

# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) compound\_2, compound\_4

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found.      CIF dictionary      Interpreting this report

## Datablock: compound\_2

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Bond precision:    C-C = 0.0024 Å

Wavelength=0.71075

Cell:                a=10.337(6)                b=10.816(6)                c=12.119(7)  
                      alpha=72.216(16)        beta=84.13(2)        gamma=69.554(17)  
Temperature:        93 K

	Calculated	Reported
Volume	1208.9(12)	1209.0(12)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	2(C30 H24 O2), C3 H6 O	C30 H24 O2, 0.5(C3 H6 O)
Sum formula	C63 H54 O5	C31.5 H27 O2.5
Mr	891.06	445.56
Dx,g cm-3	1.224	1.224
Z	1	2
Mu (mm-1)	0.076	0.076
F000	472.0	472.0
F000'	472.20	
h,k,lmax	13,14,15	13,14,15
Nref	5584	5322
Tmin,Tmax	0.985,0.985	0.853,0.985
Tmin'	0.985	

Correction method= # Reported T Limits: Tmin=0.853 Tmax=0.985  
AbsCorr = MULTI-SCAN

Data completeness= 0.953

Theta(max)= 27.531

R(reflections)= 0.0510( 4401)

wR2(reflections)= 0.1477( 5322)

S = 0.980

Npar= 329

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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

PLAT029_ALERT_3_C	_diffn_measured_fraction_theta_full value Low .	0.975	Note
PLAT041_ALERT_1_C	Calc. and Reported SumFormula Strings Differ		Please Check
PLAT906_ALERT_3_C	Large K value in the Analysis of Variance .....	6.211	Check
PLAT910_ALERT_3_C	Missing # of FCF Reflection(s) Below Theta(Min).	8	Note
PLAT911_ALERT_3_C	Missing # FCF Refl Between THmin & STh/L= 0.600	103	Report
PLAT934_ALERT_3_C	Number of (Iobs-Icalc)/SigmaW > 10 Outliers ....	1	Check



### Alert level G

PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms .....	4	Report
PLAT042_ALERT_1_G	Calc. and Reported MoietyFormula Strings Differ		Please Check
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...	0.50	Check
PLAT093_ALERT_1_G	No s.u.'s on H-positions, Refinement Reported as		mixed Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H1 is Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H2 is Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H31 is Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H32 is Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of O3 is Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C31 is Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C32 is Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C33 is Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H25 is Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H26 is Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H27 is Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H28 is Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H29 is Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H30 is Constrained at	0.5	Check
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2)..	100%	Note
PLAT789_ALERT_4_G	Atoms with Negative _atom_site_disorder_group #	10	Check
PLAT793_ALERT_4_G	The Model has Chirality at C1 (Centro SPGR)		S Verify
PLAT882_ALERT_1_G	Missing datum for _diffn_reflns_av_unetI/netI .		Please Check
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	152	Note
PLAT961_ALERT_5_G	Dataset Contains no Negative Intensities .....		Please Check
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	12	Info

- 0 **ALERT level A** = Most likely a serious problem - resolve or explain  
0 **ALERT level B** = A potentially serious problem, consider carefully  
6 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
25 **ALERT level G** = General information/check it is not something unexpected
- 5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
1 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  
18 ALERT type 4 Improvement, methodology, query or suggestion  
2 ALERT type 5 Informative message, check

## Datablock: compound\_4

Bond precision: C-C = 0.0027 A

Wavelength=0.71075

Cell: a=17.089(4) b=12.512(3) c=20.001(4)  
alpha=90 beta=107.378(2) gamma=90  
Temperature: 123 K

	Calculated	Reported
Volume	4081.4(16)	4081.5(15)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C55 H50 O3 Ru	C55 H50 O3 Ru
Sum formula	C55 H50 O3 Ru	C55 H50 O3 Ru
Mr	860.02	860.07
Dx,g cm-3	1.400	1.400
Z	4	4
Mu (mm-1)	0.431	0.431
F000	1792.0	1792.0
F000'	1787.61	
h,k,lmax	22,16,25	22,16,25
Nref	9363	9326
Tmin,Tmax	0.917,0.917	0.764,0.917
Tmin'	0.917	

Correction method= # Reported T Limits: Tmin=0.764 Tmax=0.917  
AbsCorr = MULTI-SCAN

Data completeness= 0.996                      Theta(max)= 27.494

R(reflections)= 0.0332( 8496)              wR2(reflections)= 0.0795( 9326)

S = 1.359                                      Npar= 539

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**test-name\_ALERT\_alert-type\_alert-level.**

Click on the hyperlinks for more details of the test.



#### Alert level B

PLAT420_ALERT_2_B D-H Without Acceptor	O2	-- H1	...	Please Check
PLAT420_ALERT_2_B D-H Without Acceptor	O3	-- H2	...	Please Check
PLAT910_ALERT_3_B Missing # of FCF Reflection(s) Below Theta(Min).				14 Note
PLAT934_ALERT_3_B Number of (Iobs-Icalc)/SigmaW > 10 Outliers ....				2 Check



#### Alert level C

PLAT220_ALERT_2_C Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range	3.2	Ratio
PLAT222_ALERT_3_C Non-Solvent Resd 1 H Uiso(max)/Uiso(min) Range	4.1	Ratio
PLAT906_ALERT_3_C Large K value in the Analysis of Variance .....	4.491	Check
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L= 0.600	13	Report



#### Alert level G

PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms .....	2	Report
PLAT793_ALERT_4_G The Model has Chirality at C16 (Centro SPGR)	S	Verify
PLAT793_ALERT_4_G The Model has Chirality at C17 (Centro SPGR)	R	Verify
PLAT882_ALERT_1_G Missing datum for _diffn_reflms_av_unetI/netI .	Please	Check
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600	11	Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....	2	Note
PLAT961_ALERT_5_G Dataset Contains no Negative Intensities .....	Please	Check

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### Publication of your CIF

You should attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the nature of your study may justify the reported deviations from journal submission requirements and the more serious of these should be commented upon in the discussion or experimental section of a paper or in the "special\_details" fields of the CIF. *checkCIF* was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

If you wish to submit your CIF for publication in Acta Crystallographica Section C or E, you should upload your CIF via the web. If you wish to submit your CIF for publication in IUCrData you should upload your CIF via the web. If your CIF is to form part of a submission to another IUCr journal, you will be asked, either during electronic submission or by the Co-editor handling your paper, to upload your CIF via our web site.



