

# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) Coesite-III\_27.9GPa

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: Coesite-III\_27.9GPa

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Bond precision:    Si- O = 0.0401 A                      Wavelength=0.29004

Cell:                      a=6.571(3)                      b=17.790(7)                      c=6.766(4)  
                                    alpha=82.14(4)                      beta=120.81(6)                      gamma=87.13(3)  
Temperature:            296 K

	Calculated	Reported
Volume	666.2(7)	666.2(6)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	O24 Si12	O2 Si
Sum formula	O24 Si12	O2 Si
Mr	721.08	60.09
Dx,g cm-3	3.595	3.595
Z	2	24
Mu (mm-1)	0.149	0.149
F000	720.0	720.0
F000'	720.06	
h,k,lmax	8,23,8	8,23,7
Nref	3289	833
Tmin,Tmax		0.172,1.000
Tmin'		

Correction method= # Reported T Limits: Tmin=0.172 Tmax=1.000  
AbsCorr = MULTI-SCAN

Data completeness= 0.253                      Theta(max)= 11.146


R(reflections)= 0.1364( 681)                      wR2(reflections)= 0.3632( 833)

S = 1.625                      Npar= 143

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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.

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 **Alert level A**

ATOM007\_ALERT\_1\_A \_atom\_site\_aniso\_label is missing  
Unique label identifying the atom site.

**Author Response: Due to incompleteness of the dataset thermal parameters were refined in isotropic approximation.**

PLAT029\_ALERT\_3\_A \_diffrn\_measured\_fraction\_theta\_full value Low . 0.253 Why?

**Author Response: The dataset was incomplete since the data were collected in a diamond anvil cell metallic body of which shadows more than 60% of the reflections.**


PLAT088\_ALERT\_3\_A Poor Data / Parameter Ratio ..... 5.83 Note

**Author Response: Poor data/parameter ratio is due to low symmetry of the structure (P-1), big amount of the parameters to refine (27 atoms) and incompleteness of the dataset (measurement in a diamond anvil cell).**

PLAT910\_ALERT\_3\_A Missing # of FCF Reflection(s) Below Theta(Min). 52 Note

**Author Response: Certain part of the reflections is missing due to geometry of the experiment. The metallic body of the diamond anvil cell absorbs more than 60% of the reflections.**

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 **Alert level B**

DIFMN02\_ALERT\_2\_B The minimum difference density is < -0.1\*ZMAX\*1.00  
\_refine\_diff\_density\_min given = -1.421  
Test value = -1.400

**Author Response: Due to partial overlap of the reflections with those belonging to low-pressure phase (coesite-II) and poor data/parameter ratio.**

PLAT084\_ALERT\_3\_B High wR2 Value (i.e. > 0.25) ..... 0.36 Report

**Author Response: Due to partial overlap of the reflections with those belonging to low-pressure phase (coesite-II).**

PLAT098\_ALERT\_2\_B Large Reported Min. (Negative) Residual Density -1.42 eA-3

**Author Response: Due to partial overlap of the reflections with those belonging to low-pressure phase (coesite-II) and poor data/parameter ratio.**

**Author Response: Certain part of the reflections is missing due to geometry of the experiment. The metallic body of the diamond anvil cell absorbs more than 60% of the reflections.**

● **Alert level C**

DIFMN03\_ALERT\_1\_C The minimum difference density is < -0.1\*ZMAX\*0.75  
 The relevant atom site should be identified.

DIFMX02\_ALERT\_1\_C The maximum difference density is > 0.1\*ZMAX\*0.75  
 The relevant atom site should be identified.

PLAT082\_ALERT\_2\_C High R1 Value ..... 0.14 Report

PLAT097\_ALERT\_2\_C Large Reported Max. (Positive) Residual Density 1.18 eA-3

PLAT155\_ALERT\_4\_C The Triclinic Unitcell is NOT Reduced ..... Please Do !

PLAT906\_ALERT\_3\_C Large K Value in the Analysis of Variance ..... 4.738 Check

PLAT913\_ALERT\_3\_C Missing # of Very Strong Reflections in FCF .... 9 Note

PLAT975\_ALERT\_2\_C Check Calcd Resid. Dens. 0.65A From O3 1.04 eA-3

PLAT976\_ALERT\_2\_C Check Calcd Resid. Dens. 0.92A From O21 -0.96 eA-3

● **Alert level G**

ABSMU01\_ALERT\_1\_G Calculation of \_exptl\_absorpt\_correction\_mu  
 not performed for this radiation type.

PLAT004\_ALERT\_5\_G Polymeric Structure Found with Maximum Dimension 3 Info

PLAT012\_ALERT\_1\_G N.O.K. \_shelx\_res\_checksum Found in CIF ..... Please Check

PLAT042\_ALERT\_1\_G Calc. and Reported MoietyFormula Strings Differ Please Check

PLAT045\_ALERT\_1\_G Calculated and Reported Z Differ by a Factor ... 0.08 Check

PLAT072\_ALERT\_2\_G SHELXL First Parameter in WGHT Unusually Large 0.20 Report

PLAT396\_ALERT\_2\_G Deviating Si-O-Si Angle From 150 for O1 180.0 Degree

PLAT396\_ALERT\_2\_G Deviating Si-O-Si Angle From 150 for O2 180.0 Degree

PLAT396\_ALERT\_2\_G Deviating Si-O-Si Angle From 150 for O3 126.9 Degree

PLAT396\_ALERT\_2\_G Deviating Si-O-Si Angle From 150 for O4 136.9 Degree

PLAT396\_ALERT\_2\_G Deviating Si-O-Si Angle From 150 for O5 129.4 Degree

PLAT396\_ALERT\_2\_G Deviating Si-O-Si Angle From 150 for O6 120.5 Degree

PLAT396\_ALERT\_2\_G Deviating Si-O-Si Angle From 150 for O7 125.1 Degree

PLAT396\_ALERT\_2\_G Deviating Si-O-Si Angle From 150 for O8 124.6 Degree

PLAT396\_ALERT\_2\_G Deviating Si-O-Si Angle From 150 for O9 136.2 Degree

PLAT396\_ALERT\_2\_G Deviating Si-O-Si Angle From 150 for O11 171.4 Degree

PLAT396\_ALERT\_2\_G Deviating Si-O-Si Angle From 150 for O12 128.1 Degree

PLAT396\_ALERT\_2\_G Deviating Si-O-Si Angle From 150 for O13 130.1 Degree

PLAT396\_ALERT\_2\_G Deviating Si-O-Si Angle From 150 for O14 135.0 Degree

PLAT396\_ALERT\_2\_G Deviating Si-O-Si Angle From 150 for O15 122.6 Degree

PLAT396\_ALERT\_2\_G Deviating Si-O-Si Angle From 150 for O16 120.9 Degree

PLAT396\_ALERT\_2\_G Deviating Si-O-Si Angle From 150 for O19 135.1 Degree

PLAT396\_ALERT\_2\_G Deviating Si-O-Si Angle From 150 for O20 134.8 Degree

PLAT396\_ALERT\_2\_G Deviating Si-O-Si Angle From 150 for O21 132.5 Degree

PLAT396\_ALERT\_2\_G Deviating Si-O-Si Angle From 150 for O22 124.6 Degree

PLAT396\_ALERT\_2\_G Deviating Si-O-Si Angle From 150 for O23 127.6 Degree

PLAT396\_ALERT\_2\_G Deviating Si-O-Si Angle From 150 for O25 135.2 Degree

PLAT432\_ALERT\_2\_G Short Inter X...Y Contact Si1 ..025 2.67 Ang.

PLAT432\_ALERT\_2\_G Short Inter X...Y Contact Si1 ..02 3.39 Ang.

PLAT432\_ALERT\_2\_G Short Inter X...Y Contact Si1 ..Si1 3.49 Ang.

PLAT432\_ALERT\_2\_G Short Inter X...Y Contact Si2 ..03 3.38 Ang.

PLAT432\_ALERT\_2\_G Short Inter X...Y Contact Si3 ..Si5 3.56 Ang.

PLAT432\_ALERT\_2\_G Short Inter X...Y Contact Si5 ..020 2.81 Ang.

PLAT432\_ALERT\_2\_G Short Inter X...Y Contact Si11 ..03 3.11 Ang.

PLAT432\_ALERT\_2\_G Short Inter X...Y Contact Si11 ..05 3.37 Ang.

PLAT432_ALERT_2_G	Short Inter X...Y Contact	Si12	..Si12	3.14	Ang.
PLAT793_ALERT_4_G	Model has Chirality at	Si3	(Centro SPGR)	R	Verify
PLAT793_ALERT_4_G	Model has Chirality at	Si5	(Centro SPGR)	R	Verify
PLAT793_ALERT_4_G	Model has Chirality at	Si7	(Centro SPGR)	S	Verify
PLAT793_ALERT_4_G	Model has Chirality at	Si8	(Centro SPGR)	R	Verify
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above	S <sub>Th</sub> /L= 0.600		571	Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded	.res File ...		5	Note

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

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

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**PLATON version of 30/01/2018; check.def file version of 30/01/2018**

