

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) gu2

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: gu2

Bond precision:	= 0.0000 A	Wavelength=0.71073	
Cell:	a=8.0898 (1) alpha=90	b=8.0898 (1) beta=90	c=8.0898 (1) gamma=90
Temperature:	293 K		
	Calculated	Reported	
Volume	529.44 (2)	529.44 (2)	
Space group	F d -3 m	F d -3 m	
Hall group	-F 4vw 2vw	-F 4vw 2vw	
Moiety formula	Co23.20 Cu0.16 Mn0.24 O32 Si0.16	0.25 (Co11.6 Cu0.08 Mn0.12 O16 Si0.08)	
Sum formula	Co23.20 Cu0.16 Mn0.24 O32 Si0.16	Co2.90 Cu0.02 Mn0.03 O4 Si0.02	
Mr	1906.95	238.38	
Dx, g cm-3	5.981	5.981	
Z	1	8	
Mu (mm-1)	18.070	18.071	
F000	895.2	895.0	
F000'	903.85		
h, k, lmax	12, 12, 12	12, 12, 11	
Nref	67	69	
Tmin, Tmax	0.699, 0.805	0.697, 1.000	
Tmin'	0.576		

Correction method= # Reported T Limits: Tmin=0.697 Tmax=1.000

AbsCorr = MULTI-SCAN

Data completeness= 1.030

Theta(max)= 33.154

R(reflections)= 0.0124(66)

wR2(reflections)=
0.0352(69)

S = 1.258

Npar= 7

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 ...	1.030
PLAT077_ALERT_4_C	Unitcell Contains Non-integer Number of Atoms ..	Please Check
PLAT088_ALERT_3_C	Poor Data / Parameter Ratio	9.86 Note
PLAT313_ALERT_2_C	Oxygen with Three Covalent Bonds (rare)	0003 Check



Alert level G

PLAT042_ALERT_1_G	Calc. and Reported Moiety Formula Strings Differ	Please Check
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...	0.1250 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	2 Report
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records	2 Report
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature (K)	293 Check
PLAT200_ALERT_1_G	Reported _diffn_ambient_temperature (K)	293 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Cu1 Constrained at	0.0199 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Co1 Constrained at	0.9199 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Co2 Constrained at	0.99 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Mn1 Constrained at	0.0101 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Mn2 Constrained at	0.01 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Si1 Constrained at	0.0199 Check
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)	89% Note
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in (Resd 1)	20.04 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact Si1 ..0003	3.39 Ang.
	-1/4+y,-1/4+x,2-z =	37_446 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact Si1 ..0003	3.39 Ang.
	1-y,1-x,2-z =	14_667 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact Si1 ..0003	3.39 Ang.
	1-x,1/4+y,1/4+z =	148_665 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact Si1 ..0003	3.39 Ang.
	1-z,1/4+x,1/4+y =	150_665 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact Si1 ..0003	3.39 Ang.
	1/2-y,-1/4+x,1/4+z =	16_545 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact Si1 ..0003	3.39 Ang.
	1/4+x,1-z,1/4+y =	44_554 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact Si1 ..0003	3.39 Ang.
	-1/4+x,-3/4+z,3/2-y =	17_446 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact Si1 ..0003	3.39 Ang.
	1/4+y,1-x,1/4+z =	39_554 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact Si1 ..0003	3.39 Ang.
	1/2-x,-1/4+z,1/4+y =	18_545 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact Si1 ..0003	3.39 Ang.
	-1/4+z,1/2-x,1/4+y =	104_566 Check
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	1 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 !

PLAT955_ALERT_1_G Reported (CIF) and Actual (FCF) Lmax Differ by . 1 Units
PLAT961_ALERT_5_G Dataset Contains no Negative Intensities Please Check

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

7 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
11 ALERT type 2 Indicator that the structure model may be wrong or deficient
2 ALERT type 3 Indicator that the structure quality may be low
12 ALERT type 4 Improvement, methodology, query or suggestion
2 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.

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