

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 4c_benzo_mes_SbF6_2

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: 4c_benzo_mes_SbF6_2

Bond precision:	C-C = 0.0104 Å	Wavelength=0.71073
Cell:	a=9.6256(10)	b=11.6000(13) c=22.777(3)
	alpha=86.362(4)	beta=78.497(4) gamma=75.573(4)
Temperature:	150 K	
	Calculated	Reported
Volume	2413.3(5)	2413.3(5)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C47 H51 N O, 2(F6 Sb) [+ solvent]	C47 H51 N O, 2(F6 Sb) [+ solvent]
Sum formula	C47 H51 F12 N O Sb2 [+ solvent]	C47 H51 F12 N O Sb2
Mr	1117.41	1117.39
Dx, g cm ⁻³	1.538	1.538
Z	2	2
Mu (mm ⁻¹)	1.200	1.200
F000	1116.0	1116.0
F000'	1114.31	
h, k, lmax	11, 14, 27	11, 14, 27
Nref	9165	9156
Tmin, Tmax	0.759, 0.942	0.816, 0.942
Tmin'	0.759	

Correction method= # Reported T Limits: Tmin=0.816 Tmax=0.942
AbsCorr = MULTI-SCAN

Data completeness= 0.999 Theta(max)= 25.681

R(reflections)= 0.0726(7655)

wR2(reflections)=
0.2038(9156)

S = 1.051

Npar= 641

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

PLAT971_ALERT_2_A Check Calcd Resid. Dens. 0.57Ang From F9B 3.67 eA-3

Author Response: A disorder is already modeled on this counter ion. This residual electronic density cannot be reliably interpreted.



Alert level B

PLAT972_ALERT_2_B Check Calcd Resid. Dens. 0.38Ang From Sb3B -2.86 eA-3

Author Response: A disorder is already modeled on this counter ion. This residual electronic density cannot be reliably interpreted.

PLAT972_ALERT_2_B Check Calcd Resid. Dens. 0.61Ang From Sb3B -2.78 eA-3

Author Response: A disorder is already modeled on this counter ion. This residual electronic density cannot be reliably interpreted.



Alert level C

PLAT220_ALERT_2_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 3.9 Ratio
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds 0.01042 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 2.722 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 7 Report
-2 2 0, 0 -1 1, 1 0 1, 0 2 1, -2 0 2, -2 2 2,
2 4 8,
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) . 1 Check
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.44Ang From Sb1A 1.86 eA-3

Author Response: A disorder is already modeled on this counter ion. This residual electronic density cannot be reliably interpreted.

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.47Ang From Sb1B 1.73 eA-3

Author Response: A disorder is already modeled on this counter ion. This residual electronic density cannot be reliably interpreted.


```

      1 0 1, 0 2 1, 2 4 8, -2 2 0, -2 2 2,
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ..... 3.6 Low
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ..... 4.407 Note
      Predicted wR2: Based on SigI**2 4.62 or SHELX Weight 19.48
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 0 Info

```

```

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

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
14 ALERT type 2 Indicator that the structure model may be wrong or deficient
13 ALERT type 3 Indicator that the structure quality may be low
24 ALERT type 4 Improvement, methodology, query or suggestion
1 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. 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.

