checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 4

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: 4

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Bond precision:    P- O = 0.0017 A            Wavelength=1.54184

Cell:              a=27.9777(7)      b=27.9777(7)       c=27.9777(7)
                   alpha=90          beta=90            gamma=90
Temperature:       100 K

                   Calculated                 Reported
Volume             21899.6(16)                21899.6(17)
Space group        F d -3 c                   F d -3 c
Hall group         -F 4cvw 2vw                -F 4cvw 2vw
                   4(O4 P), 2(F), 36(H2 O),   0.06(F16 H576 Na103.9 O320
Moiety formula     3(O), 13(Na)               P8), 1.5(O4 P), 1.51(O)
Sum formula        F2 H72 Na13 O55 P4         F H36 Na6.49 O27.51 P2
Mr                 1413.32                    706.60
Dx,g cm-3          1.715                      1.715
Z                  16                         32
Mu (mm-1)          3.514                      3.514
F000               11727.9                    11727.0
F000'              11818.69
h,k,lmax           35,35,35                   34,33,28
Nref               968                        939
Tmin,Tmax          0.776,0.869                0.452,1.000
Tmin'              0.755

Correction method= # Reported T Limits: Tmin=0.452 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.970            Theta(max)= 76.283

R(reflections)= 0.0425( 812)        wR2(reflections)= 0.1100( 939)

S = 1.122                  Npar= 92
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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

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PLAT041_ALERT_1_C Calc. and Reported SumFormula    Strings  Differ      Please Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      2.902 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600          14 Report
PLAT975_ALERT_2_C Check Calcd Resid. Dens.  0.88A    From O1             0.80 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens.  0.88A    From O1             0.80 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens.  0.88A    From O1             0.80 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens.  0.88A    From O1             0.80 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens.  0.90A    From O1             0.80 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens.  0.60A    From O1             0.41 eA-3
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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:   H36 F1 Na6.49 O27.51 P2
           Atom count from _chemical_formula_moiety:H34.56 F0.96 Na6.234 O26.71 P
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:H36 F1 Na6.49 O27.51 P2
           Atom count from the _atom_site data:  H36.00428 F1.004979 Na6.499869 O
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    32
           From the CIF: _chemical_formula_sum  F H36 Na6.49 O27.51 P2
           TEST: Compare cell contents of formula and atom_site data

           atom     Z*formula   cif sites diff
           F          32.00      32.00    0.00
           H        1152.02    1152.00    0.02
           Na        207.68     208.00   -0.32
           O         880.34     879.99    0.34
           P          64.00      64.00    0.00
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
PLAT068_ALERT_1_G Reported F000 Differs from Calcd (or Missing)...   Please Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large   107.49 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
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     0.65 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H5B        Constrained at     0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H5C        Constrained at      0.6 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
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600       14 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....        1 Note
PLAT951_ALERT_5_G Calculated (ThMax) and CIF-Reported Kmax Differ         2 Units
PLAT952_ALERT_5_G Calculated (ThMax) and CIF-Reported Lmax Differ         7 Units
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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
   9 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

   8 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   9 ALERT type 2 Indicator that the structure model may be wrong or deficient
   4 ALERT type 3 Indicator that the structure quality may be low
  12 ALERT type 4 Improvement, methodology, query or suggestion
   2 ALERT type 5 Informative message, check
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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.

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