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: try

Bond precision: Si- O = 0.0412 A   Wavelength=0.71073

Cell: a=24.8510(6)   b=24.8510(6)   c=60.8811(12)
                alpha=90   beta=90   gamma=120
Temperature: 100 K

	Calculated	Reported
Volume	32561(2)	32561.2(13)
Space group	R -3	R-3
Hall group	-R 3	?
Moiety formula	Co16 O164 P4 Si4 W36, 36.75(O), 12(Na)	?
Sum formula	Co16 Na12 O200.75 P4 Si4 W36	H168 Co16 Na32 O242 P4 Si4 W36
Mr	11285.24	12574.75
Dx,g cm-3	3.453	3.848
Z	6	6
Mu (mm-1)	20.354	20.423
F000	29700.0	34008.0
F000'	29599.93	
h,k,lmax	26,26,64	26,26,64
Nref	8836	8821
Tmin,Tmax	0.000,0.294	0.045,0.374
Tmin'	0.000	

Correction method= MULTI-SCAN

Data completeness= 0.998   Theta(max)= 21.960

R(reflections)= 0.0934(6472)   wR2(reflections)= 0.2860(8821)

S = 1.003   Npar= Npar = 501

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 A**

CHEMW03_ALERT_2_A ALERT: The ratio of given/expected molecular weight as
           calculated from the _atom_site* data lies outside
           the range 0.90 <> 1.10
           From the CIF: _cell_formula_units_Z   6
           From the CIF: _chemical_formula_weight   *******
           TEST: Calculate formula weight from _atom_site_*

atom	mass	num	sum
O	16.00	200.75	3211.80
H	1.01	0.00	0.00
Na	22.99	12.00	275.88
Si	28.09	4.00	112.34
P	30.97	4.00	123.90
Co	58.93	16.00	942.93
W	183.85	36.00	6618.60

           Calculated formula weight   11285.45
THETM01_ALERT_3_A The value of sine(theta_max)/wavelength is less than 0.550
           Calculated sin(theta_max)/wavelength =   0.5262
PLAT043_ALERT_1_A Calculated and Reported Mol. Weight Differ by ..   1289.51 Check
PLAT601_ALERT_2_A Structure Contains Solvent Accessible VOIDS of .   5142 Ang3

🟠 **Alert level B**

CHEMS01_ALERT_1_B The sum formula contains elements in the wrong order.
           H precedes Co
           Sequence must be alphabetical for inorganic structures.
SYMMS02_ALERT_1_B The unit-cell lengths a and c should be equal for a
           rhombohedral cell
  Cell   24.8510   24.8510   60.8811
  Angles   90.0000   90.0000 120.0000
SYMMS02_ALERT_1_B Cell angles alpha and gamma should be equal for a
           rhombohedral cell
  Cell   24.8510   24.8510   60.8811
  Angles   90.0000   90.0000 120.0000
SYMMS02_ALERT_1_B All angles should not be 90 for a rhombohedral cell
  Cell   24.8510   24.8510   60.8811
  Angles   90.0000   90.0000 120.0000
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) ....   O1W Check
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) ....   O2W Check
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) ....   O3W Check
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) ....   O4W Check
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) ....   O5W Check
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) ....   O6W Check

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🟡 **Alert level C**

RFACR01_ALERT_3_C The value of the weighted R factor is > 0.25
           Weighted R factor given   0.286
RINTA01_ALERT_3_C The value of Rint is greater than 0.12
           Rint given   0.143
PLAT020_ALERT_3_C The value of Rint is greater than 0.12 ....   0.143
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
PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) ....   0.29 Why ?
PLAT202_ALERT_3_C Isotropic non-H Atoms in Anion/Solvent   13

⬤ Alert level G

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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:H168 Co16 Na32 O242 P4 Si4 W36
             Atom count from the _atom_site data:  Co16 Na12 O200.7499 P4 Si4 W36
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    6
            From the CIF: _chemical_formula_sum  H168 Co16 Na32 O242 P4 Si4 W36
            TEST: Compare cell contents of formula and atom_site data

            atom     Z*formula  cif sites diff
            H         1008.00       0.00 1008.00
            Co          96.00      96.00    0.00
            Na         192.00      72.00  120.00
            O         1452.00    1204.50  247.50
            P           24.00      24.00    0.00
            Si          24.00      24.00    0.00
            W          216.00     216.00    0.00
PLAT005_ALERT_5_G No _iucr_refine_instructions_details  in the CIF      Please Do !
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large.   20000.00 Why ?
PLAT104_ALERT_1_G The Reported Crystal System is Inconsistent with        R-3 Check
PLAT112_ALERT_2_G ADDSYM Detects Additional (Pseudo) Symm. Elem...         n Check
PLAT112_ALERT_2_G ADDSYM Detects Additional (Pseudo) Symm. Elem...         a Check
PLAT112_ALERT_2_G ADDSYM Detects Additional (Pseudo) Symm. Elem...         n Check
PLAT112_ALERT_2_G ADDSYM Detects Additional (Pseudo) Symm. Elem...         3 Check
PLAT112_ALERT_2_G ADDSYM Detects Additional (Pseudo) Symm. Elem...         3 Check
PLAT112_ALERT_2_G ADDSYM Detects Additional (Pseudo) Symm. Elem...         3 Check
PLAT113_ALERT_2_G ADDSYM Suggests Possible Pseudo/New Space-group.      Fd-3 Check
PLAT152_ALERT_1_G The Supplied and Calc. Volume s.u. Differ by ...        7 Units
PLAT302_ALERT_4_G Anion/Solvent Disorder ............ Percentage =       63 Note
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....      O7W Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....      O8W Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....      O9W Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....     O10W Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....     O11W Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....     O12W Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....     O13W Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....     O14W Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....     O15W Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....     O16W Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....     O17W Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........       11 Note
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #        2 Note
            O
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #        3 Note
            O
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #        4 Note
            O
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #        5 Note
            O
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #        6 Note
            O
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #        7 Note
            O
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #        8 Note
            O
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #        9 Note
            O
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #       10 Note
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                  O
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #      11 Note
                  O
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #      13 Note
                  O
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #      15 Note
                  O
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #      16 Note
                  O
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #      17 Note
                  O
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #      18 Note
                  O
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #      20 Note
                  Na
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #      22 Note
                  Na
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #      23 Note
                  Na
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #      24 Note
                  Na
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #      25 Note
                  Na
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #      26 Note
                  Na
PLAT793_ALERT_4_G The Model has Chirality at P1      .............     S Verify
PLAT793_ALERT_4_G The Model has Chirality at P2      .............     R Verify
PLAT793_ALERT_4_G The Model has Chirality at Si1     .............     R Verify
PLAT793_ALERT_4_G The Model has Chirality at Si2     .............     R Verify
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   4 ALERT level A = Most likely a serious problem - resolve or explain
  10 ALERT level B = A potentially serious problem, consider carefully
   7 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  52 ALERT level G = General information/check it is not something unexpected

  11 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  28 ALERT type 2 Indicator that the structure model may be wrong or deficient
   6 ALERT type 3 Indicator that the structure quality may be low
  27 ALERT type 4 Improvement, methodology, query or suggestion
   1 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*, 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 05/02/2014; check.def file version of 05/02/2014