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: seab017

Bond precision: C-C = 0.0117 AWavelength=0.71073 a=11.6299(10) b=11.7654(11) Cell: c=17.0791(15)alpha=90 beta=102.119(1) gamma=90 200 K Temperature: Calculated Reported Volume 2284.9(4) 2284.9(4)Space group P 21/n P2(1)/n Hall group -P 2yn ? Moiety formula C15 H32 Cu N3 Si2 ? Sum formula C15 H32 Cu N3 Si2 C15 H32 Cu N3 Si2 Mr 374.17 374.16 Dx,g cm-3 1.088 1.088 Ζ 4 4 Mu (mm-1) 1.059 1.059 F000 800.0 800.0 F000′ 802.03 h,k,lmax 15,15,22 15,15,22 Nref 5256 5245 Tmin,Tmax 0.881,0.919 0.883,0.920 Tmin′ 0.881 Correction method= MULTI-SCAN Data completeness= 0.998 Theta(max) = 27.530R(reflections) = 0.0818(3832) wR2(reflections) = 0.2674(5245) S = 1.046Npar= 225

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.

Hirshfeld Dif	fference Sil	C11′		0.17	Ang.
Hirshfeld Dif	fference Si2	C14′		0.16	Ang.
High Ueo	q as Compared	l to Neighbors	for	C3	
Low Ueo	q as Compared	l to Neighbors	for	Cu	
Low Ueo	q as Compared	l to Neighbors	for	Sil	
Low Ueo	q as Compared	l to Neighbors	for	Si2	
Low Ueo	q as Compared	l to Neighbors	for	N3	
Low Ueo	q as Compared	l to Neighbors	for	C4	
nd Precision	on C-C Bond	ls		0.0117	Ang
Inter XH3	XHn H3A	H11B		2.13	Ang.
Inter XH3	XHn H6A	H8B	••	2.10	Ang.
	Hirshfeld Di Hirshfeld Di High Ue Low Ue Low Ue Low Ue Low Ue Low Ue nd Precision Inter XH3	Hirshfeld Difference SilHirshfeld Difference Si2HighUeq as ComparedLowUeq as ComparedLow <t< td=""><td>Hirshfeld Difference Si1 Cll' Hirshfeld Difference Si2 Cl4' High Ueq as Compared to Neighbors Low Ueq as Compared to Neighbors</td><td>Hirshfeld Difference Si1Cll'Hirshfeld Difference Si2Cl4'HighUeq as Compared to Neighbors forLowUeq as Compared to Neighbors forLowUeq as Compared to Neighbors forUeq as Compared to Neighbors forLowUeq as Compared to Neighbors for<</td><td>Hirshfeld Difference Si1 Cl1'0.17Hirshfeld Difference Si2 Cl4'0.16HighUeq as Compared to Neighbors forC3LowUeq as Compared to Neighbors forCuLowUeq as Compared to Neighbors forSi1LowUeq as Compared to Neighbors forSi2LowUeq as Compared to Neighbors forN3LowUeq as Compared to Neighbors forC4LowUeq as Compared to Neighbors forC4LowUeq as Compared to Neighbors for0.0117Inter XH3XHnH3AH11B2.13Inter XH3XHnH6AH8B2.10</td></t<>	Hirshfeld Difference Si1 Cll' Hirshfeld Difference Si2 Cl4' High Ueq as Compared to Neighbors Low Ueq as Compared to Neighbors	Hirshfeld Difference Si1Cll'Hirshfeld Difference Si2Cl4'HighUeq as Compared to Neighbors forLowUeq as Compared to Neighbors forLowUeq as Compared to Neighbors forUeq as Compared to Neighbors forLowUeq as Compared to Neighbors for<	Hirshfeld Difference Si1 Cl1'0.17Hirshfeld Difference Si2 Cl4'0.16HighUeq as Compared to Neighbors forC3LowUeq as Compared to Neighbors forCuLowUeq as Compared to Neighbors forSi1LowUeq as Compared to Neighbors forSi2LowUeq as Compared to Neighbors forN3LowUeq as Compared to Neighbors forC4LowUeq as Compared to Neighbors forC4LowUeq as Compared to Neighbors for0.0117Inter XH3XHnH3AH11B2.13Inter XH3XHnH6AH8B2.10

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Alert level G	
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite	13
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained Atom Sites	30
PLAT005_ALERT_5_G No _iucr_refine_instructions_details in CIF	?
PLAT007_ALERT_5_G Note: Number of Unrefined D-H Atoms	1
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large.	0.14
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Cu C8	6.1 su
PLAT301_ALERT_3_G Note: Main Residue Disorder	43 Perc.
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels	3
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF #	10
C10'-SI1 -C10 1.555 1.555 1.555	8.00 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF #	12
C11 -SI1 -C11′ 1.555 1.555 1.555	26.90 Deg.
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms	!
PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints	270

0 ALERT level A = Most likely a serious problem - resolve or explain 0 ALERT level B = A potentially serious problem, consider carefully 14 ALERT level C = Check. Ensure it is not caused by an omission or oversight 12 ALERT level G = General information/check it is not something unexpected 0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data 14 ALERT type 2 Indicator that the structure model may be wrong or deficient 4 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

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*, 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 04/07/2012; check.def file version of 28/06/2012

Datablock seab017 - ellipsoid plot



