

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) s-cu4au8

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: s-cu4au8

Bond precision:	C-C = 0.0580 A	Wavelength=1.54184	
Cell:	a=16.6336 (2) alpha=90	b=26.8950 (3) beta=91.346 (1)	c=31.7629 (4) gamma=90
Temperature:	200 K		
	Calculated	Reported	
Volume	14205.6 (3)	14205.6 (3)	
Space group	P 21	P 1 21 1	
Hall group	P 2yb	P 2yb	
Moiety formula	C144 H96 Au8 Cu4 N6 P6 S6 [+ solvent]	C144 H96 Au8 Cu4 N6 P6 S6	
Sum formula	C144 H96 Au8 Cu4 N6 P6 S6 [+ solvent]	C144 H96 Au8 Cu4 N6 P6 S6	
Mr	4118.41	4118.33	
Dx, g cm ⁻³	1.926	1.926	
Z	4	4	
Mu (mm ⁻¹)	17.577	17.577	
F000	7744.0	7744.0	
F000'	7600.06		
h, k, lmax	20, 33, 39	20, 33, 39	
Nref	57792 [29541]	53322	
Tmin, Tmax	0.119, 0.121	0.531, 1.000	
Tmin'	0.020		

Correction method= # Reported T Limits: Tmin=0.531 Tmax=1.000

AbsCorr = MULTI-SCAN

Data completeness= 1.81/0.92

Theta (max)= 74.127

R(reflections)= 0.0808(42412)

wR2(reflections)=
0.2239(53322)

S = 1.043

Npar= 3121

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 B**

PLAT342_ALERT_3_B Low Bond Precision on C-C Bonds 0.058 Ang.

 **Alert level C**

PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density	2.28	Report
PLAT213_ALERT_2_C	Atom C222 has ADP max/min Ratio	3.9	prolat
PLAT220_ALERT_2_C	NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range	3.8	Ratio
PLAT220_ALERT_2_C	NonSolvent Resd 2 C Ueq(max)/Ueq(min) Range	3.1	Ratio
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C31	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C54	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C61	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C86	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C88	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C102	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C118	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C141	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C161	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C167	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C207	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C210	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C215	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C240	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C241	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C247	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C249	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C254	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C287	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C1	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C3	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C152	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C162	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C208	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C211	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C221	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C239	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C246	Check
PLAT331_ALERT_2_C	Small Aver Phenyl C-C Dist C201 --C206 .	1.37	Ang.
PLAT332_ALERT_2_C	Large Phenyl C-C Range C163 -C168 .	0.16	Ang.
PLAT332_ALERT_2_C	Large Phenyl C-C Range C189 -C194 .	0.18	Ang.
PLAT332_ALERT_2_C	Large Phenyl C-C Range C251 -C256 .	0.17	Ang.
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	51	Report
PLAT977_ALERT_2_C	Check Negative Difference Density on H22 .	-0.37	eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on H27 .	-0.33	eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on H30 .	-0.45	eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on H37 .	-0.34	eA-3

PLAT977_ALERT_2_C	Check Negative Difference Density on H64	.	-0.43 eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on H66	.	-0.48 eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on H74	.	-0.31 eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on H83	.	-0.48 eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on H84	.	-0.41 eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on H89	.	-0.38 eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on H111	.	-0.31 eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on H131	.	-0.44 eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on H158	.	-0.49 eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on H161	.	-0.40 eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on H170	.	-0.59 eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on H175	.	-0.32 eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on H176	.	-0.33 eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on H186	.	-0.47 eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on H187	.	-0.43 eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on H210	.	-0.57 eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on H211	.	-0.32 eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on H220	.	-0.34 eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on H225	.	-0.33 eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on H240	.	-0.63 eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on H259	.	-0.33 eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on H271	.	-0.61 eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on H286	.	-0.34 eA-3

Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite		52	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...		98	Report
PLAT072_ALERT_2_G	SHELXL First Parameter in WGHT Unusually Large		0.13	Report
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large		148.53	Why ?
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records		11	Report
PLAT177_ALERT_4_G	The CIF-Embedded .res File Contains DELU Records		1	Report
PLAT186_ALERT_4_G	The CIF-Embedded .res File Contains ISOR Records		16	Report
PLAT335_ALERT_2_G	Check Large C6 Ring C-C Range C69	-C78	0.16	Ang.
PLAT335_ALERT_2_G	Check Large C6 Ring C-C Range C79	-C88	0.16	Ang.
PLAT335_ALERT_2_G	Check Large C6 Ring C-C Range C267	-C276	0.18	Ang.
PLAT606_ALERT_4_G	Solvent Accessible VOID(S) in Structure		!	Info
PLAT722_ALERT_1_G	Angle Calc 121.00, Rep 119.80 Dev...		1.20	Degree
	C199 -C198 -H198 1_555 1_555 1_555	#	930	Check
PLAT722_ALERT_1_G	Angle Calc 117.00, Rep 118.40 Dev...		1.40	Degree
	C256 -C255 -H255 1_555 1_555 1_555	#	961	Check
PLAT722_ALERT_1_G	Angle Calc 123.00, Rep 124.10 Dev...		1.10	Degree
	C144 -C143 -H143 1_555 1_555 1_555	#	1275	Check
PLAT722_ALERT_1_G	Angle Calc 120.00, Rep 118.70 Dev...		1.30	Degree
	C137 -C136 -H136 1_555 1_555 1_555	#	1288	Check
PLAT794_ALERT_5_G	Tentative Bond Valency for Cu3 (I)	.	1.00	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints		651	Note
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary	.	Please	Do !
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).		2	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600		593	Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File		9	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity		4.3	Low
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.		0	Info
PLAT992_ALERT_5_G	Repd & Actual _reflns_number_gt Values Differ by		3	Check

0 **ALERT level A** = Most likely a serious problem - resolve or explain

1 **ALERT level B** = A potentially serious problem, consider carefully
64 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
24 **ALERT level G** = General information/check it is not something unexpected

5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
72 ALERT type 2 Indicator that the structure model may be wrong or deficient
5 ALERT type 3 Indicator that the structure quality may be low
5 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.

PLATON version of 20/01/2022; check.def file version of 19/01/2022

