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: 22_06_2020_dt_btmaptcl61to2_n

Bond precision: C-C = 0.0053 A Wavelength=1.54184

Cell: a=10.9703(2) b=11.9807(3) c=9.6767(2)
alpha=90 beta=91.7727(19) gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	1271.22(5)	1271.22(5)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	2(C10 H16 N), Cl6 Pt	2(C10 H16 N), Cl6 Pt
Sum formula	C20 H32 Cl6 N2 Pt	C20 H32 Cl6 N2 Pt
Mr	708.26	708.26
Dx,g cm-3	1.850	1.850
Z	2	2
Mu (mm-1)	16.206	16.206
F000	692.0	692.0
F000'	688.26	
h,k,lmax	13,14,11	13,14,11
Nref	2327	2327
Tmin,Tmax	0.358,0.445	0.109,0.545
Tmin'	0.002	

Correction method= # Reported T Limits: Tmin=0.109 Tmax=0.545
AbsCorr = ANALYTICAL

Data completeness= 1.000 Theta(max)= 68.223

R(reflections)= 0.0203(2180) wR2(reflections)= 0.0481(2327)

S = 1.072 Npar= 136

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
PLAT794_ALERT_5_G Tentative Bond Valency for Pt12 (II) . 2.89 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
0 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
2 **ALERT level G** = General information/check it is not something unexpected

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
0 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
0 ALERT type 4 Improvement, methodology, query or suggestion
1 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 22_06_2020_dt_btmaptcl61to2_n - ellipsoid plot

