



## checkCIF/PLATON report

Structure factors have been supplied for datablock(s) Exp1\_p10\_MHIIb, Exp1\_p11\_MHIIb, Exp1\_p12\_MHIIb, Exp1\_p13\_MHIIb, Exp1\_p14\_MHIIb, Exp1\_p15\_MHIIb, Exp1\_p1\_MHI, Exp1\_p2\_MHI, Exp1\_p3\_MHI, Exp1\_p4\_MHI, Exp1\_p5\_MHI, Exp1\_p5\_MHIIa, Exp1\_p6\_MHIIa, Exp1\_p7\_MHIIa, Exp1\_p8\_MHIIa, Exp1\_p9\_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: Exp1\_p1\_MHI

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Bond precision:	= 0.0000 A	Wavelength=0.71075	
Cell:	a=11.7623 (4)	b=11.7623 (4)	c=11.7623 (4)
	alpha=90	beta=90	gamma=90
Temperature:	296 K		
	Calculated	Reported	
Volume	1627.33 (17)	1627.33 (18)	
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), 7.8 (C)	
Sum formula	C0.17 O	C7.80 O46	
Mr	18.04	829.68	
Dx, g cm <sup>-3</sup>	0.847	0.847	
Z	46	1	
Mu (mm <sup>-1</sup> )	0.097	0.097	
F000	414.8	415.0	
F000'	415.28		
h, k, lmax	15, 15, 15	15, 15, 9	
Nref	391	387	
Tmin, Tmax	0.999, 0.999	0.056, 1.000	
Tmin'	0.999		



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 ..... 0.8466 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), 7.8(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) ..... 0.32 Report  
PLAT094\_ALERT\_2\_C Ratio of Maximum / Minimum Residual Density .... 3.16 Report  
PLAT905\_ALERT\_3\_C Negative K value in the Analysis of Variance ... -3.085 Report  
PLAT939\_ALERT\_3\_C Large Value of Not (SHELXL) Weight Optimized S . 12.18 Check

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**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 0.996 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 ... 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 0.20 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  
PLAT883\_ALERT\_1\_G Absent Datum for \_atom\_sites\_solution\_primary .. Please Do !  
PLAT910\_ALERT\_3\_G Missing FCF Reflection(s) Below Theta (Min) [Deg]= 4.24 Note  
0 1 1, 0 0 2, 0 1 2,  
PLAT941\_ALERT\_3\_G Average HKL Measurement Multiplicity ..... 2.0 Low  
PLAT952\_ALERT\_5\_G Calculated (ThMax) and CIF-Reported Lmax Differ. 6 Units  
PLAT955\_ALERT\_1\_G Reported (CIF) and Actual (FCF) Lmax Differ by . 6 Units  
PLAT969\_ALERT\_5\_G The 'Henn et al.' R-Factor-gap value ..... 19.101 Note  
Predicted wR2: Based on SigI\*\*2 1.70 or SHELX Weight 25.30

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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**

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 ..... 0.8530 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), 7.802(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)	.....	0.26 Report
PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density	....	2.69 Report

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**Alert level G**

ABSMU01_ALERT_1_G	Calculation of _exptl_absorpt_correction_mu		
	not performed for this radiation type.		
PLAT019_ALERT_1_G	_diffn_measured_fraction_theta_full/*_max < 1.0		0.996 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	...	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		0.16 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
PLAT883_ALERT_1_G	Absent Datum for _atom_sites_solution_primary	..	Please Do !
PLAT910_ALERT_3_G	Missing FCF Reflection(s) Below Theta(Min) [Deg]=		4.25 Note
	0 1 1, 0 0 2, 0 1 2,		
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	.....	3.0 Low
PLAT952_ALERT_5_G	Calculated (ThMax) and CIF-Reported Lmax Differ.		6 Units
PLAT955_ALERT_1_G	Reported (CIF) and Actual (FCF) Lmax Differ by	.	6 Units
PLAT969_ALERT_5_G	The 'Henn et al.' R-Factor-gap value	.....	13.997 Note
	Predicted wR2: Based on SigI**2 1.89 or SHELX Weight	24.96	

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- 8 **ALERT level A** = Most likely a serious problem - resolve or explain  
1 **ALERT level B** = A potentially serious problem, consider carefully  
5 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
19 **ALERT level G** = General information/check it is not something unexpected
- 18 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  
4 ALERT type 3 Indicator that the structure quality may be low  
7 ALERT type 4 Improvement, methodology, query or suggestion  
2 ALERT type 5 Informative message, check
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**Datablock: Exp1\_p3\_MHI**

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Bond precision: = 0.0000 A Wavelength=0.71075  
Cell: a=11.6876(5) b=11.6876(5) c=11.6876(5)  
alpha=90 beta=90 gamma=90  
Temperature: 296 K

	Calculated	Reported
Volume	1596.5(2)	1596.5(2)
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), 7.835(C)
Sum formula	C0.17 O	C7.83 O46
Mr	18.05	830.04
Dx, g cm-3	0.863	0.863
Z	46	1
Mu (mm-1)	0.099	0.099
F000	415.0	415.0
F000'	415.52	
h, k, lmax	15, 15, 15	15, 15, 8
Nref	384	378
Tmin, Tmax	0.999, 0.999	0.242, 1.000
Tmin'	0.999	

Correction method= # Reported T Limits: Tmin=0.242 Tmax=1.000  
AbsCorr = MULTI-SCAN


Data completeness= 0.984 Theta(max)= 28.230

R(reflections)= 0.0703( 251) wR2(reflections)=  
0.2364( 378)  
S = 1.050 Npar= 15

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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**

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<sup>-3</sup> ..... 0.8635 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.: C7.83 O46  
PLAT042\_ALERT\_1\_C Calc. and Reported MoietyFormula Strings Differ Please Check  
Calc: O, 0.17(C)  
Rep.: 46(O), 7.835(C)  
PLAT077\_ALERT\_4\_C Unit-Cell Contains Non-integer Number of Atoms . Please Check  
PLAT911\_ALERT\_3\_C Missing FCF Refl Between Thmin & STh/L= 0.600 2 Report  
4 4 4, 8 8 8,

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	Calculated	Reported
Volume	1582.2(2)	1582.2(2)
Space group	P m -3 n	P m -3 n
Hall group	-P 4n 2 3	-P 4n 2 3
Moiety formula	O, 0.171(C)	46(O), 7.858(C)
Sum formula	C0.17 O	C7.86 O46
Mr	18.05	830.40
Dx, g cm-3	0.872	0.872
Z	46	1
Mu (mm-1)	0.100	0.100
F000	415.2	415.0
F000'	415.64	
h, k, lmax	15, 15, 15	15, 15, 8
Nref	377	374
Tmin, Tmax	0.999, 0.999	0.186, 1.000
Tmin'	0.999	


Correction method= # Reported T Limits: Tmin=0.186 Tmax=1.000  
AbsCorr = MULTI-SCAN

Data completeness= 0.992                      Theta(max)= 28.258

R(reflections)= 0.0698( 247)                      wR2(reflections)=  
0.2391( 374)

S = 1.102                      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 ..... 0.8715 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.: C7.86 O46  
PLAT042\_ALERT\_1\_C Calc. and Reported MoietyFormula Strings Differ Please Check  
Calc: O, 0.171(C)  
Rep.: 46(O), 7.858(C)  
PLAT077\_ALERT\_4\_C Unit-Cell Contains Non-integer Number of Atoms . Please Check  
PLAT911\_ALERT\_3\_C Missing FCF Refl Between Thmin & STh/L= 0.600 2 Report  
4 4 4, 8 8 8,

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**Alert level G**

ABSMU01\_ALERT\_1\_G Calculation of \_exptl\_absorpt\_correction\_mu  
not performed for this radiation type.  
PLAT019\_ALERT\_1\_G \_diffn\_measured\_fraction\_theta\_full/\*\_max < 1.0 0.998 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 ... 46 Check



	Calculated	Reported
Volume	1573.2(2)	1573.2(2)
Space group	P m -3 n	P m -3 n
Hall group	-P 4n 2 3	-P 4n 2 3
Moiety formula	O, 0.172(C)	46(O), 7.896(C)
Sum formula	C0.17 O	C7.89 O46
Mr	18.06	830.76
Dx, g cm-3	0.877	0.877
Z	46	1
Mu (mm-1)	0.101	0.101
F000	415.4	415.0
F000'	415.88	
h, k, lmax	15, 15, 15	15, 15, 8
Nref	377	371
Tmin, Tmax	0.999, 0.999	0.465, 1.000
Tmin'	0.999	


Correction method= # Reported T Limits: Tmin=0.465 Tmax=1.000  
AbsCorr = MULTI-SCAN

Data completeness= 0.984                      Theta(max)= 28.124

R(reflections)= 0.0657( 237)                      wR2(reflections)=  
0.2357( 371)

S = 1.064                      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 ..... 0.8770 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.: C7.89 O46  
PLAT042\_ALERT\_1\_C Calc. and Reported MoietyFormula Strings Differ Please Check  
Calc: O, 0.172(C)  
Rep.: 46(O), 7.896(C)  
PLAT077\_ALERT\_4\_C Unit-Cell Contains Non-integer Number of Atoms . Please Check  
PLAT906\_ALERT\_3\_C Large K Value in the Analysis of Variance ..... 3.545 Check  
PLAT906\_ALERT\_3\_C Large K Value in the Analysis of Variance ..... 2.689 Check  
PLAT911\_ALERT\_3\_C Missing FCF Refl Between Thmin & STh/L= 0.600 2 Report  
4 4 4, 8 8 8,

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**Alert level G**

ABSMU01\_ALERT\_1\_G Calculation of \_exptl\_absorpt\_correction\_mu  
not performed for this radiation type.  
PLAT019\_ALERT\_1\_G \_diffn\_measured\_fraction\_theta\_full/\*\_max < 1.0 0.998 Report



	Calculated	Reported
Volume	1240.5(8)	1240.4(7)
Space group	P 6/m m m	P 6/m m m
Hall group	-P 6 2	-P 6 2
Moiety formula	O, 0.168(C)	34(O), 5.692(C1)
Sum formula	C0.17 O	C5.69 O34
Mr	18.01	612.34
Dx, g cm <sup>-3</sup>	0.820	0.820
Z	34	1
Mu (mm <sup>-1</sup> )	0.094	0.094
F000	306.2	306.0
F000'	306.55	
h, k, lmax	15, 15, 13	15, 15, 5
Nref	664	310
Tmin, Tmax	0.997, 0.997	0.110, 1.000
Tmin'	0.997	

Correction method= # Reported T Limits: Tmin=0.110 Tmax=1.000  
AbsCorr = MULTI-SCAN

Data completeness= 0.467                      Theta(max)= 28.244

R(reflections)= 0.0707( 259)                      wR2(reflections)=  
0.2445( 310)

S = 1.152                      Npar= 27

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**

PLAT029\_ALERT\_3\_A \_diffn\_measured\_fraction\_theta\_full value Low . 0.482 Why?

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

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**Alert level B**

PLAT049\_ALERT\_1\_B Calculated Density Less Than 1.0 gcm<sup>-3</sup> ..... 0.8198 Check  
C1 C2 C3

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

PLAT601\_ALERT\_2\_B Unit-Cell Contains Solvent Accessible VOIDS .LE. 166 Ang\*\*3  
PLAT911\_ALERT\_3\_B Missing FCF Refl Between Thmin & STh/L= 0.600 74 Report  
0 4 1, -1 9 1, 0 1 2, -1 2 2, 0 2 2, -1 3 2,  
0 3 2, 0 0 3, 0 1 3, -1 2 3, 0 2 3, -1 3 3,  
0 3 3, -2 4 3, -1 4 3, 0 4 3, -2 5 3, -1 5 3,  
0 0 4, 0 1 4, -1 2 4, 0 2 4, -1 3 4, 0 3 4,  
-2 4 4, -1 4 4, 0 4 4, -2 5 4, -1 5 4, 0 5 4,  
( 44 More Missing: see the .ckf listing file)

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**Alert level C**

PLAT041\_ALERT\_1\_C Calc. and Reported SumFormula Strings Differ Please Check  
Calc.: C0.17 O  
Rep.: C5.69 O34

PLAT042\_ALERT\_1\_C Calc. and Reported MoietyFormula Strings Differ Please Check  
 Calc: 0, 0.168(C)  
 Rep.: 34(O), 5.692(C1)

PLAT077\_ALERT\_4\_C Unit-Cell Contains Non-integer Number of Atoms . Please Check

PLAT906\_ALERT\_3\_C Large K Value in the Analysis of Variance ..... 2.294 Check

PLAT910\_ALERT\_3\_C Missing FCF Reflection(s) Below Theta(Min) [Deg]= 4.43 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: C5.69 O34  
 Atom count from the \_atom\_site data: C5.7 O34

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 ... 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

PLAT301\_ALERT\_3\_G Main Residue Disorder .....(Resd 5) 100% Note

PLAT301\_ALERT\_3\_G Main Residue Disorder .....(Resd 6) 100% Note

PLAT301\_ALERT\_3\_G Main Residue Disorder .....(Resd 7) 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) 0.11 Check

PLAT304\_ALERT\_4\_G Non-Integer Number of Atoms in ..... (Resd 6) 0.08 Check

PLAT304\_ALERT\_4\_G Non-Integer Number of Atoms in ..... (Resd 7) 0.05 Check

PLAT802\_ALERT\_4\_G CIF Input Record(s) with more than 80 Characters 8 Info

PLAT883\_ALERT\_1\_G Absent Datum for \_atom\_sites\_solution\_primary .. Please Do !

PLAT933\_ALERT\_2\_G Number of HKL-OMIT Records in Embedded .res File 2 Note  
 -1 9 1, 0 4 1,

PLAT941\_ALERT\_3\_G Average HKL Measurement Multiplicity ..... 2.0 Low

PLAT952\_ALERT\_5\_G Calculated (ThMax) and CIF-Reported Lmax Differ. 8 Units

PLAT958\_ALERT\_1\_G Calculated (ThMax) and Actual (FCF) Lmax Differ. 8 Units

PLAT969\_ALERT\_5\_G The 'Henn et al.' R-Factor-gap value ..... 6.917 Note  
 Predicted wR2: Based on SigI\*\*2 3.53 or SHELX Weight 21.22

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

17 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
 4 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  
 9 ALERT type 4 Improvement, methodology, query or suggestion  
 2 ALERT type 5 Informative message, check

**Datablock: Exp1\_p6\_MHIIa**

Bond precision: = 0.0000 A Wavelength=0.37380  
Cell: a=11.9157(7) b=11.9157(7) c=9.992(5)  
alpha=90 beta=90 gamma=120  
Temperature: 296 K

	Calculated	Reported
Volume	1228.6(6)	1228.6(7)
Space group	P 6/m m m	P 6/m m m
Hall group	-P 6 2	-P 6 2
Moiety formula	O, 0.169(C)	34(O), 5.737(C)
Sum formula	C0.17 O	C5.74 O34
Mr	18.03	612.94
Dx, g cm <sup>-3</sup>	0.828	0.828
Z	34	1
Mu (mm <sup>-1</sup> )	0.027	0.026
F000	306.4	306.0
F000'	306.44	
h, k, lmax	15, 15, 13	15, 15, 5
Nref	657	307
Tmin, Tmax	0.999, 0.999	0.296, 1.000
Tmin'	0.999	

Correction method= # Reported T Limits: Tmin=0.296 Tmax=1.000  
AbsCorr = MULTI-SCAN

Data completeness= 0.467 Theta(max)= 14.421

R(reflections)= 0.0701( 235)

wR2(reflections)=  
0.2271( 307)

S = 1.098

Npar= 27

---

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**

EXPT010\_ALERT\_1\_A \_expt1\_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**

PLAT029\_ALERT\_3\_A \_diffn\_measured\_fraction\_theta\_full value Low . 0.481 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 ..... 0.8284 Check  
C1 C3

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

PLAT601\_ALERT\_2\_B Unit-Cell Contains Solvent Accessible VOIDS .LE. 156 Ang\*\*3  
PLAT911\_ALERT\_3\_B Missing FCF Refl Between Thmin & STh/L= 0.600 75 Report  
0 4 1, -1 9 1, 0 1 2, -1 2 2, 0 2 2, -1 3 2,  
0 3 2, 0 0 3, 0 1 3, -1 2 3, 0 2 3, -1 3 3,  
0 3 3, -2 4 3, -1 4 3, 0 4 3, -2 5 3, -1 5 3,  
0 0 4, 0 1 4, -1 2 4, 0 2 4, -1 3 4, 0 3 4,  
-2 4 4, -1 4 4, 0 4 4, -2 5 4, -1 5 4, 0 5 4,  
( 45 More Missing: see the .ckf listing file)

---

**Alert level C**

PLAT041\_ALERT\_1\_C Calc. and Reported SumFormula Strings Differ Please Check  
Calc: C0.17 O  
Rep.: C5.74 O34

PLAT042\_ALERT\_1\_C Calc. and Reported MoietyFormula Strings Differ Please Check  
Calc: O, 0.169(C)  
Rep.: 34(O), 5.737(C)

PLAT077\_ALERT\_4\_C Unit-Cell Contains Non-integer Number of Atoms . Please Check

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 ..... 2.992 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,

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**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 ... 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

PLAT301\_ALERT\_3\_G Main Residue Disorder .....(Resd 5) 100% Note

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) 0.08 Check

PLAT304\_ALERT\_4\_G Non-Integer Number of Atoms in ..... (Resd 7) 0.05 Check

PLAT802\_ALERT\_4\_G CIF Input Record(s) with more than 80 Characters 8 Info

PLAT883\_ALERT\_1\_G Absent Datum for \_atom\_sites\_solution\_primary .. Please Do !

PLAT933\_ALERT\_2\_G Number of HKL-OMIT Records in Embedded .res File 3 Note  
-3 11 5, -1 9 1, 0 4 1,

PLAT941\_ALERT\_3\_G Average HKL Measurement Multiplicity ..... 2.3 Low

PLAT952\_ALERT\_5\_G Calculated (ThMax) and CIF-Reported Lmax Differ. 8 Units

PLAT958\_ALERT\_1\_G Calculated (ThMax) and Actual (FCF) Lmax Differ. 8 Units

PLAT969\_ALERT\_5\_G The 'Henn et al.' R-Factor-gap value ..... 7.837 Note  
Predicted wR2: Based on SigI\*\*2 2.90 or SHELX Weight 20.69

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- 9 **ALERT level A** = Most likely a serious problem - resolve or explain
- 3 **ALERT level B** = A potentially serious problem, consider carefully
- 6 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
- 22 **ALERT level G** = General information/check it is not something unexpected
- 
- 17 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
- 10 ALERT type 4 Improvement, methodology, query or suggestion
- 2 ALERT type 5 Informative message, check
-



**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 ..... 0.8736 Check  
C1 C2

**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 73 Report  
0 4 1, 0 1 2, -1 2 2, 0 2 2, -1 3 2, 0 3 2,  
0 0 3, 0 1 3, -1 2 3, 0 2 3, -1 3 3, 0 3 3,  
-2 4 3, -1 4 3, 0 4 3, -2 5 3, -1 5 3, 0 0 4,  
0 1 4, -1 2 4, 0 2 4, -1 3 4, 0 3 4, -2 4 4,  
-1 4 4, 0 4 4, -2 5 4, -1 5 4, 0 5 4, -3 6 4,  
( 43 More Missing: see the .ckf listing file)

---

**Alert level C**

ABSMU01\_ALERT\_1\_C The ratio of given/expected absorption coefficient lies  
outside the range 0.99 <> 1.01  
Calculated value of mu = 0.098  
Value of mu given = 0.097  
PLAT041\_ALERT\_1\_C Calc. and Reported SumFormula Strings Differ Please Check  
Calc: C0.24 O  
Rep.: C8.10 O34  
PLAT042\_ALERT\_1\_C Calc. and Reported MoietyFormula Strings Differ Please Check  
Calc: O, 0.238(C)  
Rep.: 34(O), 8.096(C)  
PLAT076\_ALERT\_1\_C Occupancy 0.250 Less Than 1.0 for Sp.pos . C4  
PLAT202\_ALERT\_3\_C Isotropic non-H Atoms in Anion/Solvent ..... 1 Check  
C3  
PLAT260\_ALERT\_2\_C Large Average Ueq of Residue Including O4 0.103 Check  
PLAT910\_ALERT\_3\_C Missing FCF Reflection(s) Below Theta(Min) [Deg]= 4.46 Note  
0 1 0, -1 2 0, 0 2 0, 0 0 1, 0 1 1, -1 2 1,  
0 0 2,

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**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: C8.1 O34  
Atom count from the \_atom\_site data: C8.08 O34  
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 0.13 Report  
PLAT301\_ALERT\_3\_G Main Residue Disorder .....(Resd 5) 100% Note  
PLAT301\_ALERT\_3\_G Main Residue Disorder .....(Resd 8) 100% Note  
PLAT302\_ALERT\_4\_G Anion/Solvent/Minor-Residue Disorder (Resd 7) 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



	Calculated	Reported
Volume	1210.7(9)	1210.8(8)
Space group	P 6/m m m	P 6/m m m
Hall group	-P 6 2	-P 6 2
Moiety formula	O, 0.254(C)	34(O), 8.63(C)
Sum formula	C0.25 O	C8.62 O34
Mr	19.04	647.53
Dx, g cm <sup>-3</sup>	0.888	0.888
Z	34	1
Mu (mm <sup>-1</sup> )	0.099	0.099
F000	323.7	324.0
F000'	324.08	
h, k, lmax	15, 15, 13	15, 15, 5
Nref	651	306
Tmin, Tmax	0.996, 0.997	0.268, 1.000
Tmin'	0.996	

Correction method= # Reported T Limits: Tmin=0.268 Tmax=1.000  
AbsCorr = MULTI-SCAN

Data completeness= 0.470                      Theta(max)= 28.208

R(reflections)= 0.0718( 242)                      wR2(reflections)=  
0.2265( 306)

S = 1.058                      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 .                      0.487 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<sup>-3</sup> .....                      0.8881 Check  
O4A                      C1                      C2                      C3

**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 72 Report  
0 4 1, 0 1 2, -1 2 2, 0 2 2, -1 3 2, 0 3 2,  
0 0 3, 0 1 3, -1 2 3, 0 2 3, -1 3 3, 0 3 3,  
-2 4 3, -1 4 3, 0 4 3, -2 5 3, -1 5 3, 0 0 4,  
0 1 4, -1 2 4, 0 2 4, -1 3 4, 0 3 4, -2 4 4,  
-1 4 4, 0 4 4, -2 5 4, -1 5 4, 0 5 4, -3 6 4,  
( 42 More Missing: see the .ckf listing file)

---

**Alert level C**

PLAT041\_ALERT\_1\_C Calc. and Reported SumFormula Strings Differ Please Check  
Calc: C0.25 O  
Rep.: C8.62 O34  
PLAT042\_ALERT\_1\_C Calc. and Reported MoietyFormula Strings Differ Please Check  
Calc: O, 0.254(C)  
Rep.: 34(O), 8.63(C)  
PLAT077\_ALERT\_4\_C Unit-Cell Contains Non-integer Number of Atoms . Please Check  
PLAT906\_ALERT\_3\_C Large K Value in the Analysis of Variance ..... 3.172 Check  
PLAT910\_ALERT\_3\_C Missing FCF Reflection(s) Below Theta(Min) [Deg]= 4.47 Note  
0 1 0, -1 2 0, 0 2 0, 0 0 1, 0 1 1, -1 2 1,  
0 0 2,  
PLAT939\_ALERT\_3\_C Large Value of Not (SHELXL) Weight Optimized S . 14.31 Check

---

**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 ... 34 Check  
PLAT072\_ALERT\_2\_G SHELXL First Parameter in WGHT Unusually Large 0.16 Report  
PLAT171\_ALERT\_4\_G The CIF-Embedded .res File Contains EADP Records 1 Report  
PLAT301\_ALERT\_3\_G Main Residue Disorder .....(Resd 4) 100% Note  
PLAT301\_ALERT\_3\_G Main Residue Disorder .....(Resd 5) 100% Note  
PLAT301\_ALERT\_3\_G Main Residue Disorder .....(Resd 9) 100% Note  
PLAT304\_ALERT\_4\_G Non-Integer Number of Atoms in ..... (Resd 1) 0.25 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) 0.26 Check  
PLAT304\_ALERT\_4\_G Non-Integer Number of Atoms in ..... (Resd 5) 0.24 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  
PLAT304\_ALERT\_4\_G Non-Integer Number of Atoms in ..... (Resd 9) 0.07 Check  
PLAT432\_ALERT\_2\_G Short Inter X...Y Contact C4 ..C4 . 2.00 Ang.  
y, -x+y, z = 5\_555 Check  
PLAT432\_ALERT\_2\_G Short Inter X...Y Contact C4 ..C4 . 2.00 Ang.  
x-y, x, z = 6\_555 Check  
PLAT773\_ALERT\_2\_G Check long C-C Bond in CIF: C4 --C4 2.00 Ang.  
PLAT773\_ALERT\_2\_G Check long C-C Bond in CIF: C4 --C4 2.00 Ang.  
PLAT802\_ALERT\_4\_G CIF Input Record(s) with more than 80 Characters 2 Info  
PLAT883\_ALERT\_1\_G Absent Datum for \_atom\_sites\_solution\_primary .. Please Do !  
PLAT933\_ALERT\_2\_G Number of HKL-OMIT Records in Embedded .res File 2 Note  
-3 11 5, 0 4 1,



Data completeness= 0.82/0.47                      Theta(max)= 28.266

R(reflections)= 0.0923( 442)

wR2(reflections)=  
0.2390( 537)

S = 1.090

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 .                      0.467 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 .....                      0.8999 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                      80 Report  
0 4 0, -2 7 0, 0 3 1, 0 4 1, -3 12 1, -6 13 1,  
0 1 2, -1 2 2, 0 2 2, -1 3 2, 0 3 2, 0 0 3,  
0 1 3, -1 2 3, 0 2 3, -1 3 3, 0 3 3, -2 4 3,  
-1 4 3, 0 4 3, -2 5 3, -1 5 3, -3 7 3, -5 10 3,

0 0 4, 0 1 4, -1 2 4, 0 2 4, -1 3 4, 0 3 4,  
( 50 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` -0.600  
From the CIF: `_refine_ls_abs_structure_Flack_su` 1.000  
PLAT041\_ALERT\_1\_C Calc. and Reported SumFormula Strings Differ Please Check  
Calc: C0.26 O  
Rep.: C8.97 O34  
PLAT042\_ALERT\_1\_C Calc. and Reported MoietyFormula Strings Differ Please Check  
Calc: O, 0.264(C)  
Rep.: 34(O), 8.974(C)  
PLAT910\_ALERT\_3\_C Missing FCF Reflection(s) Below Theta(Min) [Deg]= 4.48 Note  
0 1 0, -1 2 0, 0 2 0, 0 0 1, 0 1 1, -1 2 1,  
0 0 2,

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**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`: C8.97 O34  
Atom count from the `_atom_site` data: C8.98 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 0.18 Report  
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) 0.17 Check  
PLAT802\_ALERT\_4\_G CIF Input Record(s) with more than 80 Characters 8 Info  
PLAT883\_ALERT\_1\_G Absent Datum for `_atom_sites_solution_primary` .. Please Do !  
PLAT912\_ALERT\_4\_G Missing # of FCF Reflections Above STh/L= 0.600 1 Note  
PLAT915\_ALERT\_3\_G No Flack x Check Done: Low Friedel Pair Coverage 48 %  
PLAT916\_ALERT\_2\_G Hooft y and Flack x Parameter Values Differ by . 0.20 Check  
PLAT933\_ALERT\_2\_G Number of HKL-OMIT Records in Embedded .res File 23 Note  
-6 13 1, -5 10 3, -5 14 0, -4 8 4, -4 11 4, -3 7 3,  
-3 11 5, -3 12 1, -3 13 4, -2 7 0, -2 14 3, 0 3 1,  
0 4 0, 0 4 1, 2 5 0, 3 4 3, 3 9 1, 3 10 4,  
4 7 4, 5 5 3, 5 8 1, 6 7 1, 7 8 1,  
PLAT941\_ALERT\_3\_G Average HKL Measurement Multiplicity ..... 2.3 Low  
PLAT952\_ALERT\_5\_G Calculated (ThMax) and CIF-Reported Lmax Differ. 8 Units  
PLAT958\_ALERT\_1\_G Calculated (ThMax) and Actual (FCF) Lmax Differ. 8 Units  
PLAT969\_ALERT\_5\_G The 'Henn et al.' R-Factor-gap value ..... 10.153 Note  
Predicted wR2: Based on SigI\*\*2 2.35 or SHELX Weight 21.93  
PLAT992\_ALERT\_5\_G Repd & Actual `_reflns_number_gt` Values Differ by 2 Check



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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 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 . 0.485 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 ..... 0.9182 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 71 Report  
0 1 2, -1 2 2, 0 2 2, -1 3 2, 0 3 2, 0 0 3,  
0 1 3, -1 2 3, 0 2 3, -1 3 3, 0 3 3, -2 4 3,  
-1 4 3, 0 4 3, -2 5 3, -1 5 3, 0 0 4, 0 1 4,  
-1 2 4, 0 2 4, -1 3 4, 0 3 4, -2 4 4, -1 4 4,  
0 4 4, -2 5 4, -1 5 4, 0 5 4, -3 6 4, -2 6 4,  
( 41 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 -3.900

From the CIF: `_refine_ls_abs_structure_Flack_su` 1.000  
 PLAT041\_ALERT\_1\_C Calc. and Reported SumFormula Strings Differ Please Check  
     Calc: C0.29 O  
     Rep.: C9.80 O34  
 PLAT042\_ALERT\_1\_C Calc. and Reported MoietyFormula Strings Differ Please Check  
     Calc: O, 0.288(C)  
     Rep.: 34(O), 9.804(C)  
 PLAT077\_ALERT\_4\_C Unit-Cell Contains Non-integer Number of Atoms . Please Check  
 PLAT910\_ALERT\_3\_C Missing FCF Reflection(s) Below Theta (Min) [Deg]= 4.49 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.  
 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 0.16 Report  
 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) 0.23 Check  
 PLAT802\_ALERT\_4\_G CIF Input Record(s) with more than 80 Characters 8 Info  
 PLAT883\_ALERT\_1\_G Absent Datum for `_atom_sites_solution_primary` .. Please Do !  
 PLAT915\_ALERT\_3\_G No Flack x Check Done: Low Friedel Pair Coverage 51 %  
 PLAT916\_ALERT\_2\_G Hooft y and Flack x Parameter Values Differ by . 2.60 Check  
 PLAT941\_ALERT\_3\_G Average HKL Measurement Multiplicity ..... 2.3 Low  
 PLAT952\_ALERT\_5\_G Calculated (ThMax) and CIF-Reported Lmax Differ. 8 Units  
 PLAT958\_ALERT\_1\_G Calculated (ThMax) and Actual (FCF) Lmax Differ. 8 Units  
 PLAT969\_ALERT\_5\_G The 'Henn et al.' R-Factor-gap value ..... 10.218 Note  
     Predicted wR2: Based on SigI\*\*2 2.03 or SHELX Weight 19.12

- 5 **ALERT level A** = Most likely a serious problem - resolve or explain  
 2 **ALERT level B** = A potentially serious problem, consider carefully  
 5 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
 23 **ALERT level G** = General information/check it is not something unexpected
- 13 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  
 6 ALERT type 3 Indicator that the structure quality may be low  
 12 ALERT type 4 Improvement, methodology, query or suggestion  
 2 ALERT type 5 Informative message, check

**Datablock: Exp1\_p11\_MHIIb**

Bond precision: = 0.0000 A Wavelength=0.71075  
Cell: a=11.7769(6) b=11.7769(6) c=9.896(4)  
alpha=90 beta=90 gamma=120  
Temperature: 296 K

	Calculated	Reported
Volume	1188.7(5)	1188.7(5)
Space group	P -6 2 m	P -6 2 m
Hall group	P -6 -2	P -6 -2
Moiety formula	17(O), 5(C)	34(O), 10(C)
Sum formula	C5 O17	C10 O34
Mr	332.05	664.10
Dx, g cm <sup>-3</sup>	0.928	0.928
Z	2	1
Mu (mm <sup>-1</sup> )	0.103	0.103
F000	332.0	332.0
F000'	332.37	
h, k, lmax	15, 15, 13	15, 15, 5
Nref	1125[ 639]	553
Tmin, Tmax	0.996, 0.997	0.445, 1.000
Tmin'	0.996	

Correction method= # Reported T Limits: Tmin=0.445 Tmax=1.000  
AbsCorr = MULTI-SCAN


Data completeness= 0.87/0.49 Theta(max)= 28.253

R(reflections)= 0.0691( 499) wR2(reflections)=  
0.1815( 553)  
S = 1.078 Npar= 38

---

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 \_expt1\_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 . 0.484 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<sup>-3</sup> ..... 0.9277 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 71 Report  
0 1 2, -1 2 2, 0 2 2, -1 3 2, 0 3 2, 0 0 3,  
0 1 3, -1 2 3, 0 2 3, -1 3 3, 0 3 3, -2 4 3,  
-1 4 3, 0 4 3, -2 5 3, -1 5 3, 0 0 4, 0 1 4,  
-1 2 4, 0 2 4, -1 3 4, 0 3 4, -2 4 4, -1 4 4,  
0 4 4, -2 5 4, -1 5 4, 0 5 4, -3 6 4, -2 6 4,  
( 41 More Missing: see the .ckf listing file)

---

**Alert level C**

STRVA01\_ALERT\_2\_C Chirality of atom sites is inverted?  
From the CIF: \_refine\_ls\_abs\_structure\_Flack 2.700  
From the CIF: \_refine\_ls\_abs\_structure\_Flack\_su 1.000  
PLAT041\_ALERT\_1\_C Calc. and Reported SumFormula Strings Differ Please Check  
Calc: C5 O17  
Rep.: C10 O34  
PLAT042\_ALERT\_1\_C Calc. and Reported MoietyFormula Strings Differ Please Check  
Calc: 17(O), 5(C)  
Rep.: 34(O), 10(C)  
PLAT907\_ALERT\_2\_C Flack x > 0.5, Structure Needs to be Inverted? . 2.70 Check  
PLAT910\_ALERT\_3\_C Missing FCF Reflection(s) Below Theta(Min) [Deg]= 4.50 Note  
0 1 0, -1 2 0, 0 2 0, 0 0 1, 0 1 1, -1 2 1,  
0 0 2,  
PLAT939\_ALERT\_3\_C Large Value of Not (SHELXL) Weight Optimized S . 11.56 Check

---

**Alert level G**

ABSMU01\_ALERT\_1\_G Calculation of \_exptl\_absorpt\_correction\_mu  
not performed for this radiation type.





GEOM003\_ALERT\_1\_A \_geom\_bond\_distance is missing  
Distance between atom sites 1 and 2.

**Author Response: <https://doi.org/10.1515/ESRF-ES-1803920850>**

PLAT029\_ALERT\_3\_A \_diffrn\_measured\_fraction\_theta\_full value Low . 0.492 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<sup>-3</sup> ..... 0.9372 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 70 Report  
0 1 2, -1 2 2, 0 2 2, -1 3 2, 0 3 2, 0 0 3,  
0 1 3, -1 2 3, 0 2 3, -1 3 3, 0 3 3, -2 4 3,  
-1 4 3, 0 4 3, -2 5 3, -1 5 3, 0 0 4, 0 1 4,  
-1 2 4, 0 2 4, -1 3 4, 0 3 4, -2 4 4, -1 4 4,  
0 4 4, -2 5 4, -1 5 4, 0 5 4, -3 6 4, -2 6 4,  
( 40 More Missing: see the .ckf listing file)

---

**Alert level C**

STRVA01\_ALERT\_4\_C Flack test results are ambiguous.  
From the CIF: \_refine\_ls\_abs\_structure\_Flack 0.600  
From the CIF: \_refine\_ls\_abs\_structure\_Flack\_su 1.000  
PLAT041\_ALERT\_1\_C Calc. and Reported SumFormula Strings Differ Please Check  
Calc: C5 O17  
Rep.: C10 O34  
PLAT042\_ALERT\_1\_C Calc. and Reported MoietyFormula Strings Differ Please Check  
Calc: 17(O), 5(C)  
Rep.: 34(O), 10(C)  
PLAT907\_ALERT\_2\_C Flack x > 0.5, Structure Needs to be Inverted? . 0.60 Check  
PLAT910\_ALERT\_3\_C Missing FCF Reflection(s) Below Theta(Min) [Deg]= 4.51 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.  
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 ... 2 Check  
PLAT072\_ALERT\_2\_G SHELXL First Parameter in WGHT Unusually Large 0.15 Report  
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





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 . 0.486 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 ..... 0.9469 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 70 Report  
0 1 2, -1 2 2, 0 2 2, -1 3 2, 0 3 2, 0 0 3,  
0 1 3, -1 2 3, 0 2 3, -1 3 3, 0 3 3, -2 4 3,  
-1 4 3, 0 4 3, -2 5 3, -1 5 3, 0 0 4, 0 1 4,  
-1 2 4, 0 2 4, -1 3 4, 0 3 4, -2 4 4, -1 4 4,  
0 4 4, -2 5 4, -1 5 4, 0 5 4, -3 6 4, -2 6 4,  
( 40 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 -2.500  
From the CIF: \_refine\_ls\_abs\_structure\_Flack\_su 1.000  
PLAT041\_ALERT\_1\_C Calc. and Reported SumFormula Strings Differ Please Check  
Calc: C5 O17  
Rep.: C10 O34  
PLAT042\_ALERT\_1\_C Calc. and Reported MoietyFormula Strings Differ Please Check  
Calc: 17(O), 5(C)  
Rep.: 34(O), 10(C)  
PLAT910\_ALERT\_3\_C Missing FCF Reflection(s) Below Theta(Min) [Deg]= 4.53 Note  
0 1 0, -1 2 0, 0 2 0, 0 0 1, 0 1 1, -1 2 1,  
0 0 2,

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**Alert level G**

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 ... 2 Check  
PLAT072\_ALERT\_2\_G SHELXL First Parameter in WGHT Unusually Large 0.15 Report  
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



	Calculated	Reported
Volume	1156.4(6)	1156.4(6)
Space group	P -6 2 m	P -6 2 m
Hall group	P -6 -2	P -6 -2
Moiety formula	17(O), 5(C)	34(O), 10(C)
Sum formula	C5 O17	C10 O34
Mr	332.05	664.10
Dx, g cm <sup>-3</sup>	0.954	0.954
Z	2	1
Mu (mm <sup>-1</sup> )	0.105	0.106
F000	332.0	332.0
F000'	332.37	
h, k, lmax	15, 15, 13	15, 15, 5
Nref	1097 [ 624]	528
Tmin, Tmax	0.996, 0.997	0.253, 1.000
Tmin'	0.996	

Correction method= # Reported T Limits: Tmin=0.253 Tmax=1.000  
AbsCorr = MULTI-SCAN

Data completeness= 0.85/0.48                      Theta(max)= 28.239

R(reflections)= 0.0668 ( 433)

wR2(reflections)=  
0.1871 ( 528)

S = 1.062

Npar= 38

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 . 0.482 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 ..... 0.9536 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 71 Report  
0 1 2, -1 2 2, 0 2 2, -1 3 2, 0 3 2, 0 0 3,  
0 1 3, -1 2 3, 0 2 3, -1 3 3, 0 3 3, -2 4 3,  
-1 4 3, 0 4 3, -2 5 3, -1 5 3, 0 0 4, 0 1 4,  
-1 2 4, 0 2 4, -1 3 4, 0 3 4, -2 4 4, -1 4 4,  
0 4 4, -2 5 4, -1 5 4, 0 5 4, -3 6 4, -2 6 4,  
( 41 More Missing: see the .ckf listing file)

---

**Alert level C**

STRVA01\_ALERT\_2\_C Chirality of atom sites is inverted?  
From the CIF: \_refine\_ls\_abs\_structure\_Flack 5.000  
From the CIF: \_refine\_ls\_abs\_structure\_Flack\_su 1.000  
PLAT041\_ALERT\_1\_C Calc. and Reported SumFormula Strings Differ Please Check  
Calc: C5 O17  
Rep.: C10 O34  
PLAT042\_ALERT\_1\_C Calc. and Reported MoietyFormula Strings Differ Please Check  
Calc: 17(O), 5(C)  
Rep.: 34(O), 10(C)  
PLAT907\_ALERT\_2\_C Flack x > 0.5, Structure Needs to be Inverted? . 5.00 Check  
PLAT910\_ALERT\_3\_C Missing FCF Reflection(s) Below Theta(Min) [Deg]= 4.54 Note  
0 1 0, -1 2 0, 0 2 0, 0 0 1, 0 1 1, -1 2 1,  
0 0 2,

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**Alert level G**

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 ... 2 Check  
PLAT072\_ALERT\_2\_G SHELXL First Parameter in WGHT Unusually Large 0.14 Report  
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)	0.25	Check
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters		8	Info
PLAT883_ALERT_1_G Absent Datum for _atom_sites_solution_primary ..			Please Do !
PLAT915_ALERT_3_G No Flack x Check Done: Low Friedel Pair Coverage		49	%
PLAT916_ALERT_2_G Hooft y and Flack x Parameter Values Differ by .		3.20	Check
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File		2	Note
	-2 -2 0, 2 2 0,		
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity .....		2.3	Low
PLAT952_ALERT_5_G Calculated (ThMax) and CIF-Reported Lmax Differ.		8	Units
PLAT958_ALERT_1_G Calculated (ThMax) and Actual (FCF) Lmax Differ.		8	Units
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value .....		4.429	Note
	Predicted wR2: Based on SigI**2 4.23 or SHELX Weight 17.61		

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

12 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  
5 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

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## Datablock: Exp1\_p15\_MHIib

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Bond precision:	= 0.0000 A		Wavelength=0.71075
Cell:	a=11.6203(10)	b=11.6203(10)	c=9.836(8)
	alpha=90	beta=90	gamma=120
Temperature:	296 K		



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 . 0.483 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 ..... 0.9588 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 71 Report  
0 1 2, -1 2 2, 0 2 2, -1 3 2, 0 3 2, 0 0 3,  
0 1 3, -1 2 3, 0 2 3, -1 3 3, 0 3 3, -2 4 3,  
-1 4 3, 0 4 3, -2 5 3, -1 5 3, 0 0 4, 0 1 4,  
-1 2 4, 0 2 4, -1 3 4, 0 3 4, -2 4 4, -1 4 4,  
0 4 4, -2 5 4, -1 5 4, 0 5 4, -3 6 4, -2 6 4,  
( 41 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 -3.700  
From the CIF: \_refine\_ls\_abs\_structure\_Flack\_su 1.000  
PLAT041\_ALERT\_1\_C Calc. and Reported SumFormula Strings Differ Please Check  
Calc: C5 O17  
Rep.: C10 O34  
PLAT042\_ALERT\_1\_C Calc. and Reported MoietyFormula Strings Differ Please Check  
Calc: 17(O), 5(C)  
Rep.: 34(O), 10(C)  
PLAT910\_ALERT\_3\_C Missing FCF Reflection(s) Below Theta(Min) [Deg]= 4.55 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.  
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 ... 2 Check  
PLAT072\_ALERT\_2\_G SHELXL First Parameter in WGHT Unusually Large 0.14 Report  
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)	0.25	Check
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters		8	Info
PLAT883_ALERT_1_G Absent Datum for _atom_sites_solution_primary ..			Please Do !
PLAT915_ALERT_3_G No Flack x Check Done: Low Friedel Pair Coverage		49	%
PLAT916_ALERT_2_G Hooft y and Flack x Parameter Values Differ by .		2.80	Check
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File		2	Note
	-2 -2 0, 2 2 0,		
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity .....		2.3	Low
PLAT952_ALERT_5_G Calculated (ThMax) and CIF-Reported Lmax Differ.		8	Units
PLAT958_ALERT_1_G Calculated (ThMax) and Actual (FCF) Lmax Differ.		8	Units
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value .....		4.364	Note
	Predicted wR2: Based on SigI**2 4.33 or SHELX Weight 17.96		

- 
- 5 **ALERT level A** = Most likely a serious problem - resolve or explain  
2 **ALERT level B** = A potentially serious problem, consider carefully  
4 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
22 **ALERT level G** = General information/check it is not something unexpected
- 12 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  
5 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
- 

## 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.

```
# 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_Exp1_p1_MHI
;
PROBLEM: _exptl_crystal_colour (_pd_char_colour for powder) is missing
RESPONSE: ...
;
_vrf_GEOM005_Exp1_p1_MHI
;
PROBLEM: _geom_angle_atom_site_label_1 is missing
RESPONSE: ...
;
_vrf_EXPT010_Exp1_p2_MHI
;
PROBLEM: _exptl_crystal_colour (_pd_char_colour for powder) is missing
RESPONSE: ...
;
_vrf_GEOM005_Exp1_p2_MHI
;
PROBLEM: _geom_angle_atom_site_label_1 is missing
RESPONSE: ...
;
_vrf_EXPT010_Exp1_p3_MHI
;
PROBLEM: _exptl_crystal_colour (_pd_char_colour for powder) is missing
RESPONSE: ...
;
_vrf_GEOM005_Exp1_p3_MHI
;
PROBLEM: _geom_angle_atom_site_label_1 is missing
RESPONSE: ...
;
_vrf_EXPT010_Exp1_p4_MHI
;
PROBLEM: _exptl_crystal_colour (_pd_char_colour for powder) is missing
RESPONSE: ...
;
_vrf_GEOM005_Exp1_p4_MHI
;
PROBLEM: _geom_angle_atom_site_label_1 is missing
RESPONSE: ...
;
_vrf_EXPT010_Exp1_p5_MHI
;
PROBLEM: _exptl_crystal_colour (_pd_char_colour for powder) is missing
RESPONSE: ...
;
_vrf_GEOM005_Exp1_p5_MHI
;
PROBLEM: _geom_angle_atom_site_label_1 is missing
RESPONSE: ...
;
_vrf_EXPT010_Exp1_p5_MHIIa
;
PROBLEM: _exptl_crystal_colour (_pd_char_colour for powder) is missing
RESPONSE: ...
;
```

```
_vrf_GEOM005_Expl_p5_MHIIa
;
PROBLEM: _geom_angle_atom_site_label_1 is missing
RESPONSE: ...
;
_vrf_EXPT010_Expl_p6_MHIIa
;
PROBLEM: _exptl_crystal_colour (_pd_char_colour for powder) is missing
RESPONSE: ...
;
_vrf_GEOM005_Expl_p6_MHIIa
;
PROBLEM: _geom_angle_atom_site_label_1 is missing
RESPONSE: ...
;
_vrf_EXPT010_Expl_p7_MHIIa
;
PROBLEM: _exptl_crystal_colour (_pd_char_colour for powder) is missing
RESPONSE: ...
;
_vrf_EXPT010_Expl_p8_MHIIa
;
PROBLEM: _exptl_crystal_colour (_pd_char_colour for powder) is missing
RESPONSE: ...
;
_vrf_EXPT010_Expl_p9_MHIIb
;
PROBLEM: _exptl_crystal_colour (_pd_char_colour for powder) is missing
RESPONSE: ...
;
_vrf_EXPT010_Expl_p10_MHIIb
;
PROBLEM: _exptl_crystal_colour (_pd_char_colour for powder) is missing
RESPONSE: ...
;
_vrf_EXPT010_Expl_p11_MHIIb
;
PROBLEM: _exptl_crystal_colour (_pd_char_colour for powder) is missing
RESPONSE: ...
;
_vrf_EXPT010_Expl_p12_MHIIb
;
PROBLEM: _exptl_crystal_colour (_pd_char_colour for powder) is missing
RESPONSE: ...
;
_vrf_EXPT010_Expl_p13_MHIIb
;
PROBLEM: _exptl_crystal_colour (_pd_char_colour for powder) is missing
RESPONSE: ...
;
_vrf_EXPT010_Expl_p14_MHIIb
;
PROBLEM: _exptl_crystal_colour (_pd_char_colour for powder) is missing
RESPONSE: ...
;
_vrf_EXPT010_Expl_p15_MHIIb
;
```

PROBLEM: \_exptl\_crystal\_colour (\_pd\_char\_colour for powder) is missing  
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.

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

Datablock Exp1\_p1\_MHI - ellipsoid plot

