

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) Co-dcbdt

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: Co-dcbdt

Bond precision:	C-C = 0.0064 Å	Wavelength=1.54184	
Cell:	a=22.1038 (3) alpha=90	b=22.5058 (3) beta=90	c=14.2421 (2) gamma=90
Temperature:	150 K		
	Calculated	Reported	
Volume	7084.93 (17)	7084.93 (17)	
Space group	P b c n	P b c n	
Hall group	-P 2n 2ab	-P 2n 2ab	
Moiety formula	C16 H8 Co2 O10 S4, 3 (C4 H10 O)	C16 H8 Co2 O10 S4, 3 (C4 H10 O)	
Sum formula	C28 H38 Co2 O13 S4	C28 H38 Co2 O13 S4	
Mr	828.68	828.68	
Dx, g cm ⁻³	1.554	1.554	
Z	8	8	
Mu (mm ⁻¹)	10.069	10.069	
F000	3424.0	3424.0	
F000'	3406.51		
h, k, lmax	27, 28, 18	27, 28, 17	
Nref	7520	7316	
Tmin, Tmax		0.188, 1.000	
Tmin'			

Correction method= # Reported T Limits: Tmin=0.188 Tmax=1.000
AbsCorr = ?

Data completeness= 0.973 Theta(max)= 77.409

R(reflections)= 0.0906 (5542)

wR2(reflections)=
0.2776 (7316)

S = 1.070

Npar= 433

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

PLAT430_ALERT_2_B	Short Inter D...A Contact	O2	..O13	.	2.73 Ang.
			x,y,z =		1_555 Check
PLAT430_ALERT_2_B	Short Inter D...A Contact	O5	..O11	.	2.75 Ang.
			x,y,z =		1_555 Check
PLAT430_ALERT_2_B	Short Inter D...A Contact	O6	..O13	.	2.80 Ang.
			x,1-y,-1/2+z =		7_565 Check
PLAT430_ALERT_2_B	Short Inter D...A Contact	O7	..O10	.	2.84 Ang.
			x,1-y,1/2+z =		7_566 Check
PLAT430_ALERT_2_B	Short Inter D...A Contact	O11	..O12	.	2.84 Ang.
			3/2-x,3/2-y,1/2+z =		2_665 Check

Alert level C

RINTA01_ALERT_3_C The value of Rint is greater than 0.12

Rint given 0.167

PLAT020_ALERT_3_C	The Value of Rint is Greater Than 0.12	0.167	Report
PLAT052_ALERT_1_C	Info on Absorption Correction Method Not Given		Please Do !
PLAT053_ALERT_1_C	Minimum Crystal Dimension Missing (or Error) ...		Please Check
PLAT054_ALERT_1_C	Medium Crystal Dimension Missing (or Error) ...		Please Check
PLAT055_ALERT_1_C	Maximum Crystal Dimension Missing (or Error) ...		Please Check
PLAT084_ALERT_3_C	High wR2 Value (i.e. > 0.25)	0.28	Report
PLAT213_ALERT_2_C	Atom Col has ADP max/min Ratio	3.1	prolat
PLAT243_ALERT_4_C	High 'Solvent' Ueq as Compared to Neighbors of	C19	Check
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of	O13	Check
PLAT250_ALERT_2_C	Large U3/U1 Ratio for <U(i,j)> Tensor(Resd 1)	2.2	Note
PLAT341_ALERT_3_C	Low Bond Precision on C-C Bonds	0.00642	Ang.
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	2.915	Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	5	Report
	0 0 2, 0 0 4, 23 10 4, 22 11 4, 23 11 4,		
PLAT971_ALERT_2_C	Check Calcd Resid. Dens. 1.19Ang From Co1	1.58	eA-3
PLAT972_ALERT_2_C	Check Calcd Resid. Dens. 0.93Ang From Co3	-2.37	eA-3
PLAT972_ALERT_2_C	Check Calcd Resid. Dens. 1.06Ang From Co1	-2.24	eA-3
PLAT972_ALERT_2_C	Check Calcd Resid. Dens. 0.91Ang From Co2	-2.17	eA-3
PLAT972_ALERT_2_C	Check Calcd Resid. Dens. 1.02Ang From Co1	-2.14	eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on H8B .	-0.66	eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on H19B .	-0.33	eA-3

Alert level G

PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	32	Report
PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	2	Info
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	4	Report
	H8A H8B H9A H9B		
PLAT072_ALERT_2_G	SHELXL First Parameter in WGHT Unusually Large	0.20	Report
PLAT186_ALERT_4_G	The CIF-Embedded .res File Contains ISOR Records	3	Report
PLAT794_ALERT_5_G	Tentative Bond Valency for Co1 (II) .	1.97	Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Co2 (II) .	2.17	Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Co3 (II) .	2.19	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	192	Note

PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=	0.600	195	Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF		1	Note
0 0 4,			
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity		4.9	Low
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value		2.83	Note
Predicted wR2: Based on SigI**2	9.79 or SHELX Weight	26.74	
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.		0	Info

0	ALERT level A	= Most likely a serious problem - resolve or explain
5	ALERT level B	= A potentially serious problem, consider carefully
21	ALERT level C	= Check. Ensure it is not caused by an omission or oversight
14	ALERT level G	= General information/check it is not something unexpected
4	ALERT type 1	CIF construction/syntax error, inconsistent or missing data
17	ALERT type 2	Indicator that the structure model may be wrong or deficient
9	ALERT type 3	Indicator that the structure quality may be low
4	ALERT type 4	Improvement, methodology, query or suggestion
6	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.

