

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) shelx

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: shelx

| | | |
|-----------------|-------------------------|----------------------------------|
| Bond precision: | S- S = 0.0002 A | Wavelength=0.71073 |
| Cell: | a=5.61826 (6) | b=5.61826 (6) c=5.61826 (6) |
| | alpha=90 | beta=90 gamma=90 |
| Temperature: | 298 K | |
| | Calculated | Reported |
| Volume | 177.340 (6) | 177.340 (6) |
| Space group | P a -3 | P a -3 |
| Hall group | -P 2ac 2ab | -P 2ac 2ab |
| Moiety formula | Os1.33 Rh0.27 Ru2.40 S8 | ? |
| Sum formula | Os1.33 Rh0.27 Ru2.40 S8 | Os0.33 Rh0.07 Ru0.60 S2 |
| Mr | 779.66 | 194.90 |
| Dx, g cm-3 | 7.300 | 7.300 |
| Z | 1 | 4 |
| Mu (mm-1) | 31.601 | 31.657 |
| F000 | 346.8 | 347.0 |
| F000' | 343.00 | |
| h, k, lmax | 11, 11, 11 | 11, 11, 11 |
| Nref | 278 | 281 |
| Tmin, Tmax | 0.333, 0.566 | 0.452, 0.706 |
| Tmin' | 0.271 | |

Correction method= # Reported T Limits: Tmin=0.452 Tmax=0.706
AbsCorr = GAUSSIAN

Data completeness= 1.011 Theta(max)= 47.530

| | |
|-------------------------------|---------------------------------|
| R(reflections)= 0.0088 (242) | wR2(reflections)= 0.0204 (281) |
| S = 1.083 | Npar= 8 |

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

| | | |
|-------------------|--|--------------|
| PLAT021_ALERT_4_C | Ratio Unique / Expected Reflections too High ... | 1.011 |
| PLAT077_ALERT_4_C | Unitcell Contains Non-integer Number of Atoms .. | Please Check |
| PLAT731_ALERT_1_C | Bond Calc 2.2123(2), Rep 2.2123(7) | 4 su-Rat |
| S | -S 1_555 13_546 | # 7 Check |



Alert level G

| | | |
|-------------------|--|--------------|
| PLAT004_ALERT_5_G | Polymeric Structure Found with Maximum Dimension | 3 Info |
| PLAT045_ALERT_1_G | Calculated and Reported Z Differ by a Factor ... | 0.250 Check |
| PLAT068_ALERT_1_G | Reported F000 Differs from Calcd (or Missing)... | Please Check |
| PLAT168_ALERT_4_G | The CIF-Embedded .res File Contains EXYZ Records | 1 Report |
| PLAT171_ALERT_4_G | The CIF-Embedded .res File Contains EADP Records | 1 Report |
| PLAT300_ALERT_4_G | Atom Site Occupancy of Rh Constrained at | 0.067 Check |
| PLAT301_ALERT_3_G | Main Residue Disorder(Resd 1) | 65% Note |
| PLAT811_ALERT_5_G | No ADDSYM Analysis: Too Many Excluded Atoms | ! Info |
| PLAT883_ALERT_1_G | No Info/Value for _atom_sites_solution_primary . | Please Do ! |
| PLAT967_ALERT_5_G | Note: Two-Theta Cutoff Value in Embedded .res .. | 95.3 Degree |

- 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
10 **ALERT level G** = General information/check it is not something unexpected

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

