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: c___3369

Bond precision: C-C = 0.0050 A Wavelength=0.71073

Cell: a=19.4549(2) b=19.8966(3) c=19.9214(3)
alpha=90.301(1) beta=96.296(1) gamma=115.612(1)
Temperature: 123 K

	Calculated	Reported
Volume	6899.73(17)	6899.72(17)
Space group	P -1	P-1
Hall group	-P 1	?
Moiety formula	C72 H60 Cl2 Dy O4 P4, Cl4 Fe	?
Sum formula	C72 H60 Cl6 Dy Fe O4 P4	C72 H60 Cl6 Dy Fe O4 P4
Mr	1544.13	1544.13
Dx,g cm-3	1.487	1.486
Z	4	4
Mu (mm-1)	1.658	1.658
F000	3112.0	3112.0
F000’	3118.65	
h,k,lmax	25,25,25	25,25,25
Nref	31688	31378
Tmin,Tmax	0.556,0.847	0.556,0.847
Tmin’	0.510	

Correction method= # Reported T Limits: Tmin=0.556 Tmax=0.847
AbsCorr = MULTI-SCAN

Data completeness= 0.990 Theta(max)= 27.500

R(reflections)= 0.0377(26632) wR2(reflections)= 0.0745(31378)

S = 1.064 Npar= 1585

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 C

PLAT220_ALERT_2_C Non-Solvent Resd 2 C Ueq(max)/Ueq(min) Range 3.2 Ratio
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of Fe15 Check
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of Fe16 Check
PLAT601_ALERT_2_C Structure Contains Solvent Accessible VOIDS of . 31 Ang**3

Alert level G

PLAT005_ALERT_5_G No Embedded Refinement Details Found in the CIF Please Do !
PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical ? Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 9.45 Why ?
PLAT093_ALERT_1_G No s.u.'s on H-positions, Refinement Reported as mixed Check
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note) 0.001 Degree
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Dy1 --Cl5 . 5.0 s.u.
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. # 4 Note
Cl4 Fe
PLAT794_ALERT_5_G Tentative Bond Valency for Dy1 (III) . 3.25 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Dy2 (III) . 3.21 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Fe15 (III) . 3.06 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Fe16 (III) . 3.06 Info
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters 2 Info
PLAT899_ALERT_4_G SHELXL97 is Deprecated and Succeeded by SHELXL 2018 Note

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0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
4 **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

3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
4 ALERT type 2 Indicator that the structure model may be wrong or deficient
0 ALERT type 3 Indicator that the structure quality may be low
5 ALERT type 4 Improvement, methodology, query or suggestion
5 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 23/04/2018; check.def file version of 23/04/2018

Datablock c___3369 - ellipsoid plot