checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: 2

```
Bond precision:  C-C = 0.0040 A          Wavelength=0.71073

Cell:            a=8.6148(2)    b=31.8694(4)        c=14.8246(3)
                 alpha=90       beta=93.7902(5)     gamma=90
Temperature:     150 K
```

	Calculated	Reported
Volume	4061.17(14)	4061.17(14)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	?
Moiety formula	C26 H24 N2 Th	?
Sum formula	C26 H24 N2 Th	C26 H24 N2 Th
Mr	596.51	596.51
Dx,g cm-3	1.951	1.951
Z	8	8
Mu (mm-1)	7.358	7.358
F000	2272.0	2272.0
F000’	2215.54	
h,k,lmax	12,45,21	12,45,21
Nref	12411	12383
Tmin,Tmax	0.298,0.516	0.371,0.516
Tmin’	0.275	

```
Correction method= MULTI-SCAN

Data completeness= 0.998          Theta(max)= 30.510

R(reflections)= 0.0248( 10609)    wR2(reflections)= 0.0547( 12383)

S = 0.988                 Npar= 523
```

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

```
PLAT048_ALERT_1_C MoietyFormula Not Given .....................        ?
PLAT125_ALERT_4_C No ’_symmetry_space_group_name_Hall’ Given .....     ?
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for      Th2
```

Alert level G
PLAT005_ALERT_5_G No _iucr_refine_instructions_details in the CIF ?

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

1 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
0 ALERT type 3 Indicator that the structure quality may be low
1 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check

Datablock: 3py2

Bond precision: C-C = 0.0035 A Wavelength=0.71073

Cell: a=10.4981(5) b=9.3769(2) c=15.0666(7)
alpha=90 beta=98.436(2) gamma=90
Temperature: 150 K

	Calculated	Reported
Volume	1467.10(10)	1467.10(10)
Space group	P 21/m	P 21/m
Hall group	-P 2yb	?
Moiety formula	C26 H24 N2 Th, C5 H5 K N, C5 H5 N	?
Sum formula	C36 H34 K N4 Th	C36 H34 K N4 Th
Mr	793.81	793.81
Dx,g cm-3	1.797	1.797
Z	2	2
Mu (mm-1)	5.257	5.257
F000	774.0	774.0
F000’	760.27	
h,k,lmax	14,13,21	14,13,21
Nref	4725	4721
Tmin,Tmax	0.505,0.729	0.460,0.729
Tmin’	0.427	

Correction method= MULTI-SCAN

Data completeness= 0.999 Theta(max)= 30.510

R(reflections)= 0.0237(4199) wR2(reflections)= 0.0438(4721)

S = 0.973 Npar= 218

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

PLAT048_ALERT_1_C MoietyFormula Not Given ..... ?
PLAT125_ALERT_4_C No '_symmetry_space_group_name_Hall' Given ..... ?

Alert level G

PLAT005_ALERT_5_G No _iucr_refine_instructions_details in the CIF ?
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) . 1.45 Ratio
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. # 2
C5 H5 K N
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. # 3
C5 H5 N

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

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
0 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
4 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check

checkCIF publication errors

Alert level A

PUBL004_ALERT_1_A The contact author's name and address are missing,
_publ_contact_author_name and _publ_contact_author_address.
PUBL005_ALERT_1_A _publ_contact_author_email, _publ_contact_author_fax and
_publ_contact_author_phone are all missing.
At least one of these should be present.
PUBL006_ALERT_1_A _publ_requested_journal is missing
e.g. 'Acta Crystallographica Section C'
PUBL008_ALERT_1_A _publ_section_title is missing. Title of paper.
PUBL009_ALERT_1_A _publ_author_name is missing. List of author(s) name(s).
PUBL010_ALERT_1_A _publ_author_address is missing. Author(s) address(es).
PUBL012_ALERT_1_A _publ_section_abstract is missing.
Abstract of paper in English.

Alert level G

PUBL013_ALERT_1_G The _publ_section_comment (discussion of study) is
missing. This is required for a full paper submission (but is
optional for an electronic paper).
PUBL017_ALERT_1_G The _publ_section_references section is missing or
empty.

```
   7 ALERT level A = Data missing that is essential or data in wrong format
   2 ALERT level G = General alerts. Data that may be required is missing
```

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 level A alerts remain, which you believe to be justified deviations, and you intend to submit this CIF for publication in Acta Crystallographica Section C or Section E, you should additionally insert an explanation in your CIF using the Validation Reply Form (VRF) below. Your explanation will be considered as part of the review process.

If you intend to submit to another section of Acta Crystallographica or Journal of Applied Crystallography or Journal of Synchrotron Radiation, you should make sure that at least a basic structural check is run on the final version of your CIF prior to submission.

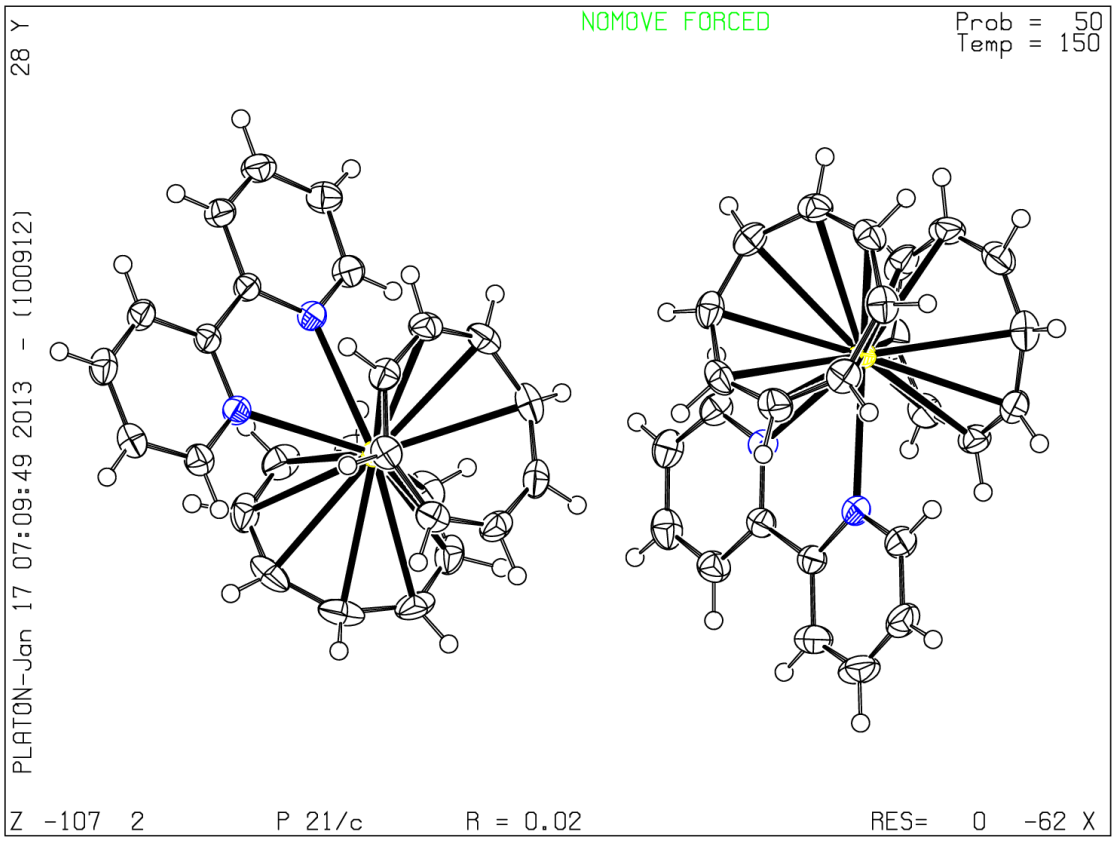
```
# start Validation Reply Form
_vrf_PUBL004_GLOBAL
;
PROBLEM: The contact author’s name and address are missing,
RESPONSE: ...
;
_vrf_PUBL005_GLOBAL
;
PROBLEM: _publ_contact_author_email, _publ_contact_author_fax and
RESPONSE: ...
;
_vrf_PUBL006_GLOBAL
;
PROBLEM: _publ_requested_journal is missing
RESPONSE: ...
;
_vrf_PUBL008_GLOBAL
;
PROBLEM: _publ_section_title is missing. Title of paper.
RESPONSE: ...
;
_vrf_PUBL009_GLOBAL
;
PROBLEM: _publ_author_name is missing. List of author(s) name(s).
RESPONSE: ...
;
_vrf_PUBL010_GLOBAL
;
PROBLEM: _publ_author_address is missing. Author(s) address(es).
```

```
RESPONSE: ...
;
_vrf_PUBL012_GLOBAL
;
PROBLEM: _publ_section_abstract is missing.
RESPONSE: ...
;
# end Validation Reply Form
```

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 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.

PLATON version of 05/11/2012; check.def file version of 05/11/2012

Datablock 2 - ellipsoid plot



Datablock 3py2 - ellipsoid plot