



## Alert level A

EXPT005\_ALERT\_1\_A \_exptl\_crystal\_description is missing  
Crystal habit description.  
The following tests will not be performed.  
CRYSR\_01

DIFF003\_ALERT\_1\_A \_diffrn\_measurement\_device\_type is missing  
Diffractometer make and type. Replaces \_diffrn\_measurement\_type.

ATOM007\_ALERT\_1\_A \_atom\_site\_aniso\_label is missing  
Unique label identifying the atom site.

GEOM001\_ALERT\_1\_A \_geom\_bond\_atom\_site\_label\_1 is missing  
Label identifying the atom site 1.

GEOM002\_ALERT\_1\_A \_geom\_bond\_atom\_site\_label\_2 is missing  
Label identifying the atom site 2.

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

GEOM006\_ALERT\_1\_A \_geom\_angle\_atom\_site\_label\_2 is missing  
Label identifying the atom site 2.

GEOM007\_ALERT\_1\_A \_geom\_angle\_atom\_site\_label\_3 is missing  
Label identifying the atom site 3.

SYMMG01\_ALERT\_1\_A Unrecognised \_symmetry\_space\_group\_name\_H-M  
From the CIF: \_symmetry\_Int\_Tables\_number 227  
From the CIF: \_symmetry\_space\_group\_name\_H-M F 41/d -3 2/m (origin  
Int. Tables space group number for F 41/d -3 2/m (origin choice 2) is

SYMMG02\_ALERT\_1\_A Supplied \_symmetry\_space\_group\_name\_H-M not recognised  
From the CIF: \_symmetry\_equiv\_pos\_as\_xyz  
x,y,z  
x,-y+1/4,-z+1/4  
-x+1/4,y,-z+1/4  
-x+1/4,-y+1/4,z  
y,z,x  
y,-z+1/4,-x+1/4  
-y+1/4,z,-x+1/4  
-y+1/4,-z+1/4,x  
z,x,y  
z,-x+1/4,-y+1/4  
-z+1/4,x,-y+1/4  
-z+1/4,-x+1/4,y  
-y,-x,-z  
-y,x+1/4,z+1/4  
y+1/4,-x,z+1/4  
y+1/4,x+1/4,-z  
-x,-z,-y  
-x,z+1/4,y+1/4  
x+1/4,-z,y+1/4  
x+1/4,z+1/4,-y  
-z,-y,-x  
-z,y+1/4,x+1/4  
z+1/4,-y,x+1/4  
z+1/4,y+1/4,-x  
-x,-y,-z  
-x,y+1/4,z+1/4  
x+1/4,-y,z+1/4  
x+1/4,y+1/4,-z  
-y,-z,-x  
-y,z+1/4,x+1/4  
y+1/4,-z,x+1/4  
y+1/4,z+1/4,-x  
-z,-x,-y  
-z,x+1/4,y+1/4  
z+1/4,-x,y+1/4  
z+1/4,x+1/4,-y

$y, x, z$   
 $y, -x+1/4, -z+1/4$   
 $-y+1/4, x, -z+1/4$   
 $-y+1/4, -x+1/4, z$   
 $x, z, y$   
 $x, -z+1/4, -y+1/4$   
 $-x+1/4, z, -y+1/4$   
 $-x+1/4, -z+1/4, y$   
 $z, y, x$   
 $z, -y+1/4, -x+1/4$   
 $-z+1/4, y, -x+1/4$   
 $-z+1/4, -y+1/4, x$   
 $x, y+1/2, z+1/2$   
 $x, -y+3/4, -z+3/4$   
 $-x+1/4, y+1/2, -z+3/4$   
 $-x+1/4, -y+3/4, z+1/2$   
 $y, z+1/2, x+1/2$   
 $y, -z+3/4, -x+3/4$   
 $-y+1/4, z+1/2, -x+3/4$   
 $-y+1/4, -z+3/4, x+1/2$   
 $z, x+1/2, y+1/2$   
 $z, -x+3/4, -y+3/4$   
 $-z+1/4, x+1/2, -y+3/4$   
 $-z+1/4, -x+3/4, y+1/2$   
 $-y, -x+1/2, -z+1/2$   
 $-y, x+3/4, z+3/4$   
 $y+1/4, -x+1/2, z+3/4$   
 $y+1/4, x+3/4, -z+1/2$   
 $-x, -z+1/2, -y+1/2$   
 $-x, z+3/4, y+3/4$   
 $x+1/4, -z+1/2, y+3/4$   
 $x+1/4, z+3/4, -y+1/2$   
 $-z, -y+1/2, -x+1/2$   
 $-z, y+3/4, x+3/4$   
 $z+1/4, -y+1/2, x+3/4$   
 $z+1/4, y+3/4, -x+1/2$   
 $-x, -y+1/2, -z+1/2$   
 $-x, y+3/4, z+3/4$   
 $x+1/4, -y+1/2, z+3/4$   
 $x+1/4, y+3/4, -z+1/2$   
 $-y, -z+1/2, -x+1/2$   
 $-y, z+3/4, x+3/4$   
 $y+1/4, -z+1/2, x+3/4$   
 $y+1/4, z+3/4, -x+1/2$   
 $-z, -x+1/2, -y+1/2$   
 $-z, x+3/4, y+3/4$   
 $z+1/4, -x+1/2, y+3/4$   
 $z+1/4, x+3/4, -y+1/2$   
 $y, x+1/2, z+1/2$   
 $y, -x+3/4, -z+3/4$   
 $-y+1/4, x+1/2, -z+3/4$   
 $-y+1/4, -x+3/4, z+1/2$   
 $x, z+1/2, y+1/2$   
 $x, -z+3/4, -y+3/4$   
 $-x+1/4, z+1/2, -y+3/4$   
 $-x+1/4, -z+3/4, y+1/2$   
 $z, y+1/2, x+1/2$   
 $z, -y+3/4, -x+3/4$   
 $-z+1/4, y+1/2, -x+3/4$   
 $-z+1/4, -y+3/4, x+1/2$   
 $x+1/2, y, z+1/2$   
 $x+1/2, -y+1/4, -z+3/4$

-x+3/4, y, -z+3/4  
-x+3/4, -y+1/4, z+1/2  
y+1/2, z, x+1/2  
y+1/2, -z+1/4, -x+3/4  
-y+3/4, z, -x+3/4  
-y+3/4, -z+1/4, x+1/2  
z+1/2, x, y+1/2  
z+1/2, -x+1/4, -y+3/4  
-z+3/4, x, -y+3/4  
-z+3/4, -x+1/4, y+1/2  
-y+1/2, -x, -z+1/2  
-y+1/2, x+1/4, z+3/4  
y+3/4, -x, z+3/4  
y+3/4, x+1/4, -z+1/2  
-x+1/2, -z, -y+1/2  
-x+1/2, z+1/4, y+3/4  
x+3/4, -z, y+3/4  
x+3/4, z+1/4, -y+1/2  
-z+1/2, -y, -x+1/2  
-z+1/2, y+1/4, x+3/4  
z+3/4, -y, x+3/4  
z+3/4, y+1/4, -x+1/2  
-x+1/2, -y, -z+1/2  
-x+1/2, y+1/4, z+3/4  
x+3/4, -y, z+3/4  
x+3/4, y+1/4, -z+1/2  
-y+1/2, -z, -x+1/2  
-y+1/2, z+1/4, x+3/4  
y+3/4, -z, x+3/4  
y+3/4, z+1/4, -x+1/2  
-z+1/2, -x, -y+1/2  
-z+1/2, x+1/4, y+3/4  
z+3/4, -x, y+3/4  
z+3/4, x+1/4, -y+1/2  
y+1/2, x, z+1/2  
y+1/2, -x+1/4, -z+3/4  
-y+3/4, x, -z+3/4  
-y+3/4, -x+1/4, z+1/2  
x+1/2, z, y+1/2  
x+1/2, -z+1/4, -y+3/4  
-x+3/4, z, -y+3/4  
-x+3/4, -z+1/4, y+1/2  
z+1/2, y, x+1/2  
z+1/2, -y+1/4, -x+3/4  
-z+3/4, y, -x+3/4  
-z+3/4, -y+1/4, x+1/2  
x+1/2, y+1/2, z  
x+1/2, -y+3/4, -z+1/4  
-x+3/4, y+1/2, -z+1/4  
-x+3/4, -y+3/4, z  
y+1/2, z+1/2, x  
y+1/2, -z+3/4, -x+1/4  
-y+3/4, z+1/2, -x+1/4  
-y+3/4, -z+3/4, x  
z+1/2, x+1/2, y  
z+1/2, -x+3/4, -y+1/4  
-z+3/4, x+1/2, -y+1/4  
-z+3/4, -x+3/4, y  
-y+1/2, -x+1/2, -z  
-y+1/2, x+3/4, z+1/4  
y+3/4, -x+1/2, z+1/4  
y+3/4, x+3/4, -z

$-x+1/2, -z+1/2, -y$   
 $-x+1/2, z+3/4, y+1/4$   
 $x+3/4, -z+1/2, y+1/4$   
 $x+3/4, z+3/4, -y$   
 $-z+1/2, -y+1/2, -x$   
 $-z+1/2, y+3/4, x+1/4$   
 $z+3/4, -y+1/2, x+1/4$   
 $z+3/4, y+3/4, -x$   
 $-x+1/2, -y+1/2, -z$   
 $-x+1/2, y+3/4, z+1/4$   
 $x+3/4, -y+1/2, z+1/4$   
 $x+3/4, y+3/4, -z$   
 $-y+1/2, -z+1/2, -x$   
 $-y+1/2, z+3/4, x+1/4$   
 $y+3/4, -z+1/2, x+1/4$   
 $y+3/4, z+3/4, -x$   
 $-z+1/2, -x+1/2, -y$   
 $-z+1/2, x+3/4, y+1/4$   
 $z+3/4, -x+1/2, y+1/4$   
 $z+3/4, x+3/4, -y$   
 $y+1/2, x+1/2, z$   
 $y+1/2, -x+3/4, -z+1/4$   
 $-y+3/4, x+1/2, -z+1/4$   
 $-y+3/4, -x+3/4, z$   
 $x+1/2, z+1/2, y$   
 $x+1/2, -z+3/4, -y+1/4$   
 $-x+3/4, z+1/2, -y+1/4$   
 $-x+3/4, -z+3/4, y$   
 $z+1/2, y+1/2, x$   
 $z+1/2, -y+3/4, -x+1/4$   
 $-z+3/4, y+1/2, -x+1/4$   
 $-z+3/4, -y+3/4, x$

These symops generate the Hall space group symbol  $-f_4vw_2vw_3$   
 which is equivalent to the H-M space group symbol  $f_d-3_m$

PLAT029_ALERT_3_A	_diffrn_measured_fraction_theta_full	value Low	0.000	Why?
PLAT043_ALERT_1_A	Calculated and Reported Mol. Weight	Differ by ..	364.95	Check
PLAT129_ALERT_4_A	Unusual Space Group Specified	.....	F41/D-3	Check
PLAT183_ALERT_1_A	Missing _cell_measurement_reflns_used	Value ....		Please Do !
PLAT184_ALERT_1_A	Missing _cell_measurement_theta_min	Value .....		Please Do !
PLAT185_ALERT_1_A	Missing _cell_measurement_theta_max	Value .....		Please Do !
PLAT197_ALERT_1_A	Missing _cell_measurement_temperature	Datum ....		Please Add
PLAT198_ALERT_1_A	Missing _diffrn_ambient_temperature	Datum ....		Please Add
PLAT880_ALERT_1_A	NO datum for _diffrn_reflns_number	.....		Please Do !
PLAT881_ALERT_1_A	No Datum for _diffrn_reflns_av_R	equivalents ...		Please Do !

**Alert level C**

PLAT141_ALERT_4_C	s.u. on a - Axis Small or Missing	.....	0.00000	Ang.
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**Alert level G**

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension		3	Info
PLAT005_ALERT_5_G	No Embedded Refinement Details Found	in the CIF		Please Do !
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor	...	0.00	Check
PLAT120_ALERT_1_G	Reported F41/d-3	Inconsistent with Explicit	Fd-3m	Check
PLAT794_ALERT_5_G	Tentative Bond Valency for Zn1	(II)	1.54	Info
PLAT808_ALERT_5_G	No Parseable SHELXL Style Weighting Scheme Found			Please Check
PLAT882_ALERT_1_G	No Datum for _diffrn_reflns_av_unetI/netI	.....		Please Do !
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary			Please Do !
PLAT980_ALERT_1_G	No Anomalous Scattering Factors Found in CIF	...		Please Check

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

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

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It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special\_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

### **Publication of your CIF in IUCr journals**

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

### **Publication of your CIF in other journals**

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

