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 refined isotropically. The final cycle of full-matrix least-squares refinement[3] was based on 7528 observed reflections ($I > 3.00\sigma(I)$) and 728 variable parameters and converged (largest parameter shift was 9.20 times its esd) with unweighted and weighted agreement factors of:

$$R = \Sigma||Fo| - |Fc||/\Sigma|Fo| = 0.050$$

$$R_w = \sqrt{\Sigma w(|Fo| - |Fc|)^2/\Sigma wFo^2} = 0.062$$

The standard deviation of an observation of unit weight[4] was 1.22. The weighting scheme was based on counting statistics and included a factor (p = 0.060) 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 0.83 and -0.31 $e^-/\AA^3$, respectively.

Neutral atom scattering factors were taken from Cromer and Waber[5] . Anomalous dispersion effects were included in Fcalc[6]; the values for Δf' and Δf" 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) SIR92: Altomare, A., Burla, M.C., Camalli, M., Cascarano, M., Giacovazzo, C., Guagliardi, A., Polidori, G., (1994), J. Appl. Cryst., 27, 435

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

where w = $\frac{1}{\sigma^2(Fo)} = [\sigma_c^2(Fo) + \frac{p^2}{4}Fo^2]^{-1}$

$\sigma_c(Fo)$ = e.s.d. based on counting statistics

p = p-factor

(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

Del

(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	$C_{35}H_{42}O_{12}N_6CuF_6S_2$
Formula Weight	980.41
Crystal Color, Habit	green, plate
Crystal Dimensions	0.33 X 0.75 X 0.13 mm
Crystal System	monoclinic
Lattice Type	Primitive
No. of Reflections Used for Unit Cell Determination (2θ range)	24 (38.8 - 39.9°)
Omega Scan Peak Width at Half-height	0.31°
Lattice Parameters	a = 7.493(3)Å b = 13.001(4) Å c = 20.876(2) Å β = 95.77(2)°
	V = 2023.3(10) Å^3
Space Group	$P2_1$ (#4)
Z value	4
D_{calc}	3.218 g/cm^3
F_{000}	2020.00
μ(MoKα)	14.80 cm^{-1}

B. Intensity Measurements

Diffractometer	Rigaku AFC5R
Radiation	MoKα (λ = 0.71069 Å) graphite monochromated

Attenuator	Zr foil (factors = 1.00, 3.40, 11.34, 38.03)
Take-off Angle	6.0°
Detector Aperture	9.0 mm horizontal 13.0 mm vertical
Crystal to Detector Distance	258 mm
Temperature	-100.0°C
Scan Type	ω-2θ
Scan Rate	8.0°/min (in ω) (up to 10 scans)
Scan Width	$(1.10 + 0.30 \tan \theta)°$
$2\theta_{max}$	55.0°
No. of Reflections Measured	Total: 10426 Unique: 4850 (R_{int} = 0.048)
Corrections	Lorentz-polarization Absorption (trans. factors: 0.8512 - 0.9980) Decay (3.69% decline)

C. Structure Solution and Refinement

Structure Solution	Direct Methods (SIR92)
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	0.0600
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (I>3.00σ(I))	7528
No. Variables	728
Reflection/Parameter Ratio	10.34
Residuals: R; Rw	0.050 ; 0.062
Residuals: R1	0.050

No. of Reflections to calc R1	7528
Goodness of Fit Indicator	1.22
Max Shift/Error in Final Cycle	9.20
Maximum peak in Final Diff. Map	0.83 $e^-/\AA^3$
Minimum peak in Final Diff. Map	-0.31 $e^-/\AA^3$

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

atom	x	y	z	B_{eq}
Cu(1)	0.03074(5)	0.1523(3)	0.25708(2)	1.879(7)
S(1)	0.5103(2)	0.2151(3)	0.61269(6)	3.48(2)
S(2)	0.3502(2)	0.0843(4)	0.92852(6)	3.72(3)
F(1)	0.1837(4)	0.1413(5)	0.6100(2)	5.36(8)
F(2)	0.3326(5)	0.0817(5)	0.5383(2)	6.9(1)
F(3)	0.3874(5)	0.0322(4)	0.6360(2)	6.8(1)
F(4)	0.5425(8)	0.2515(4)	0.9349(3)	8.4(1)
F(5)	0.4867(5)	0.1918(5)	0.8395(2)	6.26(9)
F(6)	0.6835(4)	0.1205(4)	0.9050(2)	4.77(8)
O(1)	-0.1488(4)	0.3585(4)	0.2654(2)	3.14(7)
O(2)	0.3374(4)	0.0748(4)	0.1924(2)	2.84(6)
O(3)	-0.1129(4)	0.1625(4)	0.1018(1)	3.45(6)
O(4)	0.1105(5)	-0.0299(4)	0.3422(1)	3.38(7)
O(5)	-0.3169(4)	0.0614(4)	0.2705(1)	3.07(7)
O(6)	0.2968(4)	0.2894(4)	0.3676(2)	3.43(7)
O(7)	0.4526(8)	0.2885(5)	0.5668(3)	7.9(1)
O(8)	0.4984(6)	0.2434(5)	0.6780(2)	5.6(1)
O(9)	0.6774(4)	0.1659(5)	0.6030(2)	5.32(9)
O(10)	0.2015(7)	0.1511(6)	0.9316(3)	8.4(1)
O(11)	0.3283(6)	0.0071(5)	0.8791(2)	5.9(1)
O(12)	0.4303(7)	0.0468(5)	0.9887(2)	5.7(1)
N(1)	-0.0136(5)	0.3035(4)	0.2370(2)	2.44(6)
N(2)	0.2588(4)	0.1667(4)	0.2140(1)	2.21(6)
N(3)	-0.0853(4)	0.0961(4)	0.1571(2)	2.43(6)

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

atom	x	y	z	B_{eq}
N(4)	0.0788(4)	0.0010(4)	0.2766(2)	2.34(6)
N(5)	-0.1937(4)	0.1321(4)	0.3013(2)	2.17(6)
N(6)	0.1477(5)	0.2212(4)	0.3596(2)	2.77(7)
C(1)	0.2610(6)	0.3485(5)	0.1847(2)	2.59(7)
C(2)	0.0821(6)	0.3666(5)	0.2082(2)	2.40(7)
C(3)	-0.1000(7)	0.4684(5)	0.2637(2)	3.02(9)
C(4)	0.0414(7)	0.4768(5)	0.2168(2)	2.99(8)
C(5)	0.2300(8)	0.5193(5)	0.2384(3)	3.9(1)
C(6)	0.3673(7)	0.4356(5)	0.2235(3)	3.3(1)
C(7)	0.3340(6)	0.2435(5)	0.1921(2)	2.56(8)
C(8)	0.4423(7)	0.1050(6)	0.1394(3)	3.41(9)
C(9)	0.4723(7)	0.2186(6)	0.1475(3)	3.46(9)
C(10)	0.424(1)	0.2938(6)	0.0922(3)	5.0(1)
C(11)	0.2613(9)	0.3575(6)	0.1103(2)	4.1(1)
C(12)	-0.0198(6)	-0.0901(5)	0.1737(2)	2.86(8)
C(13)	-0.0843(5)	0.0050(5)	0.1382(2)	2.68(7)
C(14)	-0.071(1)	0.1002(7)	0.0468(3)	4.8(1)
C(15)	-0.1033(7)	-0.0095(6)	0.0662(2)	4.26(10)
C(16)	0.032(1)	-0.0978(7)	0.0585(3)	5.2(2)
C(17)	0.1069(7)	-0.1331(6)	0.1253(3)	4.0(1)
C(18)	0.0617(6)	-0.0786(5)	0.2415(2)	2.64(8)
C(19)	0.0517(9)	-0.1379(5)	0.3442(3)	4.2(1)
C(20)	0.0660(8)	-0.1781(5)	0.2769(3)	3.79(10)
C(21)	-0.0932(9)	-0.2385(5)	0.2391(4)	5.0(1)

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

atom	x	y	z	B_{eq}
C(22)	-0.1714(7)	-0.1675(5)	0.1868(3)	4.1(1)
C(23)	-0.1309(6)	0.1977(5)	0.4140(2)	2.83(8)
C(24)	-0.2363(5)	0.1516(5)	0.3576(2)	2.41(6)
C(25)	-0.4130(6)	0.0147(5)	0.3214(2)	3.22(9)
C(26)	-0.3926(7)	0.0910(5)	0.3768(3)	3.60(10)
C(27)	-0.325(1)	0.0566(6)	0.4452(3)	5.6(1)
C(28)	-0.1416(10)	0.1047(6)	0.4618(3)	4.6(1)
C(29)	0.0553(6)	0.2324(5)	0.4063(2)	2.61(8)
C(30)	0.2629(7)	0.3639(5)	0.4186(3)	3.7(1)
C(31)	0.1143(7)	0.3168(5)	0.4525(2)	3.16(9)
C(32)	-0.0649(9)	0.3737(6)	0.4574(3)	4.4(1)
C(33)	-0.2168(7)	0.3000(5)	0.4378(3)	4.2(1)
C(34)	0.3469(7)	0.1122(5)	0.5989(3)	3.89(9)
C(35)	0.5219(7)	0.1665(6)	0.9013(3)	4.34(9)
H(1)	-0.047(7)	0.488(4)	0.311(2)	3.1(9)
H(2)	-0.202(7)	0.494(4)	0.250(2)	3.1(9)
H(3)	-0.006(5)	0.504(3)	0.180(2)	1.3(7)
H(4)	0.231(7)	0.539(4)	0.281(3)	3.7(10)
H(5)	0.261(8)	0.574(5)	0.219(3)	5(1)
H(6)	0.430(8)	0.405(5)	0.268(3)	5.0(10)
H(7)	0.438(9)	0.447(5)	0.210(3)	3(1)
H(8)	0.162(10)	0.337(6)	0.090(4)	6(1)
H(9)	0.254(7)	0.426(4)	0.096(3)	3.5(9)
H(10)	0.416(7)	0.257(4)	0.057(3)	4.1(10)

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

atom	x	y	z	B_{eq}
H(11)	0.520(9)	0.337(5)	0.090(3)	4(1)
H(12)	0.594(8)	0.226(4)	0.169(3)	4(1)
H(13)	0.363(7)	0.090(4)	0.103(3)	3.3(9)
H(14)	0.551(8)	0.065(5)	0.146(3)	4(1)
H(15)	0.05(1)	0.104(6)	0.042(4)	7(1)
H(16)	-0.159(9)	0.131(6)	0.014(3)	6(1)
H(17)	-0.220(7)	-0.035(4)	0.057(2)	3.6(8)
H(18)	0.088(10)	-0.082(5)	0.040(3)	6(1)
H(19)	-0.03(1)	-0.156(7)	0.028(5)	9(1)
H(20)	0.208(8)	-0.106(4)	0.140(3)	4(1)
H(21)	0.121(7)	-0.208(5)	0.134(3)	4.6(10)
H(22)	-0.284(8)	-0.126(4)	0.205(3)	4(1)
H(23)	-0.24(1)	-0.186(6)	0.149(4)	7(1)
H(24)	-0.186(7)	-0.253(4)	0.271(3)	3.6(9)
H(25)	-0.045(9)	-0.309(5)	0.223(3)	6(1)
H(26)	0.184(8)	-0.205(5)	0.282(3)	4.1(9)
H(27)	0.126(7)	-0.167(4)	0.377(2)	2.7(9)
H(28)	-0.077(8)	-0.136(4)	0.357(3)	3.7(9)
H(29)	-0.359(8)	-0.059(4)	0.328(3)	4.0(9)
H(30)	-0.529(7)	-0.002(4)	0.304(3)	3.9(10)
H(31)	-0.501(9)	0.133(6)	0.371(3)	6(1)
H(32)	-0.352(9)	-0.007(5)	0.446(3)	5(1)
H(33)	-0.44(2)	0.07(2)	0.458(8)	17(3)
H(34)	-0.052(8)	0.057(5)	0.451(3)	3(1)

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

atom	x	y	z	B_{eq}
H(35)	-0.12(1)	0.147(8)	0.512(4)	10(1)
H(36)	-0.288(9)	0.325(5)	0.402(3)	5(1)
H(37)	-0.20(4)	0.19(2)	0.40(1)	46(8)
H(38)	-0.06(2)	0.38(1)	0.493(9)	12(3)
H(39)	-0.05(1)	0.442(7)	0.449(5)	8(2)
H(40)	0.136(6)	0.285(4)	0.495(2)	2.9(9)
H(41)	0.409(9)	0.375(5)	0.441(3)	6(1)
H(42)	0.223(8)	0.431(4)	0.398(3)	3.8(8)

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

Table 2. Anisotropic Displacement Parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Cu(1)	0.0197(2)	0.0274(2)	0.0251(2)	0.0006(2)	0.0058(1)	0.0009(2)
S(1)	0.0460(6)	0.0464(6)	0.0389(6)	-0.0108(5)	0.0009(5)	0.0003(5)
S(2)	0.0574(7)	0.0530(7)	0.0334(6)	0.0158(6)	0.0167(5)	0.0064(5)
F(1)	0.037(1)	0.086(3)	0.082(2)	-0.006(2)	0.012(1)	-0.007(2)
F(2)	0.079(2)	0.119(3)	0.069(2)	-0.050(2)	0.031(2)	-0.052(2)
F(3)	0.074(2)	0.052(2)	0.132(4)	-0.005(2)	0.009(2)	0.035(2)
F(4)	0.161(4)	0.051(2)	0.118(4)	-0.020(2)	0.078(3)	-0.026(2)
F(5)	0.065(2)	0.117(3)	0.060(2)	0.043(2)	0.029(2)	0.042(2)
F(6)	0.048(2)	0.075(2)	0.057(2)	0.008(1)	-0.001(1)	0.004(2)
O(1)	0.040(2)	0.031(1)	0.052(2)	0.005(1)	0.021(1)	0.001(1)
O(2)	0.024(1)	0.045(2)	0.040(2)	0.000(1)	0.009(1)	-0.010(1)
O(3)	0.044(2)	0.060(2)	0.026(1)	0.002(2)	0.000(1)	0.008(1)
O(4)	0.055(2)	0.043(2)	0.031(1)	0.012(1)	0.004(1)	0.005(1)
O(5)	0.028(1)	0.054(2)	0.035(2)	-0.013(1)	0.001(1)	0.002(1)
O(6)	0.032(2)	0.053(2)	0.045(2)	-0.006(1)	0.005(1)	-0.014(1)
O(7)	0.114(4)	0.066(3)	0.107(4)	-0.030(3)	-0.047(3)	0.046(3)
O(8)	0.061(2)	0.105(4)	0.046(2)	0.001(2)	0.006(2)	-0.033(2)
O(9)	0.040(2)	0.099(3)	0.066(2)	-0.020(2)	0.018(2)	-0.031(3)
O(10)	0.095(3)	0.100(3)	0.138(4)	0.062(3)	0.090(3)	0.056(4)
O(11)	0.062(2)	0.110(4)	0.053(2)	-0.015(2)	0.009(2)	-0.038(2)
O(12)	0.112(4)	0.070(3)	0.032(2)	-0.010(3)	0.003(2)	0.012(2)
N(1)	0.029(2)	0.033(1)	0.032(2)	0.001(1)	0.009(1)	0.002(1)
N(2)	0.021(1)	0.037(2)	0.026(1)	0.000(1)	0.003(1)	-0.010(1)
N(3)	0.023(2)	0.045(2)	0.024(2)	-0.003(1)	0.001(1)	0.000(1)

Table 2. Anisotropic Displacement Parameters (continued)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
N(4)	0.028(2)	0.033(1)	0.029(1)	0.002(1)	0.005(1)	0.002(1)
N(5)	0.023(1)	0.033(2)	0.027(1)	0.001(1)	0.004(1)	0.008(1)
N(6)	0.034(2)	0.038(2)	0.034(2)	0.003(1)	0.005(1)	-0.006(2)
C(1)	0.035(2)	0.042(2)	0.023(2)	-0.014(2)	0.009(2)	-0.001(2)
C(2)	0.035(2)	0.035(2)	0.021(2)	-0.009(2)	0.002(1)	-0.003(1)
C(3)	0.037(2)	0.031(2)	0.046(3)	0.004(2)	0.003(2)	0.000(2)
C(4)	0.056(2)	0.029(2)	0.028(2)	-0.001(2)	0.001(2)	0.004(2)
C(5)	0.060(3)	0.041(2)	0.049(3)	-0.026(2)	0.021(2)	-0.012(2)
C(6)	0.046(3)	0.046(2)	0.036(2)	-0.019(2)	0.007(2)	-0.004(2)
C(7)	0.027(2)	0.044(2)	0.028(2)	-0.010(2)	0.008(2)	-0.009(2)
C(8)	0.033(2)	0.064(2)	0.035(2)	0.003(2)	0.012(2)	-0.007(2)
C(9)	0.034(2)	0.063(2)	0.038(2)	-0.015(2)	0.021(2)	-0.015(2)
C(10)	0.100(5)	0.053(3)	0.048(3)	-0.005(3)	0.050(3)	0.001(2)
C(11)	0.065(3)	0.064(3)	0.026(2)	-0.020(2)	0.011(2)	-0.003(2)
C(12)	0.032(2)	0.038(2)	0.040(2)	-0.010(1)	0.010(2)	-0.015(2)
C(13)	0.021(2)	0.052(2)	0.029(2)	-0.010(2)	0.005(1)	-0.010(2)
C(14)	0.071(4)	0.087(3)	0.025(2)	0.011(3)	0.005(2)	-0.001(2)
C(15)	0.040(2)	0.090(3)	0.032(2)	-0.015(2)	0.004(2)	-0.024(2)
C(16)	0.082(5)	0.073(4)	0.049(3)	-0.008(3)	0.027(3)	-0.029(3)
C(17)	0.038(3)	0.058(3)	0.059(3)	-0.008(2)	0.021(2)	-0.026(2)
C(18)	0.030(2)	0.033(2)	0.039(2)	0.001(2)	0.012(2)	-0.001(1)
C(19)	0.069(4)	0.043(2)	0.052(2)	0.014(2)	0.018(3)	0.024(2)
C(20)	0.057(3)	0.031(2)	0.060(3)	0.012(2)	0.023(2)	0.007(2)
C(21)	0.064(3)	0.036(3)	0.093(4)	-0.008(2)	0.022(3)	0.004(2)

Table 2. Anisotropic Displacement Parameters (continued)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(22)	0.044(3)	0.052(3)	0.060(3)	-0.020(2)	0.013(2)	-0.015(2)
C(23)	0.042(2)	0.036(2)	0.032(2)	0.005(2)	0.012(2)	0.002(1)
C(24)	0.030(2)	0.027(2)	0.036(2)	0.009(2)	0.012(1)	0.006(2)
C(25)	0.029(2)	0.048(3)	0.044(2)	-0.012(2)	0.001(2)	0.017(2)
C(26)	0.038(2)	0.044(2)	0.060(3)	-0.003(2)	0.030(2)	0.005(2)
C(27)	0.119(5)	0.057(4)	0.041(3)	-0.042(4)	0.035(3)	-0.005(2)
C(28)	0.091(4)	0.052(3)	0.037(3)	0.006(3)	0.021(3)	0.017(2)
C(29)	0.040(2)	0.033(2)	0.026(2)	0.012(2)	0.003(1)	-0.001(1)
C(30)	0.036(2)	0.054(3)	0.051(3)	0.004(2)	0.003(2)	-0.017(2)
C(31)	0.053(2)	0.039(2)	0.027(2)	0.004(2)	0.001(2)	-0.002(2)
C(32)	0.059(3)	0.048(3)	0.060(4)	0.007(2)	0.014(3)	-0.020(3)
C(33)	0.046(3)	0.048(3)	0.065(4)	0.011(2)	0.014(3)	-0.019(3)
C(34)	0.042(2)	0.051(2)	0.057(2)	-0.010(2)	0.014(2)	-0.006(2)
C(35)	0.063(2)	0.055(3)	0.050(2)	0.013(2)	0.023(2)	0.008(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
Cu(1)	N(1)	2.030(4)	Cu(1)	N(2)	2.018(3)
Cu(1)	N(3)	2.299(4)	Cu(1)	N(4)	2.033(4)
Cu(1)	N(5)	2.015(3)	S(1)	O(7)	1.390(5)
S(1)	O(8)	1.425(4)	S(1)	O(9)	1.438(5)
S(1)	C(34)	1.817(6)	S(2)	O(10)	1.419(5)
S(2)	O(11)	1.437(4)	S(2)	O(12)	1.423(4)
S(2)	C(35)	1.807(7)	F(1)	C(34)	1.323(6)
F(2)	C(34)	1.319(7)	F(3)	C(34)	1.314(7)
F(4)	C(35)	1.309(8)	F(5)	C(35)	1.332(7)
F(6)	C(35)	1.347(7)	O(1)	N(1)	1.418(5)
O(1)	C(3)	1.477(6)	O(2)	N(2)	1.425(5)
O(2)	C(8)	1.473(6)	O(3)	N(3)	1.440(5)
O(3)	C(14)	1.463(7)	O(4)	N(4)	1.424(5)
O(4)	C(19)	1.473(7)	O(5)	N(5)	1.411(5)
O(5)	C(25)	1.472(6)	O(6)	N(6)	1.423(5)
O(6)	C(30)	1.479(6)	N(1)	C(2)	1.278(6)
N(2)	C(7)	1.255(6)	N(3)	C(13)	1.248(6)
N(4)	C(18)	1.268(6)	N(5)	C(24)	1.273(5)
N(6)	C(29)	1.260(6)	C(1)	C(2)	1.492(6)
C(1)	C(6)	1.564(7)	C(1)	C(7)	1.473(7)
C(1)	C(11)	1.557(7)	C(2)	C(4)	1.480(7)
C(3)	C(4)	1.517(7)	C(3)	H(1)	1.05(6)
C(3)	H(2)	0.86(6)	C(4)	C(5)	1.542(8)
C(4)	H(3)	0.89(4)	C(5)	C(6)	1.550(9)

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

atom	atom	distance	atom	atom	distance
C(5)	H(4)	0.91(6)	C(5)	H(5)	0.86(7)
C(6)	H(6)	1.08(7)	C(6)	H(7)	0.64(7)
C(7)	C(9)	1.496(7)	C(8)	C(9)	1.501(8)
C(8)	H(13)	0.93(6)	C(8)	H(14)	0.96(7)
C(9)	C(10)	1.529(10)	C(9)	H(12)	0.98(7)
C(10)	C(11)	1.55(1)	C(10)	H(10)	0.87(6)
C(10)	H(11)	0.92(8)	C(11)	H(8)	0.86(8)
C(11)	H(9)	0.94(6)	C(12)	C(13)	1.496(7)
C(12)	C(17)	1.557(7)	C(12)	C(18)	1.492(7)
C(12)	C(22)	1.562(7)	C(13)	C(15)	1.508(7)
C(14)	C(15)	1.51(1)	C(14)	H(15)	0.95(9)
C(14)	H(16)	0.99(8)	C(15)	C(16)	1.55(1)
C(15)	H(17)	0.94(6)	C(16)	C(17)	1.52(1)
C(16)	H(18)	0.63(7)	C(16)	H(19)	1.1(1)
C(17)	H(20)	0.86(7)	C(17)	H(21)	0.99(7)
C(18)	C(20)	1.490(7)	C(19)	C(20)	1.512(9)
C(19)	H(27)	0.92(6)	C(19)	H(28)	1.03(6)
C(20)	C(21)	1.57(1)	C(20)	H(26)	0.94(7)
C(21)	C(22)	1.50(1)	C(21)	H(24)	1.03(6)
C(21)	H(25)	1.05(8)	C(22)	H(22)	1.10(6)
C(22)	H(23)	0.93(9)	C(23)	C(24)	1.477(7)
C(23)	C(28)	1.575(7)	C(23)	C(29)	1.490(7)
C(23)	C(33)	1.580(7)	C(23)	H(37)	0.6(3)
C(24)	C(26)	1.500(6)	C(24)	H(37)	1.1(3)

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

atom	atom	distance	atom	atom	distance
C(25)	C(26)	1.520(8)	C(25)	H(29)	1.04(6)
C(25)	H(30)	0.93(6)	C(26)	C(27)	1.53(1)
C(26)	H(31)	0.98(8)	C(27)	C(28)	1.52(1)
C(27)	H(32)	0.86(8)	C(27)	H(33)	1.0(2)
C(28)	H(34)	0.96(6)	C(28)	H(35)	1.2(1)
C(29)	C(31)	1.498(7)	C(30)	C(31)	1.508(8)
C(30)	H(41)	1.16(7)	C(30)	H(42)	1.01(6)
C(31)	C(32)	1.546(8)	C(31)	H(40)	0.97(6)
C(32)	C(33)	1.512(10)	C(32)	H(38)	0.7(2)
C(32)	H(39)	0.9(1)	C(33)	H(36)	0.93(7)

Table 4. Bond Angles(°)

atom	atom	atom	angle	atom	atom	atom	angle
N(1)	Cu(1)	N(2)	86.9(2)	N(1)	Cu(1)	N(3)	94.6(2)
N(1)	Cu(1)	N(4)	179.1(2)	N(1)	Cu(1)	N(5)	95.4(1)
N(2)	Cu(1)	N(3)	83.4(1)	N(2)	Cu(1)	N(4)	92.2(2)
N(2)	Cu(1)	N(5)	177.7(2)	N(3)	Cu(1)	N(4)	85.3(1)
N(3)	Cu(1)	N(5)	96.8(1)	N(4)	Cu(1)	N(5)	85.5(1)
O(7)	S(1)	O(8)	115.9(4)	O(7)	S(1)	O(9)	115.1(4)
O(7)	S(1)	C(34)	103.8(3)	O(8)	S(1)	O(9)	112.9(3)
O(8)	S(1)	C(34)	103.7(3)	O(9)	S(1)	C(34)	103.4(3)
O(10)	S(2)	O(11)	115.2(4)	O(10)	S(2)	O(12)	115.7(3)
O(10)	S(2)	C(35)	103.9(3)	O(11)	S(2)	O(12)	113.7(3)
O(11)	S(2)	C(35)	102.8(3)	O(12)	S(2)	C(35)	103.3(3)
N(1)	O(1)	C(3)	106.8(3)	N(2)	O(2)	C(8)	106.4(4)
N(3)	O(3)	C(14)	105.8(4)	N(4)	O(4)	C(19)	106.0(4)
N(5)	O(5)	C(25)	106.6(3)	N(6)	O(6)	C(30)	107.6(4)
Cu(1)	N(1)	O(1)	120.7(3)	Cu(1)	N(1)	C(2)	129.1(3)
O(1)	N(1)	C(2)	109.4(4)	Cu(1)	N(2)	O(2)	117.3(3)
Cu(1)	N(2)	C(7)	131.8(3)	O(2)	N(2)	C(7)	109.7(3)
Cu(1)	N(3)	O(3)	123.3(3)	Cu(1)	N(3)	C(13)	125.0(3)
O(3)	N(3)	C(13)	108.7(4)	Cu(1)	N(4)	O(4)	118.4(3)
Cu(1)	N(4)	C(18)	131.9(3)	O(4)	N(4)	C(18)	108.9(4)
Cu(1)	N(5)	O(5)	114.5(3)	Cu(1)	N(5)	C(24)	134.0(3)
O(5)	N(5)	C(24)	109.7(3)	O(6)	N(6)	C(29)	108.8(4)
C(2)	C(1)	C(6)	98.2(4)	C(2)	C(1)	C(7)	116.6(4)
C(2)	C(1)	C(11)	114.1(4)	C(6)	C(1)	C(7)	116.9(4)

Table 4. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C(6)	C(1)	C(11)	114.2(4)	C(7)	C(1)	C(11)	97.9(4)
N(1)	C(2)	C(1)	128.2(4)	N(1)	C(2)	C(4)	115.6(4)
C(1)	C(2)	C(4)	113.3(4)	O(1)	C(3)	C(4)	106.0(4)
O(1)	C(3)	H(1)	106(3)	O(1)	C(3)	H(2)	100(3)
C(4)	C(3)	H(1)	111(2)	C(4)	C(3)	H(2)	113(3)
H(1)	C(3)	H(2)	117(4)	C(2)	C(4)	C(3)	100.0(4)
C(2)	C(4)	C(5)	100.9(4)	C(2)	C(4)	H(3)	110(2)
C(3)	C(4)	C(5)	121.1(4)	C(3)	C(4)	H(3)	110(2)
C(5)	C(4)	H(3)	112(2)	C(4)	C(5)	C(6)	107.3(4)
C(4)	C(5)	H(4)	107(3)	C(4)	C(5)	H(5)	116(4)
C(6)	C(5)	H(4)	116(3)	C(6)	C(5)	H(5)	105(4)
H(4)	C(5)	H(5)	104(5)	C(1)	C(6)	C(5)	107.4(5)
C(1)	C(6)	H(6)	109(3)	C(1)	C(6)	H(7)	109(6)
C(5)	C(6)	H(6)	109(3)	C(5)	C(6)	H(7)	121(6)
H(6)	C(6)	H(7)	99(7)	N(2)	C(7)	C(1)	126.9(4)
N(2)	C(7)	C(9)	114.7(5)	C(1)	C(7)	C(9)	114.1(4)
O(2)	C(8)	C(9)	105.2(4)	O(2)	C(8)	H(13)	101(3)
O(2)	C(8)	H(14)	104(4)	C(9)	C(8)	H(13)	112(3)
C(9)	C(8)	H(14)	113(4)	H(13)	C(8)	H(14)	117(5)
C(7)	C(9)	C(8)	100.3(4)	C(7)	C(9)	C(10)	101.8(5)
C(7)	C(9)	H(12)	111(3)	C(8)	C(9)	C(10)	121.5(6)
C(8)	C(9)	H(12)	105(3)	C(10)	C(9)	H(12)	115(3)
C(9)	C(10)	C(11)	106.9(4)	C(9)	C(10)	H(10)	105(3)
C(9)	C(10)	H(11)	107(4)	C(11)	C(10)	H(10)	120(3)

Table 4. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C(11)	C(10)	H(11)	109(4)	H(10)	C(10)	H(11)	106(5)
C(1)	C(11)	C(10)	106.4(5)	C(1)	C(11)	H(8)	111(5)
C(1)	C(11)	H(9)	112(3)	C(10)	C(11)	H(8)	112(5)
C(10)	C(11)	H(9)	117(3)	H(8)	C(11)	H(9)	97(6)
C(13)	C(12)	C(17)	99.4(4)	C(13)	C(12)	C(18)	117.8(4)
C(13)	C(12)	C(22)	114.5(4)	C(17)	C(12)	C(18)	115.6(4)
C(17)	C(12)	C(22)	112.6(4)	C(18)	C(12)	C(22)	97.7(4)
N(3)	C(13)	C(12)	129.8(4)	N(3)	C(13)	C(15)	115.5(5)
C(12)	C(13)	C(15)	112.5(5)	O(3)	C(14)	C(15)	105.1(5)
O(3)	C(14)	H(15)	110(5)	O(3)	C(14)	H(16)	97(4)
C(15)	C(14)	H(15)	105(5)	C(15)	C(14)	H(16)	117(4)
H(15)	C(14)	H(16)	119(6)	C(13)	C(15)	C(14)	98.5(5)
C(13)	C(15)	C(16)	101.5(5)	C(13)	C(15)	H(17)	104(3)
C(14)	C(15)	C(16)	123.2(6)	C(14)	C(15)	H(17)	116(3)
C(16)	C(15)	H(17)	108(3)	C(15)	C(16)	C(17)	108.2(5)
C(15)	C(16)	H(18)	108(7)	C(15)	C(16)	H(19)	108(5)
C(17)	C(16)	H(18)	116(8)	C(17)	C(16)	H(19)	115(5)
H(18)	C(16)	H(19)	99(8)	C(12)	C(17)	C(16)	107.1(5)
C(12)	C(17)	H(20)	101(4)	C(12)	C(17)	H(21)	107(3)
C(16)	C(17)	H(20)	115(4)	C(16)	C(17)	H(21)	118(3)
H(20)	C(17)	H(21)	105(5)	N(4)	C(18)	C(12)	129.8(5)
N(4)	C(18)	C(20)	115.2(5)	C(12)	C(18)	C(20)	111.7(4)
O(4)	C(19)	C(20)	104.7(4)	O(4)	C(19)	H(27)	104(3)
O(4)	C(19)	H(28)	105(3)	C(20)	C(19)	H(27)	116(3)

Table 4. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C(20)	C(19)	H(28)	113(3)	H(27)	C(19)	H(28)	109(4)
C(18)	C(20)	C(19)	99.3(4)	C(18)	C(20)	C(21)	101.9(5)
C(18)	C(20)	H(26)	110(3)	C(19)	C(20)	C(21)	121.2(6)
C(19)	C(20)	H(26)	99(4)	C(21)	C(20)	H(26)	121(4)
C(20)	C(21)	C(22)	106.2(5)	C(20)	C(21)	H(24)	106(3)
C(20)	C(21)	H(25)	108(4)	C(22)	C(21)	H(24)	110(3)
C(22)	C(21)	H(25)	115(4)	H(24)	C(21)	H(25)	108(4)
C(12)	C(22)	C(21)	106.6(5)	C(12)	C(22)	H(22)	110(3)
C(12)	C(22)	H(23)	111(5)	C(21)	C(22)	H(22)	107(3)
C(21)	C(22)	H(23)	127(5)	H(22)	C(22)	H(23)	92(5)
C(24)	C(23)	C(28)	97.9(4)	C(24)	C(23)	C(29)	117.9(4)
C(24)	C(23)	C(33)	113.0(4)	C(24)	C(23)	H(37)	42(32)
C(28)	C(23)	C(29)	114.1(5)	C(28)	C(23)	C(33)	113.5(5)
C(28)	C(23)	H(37)	94(32)	C(29)	C(23)	C(33)	101.2(4)
C(29)	C(23)	H(37)	149(31)	C(33)	C(23)	H(37)	76(34)
N(5)	C(24)	C(23)	130.8(4)	N(5)	C(24)	C(26)	114.7(5)
N(5)	C(24)	H(37)	147(16)	C(23)	C(24)	C(26)	111.6(4)
C(23)	C(24)	H(37)	20(16)	C(26)	C(24)	H(37)	97(16)
O(5)	C(25)	C(26)	105.1(4)	O(5)	C(25)	H(29)	104(3)
O(5)	C(25)	H(30)	108(3)	C(26)	C(25)	H(29)	119(3)
C(26)	C(25)	H(30)	118(3)	H(29)	C(25)	H(30)	99(4)
C(24)	C(26)	C(25)	99.2(4)	C(24)	C(26)	C(27)	102.1(5)
C(24)	C(26)	H(31)	109(4)	C(25)	C(26)	C(27)	121.1(5)
C(25)	C(26)	H(31)	104(4)	C(27)	C(26)	H(31)	118(4)

Table 4. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C(26)	C(27)	C(28)	107.5(5)	C(26)	C(27)	H(32)	103(4)
C(26)	C(27)	H(33)	88(11)	C(28)	C(27)	H(32)	127(5)
C(28)	C(27)	H(33)	134(12)	H(32)	C(27)	H(33)	86(12)
C(23)	C(28)	C(27)	105.9(5)	C(23)	C(28)	H(34)	105(3)
C(23)	C(28)	H(35)	100(5)	C(27)	C(28)	H(34)	108(3)
C(27)	C(28)	H(35)	114(4)	H(34)	C(28)	H(35)	119(6)
N(6)	C(29)	C(23)	129.9(5)	N(6)	C(29)	C(31)	115.7(5)
C(23)	C(29)	C(31)	111.8(4)	O(6)	C(30)	C(31)	105.1(4)
O(6)	C(30)	H(41)	99(3)	O(6)	C(30)	H(42)	108(3)
C(31)	C(30)	H(41)	124(3)	C(31)	C(30)	H(42)	110(3)
H(41)	C(30)	H(42)	106(4)	C(29)	C(31)	C(30)	100.3(4)
C(29)	C(31)	C(32)	101.1(4)	C(29)	C(31)	H(40)	106(3)
C(30)	C(31)	C(32)	121.6(5)	C(30)	C(31)	H(40)	122(3)
C(32)	C(31)	H(40)	102(3)	C(31)	C(32)	C(33)	108.3(5)
C(31)	C(32)	H(38)	102(15)	C(31)	C(32)	H(39)	111(6)
C(33)	C(32)	H(38)	110(15)	C(33)	C(32)	H(39)	129(6)
H(38)	C(32)	H(39)	90(13)	C(23)	C(33)	C(32)	107.4(5)
C(23)	C(33)	H(36)	105(4)	C(32)	C(33)	H(36)	110(4)
S(1)	C(34)	F(1)	112.4(4)	S(1)	C(34)	F(2)	111.2(4)
S(1)	C(34)	F(3)	112.2(4)	F(1)	C(34)	F(2)	105.4(5)
F(1)	C(34)	F(3)	106.6(5)	F(2)	C(34)	F(3)	108.7(5)
S(2)	C(35)	F(4)	112.4(4)	S(2)	C(35)	F(5)	111.9(5)
S(2)	C(35)	F(6)	112.5(4)	F(4)	C(35)	F(5)	108.1(6)
F(4)	C(35)	F(6)	106.7(6)	F(5)	C(35)	F(6)	104.8(4)

Table 5. Torsion Angles(°)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
Cu(1)	N(1)	O(1)	C(3)	157.2(3)	Cu(1)	N(1)	C(2)	C(1)	-4.1(7)
Cu(1)	N(1)	C(2)	C(4)	-163.6(3)	Cu(1)	N(2)	O(2)	C(8)	154.5(3)
Cu(1)	N(2)	C(7)	C(1)	-8.2(7)	Cu(1)	N(2)	C(7)	C(9)	-163.4(4)
Cu(1)	N(3)	O(3)	C(14)	143.6(4)	Cu(1)	N(3)	C(13)	C(12)	3.2(7)
Cu(1)	N(3)	C(13)	C(15)	-158.5(3)	Cu(1)	N(4)	O(4)	C(19)	152.4(3)
Cu(1)	N(4)	C(18)	C(12)	-7.6(8)	Cu(1)	N(4)	C(18)	C(20)	-164.9(4)
Cu(1)	N(5)	O(5)	C(25)	150.2(3)	Cu(1)	N(5)	C(24)	C(23)	-0.6(8)
Cu(1)	N(5)	C(24)	C(26)	-159.3(3)	F(1)	C(34)	S(1)	O(7)	-63.8(6)
F(1)	C(34)	S(1)	O(8)	57.7(5)	F(1)	C(34)	S(1)	O(9)	175.7(4)
F(2)	C(34)	S(1)	O(7)	54.1(6)	F(2)	C(34)	S(1)	O(8)	175.7(5)
F(2)	C(34)	S(1)	O(9)	-66.3(5)	F(3)	C(34)	S(1)	O(7)	176.0(5)
F(3)	C(34)	S(1)	O(8)	-62.4(5)	F(3)	C(34)	S(1)	O(9)	55.5(5)
F(4)	C(35)	S(2)	O(10)	49.7(6)	F(4)	C(35)	S(2)	O(11)	170.1(5)
F(4)	C(35)	S(2)	O(12)	-71.4(6)	F(5)	C(35)	S(2)	O(10)	-72.2(5)
F(5)	C(35)	S(2)	O(11)	48.2(5)	F(5)	C(35)	S(2)	O(12)	166.7(4)
F(6)	C(35)	S(2)	O(10)	170.2(5)	F(6)	C(35)	S(2)	O(11)	-69.4(5)
F(6)	C(35)	S(2)	O(12)	49.1(5)	O(1)	N(1)	Cu(1)	N(2)	-167.9(3)
O(1)	N(1)	Cu(1)	N(3)	109.0(3)	O(1)	N(1)	Cu(1)	N(4)	-166(11)
O(1)	N(1)	Cu(1)	N(5)	11.7(3)	O(1)	N(1)	C(2)	C(1)	164.9(4)
O(1)	N(1)	C(2)	C(4)	5.5(6)	O(1)	C(3)	C(4)	C(2)	-11.4(5)
O(1)	C(3)	C(4)	C(5)	-120.6(5)	O(2)	N(2)	Cu(1)	N(1)	-160.2(3)
O(2)	N(2)	Cu(1)	N(3)	-65.2(3)	O(2)	N(2)	Cu(1)	N(4)	19.8(3)
O(2)	N(2)	Cu(1)	N(5)	28(3)	O(2)	N(2)	C(7)	C(1)	158.8(5)
O(2)	N(2)	C(7)	C(9)	3.6(5)	O(2)	C(8)	C(9)	C(7)	-16.3(6)

Table 5. Torsion Angles(°) (continued)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
O(2)	C(8)	C(9)	C(10)	-127.1(5)	O(3)	N(3)	Cu(1)	N(1)	16.8(3)
O(3)	N(3)	Cu(1)	N(2)	-69.6(3)	O(3)	N(3)	Cu(1)	N(4)	-162.4(3)
O(3)	N(3)	Cu(1)	N(5)	112.8(3)	O(3)	N(3)	C(13)	C(12)	164.2(4)
O(3)	N(3)	C(13)	C(15)	2.5(5)	O(3)	C(14)	C(15)	C(13)	-22.4(6)
O(3)	C(14)	C(15)	C(16)	-132.2(6)	O(4)	N(4)	Cu(1)	N(1)	113(11)
O(4)	N(4)	Cu(1)	N(2)	114.8(3)	O(4)	N(4)	Cu(1)	N(3)	-162.0(3)
O(4)	N(4)	Cu(1)	N(5)	-64.8(3)	O(4)	N(4)	C(18)	C(12)	161.5(4)
O(4)	N(4)	C(18)	C(20)	4.1(6)	O(4)	C(19)	C(20)	C(18)	-21.0(6)
O(4)	C(19)	C(20)	C(21)	-131.1(5)	O(5)	N(5)	Cu(1)	N(1)	117.0(3)
O(5)	N(5)	Cu(1)	N(2)	-71(3)	O(5)	N(5)	Cu(1)	N(3)	21.7(3)
O(5)	N(5)	Cu(1)	N(4)	-63.0(3)	O(5)	N(5)	C(24)	C(23)	162.5(5)
O(5)	N(5)	C(24)	C(26)	3.8(5)	O(5)	C(25)	C(26)	C(24)	-18.5(5)
O(5)	C(25)	C(26)	C(27)	-128.7(5)	O(6)	N(6)	C(29)	C(23)	165.0(4)
O(6)	N(6)	C(29)	C(31)	5.0(6)	O(6)	C(30)	C(31)	C(29)	-12.3(5)
O(6)	C(30)	C(31)	C(32)	-122.2(5)	N(1)	Cu(1)	N(2)	C(7)	6.0(4)
N(1)	Cu(1)	N(3)	C(13)	175.1(4)	N(1)	Cu(1)	N(4)	C(18)	-78(11)
N(1)	Cu(1)	N(5)	C(24)	-80.5(5)	N(1)	O(1)	C(3)	C(4)	15.1(5)
N(1)	C(2)	C(1)	C(6)	-122.2(5)	N(1)	C(2)	C(1)	C(7)	3.5(7)
N(1)	C(2)	C(1)	C(11)	116.5(6)	N(1)	C(2)	C(4)	C(3)	4.1(6)
N(1)	C(2)	C(4)	C(5)	128.6(5)	N(2)	Cu(1)	N(1)	C(2)	0.1(4)
N(2)	Cu(1)	N(3)	C(13)	88.7(4)	N(2)	Cu(1)	N(4)	C(18)	-77.0(4)
N(2)	Cu(1)	N(5)	C(24)	90(3)	N(2)	O(2)	C(8)	C(9)	19.4(5)
N(2)	C(7)	C(1)	C(2)	2.9(7)	N(2)	C(7)	C(1)	C(6)	118.5(5)
N(2)	C(7)	C(1)	C(11)	-119.2(5)	N(2)	C(7)	C(9)	C(8)	8.5(6)

Table 5. Torsion Angles(°) (continued)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
N(2)	C(7)	C(9)	C(10)	134.0(5)	N(3)	Cu(1)	N(1)	C(2)	-83.0(4)
N(3)	Cu(1)	N(2)	C(7)	101.1(4)	N(3)	Cu(1)	N(4)	C(18)	6.2(4)
N(3)	Cu(1)	N(5)	C(24)	-175.9(4)	N(3)	O(3)	C(14)	C(15)	25.5(6)
N(3)	C(13)	C(12)	C(17)	-127.7(5)	N(3)	C(13)	C(12)	C(18)	-2.0(7)
N(3)	C(13)	C(12)	C(22)	112.1(6)	N(3)	C(13)	C(15)	C(14)	13.1(6)
N(3)	C(13)	C(15)	C(16)	139.6(5)	N(4)	Cu(1)	N(1)	C(2)	1(11)
N(4)	Cu(1)	N(2)	C(7)	-173.9(4)	N(4)	Cu(1)	N(3)	C(13)	-4.0(4)
N(4)	Cu(1)	N(5)	C(24)	99.4(5)	N(4)	O(4)	C(19)	C(20)	24.8(6)
N(4)	C(18)	C(12)	C(13)	3.9(7)	N(4)	C(18)	C(12)	C(17)	121.2(6)
N(4)	C(18)	C(12)	C(22)	-119.1(6)	N(4)	C(18)	C(20)	C(19)	11.2(6)
N(4)	C(18)	C(20)	C(21)	136.1(5)	N(5)	Cu(1)	N(1)	C(2)	179.7(4)
N(5)	Cu(1)	N(2)	C(7)	-165(3)	N(5)	Cu(1)	N(3)	C(13)	-88.9(4)
N(5)	Cu(1)	N(4)	C(18)	103.4(4)	N(5)	O(5)	C(25)	C(26)	22.1(5)
N(5)	C(24)	C(23)	C(28)	-120.1(6)	N(5)	C(24)	C(23)	C(29)	2.6(8)
N(5)	C(24)	C(23)	C(33)	120.2(6)	N(5)	C(24)	C(26)	C(25)	9.8(6)
N(5)	C(24)	C(26)	C(27)	134.6(5)	N(6)	O(6)	C(30)	C(31)	16.0(5)
N(6)	C(29)	C(23)	C(24)	-6.8(8)	N(6)	C(29)	C(23)	C(28)	107.2(6)
N(6)	C(29)	C(23)	C(33)	-130.6(6)	N(6)	C(29)	C(31)	C(30)	5.0(6)
N(6)	C(29)	C(31)	C(32)	130.3(5)	C(1)	C(2)	C(4)	C(3)	-158.5(4)
C(1)	C(2)	C(4)	C(5)	-33.9(5)	C(1)	C(6)	C(5)	C(4)	7.2(6)
C(1)	C(7)	C(9)	C(8)	-149.9(5)	C(1)	C(7)	C(9)	C(10)	-24.4(6)
C(1)	C(11)	C(10)	C(9)	20.6(7)	C(2)	N(1)	O(1)	C(3)	-13.0(5)
C(2)	C(1)	C(6)	C(5)	-25.1(5)	C(2)	C(1)	C(7)	C(9)	158.1(4)
C(2)	C(1)	C(11)	C(10)	-156.4(5)	C(2)	C(4)	C(5)	C(6)	14.3(6)

Table 5. Torsion Angles(°) (continued)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
C(3)	C(4)	C(5)	C(6)	123.1(5)	C(4)	C(2)	C(1)	C(6)	37.6(5)
C(4)	C(2)	C(1)	C(7)	163.3(4)	C(4)	C(2)	C(1)	C(11)	-83.6(5)
C(5)	C(6)	C(1)	C(7)	-150.5(4)	C(5)	C(6)	C(1)	C(11)	96.1(6)
C(6)	C(1)	C(7)	C(9)	-86.2(5)	C(6)	C(1)	C(11)	C(10)	91.7(6)
C(7)	N(2)	O(2)	C(8)	-14.7(5)	C(7)	C(1)	C(11)	C(10)	-32.6(6)
C(7)	C(9)	C(10)	C(11)	0.7(7)	C(8)	C(9)	C(10)	C(11)	110.8(6)
C(9)	C(7)	C(1)	C(11)	36.1(5)	C(12)	C(13)	C(15)	C(14)	-151.8(5)
C(12)	C(13)	C(15)	C(16)	-25.2(6)	C(12)	C(17)	C(16)	C(15)	16.1(8)
C(12)	C(18)	C(20)	C(19)	-150.2(5)	C(12)	C(18)	C(20)	C(21)	-25.4(6)
C(12)	C(22)	C(21)	C(20)	23.9(7)	C(13)	N(3)	O(3)	C(14)	-17.8(5)
C(13)	C(12)	C(17)	C(16)	-29.4(6)	C(13)	C(12)	C(18)	C(20)	161.9(4)
C(13)	C(12)	C(22)	C(21)	-162.4(5)	C(13)	C(15)	C(16)	C(17)	4.4(7)
C(14)	C(15)	C(16)	C(17)	112.7(7)	C(15)	C(13)	C(12)	C(17)	34.5(5)
C(15)	C(13)	C(12)	C(18)	160.2(4)	C(15)	C(13)	C(12)	C(22)	-85.8(5)
C(16)	C(17)	C(12)	C(18)	-156.6(5)	C(16)	C(17)	C(12)	C(22)	92.2(7)
C(17)	C(12)	C(18)	C(20)	-80.8(6)	C(17)	C(12)	C(22)	C(21)	84.9(6)
C(18)	N(4)	O(4)	C(19)	-18.4(5)	C(18)	C(12)	C(22)	C(21)	-37.0(6)
C(18)	C(20)	C(21)	C(22)	-0.3(6)	C(19)	C(20)	C(21)	C(22)	108.3(6)
C(20)	C(18)	C(12)	C(22)	38.9(5)	C(23)	C(24)	C(26)	C(25)	-152.9(4)
C(23)	C(24)	C(26)	C(27)	-28.2(6)	C(23)	C(28)	C(27)	C(26)	19.7(7)
C(23)	C(29)	C(31)	C(30)	-158.6(4)	C(23)	C(29)	C(31)	C(32)	-33.2(6)
C(23)	C(33)	C(32)	C(31)	-5.1(7)	C(24)	N(5)	O(5)	C(25)	-16.5(5)
C(24)	C(23)	C(28)	C(27)	-34.4(6)	C(24)	C(23)	C(29)	C(31)	153.8(4)
C(24)	C(23)	C(33)	C(32)	-141.1(5)	C(24)	C(26)	C(27)	C(28)	3.5(7)

Table 5. Torsion Angles(°) (continued)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
C(25)	C(26)	C(27)	C(28)	112.1(6)	C(26)	C(24)	C(23)	C(28)	39.1(5)
C(26)	C(24)	C(23)	C(29)	161.8(4)	C(26)	C(24)	C(23)	C(33)	-80.6(5)
C(27)	C(28)	C(23)	C(29)	-159.8(5)	C(27)	C(28)	C(23)	C(33)	85.0(6)
C(28)	C(23)	C(29)	C(31)	-92.2(5)	C(28)	C(23)	C(33)	C(32)	108.6(6)
C(29)	N(6)	O(6)	C(30)	-13.3(5)	C(29)	C(23)	C(33)	C(32)	-14.0(6)
C(29)	C(31)	C(32)	C(33)	22.0(7)	C(30)	C(31)	C(32)	C(33)	131.5(6)
C(31)	C(29)	C(23)	C(33)	30.0(5)					

Table 6. Non-bonded Contacts out to 3.60 Å

atom	atom	distance	ADC	atom	atom	distance	ADC
S(1)	H(27)	3.11(5)	65602	S(1)	H(26)	3.18(7)	65602
S(1)	H(29)	3.43(6)	55602	S(2)	H(11)	3.39(8)	64602
S(2)	H(15)	3.41(9)	55601	S(2)	H(3)	3.42(5)	54602
S(2)	H(23)	3.46(9)	55602	S(2)	H(10)	3.50(6)	55601
F(1)	H(24)	2.84(6)	55602	F(1)	H(1)	2.85(6)	54602
F(1)	H(35)	2.9(1)	1	F(1)	H(39)	3.0(1)	54602
F(1)	H(40)	3.04(6)	1	F(1)	H(28)	3.10(6)	55602
F(1)	H(27)	3.43(5)	55602	F(1)	H(2)	3.49(6)	54602
F(1)	C(19)	3.551(7)	55602	F(1)	C(3)	3.568(7)	54602
F(2)	H(33)	2.5(2)	65501	F(2)	H(39)	2.8(1)	54602
F(2)	H(40)	3.12(6)	1	F(2)	H(34)	3.27(6)	1
F(2)	H(38)	3.3(2)	54602	F(2)	H(41)	3.31(7)	64602
F(2)	C(32)	3.373(8)	54602	F(2)	C(27)	3.388(9)	65501
F(2)	H(32)	3.41(7)	65501	F(2)	H(35)	3.5(1)	1
F(2)	H(36)	3.58(7)	54602	F(3)	H(6)	2.84(7)	64602
F(3)	H(36)	2.88(7)	54602	F(3)	H(2)	2.92(6)	54602
F(3)	H(1)	2.94(5)	54602	F(3)	H(41)	3.10(7)	64602
F(3)	H(39)	3.1(1)	54602	F(3)	H(4)	3.20(6)	64602
F(3)	C(3)	3.257(7)	54602	F(3)	H(42)	3.34(6)	64602
F(3)	H(7)	3.52(7)	64602	F(3)	C(6)	3.531(7)	64602
F(3)	C(33)	3.567(9)	54602	F(3)	C(32)	3.598(9)	54602
F(4)	H(10)	2.82(6)	55601	F(4)	H(23)	2.84(9)	55602
F(4)	H(16)	3.07(8)	65601	F(4)	H(21)	3.07(6)	65602
F(4)	H(20)	3.16(6)	65602	F(4)	C(17)	3.375(8)	65602

Table 6. Non-bonded Contacts out to 3.60 Å (continued)

atom	atom	distance	ADC	atom	atom	distance	ADC
F(4)	H(11)	3.44(7)	55601	F(4)	H(18)	3.51(8)	65602
F(4)	C(10)	3.531(8)	55601	F(5)	H(23)	2.47(9)	55602
F(5)	H(5)	2.81(7)	64602	F(5)	H(22)	2.91(6)	55602
F(5)	C(22)	2.995(6)	55602	F(5)	H(24)	3.15(6)	55602
F(5)	H(21)	3.21(6)	65602	F(5)	C(21)	3.352(9)	55602
F(5)	H(7)	3.41(7)	64602	F(5)	H(25)	3.43(7)	55602
F(5)	O(8)	3.447(6)	1	F(5)	H(20)	3.49(6)	65602
F(5)	C(5)	3.588(7)	64602	F(6)	H(16)	2.46(8)	65601
F(6)	H(9)	2.57(6)	64602	F(6)	H(5)	2.73(7)	64602
F(6)	H(21)	2.83(7)	65602	F(6)	C(14)	3.334(8)	65601
F(6)	H(7)	3.35(8)	64602	F(6)	C(5)	3.392(7)	64602
F(6)	C(11)	3.462(8)	64602	F(6)	H(3)	3.48(4)	64602
F(6)	C(6)	3.594(7)	64602	O(1)	H(12)	3.16(7)	45501
O(1)	H(6)	3.22(7)	45501	O(1)	H(7)	3.39(7)	45501
O(2)	H(30)	2.64(6)	65501	O(2)	O(5)	2.924(5)	65501
O(2)	C(25)	3.217(6)	65501	O(3)	H(12)	2.85(6)	45501
O(3)	H(14)	3.05(7)	45501	O(3)	C(9)	3.421(6)	45501
O(3)	H(11)	3.55(7)	45501	O(3)	C(8)	3.579(7)	45501
O(4)	H(30)	2.92(6)	65501	O(5)	H(14)	2.69(7)	45501
O(5)	H(12)	3.03(6)	45501	O(5)	C(8)	3.174(7)	45501
O(5)	C(9)	3.528(8)	45501	O(5)	N(2)	3.552(5)	45501
O(6)	H(31)	2.53(8)	65501	O(6)	H(36)	3.16(8)	65501
O(6)	C(26)	3.466(7)	65501	O(7)	H(40)	2.68(5)	1
O(7)	H(32)	2.76(8)	55602	O(7)	H(41)	2.84(7)	1

Table 6. Non-bonded Contacts out to 3.60 Å (continued)

atom	atom	distance	ADC	atom	atom	distance	ADC
O(7)	H(29)	3.10(6)	55602	O(7)	H(27)	3.30(6)	65602
O(7)	C(31)	3.322(8)	1	O(7)	C(30)	3.417(8)	1
O(7)	H(28)	3.51(6)	55602	O(8)	H(26)	2.53(7)	65602
O(8)	H(24)	2.67(6)	55602	O(8)	H(29)	2.77(6)	55602
O(8)	H(30)	3.33(6)	55602	O(8)	H(27)	3.35(5)	65602
O(8)	H(4)	3.40(6)	64602	O(8)	C(20)	3.458(8)	65602
O(8)	H(5)	3.46(7)	64602	O(8)	H(22)	3.49(6)	55602
O(8)	H(28)	3.54(6)	55602	O(8)	C(25)	3.585(8)	55602
O(9)	H(35)	2.5(1)	65501	O(9)	H(27)	2.63(5)	65602
O(9)	H(4)	2.96(6)	64602	O(9)	H(26)	3.02(6)	65602
O(9)	H(42)	3.14(6)	64602	O(9)	H(33)	3.3(2)	65501
O(9)	C(19)	3.376(8)	65602	O(9)	C(28)	3.459(8)	65501
O(9)	C(27)	3.587(8)	65501	O(10)	H(15)	2.72(9)	55601
O(10)	H(23)	2.74(9)	55602	O(10)	H(19)	3.0(1)	55602
O(10)	H(21)	3.22(7)	55602	O(10)	H(10)	3.24(6)	55601
O(10)	H(3)	3.24(5)	54602	O(10)	H(16)	3.35(7)	55601
O(10)	H(25)	3.37(7)	55602	O(10)	C(14)	3.374(8)	55601
O(10)	C(22)	3.407(8)	55602	O(11)	H(11)	2.54(8)	64602
O(11)	H(3)	2.60(4)	54602	O(11)	H(2)	2.76(6)	54602
O(11)	H(7)	2.79(7)	64602	O(11)	C(4)	3.274(7)	54602
O(11)	H(9)	3.30(6)	64602	O(11)	C(3)	3.323(7)	54602
O(11)	C(10)	3.36(1)	64602	O(11)	C(6)	3.411(7)	64602
O(12)	H(13)	2.56(6)	55601	O(12)	H(17)	3.04(6)	65601
O(12)	H(10)	3.09(6)	55601	O(12)	H(15)	3.22(10)	55601

Table 6. Non-bonded Contacts out to 3.60 Å (continued)

atom	atom	distance	ADC	atom	atom	distance	ADC
O(12)	H(11)	3.22(8)	64602	O(12)	C(8)	3.228(7)	55601
O(12)	H(16)	3.26(8)	65601	O(12)	H(14)	3.32(7)	55601
O(12)	H(18)	3.33(8)	55601	O(12)	H(9)	3.47(6)	64602
N(1)	H(12)	3.29(7)	45501	N(2)	H(30)	3.21(6)	65501
N(3)	H(14)	2.74(7)	45501	N(3)	H(12)	2.97(6)	45501
N(3)	C(8)	3.524(7)	45501	N(4)	H(30)	2.94(6)	65501
N(5)	H(12)	3.28(6)	45501	N(6)	H(31)	2.86(8)	65501
C(3)	H(25)	3.06(8)	56501	C(3)	H(7)	3.54(7)	45501
C(4)	H(25)	2.87(8)	56501	C(5)	H(25)	3.04(8)	56501
C(6)	H(2)	3.31(6)	65501	C(11)	H(19)	3.2(1)	2
C(13)	H(14)	2.87(7)	45501	C(15)	H(14)	3.36(7)	45501
C(15)	H(9)	3.57(6)	54502	C(16)	H(8)	3.40(8)	54502
C(18)	H(30)	3.36(6)	65501	C(19)	H(38)	3.4(2)	54602
C(21)	H(2)	3.58(6)	54501	C(27)	H(41)	3.44(7)	54602
C(28)	H(39)	3.1(1)	54602	C(28)	H(38)	3.3(2)	54602
C(30)	H(32)	3.30(7)	55602	C(30)	H(36)	3.45(8)	65501
C(31)	H(32)	3.48(7)	55602	C(32)	H(34)	3.12(7)	55602
C(32)	H(27)	3.58(5)	55602	C(33)	H(41)	2.98(7)	45501
C(34)	H(39)	3.2(1)	54602	C(34)	H(40)	3.40(6)	1
C(34)	H(1)	3.47(5)	54602	C(34)	H(33)	3.5(2)	65501
C(34)	H(24)	3.55(6)	55602	C(35)	H(23)	2.97(9)	55602
C(35)	H(16)	3.21(8)	65601	C(35)	H(21)	3.28(6)	65602
C(35)	H(5)	3.35(7)	64602	C(35)	H(9)	3.55(6)	64602
H(1)	H(25)	3.22(9)	56501	H(2)	H(7)	2.81(9)	45501

Table 6. Non-bonded Contacts out to 3.60 Å (continued)

atom	atom	distance	ADC
H(2)	H(25)	2.89(9)	56501
H(2)	H(24)	3.32(8)	56501
H(4)	H(25)	3.02(10)	56501
H(5)	H(25)	2.77(10)	56501
H(5)	H(21)	3.46(10)	56501
H(8)	H(19)	2.6(1)	2
H(8)	H(17)	3.6(1)	2
H(9)	H(17)	3.22(9)	2
H(10)	H(19)	3.4(1)	2
H(14)	H(22)	2.99(9)	65501
H(15)	H(19)	3.4(1)	2
H(26)	H(30)	3.41(9)	65501
H(27)	H(35)	3.4(1)	54602
H(28)	H(38)	3.2(2)	54602
H(31)	H(41)	3.6(1)	45501
H(32)	H(40)	3.32(9)	54602
H(32)	H(38)	3.5(2)	54602
H(34)	H(38)	2.6(2)	54602
H(35)	H(39)	3.1(2)	54602
H(36)	H(41)	2.6(1)	45501
H(2)	H(6)	3.06(9)	45501
H(3)	H(25)	2.63(9)	56501
H(4)	H(26)	3.35(9)	56501
H(5)	H(26)	3.24(10)	56501
H(6)	H(36)	3.5(1)	65501
H(8)	H(18)	3.3(1)	2
H(9)	H(19)	3.1(1)	2
H(9)	H(16)	3.5(1)	2
H(14)	H(17)	2.96(9)	65501
H(14)	H(30)	3.52(9)	65501
H(16)	H(19)	3.3(1)	2
H(27)	H(38)	2.9(2)	54602
H(27)	H(40)	3.53(8)	54602
H(28)	H(40)	3.33(8)	54602
H(32)	H(41)	2.9(1)	54602
H(32)	H(42)	3.41(9)	54602
H(33)	H(41)	3.3(2)	54602
H(34)	H(39)	2.6(1)	54602
H(35)	H(42)	3.5(1)	54602

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,	1/2+Y,	-Z