)	H(35)	119.9	C(40)	C(41)	H(35)	119.2
Cl(4)	C(42)	H(36)	108.3	Cl(4)	C(42)	H(37)	108.2
Cl(5)	C(42)	H(36)	109.0	Cl(5)	C(42)	H(37)	108.9
H(36)	C(42)	H(37)	109.3				

Table 9. Torsion Angles(°)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
P(1)	N(2)	P(2)	C(24)	-108.2(6)	P(1)	N(2)	P(2)	C(30)	133.4(6)
P(1)	N(2)	P(2)	C(36)	13.3(7)	P(1)	C(6)	C(7)	C(8)	-176.7(6)
P(1)	C(6)	C(11)	C(10)	175.4(6)	P(1)	C(12)	C(13)	C(14)	177.9(6)
P(1)	C(12)	C(17)	C(16)	-176.7(6)	P(1)	C(18)	C(19)	C(20)	-177.0(6)
P(1)	C(18)	C(23)	C(22)	177.6(5)	P(2)	N(2)	P(1)	C(6)	-68.6(6)
P(2)	N(2)	P(1)	C(12)	56.1(7)	P(2)	N(2)	P(1)	C(18)	173.8(5)
P(2)	C(24)	C(25)	C(26)	-177.2(6)	P(2)	C(24)	C(29)	C(28)	176.9(5)
P(2)	C(30)	C(31)	C(32)	-178.7(6)	P(2)	C(30)	C(35)	C(34)	178.0(6)
P(2)	C(36)	C(37)	C(38)	-171.6(7)	P(2)	C(36)	C(41)	C(40)	170.9(6)
N(2)	P(1)	C(6)	C(7)	5.5(7)	N(2)	P(1)	C(6)	C(11)	-170.7(6)
N(2)	P(1)	C(12)	C(13)	-121.6(6)	N(2)	P(1)	C(12)	C(17)	56.4(7)
N(2)	P(1)	C(18)	C(19)	-156.2(5)	N(2)	P(1)	C(18)	C(23)	25.6(6)
N(2)	P(2)	C(24)	C(25)	-19.2(7)	N(2)	P(2)	C(24)	C(29)	164.5(5)
N(2)	P(2)	C(30)	C(31)	-12.8(7)	N(2)	P(2)	C(30)	C(35)	167.8(6)
N(2)	P(2)	C(36)	C(37)	111.6(6)	N(2)	P(2)	C(36)	C(41)	-59.2(6)
C(1)	C(2)	C(3)	C(4)	0(1)	C(1)	C(5)	C(4)	C(3)	2(1)
C(2)	C(1)	C(5)	C(4)	-2(1)	C(2)	C(3)	C(4)	C(5)	-1(1)
C(3)	C(2)	C(1)	C(5)	1(1)	C(6)	P(1)	C(12)	C(13)	5.3(7)
C(6)	P(1)	C(12)	C(17)	-176.7(5)	C(6)	P(1)	C(18)	C(19)	82.0(6)
C(6)	P(1)	C(18)	C(23)	-96.3(6)	C(6)	C(7)	C(8)	C(9)	1(1)
C(6)	C(11)	C(10)	C(9)	1(1)	C(7)	C(6)	P(1)	C(12)	-121.4(6)
C(7)	C(6)	P(1)	C(18)	124.1(6)	C(7)	C(6)	C(11)	C(10)	0(1)
C(7)	C(8)	C(9)	C(10)	0(1)	C(8)	C(7)	C(6)	C(11)	0(1)
C(8)	C(9)	C(10)	C(11)	0(1)	C(11)	C(6)	P(1)	C(12)	62.4(7)

Table 9. Torsion Angles(°) (continued)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
C(11)	C(6)	P(1)	C(18)	-52.1(7)	C(12)	P(1)	C(18)	C(19)	-34.3(6)
C(12)	P(1)	C(18)	C(23)	147.4(5)	C(12)	C(13)	C(14)	C(15)	-1(1)
C(12)	C(17)	C(16)	C(15)	-1(1)	C(13)	C(12)	P(1)	C(18)	119.8(6)
C(13)	C(12)	C(17)	C(16)	1(1)	C(13)	C(14)	C(15)	C(16)	0(1)
C(14)	C(13)	C(12)	C(17)	0(1)	C(14)	C(15)	C(16)	C(17)	0(1)
C(17)	C(12)	P(1)	C(18)	-62.2(6)	C(18)	C(19)	C(20)	C(21)	-1(1)
C(18)	C(23)	C(22)	C(21)	0(1)	C(19)	C(18)	C(23)	C(22)	0(1)
C(19)	C(20)	C(21)	C(22)	1(1)	C(20)	C(19)	C(18)	C(23)	1(1)
C(20)	C(21)	C(22)	C(23)	0(1)	C(24)	P(2)	C(30)	C(31)	-132.1(6)
C(24)	P(2)	C(30)	C(35)	48.4(7)	C(24)	P(2)	C(36)	C(37)	-125.4(6)
C(24)	P(2)	C(36)	C(41)	63.8(6)	C(24)	C(25)	C(26)	C(27)	1(1)
C(24)	C(29)	C(28)	C(27)	0(1)	C(25)	C(24)	P(2)	C(30)	98.8(6)
C(25)	C(24)	P(2)	C(36)	-145.4(6)	C(25)	C(24)	C(29)	C(28)	0(1)
C(25)	C(26)	C(27)	C(28)	0(1)	C(26)	C(25)	C(24)	C(29)	0(1)
C(26)	C(27)	C(28)	C(29)	0(1)	C(29)	C(24)	P(2)	C(30)	-77.5(6)
C(29)	C(24)	P(2)	C(36)	38.2(6)	C(30)	P(2)	C(36)	C(37)	-8.9(7)
C(30)	P(2)	C(36)	C(41)	-179.8(5)	C(30)	C(31)	C(32)	C(33)	0(1)
C(30)	C(35)	C(34)	C(33)	1(1)	C(31)	C(30)	P(2)	C(36)	112.3(6)
C(31)	C(30)	C(35)	C(34)	-1(1)	C(31)	C(32)	C(33)	C(34)	0(1)
C(32)	C(31)	C(30)	C(35)	0(1)	C(32)	C(33)	C(34)	C(35)	0(1)
C(35)	C(30)	P(2)	C(36)	-67.2(7)	C(36)	C(37)	C(38)	C(39)	2(1)
C(36)	C(41)	C(40)	C(39)	0(1)	C(37)	C(36)	C(41)	C(40)	0(1)
C(37)	C(38)	C(39)	C(40)	-3(1)	C(38)	C(37)	C(36)	C(41)	0(1)
C(38)	C(39)	C(40)	C(41)	1(1)					

Table 10. Non-bonded Contacts out to 3.80 Å

atom	atom	distance	ADC
Cl(1)	C(26)	3.658(9)	65601
Cl(2)	C(9)	3.548(9)	1
Cl(2)	C(35)	3.660(8)	55602
Cl(3)	C(9)	3.44(2)	1
Cl(3)	C(13)	3.66(1)	66602
O(1a)	C(32)	3.42(3)	65501
O(1b)	C(14)	3.37(3)	55601
O(1b)	C(8)	3.46(4)	1
O(1c)	C(13)	3.34(3)	66602
O(1c)	C(10)	3.40(3)	1
N(1b)	C(9)	3.59(4)	1
C(4)	C(22)	3.40(1)	65601
C(5)	C(21)	3.56(1)	65601
C(33)	C(33)	3.54(2)	45602
Cl(1)	H(17)	2.83	66602
Cl(1)	H(37)	2.83	1
Cl(2)	H(8)	2.80	1
Cl(3)	H(8)	2.66	1
Cl(3)	H(10)	2.95	66602
O(1a)	H(27)	2.55	65501
O(1a)	H(17)	2.72	66602
O(1b)	H(13)	2.58	55601
O(1b)	H(7)	2.80	1
O(1b)	H(8)	2.83	1

atom	atom	distance	ADC
Cl(1)	C(32)	3.677(8)	65501
Cl(2)	C(14)	3.650(9)	55601
Cl(2)	C(15)	3.69(1)	55601
Cl(3)	C(42)	3.66(2)	1
O(1a)	C(26)	3.33(3)	65601
O(1b)	C(15)	3.27(3)	55601
O(1b)	C(35)	3.44(4)	55602
O(1b)	C(9)	3.47(4)	1
O(1c)	C(9)	3.36(4)	1
O(1c)	C(11)	3.41(2)	66602
N(1c)	C(9)	3.53(5)	1
C(4)	C(23)	3.42(1)	65601
C(16)	C(39)	3.43(1)	2
Cl(1)	H(27)	2.80	65501
Cl(1)	H(22)	2.83	65601
Cl(2)	H(30)	2.79	55602
Cl(2)	H(12)	2.97	55601
Cl(3)	H(36)	2.87	1
Cl(3)	H(16)	2.96	66602
O(1a)	H(22)	2.59	65601
O(1b)	H(30)	2.57	55602
O(1b)	H(12)	2.78	55601
O(1b)	H(25)	2.80	55602
O(1c)	H(10)	2.57	66602

Table 10. Non-bonded Contacts out to 3.80 Å (continued)

atom	atom	distance	ADC	atom	atom	distance	ADC
O(1c)	H(8)	2.70	1	O(1c)	H(9)	2.78	1
O(1c)	H(36)	2.84	1	N(1a)	H(37)	2.88	1
N(1b)	H(8)	2.74	1	N(1c)	H(8)	2.66	1
C(10)	H(19)	2.98	56602	C(11)	H(19)	2.91	56602
C(16)	H(5)	2.99	66602	C(29)	H(34)	2.90	2
C(33)	H(33)	2.92	55602	H(3)	H(21)	2.57	65601
H(4)	H(15)	2.38	65601	H(12)	H(25)	2.64	2
H(31)	H(32)	2.47	55602	H(34)	H(35)	2.63	2

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

Table 11. Least Squares Planes

Plane number 1

Atoms defining plane	Distance
C(1)	0.013(8)
C(2)	-0.005(8)
C(3)	-0.006(9)
C(4)	0.014(8)
C(5)	-0.016(8)
Additional Atoms	**Distance**
Cr(1)	-1.881

Plane number 2

Atoms defining plane	Distance
C(6)	-0.001(6)
C(7)	-0.005(7)
C(8)	0.007(8)
C(9)	0.001(8)
C(10)	-0.008(8)
C(11)	0.007(7)
Additional Atoms	**Distance**
P(1)	-0.106

Plane number 3

Atoms defining plane	Distance
C(12)	-0.004(7)
C(13)	-0.003(7)
C(14)	0.008(8)
C(15)	-0.003(9)
C(16)	-0.007(8)
C(17)	0.009(7)
Additional Atoms	**Distance**
P(1)	-0.073

Plane number 4

Atoms defining plane	Distance
C(18)	0.003(6)
C(19)	-0.006(7)
C(20)	0.006(8)
C(21)	-0.002(8)
C(22)	0.000(7)
C(23)	-0.001(7)
Additional Atoms	Distance
P(1)	0.066

Plane number 5

Atoms defining plane	Distance
C(24)	0.002(6)
C(25)	-0.004(8)
C(26)	0.004(8)
C(27)	-0.002(8)
C(28)	0.001(7)
C(29)	-0.001(7)
Additional Atoms	Distance
P(2)	-0.084

Plane number 6

Atoms defining plane	Distance
C(30)	0.005(7)
C(31)	-0.002(7)
C(32)	-0.004(8)
C(33)	0.004(9)
C(34)	0.003(9)
C(35)	-0.008(8)
Additional Atoms	Distance
P(2)	0.045

Plane number 7

Atoms defining plane	Distance
C(36)	0.003(6)
C(37)	0.005(8)
C(38)	-0.016(9)
C(39)	0.012(9)
C(40)	-0.001(8)
C(41)	-0.005(7)

Additional Atoms	Distance
P(2)	0.247

Summary

plane	mean deviation	χ^2
1	0.0107	7.9
2	0.0049	2.9
3	0.0055	3.6
4	0.0031	1.5
5	0.0024	0.7
6	0.0043	2.0
7	0.0072	5.6

Dihedral angles between planes (°)

plane	1	2	3	4	5	6
2	114.7					
3	72.2	115.6				
4	12.3	102.5	78.1			
5	103.1	42.3	73.3	95.0		
6	55.5	60.1	103.6	43.2	69.9	
7	38.3	116.6	34.5	43.6	82.4	75.8