X-ray Structure Report

February 26, 2003

Experimental

Data Collection

A red prism crystal of $S_40_2NC_20H_{19}$ having approximate dimensions of 0.30 x 0.25 x 0.25 mm was mounted on a glass fiber. All measurements were made on a Rigaku RAXIS imaging plate area detector with graphite monochromated Mo-Kα radiation.

lndexing was performed from 2 stills which were exposed for 5 seconds. The crystal-to-detector distance was 127.40 mm.

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

a = 17.783(1) Å
b = 23.259(2) Å
c = 10.0808(8) Å
V = 4169.5(5) Å^3

For Z = 8 and F.W. = 433.62, the calculated density is 1.38 g/cm^3. The systematic absences of:

Okl: k±2n
hOl: l±2n
hkO: h±2n

uniquely determine the space group to be:

Pbca (#61)

The data were collected at a temperature of 23±1^{O}C to a maximum 20 value of 55.0°. A total of 44 oscillation images were collected. A sweep of data was done using ω scans from 130.0 to 190.0^O in 5.0^O step, at χ=45.0^O and 4, = 0.0^O. The exposure rate was 1.5 [sec./ ^{O}]. The detector at the zero swing position. A second sweep was performed using o scans from 0.0 to 160.0^O in 5.0^O step, at χ =45.0^O and ϕ= 180.0^O. The exposure rate was 1.5 [sec./^{O}]. The detector at the zero swing position. The crystal-to-detector distance was 127.40 mm. Readout was performed in the 0.1 00 mm pixel mode.

Data Reduction

Of the 9479 reflections which were collected, 4748 were unique (R_{int} = 0.053); equivalent reflections were merged.

The linear absorption coefficient, μ, for Mo-Kα radiation is 4.7 cm^{-1}. was applied which resulted in

transmission factors ranging from 0.80 to 1.22. 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 reined anisotropically. Hydrogen atoms were refined isotropically. The final cycle of full-matrix least-squares refinement[3] on F was based on 2723 observed reflections ($I > 0.90\sigma(I)$) and 263 variable parameters and converged (largest parameter shift was 0.03 times its esd) with unweighted and weighted agreement factors of:

$$R = = \Sigma \, ||Fo| - |Fc|| / \Sigma \, |Fo| = 0.036$$

$$R_w = [\Sigma \, w \, (|Fo| - |Fc|)^2 / \Sigma \, w \, Fo^2]^{1/2} = 0.043$$

The standard deviation of an observation of unit weight[4] was 0.86. The weighting scheme was based on computing[5]. 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 0.38 and -0.36 $e^-/Å^3$, respectively.

Neutral atom scattering factors were taken from Cromer and Waber[6]. Anomalous dispersion effects were included in Fcalc[7]; the values for Δf and $\Delta f''$ were those of Creagh and McAuley[8]. The values for the mass attenuation coefficients are those of Creagh and Hubbell[9]. All calculations were performed using the CrystalStructure[10,11] crystallographic software Package.

References

(1) SIR92: Altomare, A., Cascarano, G., Giacovazzo, C., Guagliardi, A., Burla, M., Polidori, G., and Camalli, M. (1994) J. Appl. Cryst., 27, 435.

(2) DIRDIF99: Beurskens, P.T., Admiraal, G., Beurskens, G., Bosman, W.P., de Gelder, R., Israel, R. and Smits, J.M.M. (1999). The DIRDIF-99 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= Least Squares weights.

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

$[\Sigma w(|Fo|-|Fc|)^2/(N_o-N_v)]^{1/2}$

where: N_o = number of observations

N_v = number of variables

(5) Carruthers, J.R. and Watkin, D.J. (1979), Acta Cryst, A35, 698-699

(6) Cromer, D. T. & Waber, J. T.; "International Tables for X-ray Crystallography", Vol. IV, The Kynoch Press, Birmingham, England, Table 2.2 A (1974).

(7) Ibers, J. A. & Hamilton, W. C.; Acta CrystaIIogr., 17, 781 (1964).

(8) Creagh, D. C. & McAuley, W.J.; "International Tables for CrystaIIography", VoI C, (A.J.C. Wilson, ed.) Kluwer Academic Publishers, Boston, Table 4.2.6.8, pages 219-222 (1 992).

(9) Creagh, D. C. & HubbeII, J.H..; "lnternationaI Tables for Crystallography", VoI C, (A.J.C. Wilson, ed.) KIuwer Academic Publishers, Boston, Table 4.2.4.3, pages 200-206 (1 992).

(10) CrystalStructure 2.00: Crystal Structure Analysis Package, Rigaku and MSC (2001).

(11) CRYSTALS Issue 10: Watkin, D.J., Prout, C.K. Carruthers, J.R. & Betteridge, P.W. Chemical Crystallography Laboratory, Oxford, UK.

EXPERIMENTAL DETAILS

A. Crystal Data

Empirical Formula	$S_4O_2NC_{20}H_{19}$
Formula Weight	433.62
Crystal Color, Habit	red, prism
Crystal Dimensions	0.30 X 0.25 X 0.25 mm
Crystal System	orthorhombic
Lattice Type	Primitive
Indexing Images	2 stills @ 5.0 seconds
Detector Position	127.40 mm
Pixel Size	0.100 mm
Lattice Parameters	a= 17.783(1) Å b= 23.259(2) Å c= 10.0808(8) Å V = 4169.5(5) Å^3
Space Group	Pbca (#61)
Z value	8
Dcalc	1.381 g/cm^3
F_{000}	1808.00
μ(Mo Kα)	4.71 cm^{-1}

B. Intensity Measurements

Diffractometer	Rigaku RAXIS-RAPID
Radiation	MoKα (λ = 0.71069 Å) graphite monochromated
Detector Aperture	270 mm x256 mm
Data Images	44 exposures
ω oscillation Range (χ=45.0, ϕ=0.0)	130.0 - 190.0^{O}
Exposure Rate	1.5 sec./^{O}
Detector Swing Angle	0.00^{O}
ω oscillation Range (χ=45.0, ϕ=1 80.0)	0.0- 160.0^{O}
Exposure Rate	1.5 sec. /^{O}
Detector Swing Angle	0.00^{O}
Detector Position	127.40 mm
Pixel Size	0.100 mm
$2\theta_{max}$	55.0^{O}
No. of Reflections Measured	Total: 9479
Corrections	Unique: 4748 (R_{int} = 0.053) Lorentz-polarization Absorption (trans. factors: 0.7975 - 1.2208)

C. Structure Solution and Refinement

Structure Solution	Direct Methods (SIR92)
Refinement	Full-matrix least-squares on F
Function Minimized	$\Sigma w(IFol - IFcl)^2$
Least Squares Weights	Chebychev polynomial with 3 parameters 0.090,0.071,0.038,
Anomalous Dispersion	2723
No. Observations ($I>0.90\sigma(I)$)	263
No. Variables	All non-hydrogen atoms
Reflection/Parameter Ratio	10.35
Residuals: R; R_w	0.036 ; 0.043
Goodness of Fit Indicator	0.86
Max Shift/Error in Final Cycle	0.03
Maximum peak in Final Diff. Map	0.38 $e^-/Å^3$
Minimum peak in Final Diff. Map	-0.36 $e^-/Å^3$

Table 1. Atomic coordinates and Biso/Beq

atom	x	y	Z	Beq
S(1)	0.3781 4(6)	0.06381 (4)	0.5730(1)	3.46(2)
S(2)	0.1 6260m	0.1 5998(6)	0.9440(1)	4.63(3)
S(3)	0.06407(6)	0.1 9379 (5)	0.7158(1)	3.69(2)
S(4)	0.21791 m	-0.01 186 (5)	0.4777(1)	5.11(3)
0(1)	0.3835(2)	0.0651(1)	0.4315(3)	5.46(8)
0(2)	0.4261 (2)	0.1 017(1)	0.6457(4)	6.05(9)
N(1)	0.1831 (1)	0.1293(1)	0.6893(3)	2.51 (6)
C(1)	0.2859(2)	0.2309(2)	0.7087(4)	3.36(9)
C(2)	0.31 92(2)	0.2777(2)	0.7730(5)	4.3(1)
C(3)	0.3665(3)	0.2686(2)	0.8797(5)	4.8(1)
C(4)	0.381 9(2)	0.21 32(2)	0.91 99(4)	4.6(1)
C(5)	0.351 0(2)	0.1 664(2)	0.8564(4)	3.59(9)
C(6)	0.3016(2)	0.1 748(1)	0.7508(3)	2.63(7)
C(7)	0.2599(2)	0.1 268(1)	0.6892(3)	2.52(7)
C(8)	0.2840(2)	0.0789(1)	0.61 78(4)	2.63(7)
C(9)	0.3939(3)	-0.0072(2)	0.6280(5)	5.1(1)
C(10)	0.221 1 (2)	0.0470(1)	0.5689(4)	2.82(7)
C(11)	0.1497(2)	0.0788(1)	0.6145(4)	2.60(7)
C(12)	0.1 049(2)	0.0410(2)	0.7096(4)	4.0(1)
C(13)	0.1402(2)	0.1 598(1)	0.7869(4)	2.75(8)
C(14)	0.0141 (2)	0.2190(2)	0.8596(4)	4.4(1)
C(15)	0.1 068(2)	0.1 005(1)	0.4921 (4)	2.84(8)
C(1 6)	0.0332(2)	0.0850(2)	0.4662(4)	3.9(1)
C(17)	-0.0017(3)	0.1 043(2)	0.3492(5)	5.2(1)
C(1 8)	0.0370(3)	0.1 374(2)	0.2607(5)	5.6(1)
C(19)	0.1 100(3)	0.1533(2)	0.2865 (4)	5.0(1)
C(20)	0.1 442(2)	0.1 354(2)	0.401 8(4)	3.8(1)
H(1)	0.3830(3)	-0.0097(2)	0.7200(5)	6.2(2)
H(2)	0.3621 (3)	-0.0327(2)	0.5803(5)	6.2(2)
H(3)	0.4450(3)	-0.01 73(2)	0.6131 (5)	6.2(2)
H(4)	0.0454(2)	0.2443(2)	0.9086 (4)	5.3(1)
H(5)	-0.0302(2)	0.2387(2)	0.8331 (4)	5.3(1)
H(6)	0.0008(2)	0.1 870(2)	0.91 34(4)	5.3(1)
H(7)	0.0654(2)	0.0628(2)	0.7483(4)	4.8(1)
H(8)	0.0842(2)	0.0095 (2)	0.6621 (4)	4.8(1)
H(9)	0.1 372(2)	0.0271 (2)	0.7773(4)	4.8(1)
H(10)	0.3881(3)	0.3002(2)	0.9258(5)	5.7(1)

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

atom	x	y	z	B_{eq}
H(11)	0.3101 (2)	0.31 59(2)	0.7437(5)	5.1(1)
H(12)	0.2520(2)	0.2370(2)	0.6372(4)	4.0(1)
H(13)	0.4151 (2)	0.2071 (2)	0.9925(4)	5.5(1)
H(14)	0.3625(2)	0.1 284(2)	0.8841 (4)	4.3(1)
H(15)	-0.0525(3)	0.0944(2)	0.3312(5)	6.2(2)
H(16)	0.0065(2)	0.0616(2)	0.5274(4)	4.7(1)
H(17)	0.01 35(3)	0.1491 (2)	0.1 805(5)	6.7(2)
H(18)	0.1 364(3)	0.1 769(2)	0.2255(4)	6.0(1)
H(19)	0.1 942(2)	0.1 472(2)	0.4209(4)	4.5(1)

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

Table 2. Anisotropic Displacement Parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
S(1)	0.0376(5)	0.0406(5)	0.0535(6)	0.0032(5)	0.0078(5)	-0.0097(5)
S(2)	0.0594m	0.0887(9)	0.0280(5)	0.01 43m	0.0034(5)	-0.0034(6)
S(3)	0.0436(6)	0.0574(6)	0.0391 (5)	0.01 58(5)	0.0003(5)	-0.0058(5)
S(4)	0.061 8m	0.0482(6)	0.0843(9)	0.0046(6)	-0.01 42m	-0.0336(6)
0(1)	0.077(2)	0.071 (2)	0.059(2)	0.006(2)	0.024(2)	-0.001 (2)
0(2)	0.038(2)	0.074(2)	0.1 1 8(3)	-0.004(2)	0.005(2)	-0.047(2)
N(1)	0.031 (2)	0.034(2)	0.030(1)	-0.001 (1)	0.000(1)	-0.006(1)
C(1)	0.038(2)	0.043(2)	0.046(2)	0.000(2)	0.004(2)	-0.004(2)
C(2)	0.053(3)	0.036(2)	0.073(3)	-0.007(2)	0.021 (3)	-0.01 1 (2)
C(3)	0.052(3)	0.066(3)	0.062(3)	-0.02 1 (2)	0.009(2)	-0.038(3)
C(4)	0.043(2)	0.082(3)	0.048(3)	-0.01 1 (2)	-0.001 (2)	-0.023(3)
C(5)	0.042(2)	0.056(3)	0.039(2)	-0.003(2)	-0.002(2)	-0.008(2)
C(6)	0.032(2)	0.038(2)	0.030(2)	-0.001 (2)	0.004(2)	-0.01 0(2)
C(7)	0.034(2)	0.036(2)	0.026(2)	-0.001 (2)	-0.000(2)	0.003(2)
C(8)	0.032(2)	0.032(2)	0.036(2)	-0.000(2)	-0.001 (2)	-0.005(2)
C(9)	0.058(3)	0.053(3)	0.084(4)	0.020(2)	-0.004(3)	0.002(3)
C(10)	0.041 (2)	0.030(2)	0.036(2)	0.001 (2)	-0.003(2)	-0.002(2)
C(11)	0.034(2)	0.030(2)	0.035(2)	-0.005(2)	-0.001 (2)	-0.001 (2)
C(12)	0.053(3)	0.048(2)	0.052(3)	-0.01 1 (2)	-0.001 (2)	0.009(2)
C(13)	0.035(2)	0.036(2)	0.034(2)	-0.004(2)	0.004(2)	-0.001 (2)
C(14)	0.047(3)	0.066(3)	0.055(3)	0.01 2(2)	0.01 0(2)	-0.01 1 (2)
C(15)	0.038(2)	0.038(2)	0.032(2)	0.001 (2)	-0.003(2)	-0.008(2)
C(16)	0.044(2)	0.043(2)	0.061 (3)	-0.004(2)	-0.011 (2)	-0.004(2)
C(17)	0.058(3)	0.059(3)	0.080(4)	0.007(3)	-0.039(3)	-0.01 8(3)
C(18)	0.1 01 (4)	0.062(3)	0.050(3)	0.028(3)	-0.029(3)	-0.006(3)
C(19)	0.079(4)	0.070(3)	0.041 (2)	0.01 3(3)	0.004(3)	0.007(2)
C(20)	0.051 (3)	0.058(3)	0.034(2)	0.006(2)	0.000(2)	0.001 (2)

The general temperature factor expression: $\exp(-2\pi^2(a^{*\prime}2U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^{*\prime}U_{23}kl))$

able 3. Bond lengths (Å)

atom	atom	distanee	atom	atom	dista nce
S(1)	O(1)	1.430(3)	S(1)	O(2)	1.428(3)
S(1)	C(8)	1.769(4)	S(1)	C(9)	1.764(4)
S(2)	C(13)	1.634(4)	S(3)	C(13)	1.724(4)
S(3)	C(14)	1.798(4)	S(4)	C(10)	1.650(4)
N(1)	C(7)	1.368(4)	N(1)	C(11)	1.517(4)
N(1)	C(13)	1.432(4)	C(1)	C(2)	1.399(5)
C(1)	C(6)	1.400(5)	C(2)	C(3)	1.382(6)
C(3)	C(4)	1.380(6)	C(4)	C(5)	1.377(5)
C(5)	C(6)	1.393(5)	C(6)	C(7)	1.478(5)
C(7)	C(8)	1.394(5)	C(8)	C(10)	1.429(5)
C(10)	C(11)	1.540(5)	C(11)	C(12)	1.525(5)
C(11)	C(15)	1.535(5)	C(15)	C(16)	1.383(5)
C(15)	C(20)	1.389(5)	C(16)	C(17)	1.407(6)
C(17)	C(18)	1.364(7)	C(18)	C(19)	1.373(7)
C(19)	C(20)	1.377(6)			

able 4. Bond lengths involving hydrogens (Å)

atom	atom	distance	atom	atom	distance
C(1)	H(12)	0.95	C(2)	H(11)	0.95
C(3)	H(10)	0.950(6)	C(4)	H(13)	0.95
C(5)	H(14)	0.95	C(9)	H(1)	0.95
C(9)	H(2)	0.95	C(9)	H(3)	0.95
C(12)	H(7)	0.950(5)	C(12)	H(8)	0.950(5)
C(12)	H(9)	0.950(5)	C(14)	H(4)	0.950(5)
C(14)	H(5)	0.95	C(14)	H(6)	0.95
C(16)	H(16)	0.950(6)	C(17)	H(15)	0.95
C(18)	H(17)	0.95	C(19)	H(18)	0.950(6)
C(20)	H(19)	0.95			

Table 5. Bond angles(°)

atom	atom	atom	angle	atom	atom	atom	angle
O(1)	S(1)	O(2)	117.4(2)	O(1)	S(1)	C(8)	108.3(2)
O(2)	S(1)	C(8)	108.2(2)	O(1)	S(1)	C(9)	108.8(2)
O(2)	S(1)	C(9)	108.7(2)	C(8)	S(1)	C(9)	104.8(2)
C(13)	S(3)	C(14)	101.7(2)	C(7)	N(1)	C(11)	111.0(3)
C(7)	N(1)	C(13)	123.6(3)	C(11)	N(1)	C(13)	121.1(3)
C(2)	C(1)	C(6)	120.0(4)	C(1)	C(2)	C(3)	119.9(4)
C(2)	C(3)	C(4)	119.6(4)	C(3)	C(4)	C(5)	121.5(4)
C(4)	C(5)	C(6)	119.8(4)	C(1)	C(6)	C(5)	119.2(4)
C(1)	C(6)	C(7)	118.5(3)	C(5)	C(6)	C(7)	122.1(3)
N(1)	C(7)	C(6)	117.9(3)	N(1)	C(7)	C(8)	110.0(3)
C(6)	C(7)	C(8)	131.9(3)	S(1)	C(8)	C(7)	125.5(3)
S(1)	C(8)	C(10)	123.4(3)	C(7)	C(8)	C(10)	110.7(3)
S(4)	C(10)	C(8)	130.5(3)	S(4)	C(10)	C(11)	122.4(3)
C(8)	C(10)	C(11)	107.1(3)	N(1)	C(11)	C(10)	101.3(3)
N(1)	C(11)	C(12)	109.8(3)	C(10)	C(11)	C(12)	110.0(3)
N(1)	C(11)	C(15)	109.9(3)	C(10)	C(11)	C(15)	109.1(3)
C(12)	C(11)	C(15)	115.8(3)	S(2)	C(13)	S(3)	126.3(2)
S(2)	C(13)	N(1)	122.6(3)	S(3)	C(13)	N(1)	111.1(2)
C(11)	C(15)	C(16)	122.4(4)	C(11)	C(15)	C(20)	118.8(3)
C(16)	C(15)	C(20)	118.8(4)	C(15)	C(16)	C(17)	119.4(4)
C(16)	C(17)	C(18)	120.4(4)	C(17)	C(18)	C(19)	120.3(5)
C(18)	C(19)	C(20)	119.8(5)	C(15)	C(20)	C(19)	121.2(4)

Table 6. Bond angles involving hydrogens(O)

atom	atom	atom	angle	atom	atom	atom	angle
C(2)	C(1)	H(12)	120.2(3)	C(6)	C(1)	H(12)	119.7(2)
C(1)	C(2)	H(11)	120.8(3)	C(3)	C(2)	H(11)	119.3(3)
C(2)	C(3)	H(10)	120.6(3)	C(4)	C(3)	H(10)	119.9(3)
C(3)	C(4)	H(13)	119.2(3)	C(5)	C(4)	H(13)	119.3(3)
C(4)	C(5)	H(14)	120.8(3)	C(6)	C(5)	H(14)	119.4(2)
S(1)	C(9)	H(1)	109.5(2)	S(1)	C(9)	H(2)	109.3(2)
H(1)	C(9)	H(2)	109.5(2)	S(1)	C(9)	H(3)	109.6(2)
H(1)	C(9)	H(3)	109.5	H(2)	C(9)	H(3)	109.47(1)
C(11)	C(12)	H(7)	109.7(2)	C(11)	C(12)	H(8)	109.3(2)
H(7)	C(12)	H(8)	109.47(1)	C(11)	C(12)	H(9)	109.4(2)
H(7)	C(12)	H(9)	109.5	H(8)	C(12)	H(9)	109.48(1)
S(3)	C(14)	H(4)	109.4(2)	S(3)	C(14)	H(5)	109.9(1)
H(4)	C(14)	H(5)	109.47(1)	S(3)	C(14)	H(6)	109.1(2)
H(4)	C(14)	H(6)	109.47(1)	H(5)	C(14)	H(6)	109.47(1)
C(15)	C(16)	H(16)	120.0(3)	C(17)	C(16)	H(16)	120.5(3)
C(16)	C(17)	H(15)	120.1(3)	C(18)	C(17)	H(15)	119.5(3)
C(17)	C(18)	H(17)	119.7(3)	C(19)	C(18)	H(17)	120.0(3)
C(18)	C(19)	H(18)	120.1(3)	C(20)	C(19)	H(18)	120.1(3)
C(15)	C(20)	H(19)	119.0(2)	C(19)	C(20)	H(19)	119.8(3)

Table 7. Torsion Angles(°)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
O(1)	S(1)	C(8)	C(7)	-115.8(6)	O(1)	S(1)	C(8)	C(10)	55.1m
O(2)	S(1)	C(8)	C(7)	12.4(7)	O(2)	S(1)	C(8)	C(10)	-176.7(5)
C(9)	S(1)	C(8)	C(7)	128.2(6)	C(9)	S(1)	C(8)	C(10)	-60.9(7)
C(14)	S(3)	C(13)	S(2)	-7.1(7)	C(14)	S(3)	C(13)	N(1)	172.1(5)
C(11)	N(1)	C(7)	C(6)	176.2(4)	C(11)	N(1)	C(7)	C(8)	1.1(6)
C(13)	N(1)	C(7)	C(6)	-27.0(7)	C(13)	N(1)	C(7)	C(8)	157.8(4)
C(7)	N(1)	C(11)	C(10)	-0.8(5)	C(7)	N(1)	C(11)	C(12)	115.4(5)
C(7)	N(1)	C(11)	C(15)	-116.2(5)	C(13)	N(1)	C(11)	C(10)	-158.3(5)
C(13)	N(1)	C(11)	C(12)	-42.0(6)	C(13)	N(1)	C(11)	C(15)	86.4(6)
C(7)	N(1)	C(13)	S(2)	-39.7(7)	C(7)	N(1)	C(13)	S(3)	141.1(4)
C(11)	N(1)	C(13)	S(2)	114.8(5)	C(11)	N(1)	C(13)	S(3)	-64.4(5)
C(6)	C(1)	C(2)	C(3)	-1.2(8)	C(2)	C(1)	C(6)	C(5)	-0.4(8)
C(2)	C(1)	C(6)	C(7)	174.3(5)	C(1)	C(2)	C(3)	C(4)	1.6(9)
C(2)	C(3)	C(4)	C(5)	-0.2(9)	C(3)	C(4)	C(5)	C(6)	-1.5(9)
C(4)	C(5)	C(6)	C(1)	1.8(8)	C(4)	C(5)	C(6)	C(7)	-172.7(5)
C(1)	C(6)	C(7)	N(1)	-53.5(7)	C(1)	C(6)	C(7)	C(8)	120.4(6)
C(5)	C(6)	C(7)	N(1)	121.0(6)	C(5)	C(6)	C(7)	C(8)	-65.1(8)
N(1)	C(7)	C(8)	S(1)	171.1(3)	N(1)	C(7)	C(8)	C(10)	-0.8(5)
C(6)	C(7)	C(8)	S(1)	-3.2(8)	C(6)	C(7)	C(8)	C(10)	-175.1(5)
S(1)	C(8)	C(10)	S(4)	6.8(6)	S(1)	C(8)	C(10)	C(11)	-171.8(3)
C(7)	C(8)	C(10)	S(4)	178.9(4)	C(7)	C(8)	C(10)	C(11)	0.3(6)
S(4)	C(10)	C(11)	N(1)	-178.4(2)	S(4)	C(10)	C(11)	C(12)	65.5(5)
S(4)	C(10)	C(11)	C(15)	-62.5(4)	C(8)	C(10)	C(11)	N(1)	0.3(5)
C(8)	C(10)	C(11)	C(12)	-115.8(5)	C(8)	C(10)	C(11)	C(15)	116.2(5)
N(1)	C(11)	C(15)	C(16)	-127.6(5)	N(1)	C(11)	C(15)	C(20)	54.7(6)
C(10)	C(11)	C(15)	C(16)	122.1(5)	C(10)	C(11)	C(15)	C(20)	-55.6(6)
C(12)	C(11)	C(15)	C(16)	-2.6(8)	C(12)	C(11)	C(15)	C(20)	179.7(5)
C(11)	C(15)	C(16)	C(17)	-177.2(5)	C(20)	C(15)	C(16)	C(17)	0.6(8)
C(11)	C(15)	C(20)	C(19)	176.2(5)	C(16)	C(15)	C(20)	C(19)	-1.6(9)
C(15)	C(16)	C(17)	C(18)	0.9(9)	C(16)	C(17)	C(18)	C(19)	-1.4(9)
C(17)	C(18)	C(19)	C(20)	0.3(1)	C(18)	C(19)	C(20)	C(15)	1.2(9)

Table 8. Distances beyond the asymmetric unit out to 3.60 Å

atom	atom	distance	ADC	atom	atom	distance	ADC
S(1)	S(4)	3.484(2)	(1)	S(1)	O(1)	1.430(3)	(1)
S(1)	O(2)	1.428(3)	(1)	S(1)	C(6)	3.425(3)	(1)
S(1)	C(7)	2.817(4)	(1)	S(1)	C(8)	1.769(4)	(1)
S(1)	C(9)	1.764(4)	(1)	S(1)	C(10)	2.820(4)	(1)
S(2)	S(3)	2.997(2)	(1)	S(2)	N(1)	2.690(3)	(1)
S(2)	C(5)	3.468(4)	(1)	S(2)	C(6)	3.166(4)	(1)
S(2)	C(7)	3.192(4)	(1)	S(2)	C(13)	1.634(4)	(1)
S(2)	C(14)	3.096(4)	(1)	S(2)	C(19)	3.580(4)	(1,1,0,0,1)
S(3)	0(2)	3.544(3)	(J4,1,-1,0,1)	S(3)	N(1)	2.608(3)	(1)
S(3)	C(4)	3.545(4)	(4,1,-1,0,1)	S(3)	C(11)	3.242(4)	(1)
S(3)	C(13)	1.724(4)	(1)	S(3)	C(14)	1.798(4)	(1)
S(3)	C(15)	3.221(4)	(1)	S(4)	0(1)	3.477(3)	(1)
S(4)	C(8)	2.797(4)	(1)	S(4)	C(9)	3.479(5)	(1)
S(4)	C(10)	1.650(4)	(1)	S(4)	C(11)	2.797(4)	(1)
S(4)	C(12)	3.319(4)	(1)	S(4)	C(15)	3.279(4)	(1)
0(1)	0(2)	2.442(5)	(1)	O(1)	C(8)	2.600(5)	(1)
0(1)	C(9)	2.604(6)	(1)	O(1)	C(10)	3.230(5)	(1)
0(1)	C(12)	3.337(5)	(4,1,0,0,-1)	O(2)	C(5)	2.926(5)	(1)
0(2)	C(6)	2.986(4)	(1)	O(2)	C(7)	3.044(4)	(1)
0(2)	C(8)	2.597(5)	(1)	O(2)	C(9)	2.601(5)	(1)
0(2)	C(14)	3.146(5)	(-4,1,0,0,1)	N(1)	C(1)	2.994(5)	(1)
N(1)	C(5)	3.535(5)	(1)	N(1)	C(6)	2.439(4)	(1)
N(1)	C(7)	1.368(4)	(1)	N(1)	C(8)	2.262(4)	(1)
N(1)	C(10)	2.365(4)	(1)	N(1)	C(11)	1.517(4)	(1)
N(1)	C(12)	2.488(5)	(1)	N(1)	C(13)	1.432(4)	(1)
N(1)	C(15)	2.498(4)	(1)	N(1)	C(20)	2.984(5)	(1)
C(1)	C(2)	1.399(5)	(1)	C(1)	C(3)	2.407(6)	(1)
C(1)	C(4)	2.760(6)	(1)	C(1)	C(5)	2.409(6)	(1)
C(2)	C(6)	2.425(5)	(1)	C(3)	C(4)	1.380(6)	(1)
C(3)	C(5)	2.405(6)	(1)	C(3)	C(6)	2.789(5)	(1)
C(4)	C(5)	1.377(5)	(1)	C(4)	C(6)	2.396(5)	(1)
C(4)	C(14)	3.599(6)	(-2,1,0,0,2)	C(5)	C(6)	1.393(5)	(1)
C(5)	C(7)	2.512(5)	(1)	C(5)	C(8)	3.369(5)	(1)
C(6)	C(7)	1.478(5)	(1)	C(6)	C(8)	2.623(5)	(1)

Table 8. Distances beyond the asymmetric unit out to 3.60 Å (continued)

atom	atom	distance	ADC	atom	atom	distance	ADC
C(6)	C(13)	2.914(5)	(1)	C(7)	C(8)	1.394(5)	(1)
C(7)	C(10)	2.321(5)	(1)	C(7)	C(11)	2.378(5)	(1)
C(7)	C(12)	3.410(5)	(1)	C(7)	C(13)	2.468(5)	(1)
C(7)	C(15)	3.425(5)	(1)	C(7)	C(20)	3.559(5)	(1)
C(8)	C(9)	2.799(5)	(1)	C(8)	C(10)	1.429(5)	(1)
C(8)	C(11)	2.389(5)	(1)	C(8)	C(12)	3.432(5)	(1)
C(8)	C(15)	3.433(5)	(1)	C(8)	C(20)	3.556(5)	(1)
C(9)	C(10)	3.374(5)	(1)	C(9)	C(18)	3.532(6)	(4)
C(10)	C(11)	1.540(5)	(1)	C(10)	C(12)	2.511(5)	(1)
C(10)	C(15)	2.506(5)	(1)	C(10)	C(20)	2.988(5)	(1)
C(11)	C(12)	1.525(5)	(1)	C(11)	C(13)	2.568(5)	(1)
C(11)	C(15)	1.535(5)	(1)	C(11)	C(16)	2.558(5)	(1)
C(11)	C(20)	2.517(5)	(1)	C(12)	C(13)	2.938(5)	(1)
C(12)	C(15)	2.593(5)	(1)	C(12)	C(16)	2.947(6)	(1)
C(13)	C(14)	2.732(5)	(1)	C(13)	C(15)	3.329(5)	(1)
C(14)	C(18)	3.509(6)	(3)	C(14)	C(19)	3.504(6)	(3)
C(15)	C(16)	1.383(5)	(1)	C(15)	C(17)	2.410(5)	(1)
C(15)	C(18)	2.778(6)	(1)	C(15)	C(19)	2.409(6)	(1)
C(15)	C(20)	1.389(5)	(1)	C(16)	C(17)	1.407(6)	(1)
C(16)	C(18)	2.405(7)	(1)	C(16)	C(19)	2.770(7)	(1)
C(16)	C(20)	2.387(6)	(1)	C(17)	C(18)	1.364(7)	(1)
C(17)	C(19)	2.374(7)	(1)	C(17)	C(20)	2.745(6)	(1)
C(18)	C(19)	1.373(7)	(1)	C(18)	C(20)	2.379(6)	(1)
C(19)	C(20)	1.377(6)	(1)				

Table 9. Distances beyond the asymmetric unn out to 3.60 Å

atom	atom	distance	ADC	atom	atom	distance	ADC
S(1)	H(1)	2.265(5)	(1)	S(1)	H(2)	2.263(4)	(1)
S(1)	H(3)	2.267(4)	(1)	S(1)	H(10)	3.499(5)	(3,1,0,0,-1)
S(1)	H(14)	3.489(4)	(1)	S(2)	H(2)	3.294(5)	(4)
S(2)	H(4)	2.884(4)	(1)	S(2)	H(6)	2.960(4)	(1)
S(2)	H(7)	3.463(4)	(1)	S(2)	H(9)	3.546(4)	(1)
S(2)	H(12)	3.473(4)	(3)	S(2)	H(17)	3.575(6)	(1,1,0,0,1)
S(2)	H(18)	2.902(4)	(1,1,0,0,1)	S(3)	H(4)	2.295(4)	(1)
S(3)	H(4)	3.431(4)	(3,1,0,0,-1)	S(3)	H(5)	2.302(4)	(1)
S(3)	H(6)	2.292(4)	(1)	S(3)	H(7)	3.064(4)	(1)
S(3)	H(12)	3.579(4)	(1)	S(3)	H(13)	3.395(4)	(-4,1,-1,0,1)
S(3)	H(18)	3.273(5)	(3)	S(4)	H(1)	3.197(5)	(4,1,0,0,-1)
S(4)	H(2)	2.807(5)	(1)	S(4)	H(8)	3.059(4)	(1)
S(4)	H(9)	3.465(4)	(1)	S(4)	H(9)	3.293(4)	(4,1,0,0,-1)
S(4)	H(14)	3.206(4)	(4,1,0,0,-1)	O(1)	H(1)	3.389(6)	(1)
O(1)	H(2)	2.750(5)	(1)	O(1)	H(3)	2.867(5)	(1)
O(1)	H(3)	3.278(5)	(-1,1,1,0,1)	O(1)	H(8)	3.273(5)	(4,1,0,0,-1)
O(1)	H(9)	2.674(5)	(4,1,0,0,-1)	O(1)	H(10)	3.135(6)	(3,1,0,0,-1)
O(1)	H(11)	3.598(5)	(3,1,0,0,-1)	O(1)	H(15)	2.962(5)	(-4)
O(1)	H(17)	3.231(6)	(-4)	O(2)	H(1)	2.804(6)	(1)
O(2)	H(2)	3.389(5)	(1)	O(2)	H(3)	2.807(5)	(1)
O(2)	H(5)	3.288(5)	(-4,1,0,0,1)	O(2)	H(6)	2.463(6)	(-4,1,0,0,1)
O(2)	H(7)	2.845(5)	(-4,1,0,0,1)	O(2)	H(10)	3.253(6)	(3,1,0,0,-1)
O(2)	H(14)	2.728(5)	(1)	N(1)	H(7)	2.670(5)	(1)
N(1)	H(8)	3.307(5)	(1)	N(1)	H(9)	2.664(5)	(1)
N(1)	H(12)	2.838(5)	(1)	N(1)	H(19)	2.746(5)	(1)
C(1)	H(5)	3.303(6)	(-4,1,0,0,1)	C(1)	H(10)	3.269(6)	(1)
C(1)	H(10)	3.459(6)	(3,1,0,0,-1)	C(1)	H(11)	2.054(5)	(1)
C(1)	H(12)	0.95	(1)	C(1)	H(13)	3.480(6)	(3,1,0,0,-1)
C(1)	H(14)	3.266(6)	(1)	C(1)	H(18)	3.419(7)	(3)
C(2)	H(5)	3.023(6)	(-4,1,0,0,1)	C(2)	H(10)	2.036(6)	(1)
C(2)	H(11)	0.95	(1)	C(2)	H(12)	2.049(6)	(1)
C(2)	H(13)	3.240(7)	(1)	C(2)	H(13)	3.320(6)	(3,1,0,0,-1)
C(2)	H(18)	3.451(7)	(3)	C(2)	H(19)	3.195(6)	(3)
C(3)	H(5)	3.434(6)	(-2,1,0,0,2)	C(3)	H(5)	2.908(6)	(-4,1,0,0,1)
C(3)	H(6)	3.335(6)	(-2,1,0,0,2)	C(3)	H(10)	0.950(6)	(1)
C(3)	H(11)	2.024(7)	(1)	C(3)	H(12)	3.265(6)	(1)
C(3)	H(12)	3.302(6)	(3)	C(3)	H(13)	2.021(7)	(1)

*ADC (S, L, TX, TY, TZ) represents foIlowing things.

S: Symmetry operation number. -S is inversion of operation S.
(1) X,Y,Z
(2) -X+1/2,Y+1/2,Z
(3) X,-Y+1/2,Z+1/2
(4) -X+1/2,-Y,Z+1/2

L: Lattice translation.
(1) 0,0,0

TX, TY, TZ: Unit cell translation along the x, y, and z directions.