



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 325co

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: 325co

Bond precision: C-C = 0.0087 Å

Wavelength=0.71073

Cell: a=9.1977 (15) b=11.1388 (19) c=16.013 (3)
 alpha=98.096 (5) beta=95.858 (5) gamma=102.487 (5)
Temperature: 150 K

	Calculated	Reported
Volume	1570.8 (5)	1570.8 (5)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C9 H27 B6 Co N3 O13, 11 (H2 O)	C9 H27 B6 Co N3 O13, 11 (H2 O)
Sum formula	C9 H49 B6 Co N3 O24	C9 H49 B6 Co N3 O24
Mr	707.30	707.30
Dx, g cm ⁻³	1.495	1.495
Z	2	2
Mu (mm ⁻¹)	0.639	0.639
F000	746.0	746.0
F000'	747.20	
h, k, lmax	12, 14, 21	12, 14, 21
Nref	7813	7687
Tmin, Tmax	0.858, 0.950	0.644, 0.746
Tmin'	0.826	

Correction method= # Reported T Limits: Tmin=0.644 Tmax=0.746
AbsCorr = NONE

Data completeness= 0.984

Theta(max)= 28.288

R(reflections)= 0.0694(4723)

wR2(reflections)=
0.1585(7687)

S = 1.040

Npar= 439

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

PLAT057_ALERT_3_C	Correction for Absorption Required	RT(exp) ...	1.11	Do !
PLAT241_ALERT_2_C	High MainResAtom	Ueq as Compared to Neighbours	C1	Check
PLAT241_ALERT_2_C	High MainResAtom	Ueq as Compared to Neighbours	C2	Check
PLAT241_ALERT_2_C	High MainResAtom	Ueq as Compared to Neighbours	C4	Check
PLAT241_ALERT_2_C	High MainResAtom	Ueq as Compared to Neighbours	C8	Check
PLAT242_ALERT_2_C	Low MainResAtom	Ueq as Compared to Neighbours	N1	Check
PLAT242_ALERT_2_C	Low MainResAtom	Ueq as Compared to Neighbours	N2	Check
PLAT242_ALERT_2_C	Low MainResAtom	Ueq as Compared to Neighbours	N3	Check
PLAT260_ALERT_2_C	Large Average	Ueq of Residue Including O15	0.103	Check
PLAT260_ALERT_2_C	Large Average	Ueq of Residue Including O16	0.102	Check
PLAT260_ALERT_2_C	Large Average	Ueq of Residue Including O19	0.112	Check
PLAT260_ALERT_2_C	Large Average	Ueq of Residue Including O21	0.104	Check
PLAT313_ALERT_2_C	Oxygen with Three Covalent Bonds (rare)		09	Check
PLAT341_ALERT_3_C	Low Bond Precision on C-C Bonds		0.00867	Ang.
PLAT360_ALERT_2_C	Short C(sp3)-C(sp3) Bond	C1 - C2 .	1.43	Ang.
PLAT360_ALERT_2_C	Short C(sp3)-C(sp3) Bond	C4 - C5 .	1.43	Ang.
PLAT415_ALERT_2_C	Short Inter D-H..H-X	H9B ..H22B .	2.10	Ang.
		1-x,1-y,1-z =	2_666	Check
PLAT417_ALERT_2_C	Short Inter D-H..H-D	H2 ..H23A .	2.10	Ang.
		x,y,z =	1_555	Check
PLAT417_ALERT_2_C	Short Inter D-H..H-D	H4 ..H17B .	2.10	Ang.
		x,y,z =	1_555	Check
PLAT417_ALERT_2_C	Short Inter D-H..H-D	H13 ..H13 .	2.10	Ang.
		1-x,2-y,2-z =	2_677	Check
PLAT417_ALERT_2_C	Short Inter D-H..H-D	H16A ..H17B .	2.10	Ang.
		x,y,z =	1_555	Check
PLAT417_ALERT_2_C	Short Inter D-H..H-D	H19B ..H23B .	2.10	Ang.
		1-x,1-y,2-z =	2_667	Check
PLAT417_ALERT_2_C	Short Inter D-H..H-D	H20A ..H22B .	2.10	Ang.
		-x,-y,1-z =	2_556	Check
PLAT417_ALERT_2_C	Short Inter D-H..H-D	H20B ..H21B .	2.10	Ang.
		x,y,z =	1_555	Check
PLAT417_ALERT_2_C	Short Inter D-H..H-D	H21A ..H22B .	2.10	Ang.
		x,y,z =	1_555	Check
PLAT417_ALERT_2_C	Short Inter D-H..H-D	H23A ..H23A .	2.10	Ang.
		2-x,1-y,2-z =	2_767	Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance		6.303	Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.600	12	Report
	0 1 1, -5 5 1, 10 1 2, 9 -3 4, 7 4 4, 8 -5 6,			
	7 5 7, 8 1 9, 6 2 9, 7 -8 10, 6 2 11, 3 3 12,			

● Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	25	Note
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	24	Report
	H7 H13 H14A H14B H15A H15B H16A H16B		
	H17A H17B H18A H18B H19A H19B H20A H20B		
	H21A H21B H22A H22B H23A H23B H24A H24B		
PLAT154_ALERT_1_G	The s.u.'s on the Cell Angles are Equal ..(Note)	0.005	Degree
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	17	Report
PLAT173_ALERT_4_G	The CIF-Embedded .res File Contains DANG Records	6	Report
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit-Cell: Resd. #	2	Note
	H2 O		
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit-Cell: Resd. #	3	Note
	H2 O		
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit-Cell: Resd. #	9	Note
	H2 O		
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit-Cell: Resd. #	10	Note
	H2 O		
PLAT794_ALERT_5_G	Tentative Bond Valency for Col (II) .	1.90	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	23	Note
PLAT910_ALERT_3_G	Missing FCF Reflection(s) Below Theta(Min) [Deg]=	2.47	Note
	1 0 0, 0 1 0, 0 -1 1, 0 0 1,		
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	110	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	3.7	Low
PLAT969_ALERT_5_G	The 'Henn et al.' R-Factor-gap value	3.588	Note
	Predicted wR2: Based on SigI**2 4.42 or SHELX Weight 15.24		Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	0	Info

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- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
28 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
16 **ALERT level G** = General information/check it is not something unexpected
- 1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
26 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
7 ALERT type 4 Improvement, methodology, query or suggestion
3 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. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

duplicate check

No duplication found

Datablock 325co - ellipsoid plot

