Electronic Supplementary Information

Solvent-assisted coordination driven assembly of a supramolecular architecture featuring two types of connectivity from discrete nanocages

Zheng Niu\textsuperscript{a,b}, Lei Wang\textsuperscript{a}, Sheng Fang\textsuperscript{b}, Pui Ching Lan\textsuperscript{a}, Briana Aguila\textsuperscript{a}, Jason Perman\textsuperscript{a}, Jian-Gong Ma\textsuperscript{a,b}, Peng Cheng\textsuperscript{b}, Xiaopeng Li\textsuperscript{a} and Shengqian Ma\textsuperscript{*a}

\textsuperscript{a}Department of Chemistry, University of South Florida, CHE 205A, 4202 E. Fowler Avenue, Tampa, Florida 33620, U. S. A.

\textsuperscript{b}College of Chemistry, Key Laboratory of Advanced Energy Materials Chemistry (MOE), and Collaborative Innovation Center of Chemical Science and Engineering, Nankai University, Tianjin 300071, P. R. China

E-mail: sqma@usf.edu (S. Ma); mvbasten@nankai.edu.cn (J.-G. Ma)
Experimental Details

1. Materials and General methods

All chemical reagents were obtained from commercial sources and, unless otherwise noted, were used as received without further purification. Elemental analysis was performed on a Perkin–Elmer 240 CHN elemental analyzer. IR spectra were recorded on a Perkin Elmer UATR TWO FT-IR spectrophotometer. Powder X-ray diffraction measurements (PXRD) were recorded on a Bruker D8 Advance X-ray diffractometer using Cu Ka radiation. The simulated powder patterns were calculated by using Mercury 2.0. The NMR tests were performed on the Varian Unity Inova 400 spectrometer. Gas adsorption measurement was tested by Micromeritics ASAP 2020 surface area and porosity analyzer. Thermogravimetric analysis was performed on a Labsys NETZSCH TG 209 Setaram apparatus with a heating rate of 10°C min\(^{-1}\) under a nitrogen atmosphere.

2. Crystallographic studies and refinement of the crystal structures

Crystallographic data of 1 and 2 were collected with a SuperNova, Single source at offset, Eos diffractometer with a Mo Kα radiation (\(\lambda= 0.71073 \text{ Å}\)). All the structures were solved by direct methods and refined anisotropically by full-matrix least-squares techniques based on \(F^2\) using the SHELXS-97 and SHELXL-97 programs\(^1\) contained on Olex 2\(^2\). The electron density of disordered guest molecules in 1 and 2 were treated as a diffuse contribution using the program SQUEEZE\(^3\). The number of whole guest molecules in 1 and 2 was determined on the basis of TGA and EA. Anisotropic thermal parameters were assigned to all non-hydrogen atoms. The hydrogen atoms of the ligand were generated geometrically; the hydrogen atoms of the water molecules were located in Fourier-difference electron density maps and refined with isotropic temperature factors. The large amount of disorder solvent leads to the weak diffraction in the high angel area, thus makes the relative low resolution. This is very common phenomenon in the compound with big unit cell. Crystal data as well as details of data collection and refinement for the complexes are summarized in Table S1 and S2.
**Table S1.** Crystal data and structure refinement for 1 (0D nanocage, without solvent)

| Property                                      | Value                        |
|-----------------------------------------------|------------------------------|
| CCDC Number                                   | 1569639                      |
| Chemical formula                              | C$_{228}$H$_{204}$Cu$_{24}$N$_{12}$O$_{144}$ |
| Formula weight                                 | 6940.98                      |
| Radiation                                     | Mo Kα                        |
| Wavelength (Å)                                | 0.71073                      |
| Crystal system, space group                   | tetragonal, $I4/m$           |
| Unit cell parameter                           | $a = 28.6201(10)$ alpha = 90 |
|                                               | $b = 28.6201(10)$ beta = 90  |
|                                               | $c = 39.803(2)$ gamma = 90   |
| Volume (Å$^3$)                                 | 32603(3)                     |
| Z, Calculated density (g/cm$^3$)               | 2, 0.707                     |
| F(000)                                        | 7008                         |
| Crystal size (mm)                             | 0.5x0.4x0.2                  |
| Completeness (to theta)                       | 0.993 (25.01)                |
| Refinement method                             | Full-matrix least-squares on F$^2$ |
| Goodness-of-fit on F$^2$                      | 0.819                        |
| Final R indices [I>2sigma(I)]                 | $R = 0.0795$, $wR2 = 0.1971$ |
| Largest diff. Peak and hole                   | 0.53, -0.7                   |
| **Table S2.** Crystal data and structure refinement for 2 (3D nanocage architecture, without solvent) |
|---------------------------------------------------------------|
| CCDC Number | 1569640 |
| Chemical formula | C_{198}H_{145}Cu_{24}O_{139}S |
| Formula weight | 6305.15 |
| Radiation | Mo Kα |
| Wavelength (Å) | 0.71073 |
| Crystal system, space group | triclinic, P-1 |
| Unit cell parameter | $a = 24.5209(10)$  \( \alpha = 88.010(2) \)  
| | \( b = 25.3703(7) \)  \( \beta = 79.070(3) \)  
| | \( c = 37.0128(12) \)  \( \gamma = 75.949(3) \)  
| Volume (Å³) | 21930.1(13) |
| Z, Calculated density (g/cm³) | 2, 0.955 |
| F(000) | 6314 |
| Crystal size (mm) | 0.3×0.3×0.2 |
| Completeness (to theta) | 0.995 (20.816) |
| Refinement method | Full-matrix least-squares on F² |
| Goodness-of-fit on F² | 0.841 |
| Final R indices [I>2sigma(I)] | $R = 0.0840$, $wR2 = 0.2263$ |
| Largest diff. Peak and hole | 1.36, -0.67 |
Fig. S1. Connectivity between two neighboring nanocages in 2 and the orbicular connection unit.

3. The thermogravimetric analysis and powder X-ray diffraction measurement

Fig. S2. Thermogravimetric analysis of nanocage 1. The 44.06 % weight loss at 170 °C corresponds to the loss of fifty-nine guest DMF molecules and thirty-six guest MeOH molecules per cell, which is accord with the molecular formulation of 1.
Fig. S3. Thermogravimetric analysis of nanocage architecture 2. The 35.82 % weight loss at 240 °C corresponds to the loss of eighteen guest DMSO molecules and sixty-six guest MeOH molecules per cell, which is accord with the molecular formulation of 2.

Fig. S4. Comparison of experimental and simulated powder XRD patterns of 2.
Fig. S5. The powder XRD patterns of 2 before the catalysis reaction and after the catalysis reaction.

4. ESI measurements.

ESI-MS was conducted on Waters Synapt G2 mass spectrometer under the following conditions: ESI capillary voltage, 4.5 kV; sample cone voltage, 15 V; extraction cone voltage, 0.3 V; source temperature 120 °C; desolvation temperature, 150 °C; cone gas flow, 15 L/h; desolvation gas flow, 700 L/h (N₂).
Fig. S6. ESI-MS spectra of reaction mixture a) before heating and b) after heating for 1h.

Fig. S7. Isotope pattern (blue for calculated value and red for measured value) of the individual nanocage ([Cu_{24}(C_8O_5H_4)_{24}(DMF)_n(H_2O)_6+2H^+])^{2+} n=0,1,2 from left to right).
Fig. S8. Isotope pattern (blue for calculated value and red for measured value) of the nanocage dimer ([Cu$_{48}$(C$_8$O$_5$H$_4$)$_{48}$(DMSO)$_n$(H$_2$O)$_{19}$ + $3\text{H}^+$])$^{3+}$ n=1, 2, 3, 4, 5, 6 from left to right).
Fig. S9. Isotope pattern (blue for calculated value and red for measured value) of the nanocage dimer (\(\text{[Cu}_{48}(\text{C}_8\text{O}_5\text{H}_4)_{48}(\text{DMSO})_{n}(\text{H}_2\text{O})_{19}+3\text{H}^+\]^{3+}\)) \(n=1, 2, 3, 4, 5, 6\) from left to right).
5. Low-Pressure Gas Sorption Measurements.

The CO$_2$ (99.999 %) adsorption/desorption isotherms were measured volumetrically using a Micromeritics ASAP 2020 surface area analyzer. Before analysis, nanocage architecture 2 were soaked in EtOH for 6 hours with replacing the solvent with fresh EtOH every 1 hour. Then, the samples were processed by using Tousimi Samdri PVT-30 critical point dryer. After that, the samples were charged into a sample tube and activated at 40 °C for 2 hours by using the “outgas” function of the surface area analyzer, respectively. Helium (99.999 %) was used for the estimation of the free space (dead volume). In the CO$_2$ adsorption isotherms measurement at 195K, to provide the relative pressure P/P$_0$ accurately at each data point, the saturation pressure P$_0$ was monitored and measured throughout the gases’ analyses by a dedicated saturation pressure transducer. The specific surface areas were determined using the Brunauer-Emmett-Teller (BET) from the CO$_2$ sorption data. When applying the BET theory, we made sure that our analysis satisfied the two consistency criteria as detailed by Walton and co-workers$^4$.

References:

(1) G. M. Sheldrick, Acta Cryst., 2008, A64, 112.

(2) O. V. Dolomanov, L. J. Bourhis, R. J. Gildea, J. A. K. Howard and H. Puschmann, J. Appl. Cryst., 2009, 42, 339.

(3) A.L. Spek, Acta Cryst. 2009, D65, 148.
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: 1

| Bond precision: | C-C = 0.0095 Å | Wavelength=0.71073 |
|-----------------|-----------------|--------------------|
| Cell:           | a=28.6201(10)   | b=28.6201(10)      | c=39.803(2) |
| alpha=90       | beta=90        | gamma=90          |
| Temperature:    | 129 K           |                    |
| Volume          | Calculated      | Reported           |
| Space group     | I 4/m           | I 4/m              |
| Hall group      | -I 4            | -I 4               |
| Moiety formula  | C228 H204 Cu24 N12 O144 [+ solvent] | C228 H204 Cu24 N12 O144 |
| Sum formula     | C228 H204 Cu24 N12 O144 [+ solvent] | C228 H204 Cu24 N12 O144 |
| Mr              | 6941.24         | 6940.98            |
| Dx, g cm−3      | 0.707           | 0.707              |
| Z                | 2               | 2                  |
| Mu (mm−1)       | 0.810           | 0.810              |
| F000            | 7008.0          | 7008.0             |
| F000′           | 7026.99         |                    |
| h,k,lmax        | 34,34,47        | 33,34,47           |
| Nref            | 14602           | 14507              |
| Tmin,Tmax       | 0.685,0.850     | 0.754,1.000        |
| Tmin’           | 0.660           |                    |

Correction method= # Reported T Limits: Tmin=0.754 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.993  Theta(max)= 25.010

R(reflections)= 0.0795 (5010)  wR2(reflections)= 0.2265 (14507)

S = 0.819  Npar= 461
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
| Alert | Description |
|-------|-------------|
| PLAT026_ALERT_3_B | Ratio Observed / Unique Reflections (too) Low .. 35 % |
| PLAT355_ALERT_3_B | Long O-H (X0.82,N0.98A) O1D - HIDA .. 1.12 Ang. |
| PLAT369_ALERT_2_B | Long C(sp2)-C(sp2) Bond C35 - C41 .. 1.59 Ang. |
| PLAT420_ALERT_2_B | D-H Without Acceptor O1D -- H1DA ... Please Check |
| PLAT420_ALERT_2_B | D-H Without Acceptor O1D -- H1DB ... Please Check |
| PLAT420_ALERT_2_B | D-H Without Acceptor O18 -- H18 ... Please Check |
| PLAT420_ALERT_2_B | D-H Without Acceptor O34 -- H34 ... Please Check |
| PLAT420_ALERT_2_B | D-H Without Acceptor O47 -- H47 ... Please Check |
| PLAT420_ALERT_2_B | D-H Without Acceptor O51 -- *H51A ... Please Check |
| PLAT420_ALERT_2_B | D-H Without Acceptor O51 -- *H51B ... Please Check |
| PLAT990_ALERT_1_B | Deprecated .res/.hkl Input Style SQUEEZE job ... ! Note |

### Alert level C
| Alert | Description |
|-------|-------------|
| PLAT018_ALERT_1_C | _diffrn_measured_fraction_theta_max .NE. *_full ! Check |
| PLAT220_ALERT_2_C | Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range 3.6 Ratio |
| PLAT241_ALERT_2_C | High ‘MainMol’ Ueq as Compared to Neighbors of O32 Check |
| PLAT241_ALERT_2_C | High ‘MainMol’ Ueq as Compared to Neighbors of O45 Check |
| PLAT241_ALERT_2_C | High ‘MainMol’ Ueq as Compared to Neighbors of C1 Check |
| PLAT242_ALERT_2_C | Low ‘MainMol’ Ueq as Compared to Neighbors of Cu1 Check |
| PLAT242_ALERT_2_C | Low ‘MainMol’ Ueq as Compared to Neighbors of Cu2 Check |
| PLAT242_ALERT_2_C | Low ‘MainMol’ Ueq as Compared to Neighbors of Cu4 Check |
| PLAT242_ALERT_2_C | Low ‘MainMol’ Ueq as Compared to Neighbors of O5 Check |
| PLAT242_ALERT_2_C | Low ‘MainMol’ Ueq as Compared to Neighbors of N48 Check |
| PLAT242_ALERT_2_C | Low ‘MainMol’ Ueq as Compared to Neighbors of C15 Check |
| PLAT242_ALERT_2_C | Low ‘MainMol’ Ueq as Compared to Neighbors of C31 Check |
| PLAT250_ALERT_2_C | Large U3/U1 Ratio for Average U(i,j) Tensor ... 2.1 Note |
| PLAT34_ALERT_2_C | Small Average Benzene C-C Dist. C22 -C27 1.37 Ang. |
| PLAT341_ALERT_3_C | Low Bond Precision on C-C Bonds................. 0.0095 Ang. |
| PLAT369_ALERT_2_C | Long C(sp2)-C(sp2) Bond C6 - C12 .. 1.54 Ang. |
| PLAT369_ALERT_2_C | Long C(sp2)-C(sp2) Bond C10 - C15 .. 1.54 Ang. |
| PLAT369_ALERT_2_C | Long C(sp2)-C(sp2) Bond C22 - C28 .. 1.53 Ang. |
| PLAT369_ALERT_2_C | Long C(sp2)-C(sp2) Bond C26 - C31 .. 1.54 Ang. |
| PLAT369_ALERT_2_C | Long C(sp2)-C(sp2) Bond C39 - C44 .. 1.54 Ang. |

### Alert level G
| Alert | Description |
|-------|-------------|
| PLAT002_ALERT_2_G | Number of Distance or Angle Restraints on AtSite 2 Note |
| PLAT003_ALERT_2_G | Number of Uiso or Uij Restrained non-H Atoms ... 4 Report |
| PLAT005_ALERT_3_G | No Embedded Refinement Details found in the CIF Please Do ! |
| PLAT007_ALERT_5_G | Number of Unrefined Donor-H Atoms ............... 7 Report |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H51A is Constrained at 0.5 Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H51B is Constrained at 0.5 Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H53A is Constrained at 0.5 Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H53B is Constrained at 0.5 Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H53C is Constrained at 0.5 Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H55A is Constrained at 0.5 Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H55B is Constrained at 0.5 Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H55C is Constrained at 0.5 Check |
| PLAT606_ALERT_4_G |VERY LARGE Solvent Accessible VOID(S) in Structure ! Info |
| PLAT720_ALERT_4_G | Number of Unusual/Non-Standard Labels ............. 5 Note |
| PLAT789_ALERT_4_G | Atoms with Negative _atom_site_disorder_group # 3 Check |
| PLAT802_ALERT_4_G | CIF Input Record(s) with more than 80 Characters 1 Info |
0 ALERT level A = Most likely a serious problem - resolve or explain
12 ALERT level B = A potentially serious problem, consider carefully
21 ALERT level C = Check. Ensure it is not caused by an omission or oversight
18 ALERT level G = General information/check it is not something unexpected

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
29 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
13 ALERT type 4 Improvement, methodology, query or suggestion
2 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.
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: 2

Bond precision: C-C = 0.0201 Å

Wavelength=0.71073

Cell:
\[ a = 24.5209(10) \quad b = 25.3703(7) \quad c = 37.0128(12) \]
\[ \alpha = 88.010(2) \quad \beta = 79.070(3) \quad \gamma = 75.949(3) \]

Temperature: 128 K

Calculated
Reported

Volume: 21930.1(13)
21930.1(13)

Space group: P -1
P -1

Hall group: -P 1
-P 1

Moiety formula:
C198 H145 Cu24 O139 S [+ solvent]
C198 H145 Cu24 O139 S

Sum formula:
C198 H145 Cu24 O139 S [+ solvent]
C198 H145 Cu24 O139 S

Mr: 6305.33
6305.15

Dx, g cm\(^{-3}\): 0.955
0.955

Z: 2
2

\( \mu (\text{mm}^{-1}) \): 1.201
1.201

F(000): 6314.0
6314.0

F(000)': 6333.01

\( h, k, l \text{max} \): 24, 25, 37
24, 25, 36

Nref: 45941
45715

Tmin, Tmax: 0.567, 0.786
0.661, 1.000

Tmin': 0.543

Correction method= # Reported T Limits: Tmin=0.661 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.995
Theta(max)= 20.816

R(reflections)= 0.0840 (18111)
wR2(reflections)= 0.2263 (45715)

S = 0.841
Npar= 2634
The following ALERTS were generated. Each ALERT has the format
\texttt{test-name\_ALERT\_alert-type\_alert-level}.
Click on the hyperlinks for more details of the test.

### Alert level A

| ALERT | Test Name | Alert Type | Alert Level | Details |
|-------|-----------|------------|-------------|---------|
| THETM01_ALERT_3_A | The value of \(\sin(\theta_{max})/\text{wavelength}\) is less than 0.550 |
| | Calculated \(\sin(\theta_{max})/\text{wavelength} = 0.5000\) |

### Alert level B

| ALERT | Test Name | Alert Type | Alert Level | Details |
|-------|-----------|------------|-------------|---------|
| PLAT213_ALERT_2_B | Atom O115 | has ADP max/min Ratio | 4.7 prolat |
| PLAT213_ALERT_2_B | Atom O238 | has ADP max/min Ratio | 4.3 prolat |
| PLAT213_ALERT_2_B | Atom C3 | has ADP max/min Ratio | 4.2 prolat |
| PLAT213_ALERT_2_B | Atom C350 | has ADP max/min Ratio | 4.8 oblate |
| PLAT213_ALERT_2_B | Atom C732 | has ADP max/min Ratio | 4.4 prolat |
| PLAT341_ALERT_3_B | Low Bond Precision on C-C Bonds | \(\ldots\) | 0.02015 Ang. |
| PLAT369_ALERT_2_B | Long C(sp2)-C(sp2) Bond C1 - C610_g | \(\ldots\) | 1.58 Ang. |
| PLAT369_ALERT_2_B | Long C(sp2)-C(sp2) Bond C2 - C33_b | \(\ldots\) | 1.62 Ang. |
| PLAT369_ALERT_2_B | Long C(sp2)-C(sp2) Bond C14 - C489 | \(\ldots\) | 1.57 Ang. |
| PLAT369_ALERT_2_B | Long C(sp2)-C(sp2) Bond C22 - C596 | \(\ldots\) | 1.61 Ang. |
| PLAT369_ALERT_2_B | Long C(sp2)-C(sp2) Bond C42 - C275 | \(\ldots\) | 1.58 Ang. |
| PLAT369_ALERT_2_B | Long C(sp2)-C(sp2) Bond C208 - C721 | \(\ldots\) | 1.59 Ang. |
| PLAT369_ALERT_2_B | Long C(sp2)-C(sp2) Bond C231 - C695 | \(\ldots\) | 1.59 Ang. |
| PLAT369_ALERT_2_B | Long C(sp2)-C(sp2) Bond C340 - C673 | \(\ldots\) | 1.61 Ang. |
| PLAT369_ALERT_2_B | Long C(sp2)-C(sp2) Bond C425 - C715 | \(\ldots\) | 1.61 Ang. |
| PLAT369_ALERT_2_B | Long C(sp2)-C(sp2) Bond C458 - C728 | \(\ldots\) | 1.57 Ang. |
| PLAT414_ALERT_2_B | Short Intra D-H..H-X | H410 - H580 | \(\ldots\) | 1.86 Ang. |
| PLAT417_ALERT_2_B | Short Inter D-H..H-D | H6 - H117 | \(\ldots\) | 2.00 Ang. |
| PLAT420_ALERT_2_B | D-H Without Acceptor | O1 - H1 | Please Check |
| PLAT420_ALERT_2_B | D-H Without Acceptor | O2 - H2 | Please Check |
| PLAT420_ALERT_2_B | D-H Without Acceptor | O12 - H12A | Please Check |
| PLAT420_ALERT_2_B | D-H Without Acceptor | O128 - H12C | Please Check |
| PLAT420_ALERT_2_B | D-H Without Acceptor | O132 - H13A | Please Check |
| PLAT420_ALERT_2_B | D-H Without Acceptor | O132 - H13B | Please Check |
| PLAT420_ALERT_2_B | D-H Without Acceptor | O148 - H14A | Please Check |
| PLAT420_ALERT_2_B | D-H Without Acceptor | O148 - H14B | Please Check |
| PLAT420_ALERT_2_B | D-H Without Acceptor | O15 - H15A | Please Check |
| PLAT420_ALERT_2_B | D-H Without Acceptor | O15 - H15B | Please Check |
| PLAT420_ALERT_2_B | D-H Without Acceptor | O214 - H21A | Please Check |
| PLAT420_ALERT_2_B | D-H Without Acceptor | O214 - H21B | Please Check |
| PLAT420_ALERT_2_B | D-H Without Acceptor | O238 - H23A | Please Check |
| PLAT420_ALERT_2_B | D-H Without Acceptor | O238 - H23B | Please Check |
| PLAT420_ALERT_2_B | D-H Without Acceptor | O27 - H27 | Please Check |
| PLAT420_ALERT_2_B | D-H Without Acceptor | O305 - H30A | Please Check |
| PLAT420_ALERT_2_B | D-H Without Acceptor | O35 - H35 | Please Check |
| PLAT420_ALERT_2_B | D-H Without Acceptor | O41 - H41 | Please Check |
| PLAT420_ALERT_2_B | D-H Without Acceptor | O43 - H43 | Please Check |
| PLAT420_ALERT_2_B | D-H Without Acceptor | O452 - H45A | Please Check |
| PLAT420_ALERT_2_B | D-H Without Acceptor | O452 - H45B | Please Check |
| PLAT420_ALERT_2_B | D-H Without Acceptor | O50 - H50A | Please Check |
| PLAT420_ALERT_2_B | D-H Without Acceptor | O50 - H50B | Please Check |
| PLAT420_ALERT_2_B | D-H Without Acceptor | O55 - H55 | Please Check |
| PLAT420_ALERT_2_B | D-H Without Acceptor | O58 - H58A | Please Check |
| PLAT420_ALERT_2_B | D-H Without Acceptor | O58 - H58B | Please Check |
| PLAT420_ALERT_2_B | D-H Without Acceptor | O63 - H63 | Please Check |
| PLAT420_ALERT_2_B | D-H Without Acceptor | O68 - H68 | Please Check |
| PLAT420_ALERT_2_B | D-H Without Acceptor | O72 - H72A | Please Check |
| PLAT420_ALERT_2_B | D-H Without Acceptor | O72 - H72B | Please Check |
Alert level C

RINTA01_ALERT_3_C The value of Rint is greater than 0.12
Rint given 0.137

PLAT018_ALERT_1_C _diffrn_measured_fraction_theta_max .NE. *_full ! Check
PLAT020_ALERT_3_C The value of Rint is greater than 0.12 ........... 0.137 Report
PLAT026_ALERT_3_C Ratio Observed / Unique Reflections (too) Low .. 40 %
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density .... 2.02 Report
PLAT213_ALERT_2_C Atom O55 has ADP max/min Ratio ..... 4.0 prolat
PLAT213_ALERT_2_C Atom O72 has ADP max/min Ratio ...... 3.1 prolat
PLAT213_ALERT_2_C Atom O133 has ADP max/min Ratio ...... 3.2 prolat
PLAT213_ALERT_2_C Atom O206 has ADP max/min Ratio ...... 3.3 prolat
PLAT213_ALERT_2_C Atom O257 has ADP max/min Ratio ...... 3.8 prolat
PLAT213_ALERT_2_C Atom O384 has ADP max/min Ratio ...... 3.1 prolat
PLAT213_ALERT_2_C Atom C1 has ADP max/min Ratio ...... 3.5 prolat
PLAT213_ALERT_2_C Atom C17 has ADP max/min Ratio ...... 3.2 prolat
PLAT213_ALERT_2_C Atom C20 has ADP max/min Ratio ...... 3.1 prolat
PLAT213_ALERT_2_C Atom C654 has ADP max/min Ratio ...... 4.0 prolat
PLAT220_ALERT_2_C Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range 5.2 Ratio
PLAT220_ALERT_2_C Non-Solvent Resd 1 O Ueq(max)/Ueq(min) Range 5.3 Ratio
PLAT222_ALERT_3_C Non-Solvent Resd 1 H Uiso(max)/Uiso(min) Range 7.2 Ratio
PLAT241_ALERT_2_C High ‘MainMol’ Ueq as Compared to Neighbors of 08 Check
PLAT241_ALERT_2_C High ‘MainMol’ Ueq as Compared to Neighbors of 043 Check
PLAT241_ALERT_2_C High ‘MainMol’ Ueq as Compared to Neighbors of 093 Check
PLAT241_ALERT_2_C High ‘MainMol’ Ueq as Compared to Neighbors of 0133 Check
PLAT241_ALERT_2_C High ‘MainMol’ Ueq as Compared to Neighbors of 0226 Check
PLAT241_ALERT_2_C High ‘MainMol’ Ueq as Compared to Neighbors of 0270 Check
PLAT241_ALERT_2_C High ‘MainMol’ Ueq as Compared to Neighbors of 0316 Check
PLAT241_ALERT_2_C High ‘MainMol’ Ueq as Compared to Neighbors of 0363 Check
PLAT241_ALERT_2_C High ‘MainMol’ Ueq as Compared to Neighbors of 0408 Check
PLAT241_ALERT_2_C High ‘MainMol’ Ueq as Compared to Neighbors of 0543 Check
PLAT241_ALERT_2_C High ‘MainMol’ Ueq as Compared to Neighbors of 0545 Check
PLAT241_ALERT_2_C High ‘MainMol’ Ueq as Compared to Neighbors of 0607 Check
PLAT241_ALERT_2_C High ‘MainMol’ Ueq as Compared to Neighbors of 049 Check
PLAT241_ALERT_2_C High ‘MainMol’ Ueq as Compared to Neighbors of 0144 Check
PLAT241_ALERT_2_C High ‘MainMol’ Ueq as Compared to Neighbors of 0486 Check
PLAT241_ALERT_2_C High ‘MainMol’ Ueq as Compared to Neighbors of 0532 Check
PLAT241_ALERT_2_C High ‘MainMol’ Ueq as Compared to Neighbors of 0562 Check
PLAT241_ALERT_2_C High ‘MainMol’ Ueq as Compared to Neighbors of 0590 Check
PLAT241_ALERT_2_C High ‘MainMol’ Ueq as Compared to Neighbors of 0634 Check
PLAT241_ALERT_2_C High ‘MainMol’ Ueq as Compared to Neighbors of 0637 Check
PLAT241_ALERT_2_C Low ‘MainMol’ Ueq as Compared to Neighbors of Cu7 Check
| Alert level | Description |
|-------------|-------------|
| G           | Number of Distance or Angle Restraints on AtSite | 27 Note |
| G           | Number of Uiso or Uij Restained non-H Atoms ... | 82 Report |
| G           | Polymeric Structure Found with Maximum Dimension | 3 Info |
| G           | No Embedded Refinement Details found in the CIF Please Do ! | |
| G           | Number of Unrefined Donor-H Atoms .............. | 47 Report |
| G           | Check Large C6 Ring C-C Range C33 -C665 | 0.17 Ang. |
| G           | Check Large C6 Ring C-C Range C156 -C634 | 0.20 Ang. |
| G           | Check Large C6 Ring C-C Range C292 -C644 | 0.17 Ang. |
| G           | Short Inter X...Y Contact O2 .. C612 .. | 3.00 Ang. |
| G           | VERY LARGE Solvent Accessible VOID(S) in Structure ! Info |
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.

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**PLATON version of 13/08/2017; check.def file version of 27/07/2017**
