

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: lms69

Bond precision: C-C = 0.0104 Å Wavelength=0.71073

Cell: a=9.865(2) b=20.857(4) c=9.4829(19)
 alpha=90 beta=90 gamma=90

Temperature: 293 K

	Calculated	Reported
Volume	1951.2(7)	1951.1(7)
Space group	P c a 21	Pca2(1)
Hall group	P 2c -2ac	?
Moiety formula	C25 H21 Fe N O	C25H21FeNo
Sum formula	C25 H21 Fe N O	C25H21FeNo
Mr	407.28	407.28
Dx,g cm-3	1.386	1.386
Z	4	4
Mu (mm-1)	0.788	0.788
F000	848.0	848.0
F000'	849.64	
h,k,lmax	12,27,12	12,27,12
Nref	2384[4484]	4343
Tmin,Tmax	0.797,0.889	0.058,0.081
Tmin'	0.696	

Correction method= MULTI-SCAN

Data completeness= 1.82/0.97 Theta(max)= 27.510

R(reflections)= 0.0844(4006) wR2(reflections)= 0.2198(4343)

S = 1.121 Npar= 229

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

PLAT201_ALERT_2_B Isotropic non-H Atoms in Main Residue(s)

5



Alert level C

ABSTY02_ALERT_1_C An _exptl_absorpt_correction_type has been given without
a literature citation. This should be contained in the
_exptl_absorpt_process_details field.
Absorption correction given as Multi-scan

STRVA01_ALERT_2_C Chirality of atom sites is inverted?
From the CIF: _refine_ls_abs_structure_Flack 0.960
From the CIF: _refine_ls_abs_structure_Flack_su 0.040

PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ ?
PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings Differ ?
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density 2.04
PLAT220_ALERT_2_C Large Non-Solvent C Ueq(max)/Ueq(min) ... 3.1 Ratio
PLAT241_ALERT_2_C Check High Ueq as Compared to Neighbors for C1
PLAT241_ALERT_2_C Check High Ueq as Compared to Neighbors for C2
PLAT241_ALERT_2_C Check High Ueq as Compared to Neighbors for C4
PLAT241_ALERT_2_C Check High Ueq as Compared to Neighbors for C5
PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for Fe1
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds 0.0104 Ang
PLAT369_ALERT_2_C Long C(sp2)-C(sp2) Bond C1 - C2 ... 1.55 Ang.

Alert level G

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 4
From the CIF: _chemical_formula_sum C25H21FeNO
TEST: Compare cell contents of formula and atom_site data
WARNING: Unexpected atom type is in site list: Fe
WARNING: Unexpected atom type is in site list: O
WARNING: Unexpected atom type is in site list: N
WARNING: Formula and atom_type_symbol element names mismatch.

atom	Z*formula	cif sites	diff
C	100.00	100.00	0.00
H	84.00	84.00	0.00
FeNO	4.00	0.00	4.00

WARNING: Site labels do not match formula elements

REFLT03_ALERT_4_G Please check that the estimate of the number of Friedel pairs is
correct. If it is not, please give the correct count in the
_publ_section_exptl_refinement section of the submitted CIF.
From the CIF: _diffrn_reflms_theta_max 27.51
From the CIF: _reflms_number_total 4343
Count of symmetry unique reflms 2384
Completeness (_total/calc) 182.17%
TEST3: Check Friedels for noncentro structure
Estimate of Friedel pairs measured 1959
Fraction of Friedel pairs measured 0.822
Are heavy atom types Z>Si present yes

PLAT005_ALERT_5_G No _iucr_refine_instructions_details in CIF ?
PLAT033_ALERT_4_G Flack x Parameter Value Deviates from Zero 0.960
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large. 0.11
PLAT199_ALERT_1_G Check the Reported _cell_measurement_temperature 293 K
PLAT200_ALERT_1_G Check the Reported _diffrn_ambient_temperature 293 K
PLAT792_ALERT_1_G Note: The Model has Chirality at C11 (Verify) S
PLAT792_ALERT_1_G Note: The Model has Chirality at C12 (Verify) R

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

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

PLATON version of 18/07/2011; check.def file version of 04/07/2011

