checkCIF/PLATON report

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

No syntax errors found. CIF dictionary Interpreting this report

Datablock: shelxl

Bond precision: C-C = 0.0091 A Wavelength=0.71073

Cell: a=22.7345(13) b=22.7345(13) c=64.308(7)
alpha=90 beta=90 gamma=120
Temperature: 173 K

	Calculated	Reported
Volume	28785(5)	28785(4)
Space group	R -3 c	R -3c
Hall group	-R 3 2"c	-R 3 2"c
Moiety formula	C55 H48 N O16 Zn4, 1.0(C3 N), 2.01(C)	(Zn 2++)4, (O 2-), (C18 H16 O4)3, (C3 H7 N O)
Sum formula	C60 H48 N2 O16 Zn4	C63 H69 N3 O16 Zn4
Mr	1314.75	1385.69
Dx,g cm-3	0.910	0.959
Z	12	12
Mu (mm-1)	1.031	1.033
F000	8041.4	8592.0
F000’	8058.08	
h,k,lmax	30,30,85	30,30,84
Nref	7857	7806
Tmin,Tmax	0.761,0.813	
Tmin’	0.749	

Correction method= Not given

Data completeness= 0.994 Theta(max)= 28.140

R(reflections)= 0.0874(5728) wR2(reflections)= 0.2691(7806)

S = 1.102 Npar= 299

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

CHEMW03_ALERT_2_B WARNING: The ratio of given/expected molecular weight as calculated from the _atom_site* data lies outside the range 0.95 <> 1.05

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           From the CIF: _cell_formula_units_Z                  12
           From the CIF: _chemical_formula_weight          1385.69
           TEST: Calculate formula weight from _atom_site_*
           atom     mass    num     sum
           C        12.01   59.97  720.30
           H         1.01   48.00   48.38
           N        14.01    1.98   27.73
           O        16.00   16.00  255.98
           Zn       65.39    4.00  261.56
           Calculated formula weight            1313.96
PLAT043_ALERT_1_B Check Reported Molecular Weight ................    1385.69
PLAT213_ALERT_2_B Atom C8              has ADP max/min Ratio .....       4.3 prola
PLAT220_ALERT_2_B Large Non-Solvent    C     Ueq(max)/Ueq(min) ...       5.2 Ratio
PLAT220_ALERT_2_B Large Non-Solvent    O     Ueq(max)/Ueq(min) ...       5.7 Ratio
PLAT230_ALERT_2_B Hirshfeld Test Diff for    O4     --  C11     ..       8.7 su
PLAT241_ALERT_2_B Check High      Ueq as Compared to Neighbors for         O3
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Alert level C

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RFACR01_ALERT_3_C  The value of the weighted R factor is > 0.25
           Weighted R factor given   0.269
PLAT041_ALERT_1_C Calc. and Reported SumFormula    Strings  Differ         ?
PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings  Differ         ?
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)...         ?
PLAT084_ALERT_2_C High wR2 Value ................................      0.27
PLAT213_ALERT_2_C Atom O4              has ADP max/min Ratio .....       3.5 prola
PLAT214_ALERT_2_C Atom C32     (Anion/Solvent) ADP max/min Ratio         4.4 prola
PLAT222_ALERT_3_C Large Non-Solvent    H    Uiso(max)/Uiso(min) ..       5.8 Ratio
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for       Zn2
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for        C4
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for       C11
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for       C14
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for       C16
PLAT341_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.0091 Ang
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Alert level G

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FORMU01_ALERT_1_G  There is a discrepancy between the atom counts in the
           _chemical_formula_sum and _chemical_formula_moiety. This is
           usually due to the moiety formula being in the wrong format.
           Atom count from _chemical_formula_sum:   C63 H69 N3 O16 Zn4
           Atom count from _chemical_formula_moiety:C57 H55 N1 O14 Zn4
FORMU01_ALERT_2_G  There is a discrepancy between the atom counts in the
           _chemical_formula_sum and the formula from the _atom_site* data.
           Atom count from _chemical_formula_sum:C63 H69 N3 O16 Zn4
           Atom count from the _atom_site data:  C59.97 H48 N1.98 O16 Zn4
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: Large difference may be due to a
           symmetry error - see SYMMG tests
           From the CIF: _cell_formula_units_Z   12
           From the CIF: _chemical_formula_sum  C63 H69 N3 O16 Zn4
           TEST: Compare cell contents of formula and atom_site data

           atom    Z*formula  cif sites diff
           C        756.00    719.64   36.36
           H        828.00    576.00  252.00
           N         36.00     23.76   12.24
           O        192.00    192.00    0.00
           Zn        48.00     48.00    0.00
HYDTR01_ALERT_1_G  Extra text has been found in the _refine_ls_hydrogen_treatment fi
           Explanatory text should be in the _publ_section_refinement field.
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            Hydrogen treatment given as constrained
            Hydrogen treatment identified as  constr
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite          9
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained Atom Sites ....          1
PLAT004_ALERT_5_G Info: Polymeric Structure Found with Dimension .          3
PLAT005_ALERT_5_G No _iucr_refine_instructions_details in CIF ....          ?
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT Unusually Large.       0.18
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large.      68.44
PLAT194_ALERT_1_G Missing _cell_measurement_reflns_used datum ....          ?
PLAT195_ALERT_1_G Missing _cell_measurement_theta_max   datum ....          ?
PLAT196_ALERT_1_G Missing _cell_measurement_theta_min   datum ....          ?
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Zn2    --  O3      ..       30.3 su
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Zn2    --  O21     ..        7.0 su
PLAT242_ALERT_2_G Check Low       Ueq as Compared to Neighbors for        O31
PLAT301_ALERT_3_G Note: Main Residue  Disorder ...................          6 Perc.
PLAT302_ALERT_4_G Note: Anion/Solvent Disorder ...................        100 Perc.
PLAT432_ALERT_2_G Short Inter X...Y Contact  O3     ..  C21     ..       2.85 Ang.
PLAT605_ALERT_4_G Structure Contains Solvent Accessible VOIDS of .       1652 A**3
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) .       1.30 Ratio
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C22    --  C23     .       1.97 Ang.
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ....          !
PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints .......         13
PLAT869_ALERT_4_G ALERTS Related to the use of SQUEEZE Suppressed           !
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0 **ALERT level A** = Most likely a serious problem - resolve or explain
7 **ALERT level B** = A potentially serious problem, consider carefully
14 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
26 **ALERT level G** = General information/check it is not something unexpected

11 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
24 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
4 ALERT type 4 Improvement, methodology, query or suggestion
3 ALERT type 5 Informative message, check

Our explanation to Checkcif Alert level B

1. CHEMW03_ALERT_2_B WARNING: The ratio of given/expected molecular weight as
calculated from the _atom_site* data lies outside
the range 0.95 <> 1.05
From the CIF: _cell_formula_units_Z 12
From the CIF: _chemical_formula_weight 1385.69
TEST: Calculate formula weight from _atom_site_*

atom	mass	num	sum
C	12.01	59.97	720.30
H	1.01	48.00	48.38
N	14.01	1.98	27.73
O	16.00	16.00	255.98
Zn	65.39	4.00	261.56

Calculated formula weight 1313.96

Answer: One of the dimethylformamide (DMF) molecules (O21 C21 N21 C22 C23) is obviously disordered, according to the significant residual electronic density, but it is not possible to resolve it. In the refinement only one part (assumed as a half) is given. This is, along with the non-refined hydrogen molecules of the DMF molecules gives the difference.

The structure is porous. The reflexes of the disordered guest molecules were removed by SQUEEZE (Platon).

2. PLAT043_ALERT_1_B Check Reported Molecular Weight 1385.69

See 1.

3. PLAT214_ALERT_2_B Atom C8 has ADP max/min Ratio ..... 4.3 prola

C8 atom is a most distant non-hydrogen atom from axis of the biphenyl molecule, which is rotationally not completely fixed. High anisotropic Ueq is natural.

4. PLAT220_ALERT_2_B Large Non-Solvent C Ueq(max)/Ueq(min) ... 5.2 Ratio
5. PLAT220_ALERT_2_B Large Non-Solvent O Ueq(max)/Ueq(min) ... 5.7 Ratio

The weakly coordinated DMF molecules are disordered, which is the source of atoms with high Ueq

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*, 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 15/02/2012; check.def file version of 10/02/2012

Datablock shelxl - ellipsoid plot