Radiation	MoKα (λ = 0.71069 $\AA$) graphite monochromated
Take-off Angle	2.8°
Detector Aperture	2.0 - 2.5 mm horizontal 2.0 mm vertical
Crystal to Detector Distance	21 mm
Temperature	20.0°C
Scan Type	ω
Scan Rate	0.0°/min (in ω) (up to 0 scans)
Scan Width	$(0.00 + 0.00 \tan \theta)°$
$2\theta_{max}$	46.5°
No. of Reflections Measured	Total: 6123 Unique: 2462 (R_{int} = 0.040)
Corrections	Lorentz-polarization

C. Structure Solution and Refinement

Structure Solution	Direct Methods (SHELXS86)
Refinement	Full-matrix least-squares
Function Minimized	$\Sigma w(\lvert Fo\rvert - \lvert Fc\rvert)^2$
Least Squares Weights	$w = \frac{1}{\sigma^2(Fo)} = [\sigma_c^2(Fo) + \frac{p^2}{4}Fo^2]^{-1}$
p-factor	0.0000
No. Observations (I>3.00σ(I))	1737
No. Variables	208
Reflection/Parameter Ratio	8.35
Residuals: R; Rw	0.055 ; 0.067
Goodness of Fit Indicator	4.39
Max Shift/Error in Final Cycle	0.00
Maximum peak in Final Diff. Map	0.20 $e^-/\AA^3$

Minimum peak in Final Diff. Map	-0.27 $e^-/Å^3$

Table 1. Atomic coordinates and B_{iso}/B_{eq}

atom	x	y	z	B_{eq}
O(1)	0.2676(3)	0.6784(2)	0.9724(1)	5.95(7)
O(2)	0.1751(2)	0.7956(2)	0.8738(1)	5.56(6)
O(3)	0.8454(2)	0.9227(2)	0.7483(1)	4.91(6)
C(1)	0.0359(4)	0.7243(4)	0.8763(2)	6.5(1)
C(2)	0.2841(4)	0.7607(3)	0.9248(2)	4.40(8)
C(3)	0.4240(3)	0.8379(3)	0.9159(2)	3.86(8)
C(4)	0.5383(4)	0.8254(3)	0.9723(2)	4.33(8)
C(5)	0.6713(4)	0.8946(3)	0.9663(2)	4.32(8)
C(6)	0.6963(3)	0.9748(3)	0.9034(2)	3.99(7)
C(7)	0.5783(3)	0.9877(3)	0.8475(2)	4.37(8)
C(8)	0.4472(4)	0.9196(3)	0.8544(2)	4.45(8)
C(9)	0.8347(3)	1.0499(3)	0.9004(2)	4.18(8)
C(10)	0.9107(3)	1.0926(3)	0.8396(2)	3.90(7)
C(11)	0.8740(3)	1.0522(3)	0.7610(2)	4.11(8)
C(12)	0.8621(4)	1.1150(3)	0.6932(2)	4.97(9)
C(13)	0.8243(4)	1.0238(4)	0.6356(2)	5.44(10)
C(14)	0.8162(4)	0.9082(4)	0.6716(2)	5.55(10)
C(15)	1.0365(3)	1.1870(3)	0.8506(2)	4.15(8)
C(16)	1.0290(3)	1.2853(3)	0.9043(2)	4.58(8)
C(17)	1.1457(4)	1.3750(3)	0.9162(2)	5.37(10)
C(18)	1.2710(4)	1.3639(4)	0.8730(2)	6.0(1)
C(19)	1.2820(4)	1.2701(4)	0.8189(2)	5.9(1)
C(20)	1.1640(4)	1.1823(3)	0.8057(2)	5.09(9)
H(1)	-0.0015	0.7335	0.9281	6.9655

Table 1. Atomic coordinates and B_{iso}/B_{eq} (continued)

atom	x	y	z	B_{eq}
H(2)	-0.0311	0.7607	0.8413	6.9655
H(3)	0.0571	0.6375	0.8673	6.9655
H(4)	0.5179	0.7726	1.0158	6.9655
H(5)	0.7448	0.8837	1.0040	6.9655
H(6)	0.5953	1.0437	0.8058	6.9655
H(7)	0.3669	0.9319	0.8175	6.9655
H(8)	0.8814	1.0686	0.9502	6.9655
H(9)	0.8717	1.2038	0.6903	6.9655
H(10)	0.8149	1.0458	0.5818	6.9655
H(11)	0.7889	0.8273	0.6490	6.9655
H(12)	0.9405	1.2926	0.9313	6.9655
H(13)	1.1311	1.4439	0.9546	6.9655
H(14)	1.3489	1.4243	0.8809	6.9655
H(15)	1.3750	1.2670	0.7896	6.9655
H(16)	1.1716	1.1191	0.7660	6.9655

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

Table 2. Anisotropic Displacement Parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
O(1)	0.074(2)	0.078(2)	0.074(2)	-0.014(1)	-0.003(1)	0.028(1)
O(2)	0.056(1)	0.079(2)	0.076(2)	-0.007(1)	-0.007(1)	0.022(1)
O(3)	0.069(2)	0.049(1)	0.067(2)	-0.003(1)	-0.011(1)	-0.004(1)
C(1)	0.058(2)	0.100(3)	0.088(3)	-0.009(2)	-0.004(2)	0.019(2)
C(2)	0.054(2)	0.057(2)	0.057(2)	0.005(2)	0.006(2)	-0.003(2)
C(3)	0.052(2)	0.047(2)	0.048(2)	0.005(1)	0.006(2)	0.001(1)
C(4)	0.058(2)	0.058(2)	0.049(2)	0.001(2)	0.004(2)	0.005(2)
C(5)	0.062(2)	0.055(2)	0.046(2)	0.002(2)	-0.002(2)	0.001(2)
C(6)	0.057(2)	0.044(2)	0.051(2)	0.001(2)	0.003(2)	-0.007(1)
C(7)	0.051(2)	0.056(2)	0.059(2)	-0.002(2)	-0.001(2)	0.010(2)
C(8)	0.054(2)	0.060(2)	0.055(2)	0.007(2)	-0.004(2)	0.006(2)
C(9)	0.057(2)	0.050(2)	0.051(2)	0.000(2)	-0.006(2)	-0.001(2)
C(10)	0.059(2)	0.040(2)	0.049(2)	0.002(2)	-0.004(2)	0.001(1)
C(11)	0.043(2)	0.051(2)	0.062(2)	-0.003(1)	-0.001(1)	0.000(2)
C(12)	0.066(2)	0.063(2)	0.060(2)	-0.010(2)	-0.003(2)	0.014(2)
C(13)	0.063(2)	0.090(3)	0.053(2)	-0.009(2)	-0.005(2)	0.003(2)
C(14)	0.059(2)	0.082(3)	0.069(3)	-0.006(2)	-0.012(2)	-0.020(2)
C(15)	0.043(2)	0.057(2)	0.057(2)	0.002(2)	-0.009(2)	0.004(2)
C(16)	0.058(2)	0.056(2)	0.059(2)	-0.004(2)	-0.010(2)	-0.002(2)
C(17)	0.065(2)	0.061(2)	0.078(3)	-0.006(2)	-0.014(2)	0.009(2)
C(18)	0.074(3)	0.070(3)	0.081(3)	-0.023(2)	-0.023(2)	0.018(2)
C(19)	0.052(2)	0.091(3)	0.080(3)	-0.009(2)	-0.005(2)	0.015(2)
C(20)	0.056(2)	0.073(2)	0.064(2)	0.000(2)	-0.003(2)	0.001(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 3. Bond Lengths(Å)

atom	atom	distance	atom	atom	distance
O(1)	C(2)	1.197(4)	O(2)	C(1)	1.440(4)
O(2)	C(2)	1.342(4)	O(3)	C(11)	1.374(3)
O(3)	C(14)	1.360(4)	C(2)	C(3)	1.488(4)
C(3)	C(4)	1.396(4)	C(3)	C(8)	1.383(4)
C(4)	C(5)	1.388(4)	C(5)	C(6)	1.396(4)
C(6)	C(7)	1.414(4)	C(6)	C(9)	1.456(4)
C(7)	C(8)	1.369(4)	C(9)	C(10)	1.347(4)
C(10)	C(11)	1.457(4)	C(10)	C(15)	1.490(4)
C(11)	C(12)	1.348(4)	C(12)	C(13)	1.407(4)
C(13)	C(14)	1.348(5)	C(15)	C(16)	1.381(4)
C(15)	C(20)	1.398(4)	C(16)	C(17)	1.399(4)
C(17)	C(18)	1.369(5)	C(18)	C(19)	1.355(5)
C(19)	C(20)	1.398(5)			

Table 4. Bond Lengths(Å)

atom	atom	distance	atom	atom	distance
C(1)	H(1)	0.98	C(1)	H(2)	0.92
C(1)	H(3)	0.93	C(4)	H(4)	0.95
C(5)	H(5)	0.92	C(7)	H(6)	0.94
C(8)	H(7)	0.95	C(9)	H(8)	0.97
C(12)	H(9)	0.92	C(13)	H(10)	0.96
C(14)	H(11)	0.95	C(16)	H(12)	0.93
C(17)	H(13)	0.99	C(18)	H(14)	0.94
C(19)	H(15)	0.99	C(20)	H(16)	0.95

Table 5. Bond Angles(°)

atom	atom	atom	angle	atom	atom	atom	angle
C(1)	O(2)	C(2)	116.5(3)	C(11)	O(3)	C(14)	107.1(3)
O(1)	C(2)	O(2)	123.1(3)	O(1)	C(2)	C(3)	124.8(3)
O(2)	C(2)	C(3)	112.1(3)	C(2)	C(3)	C(4)	118.0(3)
C(2)	C(3)	C(8)	123.4(3)	C(4)	C(3)	C(8)	118.6(3)
C(3)	C(4)	C(5)	120.2(3)	C(4)	C(5)	C(6)	121.3(3)
C(5)	C(6)	C(7)	117.6(3)	C(5)	C(6)	C(9)	119.9(3)
C(7)	C(6)	C(9)	122.3(3)	C(6)	C(7)	C(8)	120.4(3)
C(3)	C(8)	C(7)	121.8(3)	C(6)	C(9)	C(10)	130.3(3)
C(9)	C(10)	C(11)	122.9(3)	C(9)	C(10)	C(15)	120.3(3)
C(11)	C(10)	C(15)	116.8(3)	O(3)	C(11)	C(10)	117.5(3)
O(3)	C(11)	C(12)	108.4(3)	C(10)	C(11)	C(12)	134.1(3)
C(11)	C(12)	C(13)	108.4(3)	C(12)	C(13)	C(14)	105.8(3)
O(3)	C(14)	C(13)	110.4(3)	C(10)	C(15)	C(16)	120.9(3)
C(10)	C(15)	C(20)	121.6(3)	C(16)	C(15)	C(20)	117.5(3)
C(15)	C(16)	C(17)	122.2(3)	C(16)	C(17)	C(18)	118.4(3)
C(17)	C(18)	C(19)	121.4(3)	C(18)	C(19)	C(20)	120.3(3)
C(15)	C(20)	C(19)	120.2(3)				

Table 6. Bond Angles(°)

atom	atom	atom	angle	atom	atom	atom	angle
O(2)	C(1)	H(1)	107.3	O(2)	C(1)	H(2)	108.2
O(2)	C(1)	H(3)	107.9	H(1)	C(1)	H(2)	109.8
H(1)	C(1)	H(3)	109.1	H(2)	C(1)	H(3)	114.3
C(3)	C(4)	H(4)	117.3	C(5)	C(4)	H(4)	122.4
C(4)	C(5)	H(5)	118.2	C(6)	C(5)	H(5)	120.4
C(6)	C(7)	H(6)	117.1	C(8)	C(7)	H(6)	122.5
C(3)	C(8)	H(7)	118.5	C(7)	C(8)	H(7)	119.6
C(6)	C(9)	H(8)	114.3	C(10)	C(9)	H(8)	115.3
C(11)	C(12)	H(9)	121.3	C(13)	C(12)	H(9)	130.2
C(12)	C(13)	H(10)	123.1	C(14)	C(13)	H(10)	130.9
O(3)	C(14)	H(11)	122.8	C(13)	C(14)	H(11)	126.7
C(15)	C(16)	H(12)	117.4	C(17)	C(16)	H(12)	120.3
C(16)	C(17)	H(13)	117.6	C(18)	C(17)	H(13)	124.1
C(17)	C(18)	H(14)	118.3	C(19)	C(18)	H(14)	120.4
C(18)	C(19)	H(15)	117.7	C(20)	C(19)	H(15)	122.1
C(15)	C(20)	H(16)	120.5	C(19)	C(20)	H(16)	119.3

Table 7. Torsion Angles(°)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
O(1)	C(2)	O(2)	C(1)	-2.8(5)	O(1)	C(2)	C(3)	C(4)	-8.1(5)
O(1)	C(2)	C(3)	C(8)	170.9(3)	O(2)	C(2)	C(3)	C(4)	170.6(3)
O(2)	C(2)	C(3)	C(8)	-10.3(4)	O(3)	C(11)	C(10)	C(9)	-44.0(4)
O(3)	C(11)	C(10)	C(15)	137.2(3)	O(3)	C(11)	C(12)	C(13)	0.2(3)
O(3)	C(14)	C(13)	C(12)	0.6(4)	C(1)	O(2)	C(2)	C(3)	178.5(3)
C(2)	C(3)	C(4)	C(5)	179.5(3)	C(2)	C(3)	C(8)	C(7)	-179.0(3)
C(3)	C(4)	C(5)	C(6)	-1.9(5)	C(3)	C(8)	C(7)	C(6)	1.0(5)
C(4)	C(3)	C(8)	C(7)	0.0(5)	C(4)	C(5)	C(6)	C(7)	2.9(4)
C(4)	C(5)	C(6)	C(9)	177.6(3)	C(5)	C(4)	C(3)	C(8)	0.4(4)
C(5)	C(6)	C(7)	C(8)	-2.4(4)	C(5)	C(6)	C(9)	C(10)	152.0(3)
C(6)	C(9)	C(10)	C(11)	-9.1(5)	C(6)	C(9)	C(10)	C(15)	169.7(3)
C(7)	C(6)	C(9)	C(10)	-33.5(5)	C(8)	C(7)	C(6)	C(9)	-177.0(3)
C(9)	C(10)	C(11)	C(12)	136.8(4)	C(9)	C(10)	C(15)	C(16)	-37.3(4)
C(9)	C(10)	C(15)	C(20)	144.6(3)	C(10)	C(11)	O(3)	C(14)	-179.2(2)
C(10)	C(11)	C(12)	C(13)	179.4(3)	C(10)	C(15)	C(16)	C(17)	179.6(3)
C(10)	C(15)	C(20)	C(19)	-178.2(3)	C(11)	O(3)	C(14)	C(13)	-0.4(4)
C(11)	C(10)	C(15)	C(16)	141.5(3)	C(11)	C(10)	C(15)	C(20)	-36.6(4)
C(11)	C(12)	C(13)	C(14)	-0.5(4)	C(12)	C(11)	O(3)	C(14)	0.1(3)
C(12)	C(11)	C(10)	C(15)	-42.0(5)	C(15)	C(16)	C(17)	C(18)	-0.1(5)
C(15)	C(20)	C(19)	C(18)	-2.8(5)	C(16)	C(15)	C(20)	C(19)	3.6(5)
C(16)	C(17)	C(18)	C(19)	1.0(5)	C(17)	C(16)	C(15)	C(20)	-2.2(5)
C(17)	C(18)	C(19)	C(20)	0.4(6)					

Table 8. Non-bonded Contacts out to 3.60 Å

atom	atom	distance	ADC	atom	atom	distance	ADC
O(1)	C(17)	3.438(4)	44501	O(1)	C(16)	3.474(4)	67703
O(1)	C(13)	3.547(4)	46504	O(1)	C(14)	3.597(4)	46504
O(2)	C(19)	3.401(4)	64602	O(3)	C(1)	3.431(4)	65501
C(3)	C(5)	3.552(4)	67703	C(3)	C(12)	3.567(4)	64602
C(14)	C(16)	3.537(4)	64602				

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)	1/2-X,	1/2+Y,	1/2-Z
(3)	-X,	-Y,	-Z	(4)	1/2+X,	1/2-Y,	1/2+Z