checkCIF/PLATON report

Structure factors have been supplied for datablock(s) K8Co8_TeO3_12_10_D2O

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: K8Co8_TeO3_12_10_D2O

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Bond precision:   Co- O = 0.0032 A          Wavelength=0.71073

Cell:          a=9.39127(15)       b=15.4694(2)       c=16.3954(3)
               alpha=90.0096(14)   beta=89.6431(14)   gamma=90.0229(13)
Temperature:   213 K
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	Calculated	Reported
Volume	2381.83(7)	2381.83(7)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	Co8 O36 Te12, 0.5(K1.64 O2), 9(O), 7.179(K)	Co8 K8 O46 Te12
Sum formula	Co8 K8 O46 Te12	Co8 K8 O46 Te12
Mr	3051.44	3051.44
Dx,g cm-3	4.255	4.255
Z	2	2
Mu (mm-1)	10.739	10.739
F000	2720.0	2720.0
F000'	2717.44	
h,k,lmax	14,23,25	14,23,25
Nref	17985	17868
Tmin,Tmax	0.448,0.560	0.510,0.708
Tmin'	0.288	

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Correction method= # Reported T Limits: Tmin=0.510 Tmax=0.708
AbsCorr = ANALYTICAL
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Data completeness= 0.993 Theta(max)= 32.999

R(reflections)= 0.0245(16520) wR2(reflections)= 0.0505(17868)

S = 1.113 Npar= 688

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 B

PLAT306_ALERT_2_B Isolated Oxygen Atom(s) (H-atoms Missing ?) .... 9 Check
O34 O36 O39 O40 O41 O42 O43 O44
O45

Author Response: The deuterium atoms could not be reliably located from the difference Fourier maps, as the presence of the heavy Te atoms (together with K and Co) dominates the X-ray scattering, thereby obscuring the much weaker electron density associated with deuterium.

Alert level C

PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings Differ Please Check
Calc: Co8 O36 Te12, 0.5(K1.64 O2), 9(O), 7.179(K)
Rep.: Co8 K8 O46 Te12

Alert level G

PLAT003_ALERT_2_G Number of Uiso or U(i,j) Restrained non-H-Atoms 2 Report
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 3 Info
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 9.36 Why ?
PLAT112_ALERT_2_G ADDSYM Detects New (Pseudo) Symm. Elem b/2 80 %Fit
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records 1 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used 0.0100 Report
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 2) 100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 19) 100% Note
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) ..... O46 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact Te1 ..O44 . 3.29 Ang.
1-x,1-y,1-z = 2_666 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact Te4 ..O43 . 3.36 Ang.
1+x,y,z = 1_655 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact Te6 ..O46 . 3.27 Ang.
1+x,-1+y,z = 1_645 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact Te10 ..O42 . 3.37 Ang.
2-x,1-y,1-z = 2_766 Check
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 6 Note
PLAT870_ALERT_4_G ALERTS Related to Twinning Effects Suppressed .. ! Info
PLAT910_ALERT_3_G Missing FCF Reflection(s) Below Theta(Min)[Deg]= 2.17 Note
0 1 0, 0 -1 1, 0 0 1, 0 1 1,
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 113 Note

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PLAT931_ALERT_5_G CIFcalcFCF  Twin Law ( 0 1 0)         Est.d BASF       0.54 Check
PLAT931_ALERT_5_G CIFcalcFCF  Twin Law         [ 0 0 1] Est.d BASF       0.12 Check
PLAT931_ALERT_5_G CIFcalcFCF  Twin Law ( 1 0-1)         Est.d BASF       0.12 Check
PLAT967_ALERT_5_G Note: Two-Theta Cutoff Value in Embedded .res ..       66.0 Degree
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........      1.844 Note
              Predicted wR2: Based on SigI**2  2.74 or SHELX Weight  4.54
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
   1 ALERT level B = A potentially serious problem, consider carefully
   1 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

   2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   9 ALERT type 2 Indicator that the structure model may be wrong or deficient
   3 ALERT type 3 Indicator that the structure quality may be low
   5 ALERT type 4 Improvement, methodology, query or suggestion
   6 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 15/01/2026; check.def file version of 02/01/2026

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duplicate check

No duplication found

Datablock K8Co8_TeO3_12_10_D2O - ellipsoid plot