

# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) Compound\_6\_mo\_uco3\_4\_yel

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: Compound\_6\_mo\_uco3\_4\_yel

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Bond precision:	O- N = 0.0075 A	Wavelength=0.71073
Cell:	a=10.9048(2)	b=10.9944(2)      c=17.0902(3)
	alpha=73.445(2)	beta=89.421(1)      gamma=86.382(1)
Temperature:	100 K	
	Calculated	Reported
Volume	1960.06(6)	1960.06(6)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	H8 N2 O15 U2, H2 O	H8 N2 O15 U2, H2 O
Sum formula	H10 N2 O16 U2	H10 N2 O16 U2
Mr	770.16	770.16
Dx,g cm-3	3.915	3.915
Z	6	6
Mu (mm-1)	24.846	24.846
F000	2016.0	2016.0
F000'	1904.05	
h,k,lmax	14,14,22	14,14,22
Nref	9009	9006
Tmin,Tmax	0.029,0.083	0.783,1.000
Tmin'	0.001	

Correction method= # Reported T Limits: Tmin=0.783 Tmax=1.000  
AbsCorr = MULTI-SCAN

Data completeness= 1.000      Theta(max)= 27.500

R(reflections)= 0.0287( 6988)      wR2(reflections)= 0.0608( 9006)

S = 1.018      Npar= 626

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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.

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### ● Alert level C

PLAT220_ALERT_2_C	NonSolvent	Resd 1	O	Ueq(max)/Ueq(min)	Range	3.3	Ratio
PLAT222_ALERT_3_C	NonSolvent	Resd 1	H	Uiso(max)/Uiso(min)	Range	10.0	Ratio
PLAT222_ALERT_3_C	NonSolvent	Resd 2	H	Uiso(max)/Uiso(min)	Range	10.0	Ratio
PLAT222_ALERT_3_C	NonSolvent	Resd 3	H	Uiso(max)/Uiso(min)	Range	10.0	Ratio
PLAT223_ALERT_4_C	Solv./Anion	Resd 5	H	Ueq(max)/Ueq(min)	Range	10.0	Ratio
PLAT245_ALERT_2_C	U(iso) H34A	Smaller than	U(eq) O34	by	0.012	Ang**2	
PLAT245_ALERT_2_C	U(iso) H34B	Smaller than	U(eq) O34	by	0.012	Ang**2	
PLAT417_ALERT_2_C	Short Inter D-H..H-D		H45B	..H47A	.	2.14	Ang.
				x,l+y,z =	1_565	Check	
PLAT417_ALERT_2_C	Short Inter D-H..H-D		H45B	..H47B	.	2.11	Ang.
				x,l+y,z =	1_565	Check	
PLAT751_ALERT_4_C	Bond Calc	0.97000, Rep	0.97011(3)	.....	Senseless s.u.		
	O43 -H43A	1.555	1.555	.....	# 85	Check	
PLAT751_ALERT_4_C	Bond Calc	0.97000, Rep	0.96678(3)	.....	Senseless s.u.		
	O43 -H43B	1.555	1.555	.....	# 86	Check	
PLAT752_ALERT_4_C	Angle Calc	141.00, Rep	141.47(1)	.....	Senseless s.u.		
	U5 -O43 -H43A	1.555	1.555	1.555	# 217	Check	
PLAT752_ALERT_4_C	Angle Calc	114.00, Rep	113.53(1)	.....	Senseless s.u.		
	U5 -O43 -H43B	1.555	1.555	1.555	# 218	Check	
PLAT752_ALERT_4_C	Angle Calc	104.00, Rep	104.31	.....	Senseless s.u.		
	H43A -O43 -H43B	1.555	1.555	1.555	# 219	Check	
PLAT790_ALERT_4_C	Centre of Gravity not Within Unit Cell: Resd.	#			1	Note	
	H8 N2 O15 U2						
PLAT972_ALERT_2_C	Check Calcd Resid. Dens.	0.96A	From U2		-1.51	eA-3	
PLAT975_ALERT_2_C	Check Calcd Resid. Dens.	0.56A	From O39		1.02	eA-3	
PLAT975_ALERT_2_C	Check Calcd Resid. Dens.	0.75A	From O9		0.95	eA-3	
PLAT975_ALERT_2_C	Check Calcd Resid. Dens.	1.00A	From O2		0.94	eA-3	
PLAT975_ALERT_2_C	Check Calcd Resid. Dens.	0.57A	From O1		0.94	eA-3	
PLAT976_ALERT_2_C	Check Calcd Resid. Dens.	0.77A	From O43		-1.13	eA-3	
PLAT976_ALERT_2_C	Check Calcd Resid. Dens.	0.90A	From O22		-1.08	eA-3	
PLAT976_ALERT_2_C	Check Calcd Resid. Dens.	1.01A	From O3		-0.97	eA-3	
PLAT977_ALERT_2_C	Check Negative Difference Density on	H31			-0.38	eA-3	
PLAT977_ALERT_2_C	Check Negative Difference Density on	H40A			-0.31	eA-3	
PLAT977_ALERT_2_C	Check Negative Difference Density on	H44A			-0.54	eA-3	
PLAT977_ALERT_2_C	Check Negative Difference Density on	H46A			-0.31	eA-3	

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### ● Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	44	Note
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms .....	4	Report
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records	4	Report
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	31	Report
PLAT432_ALERT_2_G	Short Inter X...Y Contact O1	..N3	2.81 Ang.
		x,y,z =	1_555 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact O6	..N2	2.67 Ang.
		x,y,z =	1_555 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact O9	..N6	2.82 Ang.
		2-x,3-y,2-z =	2_787 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact O14	..N5	2.84 Ang.
		1-x,2-y,2-z =	2_677 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact O23	..N4	2.84 Ang.
		2-x,3-y,1-z =	2_786 Check
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd.	#	2 Note
	H8 N2 O15 U2		
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd.	#	3 Note
	H8 N2 O15 U2		
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd.	#	4 Note
	H2 O		
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd.	#	5 Note
	H2 O		

PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #	6	Note
	H2 O		
PLAT794_ALERT_5_G	Tentative Bond Valency for U1 (VI) .	5.98	Info
PLAT794_ALERT_5_G	Tentative Bond Valency for U2 (VI) .	6.12	Info
PLAT794_ALERT_5_G	Tentative Bond Valency for U3 (VI) .	6.05	Info
PLAT794_ALERT_5_G	Tentative Bond Valency for U4 (VI) .	6.11	Info
PLAT794_ALERT_5_G	Tentative Bond Valency for U5 (VI) .	6.05	Info
PLAT794_ALERT_5_G	Tentative Bond Valency for U6 (VI) .	6.18	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints .....	31	Note
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .		Please Do !
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	2	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	1	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity .....	2.6	Low

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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  
27 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
25 **ALERT level G** = General information/check it is not something unexpected

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
23 ALERT type 2 Indicator that the structure model may be wrong or deficient  
6 ALERT type 3 Indicator that the structure quality may be low  
15 ALERT type 4 Improvement, methodology, query or suggestion  
7 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* or *IUCrData*, 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.

