



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) tianhuixinite

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: tianhuixinite

Bond precision:	Mo- O = 0.0102 Å		Wavelength=1.54184
Cell:	a=10.5963(12)	b=10.5963(12)	c=3.7216(4)
	alpha=90	beta=90	gamma=120
Temperature:	293 K		
	Calculated	Reported	
Volume	361.88(9)	361.88(9)	
Space group	P 63/m	P 63/m	
Hall group	-P 6c	-P 6c	
Moiety formula	Mo6 O18, 2(O)	0.25(Mo12 O36), 1(O)	
Sum formula	Mo6 O20	Mo3 O10	
Mr	895.64	447.82	
Dx, g cm-3	4.110	4.110	
Z	1	2	
Mu (mm-1)	42.467	42.467	
F000	412.0	412.0	
F000'	412.77		
h, k, lmax	13, 13, 4	13, 13, 4	
Nref	309	296	
Tmin, Tmax	0.698, 0.809	0.367, 1.000	
Tmin'	0.623		

Correction method= # Reported T Limits: Tmin=0.367 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.958

Theta(max)= 78.771

R(reflections)= 0.0606(269)

wR2(reflections)=
0.1780(296)

S = 1.138

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

PLAT973_ALERT_2_A	Check Calcd Positive Resid. Density on	Mo	3.10 eA-3
PLAT975_ALERT_2_A	Check Calcd Resid. Dens. 0.93Ang From O4	.	2.03 eA-3

Alert level B

PLAT306_ALERT_2_B	Isolated Oxygen Atom (H-atoms Missing ?)	O4	Check
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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.: Mo6 O20		
	Rep.: Mo3 O10		

PLAT042_ALERT_1_C	Calc. and Reported MoietyFormula Strings Differ	Please	Check
	Calc.: Mo6 O18, 2(O)		
	Rep.: 0.25(Mo12 O36), 1(O)		

PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density	2.05	Report
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PLAT202_ALERT_3_C	Isotropic non-H Atoms in Anion/Solvent	1	Check
	O4		

PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	2.699	Check
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PLAT971_ALERT_2_C	Check Calcd Resid. Dens. 0.93Ang From O4	2.03	eA-3
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PLAT971_ALERT_2_C	Check Calcd Resid. Dens. 0.80Ang From O2	1.59	eA-3
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PLAT971_ALERT_2_C	Check Calcd Resid. Dens. 0.95Ang From Mo	1.56	eA-3
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PLAT971_ALERT_2_C	Check Calcd Resid. Dens. 1.86Ang From O3	1.53	eA-3
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PLAT975_ALERT_2_C	Check Calcd Resid. Dens. 0.89Ang From O2	.	0.89 eA-3
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PLAT975_ALERT_2_C	Check Calcd Resid. Dens. 0.63Ang From O2	.	0.75 eA-3
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PLAT975_ALERT_2_C	Check Calcd Resid. Dens. 0.60Ang From O2	.	0.75 eA-3
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PLAT975_ALERT_2_C	Check Calcd Resid. Dens. 0.88Ang From O3	.	0.49 eA-3
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PLAT975_ALERT_2_C	Check Calcd Resid. Dens. 0.99Ang From O3	.	0.45 eA-3
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PLAT975_ALERT_2_C	Check Calcd Resid. Dens. 0.56Ang From O1	.	0.43 eA-3
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PLAT976_ALERT_2_C	Check Calcd Resid. Dens. 0.82Ang From O4	.	-0.92 eA-3
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PLAT976_ALERT_2_C	Check Calcd Resid. Dens. 0.89Ang From O4	.	-0.86 eA-3
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PLAT976_ALERT_2_C	Check Calcd Resid. Dens. 1.01Ang From O1	.	-0.65 eA-3
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Alert level G

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	1	Info
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PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...	0.500	Check
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PLAT072_ALERT_2_G	SHELXL First Parameter in WGHT Unusually Large	0.12	Report
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PLAT199_ALERT_1_G	Reported _cell_measurement_temperature (K)	293	Check
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PLAT200_ALERT_1_G	Reported _diffn_ambient_temperature (K)	293	Check
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PLAT794_ALERT_5_G Tentative Bond Valency for Mo (VI) . 5.95 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]= 9.67 Note
 0 1 0, -1 2 0,
 PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 9 Note
 PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF 1 Note
 0 0 2,
 PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value 6.016 Note
 Predicted wR2: Based on SigI**2 2.96 or SHELX Weight 15.65

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- 2 **ALERT level A** = Most likely a serious problem - resolve or explain
 1 **ALERT level B** = A potentially serious problem, consider carefully
 19 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
 11 **ALERT level G** = General information/check it is not something unexpected
- 7 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 18 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
 1 ALERT type 4 Improvement, methodology, query or suggestion
 3 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. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

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

duplicate check

A reduced cell check using CCDC's cellCheckCSD service has found that one or more structures in this CIF are similar to those previously published in the CSD or the ICSD.

DATABLOCK: tianhuixinite

- ICSD number: 126845



[Cell Parameters for 126845: 10.6224,10.6224,3.723(90,90,120)]

DATABLOCK: tianhuixinite

- ICSD number: 135008



[Cell Parameters for 135008: 10.5927,10.5927,3.7241(90,90,120)]

DATABLOCK: tianhuixinite

- ICSD number: 177615



[Cell Parameters for 177615: 10.5621,10.5621,3.7184(90,90,120)]

Datablock tianhuixinite - ellipsoid plot

