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: Calcium_sebacate_hydrate

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Bond precision:    C-C = 0.0190 A              Wavelength=1.54175

Cell:           a=5.8633(4)          b=6.8363(6)          c=16.0587(16)
                alpha=79.338(11)     beta=81.318(9)       gamma=82.834(6)
Temperature:    293 K

                  Calculated                   Reported
Volume            622.21(10)                   622.21(10)
Space group       P -1                         P -1
Hall group        -P 1                         -P 1
Moiety formula    C10 H18 Ca O5                C10 H16 O4 2-, Ca 2+, H2 O
Sum formula       C10 H18 Ca O5                C10 H18 O5 Ca
Mr                258.32                       258.32
Dx,g cm-3         1.379                        1.379
Z                 2                            2
Mu (mm-1)         4.414                        0.000
F000              276.0                        0.0
F000'             277.58
h,k,lmax          6,7,18
Nref              2012
Tmin,Tmax
Tmin'

Correction method= Not given

Data completeness= 0.000              Theta(max)=

R(reflections)=                                  wR2(reflections)=
S =                          Npar=
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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.

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🔴 Alert level A

GEOM001_ALERT_1_A _geom_bond_atom_site_label_1 is missing
            Label identifying the atom site 1.
GEOM002_ALERT_1_A _geom_bond_atom_site_label_2 is missing
            Label identifying the atom site 2.
GEOM003_ALERT_1_A _geom_bond_distance is missing
            Distance between atom sites 1 and 2.
GEOM006_ALERT_1_A _geom_angle_atom_site_label_2 is missing
            Label identifying the atom site 2.
GEOM007_ALERT_1_A _geom_angle_atom_site_label_3 is missing
            Label identifying the atom site 3.
GEOM008_ALERT_1_A _geom_angle is missing
            Angle between atom sites 1, 2 and 3.
PLAT411_ALERT_2_A Short Inter H...H Contact H1AC   ..H1AC   .   1.62 Ang.
                                             -x,1-y,-z =   2_565 Check

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🟠 Alert level B

PLAT341_ALERT_3_B Low Bond Precision on C-C Bonds ....   0.019 Ang.
PLAT410_ALERT_2_B Short Intra H...H Contact H15   ..H15   .   1.83 Ang.
                                             -x,1-y,1-z =   2_566 Check
PLAT430_ALERT_2_B Short Inter D...A Contact O28   ..O28   .   2.83 Ang.
                                             1-x,-y,-z =   2_655 Check
PLAT780_ALERT_1_B Coordinates do not Form a Properly Connected Set   Please Do !

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🟡 Alert level C

REFI015_ALERT_1_C _refine_ls_shift/su_max is missing
            Maximum shift/s.u. ratio after final refinement cycle.
            The following tests will not be performed
            SHFSU_01
PLAT041_ALERT_1_C Calc. and Reported SumFormula   Strings Differ   Please Check
PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings Differ   Please Check
PLAT410_ALERT_2_C Short Intra H...H Contact H9   ..H21   .   1.92 Ang.
                                             -x,1-y,1-z =   2_566 Check
PLAT761_ALERT_1_C CIF Contains no X-H Bonds ....   Please Check
PLAT762_ALERT_1_C CIF Contains no X-Y-H or H-Y-H Angles ....   Please Check

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⚪ Alert level G

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension   3 Info
PLAT164_ALERT_4_G Nr. of Refined C-H H-Atoms in Heavy-Atom Struct.   16 Note
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ....   3 Note

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    7 **ALERT level A** = Most likely a serious problem - resolve or explain
    4 **ALERT level B** = A potentially serious problem, consider carefully
    6 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
    3 **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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4 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
2 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* 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