# Electronic Supplementary Information

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

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## 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 (λ= 0.71073 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) | |
|---|---|
| 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, *I*4/*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) | 0.5×0.4×0.2 |
| 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, *wR*2 = 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)<br>*b* = 25.3703(7) *beta* = 79.070(3)<br>*c* = 37.0128(12) *gamma* = 75.949(3) |
| Volume ($Å^3$) | 21930.1(13) |
| Z, Calculated density ($g/cm^3$) | 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 $F^2$ |
| Goodness-of-fit on $F^2$ | 0.841 |
| Final R indices [I>2sigma(I)] | *R* = 0.0840, *wR*2 = 0.2263 |
| Largest diff. Peak and hole | 1.36, -0.67 |

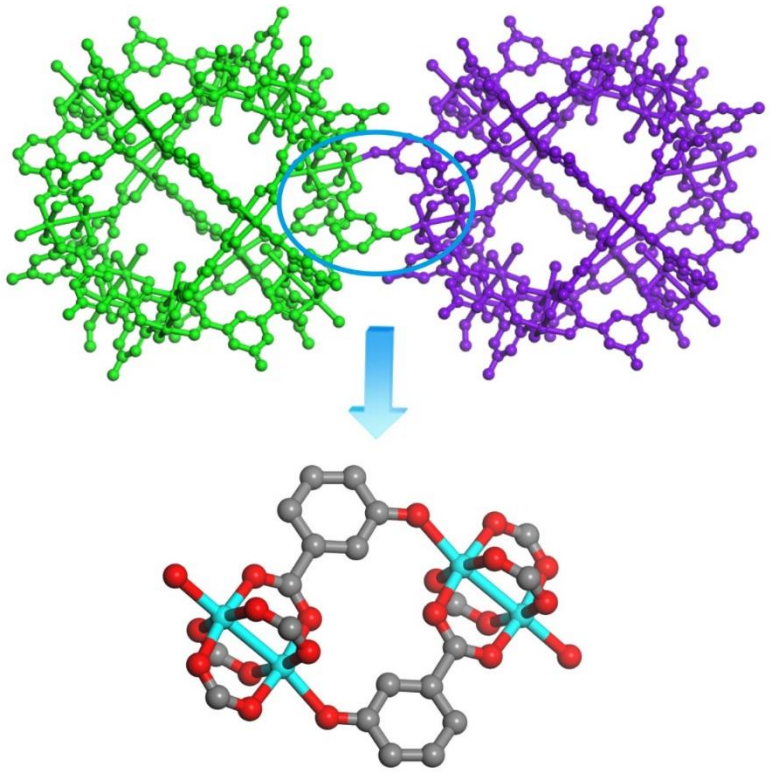

**Fig. S1.** Connectivity between two neighboring nanocages in **2** and the orbicular connection unit.

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

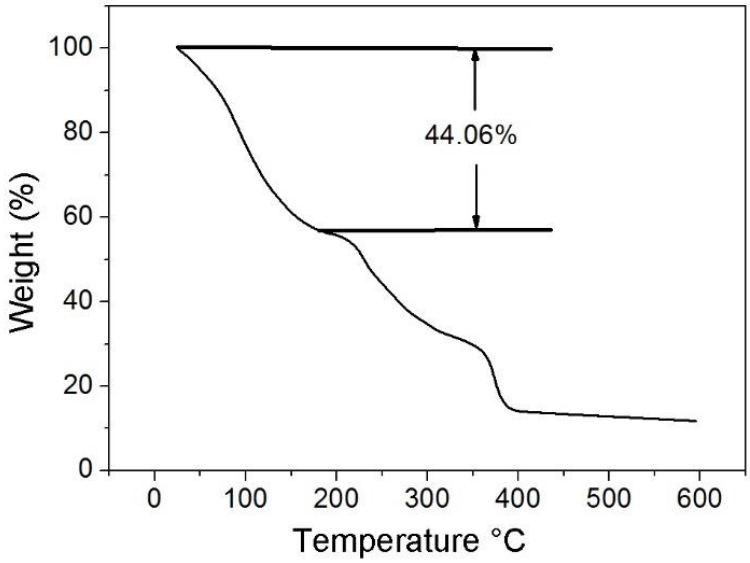


**Fig. S2.** Thermogravimetric analysis of nanocage **1**. The 44.06 % weight loss at 170 °C corresponds to the loss of fifty-nine guest DMF molecules and thirty-six guest MeOH molecules per cell, which is accord with the molecular formulation of **1.**

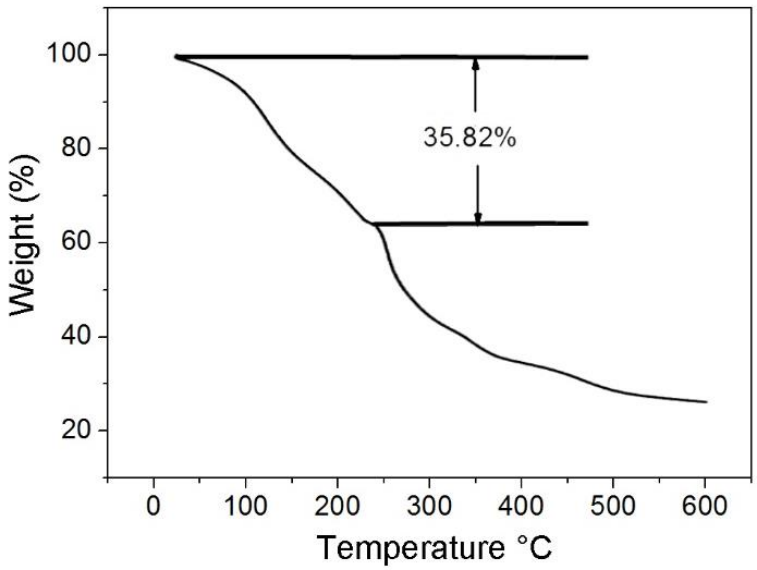


**Fig. S3.** Thermogravimetric analysis of nanocage architecture **2**. The 35.82 % weight loss at 240 °C corresponds to the loss of eighteen guest DMSO molecules and sixty-six guest MeOH molecules per cell, which is accord with the molecular formulation of **2**.

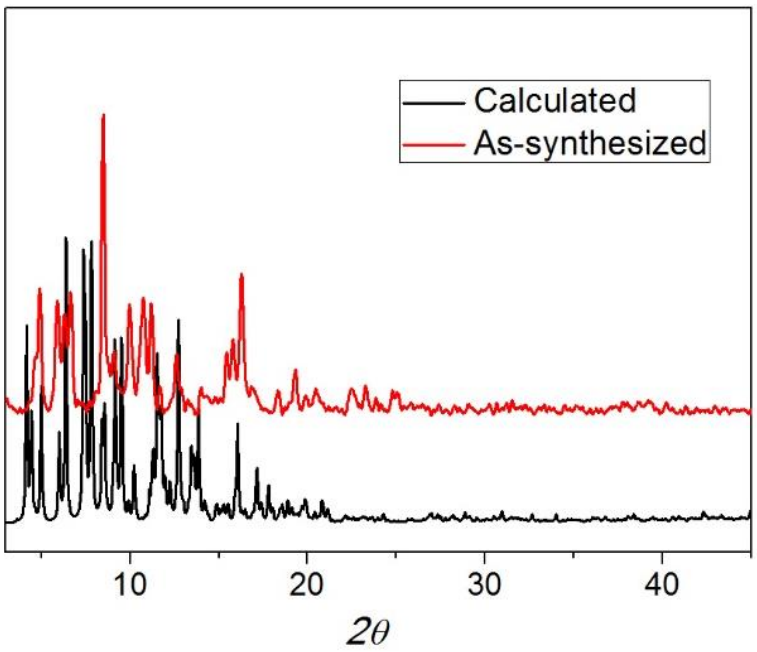


**Fig. S4.** Comparison of experimental and simulated powder XRD patterns of **2.**

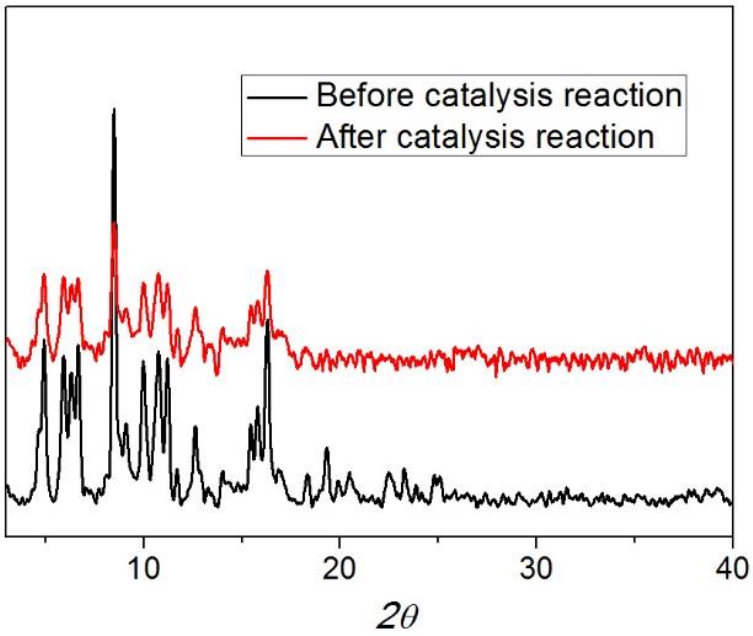


**Fig. S5.** The powder XRD patterns of **2** before the catalysis reaction and after the catalysis reaction.

**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 ºC; desolvation temperature, 150 ºC; cone gas flow, 15 L/h; desolvation gas flow, 700 L/h ($N_2$).

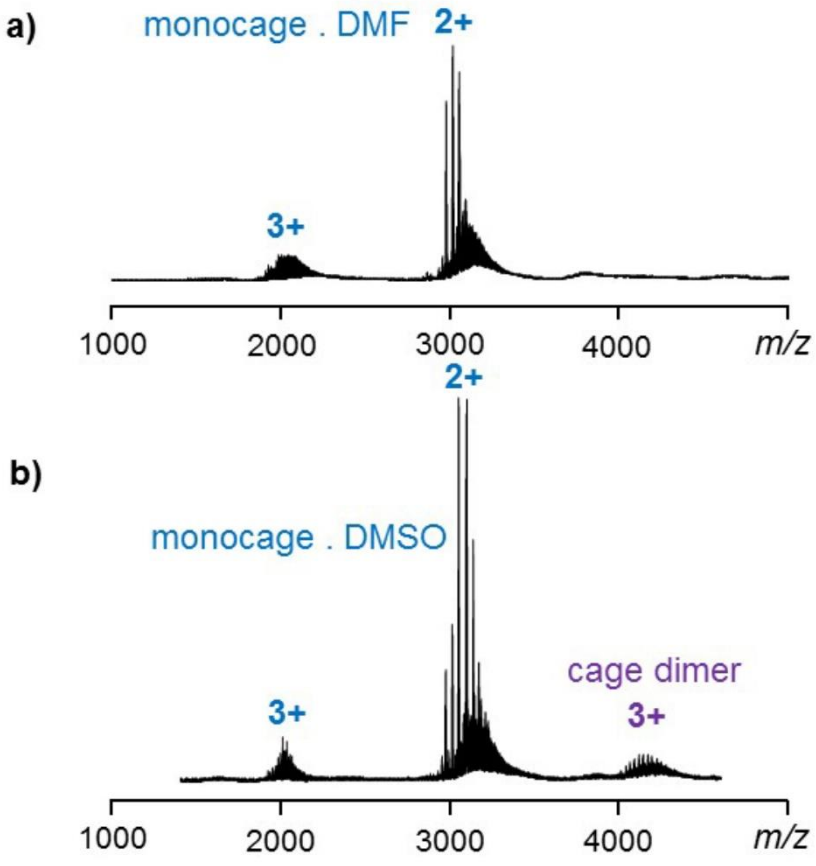


**Fig. S6.** ESI-MS spectra of reaction mixture a) before heating and b) after heating for 1h.

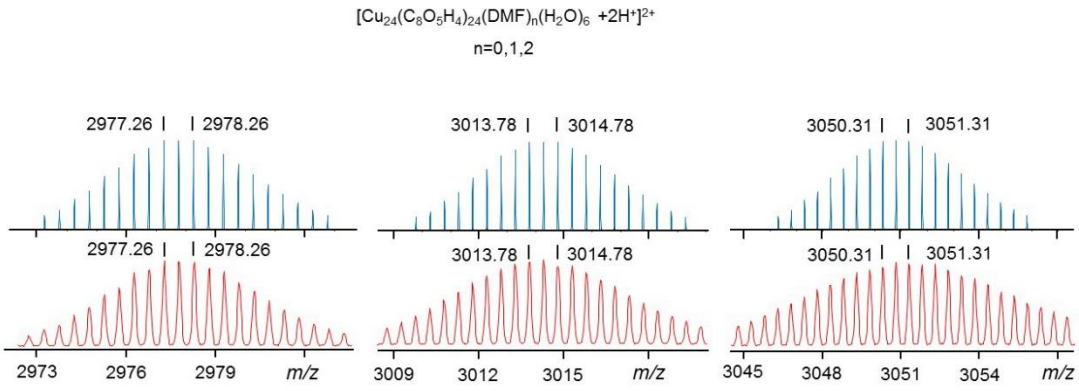


**Fig. S7.** Isotope pattern (blue for calculated value and red for measured value)of the individual nanocage ($[Cu_{24}(C_8O_5H_4)_{24}(DMF)_n(H_2O)_6 +2H^+]^{2+}$ n=0,1,2 from left to right).

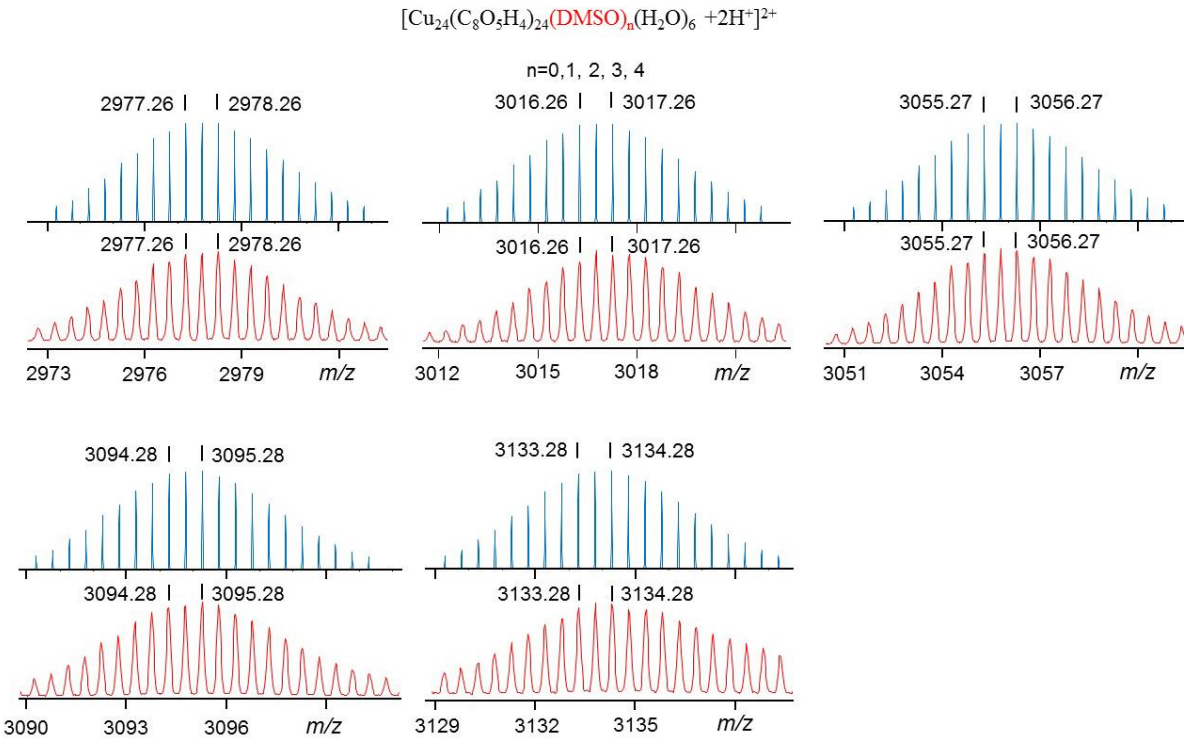


**Fig. S8.** Isotope pattern (blue for calculated value and red for measured value)of the nanocage dimer ($[Cu_{48}(C_8O_5H_4)_{48}(DMSO)_n(H_2O)_{19}+3H^+]^{3+}$ n=1,2, 3, 4, 5, 6 from left to right).

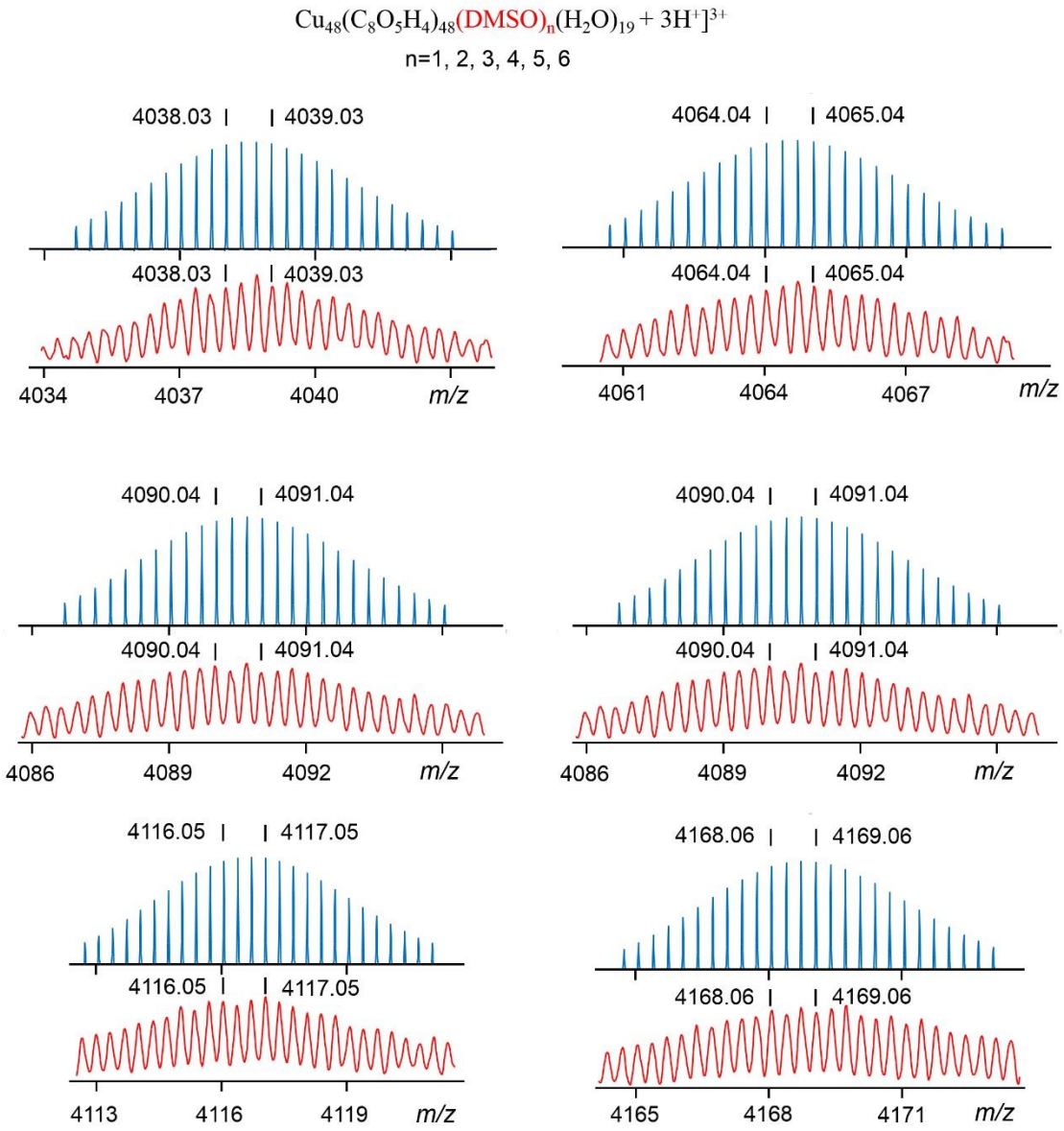


**Fig. S9.** Isotope pattern (blue for calculated value and red for measured value)of the nanocage dimer ($[Cu_{48}(C_8O_5H_4)_{48}(DMSO)_n(H_2O)_{19} + 3H^+]^{3+}$ n=1,2, 3, 4, 5, 6 from left to right).

## 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

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```
Bond precision:  C-C = 0.0095 A          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
```

| | Calculated | Reported |
|---|---|---|
| Volume | 32603(3) | 32603(3) |
| 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
```

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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.

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## Alert level B

PLAT026_ALERT_3_B Ratio Observed / Unique Reflections (too) Low .. 35 %
PLAT355_ALERT_3_B Long O-H (X0.82,N0.98A) O1D - H1DA .. 1.12 Ang.
PLAT355_ALERT_3_B Long O-H (X0.82,N0.98A) O1D - H1DB .. 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

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## Alert level C

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
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C49 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
PLAT334_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.

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## Alert level G

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_5_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

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PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        25 Note
PLAT869_ALERT_4_G ALERTS Related to the use of SQUEEZE Suppressed          ! Info
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   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
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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. 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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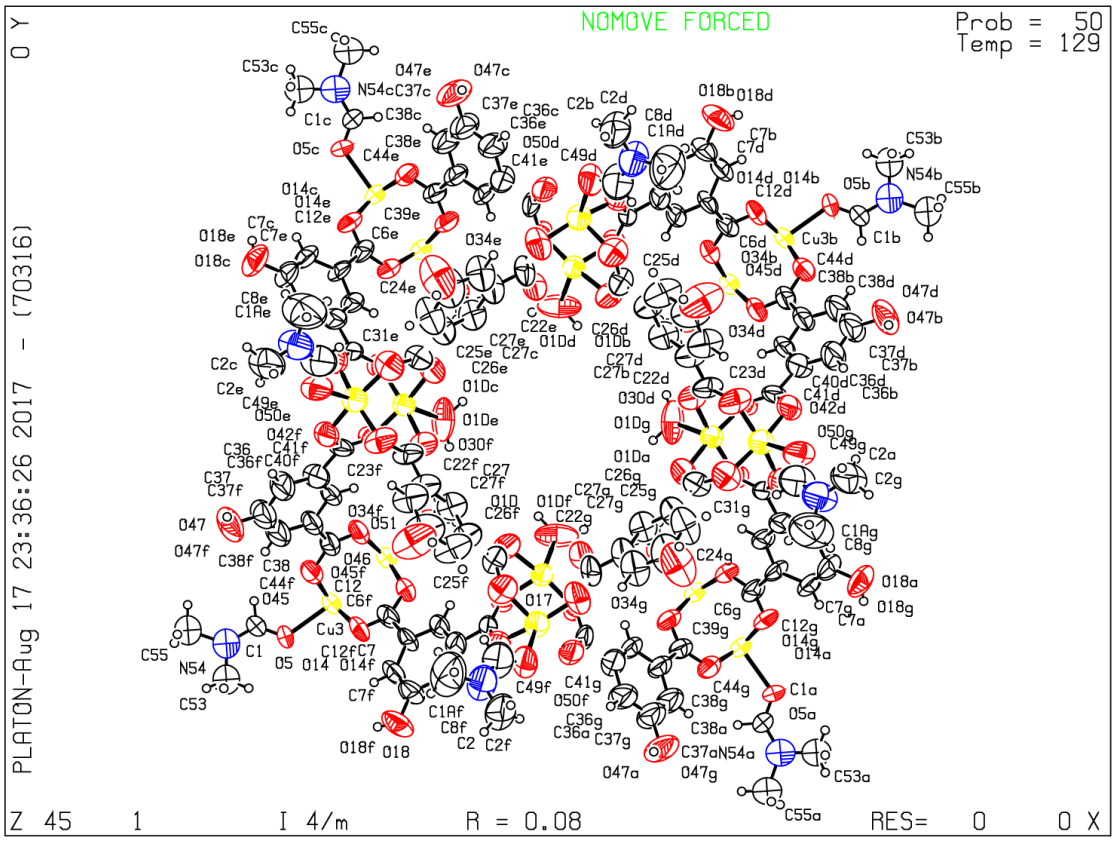
**PLATON version of 13/08/2017; check.def file version of 27/07/2017**

**Datablock 1** - ellipsoid plot



# checkCIF/PLATON report

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

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No syntax errors found. CIF dictionary Interpreting this report

# Datablock: 2

---

Bond precision: C-C = 0.0201 A Wavelength=0.71073

Cell: a=24.5209(10) b=25.3703(7) c=37.0128(12)
alpha=88.010(2) beta=79.070(3) 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 (mm-1) | 1.201 | 1.201 |
| F000 | 6314.0 | 6314.0 |
| F000’ | 6333.01 | |
| h,k,lmax | 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

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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.

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## Alert level A

THETM01_ALERT_3_A The value of sine(theta_max)/wavelength is less than 0.550
Calculated sin(theta_max)/wavelength = 0.5000

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## Alert level B

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 ..... 0.02015 Ang.
PLAT369_ALERT_2_B Long C(sp2)-C(sp2) Bond C1 - C610_g .. 1.58 Ang.
PLAT369_ALERT_2_B Long C(sp2)-C(sp2) Bond C2 - C33_b .. 1.62 Ang.
PLAT369_ALERT_2_B Long C(sp2)-C(sp2) Bond C14 - C489 .. 1.57 Ang.
PLAT369_ALERT_2_B Long C(sp2)-C(sp2) Bond C22 - C596 .. 1.61 Ang.
PLAT369_ALERT_2_B Long C(sp2)-C(sp2) Bond C42 - C275 .. 1.58 Ang.
PLAT369_ALERT_2_B Long C(sp2)-C(sp2) Bond C208 - C721 .. 1.59 Ang.
PLAT369_ALERT_2_B Long C(sp2)-C(sp2) Bond C231 - C695 .. 1.59 Ang.
PLAT369_ALERT_2_B Long C(sp2)-C(sp2) Bond C340 - C673 .. 1.61 Ang.
PLAT369_ALERT_2_B Long C(sp2)-C(sp2) Bond C425 - C715 .. 1.61 Ang.
PLAT369_ALERT_2_B Long C(sp2)-C(sp2) Bond C458 - C728 .. 1.57 Ang.
PLAT414_ALERT_2_B Short Intra D-H..H-X H410 .. H580 .. 1.86 Ang.
PLAT417_ALERT_2_B Short Inter D-H..H-D H6 .. H117 .. 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 O12 -- H12B ... Please Check
PLAT420_ALERT_2_B D-H Without Acceptor O128 -- H12C ... Please Check
PLAT420_ALERT_2_B D-H Without Acceptor O128 -- H12D ... 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

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PLAT420_ALERT_2_B D-H Without Acceptor       O75    --  H75    ...     Please Check
PLAT420_ALERT_2_B D-H Without Acceptor       O85    --  H85A   ...     Please Check
PLAT420_ALERT_2_B D-H Without Acceptor       O85    --  H85B   ...     Please Check
PLAT420_ALERT_2_B D-H Without Acceptor       O89    --  H89A   ...     Please Check
PLAT420_ALERT_2_B D-H Without Acceptor       O89    --  H89B   ...     Please Check
PLAT420_ALERT_2_B D-H Without Acceptor       O93    --  H93    ...     Please Check
PLAT420_ALERT_2_B D-H Without Acceptor       O100   --  H100   ...     Please Check
PLAT420_ALERT_2_B D-H Without Acceptor       O117   --  H117   ...     Please Check
PLAT420_ALERT_2_B D-H Without Acceptor       O186   --  H186   ...     Please Check
PLAT420_ALERT_2_B D-H Without Acceptor       O236   --  H236   ...     Please Check
PLAT420_ALERT_2_B D-H Without Acceptor       O257   --  H257   ...     Please Check
PLAT420_ALERT_2_B D-H Without Acceptor       O268   --  H268   ...     Please Check
PLAT420_ALERT_2_B D-H Without Acceptor       O314   --  H314   ...     Please Check
PLAT420_ALERT_2_B D-H Without Acceptor       O360   --  H360   ...     Please Check
PLAT420_ALERT_2_B D-H Without Acceptor       O362   --  H362   ...     Please Check
PLAT420_ALERT_2_B D-H Without Acceptor       O410   --  H410   ...     Please Check
PLAT420_ALERT_2_B D-H Without Acceptor       O556   --  H556   ...     Please Check
PLAT990_ALERT_1_B Deprecated .res/.hkl Input Style SQUEEZE job ...          ! Note
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## Alert level C

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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         O8 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        O43 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        O93 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       O133 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       O226 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       O270 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       O316 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       O363 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       O408 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       O543 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       O545 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       O607 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C49 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C144 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C486 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C532 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C562 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C590 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C634 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C637 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        Cu7 Check
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PLAT242_ALERT_2_C Low  'MainMol' Ueq as Compared to Neighbors of  Cu10 Check
PLAT242_ALERT_2_C Low  'MainMol' Ueq as Compared to Neighbors of  Cu16 Check
PLAT242_ALERT_2_C Low  'MainMol' Ueq as Compared to Neighbors of  Cu20 Check
PLAT242_ALERT_2_C Low  'MainMol' Ueq as Compared to Neighbors of  Cu22 Check
PLAT242_ALERT_2_C Low  'MainMol' Ueq as Compared to Neighbors of  Cu23 Check
PLAT242_ALERT_2_C Low  'MainMol' Ueq as Compared to Neighbors of  Cu26 Check
PLAT242_ALERT_2_C Low  'MainMol' Ueq as Compared to Neighbors of  Cu30 Check
PLAT242_ALERT_2_C Low  'MainMol' Ueq as Compared to Neighbors of  Cu31 Check
PLAT242_ALERT_2_C Low  'MainMol' Ueq as Compared to Neighbors of  Cu34 Check
PLAT242_ALERT_2_C Low  'MainMol' Ueq as Compared to Neighbors of  Cu39 Check
PLAT242_ALERT_2_C Low  'MainMol' Ueq as Compared to Neighbors of  Cu41 Check
PLAT242_ALERT_2_C Low  'MainMol' Ueq as Compared to Neighbors of  Cu48 Check
PLAT242_ALERT_2_C Low  'MainMol' Ueq as Compared to Neighbors of  C11 Check
PLAT242_ALERT_2_C Low  'MainMol' Ueq as Compared to Neighbors of  C21 Check
PLAT242_ALERT_2_C Low  'MainMol' Ueq as Compared to Neighbors of  C24 Check
PLAT242_ALERT_2_C Low  'MainMol' Ueq as Compared to Neighbors of  C201 Check
PLAT242_ALERT_2_C Low  'MainMol' Ueq as Compared to Neighbors of  C413 Check
PLAT242_ALERT_2_C Low  'MainMol' Ueq as Compared to Neighbors of  C458 Check
PLAT242_ALERT_2_C Low  'MainMol' Ueq as Compared to Neighbors of  C651 Check
PLAT242_ALERT_2_C Low  'MainMol' Ueq as Compared to Neighbors of  C659 Check
PLAT242_ALERT_2_C Low  'MainMol' Ueq as Compared to Neighbors of  C673 Check
PLAT242_ALERT_2_C Low  'MainMol' Ueq as Compared to Neighbors of  C702 Check
PLAT242_ALERT_2_C Low  'MainMol' Ueq as Compared to Neighbors of  C712 Check
PLAT242_ALERT_2_C Low  'MainMol' Ueq as Compared to Neighbors of  C723 Check
PLAT242_ALERT_2_C Low  'MainMol' Ueq as Compared to Neighbors of  C732 Check
PLAT334_ALERT_2_C Small Average Benzene  C-C Dist. C33  -C665  1.37 Ang.
PLAT334_ALERT_2_C Small Average Benzene  C-C Dist. C84  -C388  1.37 Ang.
PLAT355_ALERT_3_C Long  O-H (X0.82,N0.98A)  O15  -  H15A  ..  1.01 Ang.
PLAT355_ALERT_3_C Long  O-H (X0.82,N0.98A)  O15  -  H15B  ..  1.01 Ang.
PLAT362_ALERT_2_C Short  C(sp3)-C(sp2) Bond  C151  -  C519_d ..  1.41 Ang.
PLAT362_ALERT_2_C Short  C(sp3)-C(sp2) Bond  C503  -  C725  ..  1.35 Ang.
PLAT369_ALERT_2_C Long  C(sp2)-C(sp2) Bond  C4  -  C474  ..  1.54 Ang.
PLAT369_ALERT_2_C Long  C(sp2)-C(sp2) Bond  C5  -  C549_a ..  1.53 Ang.
PLAT369_ALERT_2_C Long  C(sp2)-C(sp2) Bond  C13  -  C594_a ..  1.54 Ang.
PLAT369_ALERT_2_C Long  C(sp2)-C(sp2) Bond  C17  -  C568_a ..  1.54 Ang.
PLAT369_ALERT_2_C Long  C(sp2)-C(sp2) Bond  C24  -  C634  ..  1.56 Ang.
PLAT369_ALERT_2_C Long  C(sp2)-C(sp2) Bond  C32  -  C630  ..  1.53 Ang.
PLAT369_ALERT_2_C Long  C(sp2)-C(sp2) Bond  C151  -  C661  ..  1.55 Ang.
PLAT369_ALERT_2_C Long  C(sp2)-C(sp2) Bond  C203  -  C583  ..  1.54 Ang.
PLAT369_ALERT_2_C Long  C(sp2)-C(sp2) Bond  C308  -  C668  ..  1.54 Ang.
PLAT369_ALERT_2_C Long  C(sp2)-C(sp2) Bond  C322  -  C698  ..  1.56 Ang.
PLAT369_ALERT_2_C Long  C(sp2)-C(sp2) Bond  C431  -  C713  ..  1.54 Ang.
PLAT369_ALERT_2_C Long  C(sp2)-C(sp2) Bond  C502  -  C582  ..  1.53 Ang.
PLAT369_ALERT_2_C Long  C(sp2)-C(sp2) Bond  C542  -  C723  ..  1.54 Ang.
PLAT369_ALERT_2_C Long  C(sp2)-C(sp2) Bond  C554  -  C677  ..  1.55 Ang.
PLAT369_ALERT_2_C Long  C(sp2)-C(sp2) Bond  C590  -  C732  ..  1.53 Ang.
PLAT369_ALERT_2_C Long  C(sp2)-C(sp2) Bond  C657  -  C693  ..  1.53 Ang.
PLAT414_ALERT_2_C Short Intra D-H..H-X  H170  ..  H413  ..  1.91 Ang.

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## Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite  27 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...  82 Report
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension  3 Info
PLAT005_ALERT_5_G No Embedded Refinement Details found  in the CIF  Please Do !
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms .....  47 Report
PLAT335_ALERT_2_G Check Large C6 Ring  C-C Range C33  -C665  0.17 Ang.
PLAT335_ALERT_2_G Check Large C6 Ring  C-C Range C156  -C634  0.20 Ang.
PLAT335_ALERT_2_G Check Large C6 Ring  C-C Range C292  -C644  0.17 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  O2  ..  C612  ..  3.00 Ang.
PLAT606_ALERT_4_G VERY LARGE Solvent Accessible VOID(S) in Structure  ! Info

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PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters          2 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        513 Note
PLAT869_ALERT_4_G ALERTS Related to the use of SQUEEZE Suppressed           ! Info
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  1 ALERT level A = Most likely a serious problem - resolve or explain
 68 ALERT level B = A potentially serious problem, consider carefully
 87 ALERT level C = Check. Ensure it is not caused by an omission or oversight
 13 ALERT level G = General information/check it is not something unexpected

  2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
152 ALERT type 2 Indicator that the structure model may be wrong or deficient
  9 ALERT type 3 Indicator that the structure quality may be low
  3 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. 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**

**Datablock 2** - ellipsoid plot