

checkCIF (basic structural check) running

Checking for embedded fcf data in CIF ...

Found embedded fcf data in CIF. Extracting fcf data from uploaded CIF, please wait

checkCIF/PLATON (basic structural check)

Structure factors have been supplied for datablock(s) L1'CuCatBr4, L1'CuCatCl4, L1HCuCatCl4

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.

Please wait while processing

[CIF dictionary](#)

[Interpreting this report](#)

[Structure factor report](#)

Datablock: L1'CuCatCl4

Bond precision:	C-C = 0.0035 Å	Wavelength=0.71070
Cell:	a=19.7412(11) b=15.9152(8) c=29.6372(2)	
	alpha=90 beta=103.9780(9) gamma=90	
Temperature:	202 K	
	Calculated	Reported
Volume	9035.8(7)	9035.8(7)
Space group	C 2/c	C 1 2/c 1
Hall group	-C 2yc	-C 2yc
Moiety formula	2(C34 H46 Cl4 Cu N6 O2), 5(C2 H3 N)	C39 H53.5 Cl4 Cu N8.5 O2
Sum formula	C78 H107 Cl8 Cu2 N17 O4	C39 H53.5 Cl4 Cu N8.5 O2
Mr	1757.51	878.77
Dx,g cm-3	1.292	1.292
Z	4	8
Mu (mm-1)	0.762	0.762

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F000          3680.0          3680.0
F000'         3688.21
h,k,lmax      25,20,38          25,20,38
Nref          10379          10131
Tmin,Tmax     0.760,0.859      0.547,0.859
Tmin'         0.710
Correction method= # Reported T Limits: Tmin=0.547 Tmax=0.859
AbsCorr = MULTI-SCAN
Data completeness= 0.976          Theta(max)= 27.481
R(reflections)= 0.0476( 9623)      wR2(reflections)= 0.1187( 10131)
S = 1.139          Npar= 504

```

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

PLAT910_ALERT_3_B Missing # of FCF Reflection(s) Below Theta(Min). 15 Note

Author Response: Reduction of beam stop mask did not yield significant improvement. Most of those missing strong reflections appeared to be very strong and were treated as overflows. This is why it was old setting for the data collections.

🟡 Alert level C

PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ Please Check
 PLAT220_ALERT_2_C NonSolvent Resd 1 C Ueq(max) / Ueq(min) Range 3.1 Ratio
 PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C17 Check
 PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of C53 Check
 PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 5.797 Check
 PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 193 Report
 PLAT934_ALERT_3_C Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers .. 1 Check

🟡 Alert level G

CHEMS02_ALERT_1_G Please check that you have entered the correct

_publ_requested_category classification of your compound;

FI or CI or EI for inorganic; FM or CM or EM for metal-organic;

FO or CO or EO for organic.

From the CIF: _publ_requested_category CHOOSE FI FM FO CI CM CO or A

From the CIF: _chemical_formula_sum : C39 H53.5 Cl4 Cu1 N8.5 O2

PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ Please Check

PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ... 0.50 Check

PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 11.85 Why ?
 PLAT143_ALERT_4_G s.u. on c - Axis Small or Missing 0.00020 Ang.
 PLAT300_ALERT_4_G Atom Site Occupancy of C55 Constrained at 0.5 Check

And 4 other PLAT300 Alerts

More ...

PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 2) 67% Note

PLAT413_ALERT_2_G Short Inter XH3 .. XHn H52A ..H56B . 1.81 Ang.
 $1/2+x, -1/2+y, z = 3_545$ Check

PLAT794_ALERT_5_G Tentative Bond Valency for Cu1 (II) . 2.18 Info

PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 42 Note

PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ... 31 Note

PLAT941_ALERT_3_G Average HKL Measurement Multiplicity 3.0 Low

PLAT961_ALERT_5_G Dataset Contains no Negative Intensities Please Check

PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 6 Info

PLAT992_ALERT_5_G Repd & Actual _reflns_number_gt Values Differ by 1 Check

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

1 **ALERT level B** = A potentially serious problem, consider carefully

7 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight

19 **ALERT level G** = General information/check it is not something unexpected

4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

6 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

9 ALERT type 4 Improvement, methodology, query or suggestion

3 ALERT type 5 Informative message, check

Datablock: L1'CuCatBr4

Bond precision: C-C = 0.0061 Å Wavelength=0.71069

Cell: a=19.8335(7) b=16.3023(5) c=29.7487(10)

alpha=90 beta=107.918(3) gamma=90

Temperature: 204 K

	Calculated	Reported
Volume	9152.2(5)	9152.2(5)
Space group	C 2/c	C 1 2/c 1
Hall group	-C 2yc	-C 2yc
Moiety formula	2(C34 H46 Br4 Cu N6 O2), 5(C2 H3 N)	C39 H53.5 Br4 Cu N8.5 O2
Sum formula	C78 H107 Br8 Cu2 N17 O4	C39 H53.5 Br4 Cu N8.5 O2
Mr	2113.11	1056.57
Dx, g cm-3	1.534	1.533

Z	4	8
Mu (mm ⁻¹)	4.012	4.022
F000	4256.0	4256.0
F000'	4250.86	
h,k,lmax	25,21,38	25,21,38
Nref	10518	10344
Tmin,Tmax	0.396,0.547	1.000,1.000
Tmin'	0.192	

Correction method= # Reported T Limits: Tmin=1.000 Tmax=1.000
 AbsCorr = REFDELTA
 Data completeness= 0.983 Theta(max)= 27.482
 R(reflections)= 0.0581(8636) wR2(reflections)= 0.1118(10344)
 S = 1.145 Npar= 504

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

PLAT213_ALERT_2_B Atom C21 has ADP max/min Ratio 4.2 prolata

Author Response: These alerts are generated because there is a large amount of disorder in the structure.

PLAT220_ALERT_2_B NonSolvent Resd 1 C Ueq(max) / Ueq(min) Range 8.9 Ratio

Author Response: These alerts are generated because there is a large amount of disorder in the structure.

PLAT242_ALERT_2_B Low 'MainMol' Ueq as Compared to Neighbors of C23 Check

Author Response: These alerts are generated because there is a large amount of disorder in the structure.

PLAT910_ALERT_3_B Missing # of FCF Reflection(s) Below Theta(Min). 15 Note

Author Response: Reduction of beam stop mask did not yield significant improvement. Most of those missing strong reflections appeared to be very strong and were treated as overflows. This is why it was old setting for the data collections.

● Alert level C

PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ Please Check
 PLAT213_ALERT_2_C Atom C22 has ADP max/min Ratio 3.6 prolatt

Author Response: These alerts are generated because there is a large amount of disorder in the structure.

PLAT222_ALERT_3_C NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range 8.9 Ratio
 PLAT234_ALERT_4_C Large Hirshfeld Difference C22 --C23 . 0.20 Ang.
 PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C27 Check

Author Response: These alerts are generated because there is a large amount of disorder in the structure.

PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of C51 Check
 PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of C53 Check
 PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds 0.00609 Ang.
 PLAT360_ALERT_2_C Short C(sp3)-C(sp3) Bond C21 - C23 . 1.39 Ang.
 PLAT413_ALERT_2_C Short Inter XH3 .. XHn H22A ..H22A . 2.10 Ang.
 2-x,y,3/2-z = 2_756 Check
 PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 13.181 Check
 PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 3.059 Check
 PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 156 Report
 PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF 49 Note

Alert level G

CHEMS02_ALERT_1_G Please check that you have entered the correct
 _publ_requested_category classification of your compound;
 FI or CI or EI for inorganic; FM or CM or EM for metal-organic;
 FO or CO or EO for organic.
 From the CIF: _publ_requested_category CHOOSE FI FM FO CI CM CO or A
 From the CIF: _chemical_formula_sum : C39 H53.5 Br4 Cu1 N8.5 O2
 PLAT019_ALERT_1_G _diffn_measured_fraction_theta_full/*_max < 1.0 0.996 Report
 PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ Please Check
 PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ... 0.50 Check
 PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 27.33 Why ?
 PLAT300_ALERT_4_G Atom Site Occupancy of C55 Constrained at 0.5 Check

And 4 other PLAT300 Alerts

More ...

PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 2) 67% Note
 PLAT794_ALERT_5_G Tentative Bond Valency for Cu1 (II) . 2.20 Info
 PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 3 Note
 PLAT941_ALERT_3_G Average HKL Measurement Multiplicity 3.5 Low
 PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 3 Info

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8 ALERT type 3 Indicator that the structure quality may be low

10 ALERT type 4 Improvement, methodology, query or suggestion

1 ALERT type 5 Informative message, check

Datablock: L1HCuCatCl4

Bond precision:	C-C = 0.0120 Å	Wavelength=0.71069
Cell:	a=15.405(7)	b=13.137(6)
	alpha=90	beta=101.852(6)
		gamma=90
Temperature:	212 K	

	Calculated	Reported
Volume	4160(3)	4160(3)
Space group	P 2/c	P 1 2/c 1
Hall group	-P 2yc	-P 2yc
Moiety formula	C33 H47 B Cl4 Cu N6 O2 [+ solvent]	C33 H47 B Cl4 Cu N6 O2
Sum formula	C33 H47 B Cl4 Cu N6 O2 [+ solvent]	C33 H47 B Cl4 Cu N6 O2
Mr	775.93	775.94
Dx,g cm-3	1.239	1.239
Z	4	4
Mu (mm-1)	0.816	0.816
F000	1620.0	1620.0
F000'	1624.04	
h,k,lmax	20,17,27	19,17,27
Nref	9534	9475
Tmin,Tmax	0.863,0.960	1.000,1.000
Tmin'	0.783	

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

AbsCorr = REFDEL

Data completeness= 0.994 Theta(max)= 27.481

R(reflections)= 0.1099(6857) wR2(reflections)= 0.2762(9475)

S = 1.110 Npar= 424

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 A

PLAT482_ALERT_4_A Small D-H...A Angle Rep for N21 ..N22 . 34.30 Degree

Author Response: The angle of N21-H21___N22 is 34.31 degree. However, in this case, this intramolecular interaction is negligible. This comes from the short distance (0.87 Å) of N21-H21 bond.

Alert level B

PLAT213_ALERT_2_B Atom C11 has ADP max/min Ratio 5.0 prolat

Author Response: This alert is generated because there is a large amount of disorder in the structure.

PLAT213_ALERT_2_B Atom C28 has ADP max/min Ratio 4.1 prolat

Author Response: This alert is generated because there is a large amount of disorder in the structure.

PLAT213_ALERT_2_B Atom C29 has ADP max/min Ratio 4.7 prolat

Author Response: This alert is generated because there is a large amount of disorder in the structure.

PLAT220_ALERT_2_B NonSolvent Resd 1 C Ueq(max) / Ueq(min) Range 10.0 Ratio

Author Response: This alert is generated because there is a large amount of disorder in the structure.

PLAT242_ALERT_2_B Low 'MainMol' Ueq as Compared to Neighbors of C13 Check

Author Response: This alert is generated because there is a large amount of disorder in the structure.

PLAT242_ALERT_2_B Low 'MainMol' Ueq as Compared to Neighbors of C27 Check

Author Response: This alert is generated because there is a large amount of disorder in the structure.

PLAT356_ALERT_3_B Short X-BH3 distance B1 - H1 . 0.99 Ang.

Author Response: This alert is generated because there is a large amount of disorder in the structure.

PLAT910_ALERT_3_B Missing # of FCF Reflection(s) Below Theta(Min). 13 Note

Author Response: Reduction of beam stop mask did not yield significant improvement. Most of those missing strong reflections appeared to be very strong and were treated as overflows. This is why it was old setting for the data collections.

● Alert level C

PLAT082_ALERT_2_C High R1 Value 0.11 Report
 PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) 0.28 Report
 PLAT213_ALERT_2_C Atom C12 has ADP max/min Ratio 3.8 prolat

Author Response: This alert is generated because there is a large amount of disorder in the structure.

PLAT222_ALERT_3_C NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range 9.4 Ratio
 PLAT234_ALERT_4_C Large Hirshfeld Difference C27 --C29 . 0.24 Ang.
 PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C17 Check

Author Response: This alert is generated because there is a large amount of disorder in the structure.

PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds 0.012 Ang.
 PLAT360_ALERT_2_C Short C(sp3)-C(sp3) Bond C11 - C13 . 1.39 Ang.
 PLAT482_ALERT_4_C Small D-H...A Angle Rep for N21 ..N32 . 99.60 Degree

Author Response: The angle of N21-H21...N22 is 34.31 degree. However, in this case, this intramolecular interaction is negligible. This comes from the short distance (0.87 Å) of N21-H21 bond.

PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 20.539 Check

And 2 other PLAT906 Alerts

More ...

PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 41 Report
 PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF 11 Note

● Alert level G

CHEMS02_ALERT_1_G Please check that you have entered the correct
 _publ_requested_category classification of your compound;
 FI or CI or EI for inorganic; FM or CM or EM for metal-organic;
 FO or CO or EO for organic.

From the CIF: _publ_requested_category CHOOSE FI FM FO CI CM CO or A

From the CIF: _chemical_formula_sum : C33 H47 B1 Cl4 Cu1 N6 O2

PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	1 Report
PLAT072_ALERT_2_G	SHELXL First Parameter in WGHT Unusually Large	0.11 Report
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	15.98 Why ?
PLAT606_ALERT_4_G	VERY LARGE Solvent Accessible VOID(S) in Structure	! Info
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF . #	185 Check
	N21 -H21 -N22 1.555 1.555 1.555 34.30 Deg.	
PLAT869_ALERT_4_G	ALERTS Related to the Use of SQUEEZE Suppressed	! Info
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	5 Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	1.0 Low
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	1 Info

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11 ALERT type 3 Indicator that the structure quality may be low

7 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. 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

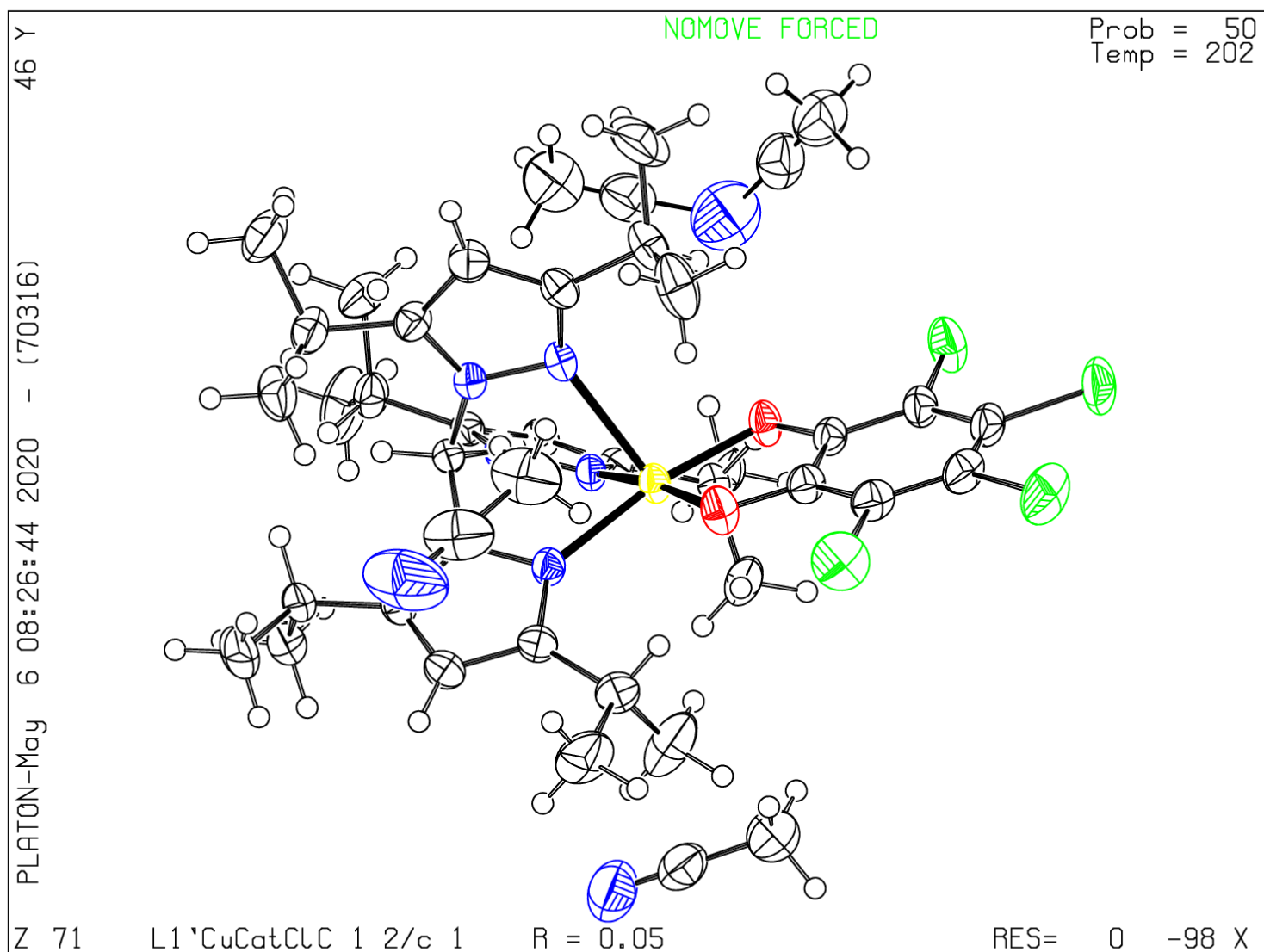
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section 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

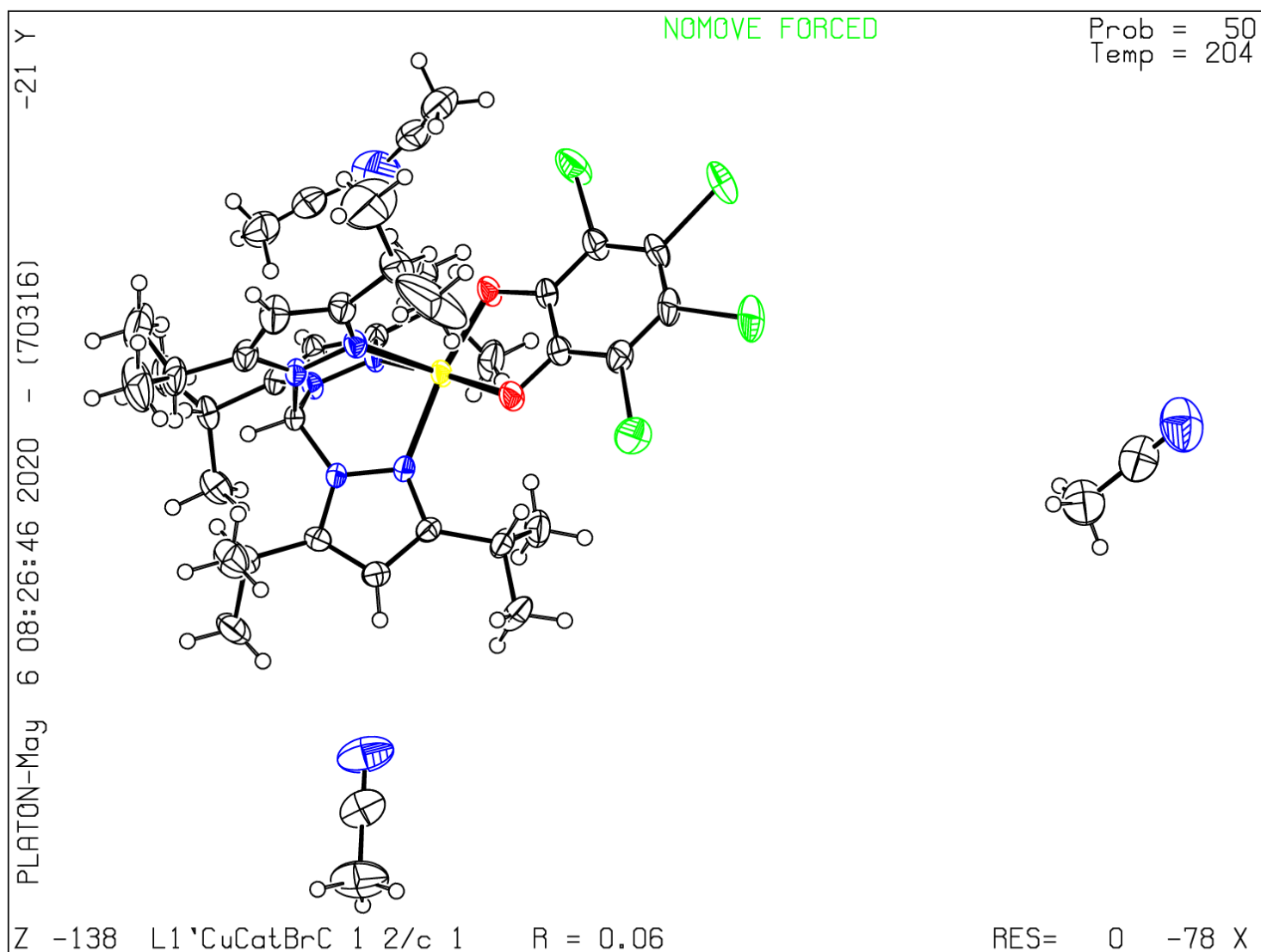
Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 22/04/2020; check.def file version of 09/03/2020

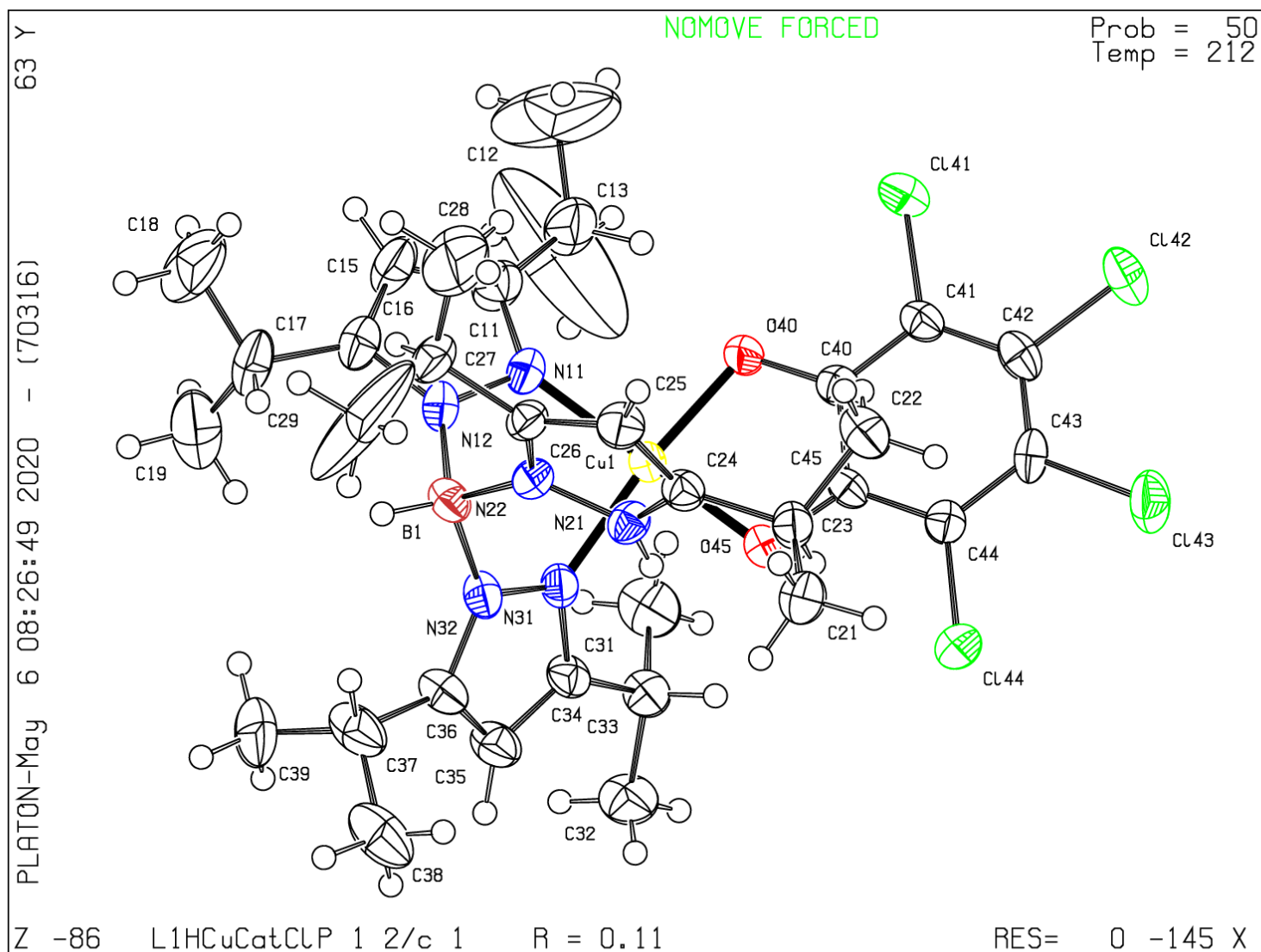
Datablock L1'CuCatCl4 - ellipsoid plot



Datablock L1'CuCatBr4 - ellipsoid plot



Datablock L1HCuCatCl4 - ellipsoid plot



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