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Experimental

Data Collection

A dark brownneedle needle crystal of $C_{26}H_{32}N_5O_4$ having approximate dimensions of 0.20 x 0.20 x 0.10 mm was mounted on a glass fiber. All measurements were made on a Rigaku RAXIS-IV imaging plate area detector with graphite monochromated Mo-Kα radiation.

Indexing was performed from 3 oscillations which were exposed for 4.0 minutes. The crystal-to-detector distance was 110.00 mm with the detector at the zero swing position. Readout was performed in the 0.100 mm pixel mode.

Cell constants and an orientation matrix for data collection corresponded to a primitive orthorhombic cell with dimensions:

a = 21.211(4) $\AA$
b = 6.1216(8) $\AA$
c = 19.01(1) $\AA$
V = 2468(3) $\AA^3$

For Z = 4 and F.W. = 478.57, the calculated density is 1.29 g/cm^3. Based on the systematic absences of:

0kl: k+l $\neq$ 2n
h0l: h $\neq$ 2n

packing considerations, a statistical analysis of intensity distribution, and the successful solution and refinement of the structure, the space group was determined to be:

$Pna2_1$ (#33)

The data were collected at a temperature of -150 $\pm$ 1°C to a maximum 2θ value of 55.0°. A total of 21 5.00° oscillation images were collected, each being exposed for 30.0 minutes. The crystal-to-detector distance was 110.00 mm with the detector at the zero swing position. Readout was performed in the 0.100 mm pixel mode.

Data Reduction

A total of 2681 reflections was collected.

The linear absorption coefficient, μ, for Mo-Kα radiation is 0.0 cm^{-1}. The data were corrected for Lorentz and polarization effects.

Structure Solution and Refinement

The structure was solved by direct methods[1] and expanded using Fourier techniques[2]. The non-hydrogen atoms were refined anisotropically. Hydrogen atoms were included but not refined. The final cycle of full-matrix least-squares refinement[3] was based on 2226 observed reflections ($I > 2.50\sigma(I)$) and 316 variable parameters and converged (largest parameter shift was 0.00 times its esd) with unweighted and weighted agreement factors of:

$$R = \Sigma||Fo| - |Fc||/\Sigma|Fo| = 0.066$$

$$R_w = \sqrt{\Sigma w(|Fo| - |Fc|)^2/\Sigma wFo^2} = 0.096$$

The standard deviation of an observation of unit weight[4] was 1.82. The weighting scheme was based on counting statistics and included a factor (p = 0.080) to downweight the intense reflections. Plots of $\Sigma w(|Fo| - |Fc|)^2$ versus $|Fo|$, 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 0.97 and -0.29 $e^-/\AA^3$, 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 Hubbel[8]. All calculations were performed using the teXsan[9] crystallographic software package of Molecular Structure Corporation.

References

(1) SHELXS86: Sheldrick, G.M. (1985). In: "Crystallographic Computing 3" (Eds G.M. Sheldrick, C. Kruger and R. Goddard) Oxford University Press, pp. 175-189.

(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: $\Sigma w(|Fo| - |Fc|)^2$

(4) Standard deviation of an observation of unit weight:

$$\sqrt{\Sigma w(|Fo| - |Fc|)^2/(No - Nv)}$$

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).

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

EXPERIMENTAL DETAILS

A. Crystal Data

Empirical Formula	$C_{26}H_{32}N_5O_4$
Formula Weight	478.57
Crystal Color, Habit	dark brownneedle, needle
Crystal Dimensions	0.20 X 0.20 X 0.10 mm
Crystal System	orthorhombic
Lattice Type	Primitive
Indexing Images	3 oscillations @ 4.0 minutes
Detector Position	110.00 mm
Detector Swing Angle	0.00°
Pixel Size	0.100 mm
Lattice Parameters	a = 21.211(4)Å b = 6.1216(8) Å c = 19.01(1) Å
	V = 2468(3) Å^3
Space Group	$Pna2_1$ (#33)
Z value	4
D_{calc}	1.288 g/cm^3
F_{000}	1020.00
μ(MoKα)	0.00 cm^{-1}

B. Intensity Measurements

Diffractometer	RAXIS-IV
Radiation	MoKα (λ = 0.71070 Å)

	graphite monochromated
Detector Aperture	300 mm x 300 mm
Data Images	21 exposures @ 30.0 minutes
Oscillation Range	5.0°
Detector Position	110.00 mm
Detector Swing Angle	0.00°
Pixel Size	0.100 mm
$2\theta_{max}$	55.0°
No. of Reflections Measured	Total: 2681
Corrections	Lorentz-polarization

C. Structure Solution and Refinement

Structure Solution	Direct Methods (SHELXS86)
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	0.0800
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (I>2.50σ(I))	2226
No. Variables	316
Reflection/Parameter Ratio	7.04
Residuals: R; Rw	0.066 ; 0.096
Goodness of Fit Indicator	1.82
Max Shift/Error in Final Cycle	0.00
Maximum peak in Final Diff. Map	0.97 $e^-/\AA^3$
Minimum peak in Final Diff. Map	-0.29 $e^-/\AA^3$

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

atom	x	y	z	B_{eq}
O(1)	0.1281(2)	0.4677(4)	0.5051(7)	3.72(8)
O(2)	0.4193(2)	0.0104(6)	0.4428(7)	3.93(9)
O(3)	0.2880(2)	-0.4023(6)	0.3014(7)	3.40(7)
O(4)	-0.1650(2)	0.0469(6)	0.5774(7)	3.17(8)
N(1)	0.1258(2)	0.2573(5)	0.5059(7)	1.82(6)
N(2)	0.3980(2)	-0.1172(5)	0.3959(7)	2.08(7)
N(3)	0.3361(2)	-0.3145(6)	0.3283(7)	1.87(7)
N(4)	-0.1462(2)	-0.0832(6)	0.6263(7)	1.94(7)
N(5)	-0.0793(2)	-0.2787(6)	0.6920(7)	2.04(8)
C(1)	0.1776(2)	0.1457(6)	0.4760(7)	1.44(7)
C(2)	0.2361(2)	0.2515(6)	0.4726(7)	1.72(8)
C(3)	0.2872(2)	0.1532(6)	0.4416(7)	1.73(8)
C(4)	0.2823(2)	-0.0555(6)	0.4117(7)	1.53(7)
C(5)	0.2222(2)	-0.1615(6)	0.4140(7)	1.55(7)
C(6)	0.1712(2)	-0.0649(6)	0.4459(7)	1.47(7)
C(7)	0.3377(2)	-0.1605(6)	0.3796(7)	1.58(7)
C(8)	0.4438(2)	-0.2751(7)	0.3597(7)	2.13(9)
C(9)	0.4010(2)	-0.3583(6)	0.2987(7)	1.88(7)
C(10)	0.5012(2)	-0.1603(8)	0.3390(7)	3.3(1)
C(11)	0.4568(3)	-0.4487(8)	0.4153(7)	3.1(1)
C(12)	0.4043(3)	-0.2212(7)	0.2322(7)	2.6(1)
C(13)	0.4071(3)	-0.5975(7)	0.2816(7)	2.80(10)
C(14)	0.0737(2)	0.1531(6)	0.5402(7)	1.47(7)
C(15)	0.0177(2)	0.2729(6)	0.5441(7)	1.51(8)

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

atom	x	y	z	B_{eq}
C(16)	-0.0340(2)	0.1806(6)	0.5767(7)	1.59(8)
C(17)	-0.0301(2)	-0.0294(6)	0.6070(7)	1.55(7)
C(18)	0.0267(2)	-0.1433(6)	0.6037(7)	1.50(7)
C(19)	0.0789(2)	-0.0537(6)	0.5705(7)	1.67(7)
C(20)	-0.0841(2)	-0.1312(6)	0.6425(7)	1.64(7)
C(21)	-0.1888(2)	-0.2385(6)	0.6634(7)	1.86(9)
C(22)	-0.1446(2)	-0.3328(7)	0.7202(7)	1.87(7)
C(23)	-0.2474(2)	-0.1115(8)	0.6918(7)	2.9(1)
C(24)	-0.2119(3)	-0.4054(8)	0.6085(7)	3.0(1)
C(25)	-0.1492(3)	-0.2176(8)	0.7920(7)	2.8(1)
C(26)	-0.1497(2)	-0.5791(7)	0.7306(7)	2.35(9)
H(1)	0.2403	0.3935	0.4915	2.0492
H(2)	0.3264	0.2277	0.4396	2.0455
H(3)	0.2176	-0.3015	0.3926	1.8569
H(4)	0.1319	-0.1384	0.4469	1.7078
H(5)	0.0153	0.4159	0.5240	1.7777
H(6)	-0.0727	0.2589	0.5779	1.8872
H(7)	0.0297	-0.2842	0.6237	1.7934
H(8)	0.1176	-0.1322	0.5676	2.0152
H(9)	0.5292	-0.2597	0.3161	3.9560
H(10)	0.4909	-0.0460	0.3065	3.9560
H(11)	0.5208	-0.1005	0.3789	3.9560
H(12)	0.4184	-0.5182	0.4273	3.7109
H(13)	0.4851	-0.5547	0.3961	3.7109

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

atom	x	y	z	B_{eq}
H(14)	0.4750	-0.3824	0.4549	3.7109
H(15)	0.4444	-0.2398	0.2099	3.0205
H(16)	0.3723	-0.2672	0.1998	3.0205
H(17)	0.3983	-0.0720	0.2430	3.0205
H(18)	0.4009	-0.6810	0.3224	3.3605
H(19)	0.3760	-0.6365	0.2471	3.3605
H(20)	0.4477	-0.6259	0.2623	3.3605
H(21)	-0.2341	-0.0047	0.7241	3.5490
H(22)	-0.2685	-0.0422	0.6532	3.5490
H(23)	-0.2753	-0.2113	0.7135	3.5490
H(24)	-0.2398	-0.5063	0.6297	3.5822
H(25)	-0.2336	-0.3312	0.5711	3.5822
H(26)	-0.1770	-0.4817	0.5887	3.5822
H(27)	-0.1178	-0.2751	0.8220	3.3836
H(28)	-0.1425	-0.0654	0.7853	3.3836
H(29)	-0.1896	-0.2420	0.8110	3.3836
H(30)	-0.1906	-0.6144	0.7470	2.8061
H(31)	-0.1433	-0.6508	0.6859	2.8061
H(32)	-0.1189	-0.6264	0.7624	2.8061

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

Table 2. Anisotropic Displacement Parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
O(1)	0.036(2)	0.015(1)	0.091(3)	-0.005(1)	0.025(2)	-0.002(2)
O(2)	0.038(2)	0.050(2)	0.061(3)	0.000(2)	-0.012(2)	-0.034(2)
O(3)	0.029(2)	0.061(2)	0.040(2)	-0.006(2)	-0.007(1)	-0.025(2)
O(4)	0.027(2)	0.049(2)	0.045(2)	0.001(2)	-0.010(2)	0.026(2)
N(1)	0.025(1)	0.016(1)	0.028(2)	0.002(1)	0.008(1)	0.003(1)
N(2)	0.021(2)	0.024(2)	0.034(2)	0.000(1)	0.004(1)	-0.004(1)
N(3)	0.024(2)	0.029(2)	0.018(2)	0.002(2)	-0.001(1)	-0.008(1)
N(4)	0.020(1)	0.027(2)	0.026(2)	0.000(1)	0.002(1)	0.006(1)
N(5)	0.022(2)	0.027(2)	0.028(2)	-0.001(2)	0.006(2)	0.004(1)
C(1)	0.023(2)	0.017(1)	0.014(2)	0.002(1)	0.001(2)	0.003(1)
C(2)	0.026(2)	0.019(2)	0.020(3)	-0.001(1)	0.000(2)	-0.002(2)
C(3)	0.018(2)	0.021(2)	0.027(2)	-0.005(2)	-0.002(2)	0.002(1)
C(4)	0.021(2)	0.022(2)	0.016(2)	-0.005(1)	0.001(2)	0.001(1)
C(5)	0.022(2)	0.018(2)	0.019(2)	-0.004(1)	-0.001(2)	-0.002(1)
C(6)	0.019(2)	0.018(2)	0.018(2)	-0.002(1)	0.001(2)	0.000(1)
C(7)	0.023(2)	0.020(2)	0.017(2)	-0.002(1)	-0.002(2)	-0.002(1)
C(8)	0.021(2)	0.034(2)	0.026(2)	0.008(2)	0.000(2)	-0.003(2)
C(9)	0.028(2)	0.020(2)	0.024(2)	-0.003(2)	0.005(2)	-0.001(1)
C(10)	0.027(2)	0.037(2)	0.062(4)	0.001(2)	0.010(2)	-0.001(2)
C(11)	0.038(3)	0.043(3)	0.036(3)	0.009(2)	-0.010(2)	0.005(2)
C(12)	0.044(3)	0.034(2)	0.020(2)	0.002(2)	0.009(2)	-0.002(2)
C(13)	0.045(3)	0.022(2)	0.039(3)	0.001(2)	0.015(2)	-0.003(2)
C(14)	0.019(2)	0.018(2)	0.019(2)	-0.001(1)	0.002(2)	-0.004(1)
C(15)	0.020(2)	0.017(2)	0.021(2)	0.003(1)	0.001(2)	0.002(1)

Table 2. Anisotropic Displacement Parameters (continued)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(16)	0.020(2)	0.019(2)	0.021(2)	0.004(2)	0.000(2)	0.002(1)
C(17)	0.022(2)	0.020(2)	0.017(2)	-0.003(1)	0.000(2)	-0.001(1)
C(18)	0.024(2)	0.018(2)	0.015(2)	0.003(1)	-0.001(2)	-0.003(1)
C(19)	0.023(2)	0.021(2)	0.019(2)	0.001(2)	-0.001(2)	-0.001(1)
C(20)	0.018(2)	0.022(2)	0.023(2)	0.001(1)	0.004(1)	-0.006(1)
C(21)	0.014(2)	0.020(2)	0.037(3)	-0.006(1)	0.002(2)	0.001(1)
C(22)	0.026(2)	0.022(2)	0.023(2)	-0.006(2)	0.007(2)	0.001(2)
C(23)	0.023(2)	0.037(3)	0.051(3)	0.004(2)	0.013(2)	-0.001(2)
C(24)	0.045(3)	0.033(2)	0.035(3)	-0.003(2)	-0.007(2)	-0.004(2)
C(25)	0.045(3)	0.037(2)	0.025(2)	-0.004(2)	0.007(2)	-0.004(2)
C(26)	0.031(2)	0.025(2)	0.033(3)	0.002(2)	-0.001(2)	0.009(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($\AA$)

atom	atom	distance	atom	atom	distance
O(1)	N(1)	1.289(5)	O(2)	N(2)	1.270(6)
O(3)	N(3)	1.261(6)	O(4)	N(4)	1.288(6)
N(1)	C(1)	1.413(8)	N(1)	C(14)	1.433(8)
N(2)	C(7)	1.341(7)	N(2)	C(8)	1.534(8)
N(3)	C(7)	1.358(7)	N(3)	C(9)	1.513(8)
N(4)	C(20)	1.384(7)	N(4)	C(21)	1.490(7)
N(5)	C(20)	1.308(8)	N(5)	C(22)	1.522(8)
C(1)	C(2)	1.400(8)	C(1)	C(6)	1.417(7)
C(2)	C(3)	1.374(8)	C(3)	C(4)	1.403(7)
C(4)	C(5)	1.431(7)	C(4)	C(7)	1.472(8)
C(5)	C(6)	1.374(8)	C(8)	C(9)	1.558(9)
C(8)	C(10)	1.461(9)	C(8)	C(11)	1.525(9)
C(9)	C(12)	1.518(9)	C(9)	C(13)	1.505(7)
C(14)	C(15)	1.398(7)	C(14)	C(19)	1.395(7)
C(15)	C(16)	1.382(8)	C(16)	C(17)	1.411(7)
C(17)	C(18)	1.392(7)	C(17)	C(20)	1.469(8)
C(18)	C(19)	1.389(8)	C(21)	C(22)	1.543(9)
C(21)	C(23)	1.562(8)	C(21)	C(24)	1.540(9)
C(22)	C(25)	1.540(9)	C(22)	C(26)	1.525(8)

Table 4. Bond Lengths($\AA$)

atom	atom	distance	atom	atom	distance
C(2)	H(1)	0.94	C(3)	H(2)	0.95
C(5)	H(3)	0.95	C(6)	H(4)	0.95
C(10)	H(9)	0.96	C(10)	H(10)	0.96
C(10)	H(11)	0.94	C(11)	H(12)	0.95
C(11)	H(13)	0.96	C(11)	H(14)	0.94
C(12)	H(15)	0.96	C(12)	H(16)	0.96
C(12)	H(17)	0.94	C(13)	H(18)	0.94
C(13)	H(19)	0.96	C(13)	H(20)	0.95
C(15)	H(5)	0.96	C(16)	H(6)	0.95
C(18)	H(7)	0.94	C(19)	H(8)	0.95
C(23)	H(21)	0.94	C(23)	H(22)	0.96
C(23)	H(23)	0.95	C(24)	H(24)	0.95
C(24)	H(25)	0.96	C(24)	H(26)	0.95
C(25)	H(27)	0.94	C(25)	H(28)	0.95
C(25)	H(29)	0.94	C(26)	H(30)	0.95
C(26)	H(31)	0.97	C(26)	H(32)	0.94

Table 5. Bond Angles(°)

atom	atom	atom	angle	atom	atom	atom	angle
O(1)	N(1)	C(1)	116.7(5)	O(1)	N(1)	C(14)	118.6(5)
C(1)	N(1)	C(14)	124.6(4)	O(2)	N(2)	C(7)	128.6(5)
O(2)	N(2)	C(8)	118.5(5)	C(7)	N(2)	C(8)	112.1(5)
O(3)	N(3)	C(7)	127.5(5)	O(3)	N(3)	C(9)	120.7(4)
C(7)	N(3)	C(9)	111.5(5)	O(4)	N(4)	C(20)	126.0(5)
O(4)	N(4)	C(21)	123.2(5)	C(20)	N(4)	C(21)	109.7(5)
C(20)	N(5)	C(22)	109.4(5)	N(1)	C(1)	C(2)	118.9(5)
N(1)	C(1)	C(6)	121.9(5)	C(2)	C(1)	C(6)	119.1(5)
C(1)	C(2)	C(3)	121.1(5)	C(2)	C(3)	C(4)	121.0(5)
C(3)	C(4)	C(5)	117.8(5)	C(3)	C(4)	C(7)	120.4(5)
C(5)	C(4)	C(7)	121.8(4)	C(4)	C(5)	C(6)	121.3(5)
C(1)	C(6)	C(5)	119.7(5)	N(2)	C(7)	N(3)	109.2(5)
N(2)	C(7)	C(4)	125.4(5)	N(3)	C(7)	C(4)	125.4(5)
N(2)	C(8)	C(9)	99.9(4)	N(2)	C(8)	C(10)	110.3(5)
N(2)	C(8)	C(11)	104.1(5)	C(9)	C(8)	C(10)	116.2(6)
C(9)	C(8)	C(11)	113.2(5)	C(10)	C(8)	C(11)	111.8(6)
N(3)	C(9)	C(8)	101.3(5)	N(3)	C(9)	C(12)	104.6(5)
N(3)	C(9)	C(13)	109.3(5)	C(8)	C(9)	C(12)	114.4(5)
C(8)	C(9)	C(13)	115.4(5)	C(12)	C(9)	C(13)	110.7(5)
N(1)	C(14)	C(15)	116.5(5)	N(1)	C(14)	C(19)	122.0(5)
C(15)	C(14)	C(19)	121.4(5)	C(14)	C(15)	C(16)	118.9(5)
C(15)	C(16)	C(17)	120.6(5)	C(16)	C(17)	C(18)	119.3(5)
C(16)	C(17)	C(20)	121.8(5)	C(18)	C(17)	C(20)	118.9(4)
C(17)	C(18)	C(19)	120.8(4)	C(14)	C(19)	C(18)	118.9(5)

Table 5. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
N(4)	C(20)	N(5)	112.5(5)	N(4)	C(20)	C(17)	123.3(5)
N(5)	C(20)	C(17)	124.2(5)	N(4)	C(21)	C(22)	101.6(4)
N(4)	C(21)	C(23)	109.2(4)	N(4)	C(21)	C(24)	107.2(5)
C(22)	C(21)	C(23)	115.3(6)	C(22)	C(21)	C(24)	114.8(5)
C(23)	C(21)	C(24)	108.2(6)	N(5)	C(22)	C(21)	103.1(5)
N(5)	C(22)	C(25)	105.7(5)	N(5)	C(22)	C(26)	109.0(5)
C(21)	C(22)	C(25)	114.3(5)	C(21)	C(22)	C(26)	114.7(5)
C(25)	C(22)	C(26)	109.5(5)				

Table 6. Bond Angles(°)

atom	atom	atom	angle	atom	atom	atom	angle
C(1)	C(2)	H(1)	119.6	C(3)	C(2)	H(1)	119.3
C(2)	C(3)	H(2)	119.9	C(4)	C(3)	H(2)	119.1
C(4)	C(5)	H(3)	119.0	C(6)	C(5)	H(3)	119.7
C(1)	C(6)	H(4)	120.5	C(5)	C(6)	H(4)	119.8
C(8)	C(10)	H(9)	109.6	C(8)	C(10)	H(10)	109.5
C(8)	C(10)	H(11)	109.8	H(9)	C(10)	H(10)	108.3
H(9)	C(10)	H(11)	109.9	H(10)	C(10)	H(11)	109.7
C(8)	C(11)	H(12)	108.9	C(8)	C(11)	H(13)	108.7
C(8)	C(11)	H(14)	109.2	H(12)	C(11)	H(13)	109.2
H(12)	C(11)	H(14)	110.9	H(13)	C(11)	H(14)	109.9
C(9)	C(12)	H(15)	110.1	C(9)	C(12)	H(16)	109.9
C(9)	C(12)	H(17)	110.4	H(15)	C(12)	H(16)	108.0
H(15)	C(12)	H(17)	109.3	H(16)	C(12)	H(17)	109.1
C(9)	C(13)	H(18)	109.8	C(9)	C(13)	H(19)	109.3
C(9)	C(13)	H(20)	109.7	H(18)	C(13)	H(19)	109.6
H(18)	C(13)	H(20)	110.2	H(19)	C(13)	H(20)	108.3
C(14)	C(15)	H(5)	120.4	C(16)	C(15)	H(5)	120.7
C(15)	C(16)	H(6)	119.3	C(17)	C(16)	H(6)	120.1
C(17)	C(18)	H(7)	119.9	C(19)	C(18)	H(7)	119.3
C(14)	C(19)	H(8)	120.2	C(18)	C(19)	H(8)	120.9
C(21)	C(23)	H(21)	109.5	C(21)	C(23)	H(22)	109.1
C(21)	C(23)	H(23)	109.2	H(21)	C(23)	H(22)	109.4
H(21)	C(23)	H(23)	110.7	H(22)	C(23)	H(23)	109.0
C(21)	C(24)	H(24)	110.1	C(21)	C(24)	H(25)	109.9

Table 6. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C(21)	C(24)	H(26)	110.2	H(24)	C(24)	H(25)	108.9
H(24)	C(24)	H(26)	109.5	H(25)	C(24)	H(26)	108.2
C(22)	C(25)	H(27)	108.6	C(22)	C(25)	H(28)	108.6
C(22)	C(25)	H(29)	108.9	H(27)	C(25)	H(28)	109.9
H(27)	C(25)	H(29)	110.7	H(28)	C(25)	H(29)	110.0
C(22)	C(26)	H(30)	109.5	C(22)	C(26)	H(31)	109.0
C(22)	C(26)	H(32)	109.8	H(30)	C(26)	H(31)	108.4
H(30)	C(26)	H(32)	110.8	H(31)	C(26)	H(32)	109.2

Table 7. Torsion Angles(°)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
O(1)	N(1)	C(1)	C(2)	24.4(10)	O(1)	N(1)	C(1)	C(6)	-152.1(7)
O(1)	N(1)	C(14)	C(15)	25(1)	O(1)	N(1)	C(14)	C(19)	-151.6(7)
O(2)	N(2)	C(7)	N(3)	-177.1(6)	O(2)	N(2)	C(7)	C(4)	3.7(9)
O(2)	N(2)	C(8)	C(9)	-169.2(5)	O(2)	N(2)	C(8)	C(10)	-46.4(8)
O(2)	N(2)	C(8)	C(11)	73.7(7)	O(3)	N(3)	C(7)	N(2)	177.1(6)
O(3)	N(3)	C(7)	C(4)	-3.7(9)	O(3)	N(3)	C(9)	C(8)	-164.4(5)
O(3)	N(3)	C(9)	C(12)	76.5(6)	O(3)	N(3)	C(9)	C(13)	-42.1(7)
O(4)	N(4)	C(20)	N(5)	-176.2(5)	O(4)	N(4)	C(20)	C(17)	2.8(8)
O(4)	N(4)	C(21)	C(22)	-174.3(5)	O(4)	N(4)	C(21)	C(23)	-52.1(8)
O(4)	N(4)	C(21)	C(24)	64.9(7)	N(1)	C(1)	C(2)	C(3)	-177.5(6)
N(1)	C(1)	C(6)	C(5)	176.4(5)	N(1)	C(14)	C(15)	C(16)	-179.8(5)
N(1)	C(14)	C(19)	C(18)	179.0(6)	N(2)	C(7)	N(3)	C(9)	-9.1(6)
N(2)	C(7)	C(4)	C(3)	24.8(8)	N(2)	C(7)	C(4)	C(5)	-154.7(5)
N(2)	C(8)	C(9)	N(3)	-23.0(5)	N(2)	C(8)	C(9)	C(12)	88.9(6)
N(2)	C(8)	C(9)	C(13)	-140.9(5)	N(3)	C(7)	N(2)	C(8)	-8.1(6)
N(3)	C(7)	C(4)	C(3)	-154.2(5)	N(3)	C(7)	C(4)	C(5)	26.3(8)
N(3)	C(9)	C(8)	C(10)	-141.5(5)	N(3)	C(9)	C(8)	C(11)	87.0(6)
N(4)	C(20)	N(5)	C(22)	-5.4(6)	N(4)	C(20)	C(17)	C(16)	27.2(8)
N(4)	C(20)	C(17)	C(18)	-153.2(5)	N(4)	C(21)	C(22)	N(5)	-18.7(5)
N(4)	C(21)	C(22)	C(25)	95.4(6)	N(4)	C(21)	C(22)	C(26)	-137.1(5)
N(5)	C(20)	N(4)	C(21)	-8.0(6)	N(5)	C(20)	C(17)	C(16)	-153.8(6)
N(5)	C(20)	C(17)	C(18)	25.7(8)	N(5)	C(22)	C(21)	C(23)	-136.7(5)
N(5)	C(22)	C(21)	C(24)	96.5(6)	C(1)	N(1)	C(14)	C(15)	-157.8(6)
C(1)	N(1)	C(14)	C(19)	24(1)	C(1)	C(2)	C(3)	C(4)	0.7(9)

Table 7. Torsion Angles(°) (continued)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
C(1)	C(6)	C(5)	C(4)	1.2(8)	C(2)	C(1)	N(1)	C(14)	-151.9(6)
C(2)	C(1)	C(6)	C(5)	0.0(8)	C(2)	C(3)	C(4)	C(5)	0.5(8)
C(2)	C(3)	C(4)	C(7)	-179.0(5)	C(3)	C(2)	C(1)	C(6)	-0.9(9)
C(3)	C(4)	C(5)	C(6)	-1.5(8)	C(4)	C(7)	N(2)	C(8)	172.8(5)
C(4)	C(7)	N(3)	C(9)	170.0(5)	C(6)	C(1)	N(1)	C(14)	31(1)
C(6)	C(5)	C(4)	C(7)	178.0(5)	C(7)	N(2)	C(8)	C(9)	20.6(6)
C(7)	N(2)	C(8)	C(10)	143.4(6)	C(7)	N(2)	C(8)	C(11)	-96.6(6)
C(7)	N(3)	C(9)	C(8)	21.4(6)	C(7)	N(3)	C(9)	C(12)	-97.7(5)
C(7)	N(3)	C(9)	C(13)	143.7(5)	C(10)	C(8)	C(9)	C(12)	-29.6(7)
C(10)	C(8)	C(9)	C(13)	100.6(6)	C(11)	C(8)	C(9)	C(12)	-161.0(6)
C(11)	C(8)	C(9)	C(13)	-30.8(8)	C(14)	C(15)	C(16)	C(17)	1.4(9)
C(14)	C(19)	C(18)	C(17)	-0.1(8)	C(15)	C(14)	C(19)	C(18)	1.5(8)
C(15)	C(16)	C(17)	C(18)	0.0(8)	C(15)	C(16)	C(17)	C(20)	179.5(5)
C(16)	C(15)	C(14)	C(19)	-2.2(9)	C(16)	C(17)	C(18)	C(19)	-0.7(8)
C(17)	C(20)	N(4)	C(21)	171.1(5)	C(17)	C(20)	N(5)	C(22)	175.6(5)
C(19)	C(18)	C(17)	C(20)	179.8(5)	C(20)	N(4)	C(21)	C(22)	17.0(6)
C(20)	N(4)	C(21)	C(23)	139.3(6)	C(20)	N(4)	C(21)	C(24)	-103.8(6)
C(20)	N(5)	C(22)	C(21)	15.8(6)	C(20)	N(5)	C(22)	C(25)	-104.5(6)
C(20)	N(5)	C(22)	C(26)	138.0(5)	C(23)	C(21)	C(22)	C(25)	-22.6(7)
C(23)	C(21)	C(22)	C(26)	105.0(6)	C(24)	C(21)	C(22)	C(25)	-149.3(6)
C(24)	C(21)	C(22)	C(26)	-21.8(8)					

Table 8. Non-bonded Contacts out to 3.60 Å

atom	atom	distance	ADC	atom	atom	distance	ADC
O(1)	C(6)	3.208(7)	56501	O(1)	C(19)	3.349(7)	56501
O(1)	C(5)	3.484(7)	56501	O(2)	C(15)	3.134(7)	4
O(2)	C(16)	3.322(7)	4	O(2)	C(11)	3.445(8)	56501
O(3)	C(26)	3.229(8)	54402	O(4)	C(2)	3.145(8)	45504
O(4)	C(3)	3.325(7)	45504	O(4)	C(24)	3.547(8)	56501
C(1)	C(25)	3.576(9)	55402	C(2)	C(24)	3.518(9)	54504
C(3)	C(24)	3.517(9)	54504	C(6)	C(25)	3.430(9)	55402
C(11)	C(16)	3.387(9)	54504	C(11)	C(15)	3.406(9)	54504

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