S1: Crystal structure data for $[(SO_4)(terpy)Mn(O)_2Mn(terpy)(O_4S)]\cdot 6H_2O$, $2\cdot 6H_2O$

Data Collection

A dark red plate crystal of $C_{30}H_{34}N_6O_{16}S_2Mn_2$ having approximate dimensions of 0.09 x 0.17 x 0.22 mm was mounted on a glass fiber. All measurements were made on an Enraf-Nonius CAD4 diffractometer with graphite monochromated Mo-KALPHA radiation.

Cell constants and an orientation matrix for data collection, obtained from a least-squares refinement using the setting angles of 25 carefully centered reflections in the range 7.18 < 2THETA < 18.00° corresponded to a C-centered monoclinic cell with dimensions:

a = 27.091(4) Å
b = 9.036(2) Å BETA = 127.42(2)°
c = 18.281(5) Å
V = 3554(1) Å^3

For Z = 4 and F.W. = 908.63, the calculated density is 1.70 g/cm^3. Based on the systematic absences of:

hkl: h+k ± 2n
h0l: l ± 2n

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

C2/c (#15)

The data were collected at a temperature of -90 ± 1°C using the OMEGA-2THETA scan technique to a maximum 2THETA value of 52.6°.Omega scans of several intense reflections, made prior to data collection, had an average width at half-height of 0.00° with a take-off angle of 2.8°. Scans of (1.34 + 1.00 tan THETA)° were made at a speed of 1.0°/min (in omega). Moving-crystal moving counter background measurements were made by scanning an additional 25 above and below the scan range. The counter aperture consisted of a variable horizontal slit with a width ranging from 2.0 to 2.5 mm and a vertical slit set to 2.0 mm. The diameter of the incident beam collimator was 0.7 mm and the crystal to detector distance was 21 cm. For intense reflections an attenuator was automatically inserted in front of the detector.

Data Reduction

Of the 3955 reflections which were collected, 3834 were unique (R_{int} = 0.115). The intensities of three representative reflection were measured after every 0 minutes of X-ray exposure time. No decay correction was applied.

The linear absorption coefficient, MU, for Mo-KALPHA radiation is 9.1 cm^{-1}. An empirical absorption correction using the program DIFABS[1] was applied which resulted in transmission factors ranging from 0.71 to 1.00. The data were corrected for Lorentz and polarization effects.

Structure Solution and Refinement

The structure was solved by heavy-atom Patterson methods[2] and expanded using Fourier techniques[3]. The non-hydrogen atoms were refined anisotropically. The hydrogen atoms of terpy were included but not refined. The final cycle of full-matrix least-squares refinement[4] was based on 1323 observed reflections (I > 3.00sigma(I)) and 253 variable parameters and converged (largest parameter shift was 0.00 times its esd) with unweighted and weighted agreement factors of:

$$R = \text{SIGMA } ||Fo| - |Fc|| / \text{SIGMA } |Fo| = 0.055$$

$$R_w = [(\text{ SIGMA w } (|Fo| - |Fc|)^2 / \text{SIGMA w } Fo^2)]^{1/2} = 0.056$$

The standard deviation of an observation of unit weight[5] was 1.58. The weighting scheme was based on counting statistics and included a factor (p = 0.026) 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 0.53 and -0.45 $e^-/Å^3$, respectively.

Neutral atom scattering factors were taken from Cromer and Waber[6]. Anomalous dispersion effects were included in Fcalc[7]; the values for DELTAf' and DELTAf" were those of Creagh and McAuley[8]. The values for the mass attenuation coefficients are those of Creagh and Hubbel[9]. All calculations were performed using the teXsan[10] crystallographic software package of Molecular Structure Corporation.

References

(1) DIFABS: Walker, N. & Stuart, Acta Cryst. A39, 158-166 (1983). An empirical absorption correction program.

(2) 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.

(3) 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.

(4) Least-Squares:

Function minimized: $Sw(|F_o|-|F_c|)^2$

where $w = 4F_o^2/\sigma^2(F_o^2) = [s^2(F_o) + (pF_o/2)^2]^{-1}$

$F_o^2 = S(C-RB)/Lp$

and $s^2(F_o^2) = [S^2(C+R^2B) + (pF_o^2)^2]/Lp^2$

S = Scan rate
C = Total integrated peak count
R = Ratio of scan time to background counting time
B = Total background count
Lp = Lorentz-polarization factor
p = p-factor

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

$[Sw(|F_o|-|F_c|)^2/(N_o-N_v)]^{1/2}$

where: N_o = number of observations

N_v = number of variables

(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 Crystallogr., 17, 781 (1964).

(8) 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).

(9) 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).

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

Table S1.1 Experimental Conditions.

A Crystal Data.	
Empirical Formula	$C_{30}H_{34}N_6O_{16}S_2Mn_2$
Formula Weight	908.63
Crystal Color, Habit	dark red, plate
Crystal Dimensions	0.09 X 0.17 X 0.22 mm
Crystal System	monoclinic
Lattice Type	C-centered
No. of Reflections Used for Unit Cell Determination (2θ range)	25 (7.2 - 18.0°)
Omega Scan Peak Width at Half-height	0.00°
Lattice Parameters	a = 27.091(4)Å b = 9.036(2) Å c = 18.281(5) Å ß = 127.42(2)° V = 3554(1) Å^3
Space Group	C2/c (#15)
Z value	4
D_{calc}	1.70 g/cm^3
F_{000}	1864.00
μ(MoKα)	9.12 cm^{-1}
B. Intensity Measurements.	
Diffractometer	CAD4
Radiation	MoKALPHA (LAMBDA = 0.71069 Å)
Attenuator	graphite monochromated Zr foil (factor = 20.40)
Take-off Angle	2.8°

Detector Aperture	2.0 - 2.5 mm horizontal 2.0 mm vertical
Crystal to Detector Distance	21 mm
Temperature	-90.0°C
Scan Type	Ω-2θ
Scan Rate	1.0°/min (in Ω) (up to 0 scans)
Scan Width	$(1.34 + 1.00 \tan \theta)^{o}$
$2\theta_{max}$	52.6°
No. of Reflections Measured (R_{int} = 0.115)	Total: 3955 Unique: 3834
Corrections	Lorentz-polarization Absorption (trans. factors: 0.7076 - 1.0000)

C. Structure Solution and Refinement.

Structure Solution	Patterson Methods (DIRDIF92 PATTY)
Refinement Function Minimized	Full-matrix least-squares SIGMA w $(\|Fo\| - \|Fc\|)^2$
Least Squares Weights	$1/^2\sigma(Fo) = 4Fo^2/\sigma^2(Fo^2)$
p-factor	0.0260
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (I>3.00sigma(I))	1323
No. Variables	253
Reflection/Parameter Ratio	5.23
Residuals: R; Rw	0.055 ; 0.056
Goodness of Fit Indicator	1.58
Max Shift/Error in Final Cycle	0.00
Maximum peak in Final Diff. Map	0.53 $e^-/Å^3$
Minimum peak in Final Diff. Map	-0.45 $e^-/Å^3$

Table S1.2 Atomic coordinates and B_{iso}/B_{eq}.

atom	x	y	z	B_{eq}
Mn(1)	0.21421(7)	0.1761(2)	0.0190(1)	1.34(4)
S(1)	0.1133(1)	0.1620(3)	0.0521(2)	1.82(7)
O(1)	0.2730(3)	0.1389(6)	0.0019(4)	1.2(2)
O(2)	0.1541(3)	0.2415(6)	0.0331(4)	1.4(2)
O(3)	0.1521(3)	0.1237(8)	0.1494(5)	3.0(2)
O(4)	0.0648(3)	0.2705(8)	0.0268(6)	3.4(2)
O(5)	0.0878(3)	0.0311(8)	-0.0060(5)	2.9(2)
O(6)	0.4654(4)	0.0060(8)	0.1041(5)	4.1(2)
O(7)	0.0296(3)	-0.2383(7)	-0.0400(5)	2.9(2)
O(8)	0.0744(4)	-0.4644(8)	-0.2120(6)	4.6(2)
N(1)	0.1442(4)	0.1069(9)	-0.1082(5)	1.4(2)
N(2)	0.2123(4)	-0.0404(8)	0.0383(6)	1.2(2)
N(3)	0.2758(3)	0.162(1)	0.1587(5)	1.5(2)
C(1)	0.1063(5)	0.202(1)	-0.1785(7)	2.4(3)
C(2)	0.0580(5)	0.149(1)	-0.2643(7)	2.9(3)
C(3)	0.0496(6)	0.000(1)	-0.2791(7)	3.0(3)
C(4)	0.0882(5)	-0.097(1)	-0.2054(8)	2.4(3)
C(5)	0.1343(5)	-0.038(1)	-0.1208(7)	1.5(2)
C(6)	0.1726(5)	-0.123(1)	-0.0373(8)	1.9(3)
C(7)	0.1750(5)	-0.277(1)	-0.0235(8)	2.2(3)
C(8)	0.2156(5)	-0.337(1)	0.0631(7)	2.1(3)
C(9)	0.2563(5)	-0.246(1)	0.1381(7)	1.6(3)
C(10)	0.2539(5)	-0.095(1)	0.1244(7)	1.5(3)
C(11)	0.2886(5)	0.022(1)	0.1926(7)	1.4(3)
C(12)	0.3323(6)	-0.004(1)	0.2864(8)	2.6(3)
C(13)	0.3600(6)	0.117(1)	0.3451(7)	2.8(3)
C(14)	0.3433(5)	0.258(1)	0.3110(7)	1.9(3)
C(15)	0.3002(5)	0.277(1)	0.2158(7)	1.8(3)
H(1)	0.1130	0.3060	-0.1687	2.9359
H(2)	0.0306	0.2158	-0.3128	3.5102
H(3)	0.0181	-0.0378	-0.3387	3.5918
H(4)	0.0826	-0.2011	-0.2136	2.8457
H(5)	0.1483	-0.3402	-0.0746	2.6333
H(6)	0.2158	-0.4405	0.0716	2.4858
H(7)	0.2852	-0.2870	0.1977	1.9030
H(8)	0.3429	-0.1016	0.3099	3.1048
H(9)	0.3908	0.1022	0.4093	3.3406
H(10)	0.3605	0.3412	0.3510	2.3020
H(11)	0.2881	0.3740	0.1913	2.1500

$B_{eq} = 8/3\ PI^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos GAMMA + 2U_{13}(aa^*cc^*)\cos BETA + 2U_{23}(bb^*cc^*)\cos ALPHA)$

Table S1.3 Anisotropic displacement parameters.

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Mn(1)	0.0196(10)	0.0146(8)	0.0156(9)	-0.0017(10)	0.0101(8)	0.0002(9)
S(1)	0.024(2)	0.025(2)	0.027(2)	-0.004(2)	0.019(2)	-0.006(2)
O(1)	0.019(4)	0.006(4)	0.017(4)	0.000(3)	0.009(4)	0.004(3)
O(2)	0.019(4)	0.022(4)	0.023(4)	-0.002(4)	0.018(4)	-0.001(3)
O(3)	0.049(5)	0.043(5)	0.018(4)	-0.008(4)	0.018(4)	0.001(4)
O(4)	0.037(5)	0.031(5)	0.077(6)	0.010(4)	0.043(5)	0.007(4)
O(5)	0.050(6)	0.031(5)	0.040(5)	-0.019(4)	0.034(5)	-0.021(4)
O(6)	0.060(6)	0.048(6)	0.030(5)	-0.001(5)	0.018(5)	-0.004(4)
O(7)	0.042(5)	0.022(4)	0.041(5)	0.003(4)	0.024(4)	0.003(4)
O(8)	0.058(6)	0.037(5)	0.058(6)	-0.001(5)	0.023(5)	-0.007(5)
N(1)	0.011(5)	0.016(5)	0.011(5)	-0.004(4)	0.000(4)	-0.002(4)
N(2)	0.013(5)	0.010(4)	0.025(6)	-0.004(4)	0.012(5)	-0.002(4)
N(3)	0.018(5)	0.025(5)	0.016(5)	-0.006(5)	0.011(4)	-0.008(5)
C(1)	0.025(7)	0.038(8)	0.025(7)	-0.002(6)	0.013(6)	0.005(6)
C(2)	0.023(7)	0.056(9)	0.018(6)	0.008(7)	0.006(6)	0.006(7)
C(3)	0.042(8)	0.048(8)	0.025(7)	-0.003(8)	0.021(7)	-0.005(7)
C(4)	0.028(7)	0.033(7)	0.027(7)	-0.006(6)	0.016(6)	-0.004(6)
C(5)	0.014(6)	0.022(6)	0.017(6)	0.002(5)	0.008(5)	0.000(5)
C(6)	0.018(7)	0.030(7)	0.030(7)	-0.006(5)	0.018(6)	-0.009(6)
C(7)	0.022(7)	0.016(6)	0.036(8)	-0.004(5)	0.013(6)	-0.013(5)
C(8)	0.032(7)	0.014(6)	0.032(7)	0.008(6)	0.019(6)	0.002(6)
C(9)	0.033(8)	0.011(6)	0.027(7)	-0.003(6)	0.024(7)	-0.004(5)
C(10)	0.026(7)	0.021(6)	0.020(7)	-0.004(6)	0.019(6)	-0.002(5)
C(11)	0.021(7)	0.017(6)	0.022(7)	0.003(5)	0.017(6)	0.004(5)
C(12)	0.050(8)	0.028(7)	0.024(7)	0.005(7)	0.025(7)	0.002(6)
C(13)	0.045(9)	0.045(8)	0.015(7)	-0.001(7)	0.018(7)	0.001(6)
C(14)	0.038(8)	0.031(7)	0.011(7)	-0.001(6)	0.018(6)	-0.004(5)
C(15)	0.032(7)	0.015(6)	0.022(7)	-0.002(5)	0.017(6)	-0.001(5)

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 S1.4 Bond lengths(Å).

atom	atom	distance	atom	atom distance
Mn(1)	Mn(1)	2.769(3)	Mn(1)	O(1) 1.833(6)
Mn(1)	O(1)	1.794(6)	Mn(1)	O(2) 1.890(6)
Mn(1)	N(1)	2.009(7)	Mn(1)	N(2) 1.994(8)
Mn(1)	N(3)	2.035(7)	S(1)	O(2) 1.526(6)
S(1)	O(3)	1.454(7)	S(1)	O(4) 1.470(7)
S(1)	O(5)	1.453(7)	N(1)	C(1) 1.36(1)
N(1)	C(5)	1.32(1)	N(2)	C(6) 1.35(1)
N(2)	C(10)	1.35(1)	N(3)	C(11) 1.36(1)
N(3)	C(15)	1.32(1)	C(1)	C(2) 1.38(1)
C(2)	C(3)	1.37(1)	C(3)	C(4) 1.40(1)
C(4)	C(5)	1.38(1)	C(5)	C(6) 1.44(1)
C(6)	C(7)	1.40(1)	C(7)	C(8) 1.38(1)
C(8)	C(9)	1.39(1)	C(9)	C(10) 1.38(1)

C(10)	C(11)	1.46(1)	C(11)	C(12)	1.39(1)
C(12)	C(13)	1.39(1)	C(13)	C(14)	1.37(1)
C(14)	C(15)	1.40(1)			

Table S1.5 Bond lengths(Å).

atom	atom	distance	atom	atom	distance
C(1)	H(1)	0.95	C(2)	H(2)	0.95
C(3)	H(3)	0.95	C(4)	H(4)	0.95
C(7)	H(5)	0.95	C(8)	H(6)	0.95
C(9)	H(7)	0.95	C(12)	H(8)	0.95
C(13)	H(9)	0.95	C(14)	H(10)	0.95
C(15)	H(11)	0.95			

Table S1.6 Bond angles(°).

atom	atom	atom	angle	atom	atom	atom	angle
Mn(1)	Mn(1)	O(1)	39.7(2)	Mn(1)	Mn(1)	O(1)	40.7(2)
Mn(1)	Mn(1)	O(2)	132.5(2)	Mn(1)	Mn(1)	N(1)	99.9(2)
Mn(1)	Mn(1)	N(2)	128.0(2)	Mn(1)	Mn(1)	N(3)	100.3(2)
O(1)	Mn(1)	O(1)	80.5(3)	O(1)	Mn(1)	O(2)	172.2(3)
O(1)	Mn(1)	N(1)	93.0(3)	O(1)	Mn(1)	N(2)	88.3(3)
O(1)	Mn(1)	N(3)	93.9(3)	O(1)	Mn(1)	O(2)	91.7(3)
O(1)	Mn(1)	N(1)	102.3(3)	O(1)	Mn(1)	N(2)	168.7(3)
O(1)	Mn(1)	N(3)	101.9(3)	O(2)	Mn(1)	N(1)	88.2(3)
O(2)	Mn(1)	N(2)	99.5(3)	O(2)	Mn(1)	N(3)	88.0(3)
N(1)	Mn(1)	N(2)	78.0(3)	N(1)	Mn(1)	N(3)	155.7(3)
N(2)	Mn(1)	N(3)	79.0(4)	O(2)	S(1)	O(3)	107.8(4)
O(2)	S(1)	O(4)	104.3(4)	O(2)	S(1)	O(5)	107.8(4)
O(3)	S(1)	O(4)	112.8(5)	O(3)	S(1)	O(5)	111.7(4)
O(4)	S(1)	O(5)	112.1(5)	Mn(1)	O(1)	Mn(1)	99.5(3)
Mn(1)	O(2)	S(1)	133.4(4)	Mn(1)	N(1)	C(1)	122.5(7)
Mn(1)	N(1)	C(5)	117.2(7)	C(1)	N(1)	C(5)	120.3(9)
Mn(1)	N(2)	C(6)	117.0(7)	Mn(1)	N(2)	C(10)	117.9(7)
C(6)	N(2)	C(10)	124.8(9)	Mn(1)	N(3)	C(11)	114.5(7)
Mn(1)	N(3)	C(15)	125.3(7)	C(11)	N(3)	C(15)	120.0(8)
N(1)	C(1)	C(2)	120(1)	C(1)	C(2)	C(3)	119(1)
C(2)	C(3)	C(4)	119(1)	C(3)	C(4)	C(5)	118(1)
N(1)	C(5)	C(4)	122.0(10)	N(1)	C(5)	C(6)	114.0(9)
C(4)	C(5)	C(6)	123(1)	N(2)	C(6)	C(5)	113.4(9)
N(2)	C(6)	C(7)	116(1)	C(5)	C(6)	C(7)	130(1)
C(6)	C(7)	C(8)	120(1)	C(7)	C(8)	C(9)	120.2(10)
C(8)	C(9)	C(10)	118(1)	N(2)	C(10)	C(9)	118.9(10)
N(2)	C(10)	C(11)	112.3(9)	C(9)	C(10)	C(11)	128(1)
N(3)	C(11)	C(10)	115.6(9)	N(3)	C(11)	C(12)	120.6(9)
C(10)	C(11)	C(12)	123.8(10)	C(11)	C(12)	C(13)	118.5(10)
C(12)	C(13)	C(14)	120(1)	C(13)	C(14)	C(15)	118.4(9)
N(3)	C(15)	C(14)	121.8(9)				

Table S1.7 Bond angles(°).

atom	atom	atom	angle	atom	atom	atom	angle
N(1)	C(1)	H(1)	119.9	C(2)	C(1)	H(1)	119.9
C(1)	C(2)	H(2)	120.1	C(3)	C(2)	H(2)	120.1
C(2)	C(3)	H(3)	120.4	C(4)	C(3)	H(3)	120.4
C(3)	C(4)	H(4)	120.9	C(5)	C(4)	H(4)	120.9
C(6)	C(7)	H(5)	119.6	C(8)	C(7)	H(5)	119.6
C(7)	C(8)	H(6)	119.9	C(9)	C(8)	H(6)	119.9
C(8)	C(9)	H(7)	120.6	C(10)	C(9)	H(7)	120.6
C(11)	C(12)	H(8)	120.7	C(13)	C(12)	H(8)	120.7
C(12)	C(13)	H(9)	119.8	C(14)	C(13)	H(9)	119.8
C(13)	C(14)	H(10)	120.8	C(15)	C(14)	H(10)	120.8
N(3)	C(15)	H(11)	119.1	C(14)	C(15)	H(11)	119.1

Table S1.8 Torsion angles(°).

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
Mn(1)	Mn(1)	O(2)	S(1)	-178.6(4)	Mn(1)	Mn(1)	N(1)	C(1)	61.6(8)
Mn(1)	Mn(1)	N(1)	C(5)	-121.0(7)	Mn(1)	Mn(1)	N(2)	C(6)	88.0(8)
Mn(1)	Mn(1)	N(2)	C(10)	-86.9(7)	Mn(1)	Mn(1)	N(3)	C(11)	121.5(7)
Mn(1)	Mn(1)	N(3)	C(15)	-62.4(8)	Mn(1)	O(1)	Mn(1)	O(1)	0.0
Mn(1)	O(1)	Mn(1)	O(2)	179.6(3)	Mn(1)	O(1)	Mn(1)	N(1)	91.1(3)
Mn(1)	O(1)	Mn(1)	N(2)	1(1)	Mn(1)	O(1)	Mn(1)	N(3)	-92.0(3)
Mn(1)	O(1)	Mn(1)	O(1)	0.0	Mn(1)	O(1)	Mn(1)	O(2)	-2(2)
Mn(1)	O(1)	Mn(1)	N(1)	-101.9(3)	Mn(1)	O(1)	Mn(1)	N(2)	-179.8(3)
Mn(1)	O(1)	Mn(1)	N(3)	101.4(3)	Mn(1)	O(2)	S(1)	O(3)	76.6(6)
Mn(1)	O(2)	S(1)	O(4)	-163.3(5)	Mn(1)	O(2)	S(1)	O(5)	-44.1(7)
Mn(1)	N(1)	C(1)	C(2)	-178.7(8)	Mn(1)	N(1)	C(5)	C(4)	-179.0(8)
Mn(1)	N(1)	C(5)	C(6)	5(1)	Mn(1)	N(2)	C(6)	C(5)	-3(1)
Mn(1)	N(2)	C(6)	C(7)	175.4(8)	Mn(1)	N(2)	C(10)	C(9)	-175.5(8)
Mn(1)	N(2)	C(10)	C(11)	7(1)	Mn(1)	N(3)	C(11)	C(10)	-3(1)
Mn(1)	N(3)	C(11)	C(12)	176.7(8)	Mn(1)	N(3)	C(15)	C(14)	-178.7(8)
S(1)	O(2)	Mn(1)	O(1)	176(1)	S(1)	O(2)	Mn(1)	O(1)	178.9(6)
S(1)	O(2)	Mn(1)	N(1)	76.7(6)	S(1)	O(2)	Mn(1)	N(2)	-0.8(6)
S(1)	O(2)	Mn(1)	N(3)	-79.2(6)	O(1)	Mn(1)	Mn(1)	O(1)	180.0
O(1)	Mn(1)	Mn(1)	O(2)	-0.5(4)	O(1)	Mn(1)	Mn(1)	N(1)	-97.3(4)
O(1)	Mn(1)	Mn(1)	N(2)	-179.7(4)	O(1)	Mn(1)	Mn(1)	N(3)	96.3(4)
O(1)	Mn(1)	O(1)	Mn(1)	0.0	O(1)	Mn(1)	N(1)	C(1)	-101.0(8)
O(1)	Mn(1)	N(1)	C(5)	81.6(8)	O(1)	Mn(1)	N(2)	C(6)	-88.2(7)
O(1)	Mn(1)	N(2)	C(10)	86.8(7)	O(1)	Mn(1)	N(3)	C(11)	-81.9(7)
O(1)	Mn(1)	N(3)	C(15)	101.9(8)	O(1)	Mn(1)	Mn(1)	O(1)	180.0
O(1)	Mn(1)	Mn(1)	O(2)	-179.5(4)	O(1)	Mn(1)	Mn(1)	N(1)	-82.7(4)
O(1)	Mn(1)	Mn(1)	N(2)	-0.3(4)	O(1)	Mn(1)	Mn(1)	N(3)	83.7(4)
O(1)	Mn(1)	O(1)	Mn(1)	0.0	O(1)	Mn(1)	N(1)	C(1)	20.1(8)
O(1)	Mn(1)	N(1)	C(5)	-162.5(7)	O(1)	Mn(1)	N(2)	C(6)	87(1)
O(1)	Mn(1)	N(2)	C(10)	-87(1)	O(1)	Mn(1)	N(3)	C(11)	163.0(7)
O(1)	Mn(1)	N(3)	C(15)	-20.9(9)	O(2)	Mn(1)	Mn(1)	O(2)	180.0
O(2)	Mn(1)	Mn(1)	N(1)	83.2(4)	O(2)	Mn(1)	Mn(1)	N(2)	0.8(5)
O(2)	Mn(1)	Mn(1)	N(3)	-83.2(4)	O(2)	Mn(1)	N(1)	C(1)	71.3(8)
O(2)	Mn(1)	N(1)	C(5)	-106.1(8)	O(2)	Mn(1)	N(2)	C(6)	91.4(7)
O(2)	Mn(1)	N(2)	C(10)	-93.7(7)	O(2)	Mn(1)	N(3)	C(11)	105.7(7)

Table S1.8 Torsion angles(°) (continued).

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
O(2)	Mn(1)	N(3)	C(15)	-70.5(8)	N(1)	Mn(1)	Mn(1)	N(1)	180.0
N(1)	Mn(1)	Mn(1)	N(2)	97.6(4)	N(1)	Mn(1)	Mn(1)	N(3)	13.6(4)
N(1)	Mn(1)	N(2)	C(6)	5.3(7)	N(1)	Mn(1)	N(2)	C(10)	-179.8(8)
N(1)	Mn(1)	N(3)	C(11)	24(1)	N(1)	Mn(1)	N(3)	C(15)	-151.8(8)
N(1)	C(1)	C(2)	C(3)	-2(1)	N(1)	C(5)	C(4)	C(3)	-2(1)
N(1)	C(5)	C(6)	N(2)	-1(1)	N(1)	C(5)	C(6)	C(7)	179(1)
N(2)	Mn(1)	Mn(1)	N(2)	-180.0	N(2)	Mn(1)	Mn(1)	N(3)	96.0(4)
N(2)	Mn(1)	N(1)	C(1)	171.4(8)	N(2)	Mn(1)	N(1)	C(5)	-5.9(7)
N(2)	Mn(1)	N(3)	C(11)	5.5(7)	N(2)	Mn(1)	N(3)	C(15)	-170.6(9)
N(2)	C(6)	C(5)	C(4)	-176.4(10)	N(2)	C(6)	C(7)	C(8)	0(1)
N(2)	C(10)	C(9)	C(8)	0(1)	N(2)	C(10)	C(11)	N(3)	-2(1)
N(2)	C(10)	C(11)	C(12)	177.3(10)	N(3)	Mn(1)	Mn(1)	N(3)	180.0
N(3)	Mn(1)	N(1)	C(1)	152.5(8)	N(3)	Mn(1)	N(1)	C(5)	-24(1)
N(3)	Mn(1)	N(2)	C(6)	177.5(8)	N(3)	Mn(1)	N(2)	C(10)	-7.6(7)
N(3)	C(11)	C(10)	C(9)	-179(1)	N(3)	C(11)	C(12)	C(13)	3(1)
N(3)	C(15)	C(14)	C(13)	0(1)	C(1)	N(1)	C(5)	C(4)	3(1)
C(1)	N(1)	C(5)	C(6)	-171.9(9)	C(1)	C(2)	C(3)	C(4)	3(1)
C(2)	C(1)	N(1)	C(5)	-1(1)	C(2)	C(3)	C(4)	C(5)	-1(1)
C(3)	C(4)	C(5)	C(6)	172(1)	C(4)	C(5)	C(6)	C(7)	4(1)
C(5)	C(6)	N(2)	C(10)	-178.6(9)	C(5)	C(6)	C(7)	C(8)	179(1)
C(6)	N(2)	C(10)	C(9)	-1(1)	C(6)	N(2)	C(10)	C(11)	-177.5(9)
C(6)	C(7)	C(8)	C(9)	-2(1)	C(7)	C(6)	N(2)	C(10)	0(1)
C(7)	C(8)	C(9)	C(10)	1(1)	C(8)	C(9)	C(10)	C(11)	175.5(10)
C(9)	C(10)	C(11)	C(12)	1(1)	C(10)	C(11)	N(3)	C(15)	173.3(9)
C(10)	C(11)	C(12)	C(13)	-176(1)	C(11)	N(3)	C(15)	C(14)	5(1)
C(11)	C(12)	C(13)	C(14)	1(1)	C(12)	C(11)	N(3)	C(15)	-6(1)
C(12)	C(13)	C(14)	C(15)	-3(1)					

Table S1.9 Non-bonded contacts out to 3.60 Å.

atom	atom	distance	ADC	atom	atom	distance	ADC
O(1)	C(8)	3.07(1)	54507	O(1)	C(7)	3.49(1)	54507
O(2)	O(6)	3.480(10)	7	O(3)	C(9)	3.31(1)	6
O(3)	C(14)	3.37(1)	54506	O(3)	C(12)	3.51(1)	6
O(4)	O(7)	2.729(10)	3	O(4)	O(6)	2.85(1)	7
O(4)	C(12)	3.47(1)	6	O(5)	O(7)	2.757(9)	1
O(5)	C(3)	3.41(1)	55402	O(6)	O(7)	2.73(1)	54507
O(6)	O(8)	2.79(1)	54507	O(6)	O(8)	2.85(1)	54508
O(7)	C(13)	3.22(1)	54506	O(7)	C(3)	3.40(1)	55402
O(7)	C(14)	3.44(1)	54506	O(8)	C(1)	3.09(1)	54501
O(8)	C(7)	3.28(1)	1	O(8)	C(4)	3.34(1)	1
O(8)	O(8)	3.37(2)	55402	O(8)	C(12)	3.54(1)	54501
O(8)	C(11)	3.55(1)	54507	O(8)	C(2)	3.58(1)	54501
N(2)	C(8)	3.59(1)	54507	C(2)	C(2)	3.48(2)	55402
C(3)	C(3)	3.44(2)	55402	C(6)	C(8)	3.36(1)	54507
C(6)	C(9)	3.58(1)	54507	C(7)	C(9)	3.55(2)	54507
C(7)	C(10)	3.57(1)	54507	C(8)	C(13)	3.37(2)	54506
C(9)	C(14)	3.35(1)	54506	C(9)	C(13)	3.57(2)	54506

The ADC (atom designator code) specifies the position of an atom in a crystal. The 5-digit number shown in the table is a composite of three one-digit numbers and one two-digit number: TA (first digit) + TB (second digit) + TC (third digit) + SN (last two digits). TA, TB and TC are the crystal lattice translation digits along cell edges a, b and c. A translation digit of 5 indicates the origin unit cell. If TA = 4, this indicates a translation of one unit cell length along the a-axis in the negative direction. Each translation digit can range in value from 1 to 9 and thus ±4 lattice translations from the origin (TA=5, TB=5, TC=5) can be represented.

The SN, or symmetry operator number, refers to the number of the symmetry operator used to generate the coordinates of the target atom. A list of symmetry operators relevant to this structure are given below.

For a given intermolecular contact, the first atom (origin atom) is located in the origin unit cell and its position can be generated using the identity operator (SN=1). Thus, the ADC for an origin atom is always 55501. The position of the second atom (target atom) can be generated using the ADC and the coordinates of the atom in the parameter table. For example, an ADC of 47502 refers to the target atom moved through symmetry operator two, then translated -1 cell translations along the a axis, +2 cell translations along the b axis, and 0 cell translations along the c axis.

An ADC of 1 indicates an intermolecular contact between two fragments (eg. cation and anion) that reside in the same asymmetric unit.

Symmetry Operators:

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