

checkCIF/PLATON report

No syntax errors found. CIF dictionary Interpreting this report

Datablock: mm05

Bond precision: C-C = 0.0018 A

Wavelength=0.71073

Cell: a=5.1333(1) b=8.1443(2) c=9.7610(2)
 alpha=73.269(1) beta=76.874(1) gamma=76.209(1)
Temperature: 150 K

	Calculated	Reported
Volume	373.988(14)	373.988(14)
Space group	P -1	P-1
Hall group	-P 1	-P 1
Moiety formula	C6 H6 F6 Mn N2 O6 S2	C6 H6 F6 Mn N2 O6 S2
Sum formula	C6 H6 F6 Mn N2 O6 S2	C6 H6 F6 Mn N2 O6 S2
Mr	435.21	435.19
Dx,g cm-3	1.932	1.932
Z	1	1
Mu (mm-1)	1.257	1.257
F000	215.0	215.0
F000'	215.76	
h,k,lmax	8,12,15	7,12,15
Nref	2989	2916
Tmin,Tmax	0.578,0.839	0.553,0.849
Tmin'	0.502	

Correction method= MULTI-SCAN

Data completeness= 0.976

Theta(max)= 33.730

R(reflections)= 0.0248(2667)

wR2(reflections)= 0.0731(2916)

S = 1.109

Npar= 106

The following ALERTS were generated. Each ALERT has the format

test-name_ALERT_alert-type_alert-level.

Click on the hyperlinks for more details of the test.

Alert level A

PLAT774_ALERT_1_A Suspect X-Y Bond in CIF: MN1 -- MN1 .. 5.13 Ang.

Alert level C

PLAT029_ALERT_3_C _diffn_measured_fraction_theta_full Low 0.98

PLAT230_ALERT_2_C Hirshfeld Test Diff for S1 -- C3 .. 6.03 su

PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X) Mn1 -- N1 .. 9.29 su
PLAT741_ALERT_1_C Bond Calc 5.13330(10), Rep 5.13330 Missing su
MN1 -MN1 1.555 1.655

● **Alert level G**

PLAT154_ALERT_1_G The su's on the Cell Angles are Equal (x 10000) 100 Deg.
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) . 1.13 Ratio

1 **ALERT level A** = In general: serious problem
0 **ALERT level B** = Potentially serious problem
4 **ALERT level C** = Check and explain
2 **ALERT level G** = General alerts; check

3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
2 ALERT type 2 Indicator that the structure model may be wrong or deficient
1 ALERT type 3 Indicator that the structure quality may be low
1 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

Datablock: pjr02

Bond precision: F- C = 0.0035 A

Wavelength=0.71073

Cell: a=18.3774(6) b=6.9991(3) c=6.5928(2)
alpha=90 beta=104.072(2) gamma=90
Temperature: 150 K

	Calculated	Reported
Volume	822.55(5)	822.55(5)
Space group	C 2/m	C2/m
Hall group	-C 2y	-C 2y
Moiety formula	H12 Mn O6, 2(C F3 O3 S)	H12 Mn O6, 2(C F3 O3 S)
Sum formula	C2 H12 F6 Mn O12 S2	C2 H12 F6 Mn O12 S2
Mr	461.20	461.18
Dx,g cm-3	1.862	1.862
Z	2	2
Mu (mm-1)	1.170	1.170
F000	462.0	462.0
F000'	463.61	
h,k,lmax	28,10,10	28,10,10
Nref	1754	1736
Tmin,Tmax	0.672,0.900	0.673,0.902
Tmin'	0.642	

Correction method= MULTI-SCAN

Data completeness= 0.990

Theta(max)= 33.720

R(reflections)= 0.0306(1479) wR2(reflections)= 0.0834(1736)

S = 1.054

Npar= 74

The following ALERTS were generated. Each ALERT has the format

test-name_ALERT_alert-type_alert-level.

Click on the hyperlinks for more details of the test.

● **Alert level C**

PLAT242_ALERT_2_C	Check Low	Ueq as Compared to Neighbors for	Mn1
PLAT242_ALERT_2_C	Check Low	Ueq as Compared to Neighbors for	S1
PLAT242_ALERT_2_C	Check Low	Ueq as Compared to Neighbors for	C1
PLAT250_ALERT_2_C	Large U3/U1 Ratio for Average U(i,j) Tensor		2.21

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0 **ALERT level G** = General alerts; check

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

4 ALERT type 2 Indicator that the structure model may be wrong or deficient

0 ALERT type 3 Indicator that the structure quality may be low

0 ALERT type 4 Improvement, methodology, query or suggestion

0 ALERT type 5 Informative message, check

Datablock: pjr03

Bond precision: C-C = 0.0029 A

Wavelength=0.71073

Cell: a=10.4628(3)

b=9.2867(2)

c=14.3842(4)

alpha=90

beta=95.981(2)

gamma=90

Temperature: 150 K

	Calculated	Reported
Volume	1390.03(6)	1390.03(6)
Space group	P n	Pn
Hall group	P -2yac	P -2yac
Moiety formula	C22 H20 F6 Mn N4 O6 S2	C22 H20 F6 Mn N4 O6 S2
Sum formula	C22 H20 F6 Mn N4 O6 S2	C22 H20 F6 Mn N4 O6 S2
Mr	669.50	669.48
Dx,g cm-3	1.600	1.600
Z	2	2
Mu (mm-1)	0.710	0.710
F000	678.0	678.0
F000'	679.59	
h,k,lmax	16,14,22	16,14,22
Nref	5568[11122]	10189
Tmin,Tmax	0.888,0.912	0.827,0.914
Tmin'	0.820	

Correction method= MULTI-SCAN

Data completeness= 1.83/0.92 Theta(max)= 33.730

R(reflections)= 0.0345(8719) wR2(reflections)= 0.0761(10189)

S = 1.023 Npar= 450

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.



Alert level C

PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X) Mn1 -- N1 .. 5.19 su



Alert level G

REFLT03_ALERT_4_G Please check that the estimate of the number of Friedel pairs is correct. If it is not, please give the correct count in the `_publ_section_exptl_refinement` section of the submitted CIF.

From the CIF: `_diffrn_reflms_theta_max` 33.73

From the CIF: `_reflms_number_total` 10189

Count of symmetry unique reflns 5568

Completeness (`_total/calc`) 182.99%

TEST3: Check Friedels for noncentro structure

Estimate of Friedel pairs measured 4621

Fraction of Friedel pairs measured 0.830

Are heavy atom types Z>Si present yes

PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints 2

PLAT033_ALERT_4_G Flack x Parameter Value Deviates from Zero 0.05

PLAT128_ALERT_4_G Non-standard setting of Space-group Pc Pn

PLAT164_ALERT_4_G Nr. of Refined C-H H-Atoms in Heavy-Atom Struct. 20

0 ALERT level A = In general: serious problem

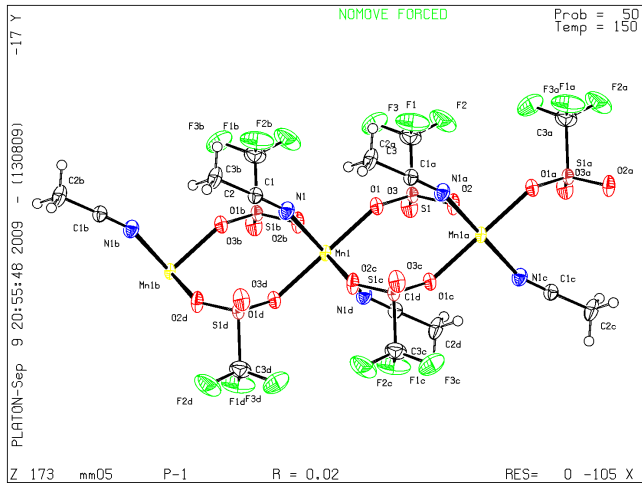
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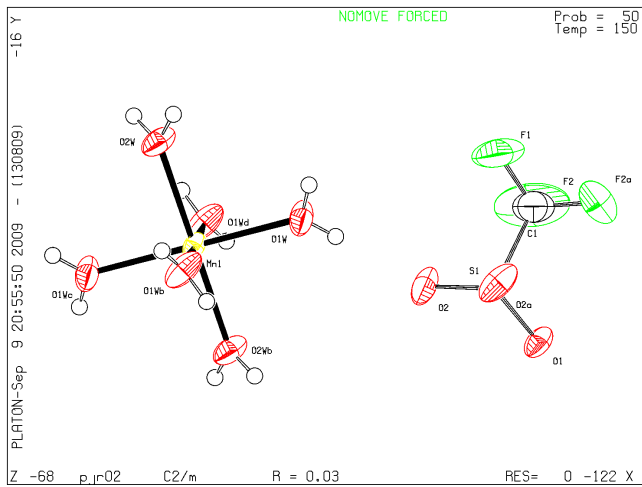
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PLATON version of 1308090: check.def file version of 13082009

Datablock mm05 - ellipsoid plot



Datablock pj02 - ellipsoid plot



Datablock pj03 - ellipsoid plot

