

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) ThRe, ThRu

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: ThRe

Bond precision:	C-C = 0.0084 Å	Wavelength=1.54184
Cell:	a=26.6348(2)	b=15.8017(1) c=20.0442(1)
	alpha=90	beta=108.307(1) gamma=90
Temperature:	150 K	
	Calculated	Reported
Volume	8009.13(10)	8009.13(10)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C34 H67 N4 Re Si3 Th	C34 H67 N4 Re Si3 Th
Sum formula	C34 H67 N4 Re Si3 Th	C34 H67 N4 Re Si3 Th
Mr	1034.44	1034.42
Dx,g cm-3	1.716	1.716
Z	8	8
Mu (mm-1)	18.769	18.769
F000	4048.0	4048.0
F000'	3987.15	
h,k,lmax	33,19,25	33,19,25
Nref	16953	16480
Tmin,Tmax	0.119,0.236	0.758,1.000
Tmin'	0.032	
Correction method= # Reported T Limits: Tmin=0.758 Tmax=1.000		
AbsCorr = GAUSSIAN		
Data completeness=	0.972	Theta(max)= 77.107
R(reflections)=	0.0307(15534)	wR2(reflections)= 0.0791(16480)
S =	1.058	Npar= 805

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**

PLAT971_ALERT_2_A Check Calcd Resid. Dens. 1.16A From Th2 4.40 eA-3

Author Response: Residual density is close to thorium and is present despite applying the correct absorption correction. It is of no chemical significance.

 **Alert level B**

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 1.16A From N3 3.32 eA-3

Author Response: Residual density is close to thorium and is present despite applying the correct absorption correction. It is of no chemical significance.

 **Alert level C**

PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density 2.52 Report
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C15 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of Si6 Check
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds 0.00836 Ang.
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 54 Report
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.94A From C15 2.40 eA-3

Author Response: Residual density is close to thorium and is present despite applying the correct absorption correction. It is of no chemical significance.

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.79A From Re1 1.58 eA-3

Author Response: Residual density is close to thorium and is present despite applying the correct absorption correction. It is of no chemical significance.

PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.86A From Th2 -1.94 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.78A From Th1 -1.74 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.71A From Th2 -1.65 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.70A From Re2 -1.53 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.77A From Th1 -1.52 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.66A From Re2 -1.51 eA-3

 **Alert level G**

PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 26.35 Why ?
PLAT142_ALERT_4_G s.u. on b - Axis Small or Missing 0.00010 Ang.
PLAT143_ALERT_4_G s.u. on c - Axis Small or Missing 0.00010 Ang.
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 419 Note

PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF	1 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity	3.3 Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.	0 Info

1 **ALERT level A** = Most likely a serious problem - resolve or explain
1 **ALERT level B** = A potentially serious problem, consider carefully
13 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
7 **ALERT level G** = General information/check it is not something unexpected

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

Datablock: ThRu

Bond precision: C-C = 0.0064 A Wavelength=0.71073

Cell: a=22.1371(8) b=23.1349(7) c=19.0421(7)
alpha=90 beta=114.222(4) gamma=90
Temperature: 150 K

	Calculated	Reported
Volume	8893.7(6)	8893.7(6)
Space group	C 2/c	C 1 2/c 1
Hall group	-C 2yc	-C 2yc
Moiety formula	C31 H62 N4 O2 Ru Si3 Th, C6 H6	C31 H62 N4 O2 Ru Si3 Th, (C6 H6)
Sum formula	C37 H68 N4 O2 Ru Si3 Th	C37 H68 N4 O2 Ru Si3 Th
Mr	1018.33	1018.33
Dx,g cm-3	1.521	1.521
Z	8	8
Mu (mm-1)	3.794	3.794
F000	4080.0	4080.0
F000'	4015.35	
h,k,lmax	30,32,26	30,31,26
Nref	12642	11275
Tmin,Tmax	0.623,0.773	0.897,0.976
Tmin'	0.181	

Correction method= # Reported T Limits: Tmin=0.897 Tmax=0.976
AbsCorr = GAUSSIAN

Data completeness= 0.892 Theta(max)= 29.699

R(reflections)= 0.0347(8861) wR2(reflections)= 0.0636(11275)

S = 1.049

Npar= 479

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 B

PLAT910_ALERT_3_B Missing # of FCF Reflection(s) Below Theta(Min). 21 Note

Author Response: Missing reflections at low angle are most likely due to obfuscation by the beamstop.

Alert level C

PLAT220_ALERT_2_C	NonSolvent	Resd 1	C	Ueq(max)/Ueq(min)	Range	3.8	Ratio
PLAT222_ALERT_3_C	NonSolvent	Resd 1	H	Uiso(max)/Uiso(min)	Range	4.8	Ratio
PLAT242_ALERT_2_C	Low	'MainMol'		Ueq as Compared to Neighbors of		C15	Check
PLAT331_ALERT_2_C	Small Aver	Phenyl	C-C	Dist C35	--C35_b	1.37	Ang.
PLAT911_ALERT_3_C	Missing FCF	Refl	Between	Thmin & STh/L=	0.600	4	Report
PLAT973_ALERT_2_C	Check Calcd	Positive	Resid.	Density on	Th1	1.25	eA-3
PLAT975_ALERT_2_C	Check Calcd	Resid.	Dens.	0.66A	From N4	0.58	eA-3

Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle	Restraints on AtSite				15	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij	Restrained non-H Atoms ...				13	Report
PLAT042_ALERT_1_G	Calc. and Reported	Moiety Formula Strings Differ					Please Check
PLAT083_ALERT_2_G	SHELXL Second	Parameter in WGHT	Unusually Large			8.06	Why ?
PLAT176_ALERT_4_G	The CIF-Embedded .res	File Contains SADI	Records			2	Report
PLAT178_ALERT_4_G	The CIF-Embedded .res	File Contains SIMU	Records			2	Report
PLAT187_ALERT_4_G	The CIF-Embedded .res	File Contains RIGU	Records			2	Report
PLAT301_ALERT_3_G	Main Residue	Disorder(Resd 1)			7%	Note
PLAT412_ALERT_2_G	Short Intra	XH3 .. XHn	H6A	..H24C	.	2.11	Ang.
				x,y,z =	1_555		Check
PLAT412_ALERT_2_G	Short Intra	XH3 .. XHn	H20B	..H23F	.	2.13	Ang.
				x,y,z =	1_555		Check
PLAT432_ALERT_2_G	Short Inter	X...Y Contact	C27	..C27		3.16	Ang.
				1-x,1-y,1-z =	5_666		Check
PLAT802_ALERT_4_G	CIF Input	Record(s) with more than 80	Characters			3	Info
PLAT860_ALERT_3_G	Number of Least-Squares	Restraints			213	Note
PLAT912_ALERT_4_G	Missing # of FCF	Reflections Above STh/L=	0.600			1332	Note
PLAT913_ALERT_3_G	Missing # of Very Strong	Reflections in FCF			2	Note
PLAT933_ALERT_2_G	Number of OMIT	Records in Embedded .res	File ...			4	Note
PLAT941_ALERT_3_G	Average HKL	Measurement Multiplicity			4.8	Low
PLAT978_ALERT_2_G	Number C-C	Bonds with Positive	Residual Density.			0	Info

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It is advisable to 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 purpose of your study may justify the reported deviations and the more serious of these should normally 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.

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* or *IUCrData*, 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 22/03/2021; check.def file version of 19/03/2021



