checkCIF/PLATON report

Structure factors have been supplied for datablock(s) rebe18

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: rebe18

Bond precision: C-C = 0.0060 A Wavelength=1.54178

Cell: a=17.7361(4) b=17.7361(4) c=17.7361(4)
    alpha=90 beta=90 gamma=90
Temperature: 100 K

 Calculated Reported
Volume 5579.2(4) 5579.2(4)
Space group P a -3 P a -3
Hall group -P 2ac 2ab -P 2ac 2ab
Moiety formula C18 H15 Br3 Ni P, C8 H20 N C18 H15 Br3 Ni P, C8 H20 N
Sum formula C26 H35 Br3 N Ni P C26 H35 Br3 N Ni P
Mr 690.90 690.96
Dx,g cm-3 1.645 1.645
Z 8 8
Mu (mm-1) 6.678 6.678
F000 2767.9 2768.0
F000’ 2733.87
h,k,lmax 21,21,21 20,21,21
Nref 1705 1703
Tmin,Tmax 0.471,0.766 0.560,0.766
Tmin’ 0.427

Correction method= # Reported T Limits: Tmin=0.560 Tmax=0.766
AbsCorr = MULTI-SCAN

Data completeness= 0.999 Theta(max)= 68.148
R(reflections)= 0.0398( 1475) wr2(reflections)= 0.1030( 1703)
S = 1.061 Npar= 159
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**

**PLAT244_ALERT_4_C** Low ‘Solvent’ Ueq as Compared to Neighbors of N1 Check

Author Response: Central nitrogen atom of a tetraethylammonium cation strongly disordered around a threefold axis.

**PLAT250_ALERT_2_C** Large U3/U1 Ratio for Average U(i,j) Tensor .... 2.2 Note

Author Response: No obvious preferred orientation of ADPs visible in packing diagrams. Eventually related with higher disorder perpendicular to the 3-fold axis.

**Alert level G**

**PLAT002_ALERT_2_G** Number of Distance or Angle Restraints on AtSite 12 Note

Author Response: The [NEt4]+ cation was found situated on a three-fold axis and was - as to be expected - highly disordered. SADI and RIGU restraints were applied to bond distances and angles in the [NEt4]+ cation. Increased ADPs and high residual charges also indicated a disorder of the bromine atoms. Most likely, a tilting of the NiBr3 moiety relativ to the Ni-P bond, so that P-Ni-Br angles become unequal. Two positions were refined for Br with SADI restraints on the Ni-Br distance, but no further restraints. Occupation factors refined to 0.54:0.46. Refinement of three bromine positions further lowered R1 and wR2 values, but yielded two practically superimposed bromine atoms with slightly different ADPs. We restricted the refinement thus to two bromine positions.

**PLAT003_ALERT_2_G** Number of Uiso or Uij Restrained non-H Atoms ... 9 Report

**PLAT083_ALERT_2_G** SHEXL Second Parameter in WGHT Unusually Large 10.84 Why ?

**PLAT176_ALERT_4_G** The CIF-Embedded .res File Contains SADI Records 4 Report

**PLAT178_ALERT_4_G** The CIF-Embedded .res File Contains SIMU Records 1 Report

**PLAT187_ALERT_4_G** The CIF-Embedded .res File Contains RIGU Records 1 Report

**PLAT232_ALERT_2_G** Hirshfeld Test Diff (M-X) Br1 --Ni1 . 8.8 s.u.

**PLAT232_ALERT_2_G** Hirshfeld Test Diff (M-X) Br2 --Ni1 . 8.5 s.u.

**PLAT300_ALERT_4_G** Atom Site Occupancy of C11 Constrained at 0.3333 Check

**PLAT300_ALERT_4_G** Atom Site Occupancy of C12 Constrained at 0.3333 Check

**PLAT300_ALERT_4_G** Atom Site Occupancy of C21 Constrained at 0.3333 Check

**PLAT300_ALERT_4_G** Atom Site Occupancy of C22 Constrained at 0.3333 Check

**PLAT300_ALERT_4_G** Atom Site Occupancy of C31 Constrained at 0.3333 Check

**PLAT300_ALERT_4_G** Atom Site Occupancy of C32 Constrained at 0.3333 Check

**PLAT300_ALERT_4_G** Atom Site Occupancy of C41 Constrained at 0.3333 Check

**PLAT300_ALERT_4_G** Atom Site Occupancy of C42 Constrained at 0.3333 Check

**PLAT300_ALERT_4_G** Atom Site Occupancy of H11A Constrained at 0.3333 Check

**PLAT300_ALERT_4_G** Atom Site Occupancy of H11B Constrained at 0.3333 Check

**PLAT300_ALERT_4_G** Atom Site Occupancy of H12A Constrained at 0.3333 Check

**PLAT300_ALERT_4_G** Atom Site Occupancy of H12B Constrained at 0.3333 Check

**PLAT300_ALERT_4_G** Atom Site Occupancy of H12C Constrained at 0.3333 Check
Atom Site Occupancy of H21A
Constrained at 0.3333

Atom Site Occupancy of H21B
Constrained at 0.3333

Atom Site Occupancy of H22A
Constrained at 0.3333

Atom Site Occupancy of H22B
Constrained at 0.3333

Atom Site Occupancy of H22C
Constrained at 0.3333

Atom Site Occupancy of H31A
Constrained at 0.3333

Atom Site Occupancy of H31B
Constrained at 0.3333

Atom Site Occupancy of H32A
Constrained at 0.3333

Atom Site Occupancy of H32B
Constrained at 0.3333

Atom Site Occupancy of H32C
Constrained at 0.3333

Atom Site Occupancy of H41A
Constrained at 0.3333

Atom Site Occupancy of H41B
Constrained at 0.3333

Atom Site Occupancy of H42A
Constrained at 0.3333

Atom Site Occupancy of H42B
Constrained at 0.3333

Atom Site Occupancy of H42C
Constrained at 0.3333

Main Residue Disorder ..........(Resd 1 ) 13% Note

Anion/Solvent/Minor-Residue Disorder (Resd 2 ) 89% Note

Atoms with Negative _atom_site_disorder_group # 30 Check

Number of Least-Squares Restraints .......... 121 Note

Percentage of I>2sig(I) Data at Theta(Max) Still 67% Note

Missing # of FCF Reflections Above STh/L= 0.600 1 Note

Number C-C Bonds with Positive Residual Density. 4 Info

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

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
7 ALERT type 2 Indicator that the structure model may be wrong or deficient
3 ALERT type 3 Indicator that the structure quality may be low
35 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.

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