

checkCIF/PLATON report

Bond distances and angles from GSAS-II had incorrect unit cell offsets prior to GSAS-II version 4876. The GSAS-II authors recommend updating. If a CIF file from the most recent GSAS-II version is still showing problems, you are encouraged to contact the software authors.

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

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: D2CO3_Complete_W2

Bond precision: O- C = 0.0500 A Wavelength=2.11754

Cell: a=5.392 (2) b=6.661 (4) c=5.6900 (12)
 alpha=90 beta=92.66 (3) gamma=90

Temperature: 298 K

	Calculated	Reported
Volume	204.13 (15)	204.12 (15)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C2 D4 O6	?
Sum formula	C2 D4 O6	C D2 O3
Mr	128.06	64.04
Dx, g cm ⁻³	2.083	2.084
Z	2	4
Mu (mm ⁻¹)	0.000	0.000
F000	149.6	0.0
F000'	127.99	
h, k, lmax		2, 3, 3
Nref		34
Tmin, Tmax		
Tmin'		

Correction method= Not given

Data completeness= Theta (max)= 0.000

R(reflections)=

wR2(reflections)=

S =

Npar=

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

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C1 Check



Alert level G

PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ... 0.500 Check
PLAT303_ALERT_2_G Full Occupancy Atom D1 with # Connections 2.00 Check
PLAT395_ALERT_2_G Deviating X-O-Y Angle From 120 for O3 . 155.3 Degree
PLAT432_ALERT_2_G Short Inter X...Y Contact O2 ..C1 . 2.48 Ang.
x,1/2-y,1/2+z = 4_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact O3 ..C1 . 2.49 Ang.
x,1/2-y,-1/2+z = 4_554 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact C1 ..C1 . 3.02 Ang.
x,1/2-y,-1/2+z = 4_554 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact C1 ..C1 . 3.02 Ang.
x,1/2-y,1/2+z = 4_555 Check
PLAT769_ALERT_4_G CIF Embedded explicitly supplied scattering data Please Note

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

- 1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
7 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
0 ALERT type 5 Informative message, check
-

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 18/05/2022; check.def file version of 17/05/2022

