



Supporting Information

for

Hydrogen-bonded macrocycle-mediated dimerization for orthogonal supramolecular polymerization

Wentao Yu, Zhiyao Yang, Chengkan Yu, Xiaowei Li and Lihua Yuan

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CheckCIF report for H2 \supset G1

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 4bp

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: 4bp

Bond precision: C-C = 0.0087 A Wavelength=0.71073

Cell: a=24.434(4) b=20.026(3) c=23.779(4)
 alpha=90 beta=118.706(2) gamma=90

Temperature: 123 K

	Calculated	Reported
Volume	10205(3)	10205(3)
Space group	P 21/c	P2(1)/c
Hall group	-P 2ybc	?
Moiety formula	C84 H108 N6 O18, C12 H13 N2, F6 P	?
Sum formula	C96 H121 F6 N8 O18 P	C96 H121 F6 N8 O18 P
Mr	1819.98	1819.98
Dx, g cm ⁻³	1.185	1.185
Z	4	4
Mu (mm ⁻¹)	0.103	0.103
F000	3864.0	3864.0
F000'	3866.48	
h,k,lmax	29,23,28	29,23,28
Nref	18170	17763
Tmin,Tmax	0.974,0.982	0.972,0.982
Tmin'	0.972	

Correction method= # Reported T Limits: Tmin=0.972 Tmax=0.982
AbsCorr = MULTI-SCAN

Data completeness= 0.978 Theta(max)= 25.100

R(reflections)= 0.1072(8898) wR2(reflections)= 0.3153(17763)

S = 1.173 Npar= 1263

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

PLAT220_ALERT_2_B	Large Non-Solvent	C	Ueq(max)/Ueq(min) Range	7.1	Ratio
PLAT222_ALERT_3_B	Large Non-Solvent	H	Uiso(max)/Uiso(min) ...	8.1	Ratio
PLAT250_ALERT_2_B	Large U3/U1 Ratio for Average U(i,j) Tensor		4.6	Note

● Alert level C

CRYSC01_ALERT_1_C The word below has not been recognised as a standard identifier.

?

CRYSC01_ALERT_1_C No recognised colour has been given for crystal colour.

RFACG01_ALERT_3_C The value of the R factor is > 0.10

R factor given 0.107

RFACR01_ALERT_3_C The value of the weighted R factor is > 0.25

Weighted R factor given 0.315

PLAT029_ALERT_3_C	_diffrn_measured_fraction_theta_full Low		0.978	Note
PLAT082_ALERT_2_C	High R1 Value		0.11	Report
PLAT084_ALERT_3_C	High wR2 Value (i.e. > 0.25)		0.32	Report
PLAT213_ALERT_2_C	Atom O1A	has ADP max/min Ratio	3.7	prolat
PLAT213_ALERT_2_C	Atom C66A	has ADP max/min Ratio	3.2	prolat
PLAT220_ALERT_2_C	Large Non-Solvent	O	Ueq(max)/Ueq(min) Range	5.4	Ratio
PLAT234_ALERT_4_C	Large Hirshfeld Difference	O1A -- C57A	..	0.17	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	C21A -- C22A	..	0.18	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	C80A -- C81A	..	0.18	Ang.
PLAT241_ALERT_2_C	High	Ueq as Compared to Neighbors for	C25A	Check
PLAT241_ALERT_2_C	High	Ueq as Compared to Neighbors for	C73A	Check
PLAT241_ALERT_2_C	High	Ueq as Compared to Neighbors for	N2	Check
PLAT242_ALERT_2_C	Low	Ueq as Compared to Neighbors for	O4A	Check
PLAT242_ALERT_2_C	Low	Ueq as Compared to Neighbors for	O5A	Check
PLAT242_ALERT_2_C	Low	Ueq as Compared to Neighbors for	N1A	Check
PLAT242_ALERT_2_C	Low	Ueq as Compared to Neighbors for	C24A	Check
PLAT242_ALERT_2_C	Low	Ueq as Compared to Neighbors for	C57A	Check
PLAT242_ALERT_2_C	Low	Ueq as Compared to Neighbors for	C75A	Check
PLAT242_ALERT_2_C	Low	Ueq as Compared to Neighbors for	C80A	Check
PLAT250_ALERT_2_C	Large U3/U1 Ratio for Average U(i,j) Tensor		3.3	Note
PLAT340_ALERT_3_C	Low Bond Precision on C-C Bonds		0.0087	Ang.
PLAT360_ALERT_2_C	Short C(sp3)-C(sp3) Bond	C81A - C82A	..	1.38	Ang.
PLAT410_ALERT_2_C	Short Intra H...H Contact	H5 .. H9	..	1.99	Ang.
PLAT412_ALERT_2_C	Short Intra XH3 .. XHn	H73A .. H78C	..	1.86	Ang.
PLAT412_ALERT_2_C	Short Intra XH3 .. XHn	H75A .. H78A	..	1.88	Ang.
PLAT413_ALERT_2_C	Short Inter XH3 .. XHn	H11 .. H28A	..	2.01	Ang.

● Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite			22	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms	...		138	Report
PLAT005_ALERT_5_G	No _iucr_refine_instructions_details in the CIF			Please Do !	
PLAT066_ALERT_1_G	Predicted and Reported Tmin&Tmax Range Identical			?	Check
PLAT072_ALERT_2_G	SHELXL First Parameter in WGHT Unusually Large.			0.15	Report
PLAT300_ALERT_4_G	Atom Site Occupancy of *C77A	is Constrained at		0.500	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *C77B	is Constrained at		0.500	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *C78A	is Constrained at		0.500	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *C78B	is Constrained at		0.500	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *H77A	is Constrained at		0.500	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *H77B	is Constrained at		0.500	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *H77C	is Constrained at		0.500	Check

PLAT300_ALERT_4_G	Atom Site Occupancy of *H77D	is Constrained at	0.500	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *H78A	is Constrained at	0.500	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *H78B	is Constrained at	0.500	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *H78C	is Constrained at	0.500	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *H78D	is Constrained at	0.500	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *H78E	is Constrained at	0.500	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *H78F	is Constrained at	0.500	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *F1	is Constrained at	0.500	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *F2	is Constrained at	0.500	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *F3	is Constrained at	0.500	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *F4	is Constrained at	0.500	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *F5	is Constrained at	0.500	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *F6	is Constrained at	0.500	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *F1'	is Constrained at	0.500	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *F1'	is Constrained at	0.500	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *F2'	is Constrained at	0.500	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *F3'	is Constrained at	0.500	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *F4'	is Constrained at	0.500	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *F5'	is Constrained at	0.500	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *F6'	is Constrained at	0.500	Check
PLAT301_ALERT_3_G	Main Residue Disorder	Percentage =	2	Note
PLAT302_ALERT_4_G	Anion/Solvent Disorder	Percentage =	100	Note
PLAT304_ALERT_4_G	Non-Integer Number of Atoms (3.50) in Resd. #		3	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms (3.50) in Resd. #		4	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact F1' .. C66A ..		2.68	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact F4' .. C25A ..		2.92	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact O10A .. C4 ..		2.98	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact O13A .. C10A ..		3.01	Ang.
PLAT606_ALERT_4_G	VERY LARGE Solvent Accessible VOID(S) in Structure		!	Info
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels		3	Note
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF #		356	Check
	C77A -C74A -C77B 1.555 1.555 1.555		12.00	Deg.
PLAT860_ALERT_3_G	Number of Least-Squares Restraints		2166	Note
PLAT869_ALERT_4_G	ALERTS Related to the use of SQUEEZE Suppressed		!	Info
PLAT899_ALERT_4_G	SHELXL97 is Deprecated and Succeeded by SHELXL		2014	Note

0 **ALERT level A** = Most likely a serious problem - resolve or explain
3 **ALERT level B** = A potentially serious problem, consider carefully
30 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
47 **ALERT level G** = General information/check it is not something unexpected

3 **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
8 **ALERT type 3** Indicator that the structure quality may be low
39 **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*, 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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