checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 3

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: 3

Bond precision: P- O = 0.0020 A   Wavelength=1.54184

Cell: a=28.1150(12)   b=28.1150(12)   c=28.1150(12)
               alpha=90   beta=90   gamma=90
Temperature: 293 K

	Calculated	Reported
Volume	22224(3)	22224(3)
Space group	F d -3 c	F d -3 c
Hall group	-F 4cvw 2vw	-F 4cvw 2vw
Moiety formula	4(O4 P), 2(F), 36(H2 O), 3(O), 13(Na)	0.03(F32 H1152 Na208 O640 P16), 1.5(O4 P), 1.5(O)
Sum formula	F2 H72 Na13 O55 P4	F H36 Na6.50 O27.50 P2
Mr	1413.32	706.65
Dx,g cm-3	1.690	1.690
Z	16	32
Mu (mm-1)	3.463	3.463
F000	11728.0	11728.0
F000'	11818.71	
h,k,lmax	34,34,34	33,26,33
Nref	930	890
Tmin,Tmax	0.847,0.933	0.715,1.000
Tmin'	0.812	

Correction method= # Reported T Limits: Tmin=0.715 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.957   Theta(max)= 72.369

R(reflections)= 0.0439(669)   wR2(reflections)= 0.1229(890)

S = 1.118   Npar= 90

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**
PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full value Low .   0.968 Why?
PLAT088_ALERT_3_C Poor Data / Parameter Ratio ....   9.89 Note
PLAT245_ALERT_2_C U(iso) H5A   Smaller than U(eq) O5   by   0.016 Ang**2
PLAT905_ALERT_3_C Negative K value in the Analysis of Variance ...   -0.338 Report
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=   0.600   27 Report

---

⚪ **Alert level G**
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: H36 F1 Na6.5 O27.5 P2
            Atom count from _chemical_formula_moiety:H34.56 F0.96 Na6.24 O26.7 P1.
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite   10 Note
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ   Please Check
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...   0.50 Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large   46.67 Why ?
PLAT168_ALERT_4_G The CIF-Embedded .res File Contains EXYZ Records   1 Report
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records   1 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records   1 Report
PLAT180_ALERT_4_G Check Cell Rounding: # of Values Ending with 0 =   3 Note
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)   293 Check
PLAT200_ALERT_1_G Reported   _diffrn_ambient_temperature ..... (K)   293 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O1   Constrained at   0.3333 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H5A   Constrained at   0.6667 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H5B   Constrained at   0.6667 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H5C   Constrained at   0.6667 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O6   Constrained at   0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Na2   Constrained at   0.25 Check
PLAT301_ALERT_3_G Main Residue Disorder ....(Resd 1)   80% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 7)   100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 9)   100% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd 3)   0.17 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd 7)   0.25 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd 9)   0.08 Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....   O6 Check
PLAT860_ALERT_3_G Number of Least-Squares Restraints ....   7 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600   5 Note
PLAT951_ALERT_5_G Calculated (ThMax) and CIF-Reported Kmax Differ   8 Units
PLAT960_ALERT_3_G Number of Intensities with I <   - 2*sig(I) ...   1 Check

---

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

   5 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
   7 ALERT type 3 Indicator that the structure quality may be low
  16 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* 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 05/12/2020; check.def file version of 05/12/2020

NOMOVE FORCED

Prob = 50
Temp = 293

74 Y

PLATON-Jan 13 17:19:32 2021 - (51220)

O1_h   O1_b
O1_e
O1_a   O1_k
O1
O1_d   O1_c   O1_l

O2
O2_l   P2
O2_n   O2_m

O3
O5
O4

Na2   O6

Na1

F

Z 76   3   F d -3 c   R = 0.04   RES= 0   -1 X