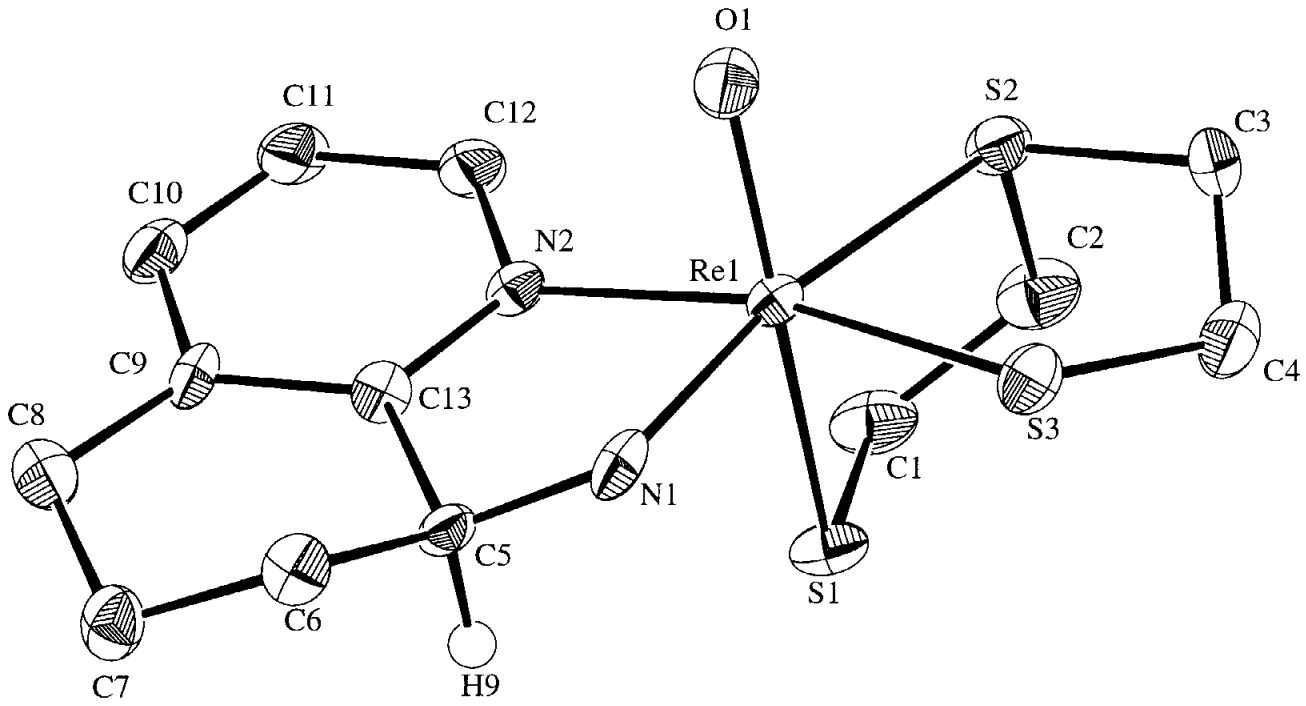
O1
C11
C12
S2
C3
C10
N2
Re1
C2
C9
C13
C4
C8
S3
C1
N1
C5
S1
C6
C7
H9

Experimental

Data Collection

A brown platelet crystal of $C_{13}H_{19}N_2OS_3Re$ having approximate dimensions of 0.10 x 0.10 x 0.05 mm was mounted on a glass fiber. All measurements were made on a Rigaku/ADSC CCD area detector with graphite monochromated Mo-Kα radiation.

Cell constants based on 4636 reflections with 2θ = 4.5 - 57.5° corresponded to a primitive monoclinic cell with dimensions:

a = 7.7579(6) $\AA$
b = 8.9622(6) $\AA$ β = 96.986(5)°
c = 11.1796(6) $\AA$
V = 771.52(8) $\AA^3$

For Z = 2 and F.W. = 501.69, the calculated density is 2.16 g/cm^3. Based on the systematic absences of:

0k0: k $\neq$ 2n

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

$P2_1$ (#4)

The data were collected at a temperature of -75 $\pm$ 1°C to a maximum 2θ value of 57.5°. Data were collected in 0.50° oscillations with 39.0 second exposures. A sweep of data was done using ϕ oscillations from 0.0 to 190.0° at χ=-90.0° and a second sweep was performed using ω oscillations between -22.0 and 18.0° at χ=-90.0°. The crystal-to-detector distance was 38.36 mm . The detector swing angle was -10.46°.

Data Reduction

Of the 6628 reflections which were collected, 3143 were unique (R_{int} = 0.065; Friedels not merged); equivalent reflections were merged. Data were collected and processed using the d*TREK program[10]. Net intensities and sigmas were derived as follows:

$$F^2 = [\sum_{i=1}^{m}(P_i - mB_{ave})] \cdot Lp$$

where P_i is the value in counts of the i^{th} pixel

m is the number of pixels in the integration area

B_{ave} is the background average

Lp is the Lorentz and polarization factor

$$B_{ave} = \frac{\sum_{j=1}^{n} B_j}{n}$$

where n is the number of pixels in the background area

B_j is the value of the j^{th} pixel in counts

$$\sigma^2(F_{hkl}^2) = [(\sum_{i=1}^{m} P_i) + m(\frac{\sum_{j=1}^{n}(B_{ave} - B_j)^2}{n-1})] \cdot Lp \cdot errmul + (erradd \cdot F^2)^2$$

where $erradd = 0.05$

$errmul = 1.90$

The linear absorption coefficient, μ, for Mo-Kα radiation is 82.8 cm^{-1}. The data were corrected for Lorentz and polarization effects.

Structure Solution and Refinement

The structure was solved by heavy-atom Patterson methods[1] and expanded using Fourier techniques[2]. This configuration was chosen based on the results of a parallel refinement of both enantiomers. The absolute configutation of C(5) was determined to be S. The non-hydrogen atoms were refined anisotropically. Some hydrogen atoms were refined isotropically, the rest were included in fixed positions. The final cycle of full-matrix least-squares refinement[3] was based on 3143 observed reflections ($I > 0.00\sigma(I)$) and 184 variable parameters and converged (largest parameter shift was 0.02 times its esd) with unweighted and weighted agreement factors of:

$$R1 = \frac{\Sigma||Fo| - |Fc||}{\Sigma|Fo|} = 0.051$$

$$wR2 = \sqrt{\frac{\Sigma(Fo^2 - Fc^2)^2}{\Sigma w(Fo^2)^2}} = 0.067$$

The standard deviation of an observation of unit weight[4] was 0.75. The weighting scheme was based on counting statistics. 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 1.59 and -1.51 $e^-/\AA^3$, 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 Hubbell[8]. All calculations were performed using the teXsan[9] crystallographic software package of Molecular Structure Corporation.

References

(1) PATTY: Beurskens, P.T., Admiraal, G., Beurskens, G., Bosman, W.P., Garcia-Granda, S., Gould, R.O., Smits, J.M.M. and Smykalla, C. (1992). The DIRDIF program system, Technical Report of the Crystallography Laboratory, University of Nijmegen, The Netherlands.

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

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

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

where: No = number of observations

Nv = number of variables

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

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

(7) Creagh, D. C. & McAuley, W.J .; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.6.8, pages 219-222 (1992).

(8) Creagh, D. C. & Hubbell, J.H..; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.4.3, pages 200-206 (1992).

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

(10) d*TREK: Area Detector Software. Version 4.13. Molecular Structure Corporation. (1996-1998).

EXPERIMENTAL DETAILS

A. Crystal Data

Empirical Formula	$C_{13}H_{19}N_2OS_3Re$
Formula Weight	501.69
Crystal Color, Habit	brown, platelet
Crystal Dimensions	0.10 X 0.10 X 0.05 mm
Crystal System	monoclinic
Lattice Type	Primitive
Lattice Parameters	a = 7.7579(6)Å b = 8.9622(6) Å c = 11.1796(6) Å β = 96.986(5)°
	V = 771.52(8) Å^3
Space Group	$P2_1$ (#4)
Z value	2
D_{calc}	2.159 g/cm^3
F_{000}	484.00
μ(MoKα)	82.80 cm^{-1}

B. Intensity Measurements

Diffractometer	Rigaku/ADSC CCD
Radiation	MoKα (λ = 0.71069 Å) graphite monochromated
Detector Aperture	94 mm x 94 mm
Data Images	460 exposures @ 39.0 seconds
ϕ oscillation Range (χ=-90.0)	0.0 - 190.0°

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

atom	x	y	z	B_{eq}
Re(1)	0.81304(4)	0.4980	0.75808(2)	1.318(5)
S(1)	1.0084(3)	0.6245(3)	0.9198(2)	1.86(5)
S(2)	0.6793(3)	0.7524(2)	0.7477(2)	1.81(4)
S(3)	0.6152(3)	0.4402(3)	0.8888(2)	1.98(5)
O(1)	0.6999(7)	0.480(1)	0.6167(5)	2.1(1)
N(1)	0.942(1)	0.3150(8)	0.7988(6)	1.7(2)
N(2)	1.0412(9)	0.5253(9)	0.6636(6)	1.3(2)
C(1)	1.003(1)	0.812(1)	0.8652(9)	2.4(2)
C(2)	0.818(1)	0.873(1)	0.8477(9)	2.5(2)
C(3)	0.493(1)	0.725(1)	0.8299(9)	2.5(2)
C(4)	0.531(1)	0.617(1)	0.9348(9)	2.3(2)
C(5)	1.120(1)	0.3019(9)	0.7761(7)	1.5(2)
C(6)	1.176(1)	0.1437(9)	0.7460(9)	1.9(2)
C(7)	1.363(1)	0.143(1)	0.7145(9)	2.1(2)
C(8)	1.385(1)	0.245(1)	0.6086(9)	2.0(2)
C(9)	1.283(1)	0.387(1)	0.6040(8)	1.6(2)
C(10)	1.3049(9)	0.502(2)	0.5206(6)	1.9(1)
C(11)	1.199(1)	0.623(1)	0.5124(8)	2.1(2)
C(12)	1.064(1)	0.632(1)	0.5814(8)	1.9(2)
C(13)	1.151(1)	0.4083(9)	0.6766(7)	1.3(2)
H(1)	1.0748	0.8743	0.9239	2.8868
H(2)	1.0510	0.8139	0.7882	2.8868
H(3)	0.8181	0.9735	0.8123	3.0014
H(4)	0.7726	0.8788	0.9258	3.0014

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

atom	x	y	z	B_{eq}
H(5)	0.4594	0.8217	0.8610	2.9981
H(6)	0.3965	0.6852	0.7743	2.9981
H(7)	0.4232	0.5994	0.9703	2.7936
H(8)	0.6169	0.6632	0.9956	2.7936
H(9)	1.1939	0.3337	0.8491	1.7644
H(10)	1.1678	0.0788	0.8154	2.2327
H(11)	1.0977	0.1064	0.6765	2.2327
H(12)	1.4409	0.1762	0.7850	2.5711
H(13)	1.3937	0.0408	0.6936	2.5711
H(14)	1.5083	0.2715	0.6130	2.3767
H(15)	1.3496	0.1899	0.5342	2.3767
H(16)	1.3965	0.4947	0.4679	2.3141
H(17)	1.2195	0.7052	0.4575	2.5355
H(18)	0.9831	0.7158	0.5705	2.2406
H(19)	0.836(7)	0.366(6)	0.769(5)	-2.2(6)

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

Table 2. Anisotropic Displacement Parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Re(1)	0.0191(1)	0.0169(1)	0.0142(1)	-0.0020(3)	0.00250(8)	0.0003(4)
S(1)	0.031(1)	0.021(1)	0.017(1)	-0.0044(9)	-0.0040(8)	0.0007(9)
S(2)	0.029(1)	0.021(1)	0.018(1)	0.003(1)	0.0024(8)	0.000(1)
S(3)	0.027(1)	0.027(1)	0.023(1)	-0.0044(9)	0.0095(9)	0.0023(9)
O(1)	0.023(3)	0.031(5)	0.026(3)	-0.003(4)	0.004(2)	-0.006(4)
N(1)	0.021(4)	0.029(4)	0.017(4)	0.003(3)	0.007(3)	-0.004(3)
N(2)	0.023(3)	0.012(6)	0.015(3)	-0.001(3)	0.003(2)	-0.002(3)
C(1)	0.038(6)	0.027(5)	0.024(5)	-0.006(4)	-0.006(4)	-0.004(4)
C(2)	0.040(6)	0.026(5)	0.027(5)	-0.004(4)	-0.002(4)	-0.006(4)
C(3)	0.022(5)	0.044(6)	0.029(5)	0.013(4)	0.006(4)	-0.005(5)
C(4)	0.030(5)	0.036(6)	0.025(5)	-0.002(4)	0.009(4)	-0.007(4)
C(5)	0.026(5)	0.018(4)	0.012(4)	0.002(3)	0.004(3)	0.003(3)
C(6)	0.031(5)	0.014(4)	0.027(5)	-0.003(4)	0.006(3)	-0.001(4)
C(7)	0.033(5)	0.020(5)	0.029(5)	0.005(4)	0.009(4)	-0.002(4)
C(8)	0.022(5)	0.023(5)	0.030(5)	0.001(4)	0.002(4)	-0.004(4)
C(9)	0.022(5)	0.026(5)	0.016(4)	-0.003(3)	0.009(3)	-0.004(4)
C(10)	0.023(4)	0.034(4)	0.017(3)	-0.005(8)	0.005(2)	-0.002(9)
C(11)	0.023(5)	0.038(6)	0.021(5)	-0.003(4)	0.006(4)	0.010(4)
C(12)	0.025(5)	0.025(5)	0.021(5)	0.002(4)	0.003(3)	0.006(4)
C(13)	0.016(4)	0.012(4)	0.021(5)	-0.008(3)	0.004(3)	0.000(3)

The general temperature factor expression:

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

Table 3. Bond Lengths($\AA$)

atom	atom	distance	atom	atom	distance
Re(1)	S(1)	2.487(2)	Re(1)	S(2)	2.502(2)
Re(1)	S(3)	2.303(2)	Re(1)	O(1)	1.719(5)
Re(1)	N(1)	1.947(8)	Re(1)	N(2)	2.183(7)
S(1)	C(1)	1.78(1)	S(2)	C(2)	1.81(1)
S(2)	C(3)	1.82(1)	S(3)	C(4)	1.82(1)
N(1)	C(5)	1.44(1)	N(2)	C(12)	1.35(1)
N(2)	C(13)	1.35(1)	C(1)	C(2)	1.53(1)
C(3)	C(4)	1.52(1)	C(5)	C(6)	1.53(1)
C(5)	C(13)	1.51(1)	C(6)	C(7)	1.54(1)
C(7)	C(8)	1.52(1)	C(8)	C(9)	1.49(1)
C(9)	C(10)	1.42(2)	C(9)	C(13)	1.40(1)
C(10)	C(11)	1.36(2)	C(11)	C(12)	1.38(1)

Table 4. Bond Lengths($\AA$)

atom	atom	distance	atom	atom	distance
Re(1)	H(19)	1.20(5)	N(1)	H(19)	0.97(5)
C(1)	H(1)	0.98	C(1)	H(2)	0.98
C(2)	H(3)	0.98	C(2)	H(4)	0.98
C(3)	H(5)	0.98	C(3)	H(6)	0.98
C(4)	H(7)	0.98	C(4)	H(8)	0.98
C(5)	H(9)	0.98	C(6)	H(10)	0.98
C(6)	H(11)	0.98	C(7)	H(12)	0.98
C(7)	H(13)	0.98	C(8)	H(14)	0.98
C(8)	H(15)	0.98	C(10)	H(16)	0.98
C(11)	H(17)	0.98	C(12)	H(18)	0.98

Table 5. Bond Angles(°)

atom	atom	atom	angle	atom	atom	atom	angle
S(1)	Re(1)	S(2)	80.25(8)	S(1)	Re(1)	S(3)	92.05(8)
S(1)	Re(1)	O(1)	155.4(4)	S(1)	Re(1)	N(1)	87.9(2)
S(1)	Re(1)	N(2)	80.9(2)	S(2)	Re(1)	S(3)	85.97(8)
S(2)	Re(1)	O(1)	83.2(4)	S(2)	Re(1)	N(1)	167.8(2)
S(2)	Re(1)	N(2)	103.4(2)	S(3)	Re(1)	O(1)	104.9(2)
S(3)	Re(1)	N(1)	91.5(2)	S(3)	Re(1)	N(2)	167.0(2)
O(1)	Re(1)	N(1)	108.9(4)	O(1)	Re(1)	N(2)	85.4(3)
N(1)	Re(1)	N(2)	77.5(3)	Re(1)	S(1)	C(1)	101.1(3)
Re(1)	S(2)	C(2)	107.8(3)	Re(1)	S(2)	C(3)	101.8(3)
C(2)	S(2)	C(3)	102.5(5)	Re(1)	S(3)	C(4)	105.9(3)
Re(1)	N(1)	C(5)	120.3(6)	Re(1)	N(2)	C(12)	126.1(6)
Re(1)	N(2)	C(13)	113.5(5)	C(12)	N(2)	C(13)	119.4(7)
S(1)	C(1)	C(2)	111.5(7)	S(2)	C(2)	C(1)	109.8(7)
S(2)	C(3)	C(4)	112.4(6)	S(3)	C(4)	C(3)	112.3(7)
N(1)	C(5)	C(6)	114.5(7)	N(1)	C(5)	C(13)	108.6(7)
C(6)	C(5)	C(13)	110.6(7)	C(5)	C(6)	C(7)	110.7(7)
C(6)	C(7)	C(8)	111.8(7)	C(7)	C(8)	C(9)	115.6(8)
C(8)	C(9)	C(10)	122.6(9)	C(8)	C(9)	C(13)	121.4(8)
C(10)	C(9)	C(13)	115.8(9)	C(9)	C(10)	C(11)	120.7(7)
C(10)	C(11)	C(12)	119.9(9)	N(2)	C(12)	C(11)	121.0(8)
N(2)	C(13)	C(5)	114.9(7)	N(2)	C(13)	C(9)	123.0(8)
C(5)	C(13)	C(9)	122.2(8)				

Table 6. Bond Angles(°)

atom	atom	atom	angle	atom	atom	atom	angle
S(1)	Re(1)	H(19)	108(2)	S(2)	Re(1)	H(19)	163(3)
S(3)	Re(1)	H(19)	79(3)	O(1)	Re(1)	H(19)	93(2)
N(1)	Re(1)	H(19)	23(3)	N(2)	Re(1)	H(19)	92(3)
Re(1)	N(1)	H(19)	29(3)	C(5)	N(1)	H(19)	141(3)
S(1)	C(1)	H(1)	108.6	S(1)	C(1)	H(2)	109.0
C(2)	C(1)	H(1)	109.0	C(2)	C(1)	H(2)	109.5
H(1)	C(1)	H(2)	109.2	S(2)	C(2)	H(3)	109.2
S(2)	C(2)	H(4)	109.4	C(1)	C(2)	H(3)	109.4
C(1)	C(2)	H(4)	109.6	H(3)	C(2)	H(4)	109.4
S(2)	C(3)	H(5)	108.7	S(2)	C(3)	H(6)	108.7
C(4)	C(3)	H(5)	108.8	C(4)	C(3)	H(6)	108.6
H(5)	C(3)	H(6)	109.6	S(3)	C(4)	H(7)	109.0
S(3)	C(4)	H(8)	108.9	C(3)	C(4)	H(7)	108.7
C(3)	C(4)	H(8)	108.7	H(7)	C(4)	H(8)	109.2
N(1)	C(5)	H(9)	107.8	C(6)	C(5)	H(9)	107.5
C(13)	C(5)	H(9)	107.6	C(5)	C(6)	H(10)	109.3
C(5)	C(6)	H(11)	109.1	C(7)	C(6)	H(10)	109.2
C(7)	C(6)	H(11)	108.9	H(10)	C(6)	H(11)	109.5
C(6)	C(7)	H(12)	108.7	C(6)	C(7)	H(13)	108.8
C(8)	C(7)	H(12)	109.0	C(8)	C(7)	H(13)	109.0
H(12)	C(7)	H(13)	109.5	C(7)	C(8)	H(14)	107.7
C(7)	C(8)	H(15)	107.9	C(9)	C(8)	H(14)	108.0
C(9)	C(8)	H(15)	108.1	H(14)	C(8)	H(15)	109.4
C(9)	C(10)	H(16)	120.1	C(11)	C(10)	H(16)	119.2

Table 6. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C(10)	C(11)	H(17)	120.0	C(12)	C(11)	H(17)	120.1
N(2)	C(12)	H(18)	119.6	C(11)	C(12)	H(18)	119.4

Table 7. Torsion Angles(°)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
Re(1)	S(1)	C(1)	C(2)	58.4(7)	Re(1)	S(2)	C(2)	C(1)	24.3(7)
Re(1)	S(2)	C(3)	C(4)	35.8(7)	Re(1)	S(3)	C(4)	C(3)	42.7(7)
Re(1)	N(1)	C(5)	C(6)	-148.5(6)	Re(1)	N(1)	C(5)	C(13)	-24.4(9)
Re(1)	N(2)	C(12)	C(11)	-168.8(7)	Re(1)	N(2)	C(13)	C(5)	-14.7(8)
Re(1)	N(2)	C(13)	C(9)	165.5(6)	S(1)	Re(1)	S(2)	C(2)	6.6(4)
S(1)	Re(1)	S(2)	C(3)	-100.8(3)	S(1)	Re(1)	S(3)	C(4)	65.0(3)
S(1)	Re(1)	N(1)	C(5)	-67.5(6)	S(1)	Re(1)	N(2)	C(12)	-100.7(7)
S(1)	Re(1)	N(2)	C(13)	91.2(5)	S(1)	C(1)	C(2)	S(2)	-56.2(8)
S(2)	Re(1)	S(1)	C(1)	-30.5(4)	S(2)	Re(1)	S(3)	C(4)	-15.1(3)
S(2)	Re(1)	N(1)	C(5)	-82(1)	S(2)	Re(1)	N(2)	C(12)	-23.0(7)
S(2)	Re(1)	N(2)	C(13)	168.8(5)	S(2)	C(3)	C(4)	S(3)	-53.7(9)
S(3)	Re(1)	S(1)	C(1)	-116.1(4)	S(3)	Re(1)	S(2)	C(2)	99.4(4)
S(3)	Re(1)	S(2)	C(3)	-8.0(3)	S(3)	Re(1)	N(1)	C(5)	-159.5(6)
S(3)	Re(1)	N(2)	C(12)	-158.4(7)	S(3)	Re(1)	N(2)	C(13)	33(1)
O(1)	Re(1)	S(1)	C(1)	17.9(7)	O(1)	Re(1)	S(2)	C(2)	-155.1(4)
O(1)	Re(1)	S(2)	C(3)	97.5(4)	O(1)	Re(1)	S(3)	C(4)	-97.0(5)
O(1)	Re(1)	N(1)	C(5)	94.2(7)	O(1)	Re(1)	N(2)	C(12)	58.9(8)
O(1)	Re(1)	N(2)	C(13)	-109.3(7)	N(1)	Re(1)	S(1)	C(1)	152.5(4)
N(1)	Re(1)	S(2)	C(2)	21(1)	N(1)	Re(1)	S(2)	C(3)	-86(1)
N(1)	Re(1)	S(3)	C(4)	153.0(4)	N(1)	Re(1)	N(2)	C(12)	169.5(7)
N(1)	Re(1)	N(2)	C(13)	1.3(5)	N(1)	C(5)	C(6)	C(7)	176.0(8)
N(1)	C(5)	C(13)	N(2)	24(1)	N(1)	C(5)	C(13)	C(9)	-156.0(8)
N(2)	Re(1)	S(1)	C(1)	74.8(4)	N(2)	Re(1)	S(2)	C(2)	-71.6(4)
N(2)	Re(1)	S(2)	C(3)	-179.0(4)	N(2)	Re(1)	S(3)	C(4)	121.7(9)

Table 7. Torsion Angles(°) (continued)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
N(2)	Re(1)	N(1)	C(5)	13.6(6)	N(2)	C(12)	C(11)	C(10)	5(1)
N(2)	C(13)	C(5)	C(6)	150.7(7)	N(2)	C(13)	C(9)	C(8)	-170.9(8)
N(2)	C(13)	C(9)	C(10)	5(1)	C(1)	C(2)	S(2)	C(3)	131.2(7)
C(2)	S(2)	C(3)	C(4)	-75.6(8)	C(5)	C(6)	C(7)	C(8)	-58(1)
C(5)	C(13)	N(2)	C(12)	176.3(8)	C(5)	C(13)	C(9)	C(8)	9(1)
C(5)	C(13)	C(9)	C(10)	-175.1(8)	C(6)	C(5)	C(13)	C(9)	-30(1)
C(6)	C(7)	C(8)	C(9)	37(1)	C(7)	C(6)	C(5)	C(13)	53(1)
C(7)	C(8)	C(9)	C(10)	171.9(9)	C(7)	C(8)	C(9)	C(13)	-13(1)
C(8)	C(9)	C(10)	C(11)	174.3(9)	C(9)	C(10)	C(11)	C(12)	-3(2)
C(9)	C(13)	N(2)	C(12)	-4(1)	C(11)	C(10)	C(9)	C(13)	-1(1)
C(11)	C(12)	N(2)	C(13)	-1(1)					

Table 8. Non-bonded Contacts out to 3.60 $\AA$

atom	atom	distance	ADC	atom	atom	distance	ADC
S(1)	N(1)	3.559(8)	75702	S(1)	C(2)	3.58(1)	74702
O(1)	C(10)	3.128(9)	45501	O(1)	C(8)	3.22(1)	45501
O(1)	C(9)	3.33(1)	45501	O(1)	C(8)	3.47(1)	75602
C(1)	C(6)	3.59(1)	56501				

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

h	k	l	Fo	Fc	sigF	h	k	l	Fo	Fc	sigF	h	k	l	Fo	Fc	sigF	h	k	l	Fo	Fc	sigF	h	k	l	Fo	Fc	sigF
1	-6	-6	13	9	6*	1	-4	5	83	86	3	1	-2	12	57	59	3	1	-1	8	58	59	2	1	2	-10	12	11	6*
1	-6	-5	64	65	2	1	-4	6	38	38	2	1	-1	-13	6	10	7*	1	-1	9	55	55	2	1	2	-9	61	60	2
1	-6	-4	12	14	6*	1	-4	7	87	87	3	1	-1	-12	52	53	2	1	-1	10	45	45	2	1	2	-8	9	6	6*
1	-6	-3	75	76	2	1	-4	8	49	49	2	1	-1	-11	0	10	7*	1	-1	11	57	58	2	1	2	-7	100	101	5
1	-6	-2	46	47	2	1	-4	9	48	49	2	1	-1	-10	66	65	2	1	-1	12	22	20	5*	1	2	-6	12	14	4*
1	-6	-1	80	82	2	1	-4	10	53	52	2	1	-1	-9	22	24	4*	1	0	-13	62	61	3	1	2	-5	95	94	3
1	-6	0	57	59	2	1	-4	11	31	32	3	1	-1	-8	108	106	3	1	0	-12	11	10	7*	1	2	-4	31	32	2
1	-6	1	59	59	2	1	-3	-12	59	60	3	1	-1	-7	18	19	4*	1	0	-11	74	76	2	1	2	-3	59	62	2
1	-6	2	38	39	2	1	-3	-11	8	7	7*	1	-1	-6	133	132	3	1	0	-10	5	11	6*	1	2	-2	50	50	2
1	-6	3	48	51	2	1	-3	-10	70	72	2	1	-1	-5	30	29	2	1	0	-9	102	102	3	1	2	-1	102	104	3
1	-6	4	45	45	2	1	-3	-9	14	10	6*	1	-1	-4	91	92	2	1	0	-8	24	26	3	1	2	0	51	52	1
1	-6	5	43	43	2	1	-3	-8	82	82	2	1	-1	-3	71	70	2	1	0	-7	142	142	4	1	2	1	131	134	3
1	-6	6	70	69	2	1	-3	-7	22	20	3	1	-1	-2	123	122	3	1	0	-6	3	7	5*	1	2	2	91	92	2
1	-6	7	43	40	2	1	-3	-6	106	106	3	1	-1	0	129	132	3	1	0	-5	109	110	3	1	2	3	94	94	2
1	-6	8	50	49	2	1	-3	-5	17	11	6*	-1	10	2	28	27	4	1	0	-4	26	21	2	1	2	4	77	76	2
1	-6	9	29	26	3	1	-3	-4	82	85	2	-1	10	1	48	46	3	1	0	-3	126	127	5	1	2	5	63	64	2
1	-5	-11	20	20	5*	1	-3	-3	35	37	2	-1	9	5	9	4	7*	1	0	1	126	130	3	1	2	6	75	77	3
1	-5	-10	65	64	2	1	-3	-2	92	95	4	-1	9	4	54	51	2	1	0	2	118	114	3	1	2	7	76	74	2
1	-5	-9	7	12	7*	1	-3	-1	39	41	2	-1	9	3	22	14	4*	1	0	3	105	108	3	1	2	8	56	56	2
1	-5	-8	71	71	2	1	-3	0	128	132	3	-1	9	2	75	68	3	1	0	4	64	63	2	1	2	9	49	48	2
1	-5	-7	10	3	6*	1	-3	1	45	46	2	-1	9	1	31	28	3	1	0	5	86	88	2	1	2	10	67	68	2
1	-5	-6	84	86	2	1	-3	2	115	115	3	-1	9	0	47	44	2	1	0	6	63	62	2	1	2	11	28	29	3
1	-5	-5	25	25	3	1	-3	3	76	77	2	-1	8	6	0	8	6*	1	0	7	72	75	5	1	2	12	62	63	3
1	-5	-4	82	84	2	1	-3	4	66	69	2	-1	8	5	55	54	2	1	0	8	38	39	2	1	3	-12	55	56	3
1	-5	-3	42	44	2	1	-3	5	51	51	2	-1	8	4	8	7	7*	1	0	9	55	55	2	1	3	-11	0	7	7*
1	-5	-2	85	87	2	1	-3	6	82	83	3	-1	8	3	87	83	3	1	0	10	57	58	2	1	3	-10	72	70	2
1	-5	-1	42	44	2	1	-3	7	48	49	3	-1	8	2	0	8	7*	1	0	11	40	41	3	1	3	-9	7	10	6*
1	-5	0	99	101	3	1	-3	8	84	83	2	-1	8	1	86	82	3	1	0	12	49	49	3	1	3	-8	80	79	2
1	-5	1	41	41	2	1	-3	9	73	71	2	-1	7	5	12	5	6*	1	1	-13	0	13	8*	1	3	-7	20	21	3
1	-5	2	85	86	2	1	-3	10	31	32	3	-1	7	4	75	75	2	1	1	-12	57	57	3	1	3	-6	99	100	3
1	-5	3	56	57	2	1	-3	11	59	59	4	-1	7	3	15	14	5*	1	1	-11	6	12	7*	1	3	-5	17	10	3*
1	-5	4	56	57	2	1	-2	-12	18	9	5*	-1	7	2	104	102	3	1	1	-10	68	68	2	1	3	-4	79	81	2
1	-5	5	60	60	2	1	-2	-11	50	50	4	-1	7	1	39	40	2	1	1	-9	24	24	3	1	3	-3	35	37	2
1	-5	6	53	52	2	1	-2	-10	14	9	6*	-1	6	3	73	77	2	1	1	-8	111	108	4	1	3	-2	100	102	3
1	-5	7	48	47	2	1	-2	-9	61	61	2	-1	6	2	45	47	2	1	1	-7	20	20	3	1	3	-1	49	47	1
1	-5	8	47	47	2	1	-2	-8	0	6	6*	-1	6	1	79	80	2	1	1	-6	137	133	4	1	3	0	125	127	4
1	-5	9	46	47	2	1	-2	-7	101	101	3	-1	5	2	87	88	2	1	1	-5	28	27	2	1	3	1	52	53	3
1	-5	10	26	26	4	1	-2	-6	0	11	6*	-1	5	1	43	45	2	1	1	-4	93	92	3	1	3	2	108	109	3
1	-4	-12	24	24	4*	1	-2	-5	99	100	3	-1	5	-11	38	42	3	1	1	-3	68	67	4	1	3	3	75	74	2
1	-4	-11	70	70	4	1	-2	-4	34	35	2	-1	4	1	129	130	3	1	1	-2	132	130	5	1	3	4	65	68	2
1	-4	-10	0	3	8*	1	-2	-3	59	64	2	-1	4	-12	29	29	4	1	1	0	138	141	6	1	3	5	55	55	2
1	-4	-9	83	83	3	1	-2	-2	51	52	2	-1	3	-12	29	28	4	1	1	1	96	95	2	1	3	6	80	80	2
1	-4	-8	10	15	6*	1	-2	-1	108	111	3	-1	2	-13	10	15	7*	1	1	2	169	170	4	1	3	7	52	51	2
1	-4	-7	96	98	3	1	-2	0	49	50	1	-1	1	1	28	28	1	1	1	3	94	91	2	1	3	8	76	77	2
1	-4	-6	17	14	4*	1	-2	1	135	138	3	-1	1	-13	43	44	3	1	1	4	104	103	3	1	3	9	69	69	2
1	-4	-5	114	116	3	1	-2	2	96	98	4	-1	0	2	12	4	2*	1	1	5	74	75	2	1	3	10	32	32	3
1	-4	-4	32	34	2	1	-2	3	92	93	2	-1	0	1	149	145	4	1	1	6	93	95	4	1	3	11	59	61	2
1	-4	-3	102	105	3	1	-2	4	81	80	2	-1	0	-13	18	19	6*	1	1	7	48	50	2	1	4	-12	24	26	5*
1	-4	-2	55	56	2	1	-2	5	58	59	2	1	-1	1	98	96	2	1	1	8	63	63	2	1	4	-11	73	71	3
1	-4	-1	126	128	3	1	-2	6	67	69	2	1	-1	2	162	162	4	1	1	9	52	50	3	1	4	-10	6	5	7*
1	-4	0	28	30	2	1	-2	7	79	77	2	1	-1	3	104	101	3	1	1	10	49	50	2	1	4	-9	89	86	3
1	-4	1	137	138	4	1	-2	8	56	56	2	1	-1	4	97	96	3	1	1	11	56	57	2	1	4	-8	15	14	5*
1	-4	2	38	40	2	1	-2	9	53	51	3	1	-1	5	73	75	2	1	1	12	27	23	4	1	4	-7	99	97	3
1	-4	3	114	114	3	1	-2	10	70	68	2	1	-1	6	88	89	2	1	2	-12	0	5	8*	1	4	-6	16	13	4*
1	-4	4	59	61	2	1	-2	11	24	25	4*	1	-1	7	47	49	2	1	2	-11	48	48	2	1	4	-5	116	117	4

h	k	l	Fo	Fc	sigF	h	k	l	Fo	Fc	sigF	h	k	l	Fo	Fc	sigF	h	k	l	Fo	Fc	sigF	h	k	l	Fo	Fc	sigF
1	4	-4	31	32	2	1	7	-7	0	8	7*	2	-8	5	47	47	3	2	-5	3	31	32	2	2	-2	-11	31	34	4
1	4	-3	111	112	3	1	7	-6	66	66	2	2	-8	6	26	25	4	2	-5	4	77	75	2	2	-2	-10	52	52	2
1	4	-2	60	59	2	1	7	0	75	74	2	2	-8	7	41	42	3	2	-5	5	64	65	2	2	-2	-9	47	48	2
1	4	0	40	40	2	1	7	1	40	41	2	2	-7	-9	79	76	3	2	-5	6	65	64	2	2	-2	-8	69	70	2
1	4	1	134	135	4	1	7	2	71	69	2	2	-7	-8	34	32	3	2	-5	7	39	40	2	2	-2	-7	38	39	2
1	4	2	39	40	1	1	7	3	23	19	3	2	-7	-7	58	58	2	2	-5	8	62	62	2	2	-2	-6	89	90	2
1	4	3	112	113	3	1	7	4	83	80	2	2	-7	-6	32	35	3	2	-5	9	15	21	6*	2	-2	-5	69	70	2
1	4	4	56	58	4	1	7	5	48	48	2	2	-7	-5	48	47	2	2	-5	10	55	54	3	2	-2	-4	79	81	2
1	4	5	87	88	2	1	7	6	64	63	2	2	-7	-4	24	24	4	2	-4	-11	18	20	5*	2	-2	-3	92	95	2
1	4	6	37	38	2	1	7	7	48	49	2	2	-7	-3	74	74	2	2	-4	-10	64	63	2	2	-2	-2	81	81	2
1	4	7	86	85	2	1	7	8	34	34	3	2	-7	-2	58	58	2	2	-4	-9	19	17	4*	2	-2	-1	78	81	2
1	4	8	51	49	2	1	7	9	32	36	4	2	-7	-1	60	60	2	2	-4	-8	71	72	2	2	-2	0	107	108	3
1	4	9	46	45	2	1	8	-8	0	1	7*	2	-7	0	59	61	2	2	-4	-7	11	12	6*	2	-2	1	81	84	2
1	4	10	50	49	2	1	8	-7	65	63	2	2	-7	1	41	42	2	2	-4	-6	108	110	3	2	-2	2	60	60	2
1	4	11	33	33	3	1	8	0	37	35	2	2	-7	2	51	50	2	2	-4	-5	54	56	2	2	-2	3	148	146	4
1	5	-11	24	22	8*	1	8	1	58	56	2	2	-7	3	50	51	2	2	-4	-4	87	88	2	2	-2	4	47	47	2
1	5	-10	71	69	2	1	8	2	17	21	4*	2	-7	4	70	68	2	2	-4	-3	53	55	2	2	-2	5	129	126	3
1	5	-9	9	11	7*	1	8	3	74	74	2	2	-7	5	38	37	3	2	-4	-2	64	66	2	2	-2	6	32	33	2
1	5	-8	75	73	2	1	8	4	19	25	4*	2	-7	6	59	60	2	2	-4	-1	40	41	2	2	-2	7	82	82	2
1	5	-7	12	2	6*	1	8	5	73	71	2	2	-7	7	22	20	4*	2	-4	0	93	97	2	2	-2	8	27	28	3
1	5	-6	89	88	3	1	8	6	51	51	2	2	-7	8	53	54	3	2	-4	1	77	79	2	2	-2	9	73	72	2
1	5	-5	21	22	3	1	8	7	37	39	3	2	-6	-10	54	53	3	2	-4	2	61	63	2	2	-2	10	17	13	5*
1	5	-4	87	90	4	1	9	1	33	34	3	2	-6	-9	27	28	4	2	-4	3	63	63	2	2	-2	11	72	73	2
1	5	-3	43	44	2	1	9	2	49	49	2	2	-6	-8	66	65	2	2	-4	4	54	54	2	2	-1	-12	11	8	7*
1	5	0	99	100	3	1	9	3	21	17	4*	2	-6	-7	33	33	3	2	-4	5	70	68	2	2	-1	-11	49	49	2
1	5	1	36	38	2	1	9	4	55	59	2	2	-6	-6	46	47	3	2	-4	6	67	67	2	2	-1	-10	30	30	3
1	5	2	86	89	2	1	9	5	44	42	3	2	-6	-5	45	46	2	2	-4	7	75	73	2	2	-1	-9	81	79	3
1	5	3	57	56	2	1	10	1	37	36	3	2	-6	-4	57	58	2	2	-4	8	21	22	4*	2	-1	-8	38	37	2
1	5	4	66	64	2	2	-10	-1	44	44	3	2	-6	-3	61	63	2	2	-4	9	52	51	3	2	-1	-7	91	91	3
1	5	5	58	59	2	2	-10	0	39	42	3	2	-6	-2	65	67	2	2	-4	10	20	19	4*	2	-1	-6	48	50	2
1	5	6	53	54	2	2	-9	-6	27	27	4	2	-6	-1	74	77	2	2	-3	-12	11	10	7*	2	-1	-5	108	106	3
1	5	7	49	49	2	2	-9	-5	37	36	3	2	-6	0	51	53	2	2	-3	-11	70	72	4	2	-1	-4	81	83	3
1	5	8	46	46	2	2	-9	-4	30	27	4	2	-6	1	78	79	2	2	-3	-10	33	36	6	2	-1	-3	116	116	3
1	5	9	47	47	2	2	-9	-3	54	54	3	2	-6	2	39	42	2	2	-3	-9	53	54	2	2	-1	-2	111	110	3
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h	k	l	Fo	Fc	sigF	h	k	l	Fo	Fc	sigF	h	k	l	Fo	Fc	sigF	h	k	l	Fo	Fc	sigF	h	k	l	Fo	Fc	sigF
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