checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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: 2020_07_01_dt_btmacucl2hcl-1to1-2_n

Bond precision: C-C = 0.0042 A Wavelength=1.54184

Cell: a=9.49010(16) b=9.02423(19) c=27.9964(4)
alpha=90 beta=92.1082(14) gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	2396.01(7)	2396.01(8)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	2(C10 H16 N), Cl4 Cu	2(C10 H16 N), Cl4 Cu
Sum formula	C20 H32 Cl4 Cu N2	C20 H32 Cl4 Cu N2
Mr	505.83	505.81
Dx,g cm-3	1.402	1.402
Z	4	4
Mu (mm-1)	5.442	5.442
F000	1052.0	1052.0
F000'	1051.60	
h,k,lmax	11,10,33	11,10,33
Nref	4294	4294
Tmin,Tmax	0.379,0.647	0.420,0.698
Tmin'	0.236	

Correction method= # Reported T Limits: Tmin=0.420 Tmax=0.698
AbsCorr = ANALYTICAL

Data completeness= 1.000 Theta(max)= 67.079

R(reflections)= 0.0361(3992) wR2(reflections)= 0.0884(4294)

S = 1.202 Npar= 250

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 G

PLAT012_ALERT_1_G N.O.K. _shelx_res_checksum Found in CIF ..... Please Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 6.79 Why ?
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..... 10 Note
H7AA H7AB H9AA H9AB H9AC H7BA H7BB H9BA
H9BB H9BC

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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
0 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
3 **ALERT level G** = General information/check it is not something unexpected

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
1 ALERT type 2 Indicator that the structure model may be wrong or deficient
0 ALERT type 3 Indicator that the structure quality may be low
1 ALERT type 4 Improvement, methodology, query or suggestion
0 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. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

PLATON version of 26/09/2025; check.def file version of 20/09/2025

Datablock 2020_07_01_dt_btmacucl2hcl-1to1-2_n - ellipsoid plot

