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Indroduction

This Crystal Contained one macrocycle, six nitrates and two waters in the asymmetric unit. The symmetry of the crystal creates in the unit cell a total of two macrocycles, 12 nitrates and four waters.

Experimental

Data Collection

A Clear Prism crystal of $O_{20}N_{14}C_{36}H_{64}$ having approximate dimensions of 0.30 x 0.15 x 0.30 mm was mounted on a glass fiber. All measurements were made on a Rigaku AFC5R diffractometer with graphite monochromated Cu-Kα radiation and a rotating anode generator.

Cell constants and an orientation matrix for data collection, obtained from a least-squares refinement using the setting angles of 18 carefully centered reflections in the range $33.73 < 2\theta < 36.35^{o}$ corresponded to a primitive triclinic cell with dimensions:

a = 10.396(2) Å α = 95.045(9)°
b = 25.633(2) Å β = 117.766(9)°
c = 10.240(1) Å γ = 80.464(9)
V = 2381.1(6) Å^3

For Z = 2 and F.W. = 1012.98, the calculated density is 1.41 g/cm^3. Based on a statistical analysis of intensity distribution, and the successful solution and refinement of the structure, the space group was determined to be:

P $\bar{1}$ (#2)

The data were collected at a temperature of 23 ± 1°C using the ω-2θ scan technique to a maximum 2θ value of 115.1°. Omega scans of several intense reflections, made prior to data collection, had an average width at half-height of 0.24° with a take-off angle of 6.0°. Scans of $(1.47 + 0.30 \tan \theta)^{o}$ were made at a speed of 32.0°/min (in ω). The weak reflections ($I < 10.0\sigma(I)$) were rescanned (maximum of 3 scans) and the counts were accumulated to ensure good counting statistics. Stationary background counts were recorded on each side of the reflection. The ratio of peak counting time to background counting time was 2:1. The diameter of the incident beam collimator was 1.0 mm, the crystal to detector distance was 400 mm, and the detector aperture was 6.0 x 6.0 mm (horizontal x vertical).

Data Reduction

Of the 6986 reflections which were collected, 6558 were unique ($R_{int} = 0.019$); equivalent reflections were merged. The intensities of three representative reflection were measured after every 150 reflections. Over the course of data collection, the standards decreased by 2.1%. A linear correction factor was applied to the data to account for this phenomenon.

The linear absorption coefficient, μ, for Cu-Kα radiation is 9.9 cm^{-1}. An empirical absorption

correction based on azimuthal scans of several reflections was applied which resulted in transmission factors ranging from 0.80 to 1.00. 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 4691 observed reflections ($I > 3.00\sigma(I)$) and 631 variable parameters and converged (largest parameter shift was 0.00 times its esd) with unweighted and weighted agreement factors of:

$$R = \Sigma \, ||Fo| - |Fc|| \, / \, \Sigma \, |Fo| = 0.056$$

$$R_w = [(\Sigma \, w \, (|Fo| - |Fc|)^2 \, / \, \Sigma \, w \, Fo^2)]^{1/2} = 0.072$$

The standard deviation of an observation of unit weight[4] was 2.35. The weighting scheme was based on counting statistics and included a factor ($p = 0.030$) 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 0.25 and -0.36 $e^-/Å^3$, 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 Hubbell[8]. All calculations were performed using the teXsan[9] crystallographic software package of Molecular Structure Corporation.

References

(1) SIR92: Altomare, A., Cascarano, M., Giacovazzo, C., Guagliardi, A. (1993). J. Appl. Cryst., 26, 343.

(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:

$\Sigma w(|F_o|-|F_c|)^2$ where

$w = 1/[\sigma^2(Fo)] = [\sigma^2_c(Fo) + p^2Fo^2/4]^{-1}$
$\sigma_c(Fo)$ = e.s.d. based on counting statistics
p = p-factor

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

$$[\Sigma w(|F_O|-|F_C|)^2/(N_O-N_V)]^{1/2}$$

where: N_O = number of observations
N_V = 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 for Windows: Crystal Structure Analysis Package, Molecular Structure Corporation (1997).

EXPERIMENTAL DETAILS

A. Crystal Data

Empirical Formula	$O_{20}N_{14}C_{36}H_{64}$
Formula Weight	1012.98
Crystal Color, Habit	Clear, Prism
Crystal Dimensions	0.30 X 0.15 X 0.30 mm
Crystal System	triclinic
Lattice Type	Primitive
No. of Reflections Used for Unit Cell Determination (2θ range)	18 (33.7 - 36.3°)
Omega Scan Peak Width at Half-height	0.24°
Lattice Parameters	a = 10.396(2) Å b = 25.633(2) Å c = 10.240(1) Å α = 95.045(9) Å β = 117.766(9) Å γ = 80.464(9) Å V = 2381.1(6) Å^3
Space Group	P $\bar{1}$ (#2)
Z value	2
D_{calc}	1.413 g/cm^3
F_{000}	1020.00
μ(CuKα)	9.92 cm^{-1}

B. Intensity Measurements

Diffractometer	Rigaku AFC5R
Radiation	CuKα (λ = 1.54178 Å)

	graphite monochromated
Attenuator	Ni foil (factors = 1.00, 3.92, 13.58, 51.27)
Take-off Angle	6.0°
Detector Aperture	6.0 mm horizontal 6.0 mm vertical
Crystal to Detector Distance	400 mm
Voltage, Current	50kV, 150mA
Temperature	23.0°C
Scan Type	ω-2θ
Scan Rate	32.0°/min (in ω) (up to 3 scans)
Scan Width	(1.47 + 0.30 tan θ)°
$2\theta_{max}$	115.1°
No. of Reflections Measured	Total: 6986
Corrections	Unique: 6558 (R_{int} = 0.019) Lorentz-polarization Absorption (trans. factors: 0.7978 - 0.9987) Decay (2.09% decline)

C. Structure Solution and Refinement

Structure Solution	Direct Methods (SIR92)
Refinement	Full-matrix least-squares
Function Minimized	Σ w (|Fo| - |Fc|)^2
Least Squares Weights	$1/\sigma^2(Fo) = 4Fo^2/\sigma^2(Fo^2)$
p-factor	0.0300
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (I>3.00σ(I))	4691
No. Variables	631

Reflection/Parameter Ratio	7.43
Residuals: R; Rw	0.056 ; 0.072
Goodness of Fit Indicator	2.35
Max Shift/Error in Final Cycle	0.00
Maximum peak in Final Diff. Map	0.25 $e^-/Å^3$
Minimum peak in Final Diff. Map	-0.36 $e^-/Å^3$

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

atom	x	y	z	B_{eq}
O(101)	0.5638(2)	0.17805(8)	0.7711(2)	5.18(5)
O(102)	0.6401(2)	0.19238(7)	1.0063(2)	5.13(5)
O(103)	0.7923(2)	0.18567(8)	0.9145(2)	5.22(5)
O(201)	0.5186(2)	0.30772(7)	0.6917(2)	4.70(5)
O(202)	0.5927(2)	0.32157(8)	0.9259(2)	5.53(6)
O(203)	0.7480(2)	0.31397(7)	0.8377(2)	4.77(5)
O(301)	0.1477(3)	0.1016(1)	1.0028(3)	9.05(8)
O(302)	0.2362(2)	0.09965(8)	1.2374(3)	6.55(7)
O(303)	0.3772(2)	0.09965(9)	1.1376(2)	6.16(6)
O(401)	0.3211(3)	0.40912(8)	1.0452(2)	6.91(6)
O(402)	0.3767(2)	0.38131(9)	1.2585(2)	6.54(6)
O(403)	0.5463(3)	0.3953(1)	1.2135(3)	8.49(8)
O(501)	0.1098(3)	0.0378(1)	1.6426(3)	8.89(9)
O(502)	0.2594(3)	-0.0264(1)	1.6296(3)	8.92(8)
O(503)	0.1942(3)	0.0407(1)	1.4924(3)	9.79(9)
O(601)	0.0886(3)	0.5472(1)	1.4808(3)	6.89(7)
O(602)	0.1647(3)	0.4858(1)	1.3665(3)	7.94(8)
O(603)	-0.0408(3)	0.5351(1)	1.2465(3)	8.43(8)
O(701)	0.5023(4)	0.0573(1)	1.4801(3)	14.2(1)
O(801)	0.0445(2)	0.43723(9)	1.0679(3)	7.41(7)
N(1)	0.7277(2)	0.06608(7)	0.9550(2)	3.11(5)
N(2)	0.5610(2)	0.43306(7)	0.7649(2)	3.29(5)
N(3)	0.7426(2)	0.10287(8)	0.6719(2)	3.81(5)
N(4)	0.6300(2)	0.35642(8)	0.5331(2)	3.51(5)

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

atom	x	y	z	B_{eq}
N(5)	0.4057(2)	0.12744(8)	0.8905(2)	3.50(5)
N(6)	0.2974(2)	0.37844(8)	0.7568(2)	4.19(6)
N(7)	0.9472(2)	0.13977(8)	1.2026(2)	3.80(5)
N(8)	0.8340(2)	0.39091(8)	1.0741(2)	3.98(5)
N(101)	0.6652(3)	0.18611(8)	0.8964(3)	4.40(6)
N(201)	0.6202(3)	0.31363(8)	0.8183(3)	4.27(6)
N(301)	0.2517(3)	0.10098(8)	1.1227(3)	4.35(6)
N(401)	0.4154(3)	0.39495(8)	1.1710(3)	4.48(6)
N(501)	0.1868(3)	0.0170(1)	1.5867(3)	5.53(7)
N(601)	0.0707(3)	0.5222(1)	1.3654(3)	5.54(8)
C(1)	0.7439(3)	0.03492(9)	0.8328(3)	3.60(6)
C(2)	0.8326(3)	0.0581(1)	0.7758(3)	3.85(6)
C(3)	0.8323(3)	0.1274(1)	0.6215(3)	4.09(7)
C(4)	0.7453(3)	0.1730(1)	0.5194(3)	3.53(6)
C(5)	0.6345(3)	0.1643(1)	0.3797(3)	3.94(7)
C(6)	0.5603(3)	0.2063(1)	0.2828(3)	4.30(7)
C(7)	0.5983(3)	0.2565(1)	0.3248(3)	3.99(7)
C(8)	0.7068(3)	0.2659(1)	0.4660(3)	3.54(6)
C(9)	0.7779(3)	0.2235(1)	0.5621(3)	3.53(6)
C(10)	0.7481(3)	0.3203(1)	0.5153(3)	3.97(7)
C(11)	0.6743(3)	0.4094(1)	0.5961(3)	3.75(6)
C(12)	0.5571(3)	0.44445(9)	0.6240(3)	3.66(6)
C(13)	0.6052(3)	0.0498(1)	0.9689(3)	3.53(6)
C(14)	0.4542(3)	0.0730(1)	0.8526(3)	3.77(6)

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

atom	x	y	z	B_{eq}
C(15)	0.2643(3)	0.1521(1)	0.7673(3)	4.27(7)
C(16)	0.2182(3)	0.2078(1)	0.8026(3)	3.67(6)
C(17)	0.1573(3)	0.2185(1)	0.8995(3)	4.45(7)
C(18)	0.1099(3)	0.2705(1)	0.9250(3)	5.00(8)
C(19)	0.1195(3)	0.3120(1)	0.8528(3)	4.39(7)
C(20)	0.1787(3)	0.3015(1)	0.7552(3)	3.72(6)
C(21)	0.2296(3)	0.2498(1)	0.7330(3)	3.83(6)
C(22)	0.1813(3)	0.3445(1)	0.6659(3)	4.55(7)
C(23)	0.2976(3)	0.4217(1)	0.6676(3)	4.41(7)
C(24)	0.4172(3)	0.4550(1)	0.7580(3)	4.07(7)
C(25)	0.8647(3)	0.05310(9)	1.0932(3)	3.64(6)
C(26)	0.8850(3)	0.0933(1)	1.2164(3)	3.94(6)
C(27)	0.9759(3)	0.1779(1)	1.3285(3)	4.89(8)
C(28)	1.0315(3)	0.2264(1)	1.3105(3)	4.13(7)
C(29)	1.1764(3)	0.2263(1)	1.3436(3)	4.57(7)
C(30)	1.2230(3)	0.2721(1)	1.3320(3)	5.18(8)
C(31)	1.1291(3)	0.3195(1)	1.2921(3)	4.33(7)
C(32)	0.9836(3)	0.3202(1)	1.2594(3)	4.02(7)
C(33)	0.9355(3)	0.2734(1)	1.2675(3)	4.07(7)
C(34)	0.8787(3)	0.3714(1)	1.2250(3)	4.78(7)
C(35)	0.7231(3)	0.4396(1)	1.0379(3)	4.19(7)
C(36)	0.6771(3)	0.4597(1)	0.8846(3)	4.00(7)
H(1)	0.7878	-0.0090	0.8699	3.7450
H(2)	0.6345	0.0375	0.7430	3.7450

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

atom	x	y	z	B_{eq}
H(3)	0.8459	0.0288	0.7006	3.7450
H(4)	0.9309	0.0744	0.8698	3.7450
H(5)	0.6640	0.0897	0.5882	4.5612
H(6)	0.7039	0.1291	0.7208	4.5612
H(7)	0.8920	0.1000	0.5988	3.7450
H(8)	0.9144	0.1381	0.7150	3.7450
H(9)	0.5994	0.1275	0.3423	3.7450
H(10)	0.4699	0.1972	0.1816	3.7450
H(11)	0.5350	0.2873	0.2495	3.7450
H(12)	0.8642	0.2275	0.6704	3.7450
H(13)	0.7772	0.3381	0.4410	3.7450
H(14)	0.8419	0.3211	0.6133	3.7450
H(15)	0.5465	0.3615	0.4391	4.2089
H(16)	0.6054	0.3405	0.5973	4.2089
H(17)	0.6784	0.4242	0.5140	3.7450
H(18)	0.7772	0.4019	0.6941	3.7450
H(19)	0.5724	0.4856	0.6187	3.7450
H(20)	0.4472	0.4383	0.5257	3.7450
H(21)	0.6161	0.0068	0.9708	3.7450
H(22)	0.6047	0.0628	1.0647	3.7450
H(23)	0.3749	0.0490	0.8414	3.7450
H(24)	0.4587	0.0712	0.7588	3.7450
H(25)	0.3930	0.1261	0.9756	4.2517
H(26)	0.4801	0.1486	0.9103	4.2517

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

atom	x	y	z	B_{eq}
H(27)	0.1890	0.1235	0.7495	3.7450
H(28)	0.2811	0.1505	0.6676	3.7450
H(29)	0.1192	0.1836	0.9453	3.7450
H(30)	0.0336	0.2775	0.9774	3.7450
H(31)	0.0839	0.3536	0.8842	3.7450
H(32)	0.2762	0.2382	0.6599	3.7450
H(33)	0.0770	0.3691	0.6369	3.7450
H(34)	0.2158	0.3267	0.5751	3.7450
H(35)	0.2792	0.3916	0.8214	3.7450
H(36)	0.3872	0.3544	0.8136	3.7450
H(37)	0.1928	0.4476	0.6286	3.7450
H(38)	0.4335	0.4588	0.8710	3.7450
H(39)	0.3842	0.4931	0.7210	3.7450
H(40)	0.3220	0.3984	0.5851	3.7450
H(41)	0.8692	0.0168	1.1203	3.7450
H(42)	0.9685	0.0493	1.0801	3.7450
H(43)	0.9607	0.0791	1.3179	3.7450
H(44)	0.7912	0.1099	1.2133	3.7450
H(45)	1.0362	0.1242	1.1959	3.7450
H(46)	0.8753	0.1621	1.1233	3.7450
H(47)	1.0618	0.1561	1.4251	3.7450
H(48)	0.8513	0.1916	1.3100	3.7450
H(49)	1.2483	0.1886	1.3719	3.7450
H(50)	1.3213	0.2748	1.3504	3.7450

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

atom	x	y	z	B_{eq}
H(51)	1.1564	0.3587	1.2906	3.7450
H(52)	0.8233	0.2743	1.2402	3.7450
H(53)	0.9316	0.4021	1.3086	3.7450
H(54)	0.7813	0.3629	1.2160	3.7450
H(55)	0.7929	0.3640	1.0035	4.7852
H(56)	0.9206	0.3995	1.0720	4.8394
H(57)	0.6251	0.4359	1.0525	3.7450
H(58)	0.7894	0.4680	1.1138	3.7450
H(59)	0.7825	0.4534	0.8708	3.7450
H(60)	0.6532	0.5016	0.8992	3.7450
H(701)	0.4465	0.0363	1.4880	3.7450
H(702)	0.4077	0.0863	1.4331	3.7450
H(801)	0.1255	0.4233	1.0946	3.7450
H(802)	0.0638	0.4685	1.1488	3.7450

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

Table 2. Anisotropic Displacement Parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
O(101)	0.064(1)	0.064(1)	0.064(1)	-0.001(1)	0.022(1)	0.014(1)
O(102)	0.080(1)	0.080(1)	0.080(1)	-0.008(1)	0.044(1)	-0.005(1)
O(103)	0.066(1)	0.066(1)	0.066(1)	-0.018(1)	0.038(1)	0.003(1)
O(201)	0.067(1)	0.067(1)	0.067(1)	-0.019(1)	0.026(1)	-0.004(1)
O(202)	0.096(2)	0.096(2)	0.096(2)	-0.017(1)	0.047(1)	0.004(1)
O(203)	0.061(1)	0.061(1)	0.061(1)	-0.001(1)	0.031(1)	0.002(1)
O(301)	0.085(2)	0.085(2)	0.085(2)	-0.052(2)	-0.012(2)	0.041(2)
O(302)	0.099(2)	0.099(2)	0.099(2)	-0.005(1)	0.074(2)	0.004(1)
O(303)	0.058(1)	0.058(1)	0.058(1)	-0.024(1)	0.034(1)	0.004(1)
O(401)	0.127(2)	0.127(2)	0.127(2)	-0.001(1)	0.022(1)	0.005(1)
O(402)	0.066(1)	0.066(1)	0.066(1)	-0.007(1)	0.036(1)	0.029(1)
O(403)	0.075(2)	0.075(2)	0.075(2)	-0.002(2)	0.059(2)	0.048(2)
O(501)	0.091(2)	0.091(2)	0.091(2)	-0.015(2)	0.061(2)	-0.044(2)
O(502)	0.109(2)	0.109(2)	0.109(2)	0.015(2)	0.049(2)	0.013(2)
O(503)	0.117(2)	0.117(2)	0.117(2)	-0.031(2)	0.030(2)	0.040(2)
O(601)	0.091(2)	0.091(2)	0.091(2)	-0.029(1)	0.045(1)	-0.025(1)
O(602)	0.114(2)	0.114(2)	0.114(2)	0.014(2)	0.060(2)	0.004(1)
O(603)	0.102(2)	0.102(2)	0.102(2)	0.003(2)	0.030(2)	-0.003(2)
O(701)	0.173(3)	0.173(3)	0.173(3)	-0.115(3)	-0.038(2)	0.062(2)
O(801)	0.079(2)	0.079(2)	0.079(2)	-0.022(1)	0.056(1)	-0.006(1)
N(1)	0.041(1)	0.041(1)	0.041(1)	-0.0047(9)	0.018(1)	0.0032(9)
N(2)	0.048(1)	0.048(1)	0.048(1)	-0.006(1)	0.023(1)	0.0018(9)
N(3)	0.049(1)	0.049(1)	0.049(1)	-0.004(1)	0.024(1)	0.004(1)
N(4)	0.052(1)	0.052(1)	0.052(1)	-0.007(1)	0.026(1)	0.003(1)

Table 2. Anisotropic Displacement Parameters (continued)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
N(5)	0.042(1)	0.042(1)	0.042(1)	-0.004(1)	0.020(1)	0.006(1)
N(6)	0.062(1)	0.062(1)	0.062(1)	-0.005(1)	0.029(1)	0.003(1)
N(7)	0.050(1)	0.050(1)	0.050(1)	-0.007(1)	0.026(1)	-0.002(1)
N(8)	0.059(1)	0.059(1)	0.059(1)	-0.011(1)	0.028(1)	-0.004(1)
N(101)	0.064(2)	0.064(2)	0.064(2)	-0.004(1)	0.032(2)	0.008(1)
N(201)	0.073(2)	0.073(2)	0.073(2)	-0.004(1)	0.036(2)	0.006(1)
N(301)	0.060(2)	0.060(2)	0.060(2)	-0.016(1)	0.026(2)	0.004(1)
N(401)	0.070(2)	0.070(2)	0.070(2)	-0.002(1)	0.030(2)	0.003(1)
N(501)	0.058(2)	0.058(2)	0.058(2)	-0.013(2)	0.016(2)	-0.012(2)
N(601)	0.073(2)	0.073(2)	0.073(2)	-0.017(2)	0.044(2)	0.001(2)
C(1)	0.055(2)	0.055(2)	0.055(2)	-0.007(1)	0.026(1)	-0.001(1)
C(2)	0.057(2)	0.057(2)	0.057(2)	0.002(1)	0.026(1)	0.006(1)
C(3)	0.048(2)	0.048(2)	0.048(2)	-0.001(1)	0.028(1)	0.010(1)
C(4)	0.046(2)	0.046(2)	0.046(2)	-0.002(1)	0.028(1)	0.002(1)
C(5)	0.054(2)	0.054(2)	0.054(2)	-0.010(1)	0.029(1)	-0.008(1)
C(6)	0.052(2)	0.052(2)	0.052(2)	-0.006(1)	0.018(1)	-0.007(1)
C(7)	0.056(2)	0.056(2)	0.056(2)	0.001(1)	0.026(1)	0.003(1)
C(8)	0.048(2)	0.048(2)	0.048(2)	-0.007(1)	0.030(1)	-0.001(1)
C(9)	0.045(2)	0.045(2)	0.045(2)	-0.006(1)	0.020(1)	-0.001(1)
C(10)	0.049(2)	0.049(2)	0.049(2)	-0.006(1)	0.027(1)	-0.001(1)
C(11)	0.056(2)	0.056(2)	0.056(2)	-0.013(1)	0.027(1)	0.004(1)
C(12)	0.062(2)	0.062(2)	0.062(2)	-0.004(1)	0.032(1)	0.010(1)
C(13)	0.048(2)	0.048(2)	0.048(2)	-0.004(1)	0.025(1)	0.008(1)
C(14)	0.052(2)	0.052(2)	0.052(2)	-0.009(1)	0.025(1)	-0.003(1)

Table 2. Anisotropic Displacement Parameters (continued)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(15)	0.052(2)	0.052(2)	0.052(2)	-0.003(1)	0.012(1)	0.002(1)
C(16)	0.038(1)	0.038(1)	0.038(1)	-0.003(1)	0.010(1)	0.005(1)
C(17)	0.056(2)	0.056(2)	0.056(2)	-0.005(1)	0.026(2)	0.006(1)
C(18)	0.064(2)	0.064(2)	0.064(2)	-0.001(2)	0.035(2)	0.004(2)
C(19)	0.058(2)	0.058(2)	0.058(2)	-0.003(1)	0.020(1)	-0.005(1)
C(20)	0.039(1)	0.039(1)	0.039(1)	-0.007(1)	0.012(1)	0.003(1)
C(21)	0.045(2)	0.045(2)	0.045(2)	-0.002(1)	0.019(1)	0.001(1)
C(22)	0.056(2)	0.056(2)	0.056(2)	-0.014(1)	0.016(1)	0.006(1)
C(23)	0.049(2)	0.049(2)	0.049(2)	0.000(1)	0.026(1)	0.018(1)
C(24)	0.060(2)	0.060(2)	0.060(2)	0.003(1)	0.038(2)	0.004(1)
C(25)	0.044(2)	0.044(2)	0.044(2)	0.001(1)	0.017(1)	0.010(1)
C(26)	0.049(2)	0.049(2)	0.049(2)	-0.008(1)	0.018(1)	0.008(1)
C(27)	0.083(2)	0.083(2)	0.083(2)	-0.025(2)	0.034(2)	-0.014(1)
C(28)	0.060(2)	0.060(2)	0.060(2)	-0.015(2)	0.026(1)	-0.013(1)
C(29)	0.058(2)	0.058(2)	0.058(2)	-0.009(2)	0.030(2)	-0.011(1)
C(30)	0.053(2)	0.053(2)	0.053(2)	-0.020(2)	0.036(2)	-0.018(2)
C(31)	0.058(2)	0.058(2)	0.058(2)	-0.012(2)	0.034(2)	-0.008(1)
C(32)	0.056(2)	0.056(2)	0.056(2)	-0.005(1)	0.025(1)	-0.003(1)
C(33)	0.046(2)	0.046(2)	0.046(2)	-0.013(2)	0.023(1)	-0.008(1)
C(34)	0.065(2)	0.065(2)	0.065(2)	0.000(2)	0.032(2)	0.006(1)
C(35)	0.058(2)	0.058(2)	0.058(2)	-0.006(1)	0.028(1)	-0.009(1)
C(36)	0.067(2)	0.067(2)	0.067(2)	-0.016(1)	0.030(1)	-0.003(1)

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(101)	N(101)	1.251(4)	O(102)	N(101)	1.261(4)
O(103)	N(101)	1.244(4)	O(201)	N(201)	1.250(4)
O(202)	N(201)	1.254(4)	O(203)	N(201)	1.250(4)
O(301)	N(301)	1.199(4)	O(302)	N(301)	1.262(4)
O(303)	N(301)	1.235(4)	O(401)	N(401)	1.241(4)
O(402)	N(401)	1.235(4)	O(403)	N(401)	1.221(4)
O(501)	N(501)	1.218(5)	O(502)	N(501)	1.224(5)
O(503)	N(501)	1.224(5)	O(601)	N(601)	1.243(5)
O(602)	N(601)	1.230(5)	O(603)	N(601)	1.251(5)
O(701)	H(701)	0.89	O(701)	H(702)	1.06
O(801)	H(801)	0.78	O(801)	H(802)	1.07
N(1)	C(1)	1.486(5)	N(1)	C(13)	1.474(4)
N(1)	C(25)	1.480(4)	N(2)	C(12)	1.477(4)
N(2)	C(24)	1.479(5)	N(2)	C(36)	1.474(5)
N(3)	C(2)	1.502(5)	N(3)	C(3)	1.494(5)
N(3)	H(5)	0.95	N(3)	H(6)	0.95
N(4)	C(10)	1.484(5)	N(4)	C(11)	1.500(5)
N(4)	H(15)	0.95	N(4)	H(16)	0.95
N(5)	C(14)	1.485(5)	N(5)	C(15)	1.503(5)
N(5)	H(25)	0.94	N(5)	H(26)	0.95
N(6)	C(22)	1.496(5)	N(6)	C(23)	1.498(5)
N(6)	H(35)	0.80	N(6)	H(36)	0.98
N(7)	C(26)	1.492(5)	N(7)	C(27)	1.490(5)
N(7)	H(45)	0.98	N(7)	H(46)	0.96

Table 3. Bond Lengths(Å) (continued)

atom	atom	distance	atom	atom	distance
N(8)	C(34)	1.498(5)	N(8)	C(35)	1.495(5)
N(8)	H(55)	0.95	N(8)	H(56)	0.97
C(1)	C(2)	1.512(5)	C(1)	H(1)	1.17
C(1)	H(2)	1.07	C(2)	H(3)	1.07
C(2)	H(4)	1.14	C(3)	C(4)	1.503(5)
C(3)	H(7)	0.95	C(3)	H(8)	1.00
C(4)	C(5)	1.384(5)	C(4)	C(9)	1.375(5)
C(5)	C(6)	1.391(6)	C(5)	H(9)	1.04
C(6)	C(7)	1.383(5)	C(6)	H(10)	1.07
C(7)	C(8)	1.390(5)	C(7)	H(11)	1.05
C(8)	C(9)	1.395(5)	C(8)	C(10)	1.500(5)
C(9)	H(12)	1.06	C(10)	H(13)	1.10
C(10)	H(14)	1.02	C(11)	C(12)	1.513(5)
C(11)	H(17)	0.97	C(11)	H(18)	1.07
C(12)	H(19)	1.10	C(12)	H(20)	1.14
C(13)	C(14)	1.520(5)	C(13)	H(21)	1.09
C(13)	H(22)	1.01	C(14)	H(23)	1.07
C(14)	H(24)	0.98	C(15)	C(16)	1.498(5)
C(15)	H(27)	1.10	C(15)	H(28)	1.11
C(16)	C(17)	1.393(6)	C(16)	C(21)	1.391(5)
C(17)	C(18)	1.388(6)	C(17)	H(29)	1.24
C(18)	C(19)	1.391(6)	C(18)	H(30)	1.13
C(19)	C(20)	1.387(6)	C(19)	H(31)	1.14
C(20)	C(21)	1.383(5)	C(20)	C(22)	1.505(6)

Table 3. Bond Lengths(Å) (continued)

atom	atom	distance	atom	atom	distance
C(21)	H(32)	1.07	C(22)	H(33)	1.08
C(22)	H(34)	1.18	C(23)	C(24)	1.508(6)
C(23)	H(37)	1.09	C(23)	H(40)	1.09
C(24)	H(38)	1.09	C(24)	H(39)	1.02
C(25)	C(26)	1.514(5)	C(25)	H(41)	0.98
C(25)	H(42)	1.13	C(26)	H(43)	1.02
C(26)	H(44)	0.98	C(27)	C(28)	1.515(6)
C(27)	H(47)	1.09	C(27)	H(48)	1.21
C(28)	C(29)	1.381(6)	C(28)	C(33)	1.387(6)
C(29)	C(30)	1.376(6)	C(29)	H(49)	1.09
C(30)	C(31)	1.386(6)	C(30)	H(50)	0.96
C(31)	C(32)	1.385(5)	C(31)	H(51)	1.09
C(32)	C(33)	1.398(6)	C(32)	C(34)	1.513(6)
C(33)	H(52)	1.06	C(34)	H(53)	1.11
C(34)	H(54)	1.03	C(35)	C(36)	1.523(5)
C(35)	H(57)	1.12	C(35)	H(58)	1.08
C(36)	H(59)	1.15	C(36)	H(60)	1.08

Table 4. Bond Angles(°)

atom	atom	atom	angle	atom	atom	atom	angle
H(701)	O(701)	H(702)	88.4	H(801)	O(801)	H(802)	99.2
C(1)	N(1)	C(13)	108.4(3)	C(1)	N(1)	C(25)	108.0(3)
C(13)	N(1)	C(25)	108.7(3)	C(12)	N(2)	C(24)	108.2(3)
C(12)	N(2)	C(36)	108.1(3)	C(24)	N(2)	C(36)	109.5(3)
C(2)	N(3)	C(3)	111.6(3)	C(2)	N(3)	H(5)	109.0
C(2)	N(3)	H(6)	109.0	C(3)	N(3)	H(5)	108.9
C(3)	N(3)	H(6)	108.9	H(5)	N(3)	H(6)	109.4
C(10)	N(4)	C(11)	112.8(3)	C(10)	N(4)	H(15)	108.6
C(10)	N(4)	H(16)	108.7	C(11)	N(4)	H(15)	108.6
C(11)	N(4)	H(16)	108.7	H(15)	N(4)	H(16)	109.4
C(14)	N(5)	C(15)	112.2(3)	C(14)	N(5)	H(25)	108.8
C(14)	N(5)	H(26)	108.3	C(15)	N(5)	H(25)	109.2
C(15)	N(5)	H(26)	108.7	H(25)	N(5)	H(26)	109.7
C(22)	N(6)	C(23)	111.7(3)	C(22)	N(6)	H(35)	107.1
C(22)	N(6)	H(36)	106.6	C(23)	N(6)	H(35)	108.5
C(23)	N(6)	H(36)	120.9	H(35)	N(6)	H(36)	100.8
C(26)	N(7)	C(27)	112.4(3)	C(26)	N(7)	H(45)	104.1
C(26)	N(7)	H(46)	111.0	C(27)	N(7)	H(45)	113.0
C(27)	N(7)	H(46)	99.6	H(45)	N(7)	H(46)	117.0
C(34)	N(8)	C(35)	111.4(3)	C(34)	N(8)	H(55)	109.0
C(34)	N(8)	H(56)	108.3	C(35)	N(8)	H(55)	108.9
C(35)	N(8)	H(56)	108.4	H(55)	N(8)	H(56)	110.9
O(101)	N(101)	O(102)	119.9(4)	O(101)	N(101)	O(103)	120.5(4)
O(102)	N(101)	O(103)	119.6(4)	O(201)	N(201)	O(202)	119.8(4)

Table 4. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
O(201)	N(201)	O(203)	120.5(4)	O(202)	N(201)	O(203)	119.6(4)
O(301)	N(301)	O(302)	120.5(4)	O(301)	N(301)	O(303)	121.3(4)
O(302)	N(301)	O(303)	118.1(4)	O(401)	N(401)	O(402)	119.5(4)
O(401)	N(401)	O(403)	122.3(4)	O(402)	N(401)	O(403)	118.2(4)
O(501)	N(501)	O(502)	119.5(5)	O(501)	N(501)	O(503)	119.3(5)
O(502)	N(501)	O(503)	121.1(5)	O(601)	N(601)	O(602)	120.3(5)
O(601)	N(601)	O(603)	120.0(5)	O(602)	N(601)	O(603)	119.7(5)
N(1)	C(1)	C(2)	114.0(3)	N(1)	C(1)	H(1)	108.4
N(1)	C(1)	H(2)	104.9	C(2)	C(1)	H(1)	113.9
C(2)	C(1)	H(2)	105.7	H(1)	C(1)	H(2)	109.6
N(3)	C(2)	C(1)	111.7(3)	N(3)	C(2)	H(3)	100.4
N(3)	C(2)	H(4)	107.1	C(1)	C(2)	H(3)	104.3
C(1)	C(2)	H(4)	111.4	H(3)	C(2)	H(4)	121.5
N(3)	C(3)	C(4)	112.6(3)	N(3)	C(3)	H(7)	108.4
N(3)	C(3)	H(8)	103.8	C(4)	C(3)	H(7)	121.8
C(4)	C(3)	H(8)	112.9	H(7)	C(3)	H(8)	94.6
C(3)	C(4)	C(5)	120.4(4)	C(3)	C(4)	C(9)	120.3(4)
C(5)	C(4)	C(9)	119.3(4)	C(4)	C(5)	C(6)	119.9(4)
C(4)	C(5)	H(9)	123.4	C(6)	C(5)	H(9)	116.6
C(5)	C(6)	C(7)	120.3(4)	C(5)	C(6)	H(10)	115.3
C(7)	C(6)	H(10)	124.2	C(6)	C(7)	C(8)	120.3(4)
C(6)	C(7)	H(11)	117.2	C(8)	C(7)	H(11)	122.3
C(7)	C(8)	C(9)	118.5(4)	C(7)	C(8)	C(10)	121.4(4)
C(9)	C(8)	C(10)	120.2(4)	C(4)	C(9)	C(8)	121.7(4)

Table 4. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C(4)	C(9)	H(12)	115.6	C(8)	C(9)	H(12)	122.6
N(4)	C(10)	C(8)	111.8(3)	N(4)	C(10)	H(13)	109.4
N(4)	C(10)	H(14)	106.9	C(8)	C(10)	H(13)	112.8
C(8)	C(10)	H(14)	114.1	H(13)	C(10)	H(14)	101.3
N(4)	C(11)	C(12)	112.2(3)	N(4)	C(11)	H(17)	100.9
N(4)	C(11)	H(18)	106.5	C(12)	C(11)	H(17)	107.8
C(12)	C(11)	H(18)	113.2	H(17)	C(11)	H(18)	115.7
N(2)	C(12)	C(11)	113.0(3)	N(2)	C(12)	H(19)	112.4
N(2)	C(12)	H(20)	111.5	C(11)	C(12)	H(19)	106.5
C(11)	C(12)	H(20)	106.4	H(19)	C(12)	H(20)	106.6
N(1)	C(13)	C(14)	114.0(3)	N(1)	C(13)	H(21)	110.5
N(1)	C(13)	H(22)	111.8	C(14)	C(13)	H(21)	111.1
C(14)	C(13)	H(22)	103.2	H(21)	C(13)	H(22)	105.7
N(5)	C(14)	C(13)	112.8(3)	N(5)	C(14)	H(23)	107.3
N(5)	C(14)	H(24)	112.6	C(13)	C(14)	H(23)	109.6
C(13)	C(14)	H(24)	106.7	H(23)	C(14)	H(24)	107.7
N(5)	C(15)	C(16)	112.4(3)	N(5)	C(15)	H(27)	102.5
N(5)	C(15)	H(28)	107.0	C(16)	C(15)	H(27)	116.1
C(16)	C(15)	H(28)	111.1	H(27)	C(15)	H(28)	107.1
C(15)	C(16)	C(17)	121.1(4)	C(15)	C(16)	C(21)	119.9(4)
C(17)	C(16)	C(21)	118.9(4)	C(16)	C(17)	C(18)	119.7(4)
C(16)	C(17)	H(29)	122.7	C(18)	C(17)	H(29)	116.4
C(17)	C(18)	C(19)	120.9(4)	C(17)	C(18)	H(30)	117.9
C(19)	C(18)	H(30)	118.7	C(18)	C(19)	C(20)	119.5(4)

Table 4. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C(18)	C(19)	H(31)	116.6	C(20)	C(19)	H(31)	123.7
C(19)	C(20)	C(21)	119.4(4)	C(19)	C(20)	C(22)	121.6(4)
C(21)	C(20)	C(22)	118.9(4)	C(16)	C(21)	C(20)	121.5(4)
C(16)	C(21)	H(32)	114.2	C(20)	C(21)	H(32)	124.2
N(6)	C(22)	C(20)	112.1(3)	N(6)	C(22)	H(33)	106.5
N(6)	C(22)	H(34)	102.9	C(20)	C(22)	H(33)	102.9
C(20)	C(22)	H(34)	111.1	H(33)	C(22)	H(34)	121.4
N(6)	C(23)	C(24)	111.8(3)	N(6)	C(23)	H(37)	108.9
N(6)	C(23)	H(40)	100.5	C(24)	C(23)	H(37)	107.6
C(24)	C(23)	H(40)	110.3	H(37)	C(23)	H(40)	117.6
N(2)	C(24)	C(23)	113.7(3)	N(2)	C(24)	H(38)	106.9
N(2)	C(24)	H(39)	111.9	C(23)	C(24)	H(38)	110.4
C(23)	C(24)	H(39)	109.9	H(38)	C(24)	H(39)	103.6
N(1)	C(25)	C(26)	113.9(3)	N(1)	C(25)	H(41)	108.3
N(1)	C(25)	H(42)	114.0	C(26)	C(25)	H(41)	113.8
C(26)	C(25)	H(42)	105.5	H(41)	C(25)	H(42)	100.7
N(7)	C(26)	C(25)	112.2(3)	N(7)	C(26)	H(43)	102.5
N(7)	C(26)	H(44)	102.2	C(25)	C(26)	H(43)	113.0
C(25)	C(26)	H(44)	112.7	H(43)	C(26)	H(44)	113.3
N(7)	C(27)	C(28)	112.3(3)	N(7)	C(27)	H(47)	104.8
N(7)	C(27)	H(48)	99.6	C(28)	C(27)	H(47)	108.9
C(28)	C(27)	H(48)	107.2	H(47)	C(27)	H(48)	123.6
C(27)	C(28)	C(29)	122.2(4)	C(27)	C(28)	C(33)	118.8(4)
C(29)	C(28)	C(33)	118.9(4)	C(28)	C(29)	C(30)	120.0(4)

Table 4. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C(28)	C(29)	H(49)	117.4	C(30)	C(29)	H(49)	122.4
C(29)	C(30)	C(31)	121.8(4)	C(29)	C(30)	H(50)	124.7
C(31)	C(30)	H(50)	113.5	C(30)	C(31)	C(32)	118.7(4)
C(30)	C(31)	H(51)	128.0	C(32)	C(31)	H(51)	113.1
C(31)	C(32)	C(33)	119.5(4)	C(31)	C(32)	C(34)	121.0(4)
C(33)	C(32)	C(34)	119.4(4)	C(28)	C(33)	C(32)	121.1(4)
C(28)	C(33)	H(52)	120.3	C(32)	C(33)	H(52)	118.6
N(8)	C(34)	C(32)	112.0(3)	N(8)	C(34)	H(53)	109.2
N(8)	C(34)	H(54)	102.6	C(32)	C(34)	H(53)	109.4
C(32)	C(34)	H(54)	107.1	H(53)	C(34)	H(54)	116.3
N(8)	C(35)	C(36)	111.7(3)	N(8)	C(35)	H(57)	114.5
N(8)	C(35)	H(58)	100.8	C(36)	C(35)	H(57)	111.0
C(36)	C(35)	H(58)	105.2	H(57)	C(35)	H(58)	112.9
N(2)	C(36)	C(35)	113.8(3)	N(2)	C(36)	H(59)	111.1
N(2)	C(36)	H(60)	117.7	C(35)	C(36)	H(59)	105.7
C(35)	C(36)	H(60)	101.4	H(59)	C(36)	H(60)	106.0

Table 5. Non-bonded Contacts out to 3.60 Å

atom	atom	distance	ADC	atom	atom	distance	ADC
O(101)	H(6)	1.9862	1	O(101)	H(26)	2.2177	1
O(101)	H(28)	2.8131	1	O(101)	H(32)	2.8674	1
O(101)	N(3)	2.904(4)	1	O(101)	N(5)	2.955(4)	1
O(101)	H(24)	3.0845	1	O(101)	H(5)	3.1644	1
O(101)	C(15)	3.272(5)	1	O(101)	N(1)	3.321(4)	1
O(101)	O(201)	3.396(4)	1	O(101)	C(14)	3.398(5)	1
O(101)	C(21)	3.514(5)	1	O(101)	H(46)	3.5497	1
O(101)	H(2)	3.5703	1	O(101)	N(201)	3.574(4)	1
O(102)	H(26)	1.9727	1	O(102)	H(46)	2.1968	1
O(102)	H(44)	2.8304	1	O(102)	H(48)	2.8512	1
O(102)	N(5)	2.901(4)	1	O(102)	N(7)	3.020(4)	1
O(102)	H(10)	3.0351	55601	O(102)	H(52)	3.1576	1
O(102)	H(25)	3.1911	1	O(102)	C(6)	3.278(5)	55601
O(102)	N(1)	3.280(4)	1	O(102)	C(26)	3.358(5)	1
O(102)	O(202)	3.384(4)	1	O(102)	H(6)	3.4988	1
O(102)	C(27)	3.502(5)	1	O(102)	H(22)	3.5342	1
O(103)	H(46)	2.0044	1	O(103)	H(6)	2.2629	1
O(103)	N(7)	2.870(4)	1	O(103)	H(8)	2.9560	1
O(103)	N(3)	3.031(4)	1	O(103)	H(4)	3.0733	1
O(103)	H(45)	3.1445	1	O(103)	H(12)	3.2302	1
O(103)	H(29)	3.2559	65501	O(103)	N(1)	3.344(4)	1
O(103)	O(203)	3.356(4)	1	O(103)	C(3)	3.402(5)	1
O(103)	N(201)	3.451(4)	1	O(103)	C(2)	3.488(5)	1
O(103)	H(26)	3.5099	1	O(103)	H(30)	3.5267	65501

Table 5. Non-bonded Contacts out to 3.60 Å (continued)

atom	atom	distance	ADC	atom	atom	distance	ADC
O(201)	H(16)	1.9142	1	O(201)	H(36)	2.3745	1
O(201)	H(40)	2.7505	1	O(201)	H(34)	2.7678	1
O(201)	N(4)	2.851(4)	1	O(201)	N(6)	2.975(4)	1
O(201)	H(15)	3.1833	1	O(201)	H(32)	3.2007	1
O(201)	H(50)	3.2421	45401	O(201)	N(2)	3.289(4)	1
O(201)	C(23)	3.354(5)	1	O(201)	C(22)	3.367(5)	1
O(201)	H(55)	3.5326	1	O(202)	H(36)	1.9702	1
O(202)	H(55)	2.2811	1	O(202)	H(54)	2.9157	1
O(202)	N(6)	2.925(5)	1	O(202)	N(8)	3.035(4)	1
O(202)	H(57)	3.1039	1	O(202)	H(52)	3.1788	1
O(202)	H(35)	3.1844	1	O(202)	N(2)	3.318(4)	1
O(202)	C(35)	3.407(5)	1	O(202)	N(101)	3.446(4)	1
O(202)	C(34)	3.455(5)	1	O(202)	H(16)	3.5071	1
O(202)	O(403)	3.539(5)	1	O(203)	H(55)	1.9561	1
O(203)	H(16)	2.2978	1	O(203)	H(30)	2.6627	65501
O(203)	N(8)	2.877(4)	1	O(203)	H(14)	2.9133	1
O(203)	H(18)	2.9246	1	O(203)	N(4)	3.000(4)	1
O(203)	H(12)	3.1119	1	O(203)	H(56)	3.1858	1
O(203)	N(2)	3.277(4)	1	O(203)	C(10)	3.319(5)	1
O(203)	C(11)	3.372(5)	1	O(203)	C(18)	3.441(5)	65501
O(203)	C(9)	3.587(5)	1	O(301)	H(29)	2.1689	1
O(301)	H(4)	2.2172	45501	O(301)	H(1)	2.6437	65702
O(301)	H(45)	2.7021	45501	O(301)	H(25)	2.8633	1
O(301)	H(42)	2.8787	45501	O(301)	H(8)	2.9177	45501

Table 5. Non-bonded Contacts out to 3.60 Å (continued)

atom	atom	distance	ADC	atom	atom	distance	ADC
O(301)	H(27)	2.9337	1	O(301)	H(41)	3.1836	65702
O(301)	C(17)	3.296(5)	1	O(301)	C(2)	3.322(5)	45501
O(301)	H(21)	3.3279	65702	O(301)	H(23)	3.5106	1
O(301)	N(7)	3.526(6)	45501	O(301)	N(5)	3.543(5)	1
O(301)	C(15)	3.571(6)	1	O(302)	H(45)	1.9214	45501
O(302)	H(702)	1.9750	1	O(302)	H(1)	2.4817	65702
O(302)	H(49)	2.5475	45501	O(302)	O(701)	2.843(6)	1
O(302)	N(7)	2.874(4)	45501	O(302)	H(701)	2.8864	1
O(302)	H(42)	2.9427	45501	O(302)	H(47)	3.3110	45501
O(302)	O(503)	3.357(6)	1	O(302)	C(29)	3.383(5)	45501
O(302)	C(1)	3.453(5)	65702	O(302)	H(29)	3.4548	1
O(302)	H(43)	3.4553	45501	O(302)	H(46)	3.5009	45501
O(302)	C(27)	3.527(5)	45501	O(302)	H(2)	3.5364	65702
O(302)	C(26)	3.587(5)	45501	O(302)	H(9)	3.5917	55601
O(303)	H(25)	1.9301	1	O(303)	H(9)	2.4522	55601
O(303)	H(10)	2.7530	55601	O(303)	H(22)	2.7976	1
O(303)	N(5)	2.843(4)	1	O(303)	H(21)	2.8556	65702
O(303)	H(702)	2.9366	1	O(303)	H(1)	3.0849	65702
O(303)	H(29)	3.1010	1	O(303)	H(23)	3.1839	1
O(303)	C(5)	3.258(5)	55601	O(303)	O(701)	3.335(5)	1
O(303)	C(14)	3.357(5)	1	O(303)	H(26)	3.3787	1
O(303)	C(6)	3.418(5)	55601	O(303)	C(13)	3.558(5)	1
O(303)	H(27)	3.5754	1	O(401)	H(35)	2.1440	1
O(401)	H(801)	2.2813	1	O(401)	H(60)	2.3374	66702

Table 5. Non-bonded Contacts out to 3.60 Å (continued)

atom	atom	distance	ADC	atom	atom	distance	ADC
O(401)	H(31)	2.7908	1	O(401)	N(6)	2.895(4)	1
O(401)	H(36)	2.9455	1	O(401)	O(801)	2.958(5)	1
O(401)	H(38)	3.0010	1	O(401)	O(603)	3.274(5)	56702
O(401)	H(57)	3.3098	1	O(401)	C(36)	3.378(5)	66702
O(401)	C(19)	3.389(5)	1	O(401)	H(802)	3.4078	1
O(401)	H(58)	3.4430	66702	O(402)	H(15)	1.9033	55601
O(402)	H(801)	2.4692	1	O(402)	H(51)	2.6201	45501
O(402)	H(11)	2.7050	55601	O(402)	H(20)	2.8172	55601
O(402)	N(4)	2.848(4)	55601	O(402)	H(50)	3.1861	45501
O(402)	O(801)	3.219(5)	1	O(402)	H(17)	3.2988	55601
O(402)	H(16)	3.3031	55601	O(402)	H(802)	3.3863	1
O(402)	C(31)	3.395(5)	45501	O(402)	H(60)	3.4331	66702
O(402)	C(11)	3.518(5)	55601	O(402)	C(7)	3.533(5)	55601
O(402)	H(19)	3.5681	66702	O(403)	H(54)	2.4361	1
O(403)	H(57)	2.5138	1	O(403)	H(15)	2.5365	55601
O(403)	H(13)	2.7500	55601	O(403)	H(17)	2.8107	55601
O(403)	H(11)	2.8537	55601	O(403)	H(39)	3.0082	66702
O(403)	H(60)	3.0181	66702	O(403)	N(4)	3.177(5)	55601
O(403)	C(34)	3.356(6)	1	O(403)	C(10)	3.364(6)	55601
O(403)	C(35)	3.470(5)	1	O(403)	C(11)	3.507(6)	55601
O(403)	H(38)	3.5879	1	O(501)	H(7)	2.4193	45601
O(501)	H(27)	2.4580	55601	O(501)	H(23)	2.5994	55601
O(501)	H(41)	2.8122	65802	O(501)	H(3)	3.1118	45601
O(501)	H(43)	3.1385	45501	O(501)	H(8)	3.2590	45601

Table 5. Non-bonded Contacts out to 3.60 Å (continued)

atom	atom	distance	ADC	atom	atom	distance	ADC
O(501)	H(43)	3.3001	65802	O(501)	C(3)	3.309(6)	45601
O(501)	N(501)	3.332(5)	55802	O(501)	O(501)	3.428(8)	55802
O(501)	C(15)	3.433(6)	55601	O(501)	C(14)	3.437(6)	55601
O(501)	H(24)	3.4832	55601	O(501)	H(28)	3.5673	55601
O(501)	H(4)	3.5809	45601	O(501)	O(502)	3.585(6)	55802
O(502)	H(9)	2.7261	65702	O(502)	H(23)	2.7354	55601
O(502)	H(7)	2.8795	65702	O(502)	H(22)	2.9357	65802
O(502)	H(5)	2.9721	65702	O(502)	H(3)	3.0285	65702
O(502)	H(44)	3.0368	65802	O(502)	H(43)	3.1062	65802
O(502)	O(701)	3.133(8)	65802	O(502)	H(24)	3.2980	55601
O(502)	C(26)	3.349(6)	65802	O(502)	H(41)	3.3733	65802
O(502)	C(3)	3.405(6)	65702	O(502)	C(14)	3.490(6)	55601
O(502)	N(3)	3.502(5)	65702	O(502)	C(5)	3.532(6)	65702
O(502)	H(701)	3.5413	1	O(503)	H(43)	2.3508	45501
O(503)	H(3)	2.4717	65702	O(503)	H(701)	2.6280	1
O(503)	H(702)	2.9842	1	O(503)	H(24)	2.9938	55601
O(503)	H(47)	3.0390	45501	O(503)	H(23)	3.1767	55601
O(503)	H(28)	3.2240	55601	O(503)	H(27)	3.2480	55601
O(503)	C(26)	3.302(6)	45501	O(503)	O(701)	3.361(7)	1
O(503)	H(45)	3.4378	45501	O(503)	C(2)	3.512(6)	65702
O(503)	C(14)	3.537(6)	55601	O(601)	H(53)	2.4945	66802
O(601)	H(33)	2.5121	56702	O(601)	H(37)	2.5841	56702
O(601)	H(17)	2.6203	66702	O(601)	H(37)	2.8664	55601
O(601)	H(39)	3.0923	55601	O(601)	H(18)	3.1929	66702

Table 5. Non-bonded Contacts out to 3.60 Å (continued)

atom	atom	distance	ADC	atom	atom	distance	ADC
O(601)	C(11)	3.286(5)	66702	O(601)	H(13)	3.3372	66702
O(601)	C(34)	3.423(5)	66802	O(601)	O(601)	3.425(7)	56802
O(601)	C(22)	3.472(6)	56702	O(601)	N(601)	3.505(5)	56802
O(601)	C(23)	3.540(5)	56702	O(601)	H(54)	3.5547	66802
O(602)	H(802)	2.0170	1	O(602)	H(20)	2.7335	55601
O(602)	H(37)	2.8068	55601	O(602)	H(19)	2.8799	66702
O(602)	H(17)	2.8939	66702	O(602)	O(801)	2.958(6)	1
O(602)	H(801)	2.9770	1	O(602)	H(40)	2.9936	55601
O(602)	H(18)	3.2066	66702	O(602)	C(23)	3.207(6)	55601
O(602)	H(39)	3.2746	55601	O(602)	H(51)	3.2873	45501
O(602)	H(59)	3.2899	66702	O(602)	C(11)	3.298(6)	66702
O(602)	H(53)	3.3142	45501	O(603)	H(802)	2.2793	1
O(603)	H(37)	2.4258	56702	O(603)	H(58)	2.5065	45501
O(603)	H(33)	2.6809	56702	O(603)	H(35)	2.6898	56702
O(603)	H(31)	3.1345	56702	O(603)	N(6)	3.162(5)	56702
O(603)	C(23)	3.188(6)	56702	O(603)	H(18)	3.1980	66702
O(603)	O(801)	3.224(5)	1	O(603)	O(801)	3.338(5)	56702
O(603)	H(801)	3.4040	56702	O(603)	C(22)	3.421(6)	56702
O(603)	H(59)	3.4732	66702	O(603)	C(35)	3.573(6)	45501
O(701)	H(5)	1.8192	55601	O(701)	H(701)	2.3877	65802
O(701)	H(2)	2.4405	55601	O(701)	N(3)	2.730(5)	55601
O(701)	H(9)	2.9368	55601	O(701)	O(701)	3.013(9)	65802
O(701)	H(24)	3.0743	55601	O(701)	H(6)	3.0851	55601
O(701)	H(2)	3.2072	65702	O(701)	H(3)	3.2096	55601

Table 5. Non-bonded Contacts out to 3.60 Å (continued)

atom	atom	distance	ADC	atom	atom	distance	ADC
O(701)	C(1)	3.334(5)	55601	O(701)	C(2)	3.359(6)	55601
O(701)	N(301)	3.508(6)	1	O(801)	H(56)	1.7517	45501
O(801)	H(59)	2.5133	45501	O(801)	N(8)	2.684(5)	45501
O(801)	H(31)	2.8320	1	O(801)	H(51)	2.8574	45501
O(801)	H(58)	2.8779	45501	O(801)	H(802)	3.1224	56702
O(801)	C(35)	3.201(5)	45501	O(801)	H(55)	3.2564	45501
O(801)	C(36)	3.351(5)	45501	O(801)	H(53)	3.4205	45501
O(801)	O(801)	3.427(7)	56702	O(801)	H(59)	3.4336	66702
O(801)	N(401)	3.490(5)	1	O(801)	N(601)	3.515(6)	1
O(801)	C(34)	3.526(5)	45501	N(1)	N(101)	3.090(4)	1
N(2)	N(201)	3.067(4)	1	N(3)	H(702)	3.2639	55401
N(3)	N(101)	3.283(5)	1	N(3)	H(701)	3.4215	55401
N(4)	N(201)	3.259(5)	1	N(4)	N(401)	3.451(5)	55401
N(5)	H(10)	3.1831	55601	N(5)	N(101)	3.274(5)	1
N(5)	N(301)	3.587(5)	1	N(6)	N(201)	3.284(5)	1
N(7)	N(101)	3.283(5)	1	N(7)	N(301)	3.594(5)	65501
N(8)	H(802)	3.1376	65501	N(8)	H(801)	3.1821	65501
N(8)	N(201)	3.294(5)	1	N(101)	H(26)	2.3534	1
N(101)	H(6)	2.3558	1	N(101)	H(46)	2.3724	1
N(101)	N(201)	3.339(4)	1	N(101)	H(44)	3.5166	1
N(201)	H(16)	2.3524	1	N(201)	H(55)	2.3778	1
N(201)	H(36)	2.4545	1	N(201)	H(40)	3.4376	1
N(301)	H(1)	2.4734	65702	N(301)	H(45)	2.6428	45501
N(301)	H(29)	2.6579	1	N(301)	H(25)	2.7170	1

Table 5. Non-bonded Contacts out to 3.60 Å (continued)

atom	atom	distance	ADC	atom	atom	distance	ADC
N(301)	H(702)	2.8425	1	N(301)	H(21)	3.1518	65702
N(301)	H(49)	3.2569	45501	N(301)	H(42)	3.2581	45501
N(301)	H(4)	3.2698	45501	N(301)	H(9)	3.3996	55601
N(301)	H(10)	3.4507	55601	N(301)	C(1)	3.543(5)	65702
N(401)	H(15)	2.5835	55601	N(401)	H(60)	2.6994	66702
N(401)	H(801)	2.7203	1	N(401)	H(11)	2.8521	55601
N(401)	H(35)	3.1767	1	N(401)	H(57)	3.2823	1
N(401)	H(17)	3.4122	55601	N(401)	H(19)	3.5708	66702
N(401)	H(54)	3.5714	1	N(401)	H(20)	3.5814	55601
N(401)	H(31)	3.5858	1	N(501)	H(23)	2.5890	55601
N(501)	H(3)	2.9563	65702	N(501)	H(43)	3.0228	45501
N(501)	H(24)	3.0424	55601	N(501)	H(27)	3.0691	55601
N(501)	C(14)	3.284(5)	55601	N(501)	H(701)	3.4107	1
N(501)	H(7)	3.4113	65702	N(501)	H(7)	3.4757	45601
N(501)	H(41)	3.5134	65802	N(501)	H(43)	3.5264	65802
N(601)	H(802)	2.4829	1	N(601)	H(37)	2.7483	56702
N(601)	H(17)	2.8479	66702	N(601)	H(33)	2.9461	56702
N(601)	H(18)	2.9650	66702	N(601)	H(37)	3.0719	55601
N(601)	C(11)	3.272(5)	66702	N(601)	H(58)	3.2882	45501
N(601)	H(53)	3.5032	45501	N(601)	H(59)	3.5484	66702
C(1)	H(42)	3.1794	75702	C(1)	H(701)	3.4411	55401
C(1)	H(701)	3.4822	65702	C(2)	H(41)	3.1218	75702
C(2)	H(42)	3.1649	75702	C(3)	H(27)	3.2945	65501
C(4)	H(48)	2.9321	55401	C(4)	H(44)	3.5930	55401

Table 5. Non-bonded Contacts out to 3.60 Å (continued)

atom	atom	distance	ADC	atom	atom	distance	ADC
C(5)	H(48)	2.8615	55401	C(5)	H(44)	2.9859	55401
C(5)	H(702)	3.5788	55401	C(6)	H(48)	2.8686	55401
C(6)	H(50)	3.1110	45401	C(6)	H(44)	3.4188	55401
C(6)	H(25)	3.4781	55401	C(7)	H(48)	2.9305	55401
C(7)	H(52)	2.9568	55401	C(7)	H(50)	2.9693	45401
C(8)	H(48)	3.0312	55401	C(8)	H(52)	3.1050	55401
C(8)	H(50)	3.5837	45401	C(9)	H(48)	3.0281	55401
C(10)	H(52)	3.3315	55401	C(10)	H(33)	3.4619	65501
C(10)	H(54)	3.5225	55401	C(11)	H(19)	3.4869	66602
C(12)	H(19)	2.8415	66602	C(12)	H(20)	3.4777	66602
C(13)	H(21)	3.2192	65702	C(13)	H(23)	3.2477	65702
C(14)	H(21)	3.2185	65702	C(15)	H(47)	3.1366	45401
C(15)	H(8)	3.4972	45501	C(16)	H(12)	3.2388	45501
C(16)	H(10)	3.5316	55601	C(16)	H(8)	3.5947	45501
C(17)	H(12)	2.8355	45501	C(17)	H(10)	3.1863	55601
C(17)	H(8)	3.2847	45501	C(18)	H(12)	2.9596	45501
C(18)	H(14)	3.2984	45501	C(19)	H(14)	2.7709	45501
C(19)	H(12)	3.4358	45501	C(19)	H(801)	3.5975	1
C(20)	H(14)	3.0705	45501	C(22)	H(14)	3.4601	45501
C(24)	H(58)	3.3162	66702	C(24)	H(57)	3.3486	66702
C(25)	H(3)	3.2687	75702	C(25)	H(1)	3.4526	75702
C(25)	H(4)	3.5364	75702	C(27)	H(28)	3.4707	65601
C(28)	H(32)	3.3092	65601	C(29)	H(32)	2.9090	65601
C(29)	H(34)	3.2852	65601	C(30)	H(34)	2.7733	65601

Table 5. Non-bonded Contacts out to 3.60 Å (continued)

atom	atom	distance	ADC	atom	atom	distance	ADC
C(30)	H(30)	3.2281	65501	C(30)	H(32)	3.3095	65601
C(31)	H(34)	2.6024	65601	C(31)	H(30)	3.0480	65501
C(31)	H(40)	3.4334	65601	C(31)	H(801)	3.4664	65501
C(32)	H(34)	3.0123	65601	C(32)	H(30)	3.2339	65501
C(32)	H(13)	3.3934	55601	C(33)	H(13)	3.1485	55601
C(33)	H(34)	3.5068	65601	C(33)	H(30)	3.5771	65501
C(34)	H(13)	3.0888	55601	C(35)	H(38)	3.1440	66702
C(35)	H(802)	3.3696	65501	C(35)	H(39)	3.3902	66702
C(36)	H(38)	3.5944	66702	H(1)	H(42)	2.4014	75702
H(1)	H(4)	3.2197	75702	H(1)	H(45)	3.3956	75702
H(1)	H(701)	3.4137	65702	H(1)	H(702)	3.4738	65702
H(1)	H(41)	3.4924	75702	H(2)	H(701)	2.4268	55401
H(2)	H(701)	2.7864	65702	H(2)	H(702)	3.1541	55401
H(2)	H(702)	3.4971	65702	H(3)	H(41)	2.7700	75702
H(3)	H(42)	2.8714	75702	H(3)	H(43)	3.1842	75702
H(3)	H(701)	3.3757	65702	H(4)	H(41)	2.8342	75702
H(4)	H(42)	3.1770	75702	H(4)	H(29)	3.5071	65501
H(5)	H(702)	2.3957	55401	H(5)	H(701)	2.5807	55401
H(5)	H(701)	3.5096	65702	H(6)	H(702)	3.3854	55401
H(7)	H(27)	2.8796	65501	H(7)	H(43)	3.2539	55401
H(7)	H(47)	3.5437	55401	H(8)	H(29)	2.6680	65501
H(8)	H(27)	2.6734	65501	H(9)	H(44)	2.8237	55401
H(9)	H(702)	2.9234	55401	H(9)	H(22)	3.1812	55401
H(9)	H(25)	3.3462	55401	H(9)	H(48)	3.4634	55401

Table 5. Non-bonded Contacts out to 3.60 Å (continued)

atom	atom	distance	ADC	atom	atom	distance	ADC
H(10)	H(25)	2.5776	55401	H(10)	H(26)	2.9836	55401
H(10)	H(50)	3.1934	45401	H(10)	H(29)	3.3648	55401
H(10)	H(48)	3.5297	55401	H(10)	H(44)	3.5924	55401
H(11)	H(50)	2.9223	45401	H(11)	H(52)	3.0056	55401
H(11)	H(48)	3.5924	55401	H(12)	H(29)	2.9715	65501
H(12)	H(30)	3.0842	65501	H(13)	H(54)	2.4644	55401
H(13)	H(52)	2.6821	55401	H(13)	H(33)	3.0148	65501
H(13)	H(53)	3.2252	55401	H(14)	H(33)	2.8177	65501
H(14)	H(31)	2.9162	65501	H(14)	H(30)	3.4914	65501
H(15)	H(50)	3.2605	45401	H(16)	H(50)	3.4489	45401
H(17)	H(19)	3.0417	66602	H(17)	H(39)	3.1126	66602
H(17)	H(20)	3.5412	66602	H(18)	H(31)	2.9701	65501
H(18)	H(33)	3.3914	65501	H(19)	H(19)	2.2935	66602
H(19)	H(20)	2.4770	66602	H(21)	H(23)	2.4543	65702
H(21)	H(21)	2.8222	65702	H(21)	H(22)	3.0073	65702
H(21)	H(25)	3.5203	65702	H(22)	H(23)	3.0451	65702
H(23)	H(41)	3.4510	65702	H(24)	H(701)	2.7895	55401
H(24)	H(702)	3.1735	55401	H(27)	H(47)	3.0831	45401
H(28)	H(47)	2.4628	45401	H(28)	H(49)	3.1124	45401
H(28)	H(702)	3.4262	55401	H(29)	H(45)	3.5841	45501
H(30)	H(55)	3.1514	45501	H(30)	H(56)	3.3765	45501
H(30)	H(51)	3.4848	45501	H(30)	H(50)	3.5882	45501
H(31)	H(801)	2.5948	1	H(31)	H(56)	3.1539	45501
H(32)	H(49)	3.0110	45401	H(32)	H(47)	3.2953	45401

Table 5. Non-bonded Contacts out to 3.60 Å (continued)

atom	atom	distance	ADC	atom	atom	distance	ADC
H(33)	H(53)	3.1060	45401	H(34)	H(51)	2.8485	45401
H(34)	H(50)	3.0980	45401	H(34)	H(53)	3.3818	45401
H(37)	H(58)	3.2163	66702	H(37)	H(53)	3.3999	45401
H(38)	H(58)	2.7858	66702	H(38)	H(57)	2.7928	66702
H(38)	H(60)	2.9389	66702	H(38)	H(38)	3.1524	66702
H(39)	H(57)	2.8476	66702	H(39)	H(58)	3.0108	66702
H(40)	H(51)	2.8800	45401	H(41)	H(42)	3.4052	75702
H(42)	H(42)	3.0373	75702	H(45)	H(702)	3.4915	65501
H(49)	H(702)	2.8088	65501	H(51)	H(801)	2.5846	65501
H(51)	H(802)	3.0768	65501	H(53)	H(802)	3.2885	65501
H(56)	H(801)	2.2161	65501	H(56)	H(802)	2.3448	65501
H(57)	H(60)	3.2929	66702	H(58)	H(802)	2.7059	65501
H(58)	H(801)	3.5828	65501	H(59)	H(802)	2.8337	66702
H(59)	H(802)	3.0379	65501	H(59)	H(801)	3.2172	65501
H(59)	H(801)	3.3927	66702	H(60)	H(801)	3.2108	66702
H(60)	H(802)	3.4130	66702	H(701)	H(701)	1.9750	65802
H(701)	H(702)	3.2492	65802	H(801)	H(802)	3.5525	56702
H(802)	H(802)	3.1706	56702				

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

Supplemental Experimental Data

Anion exchange reaction: A solution of 0.1003 g (0.1227 mmol) $L_1 \cdot 6HCl$ in 5 mL H_2O was stirred at 23° C under atmospheric conditions with 0.1250 g (0.7360mmol) $AgNO_3$. AgCl was removed by centrifuge and the solvent of the remaining solution was removed *in vacuo*. The hexahydronitrate salt thus obtained was subsequently dissolved in a solution of 6 drops H_2O/2mL ethanol and heated at 40° C until clear. Slow ether diffusion for 7 d in a closed vial at 23° C produced clear colorless crystals suitable for X-ray diffraction. Anal. Calcd for $C_{36}H_{60}N_{14}O_{18} \cdot EtOH \cdot H_2O$: C, 43.84; H, 6.58; N, 18.84; Found: C, 43.55; H, 6.29; N, 18.85. ^1H NMR (400 MHz, D_2O) δ 2.73 (t, 12H, >NCH_2), 3.15 (t, 12H, -CH_2NH-), 4.11 (s, 12H, -CH_2Ph-), 7.25 (s, 3H, Ph), 7.47 (m, 9H, Ph); ^{13}C NMR δ 45.79 (>N*C*H_2-), 50.98 (-*C*H_2NH-), 51.81 (-*C*H_2Ph), 130.42, 131.35, 131.46, 131.77 (Ph).

Computational data: Brooks, J. P.; Bruccoleri, R.; Olafson, B.; States, D.; Swaminathan, S.; Karplus, M. *J. Comput. Chem.* **1983**, *4*, 187-217. Parameters, atomic charges and topology previously developed for this class of systems were employed to study a simplified system consisting of the macrocycle and the two internal nitrates in vacuum. The standard CHARMM Version 22 treatment of nonbonded interactions was used - a 12 Å atom-based nonbonded cutoff with a switching function between 10 Å and 12 Å for van der Waals terms and a shift function at 12 Å for electrostatics to eliminate discontinuities [charmm,pardna].

Potentiometric Data: Titrations were determined potentiometrically using a glass electrode and SCC standard electrode. The electrode was standardized and linearity of response checked by titrating standard HCl against standard NaOH. Slope, constant and electrode error were obtained from a plot of theoretical versus found pH. The pH was assumed to equal p[H] with pK_w = -13.79 under the conditions used. Standard base was checked for CO_3^{2-} contamination by Grans method and was found to be less than 2% CO_3^{2-} during all titrations. A sample of the hexahydrotosylate salt of the ligand was dissolved in 50 mL H_2O (freshly triply distilled in an all-glass still) to give a ligand concentration about 1-3 mM, and the ionic strength was adjusted to 0.1 M with potassium tosylate. The solution, maintained at 25.00 ± 0.05 °C, was then titrated with standard NaOH. The processing of three such curves in HYPERQUAD gave the protonation constants. Further titrations where KNO_3 had been added to the mixture were processed in HYPERQUAD to give the stability constant for the nitrate complexes.