



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) K8Co8_TeO3_12_10_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: K8Co8_TeO3_12_10_H2O

Bond precision: Co- O = 0.0020 A Wavelength=0.71073

Cell: a=9.39592 (17) b=15.4699 (3) c=16.3979 (3)
 alpha=89.8089 (15) beta=89.6250 (14) gamma=89.8333 (15)
Temperature: 213 K

	Calculated	Reported
Volume	2383.43 (8)	2383.43 (8)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	Co8 O36 Te12, 0.5(K1.67 O2), 9(O), 7.166(K)	Co8 K8 O46 Te12
Sum formula	Co8 K8 O46 Te12	Co8 K8 O46 Te12
Mr	3051.44	3051.44
Dx, g cm ⁻³	4.252	4.252
Z	2	2
Mu (mm ⁻¹)	10.732	10.732
F000	2720.0	2720.0
F000'	2717.44	
h, k, lmax	14, 23, 25	14, 23, 25
Nref	17990	17980
Tmin, Tmax	0.339, 0.424	0.436, 0.533
Tmin'	0.298	

Correction method= # Reported T Limits: Tmin=0.436 Tmax=0.533
AbsCorr = ANALYTICAL

Data completeness= 0.999

Theta(max)= 33.000

R(reflections)= 0.0235(16000)

wR2(reflections)=
0.0525(17980)

S = 1.153

Npar= 687

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 hydrogen 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 hydrogen.

Alert level C

PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings Differ Please Check
Calc: Co8 O36 Te12, 0.5(K1.67 O2), 9(O), 7.166(K)
Rep.: Co8 K8 O46 Te12

PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 2.917 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 5 Report
-1-10 3, -2 1 4, -3 2 5, -1 4 5, -4 3 6,

PLAT975_ALERT_2_C Check Calcd Resid. Dens. 1.01Ang From O44 . 1.17 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 1.06Ang From O39 . 1.11 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 1.00Ang From O34 . 1.00 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 0.83Ang From O43 . 0.99 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 0.78Ang From O39 . 0.98 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 0.94Ang From O36 . 0.94 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 0.90Ang From O44 . 0.92 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 0.85Ang From O39 . 0.89 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 0.86Ang From O43 . 0.84 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 0.87Ang From O45 . 0.84 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 0.78Ang From O36 . 0.81 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 0.85Ang From O41 . 0.80 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 0.96Ang From O40 . 0.80 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 0.47Ang From O43 . 0.80 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 0.91Ang From O34 . 0.79 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 0.76Ang From O42 . 0.78 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 0.84Ang From O41 . 0.77 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 0.87Ang From O40 . 0.75 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 0.77Ang From O43 . 0.74 eA-3

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		7.76	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 ?)	046	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact	Te1 ..044 .	3.29	Ang.
		1-x,1-y,1-z =	2_666	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact	Te4 ..043 .	3.37	Ang.
		1+x,y,z =	1_655	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact	Te6 ..046 .	3.28	Ang.
		1+x,-1+y,z =	1_645	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact	Te10 ..042 .	3.37	Ang.
		2-x,1-y,1-z =	2_766	Check
PLAT860_ALERT_3_G	Number of Least-Squares Restraints		6	Note
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,		
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File		5	Note
		-1-10 3, -2 1 4, -3 2 5, -1 4 5, -4 3 6,		
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		2.219	Note
	Predicted wR2: Based on SigI**2	2.37 or SHELX Weight	4.56	
PLAT994_ALERT_1_G	SHELXL .ins Contains no or MERG 0 Instruction ..			! Note

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

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
29 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
3 ALERT type 4 Improvement, methodology, query or suggestion
3 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

No duplication found

Datablock K8Co8_TeO3_12_10_H2O - ellipsoid plot

