

checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: MoO3-phen

Bond precision: C-C = 0.0199 Å Wavelength=1.54178

Cell: a=22.7233(4) b=7.7355(1) c=14.5903(10)
 alpha=90 beta=90 gamma=90

Temperature: 293 K

	Calculated	Reported
Volume	2564.63(18)	2564.63(18)
Space group	C m c a	C m c a
Hall group	-C 2bc 2	?
Moiety formula	C6 H4 Mo N O3	C6 H4 Mo1 N O3
Sum formula	C6 H4 Mo N O3	C6 H4 Mo1 N O3
Mr	234.04	234.04
Dx,g cm-3	2.425	2.425
Z	16	16
Mu (mm-1)	16.362	16.362
F000	1808.0	1808.0
F000'	1811.52	
h,k,lmax	23,8,15	23,8,15
Nref	809	808
Tmin,Tmax	0.214,0.721	0.612,1.000
Tmin'	0.095	

Correction method= EMPIRICAL

Data completeness= 0.999 Theta(max)= 54.180

R(reflections)= 0.0580(655) wR2(reflections)= 0.1795(808)

S = 1.161 Npar= 97

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

THETM01_ALERT_3_A The value of sine(theta_max)/wavelength is less than 0.550
Calculated sin(theta_max)/wavelength = 0.5259

Alert level B

PLAT031_ALERT_4_B	Refined Extinction Parameter within Range	1.000	Sigma
PLAT093_ALERT_1_B	No su's on H-atoms, but refinement reported as .	mixed	
PLAT201_ALERT_2_B	Isotropic non-H Atoms in Main Residue(s)	1	

Alert level C

REFNR01_ALERT_3_C	Ratio of reflections to parameters is < 10 for a centrosymmetric structure		
	sine(theta)/lambda	0.5259	
	Proportion of unique data used	1.0000	
	Ratio reflections to parameters	8.3299	
PLAT088_ALERT_3_C	Poor Data / Parameter Ratio	8.33	
PLAT242_ALERT_2_C	Check Low Ueq as Compared to Neighbors for	Mol	
PLAT342_ALERT_3_C	Low Bond Precision on C-C Bonds	0.0199	Ang

Alert level G

PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained Atom Sites	10	
PLAT004_ALERT_5_G	Info: Polymeric Structure Found with Dimension .	3	
PLAT005_ALERT_5_G	No _iucr_refine_instructions_details in CIF ...	?	
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large.	126.99	
PLAT199_ALERT_1_G	Check the Reported _cell_measurement_temperature	293	K
PLAT200_ALERT_1_G	Check the Reported _diffrn_ambient_temperature	293	K
PLAT764_ALERT_4_G	Overcomplete CIF Bond List Detected (Rep/Expd) .	1.20	Ratio
PLAT860_ALERT_3_G	Note: Number of Least-Squares Restraints	60	

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

- 3 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
5 ALERT type 3 Indicator that the structure quality may be low
2 ALERT type 4 Improvement, methodology, query or suggestion
2 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*, 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.

