checkCIF/PLATON report

Structure factors have been supplied for datablock(s) Ni-dcbdt

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: Ni-dcbdt

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Bond precision:   C-C = 0.0046 A          Wavelength=1.54184

Cell:             a=22.0141(2)      b=22.3831(3)      c=14.1276(1)
                  alpha=90          beta=90           gamma=90
Temperature:      293 K
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	Calculated	Reported
Volume	6961.29(12)	6961.29(12)
Space group	P b c n	P b c n
Hall group	-P 2n 2ab	-P 2n 2ab
Moiety formula	C16 H8 Ni2 O10 S4, 3(C4 H12 N)	C16 H8 Ni2 O10 S4, 3(C4 H12 N)
Sum formula	C28 H44 N3 Ni2 O10 S4	C28 H45 N3 Ni2 O10 S4
Mr	828.28	829.33
Dx,g cm-3	1.581	1.583
Z	8	8
Mu (mm-1)	4.080	4.080
F000	3464.0	3472.0
F000'	3434.91	
h,k,lmax	27,28,17	27,27,17
Nref	7447	7278
Tmin,Tmax		0.305,1.000
Tmin'		

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Correction method= # Reported T Limits: Tmin=0.305 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.977          Theta(max)= 77.964

R(reflections)= 0.0577( 6201)                    wR2(reflections)=
                                                 0.1632( 7278)
S = 1.052                 Npar= 433
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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
             Calc: C28 H44 N3 Ni2 O10 S4
             Rep.: C28 H45 N3 Ni2 O10 S4
PLAT043_ALERT_1_C Calculated and Reported Mol. Weight Differ by ..       1.05 Check
PLAT053_ALERT_1_C Minimum Crystal Dimension Missing (or Error) ...     Please Check
PLAT054_ALERT_1_C Medium  Crystal Dimension Missing (or Error) ...     Please Check
PLAT055_ALERT_1_C Maximum Crystal Dimension Missing (or Error) ...     Please Check
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)...     Please Check
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....       2.13 Report
PLAT244_ALERT_4_C Low    'Solvent' Ueq as Compared to Neighbors of         N1 Check
PLAT244_ALERT_4_C Low    'Solvent' Ueq as Compared to Neighbors of         N3 Check
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C17      - C18      .       1.43 Ang.
PLAT767_ALERT_4_C INS Embedded LIST 6 Instruction Should be LIST 4     Please Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      8.695 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      2.326 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600         10 Report
               2  2  0,   0  0  2,   0  0  4,  16  9  6,  12 11  6,  19  0 10,
              18  0 12,   0 16 12,   0 16 13,   1 17 13,
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.80Ang From C17             1.96 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.71Ang From C17             1.59 eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens.  0.96Ang From O10     .      -0.44 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H9B       .      -0.37 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H10B      .      -0.31 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:   C28 H45 N3 Ni2 O10 S4
            Atom count from _chemical_formula_moiety:C28 H44 N3 Ni2 O10 S4
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:C28 H45 N3 Ni2 O10 S4
            Atom count from the _atom_site data:  C28 H44 N3 Ni2 O10 S4
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    8
           From the CIF: _chemical_formula_sum  C28 H45 N3 Ni2 O10 S4
           TEST: Compare cell contents of formula and atom_site data

           atom    Z*formula  cif sites diff
           C        224.00    224.00    0.00
           H        360.00    352.00    8.00
           N         24.00     24.00    0.00
           Ni        16.00     16.00    0.00
           O         80.00     80.00    0.00
           S         32.00     32.00    0.00
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...          5 Report
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension          2 Info
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PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............         10 Report
              H9A   H9B   H10A  H10B  H1A   H1B   H2A   H2B   H3A   H3B
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large      24.10 Why ?
PLAT143_ALERT_4_G s.u. on c - Axis Small or Missing ..............    0.00010 Ang.
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records          2 Report
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)        293 Check
PLAT200_ALERT_1_G Reported   _diffrn_ambient_temperature ..... (K)        293 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........          2 Note
              Ni02    C00L
PLAT794_ALERT_5_G Tentative Bond Valency for Ni1       (II)      .       1.97 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Ni02      (III)     .       3.00 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Ni2       (III)     .       2.95 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............         30 Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600        147 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....          1 Note
                 0  0  4,
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File          6 Note
               12 11  6,  25  9  0,  25  9  1,  16  9  6,  19 19  0,  19  1 13,
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........        4.6 Low
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........       5.54 Note
              Predicted wR2: Based on SigI**2  2.95 or SHELX Weight 15.99
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          5 Info
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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
  19 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  24 ALERT level G = General information/check it is not something unexpected

  12 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  12 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
   7 ALERT type 4 Improvement, methodology, query or suggestion
   6 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 06/01/2024; check.def file version of 05/01/2024

Datablock Ni-dcbdt - ellipsoid plot