

checkCIF/PLATON report

No syntax errors found. CIF dictionary Interpreting this report

Datablock: te-spiro

Bond precision: O- C = 0.0052 A Wavelength=1.54184

Cell: a=15.7046(2) b=8.83038(16) c=19.1603(3)
 alpha=90 beta=90 gamma=90

Temperature: 123 K

	Calculated	Reported
Volume	2657.11(7)	2657.11(8)
Space group	P b c a	P b c a
Hall group	-P 2ac 2ab	?
Moiety formula	C14 H16 O4 Te	C14 H16 O4 Te
Sum formula	C14 H16 O4 Te	C14 H16 O4 Te
Mr	375.87	375.87
Dx,g cm-3	1.879	1.879
Z	8	8
Mu (mm-1)	17.759	17.759
F000	1472.0	1472.0
F000'	1475.02	
h,k,lmax	19,10,23	19,10,23
Nref	2676	2443
Tmin,Tmax	0.014,0.142	0.233,1.000
Tmin'	0.002	

Correction method= MULTI-SCAN

Data completeness= 0.913 Theta(max)= 73.540

R(reflections)= 0.0480(2127) wR2(reflections)= 0.1330(2443)

S = 1.039 Npar= 210

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

PLAT029_ALERT_3_A _diffn_measured_fraction_theta_full Low 0.93

Alert level C

PLAT022_ALERT_3_C Ratio Unique / Expected Reflections too Low 0.91



Alert level G

PLAT301_ALERT_3_G Note: Main Residue Disorder	39.00 Perc.
PLAT432_ALERT_2_G Short Inter X...Y Contact Te .. O2A ..	2.94 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact Te .. O2B ..	3.33 Ang.
PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints	72
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels	56
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF #	7
C1AA -TE -C1AB 1.555 1.555 1.555	1.30 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF #	13
C1BB -TE -C1BA 1.555 1.555 1.555	2.20 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF #	82
C6AB -C7A -C6AA 1.555 1.555 1.555	2.30 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF #	149
C6BB -C7B -C6BA 1.555 1.555 1.555	2.80 Deg.
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms	!

1 **ALERT level A** = In general: serious problem

0 **ALERT level B** = Potentially serious problem

1 **ALERT level C** = Check and explain

10 **ALERT level G** = General alerts; check

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

2 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

5 ALERT type 4 Improvement, methodology, query or suggestion

1 ALERT type 5 Informative message, check

Datablock te-spiro - ellipsoid plot

