checkCIF/PLATON report

Structure factors have been supplied for datablock(s) Exp2_p1_MHI, Exp2_p2_MHIIa, Exp2_p3_decompression_MHIIa, Exp2_p4_MHIIa, Exp2_p5_MHIIb

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: Exp2_p1_MHI

```
Bond precision:   = 0.0000 A                Wavelength=0.37380

Cell:               a=11.7177(4)      b=11.7177(4)      c=11.7177(4)
                    alpha=90          beta=90           gamma=90
Temperature:        296 K

                  Calculated                    Reported
Volume            1608.89(16)                   1608.89(16)
Space group       P m -3 n                      P m -3 n
Hall group        -P 4n 2 3                     -P 4n 2 3
Moiety formula    O, 0.17(C)                    46(O), 7.803(C)
Sum formula       C0.17 O                       C7.80 O46
Mr                18.04                         829.68
Dx,g cm-3         0.856                         0.856
Z                 46                            1
Mu (mm-1)         0.028                         0.027
F000              414.8                         415.0
F000'             414.80
h,k,lmax          15,15,15                      10,15,15
Nref              385                           377
Tmin,Tmax         1.000,1.000                   0.038,1.000
Tmin'             1.000

Correction method= # Reported T Limits: Tmin=0.038 Tmax=1.000
AbsCorr = MULTI-SCAN
```

Data completeness= 0.979 Theta(max)= 14.427

R(reflections)= 0.0852(282) wR2(reflections)= 0.3265(377)

S = 1.215 Npar= 15

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

EXPT010_ALERT_1_A _exptl_crystal_colour (_pd_char_colour for powder) is missing
Crystal colour.
The following tests will not be performed.
CRYSC_01

GEOM001_ALERT_1_A _geom_bond_atom_site_label_1 is missing
Label identifying the atom site 1.

Author Response: The structure consists of water and methane molecules held together by

GEOM002_ALERT_1_A _geom_bond_atom_site_label_2 is missing
Label identifying the atom site 2.

Author Response: The structure consists of water and methane molecules held together by

GEOM003_ALERT_1_A _geom_bond_distance is missing
Distance between atom sites 1 and 2.

Author Response: The structure consists of water and methane molecules held together by

GEOM005_ALERT_1_A _geom_angle_atom_site_label_1 is missing
Label identifying the atom site 1.

GEOM006_ALERT_1_A _geom_angle_atom_site_label_2 is missing
Label identifying the atom site 2.

Author Response: The structure consists of water and methane molecules held together by

GEOM007_ALERT_1_A _geom_angle_atom_site_label_3 is missing
Label identifying the atom site 3.

Author Response: The structure consists of water and methane molecules held together by

GEOM008_ALERT_1_A _geom_angle is missing
Angle between atom sites 1, 2 and 3.

Author Response: The structure consists of water and methane molecules held together by

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Alert level B

```
PLAT049_ALERT_1_B Calculated Density Less Than 1.0 gcm-3 .........     0.8563 Check
              C1      C2
```

Author Response: The structure consists of an open, porous water framework containing c

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Alert level C

```
PLAT041_ALERT_1_C Calc. and Reported SumFormula    Strings  Differ     Please Check
              Calc: C0.17 O
              Rep.: C7.80 O46
PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings  Differ     Please Check
              Calc: O, 0.17(C)
              Rep.: 46(O), 7.803(C)
PLAT077_ALERT_4_C Unit-Cell Contains Non-integer Number of Atoms .     Please Check
PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) ...................       0.33 Report
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......     12.035 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600          5 Report
                0  7  7,   0  0  8,   8  8  8,   0  9  9,   0  0 14,
```

Alert level G

```
ABSMU01_ALERT_1_G  Calculation of _exptl_absorpt_correction_mu
                not performed for this radiation type.
PLAT040_ALERT_1_G No H-atoms in this Carbon Containing Compound ..     Please Check
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...        46 Check
PLAT068_ALERT_1_G Reported F000 Differs from Calcd (or Missing)...     Please Check
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large       0.18 Report
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd    5)       100% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd    1)       0.12 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd    2)       0.33 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd    3)       0.50 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd    4)       0.12 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd    5)       0.04 Check
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters          7 Info
PLAT910_ALERT_3_G Missing FCF Reflection(s) Below Theta(Min)[Deg]=       2.24 Note
                0  1  1,   0  0  2,   0  1  2,
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600          2 Note
PLAT950_ALERT_5_G Calculated (ThMax) and CIF-Reported Hmax Differ          5 Units
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........      3.677 Note
              Predicted wR2: Based on SigI**2  8.88 or SHELX Weight 26.87
```

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

  15 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
```

```
   1 ALERT type 2 Indicator that the structure model may be wrong or deficient
   5 ALERT type 3 Indicator that the structure quality may be low
   8 ALERT type 4 Improvement, methodology, query or suggestion
   2 ALERT type 5 Informative message, check
```

Datablock: Exp2_p2_MHIIa

```
Bond precision:   = 0.0000 A                Wavelength=0.37380

Cell:             a=11.9113(17)      b=11.9113(17)      c=10.0025(7)
                  alpha=90           beta=90            gamma=120
Temperature:      296 K

                 Calculated                  Reported
Volume           1229.0(4)                   1229.0(4)
Space group      P 6/m m m                   P 6/m m m
Hall group       -P 6 2                      -P 6 2
Moiety formula   O, 0.175(C)                 34(O), 5.964(C)
Sum formula      C0.18 O                     C5.96 O34
Mr               18.11                       615.58
Dx,g cm-3        0.832                       0.832
Z                34                          1
Mu (mm-1)        0.027                       0.026
F000             307.8                       308.0
F000'            307.76
h,k,lmax         15,15,13                    15,9,13
Nref             659                         551
Tmin,Tmax        1.000,1.000                 0.190,1.000
Tmin'            1.000

Correction method= # Reported T Limits: Tmin=0.190 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.836            Theta(max)= 14.429

R(reflections)= 0.0987( 367)                wR2(reflections)=
                                            0.3305( 551)
S = 1.214                  Npar= 26
```

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

EXPT010_ALERT_1_A _exptl_crystal_colour (_pd_char_colour for powder) is missing
Crystal colour.
The following tests will not be performed.
CRYSC_01

GEOM001_ALERT_1_A _geom_bond_atom_site_label_1 is missing
Label identifying the atom site 1.

Author Response: The structure consists of water and methane molecules held together by

GEOM002_ALERT_1_A _geom_bond_atom_site_label_2 is missing
Label identifying the atom site 2.

Author Response: The structure consists of water and methane molecules held together by

GEOM003_ALERT_1_A _geom_bond_distance is missing
Distance between atom sites 1 and 2.

Author Response: The structure consists of water and methane molecules held together by

GEOM005_ALERT_1_A _geom_angle_atom_site_label_1 is missing
Label identifying the atom site 1.

GEOM006_ALERT_1_A _geom_angle_atom_site_label_2 is missing
Label identifying the atom site 2.

Author Response: The structure consists of water and methane molecules held together by

GEOM007_ALERT_1_A _geom_angle_atom_site_label_3 is missing
Label identifying the atom site 3.

Author Response: The structure consists of water and methane molecules held together by

GEOM008_ALERT_1_A _geom_angle is missing
Angle between atom sites 1, 2 and 3.

Author Response: The structure consists of water and methane molecules held together by

---

Alert level B

PLAT049_ALERT_1_B Calculated Density Less Than 1.0 gcm-3 ..... 0.8317 Check
C1 C3

Author Response: The structure consists of an open, porous water framework containing c

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PLAT601_ALERT_2_B Unit-Cell Contains Solvent Accessible VOIDS .LE.        149 Ang**3
PLAT911_ALERT_3_B Missing FCF Refl Between Thmin & STh/L=    0.600         77 Report
               -1  3  0,   0  3  0,  -2  4  0,  -1  4  0,   0  4  0,  -1  5  0,
                0  5  0,  -2  6  0,  -1  6  0,   0  6  0,  -1  7  0,   0  7  0,
               -4  8  0,  -1  8  0,   0  8  0,  -1  9  0,   0  9  0,  -2 10  0,
               -1 10  0,   0 10  0,  -1 11  0,   0 11  0,  -4 12  0,  -3 12  0,
               -1 12  0,   0 12  0,  -2 13  0,  -6 14  0,  -5 14  0,   0  3  1,
                   (   47 More Missing: see the .ckf listing file)
```

Alert level C

```
DIFMX02_ALERT_1_C  The maximum difference density is > 0.1*ZMAX*0.75
           The relevant atom site should be identified.
PLAT041_ALERT_1_C Calc. and Reported SumFormula    Strings  Differ     Please Check
              Calc: C0.18 O
              Rep.: C5.96 O34
PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings  Differ     Please Check
              Calc: O, 0.175(C)
              Rep.: 34(O), 5.964(C)
PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) ...................       0.33 Report
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....       2.40 Report
PLAT097_ALERT_2_C Large Reported Max.  (Positive) Residual Density       0.65 eA-3
PLAT202_ALERT_3_C Isotropic non-H Atoms in Anion/Solvent .........          1 Check
              C2
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      4.890 Check
PLAT910_ALERT_3_C Missing FCF Reflection(s) Below Theta(Min)[Deg]=       2.38 Note
               0  1  0,  -1  2  0,   0  2  0,   0  0  1,   0  1  1,  -1  2  1,
               0  2  1,   0  0  2,
```

Alert level G

```
ABSMU01_ALERT_1_G  Calculation of _exptl_absorpt_correction_mu
               not performed for this radiation type.
PLAT019_ALERT_1_G _diffrn_measured_fraction_theta_full/*_max < 1.0      0.993 Report
PLAT040_ALERT_1_G No H-atoms in this Carbon Containing Compound ..     Please Check
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...        34 Check
PLAT068_ALERT_1_G Reported F000 Differs from Calcd (or Missing)...     Please Check
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large       0.20 Report
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd    7)       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd    6)       100% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd    1)       0.25 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd    2)       0.17 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd    3)       0.50 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd    4)       0.50 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd    5)       0.12 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd    6)       0.07 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd    7)       0.06 Check
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters          7 Info
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600         25 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File          1 Note
               8  0  6,
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........        1.7 Low
PLAT951_ALERT_5_G Calculated (ThMax) and CIF-Reported Kmax Differ           6 Units
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PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ..... 3.629 Note
Predicted wR2: Based on SigI**2 9.11 or SHELX Weight 27.23

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

17 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
5 ALERT type 2 Indicator that the structure model may be wrong or deficient
7 ALERT type 3 Indicator that the structure quality may be low
10 ALERT type 4 Improvement, methodology, query or suggestion
2 ALERT type 5 Informative message, check

Datablock: Exp2_p4_MHIIa

Bond precision: = 0.0000 A Wavelength=0.37380

Cell: a=11.8749(10) b=11.8749(10) c=9.9707(9)
alpha=90 beta=90 gamma=120
Temperature: 296 K

	Calculated	Reported
Volume	1217.6(2)	1217.6(2)
Space group	P 6/m m m	P 6/m m m
Hall group	-P 6 2	-P 6 2
Moiety formula	0.108(C12), 34(O), 7(C)	34(O), 8.296(C)
Sum formula	C8.30 O34	C8.30 O34
Mr	643.64	643.68
Dx,g cm-3	0.878	0.878
Z	1	1
Mu (mm-1)	0.028	0.027
F000	321.8	322.0
F000'	321.77	
h,k,lmax	15,15,13	6,14,13
Nref	653	574
Tmin,Tmax	1.000,1.000	0.072,1.000
Tmin'	1.000	

Correction method= # Reported T Limits: Tmin=0.072 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.879 Theta(max)= 14.405

R(reflections)= 0.0834(355)

wR2(reflections)= 0.3114(574)

S = 1.123 Npar= 28

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

EXPT010_ALERT_1_A _exptl_crystal_colour (_pd_char_colour for powder) is missing
Crystal colour.
The following tests will not be performed.
CRYSC_01

PLAT029_ALERT_3_A _diffrn_measured_fraction_theta_full value Low . 0.882 Why?

Author Response: The low data completeness is due to the physical restrictions of the D

Alert level B

PLAT049_ALERT_1_B Calculated Density Less Than 1.0 gcm-3 ..... 0.8778 Check

Author Response: The structure consists of an open, porous water framework containing c

PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) ..... O1 Check
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) ..... O2 Check
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) ..... O3 Check
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) ..... O4 Check
PLAT911_ALERT_3_B Missing FCF Refl Between Thmin & STh/L= 0.600 51 Report
-2 4 0, -2 5 0, -3 6 0, -3 7 0, -4 8 0, -5 10 0,
-5 11 0, -6 12 0, -5 12 0, -4 12 0, -6 13 0, -5 13 0,
-4 13 0, -7 14 0, -6 14 0, -2 4 1, -3 6 1, -4 8 1,
-5 10 1, -5 11 1, -6 12 1, -5 12 1, -6 13 1, -7 14 1,
-6 14 1, -3 6 2, -4 8 2, -5 10 2, -5 11 2, -6 12 2,
(21 More Missing: see the .ckf listing file)

Alert level C

PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings Differ Please Check
Calc: 0.108(C12), 34(O), 7(C)
Rep.: 34(O), 8.296(C)
PLAT077_ALERT_4_C Unit-Cell Contains Non-integer Number of Atoms . Please Check
PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) ..... 0.31 Report
PLAT202_ALERT_3_C Isotropic non-H Atoms in Anion/Solvent ..... 3 Check
C1 C2 C3
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 4.427 Check
PLAT910_ALERT_3_C Missing FCF Reflection(s) Below Theta(Min)[Deg]= 2.34 Note
0 1 0, -1 2 0, 0 2 0, 0 0 1, 0 1 1, -1 2 1,
0 0 2,

Alert level G

```
ABSMU01_ALERT_1_G  Calculation of _exptl_absorpt_correction_mu
               not performed for this radiation type.
PLAT040_ALERT_1_G No H-atoms in this Carbon Containing Compound ..     Please Check
PLAT068_ALERT_1_G Reported F000 Differs from Calcd (or Missing)...     Please Check
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large       0.19 Report
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd    1)       100% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd    1)       0.27 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd    2)       0.25 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd    3)       0.17 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd    4)       0.50 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd    5)       0.50 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd    6)       0.12 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd    7)       0.08 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd    8)       0.08 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C4       ..C4       .       1.79 Ang.
                                                  x-y,x,z  =      6_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C4       ..C4       .       1.79 Ang.
                                                 y,-x+y,z  =      5_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C4       ..C4       .       2.51 Ang.
                                                  y,x,1-z  =      7_556 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C4       ..C4       .       2.54 Ang.
                                                -y,-x,1-z  =     10_556 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C4       ..C4       .       3.09 Ang.
                                                -x+y,-x,z  =      3_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C4       ..C4       .       3.09 Ang.
                                                 -y,x-y,z  =      2_555 Check
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C4       --C4            1.78 Ang.
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C4       --C4            1.78 Ang.
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters         2 Info
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600        22 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....         2 Note
              -2  4  0,  -3  6  0,
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File         7 Note
               0  0  4,   2  0  3,   2  1  2,   3  0  1,   3  1  0,   3  3  3,
               4  0  1,
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........       2.0 Low
PLAT950_ALERT_5_G Calculated (ThMax) and CIF-Reported Hmax Differ          9 Units
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........     6.281 Note
             Predicted wR2: Based on SigI**2  4.96 or SHELX Weight 27.73
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```
  2 ALERT level A = Most likely a serious problem - resolve or explain
  6 ALERT level B = A potentially serious problem, consider carefully
  6 ALERT level C = Check. Ensure it is not caused by an omission or oversight
 28 ALERT level G = General information/check it is not something unexpected

  6 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 14 ALERT type 2 Indicator that the structure model may be wrong or deficient
  9 ALERT type 3 Indicator that the structure quality may be low
 11 ALERT type 4 Improvement, methodology, query or suggestion
  2 ALERT type 5 Informative message, check
```

Datablock: Exp2_p5_MHIIb

Bond precision: = 0.0000 A Wavelength=0.37380

Cell: a=11.8160(8) b=11.8160(8) c=9.9420(7)
alpha=90 beta=90 gamma=120
Temperature: 296 K

	Calculated	Reported
Volume	1202.11(18)	1202.11(18)
Space group	P -6 2 m	P -6 2 m
Hall group	P -6 -2	P -6 -2
Moiety formula	O, 0.269(C)	34(O), 9.121(C)
Sum formula	C0.27 O	C9.12 O34
Mr	19.23	653.53
Dx,g cm-3	0.903	0.903
Z	34	1
Mu (mm-1)	0.029	0.028
F000	326.8	327.0
F000'	326.77	
h,k,lmax	15,15,13	12,11,13
Nref	1147[651]	860
Tmin,Tmax	0.978,0.978	0.999,0.999
Tmin'	0.978	

Correction method= # Reported T Limits: Tmin=0.999 Tmax=0.999
AbsCorr = SPHERE

Data completeness= 1.32/0.75 Theta(max)= 14.429

R(reflections)= 0.0884(583) wR2(reflections)= 0.2778(860)

S = 1.111 Npar= 39

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

EXPT010_ALERT_1_A _exptl_crystal_colour (_pd_char_colour for powder) is missing
Crystal colour.
The following tests will not be performed.
CRYSC_01

GEOM001_ALERT_1_A _geom_bond_atom_site_label_1 is missing
Label identifying the atom site 1.

Author Response: The structure consists of water and methane molecules held together by

```
GEOM002_ALERT_1_A  _geom_bond_atom_site_label_2 is missing
           Label identifying the atom site 2.
```

Author Response: The structure consists of water and methane molecules held together by

```
GEOM003_ALERT_1_A  _geom_bond_distance is missing
           Distance between atom sites 1 and 2.
```

Author Response: The structure consists of water and methane molecules held together by

```
PLAT029_ALERT_3_A _diffrn_measured_fraction_theta_full value Low .      0.868 Why?
```

Author Response: The low data completeness is due to the physical restrictions of the D

Alert level B

```
PLAT049_ALERT_1_B Calculated Density Less Than 1.0 gcm-3 .........     0.9029 Check
             C1      C2      C3      C4
```

Author Response: The structure consists of an open, porous water framework containing c

```
PLAT911_ALERT_3_B Missing FCF Refl Between Thmin & STh/L=    0.600         56 Report
                0  3  0,   0  4  0,   0  5  0,  -1  6  0,   0  6  0,  -1  7  0,
                0  7  0,  -1  8  0,   0  8  0,  -1  9  0,   0  9  0,   0 10  0,
               -1 11  0,   0 11  0,  -1 12  0,   0 12  0,  -3 13  0,   0  3  1,
                0  4  1,   0  5  1,   0  8  1,   0  9  1,   0 10  1,   0 11  1,
               -1 12  1,   0 12  1,  -2 13  1,   0  8  2,   0 10  2,  -1 11  2,
                   (   26 More Missing: see the .ckf listing file)
```

Alert level C

```
STRVA01_ALERT_4_C           Flack parameter is too small
          From the CIF: _refine_ls_abs_structure_Flack  -10.000
          From the CIF: _refine_ls_abs_structure_Flack_su    1.000
PLAT041_ALERT_1_C Calc. and Reported SumFormula    Strings  Differ     Please Check
             Calc: C0.27 O
             Rep.: C9.12 O34
PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings  Differ     Please Check
             Calc: O, 0.269(C)
             Rep.: 34(O), 9.121(C)
PLAT077_ALERT_4_C Unit-Cell Contains Non-integer Number of Atoms .     Please Check
PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) ...................       0.28 Report
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      2.155 Check
PLAT910_ALERT_3_C Missing FCF Reflection(s) Below Theta(Min)[Deg]=       2.40 Note
                0  1  0,  -1  2  0,   0  2  0,   0  0  1,   0  1  1,  -1  2  1,
                0  2  1,   0  0  2,
```

Alert level G

```
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:C9.12 O34
           Atom count from the _atom_site data:  C9.13 O34
ABSMU01_ALERT_1_G  Calculation of _exptl_absorpt_correction_mu
               not performed for this radiation type.
PLAT032_ALERT_4_G Std. Uncertainty on Flack Parameter Value High .      1.000 Report
PLAT040_ALERT_1_G No H-atoms in this Carbon Containing Compound ..     Please Check
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...        34 Check
PLAT068_ALERT_1_G Reported F000 Differs from Calcd (or Missing)...     Please Check
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large       0.17 Report
PLAT180_ALERT_4_G Check Cell Rounding: # of Values Ending with 0 =          3 Note
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd    9)       100% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd    1)       0.50 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd    2)       0.33 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd    4)       0.50 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd    5)       0.50 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd    6)       0.25 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd    7)       0.17 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd    8)       0.17 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd    9)       0.18 Check
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters          8 Info
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600         28 Note
PLAT915_ALERT_3_G No Flack x Check Done: Low Friedel Pair Coverage         60 %
PLAT916_ALERT_2_G Hooft y and Flack x Parameter Values Differ by .      10.30 Check
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........        3.0 Low
PLAT950_ALERT_5_G Calculated (ThMax) and CIF-Reported Hmax Differ           3 Units
PLAT951_ALERT_5_G Calculated (ThMax) and CIF-Reported Kmax Differ           4 Units
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........      4.866 Note
              Predicted wR2: Based on SigI**2  5.71 or SHELX Weight 25.01
```

---

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

  11 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   3 ALERT type 2 Indicator that the structure model may be wrong or deficient
   8 ALERT type 3 Indicator that the structure quality may be low
  14 ALERT type 4 Improvement, methodology, query or suggestion
   3 ALERT type 5 Informative message, check

Datablock: Exp2_p3_decompression_MHIIa

Bond precision: = 0.0000 A Wavelength=0.37380

Cell:	a=11.868(2)	b=11.868(2)	c=9.9674(15)
	alpha=90	beta=90	gamma=120
Temperature:	296 K		

	Calculated	Reported
Volume	1215.8(4)	1215.8(4)
Space group	P 6/m m m	P 6/m m m
Hall group	-P 6 2	-P 6 2
Moiety formula	0.004(C12), O, 0.188(C)	34(O), 8.021(C)
Sum formula	C0.24 O	C8.02 O34
Mr	18.85	640.32
Dx,g cm-3	0.876	0.875
Z	34	1
Mu (mm-1)	0.028	0.027
F000	320.5	320.0
F000'	320.48	
h,k,lmax	15,15,13	6,15,13
Nref	654	536
Tmin,Tmax	1.000,1.000	0.240,1.000
Tmin'	1.000	

Correction method= # Reported T Limits: Tmin=0.240 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.820 Theta(max)= 14.412

R(reflections)= 0.0786(249) wR2(reflections)= 0.2949(536)

S = 0.982 Npar= 30

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

EXPT010_ALERT_1_A _exptl_crystal_colour (_pd_char_colour for powder) is missing
Crystal colour.
The following tests will not be performed.
CRYSC_01
PLAT029_ALERT_3_A _diffrn_measured_fraction_theta_full value Low . 0.821 Why?

Author Response: The low data completeness is due to the physical restrictions of the D

Alert level B

PLAT049_ALERT_1_B Calculated Density Less Than 1.0 gcm-3 ..... 0.8755 Check

Author Response: The structure consists of an open, porous water framework containing c

```
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) .......         O1 Check
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) .......         O2 Check
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) .......         O3 Check
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) .......         O4 Check
PLAT911_ALERT_3_B Missing FCF Refl Between Thmin & STh/L=    0.600         81 Report
               -1  3  0,  -2  4  0,  -3  6  0,   0  6  0,  -3  7  0,   0  7  0,
               -4  8  0,  -5 10  0,   0 10  0,  -5 11  0,  -1 11  0,   0 11  0,
               -6 12  0,  -5 12  0,  -6 13  0,  -2 13  0,  -7 14  0,  -6 14  0,
               -5 14  0,  -2  4  1,  -3  6  1,  -3  7  1,  -4  8  1,  -4  9  1,
               -5 10  1,  -5 11  1,  -6 12  1,  -5 12  1,  -6 13  1,  -7 14  1,
                   (   51 More Missing: see the .ckf listing file)
```

Alert level C

```
PLAT041_ALERT_1_C Calc. and Reported SumFormula    Strings  Differ     Please Check
             Calc: C0.24 O
             Rep.: C8.02 O34
PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings  Differ     Please Check
             Calc: 0.004(C12), O, 0.188(C)
             Rep.: 34(O), 8.021(C)
PLAT043_ALERT_1_C Calculated and Reported Mol. Weight Differ by ..       0.02 Check
PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) ...................       0.29 Report
PLAT202_ALERT_3_C Isotropic non-H Atoms in Anion/Solvent .........          3 Check
             C1      C2      C3
PLAT905_ALERT_3_C Negative K value in the Analysis of Variance ...     -0.101 Report
PLAT910_ALERT_3_C Missing FCF Reflection(s) Below Theta(Min)[Deg]=       2.35 Note
               0  1  0,  -1  2  0,   0  2  0,   0  0  1,   0  1  1,  -1  2  1,
               0  0  2,
```

Alert level G

```
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:C8.02 O34
           Atom count from the _atom_site data:  C8.08 O34
ABSMU01_ALERT_1_G  Calculation of _exptl_absorpt_correction_mu
              not performed for this radiation type.
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: check formula stoichiometry or atom site occupancies.
           From the CIF: _cell_formula_units_Z    1
           From the CIF: _chemical_formula_sum  C8.02 O34
           TEST: Compare cell contents of formula and atom_site data

           atom    Z*formula  cif sites diff
           C          8.02      8.08   -0.06
           O         34.00     34.00    0.00
PLAT040_ALERT_1_G No H-atoms in this Carbon Containing Compound ..     Please Check
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...        34 Check
PLAT068_ALERT_1_G Reported F000 Differs from Calcd (or Missing)...     Please Check
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large       0.18 Report
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd    1)       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd    7)       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd    8)       100% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd    1)       0.35 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd    2)       0.25 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd    3)       0.17 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd    4)       0.50 Check
```

```
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd    5)       0.50 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd    6)       0.12 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd    7)       0.08 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd    8)       0.06 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  O4       ..C4       .       2.96 Ang.
                                                      x,y,z  =      1_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  O4       ..C4       .       2.96 Ang.
                                                   x-y,-y,1-z  =      8_556 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C4       ..C4       .       2.04 Ang.
                                                     x-y,x,z  =      6_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C4       ..C4       .       2.04 Ang.
                                                    y,-x+y,z  =      5_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C4       ..C4       .       2.80 Ang.
                                                    -y,-x,1-z  =     10_556 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C4       ..C4       .       2.96 Ang.
                                                     y,x,1-z  =      7_556 Check
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters          2 Info
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600         30 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....          2 Note
               -2  4  0,  -3  6  0,
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........        1.5 Low
PLAT950_ALERT_5_G Calculated (ThMax) and CIF-Reported Hmax Differ           9 Units
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........      5.108 Note
             Predicted wR2: Based on SigI**2  5.77 or SHELX Weight 30.04
```

---

2 **ALERT level A** = Most likely a serious problem - resolve or explain
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12 ALERT type 4 Improvement, methodology, query or suggestion
2 ALERT type 5 Informative message, check

---

checkCIF publication errors

Alert level A

```
PUBL004_ALERT_1_A  The contact author's name and address are missing,
           _publ_contact_author_name and _publ_contact_author_address.
PUBL005_ALERT_1_A  _publ_contact_author_email, _publ_contact_author_fax and
           _publ_contact_author_phone are all missing.
           At least one of these should be present.
PUBL006_ALERT_1_A  _publ_requested_journal is missing
           e.g. 'Acta Crystallographica Section C'
PUBL008_ALERT_1_A  _publ_section_title is missing. Title of paper.
PUBL009_ALERT_1_A  _publ_author_name is missing. List of author(s) name(s).
PUBL010_ALERT_1_A  _publ_author_address is missing. Author(s) address(es).
```

```
PUBL012_ALERT_1_A  _publ_section_abstract is missing.
            Abstract of paper in English.
```

```
   7 ALERT level A = Data missing that is essential or data in wrong format
   0 ALERT level G = General alerts. Data that may be required is missing
```

Publication of your CIF

You should 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 nature of your study may justify the reported deviations from journal submission requirements and the more serious of these should 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.

If level A alerts remain, which you believe to be justified deviations, and you intend to submit this CIF for publication in a journal, you should additionally insert an explanation in your CIF using the Validation Reply Form (VRF) below. This will allow your explanation to be considered as part of the review process.

Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_PUBL004_GLOBAL
;
PROBLEM: The contact author's name and address are missing,
RESPONSE: ...
;
_vrf_PUBL005_GLOBAL
;
PROBLEM: _publ_contact_author_email, _publ_contact_author_fax and
RESPONSE: ...
;
_vrf_PUBL006_GLOBAL
;
PROBLEM: _publ_requested_journal is missing
RESPONSE: ...
;
_vrf_PUBL008_GLOBAL
;
PROBLEM: _publ_section_title is missing. Title of paper.
RESPONSE: ...
;
```

```
_vrf_PUBL009_GLOBAL
;
PROBLEM: _publ_author_name is missing. List of author(s) name(s).
RESPONSE: ...
;
_vrf_PUBL010_GLOBAL
;
PROBLEM: _publ_author_address is missing. Author(s) address(es).
RESPONSE: ...
;
_vrf_PUBL012_GLOBAL
;
PROBLEM: _publ_section_abstract is missing.
RESPONSE: ...
;
_vrf_EXPT010_Exp2_p1_MHI
;
PROBLEM: _exptl_crystal_colour (_pd_char_colour for powder) is missing
RESPONSE: ...
;
_vrf_GEOM005_Exp2_p1_MHI
;
PROBLEM: _geom_angle_atom_site_label_1 is missing
RESPONSE: ...
;
_vrf_PLAT041_Exp2_p1_MHI
;
PROBLEM: Calc. and Reported SumFormula    Strings  Differ     Please Check
RESPONSE: ...
;
_vrf_PLAT042_Exp2_p1_MHI
;
PROBLEM: Calc. and Reported MoietyFormula Strings  Differ     Please Check
RESPONSE: ...
;
_vrf_PLAT077_Exp2_p1_MHI
;
PROBLEM: Unit-Cell Contains Non-integer Number of Atoms .     Please Check
RESPONSE: ...
;
_vrf_PLAT084_Exp2_p1_MHI
;
PROBLEM: High wR2 Value (i.e. > 0.25) ...................       0.33 Report
RESPONSE: ...
;
_vrf_PLAT906_Exp2_p1_MHI
;
PROBLEM: Large K Value in the Analysis of Variance ......     12.035 Check
RESPONSE: ...
;
_vrf_PLAT911_Exp2_p1_MHI
;
PROBLEM: Missing FCF Refl Between Thmin & STh/L=    0.600          5 Report
RESPONSE: ...
;
_vrf_EXPT010_Exp2_p2_MHIIa
;
```

```
PROBLEM: _exptl_crystal_colour (_pd_char_colour for powder) is missing
RESPONSE: ...
;
_vrf_GEOM005_Exp2_p2_MHIIa
;
PROBLEM: _geom_angle_atom_site_label_1 is missing
RESPONSE: ...
;
_vrf_DIFMX02_Exp2_p2_MHIIa
;
PROBLEM: The maximum difference density is > 0.1*ZMAX*0.75
RESPONSE: ...
;
_vrf_PLAT601_Exp2_p2_MHIIa
;
PROBLEM: Unit-Cell Contains Solvent Accessible VOIDS .LE.        149 Ang**3
RESPONSE: ...
;
_vrf_PLAT911_Exp2_p2_MHIIa
;
PROBLEM: Missing FCF Refl Between Thmin & STh/L=    0.600         77 Report
RESPONSE: ...
;
_vrf_PLAT041_Exp2_p2_MHIIa
;
PROBLEM: Calc. and Reported SumFormula    Strings  Differ     Please Check
RESPONSE: ...
;
_vrf_PLAT042_Exp2_p2_MHIIa
;
PROBLEM: Calc. and Reported MoietyFormula Strings  Differ     Please Check
RESPONSE: ...
;
_vrf_PLAT084_Exp2_p2_MHIIa
;
PROBLEM: High wR2 Value (i.e. > 0.25) ...................       0.33 Report
RESPONSE: ...
;
_vrf_PLAT094_Exp2_p2_MHIIa
;
PROBLEM: Ratio of Maximum / Minimum Residual Density ....       2.40 Report
RESPONSE: ...
;
_vrf_PLAT097_Exp2_p2_MHIIa
;
PROBLEM: Large Reported Max.  (Positive) Residual Density       0.65 eA-3
RESPONSE: ...
;
_vrf_PLAT202_Exp2_p2_MHIIa
;
PROBLEM: Isotropic non-H Atoms in Anion/Solvent .........          1 Check
RESPONSE: ...
;
_vrf_PLAT906_Exp2_p2_MHIIa
;
PROBLEM: Large K Value in the Analysis of Variance ......      4.890 Check
RESPONSE: ...
```

;
_vrf_PLAT910_Exp2_p2_MHIIa
;
PROBLEM: Missing FCF Reflection(s) Below Theta(Min)[Deg]=   2.38 Note
RESPONSE: ...
;
_vrf_EXPT010_Exp2_p4_MHIIa
;
PROBLEM: _exptl_crystal_colour (_pd_char_colour for powder) is missing
RESPONSE: ...
;
_vrf_PLAT306_Exp2_p4_MHIIa
;
PROBLEM: Isolated Oxygen Atom (H-atoms Missing ?) ....   O1 Check
RESPONSE: ...
;
_vrf_PLAT911_Exp2_p4_MHIIa
;
PROBLEM: Missing FCF Refl Between Thmin & STh/L=   0.600   51 Report
RESPONSE: ...
;
_vrf_PLAT042_Exp2_p4_MHIIa
;
PROBLEM: Calc. and Reported MoietyFormula Strings Differ   Please Check
RESPONSE: ...
;
_vrf_PLAT077_Exp2_p4_MHIIa
;
PROBLEM: Unit-Cell Contains Non-integer Number of Atoms .   Please Check
RESPONSE: ...
;
_vrf_PLAT084_Exp2_p4_MHIIa
;
PROBLEM: High wR2 Value (i.e. > 0.25) ....   0.31 Report
RESPONSE: ...
;
_vrf_PLAT202_Exp2_p4_MHIIa
;
PROBLEM: Isotropic non-H Atoms in Anion/Solvent ....   3 Check
RESPONSE: ...
;
_vrf_PLAT906_Exp2_p4_MHIIa
;
PROBLEM: Large K Value in the Analysis of Variance ......   4.427 Check
RESPONSE: ...
;
_vrf_PLAT910_Exp2_p4_MHIIa
;
PROBLEM: Missing FCF Reflection(s) Below Theta(Min)[Deg]=   2.34 Note
RESPONSE: ...
;
_vrf_EXPT010_Exp2_p5_MHIIb
;
PROBLEM: _exptl_crystal_colour (_pd_char_colour for powder) is missing
RESPONSE: ...
;
_vrf_STRVA01_Exp2_p5_MHIIb

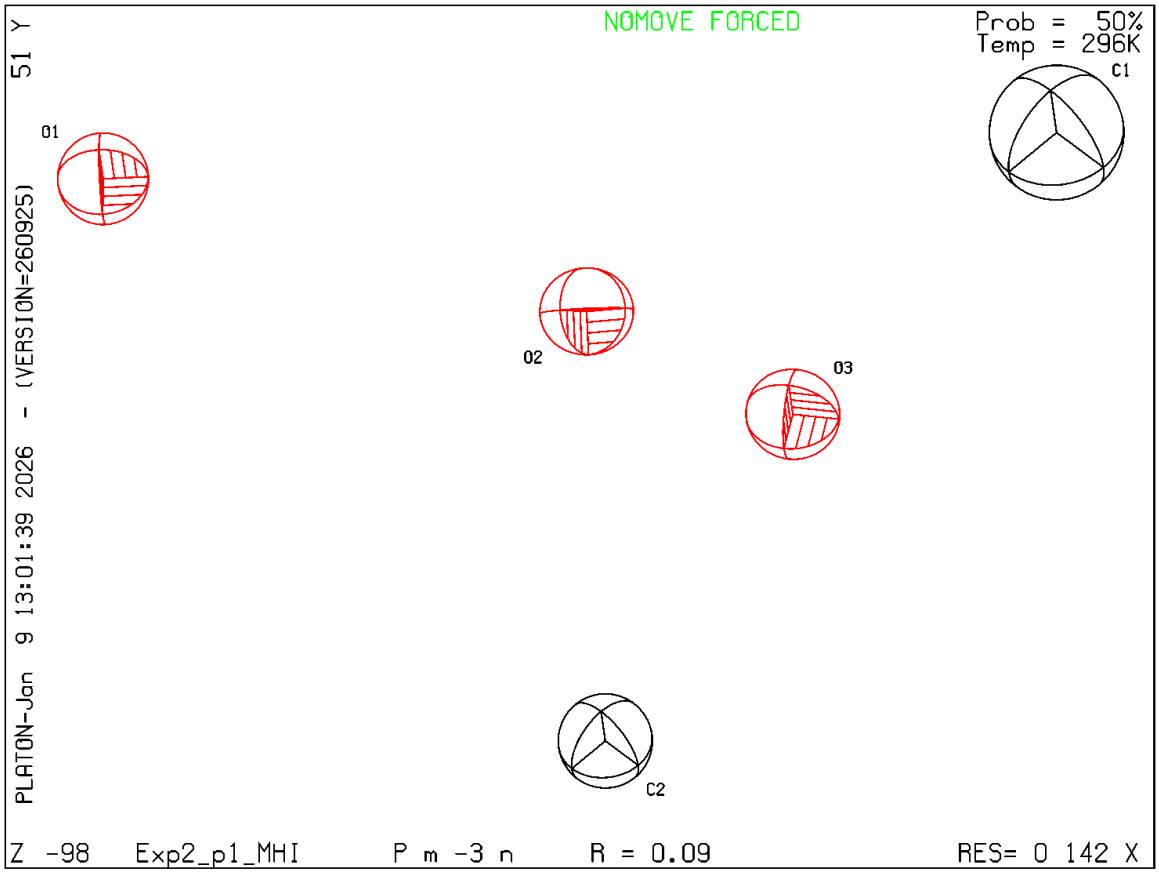
;
PROBLEM: Flack parameter is too small
RESPONSE: ...
;
_vrf_PLAT911_Exp2_p5_MHIIb
;
PROBLEM: Missing FCF Refl Between Thmin & STh/L=   0.600   56 Report
RESPONSE: ...
;
_vrf_PLAT041_Exp2_p5_MHIIb
;
PROBLEM: Calc. and Reported SumFormula   Strings Differ   Please Check
RESPONSE: ...
;
_vrf_PLAT042_Exp2_p5_MHIIb
;
PROBLEM: Calc. and Reported MoietyFormula Strings Differ   Please Check
RESPONSE: ...
;
_vrf_PLAT077_Exp2_p5_MHIIb
;
PROBLEM: Unit-Cell Contains Non-integer Number of Atoms .   Please Check
RESPONSE: ...
;
_vrf_PLAT084_Exp2_p5_MHIIb
;
PROBLEM: High wR2 Value (i.e. > 0.25) ....   0.28 Report
RESPONSE: ...
;
_vrf_PLAT906_Exp2_p5_MHIIb
;
PROBLEM: Large K Value in the Analysis of Variance ......   2.155 Check
RESPONSE: ...
;
_vrf_PLAT910_Exp2_p5_MHIIb
;
PROBLEM: Missing FCF Reflection(s) Below Theta(Min)[Deg]=   2.40 Note
RESPONSE: ...
;
_vrf_EXPT010_Exp2_p3_decompression_MHIIa
;
PROBLEM: _exptl_crystal_colour (_pd_char_colour for powder) is missing
RESPONSE: ...
;
_vrf_PLAT306_Exp2_p3_decompression_MHIIa
;
PROBLEM: Isolated Oxygen Atom (H-atoms Missing ?) ....   O1 Check
RESPONSE: ...
;
_vrf_PLAT911_Exp2_p3_decompression_MHIIa
;
PROBLEM: Missing FCF Refl Between Thmin & STh/L=   0.600   81 Report
RESPONSE: ...
;
_vrf_PLAT041_Exp2_p3_decompression_MHIIa
;
PROBLEM: Calc. and Reported SumFormula   Strings Differ   Please Check

```
RESPONSE: ...
;
_vrf_PLAT042_Exp2_p3_decompression_MHIIa
;
PROBLEM: Calc. and Reported MoietyFormula Strings  Differ     Please Check
RESPONSE: ...
;
_vrf_PLAT043_Exp2_p3_decompression_MHIIa
;
PROBLEM: Calculated and Reported Mol. Weight Differ by ..       0.02 Check
RESPONSE: ...
;
_vrf_PLAT084_Exp2_p3_decompression_MHIIa
;
PROBLEM: High wR2 Value (i.e. > 0.25) ...................       0.29 Report
RESPONSE: ...
;
_vrf_PLAT202_Exp2_p3_decompression_MHIIa
;
PROBLEM: Isotropic non-H Atoms in Anion/Solvent .........          3 Check
RESPONSE: ...
;
_vrf_PLAT905_Exp2_p3_decompression_MHIIa
;
PROBLEM: Negative K value in the Analysis of Variance ...     -0.101 Report
RESPONSE: ...
;
_vrf_PLAT910_Exp2_p3_decompression_MHIIa
;
PROBLEM: Missing FCF Reflection(s) Below Theta(Min)[Deg]=       2.35 Note
RESPONSE: ...
;
# end Validation Reply Form
```

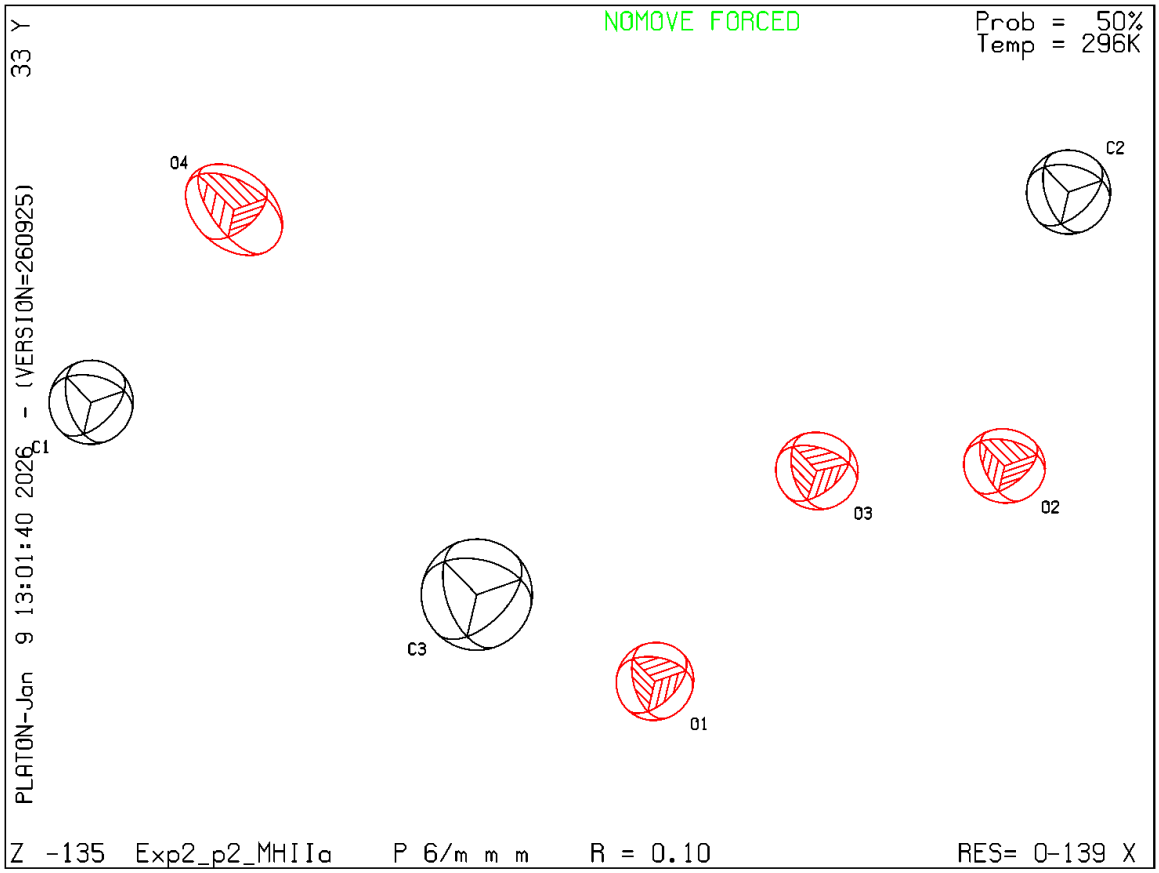
If you wish to submit your CIF for publication in Acta Crystallographica Section C or E, you should upload your CIF via the web. If you wish to submit your CIF for publication in IUCrData you should upload your CIF via the web. If your CIF is to form part of a submission to another IUCr journal, you will be asked, either during electronic submission or by the Co-editor handling your paper, to upload your CIF via our web site.

PLATON version of 26/09/2025; check.def file version of 20/09/2025

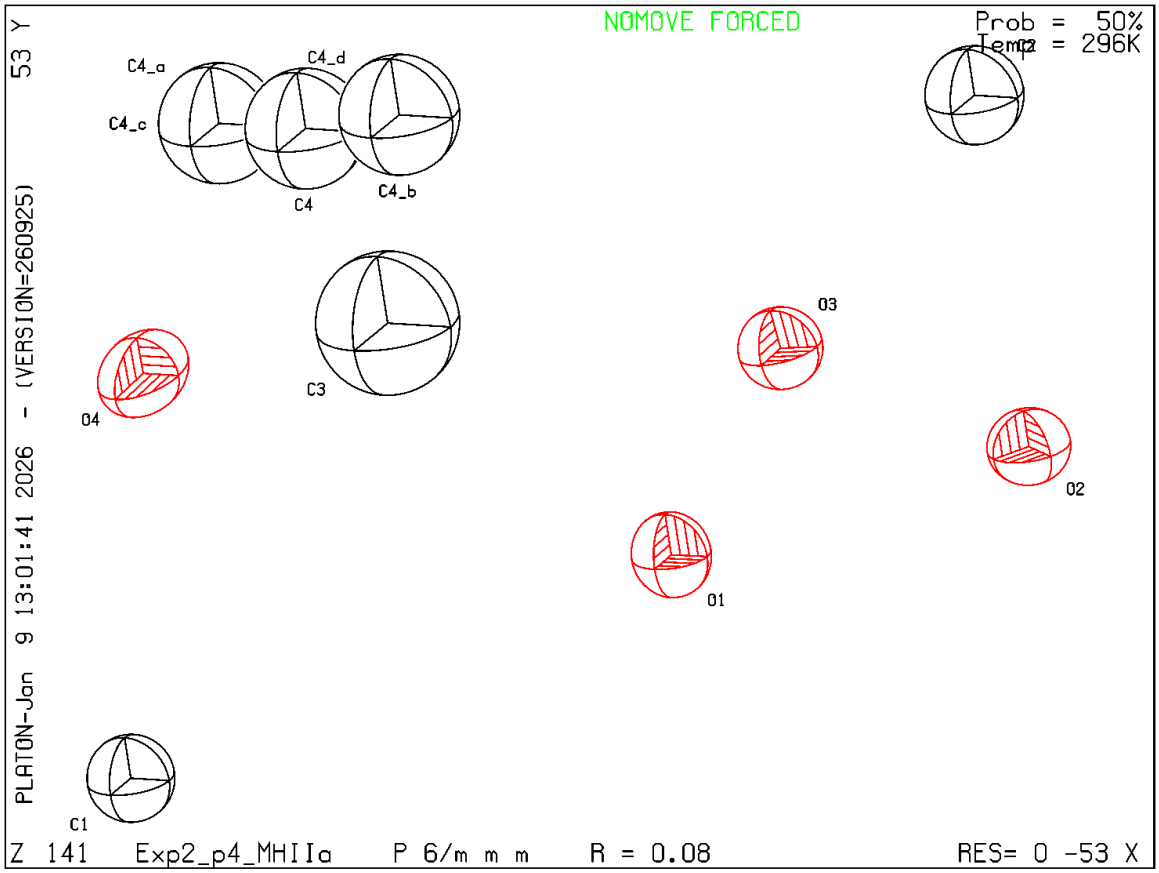
Datablock Exp2_p1_MHI - ellipsoid plot



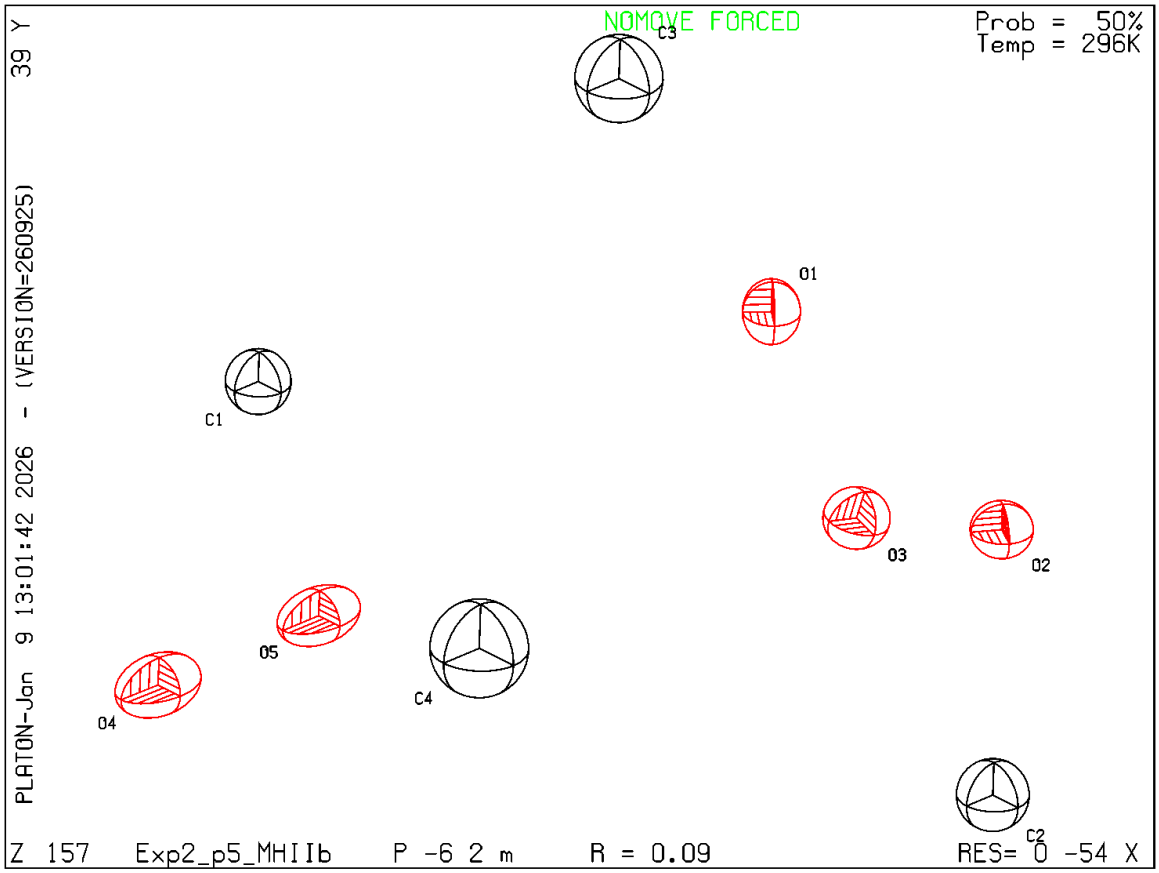
Datablock Exp2_p2_MHIIa - ellipsoid plot



Datablock Exp2_p4_MHIIa - ellipsoid plot



Datablock Exp2_p5_MHIIb - ellipsoid plot



Datablock Exp2_p3_decompression_MHIIa - ellipsoid plot