

checkCIF/PLATON report

No syntax errors found. CIF dictionary Interpreting this report

Datablock: sw224

Bond precision:	C-C = 0.0242 A	Wavelength=1.54178	
Cell:	a=17.7899(2)	b=25.2753(3)	c=43.8178(6)
	alpha=90	beta=90	gamma=90
Temperature:	100 K		
	Calculated	Reported	
Volume	19702.5(4)	19702.5(4)	
Space group	P 21 21 21	P 21 21 21	
Hall group	P 2ac 2ab	P 2ac 2ab	
Moiety formula	C74 H106 Cu3 Mo6 P12 S3, C23 H8 Al F36 O4, 2(C16 Al 3(C16 AL F36 O4), 2(F36 O4), 2(H8), C H2 CL2	C74 H106 Cu3 Mo6 P12 S3, 3(C7 H8), C H2 CL2	
Sum formula	C144 H132 Al3 Cl2 Cu3 F108 Mo6 O12 P12 S3	C144 H132 Al3 Cl2 Cu3 F108 Mo6 O12 P12 S3	
Mr	5492.48	5492.48	
Dx,g cm-3	1.852	1.852	
Z	4	4	
Mu (mm-1)	6.397	6.397	
F000	10816.0	10816.0	
F000'	10857.85		
h,k,lmax	21,30,52	21,29,52	
Nref	18683[34813]	33776	
Tmin,Tmax	0.157,0.322	0.212,0.445	
Tmin'	0.031		

Correction method= GAUSSIAN

Data completeness= 1.81/0.97 Theta(max)= 66.620

R(reflections)= 0.1392(29502) wR2(reflections)= 0.3389(33776)

S = 1.538 Npar= 2337

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

DIFMX01_ALERT_2_A The maximum difference density is > 0.1*ZMAX*2.00
_refine_diff_density_max given = 10.050
Test value = 8.400

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT097_ALERT_2_A Large Reported Max. (Positive) Residual Density. 10.05 eA-3

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT213_ALERT_2_A Atom F103 has ADP max/min Ratio 5.90 prola

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT220_ALERT_2_A Large Non-Solvent C Ueq(max)/Ueq(min) ... 8.44 Ratio

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT241_ALERT_2_A Check High Ueq as Compared to Neighbors for 07

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT241_ALERT_2_A Check High Ueq as Compared to Neighbors for 011

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT241_ALERT_2_A Check High Ueq as Compared to Neighbors for C135

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT241_ALERT_2_A Check High Ueq as Compared to Neighbors for C141

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT242_ALERT_2_A Check Low Ueq as Compared to Neighbors for Cu1

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT242_ALERT_2_A Check Low Ueq as Compared to Neighbors for C108

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT242_ALERT_2_A Check Low Ueq as Compared to Neighbors for A12

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT242_ALERT_2_A Check Low Ueq as Compared to Neighbors for C123

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT242_ALERT_2_A Check Low Ueq as Compared to Neighbors for C125

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT242_ALERT_2_A Check Low Ueq as Compared to Neighbors for C127

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT242_ALERT_2_A Check Low Ueq as Compared to Neighbors for C128

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT242_ALERT_2_A Check Low Ueq as Compared to Neighbors for C131

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT242_ALERT_2_A Check Low Ueq as Compared to Neighbors for C142

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT242_ALERT_2_A Check Low Ueq as Compared to Neighbors for C144

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT234_ALERT_4_A Large Hirshfeld Difference F18 -- C106 .. 0.33 Ang.

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT234_ALERT_4_A Large Hirshfeld Difference F45 -- C119 .. 0.42 Ang.

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT234_ALERT_4_A Large Hirshfeld Difference F46 -- C120 .. 0.32 Ang.

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT234_ALERT_4_A Large Hirshfeld Difference F51 -- C121 .. 0.46 Ang.

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT234_ALERT_4_A Large Hirshfeld Difference F52 -- C122 .. 0.39 Ang.

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT234_ALERT_4_A Large Hirshfeld Difference F54 -- C122 .. 0.35 Ang.

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT234_ALERT_4_A Large Hirshfeld Difference F63 -- C125 .. 0.31 Ang.

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT234_ALERT_4_A Large Hirshfeld Difference F65 -- C126 .. 0.39 Ang.

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT234_ALERT_4_A Large Hirshfeld Difference F72 -- C128 .. 0.45 Ang.

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT234_ALERT_4_A Large Hirshfeld Difference C113 -- C119 .. 0.35 Ang.

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT234_ALERT_4_A Large Hirshfeld Difference C114 -- C122 .. 0.34 Ang.

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT234_ALERT_4_A Large Hirshfeld Difference F73 -- C133 .. 0.41 Ang.

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT234_ALERT_4_A Large Hirshfeld Difference F97 -- C141 .. 0.31 Ang.

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT234_ALERT_4_A Large Hirshfeld Difference F98 -- C141 .. 0.40 Ang.

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT234_ALERT_4_A Large Hirshfeld Difference F104 -- C143 .. 0.42 Ang.

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT234_ALERT_4_A Large Hirshfeld Difference F105 -- C143 .. 0.36 Ang.

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

Alert level B

PLAT094_ALERT_2_B Ratio of Maximum / Minimum Residual Density 7.37
PLAT213_ALERT_2_B Atom C27 has ADP max/min Ratio 5.00 prola

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT213_ALERT_2_B Atom F3 has ADP max/min Ratio 4.10 prola

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT213_ALERT_2_B Atom F22 has ADP max/min Ratio 4.40 prola

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT213_ALERT_2_B Atom F26 has ADP max/min Ratio 4.20 prola

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT213_ALERT_2_B Atom F39 has ADP max/min Ratio 4.10 prola

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT213_ALERT_2_B Atom F49 has ADP max/min Ratio 4.90 prola

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT213_ALERT_2_B Atom F66 has ADP max/min Ratio 4.70 prola

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT213_ALERT_2_B Atom F67 has ADP max/min Ratio 4.60 prola

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT213_ALERT_2_B Atom F75 has ADP max/min Ratio 4.40 prola

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT213_ALERT_2_B Atom O11 has ADP max/min Ratio 4.60 prola

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT220_ALERT_2_B Large Non-Solvent C Ueq(max)/Ueq(min) ... 3.56 Ratio

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT220_ALERT_2_B Large Non-Solvent F Ueq(max)/Ueq(min) ... 4.00 Ratio

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT222_ALERT_3_B Large Non-Solvent H Ueq(max)/Ueq(min) ... 4.06 Ratio
PLAT230_ALERT_2_B Hirshfeld Test Diff for S1 -- P4 .. 8.77 su
PLAT230_ALERT_2_B Hirshfeld Test Diff for P2 -- P3 .. 25.23 su
PLAT232_ALERT_2_B Hirshfeld Test Diff (M-X) Mo1 -- P2 .. 19.40 su
PLAT232_ALERT_2_B Hirshfeld Test Diff (M-X) Mo2 -- S1 .. 10.95 su
PLAT232_ALERT_2_B Hirshfeld Test Diff (M-X) Mo6 -- P10 .. 16.01 su
PLAT232_ALERT_2_B Hirshfeld Test Diff (M-X) Cu1 -- C64 .. 11.59 su
PLAT232_ALERT_2_B Hirshfeld Test Diff (M-X) Cu3 -- P7 .. 10.04 su
PLAT232_ALERT_2_B Hirshfeld Test Diff (M-X) Cu3 -- P9 .. 15.74 su
PLAT241_ALERT_2_B Check High Ueq as Compared to Neighbors for P2

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT241_ALERT_2_B Check High Ueq as Compared to Neighbors for P4

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT241_ALERT_2_B Check High Ueq as Compared to Neighbors for O5

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT241_ALERT_2_B Check High Ueq as Compared to Neighbors for C122

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT242_ALERT_2_B Check Low Ueq as Compared to Neighbors for Cu2

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT242_ALERT_2_B Check Low Ueq as Compared to Neighbors for C24

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT242_ALERT_2_B Check Low Ueq as Compared to Neighbors for C99

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT242_ALERT_2_B Check Low Ueq as Compared to Neighbors for C101

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT242_ALERT_2_B Check Low Ueq as Compared to Neighbors for C109

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT242_ALERT_2_B Check Low Ueq as Compared to Neighbors for C111

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT242_ALERT_2_B Check Low Ueq as Compared to Neighbors for C115

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT242_ALERT_2_B Check Low Ueq as Compared to Neighbors for C116

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT242_ALERT_2_B Check Low Ueq as Compared to Neighbors for C117

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT242_ALERT_2_B Check Low Ueq as Compared to Neighbors for C124

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT242_ALERT_2_B Check Low Ueq as Compared to Neighbors for A13

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT242_ALERT_2_B Check Low Ueq as Compared to Neighbors for C129

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT242_ALERT_2_B Check Low Ueq as Compared to Neighbors for C136

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT342_ALERT_3_B	Low Bond Precision on C-C Bonds (x 1000)	Ang	...	24
PLAT362_ALERT_2_B	Short C(sp3)-C(sp2) Bond	C1	- C6	... 1.29 Ang.
PLAT412_ALERT_2_B	Short Intra XH3 .. XHn	H8A	.. H9C	.. 1.76 Ang.
PLAT234_ALERT_4_B	Large Hirshfeld Difference	F14	-- C105	.. 0.27 Ang.

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT234_ALERT_4_B	Large Hirshfeld Difference	F20	-- C107	.. 0.28 Ang.
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Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT234_ALERT_4_B	Large Hirshfeld Difference	C97	-- C102	.. 0.25 Ang.
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Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT234_ALERT_4_B Large Hirshfeld Difference F44 -- C119 .. 0.25 Ang.

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT234_ALERT_4_B Large Hirshfeld Difference F47 -- C120 .. 0.30 Ang.

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT234_ALERT_4_B Large Hirshfeld Difference F60 -- C124 .. 0.26 Ang.

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT234_ALERT_4_B Large Hirshfeld Difference F64 -- C126 .. 0.27 Ang.

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT234_ALERT_4_B Large Hirshfeld Difference C116 -- C126 .. 0.29 Ang.

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

● **Alert level C**

DIFMX02_ALERT_1_C The maximum difference density is > 0.1*ZMAX*0.75
The relevant atom site should be identified.

RFACG01_ALERT_3_C The value of the R factor is > 0.10
R factor given 0.139

RFACR01_ALERT_3_C The value of the weighted R factor is > 0.25
Weighted R factor given 0.339

STRVA01_ALERT_4_C Flack test results are ambiguous.
From the CIF: _refine_ls_abs_structure_Flack 0.500
From the CIF: _refine_ls_abs_structure_Flack_su 0.015

PLAT082_ALERT_2_C High R1 Value 0.14
PLAT084_ALERT_2_C High R2 Value 0.34
PLAT213_ALERT_2_C Atom Cu3 has ADP max/min Ratio 3.10 prola

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT213_ALERT_2_C Atom C1 has ADP max/min Ratio 3.30 prola

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT213_ALERT_2_C Atom C7 has ADP max/min Ratio 3.10 prola

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT213_ALERT_2_C Atom C8 has ADP max/min Ratio 3.30 prola

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT213_ALERT_2_C Atom C18 has ADP max/min Ratio 3.70 prola

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT213_ALERT_2_C Atom C26 has ADP max/min Ratio 3.50 prola

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT213_ALERT_2_C Atom C29 has ADP max/min Ratio 4.00 prola

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT213_ALERT_2_C Atom C37 has ADP max/min Ratio 3.30 prola

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT213_ALERT_2_C Atom C39 has ADP max/min Ratio 3.10 prola

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT213_ALERT_2_C Atom C40 has ADP max/min Ratio 3.40 prola

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT213_ALERT_2_C Atom C42 has ADP max/min Ratio 3.50 prola

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT213_ALERT_2_C Atom C44 has ADP max/min Ratio 3.10 prola

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT213_ALERT_2_C Atom F15 has ADP max/min Ratio 3.20 prola

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT213_ALERT_2_C Atom C98 has ADP max/min Ratio 3.50 prola

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT213_ALERT_2_C Atom F43 has ADP max/min Ratio 3.40 prola

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT213_ALERT_2_C Atom F50 has ADP max/min Ratio 3.20 prola

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT213_ALERT_2_C Atom F56 has ADP max/min Ratio 3.40 prola

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT213_ALERT_2_C Atom F61 has ADP max/min Ratio 3.10 prola

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT213_ALERT_2_C Atom F64 has ADP max/min Ratio 3.50 prola

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT213_ALERT_2_C Atom F71 has ADP max/min Ratio 3.50 prola

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT213_ALERT_2_C Atom O7 has ADP max/min Ratio 3.10 prola

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT213_ALERT_2_C Atom C122 has ADP max/min Ratio 3.10 prola

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT213_ALERT_2_C Atom F76 has ADP max/min Ratio 3.30 prola

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT213_ALERT_2_C Atom F106 has ADP max/min Ratio 3.20 oblat

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT213_ALERT_2_C Atom F107 has ADP max/min Ratio 3.20 prola

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT213_ALERT_2_C Atom C132 has ADP max/min Ratio 3.30 prola

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT213_ALERT_2_C Atom C141 has ADP max/min Ratio 3.10 prola

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT213_ALERT_2_C Atom C143 has ADP max/min Ratio 3.60 prola

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT220_ALERT_2_C Large Non-Solvent P Ueq(max)/Ueq(min) ... 3.10 Ratio

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT220_ALERT_2_C Large Non-Solvent C Ueq(max)/Ueq(min) ... 3.04 Ratio

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT220_ALERT_2_C Large Non-Solvent F Ueq(max)/Ueq(min) ... 3.32 Ratio

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT220_ALERT_2_C Large Non-Solvent C Ueq(max)/Ueq(min) ... 3.39 Ratio

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT220_ALERT_2_C Large Non-Solvent F Ueq(max)/Ueq(min) ... 3.30 Ratio

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT230_ALERT_2_C	Hirshfeld Test Diff for	C14	--	C15	..	5.65	su
PLAT230_ALERT_2_C	Hirshfeld Test Diff for	F80	--	C135	..	5.69	su
PLAT230_ALERT_2_C	Hirshfeld Test Diff for	C132	--	C142	..	6.63	su
PLAT232_ALERT_2_C	Hirshfeld Test Diff (M-X)	Mo1	--	S1	..	6.53	su
PLAT232_ALERT_2_C	Hirshfeld Test Diff (M-X)	Mo2	--	P2	..	6.06	su
PLAT232_ALERT_2_C	Hirshfeld Test Diff (M-X)	Cu1	--	P1	..	6.77	su
PLAT232_ALERT_2_C	Hirshfeld Test Diff (M-X)	Cu1	--	C65	..	7.81	su
PLAT232_ALERT_2_C	Hirshfeld Test Diff (M-X)	Cu2	--	P3	..	8.33	su
PLAT232_ALERT_2_C	Hirshfeld Test Diff (M-X)	Cu2	--	C71	..	5.79	su
PLAT241_ALERT_2_C	Check High	Ueq as Compared to Neighbors for				P7	

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT241_ALERT_2_C Check High Ueq as Compared to Neighbors for P8

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT241_ALERT_2_C Check High Ueq as Compared to Neighbors for C1

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT241_ALERT_2_C Check High Ueq as Compared to Neighbors for C52

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT241_ALERT_2_C Check High Ueq as Compared to Neighbors for C64

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT241_ALERT_2_C Check High Ueq as Compared to Neighbors for C65

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT241_ALERT_2_C Check High Ueq as Compared to Neighbors for C70

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT241_ALERT_2_C Check High Ueq as Compared to Neighbors for C71

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT241_ALERT_2_C Check High Ueq as Compared to Neighbors for O8

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for Mo2

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for Mo3

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for P1

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for C2

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for C5

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for C12

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for C13

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for C15

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for C22

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for C25

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for C32

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for C34

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for C35

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for C53

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for A11

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for C97

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for C98

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for C104

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for 06

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for C113

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for C118

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for C119

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for C120

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for C126

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for 012

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for C133

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for C134

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for C137

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for C138

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for C140

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT250_ALERT_2_C	Large U3/U1 Ratio for Average U(i,j) Tensor	3.94
PLAT250_ALERT_2_C	Large U3/U1 Ratio for Average U(i,j) Tensor	3.66
PLAT362_ALERT_2_C	Short C(sp3)-C(sp2) Bond	C11 - C16 ...	1.41 Ang.
PLAT362_ALERT_2_C	Short C(sp3)-C(sp2) Bond	C32 - C37 ...	1.40 Ang.
PLAT362_ALERT_2_C	Short C(sp3)-C(sp2) Bond	C34 - C39 ...	1.41 Ang.
PLAT363_ALERT_2_C	Long C(sp3)-C(sp2) Bond	C2 - C7 ...	1.66 Ang.
PLAT366_ALERT_2_C	Short? C(sp?)-C(sp?) Bond	C64 - C65 ...	1.39 Ang.
PLAT366_ALERT_2_C	Short? C(sp?)-C(sp?) Bond	C65 - C66 ...	1.39 Ang.
PLAT369_ALERT_2_C	Long C(sp2)-C(sp2) Bond	C41 - C42 ...	1.53 Ang.
PLAT413_ALERT_2_C	Short Inter XH3 .. XHn	H27B .. H88A ..	2.10 Ang.
PLAT420_ALERT_2_C	D-H Without Acceptor	F26 - H26 ...	?
PLAT601_ALERT_2_C	Structure Contains Solvent Accessible VOIDS of	.	100.00 A**3
PLAT033_ALERT_4_C	Flack x Parameter Value Deviates from Zero	0.50
PLAT042_ALERT_1_C	Calc. and Reported MoietyFormula Strings Differ		?
PLAT234_ALERT_4_C	Large Hirshfeld Difference Mo1	-- C4 ..	0.16 Ang.

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT234_ALERT_4_C Large Hirshfeld Difference Mo3 -- C22 .. 0.17 Ang.

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT234_ALERT_4_C Large Hirshfeld Difference Mo3 -- C23 .. 0.21 Ang.

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT234_ALERT_4_C Large Hirshfeld Difference Mo3 -- C24 .. 0.18 Ang.

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT234_ALERT_4_C Large Hirshfeld Difference Mo4 -- C33 .. 0.16 Ang.

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT234_ALERT_4_C Large Hirshfeld Difference Mo4 -- C34 .. 0.19 Ang.

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT234_ALERT_4_C Large Hirshfeld Difference Cu2 -- C70 .. 0.17 Ang.

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT234_ALERT_4_C Large Hirshfeld Difference C1 -- C5 .. 0.23 Ang.

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT234_ALERT_4_C Large Hirshfeld Difference C3 -- C4 .. 0.22 Ang.

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT234_ALERT_4_C Large Hirshfeld Difference C4 -- C5 .. 0.24 Ang.

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT234_ALERT_4_C Large Hirshfeld Difference C11 -- C16 .. 0.23 Ang.

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT234_ALERT_4_C Large Hirshfeld Difference C13 -- C14 .. 0.19 Ang.

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT234_ALERT_4_C Large Hirshfeld Difference C14 -- C19 .. 0.19 Ang.

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT234_ALERT_4_C Large Hirshfeld Difference C32 -- C33 .. 0.17 Ang.

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT234_ALERT_4_C Large Hirshfeld Difference C41 -- C42 .. 0.17 Ang.

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT234_ALERT_4_C Large Hirshfeld Difference C41 -- C45 .. 0.20 Ang.

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT234_ALERT_4_C Large Hirshfeld Difference C43 -- C44 .. 0.17 Ang.

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT234_ALERT_4_C Large Hirshfeld Difference C43 -- C48 .. 0.22 Ang.

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT234_ALERT_4_C Large Hirshfeld Difference C45 -- C50 .. 0.24 Ang.

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT234_ALERT_4_C Large Hirshfeld Difference C52 -- C53 .. 0.22 Ang.

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT234_ALERT_4_C Large Hirshfeld Difference C53 -- C54 .. 0.19 Ang.

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT234_ALERT_4_C Large Hirshfeld Difference F2 -- C101 .. 0.22 Ang.

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT234_ALERT_4_C Large Hirshfeld Difference F13 -- C105 .. 0.22 Ang.

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT234_ALERT_4_C Large Hirshfeld Difference F19 -- C107 .. 0.19 Ang.

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT234_ALERT_4_C Large Hirshfeld Difference F23 -- C108 .. 0.24 Ang.

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT234_ALERT_4_C Large Hirshfeld Difference F25 -- C109 .. 0.24 Ang.

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT234_ALERT_4_C Large Hirshfeld Difference F27 -- C109 .. 0.24 Ang.

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT234_ALERT_4_C Large Hirshfeld Difference F34 -- C112 .. 0.18 Ang.

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT234_ALERT_4_C Large Hirshfeld Difference F36 -- C112 .. 0.17 Ang.

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT234_ALERT_4_C Large Hirshfeld Difference C97 -- C101 .. 0.22 Ang.

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT234_ALERT_4_C Large Hirshfeld Difference C97 -- C103 .. 0.20 Ang.

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT234_ALERT_4_C Large Hirshfeld Difference C98 -- C105 .. 0.22 Ang.

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT234_ALERT_4_C Large Hirshfeld Difference C100 -- C112 .. 0.18 Ang.

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT234_ALERT_4_C Large Hirshfeld Difference F38 -- C117 .. 0.20 Ang.

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT234_ALERT_4_C Large Hirshfeld Difference F40 -- C118 .. 0.20 Ang.

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT234_ALERT_4_C Large Hirshfeld Difference F41 -- C118 .. 0.18 Ang.

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT234_ALERT_4_C Large Hirshfeld Difference F42 -- C118 .. 0.22 Ang.

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT234_ALERT_4_C Large Hirshfeld Difference F58 -- C124 .. 0.24 Ang.

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT234_ALERT_4_C Large Hirshfeld Difference F70 -- C128 .. 0.20 Ang.

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT234_ALERT_4_C Large Hirshfeld Difference O6 -- C114 .. 0.21 Ang.

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT234_ALERT_4_C Large Hirshfeld Difference F84 -- C136 .. 0.17 Ang.

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT234_ALERT_4_C Large Hirshfeld Difference F86 -- C137 .. 0.19 Ang.

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT234_ALERT_4_C Large Hirshfeld Difference F88 -- C138 .. 0.21 Ang.

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT234_ALERT_4_C Large Hirshfeld Difference O10 -- C130 .. 0.15 Ang.

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT234_ALERT_4_C Large Hirshfeld Difference C131 -- C139 .. 0.20 Ang.

Author Response: See "_publ_section_exptl_refinement" section of the CIF file!

PLAT243_ALERT_4_C High 'Solvent' Ueq as Compared to Neighbours of C96
PLAT380_ALERT_4_C Check Incorrectly? Oriented X(sp2)-Methyl Moiety C10
PLAT380_ALERT_4_C Check Incorrectly? Oriented X(sp2)-Methyl Moiety C26
PLAT380_ALERT_4_C Check Incorrectly? Oriented X(sp2)-Methyl Moiety C27
PLAT380_ALERT_4_C Check Incorrectly? Oriented X(sp2)-Methyl Moiety C28
PLAT380_ALERT_4_C Check Incorrectly? Oriented X(sp2)-Methyl Moiety C29
PLAT380_ALERT_4_C Check Incorrectly? Oriented X(sp2)-Methyl Moiety C30
PLAT380_ALERT_4_C Check Incorrectly? Oriented X(sp2)-Methyl Moiety C48
PLAT380_ALERT_4_C Check Incorrectly? Oriented X(sp2)-Methyl Moiety C81
PLAT775_ALERT_1_C Suspect X-Y Cont in CIF: MO1 -- CU1 .. 4.30 Ang.
PLAT775_ALERT_1_C Suspect X-Y Cont in CIF: MO1 -- CU2 .. 4.25 Ang.
PLAT775_ALERT_1_C Suspect X-Y Cont in CIF: MO2 -- CU2 .. 4.60 Ang.
PLAT775_ALERT_1_C Suspect X-Y Cont in CIF: MO2 -- CU1 .. 4.62 Ang.
PLAT775_ALERT_1_C Suspect X-Y Cont in CIF: MO3 -- CU3 .. 4.51 Ang.
PLAT775_ALERT_1_C Suspect X-Y Cont in CIF: MO3 -- CU2 .. 4.60 Ang.
PLAT775_ALERT_1_C Suspect X-Y Cont in CIF: MO4 -- CU3 .. 4.43 Ang.
PLAT775_ALERT_1_C Suspect X-Y Cont in CIF: MO4 -- CU2 .. 4.47 Ang.
PLAT775_ALERT_1_C Suspect X-Y Cont in CIF: MO5 -- CU1 .. 4.42 Ang.
PLAT775_ALERT_1_C Suspect X-Y Cont in CIF: MO5 -- CU3 .. 4.43 Ang.
PLAT775_ALERT_1_C Suspect X-Y Cont in CIF: MO6 -- CU3 .. 4.48 Ang.
PLAT775_ALERT_1_C Suspect X-Y Cont in CIF: MO6 -- CU1 .. 4.62 Ang.
PLAT775_ALERT_1_C Suspect X-Y Cont in CIF: CU1 -- C10 .. 4.13 Ang.
PLAT775_ALERT_1_C Suspect X-Y Cont in CIF: CU1 -- C48 .. 4.18 Ang.
PLAT775_ALERT_1_C Suspect X-Y Cont in CIF: CU1 -- C49 .. 4.02 Ang.
PLAT775_ALERT_1_C Suspect X-Y Cont in CIF: CU2 -- P4 .. 4.25 Ang.
PLAT775_ALERT_1_C Suspect X-Y Cont in CIF: CU2 -- C8 .. 4.03 Ang.
PLAT775_ALERT_1_C Suspect X-Y Cont in CIF: CU2 -- C26 .. 4.20 Ang.
PLAT775_ALERT_1_C Suspect X-Y Cont in CIF: CU3 -- C96 .. 4.02 Ang.
PLAT775_ALERT_1_C Suspect X-Y Cont in CIF: CU3 -- C37 .. 4.06 Ang.

PLAT775_ALERT_1_C	Suspect X-Y Cont in CIF:	CU3	--	CL2	..	4.26	Ang.
PLAT775_ALERT_1_C	Suspect X-Y Cont in CIF:	CL2	--	CU3	..	4.26	Ang.
PLAT775_ALERT_1_C	Suspect X-Y Cont in CIF:	P2	--	CU2	..	4.20	Ang.
PLAT775_ALERT_1_C	Suspect X-Y Cont in CIF:	P4	--	CU2	..	4.25	Ang.
PLAT775_ALERT_1_C	Suspect X-Y Cont in CIF:	C8	--	CU2	..	4.03	Ang.
PLAT775_ALERT_1_C	Suspect X-Y Cont in CIF:	C10	--	CU1	..	4.13	Ang.
PLAT775_ALERT_1_C	Suspect X-Y Cont in CIF:	C26	--	CU2	..	4.20	Ang.
PLAT775_ALERT_1_C	Suspect X-Y Cont in CIF:	C37	--	CU3	..	4.06	Ang.
PLAT775_ALERT_1_C	Suspect X-Y Cont in CIF:	C48	--	CU1	..	4.18	Ang.
PLAT775_ALERT_1_C	Suspect X-Y Cont in CIF:	C49	--	CU1	..	4.02	Ang.
PLAT775_ALERT_1_C	Suspect X-Y Cont in CIF:	C96	--	CU3	..	4.02	Ang.

● 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: <code>_diffrn_reflms_theta_max</code>	66.62
From the CIF: <code>_reflms_number_total</code>	33776
Count of symmetry unique reflms	18683
Completeness (<code>_total/calc</code>)	180.78%
TEST3: Check Friedels for noncentro structure	
Estimate of Friedel pairs measured	15093
Fraction of Friedel pairs measured	0.808
Are heavy atom types Z>Si present	yes

PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints 1019

PLAT328_ALERT_4_G Check for Possibly Missing H on sp3? Phosphorus. P4

PLAT328_ALERT_4_G Check for Possibly Missing H on sp3? Phosphorus. P8

PLAT328_ALERT_4_G Check for Possibly Missing H on sp3? Phosphorus. P12

34 **ALERT level A** = In general: serious problem
 50 **ALERT level B** = Potentially serious problem
 186 **ALERT level C** = Check and explain
 5 **ALERT level G** = General alerts; check

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

Publication of your CIF in IUCr journals

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 19/05/2009; check.def file version of 13/05/2009

Datablock sw224 - ellipsoid plot

