checkCIF/PLATON report

Structure factors have been supplied for datablock(s) MnH5As2O8.5

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: MnH5As2O8.5

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Bond precision:  As- O = 0.0038 A        Wavelength=0.71073

Cell:           a=4.975(1)        b=5.4747(11)     c=13.603(3)
                alpha=98.86(3)    beta=93.63(3)    gamma=99.09(3)
Temperature:    293 K

                Calculated                Reported
Volume          360.02(14)                360.02(13)
Space group     P -1                      P -1
Hall group      -P 1                      -P 1
Moiety formula  2(As2 Mn O8), O           (As2 Mn O8), 0.5(O H2)
Sum formula     As4 Mn2 O17               As2 H5 Mn O8.50
Mr              681.56                    345.82
Dx,g cm-3       3.144                     3.190
Z               1                         2
Mu (mm-1)       10.964                    10.966
F000            318.0                     328.0
F000'           319.10
h,k,lmax        6,7,19                    6,7,19
Nref            2091                      2087
Tmin,Tmax       0.108,0.769               0.526,0.748
Tmin'           0.005

Correction method= # Reported T Limits: Tmin=0.526 Tmax=0.748
AbsCorr = MULTI-SCAN

Data completeness= 0.998          Theta(max)= 29.996

R(reflections)= 0.0332( 1831)     wR2(reflections)= 0.1053( 2087)

S = 1.132                 Npar= 104
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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 B

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PLAT043_ALERT_1_B Calculated and Reported Mol. Weight Differ by ..      10.08 Check
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Alert level C

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PLAT041_ALERT_1_C Calc. and Reported SumFormula    Strings  Differ     Please Check
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)...     Please Check
PLAT220_ALERT_2_C Non-Solvent  Resd 1  O   Ueq(max)/Ueq(min) Range        4.4 Ratio
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        As2 Check
PLAT975_ALERT_2_C Check Calcd Resid. Dens.  0.71A   From Ow              1.28 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens.  0.59A   From Ow              0.81 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens.  1.00A   From O4              0.56 eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens.  0.45A   From Ow             -0.90 eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens.  0.78A   From O4             -0.59 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:   H5 As2 Mn1 O8.5
            Atom count from _chemical_formula_moiety:H1 As2 Mn1 O8.5
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:H5 As2 Mn1 O8.5
            Atom count from the _atom_site data:  As2 Mn1 O8.5
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G WARNING: H atoms missing from atom site list. Is this intentional?
           From the CIF: _cell_formula_units_Z    2
           From the CIF: _chemical_formula_sum  As2 H5 Mn O8.50
           TEST: Compare cell contents of formula and atom_site data

           atom    Z*formula  cif sites diff
           As         4.00      4.00    0.00
           H         10.00      0.00   10.00
           Mn         2.00      2.00    0.00
           O         17.00     17.00    0.00
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension          3 Info
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
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)        0.03 Degree
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 Ow         Constrained at        0.5 Check
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  2  )        100% Note
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....         Ow Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels .........          1 Note
PLAT794_ALERT_5_G Tentative Bond Valency for Mn1       (II)      .       2.03 Info
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).          3 Note
PLAT960_ALERT_3_G Number of Intensities with I  <   - 2*sig(I) ...         1 Check
PLAT992_ALERT_5_G Repd & Actual _reflns_number_gt Values Differ by         1 Check
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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
   9 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  19 ALERT level G = General information/check it is not something unexpected

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

PLATON version of 07/08/2019; check.def file version of 30/07/2019

Datablock MnH5As2O8.5 - ellipsoid plot