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: Diaspore_synchrotron_SOLEIL_structural

```
Bond precision:   Al- O = 0.0003 A         Wavelength=0.41618

Cell:              a=9.3873(2)      b=2.83254(5)      c=4.36908(19)
                   alpha=90         beta=90           gamma=90
Temperature:       293 K

                 Calculated                 Reported
Volume           116.173(6)                 116.174(6)
Space group      P n m a                    P n m a
Hall group       -P 2ac 2n                  -P 2ac 2n
Moiety formula   Al H O2                    Al H O2
Sum formula      Al H O2                    Al H O2
Mr               59.99                      59.99
Dx,g cm-3        3.430                      3.430
Z                4                          4
Mu (mm-1)        0.249                      0.248
F000             120.0                      120.0
F000'            120.06
h,k,lmax         23,7,10                    22,7,8
Nref             1042                       753
Tmin,Tmax        0.971,0.976                0.010,1.000
Tmin'            0.963

Correction method= # Reported T Limits: Tmin=0.010 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.723           Theta(max)= 31.331

R(reflections)= 0.0246( 717)                    wR2(reflections)=
                                                0.0692( 753)
S = 1.139                  Npar= 22
```

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

PLAT029_ALERT_3_A _diffrn_measured_fraction_theta_full value Low . 0.754 Why?

Author Response: Single crystal is placed in diamond anvil cell. That is why access to reciprocal space is significantly restricted. As a consequence completeness is lower than 100%.

Alert level B

PLAT430_ALERT_2_B Short Inter D...A Contact O003 ..O003 . 2.78 Ang.
3/2-x,-y,-1/2+z = 2_654 Check
PLAT430_ALERT_2_B Short Inter D...A Contact O003 ..O003 . 2.78 Ang.
3/2-x,-1/2+y,1/2+z = 8_756 Check

Alert level G

ABSMU01_ALERT_1_G Calculation of _exptl_absorpt_correction_mu
not performed for this radiation type.
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 2 Info
PLAT012_ALERT_1_G No _shelx_res_checksum Found in CIF ..... Please Check
PLAT092_ALERT_4_G Check: Wavelength Given is not Cu,Ga,Mo,Ag,In Ka 0.41618 Ang.
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 ..... 4 Note
PLAT794_ALERT_5_G Tentative Bond Valency for Al01 (III) . 2.79 Info
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters 1 Info
PLAT952_ALERT_5_G Calculated (ThMax) and CIF-Reported Lmax Differ. 2 Units
PLAT984_ALERT_1_G The Al-f'= 0.0119 Deviates from the B&C-Value 0.0199 Check
PLAT984_ALERT_1_G The O-f'= -0.0012 Deviates from the B&C-Value 0.0018 Check

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

6 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
2 ALERT type 2 Indicator that the structure model may be wrong or deficient
1 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

Datablock: Diaspore_synchrotron_SOLEIL_multipole

Bond precision: Al- O = 0.0004 A Wavelength=0.41618

Cell: a=9.3873(2) b=2.8325(1) c=4.3691(2)
alpha=90 beta=90 gamma=90
Temperature: 293 K

	Calculated	Reported
Volume	116.172(7)	116.172(7)
Space group	P n m a	P n m a
Hall group	-P 2ac 2n	-P 2ac 2n
Moiety formula	Al H O2	Al H O2
Sum formula	Al H O2	Al H O2
Mr	59.99	59.99
Dx,g cm-3	3.430	3.430
Z	4	4
Mu (mm-1)	0.249	0.248
F000	120.0	120.0
F000'	120.06	
h,k,lmax	23,7,10	22,7,8
Nref	1042	753
Tmin,Tmax	0.971,0.976	0.010,1.000
Tmin'	0.963	

Correction method= # Reported T Limits: Tmin=0.010 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.723 Theta(max)= 31.331

R(reflections)= 0.0200(717) wR2(reflections)= 0.0440(669)

S = 1.024 Npar= 35

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
PLAT029_ALERT_3_A _diffrn_measured_fraction_theta_full value Low . 0.754 Why?

Author Response: Single crystal is placed in diamond anvil cell. That is why access to reciprocal space is significantly restricted. As a consequence completeness is lower than 100%.

Alert level B

```
PLAT430_ALERT_2_B Short Inter D...A Contact  O2       ..O2       .       2.78 Ang.
                                        3/2-x,-y,-1/2+z  =      2_654 Check
PLAT430_ALERT_2_B Short Inter D...A Contact  O2       ..O2       .       2.78 Ang.
                                      3/2-x,-1/2+y,1/2+z  =      8_645 Check
```

Alert level C

```
PLAT741_ALERT_1_C Bond    Calc 2.83250(10), Rep     2.83250 ......    Missing s.u.
             AL(1)    -AL(1)           1_555   7_555 ........     #    1 Check
PLAT741_ALERT_1_C Bond    Calc 2.83250(10), Rep     2.83250 ......    Missing s.u.
             AL(1)    -AL(1)           1_555   7_575 ........     #    2 Check
```

Alert level G

```
ABSMU01_ALERT_1_G  Calculation of _exptl_absorpt_correction_mu
               not performed for this radiation type.
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension         2 Info
PLAT005_ALERT_5_G No Embedded Refinement Details Found  in the CIF     Please Do !
PLAT092_ALERT_4_G Check: Wavelength Given is not Cu,Ga,Mo,Ag,In Ka    0.41618 Ang.
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)        293 Check
PLAT200_ALERT_1_G Reported   _diffrn_ambient_temperature ..... (K)        293 Check
PLAT794_ALERT_5_G Tentative Bond Valency for Al1       (III)     .       2.79 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        12 Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT952_ALERT_5_G Calculated (ThMax) and CIF-Reported Lmax Differ.         2 Units
PLAT963_ALERT_2_G Both SHELXL WEIGHT Parameter Values Zero .......     Please Check
PLAT984_ALERT_1_G The Al-f'=    0.0119 Deviates from the B&C-Value     0.0199 Check
PLAT984_ALERT_1_G The  O-f'=   -0.0012 Deviates from the B&C-Value     0.0018 Check
```

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1 ALERT type 4 Improvement, methodology, query or suggestion
4 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

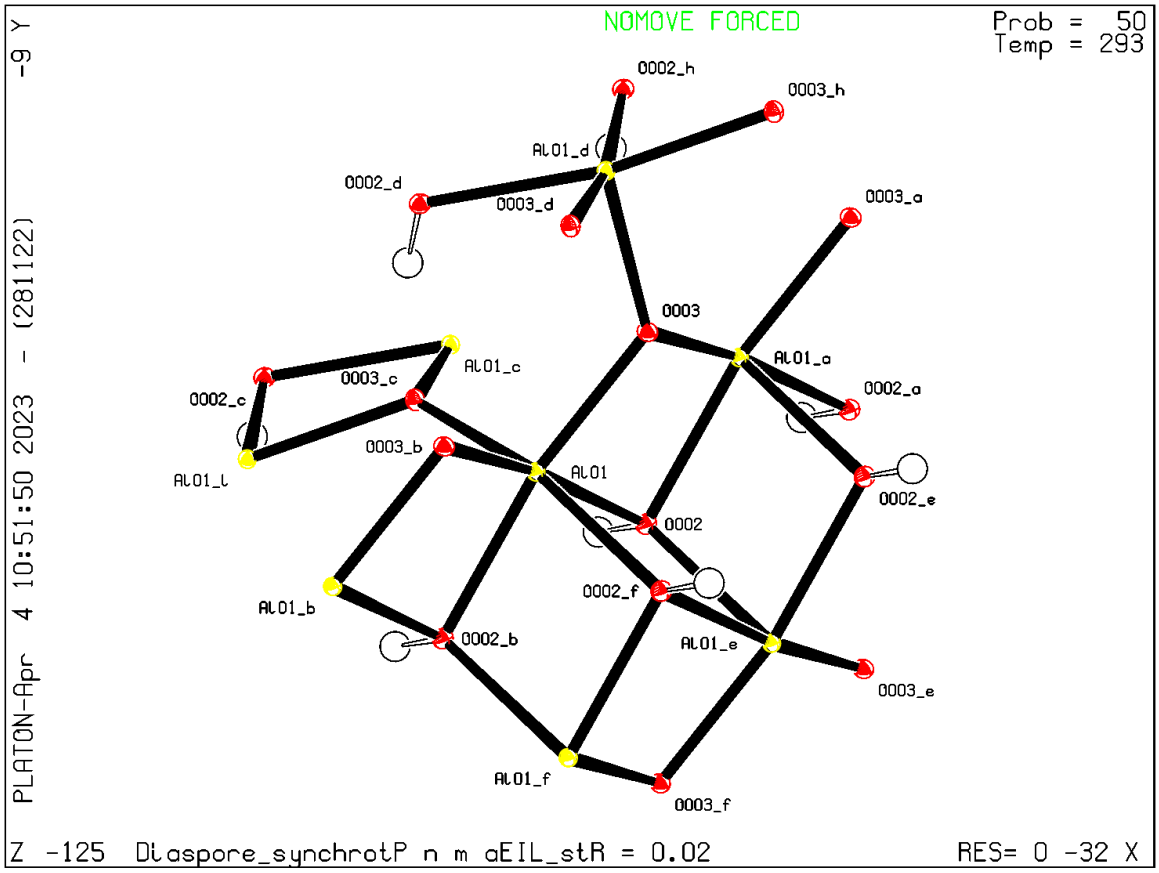
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section 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.

PLATON version of 28/11/2022; check.def file version of 28/11/2022

Datablock Diaspore_synchrotron_SOLEIL_structural - ellipsoid plot



Datablock Diaspore_synchrotron_SOLEIL_multipole - ellipsoid plot