checkCIF/PLATON report

Structure factors have been supplied for datablock(s) K8Zn8_TeO3_12_6_H2O

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: K8Zn8_TeO3_12_6_H2O

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Bond precision:   Te- O = 0.0050 A          Wavelength=1.54178

Cell:              a=9.43449(8)      b=9.43449(8)      c=7.70778(7)
                   alpha=90          beta=90           gamma=120
Temperature:       213 K
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	Calculated	Reported
Volume	594.151(11)	594.150(11)
Space group	P 63/m	P 63/m
Hall group	-P 6c	-P 6c
Moiety formula	O9 Te3 Zn2 [+ solvent]	O9 Te3 Zn2
Sum formula	O9 Te3 Zn2 [+ solvent]	O9 Te3 Zn2
Mr	657.58	657.54
Dx,g cm-3	3.676	3.675
Z	2	2
Mu (mm-1)	62.212	62.212
F000	576.0	576.0
F000'	571.06	
h,k,lmax	11,11,9	11,11,9
Nref	444	444
Tmin,Tmax	0.323,0.504	0.069,0.528
Tmin'	0.000	

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Correction method= # Reported T Limits: Tmin=0.069 Tmax=0.528
AbsCorr = ANALYTICAL
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Data completeness= 1.000 Theta(max)= 74.284

R(reflections)= 0.0236(444) wR2(reflections)= 0.0562(444)

S = 1.196 Npar= 29

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 C

PLAT975_ALERT_2_C Check Calcd Resid. Dens. 0.58Ang From O1 . 0.50 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 0.58Ang From O1 . 0.50 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 0.79Ang From O1 . 0.41 eA-3

Alert level G

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 3 Info
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 5.89 Why ?
PLAT143_ALERT_4_G s.u. on c - Axis Small or Missing ..... 0.00007 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact Te1 ..O1 . 3.28 Ang.
1-y,x-y,1/2-z = 11_656 Check
PLAT605_ALERT_4_G Largest Solvent Accessible VOID in the Structure 180 A**3
PLAT794_ALERT_5_G Tentative Bond Valency for Te1 (IV) . 3.89 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Zn1 (II) . 2.22 Info
PLAT869_ALERT_4_G ALERTS Related to the Use of SQUEEZE Suppressed ! Info
PLAT961_ALERT_5_G Dataset Contains no Negative Intensities ..... Please Check
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged Please Check
PLAT967_ALERT_5_G Note: Two-Theta Cutoff Value in Embedded .res .. 148.6 Degree
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ..... 9.893 Note
Predicted wR2: Based on SigI**2 0.57 or SHELX Weight 4.70
PLAT994_ALERT_1_G SHELXL .ins Contains no or MERG 0 Instruction .. ! Note

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

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

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 15/01/2026; check.def file version of 02/01/2026

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: K8Zn8_TeO3_12_6_H2O

- ICSD number: 24434

  [Cell Parameters for 24434: 9.41,9.41,7.64(90,90,120)]

Datablock K8Zn8_TeO3_12_6_H2O - ellipsoid plot