



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) `saber_cof-612_f_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: `saber_cof-612_f_2`

Bond precision:	C-C = 0.0311 Å		Wavelength=1.54184
Cell:	a=38.024 (2)	b=38.024 (2)	c=31.110 (4)
	alpha=90	beta=90	gamma=120
Temperature:	100 K		
	Calculated	Reported	
Volume	38954 (6)	38953 (6)	
Space group	P -6 c 2	P -6 c 2	
Hall group	P -6c 2	P -6c 2	
Moiety formula	4(C63 O6), C112 N12, C82, 12(C6), 12(C) [+ solvent]	C56 N6, C209 O12	
Sum formula	C530 N12 O24 [+ solvent]	C265 N6 O12	
Mr	6917.42	3458.71	
Dx, g cm ⁻³	0.295	0.295	
Z	1	2	
Mu (mm ⁻¹)	0.146	0.146	
F000	3456.0	3456.0	
F000'	3466.65		
h, k, lmax	23, 23, 19	23, 23, 19	
Nref	3465 [1825]	3455	
Tmin, Tmax	0.991, 0.993	0.786, 1.000	
Tmin'	0.990		

Correction method= # Reported T Limits: Tmin=0.786 Tmax=1.000
AbsCorr = MULTII-SCAN

Data completeness= 1.89/1.00 Theta(max)= 28.801

R(reflections)= 0.1074(2056) wR2(reflections)=
0.3538(3455)

S = 1.332 Npar= 162

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

THETM01_ALERT_3_A The value of sine(theta_max)/wavelength is less than 0.550
Calculated sin(theta_max)/wavelength = 0.3125

Author Response: The crystal was a weak diffractor at high angles, and the intensity of the reflections dropped below the threshold of the detector. Consequently, data collection was truncated to maintain a meaningful signal-to-noise ratio at lower resolution (1.6 ang), which is sufficient to confirm the framework connectivity.

PLAT213_ALERT_2_A Atom C1 has ADP max/min Ratio 6.7 prolat

Author Response: The ADP for atom C1 reflects the rotational freedom of the methoxy group. Given the diffraction quality at higher angles, this anisotropic model is the most reasonable representation of the electron den

PLAT250_ALERT_2_A Large U3/U1 Ratio for <U(i,j)> Tensor(Resd 4) 22.6 Note

Author Response: This exhibits high anisotropic displacement due to the flexibility of the connecting arms in the porous architecture and the low resolution of the data.

Alert level B

PLAT196_ALERT_1_B No TEMP record in '.res' and CIF 'CellTemp' .NE. 293 Degree

Author Response: The discrepancy in the TEMP record is a default setting of the refinement software (293 K) and is irrelevant to the current model, as hydrogen atoms were not included in the refinement due to the low resolution of the diffraction data.

PLAT213_ALERT_2_B Atom C006 has ADP max/min Ratio 4.2 prolat

Author Response: The ADP for atom C1 reflects the rotational freedom of the methoxy group. Given the diffraction quality at higher angles, this anisotropic model is the most reasonable representation of the electron den

PLAT213_ALERT_2_B Atom C008 has ADP max/min Ratio 4.2 prolat

Author Response: The ADP for atom C1 reflects the rotational freedom of the methoxy group. Given the diffraction quality at higher angles, this anisotropic model is the most reasonable representation of the electron den

PLAT213_ALERT_2_B Atom C00A has ADP max/min Ratio 4.2 prolat

Author Response: The ADP for atom C1 reflects the rotational freedom of the methoxy group. Given the diffraction quality at higher angles, this anisotropic model is the most reasonable representation of the electron den

PLAT213_ALERT_2_B Atom C00D has ADP max/min Ratio 4.2 prolat

Author Response: The ADP for atom C1 reflects the rotational freedom of the methoxy group. Given the diffraction quality at higher angles, this anisotropic model is the most reasonable representation of the electron den

PLAT213_ALERT_2_B Atom C00H has ADP max/min Ratio 4.2 prolat

Author Response: The ADP for atom C1 reflects the rotational freedom of the methoxy group. Given the diffraction quality at higher angles, this anisotropic model is the most reasonable representation of the electron den

PLAT213_ALERT_2_B Atom C00P has ADP max/min Ratio 4.2 prolat

Author Response: The ADP for atom C1 reflects the rotational freedom of the methoxy group. Given the diffraction quality at higher angles, this anisotropic model is the most reasonable representation of the electron den

PLAT213_ALERT_2_B Atom C00K has ADP max/min Ratio 4.2 prolat

Author Response: The ADP for atom C1 reflects the rotational freedom of the methoxy group. Given the diffraction quality at higher angles, this anisotropic model is the most reasonable representation of the electron den

PLAT241_ALERT_2_B High MainResAtom Ueq as Compared to Neighbours O1 Check

Author Response: Given the low resolution and the porous nature of the framework, this anisotropic model represents the best fit for the diffuse electron density at this position.

PLAT241_ALERT_2_B High MainResAtom Ueq as Compared to Neighbours C50 Check

Author Response: Given the low resolution and the porous nature of the framework, this anisotropic model represents the best fit for the diffuse electron density at this position.

PLAT241_ALERT_2_B High MainResAtom Ueq as Compared to Neighbours C00F Check

Author Response: Given the low resolution and the porous nature of the framework, this anisotropic model represents the best fit for the diffuse electron density at this position.

PLAT242_ALERT_2_B Low MainResAtom Ueq as Compared to Neighbours C7 Check

Author Response: Atom C7 is located in the flexible peripheral arm of the COF linker. The observed difference in compared to its neighbors is attributed to the local conformational flexibility, contrasting with the more rigid [HBC] core units. At the current resolution of 1.6 ang, this anisotropic model represents the most reasonable fit to the electron density.

PLAT242_ALERT_2_B Low MainResAtom Ueq as Compared to Neighbours C002 Check

Author Response: Atom C7 is located in the flexible peripheral arm of the COF linker. The observed difference in compared to its neighbors is attributed to the local conformational flexibility, contrasting with the more rigid [HBC] core units. At the current resolution of 1.6 ang, this anisotropic model represents the most reasonable fit to the electron density.

PLAT242_ALERT_2_B Low MainResAtom Ueq as Compared to Neighbours C00C Check

Author Response: Atom C7 is located in the flexible peripheral arm of the COF linker. The observed difference in compared to its neighbors is attributed to the local conformational flexibility, contrasting with the more rigid [HBC] core units. At the current resolution of 1.6 ang, this anisotropic model represents the most reasonable fit to the electron density.

PLAT250_ALERT_2_B Large U3/U1 Ratio for <U(i,j)> Tensor(Resd 1) 5.8 Note

Author Response: This exhibits high anisotropic displacement due to the flexibility of the connecting arms in the porous architecture and the low resolution of the data.

PLAT260_ALERT_2_B Large Average Ueq of Residue Including O1 0.306 Check

Author Response: The large average Ueq is attributed to the conformational flexibility of the peripheral arms within the large pore voids of the COF and the low resolution of the data. However, the position of O1 is chemically consistent with the expected HBC linekr structure.

PLAT260_ALERT_2_B Large Average Ueq of Residue Including C9 0.608 Check

Author Response: The large average Ueq is attributed to the conformational flexibility of the peripheral arms within the large pore voids of the COF and the low resolution of the data. However, the position of O1 is chemically consistent with the expected HBC linekr structure.

PLAT340_ALERT_3_B Low Bond Precision on C-C Bonds 0.03108 Ang.

Author Response: The low bond precision is a direct consequence of the limited resolution (1.6 ang) and the weak diffraction inherent to this porous covalent organic framework.



Alert level C

PLAT082_ALERT_2_C High R1 Value	0.11 Report
PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25)	0.35 Report
PLAT214_ALERT_2_C Atom C9 (Anion/Solvent) ADP max/min Ratio	4.8 prolat
PLAT214_ALERT_2_C Atom C10 (Anion/Solvent) ADP max/min Ratio	4.8 prolat
PLAT214_ALERT_2_C Atom C11 (Anion/Solvent) ADP max/min Ratio	4.8 prolat
PLAT214_ALERT_2_C Atom C019 (Anion/Solvent) ADP max/min Ratio	4.8 prolat
PLAT214_ALERT_2_C Atom C78 (Anion/Solvent) ADP max/min Ratio	4.8 prolat
PLAT214_ALERT_2_C Atom C105 (Anion/Solvent) ADP max/min Ratio	4.8 prolat
PLAT241_ALERT_2_C High MainResAtom Ueq as Compared to Neighbours	C3 Check

Author Response: Given the low resolution and the porous nature of the framework, this anisotropic model represents the best fit for the diffuse electron density at this position.

PLAT241_ALERT_2_C High MainResAtom Ueq as Compared to Neighbours C4 Check

Author Response: Given the low resolution and the porous nature of the framework, this anisotropic model represents the best fit for the diffuse electron density at this position.

PLAT241_ALERT_2_C High MainResAtom Ueq as Compared to Neighbours C48 Check

Author Response: Given the low resolution and the porous nature of the framework, this anisotropic model represents the best fit for the diffuse electron density at this position.

PLAT242_ALERT_2_C Low MainResAtom Ueq as Compared to Neighbours O005 Check

Author Response: Atom C7 is located in the flexible peripheral arm of the COF linker. The observed difference in compared to its neighbors is attributed to the local conformational flexibility, contrasting with the more rigid [HBC] core units. At the current resolution of 1.6 ang, this anisotropic model represents the most reasonable fit to the electron density.

PLAT242_ALERT_2_C Low MainResAtom Ueq as Compared to Neighbours C00H Check

Author Response: Atom C7 is located in the flexible peripheral arm of the COF linker. The observed difference in compared to its neighbors is attributed to the local conformational flexibility, contrasting with the more rigid [HBC] core units. At the current resolution of 1.6 ang, this anisotropic model represents the most reasonable fit to the electron density.

PLAT242_ALERT_2_C Low MainResAtom Ueq as Compared to Neighbours C009 Check

Author Response: Atom C7 is located in the flexible peripheral arm of the COF linker. The observed difference in compared to its neighbors is attributed to the local conformational flexibility, contrasting with the more rigid [HBC] core units. At the current resolution of 1.6 ang, this anisotropic model represents the most reasonable fit to the electron density.

PLAT250_ALERT_2_C Large U3/U1 Ratio for <U(i,j)> Tensor(Resd 2) 3.4 Note

Author Response: This exhibits high anisotropic displacement due to the flexibility of the connecting arms in the porous architecture and the low resolution of the data.

PLAT250_ALERT_2_C Large U3/U1 Ratio for <U(i,j)> Tensor(Resd 3) 2.6 Note

Author Response: This exhibits high anisotropic displacement due to the flexibility of the connecting arms in the porous architecture and the low resolution of the data.

PLAT260_ALERT_2_C Large Average Ueq of Residue Including N01N 0.228 Check

Author Response: The large average Ueq is attributed to the conformational flexibility of the peripheral arms within the large pore voids of the COF and the low resolution of the data. However, the position of O1 is chemically consistent with the expected HBC linekr structure.

PLAT260_ALERT_2_C Large Average Ueq of Residue Including C007 0.273 Check

Author Response: The large average Ueq is attributed to the conformational flexibility of the peripheral arms within the large pore voids of the COF and the low resolution of the data. However, the position of O1 is chemically consistent with the expected HBC linekr structure.

PLAT260_ALERT_2_C Large Average Ueq of Residue Including C000 0.210 Check

Author Response: The large average Ueq is attributed to the conformational flexibility of the peripheral arms within the large pore voids of the COF and the low resolution of the data. However, the position of O1 is chemically consistent with the expected HBC linekr structure.

PLAT767_ALERT_4_C INS Embedded LIST 6 Instruction Should be LIST 4 Please Check
 PLAT905_ALERT_3_C Negative K value in the Analysis of Variance ... -3.887 Report
 PLAT905_ALERT_3_C Negative K value in the Analysis of Variance ... -0.127 Report
 PLAT910_ALERT_3_C Missing FCF Reflection(s) Below Theta(Min) [Deg]= 3.55 Note
 0 1 0, -1 2 0, 0 2 0, -1 2 1, 0 0 2, 0 1 2,

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 8 Note
 PLAT003_ALERT_2_G Number of Uiso or U(i,j) Restrained non-H-Atoms 1 Report
 PLAT040_ALERT_1_G No H-atoms in this Carbon Containing Compound .. Please Check
 PLAT041_ALERT_1_G Calc. and Reported SumFormula Strings Differ Please Check
 Calc: C530 N12 O24
 Rep.: C265 N6 O12
 PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ Please Check
 Calc: 4(C63 O6), C112 N12, C82, 12(C6), 12(C)
 Rep.: C56 N6, C209 O12
 PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ... 0.500 Check
 PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large 0.20 Report
 PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records 10 Report
 PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 5 Report
 PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records 1 Report
 PLAT299_ALERT_4_G Atom Site Occupancy Constrained at 0.5 Check
 C6 C8 C13 C51 C54

PLAT301_ALERT_3_G	Main Residue Disorder	(Resd	3)	36% Note
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in	(Resd	2)	41.33 Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in	(Resd	3)	27.33 Check
PLAT398_ALERT_2_G	Deviating C-O-C Angle From 120 for 0005	.		97.3 Degree
PLAT432_ALERT_2_G	Short Inter X...Y Contact 0005 ..C10	.		2.95 Ang.
	x,y,z =			1_555 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact 0005 ..C78	.		2.99 Ang.
	x,y,z =			1_555 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact N01N ..C9	.		2.17 Ang.
	x,y,z =			1_555 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact N01N ..C019	.		3.04 Ang.
	x,y,z =			1_555 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C001 ..C003	.		2.38 Ang.
	x,y,3/2-z =			4_556 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C001 ..C001	.		2.63 Ang.
	1-y,x-y,3/2-z =			5_656 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C001 ..C001	.		2.63 Ang.
	1-x+y,1-x,3/2-z =			6_666 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C2 ..C78	.		2.56 Ang.
	x,y,z =			1_555 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C2 ..C105	.		2.92 Ang.
	x,y,z =			1_555 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C003 ..C003	.		2.65 Ang.
	x,y,3/2-z =			4_556 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C4 ..C78	.		2.83 Ang.
	x,y,z =			1_555 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C006 ..C006	.		2.53 Ang.
	-y,x-y,z =			2_555 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C006 ..C006	.		2.53 Ang.
	-x+y,-x,z =			3_555 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C006 ..C006	.		2.92 Ang.
	-y,-x,1-z =			10_556 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C5 ..C000	.		2.76 Ang.
	x,y,z =			1_555 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C007 ..C00J	.		2.31 Ang.
	x,y,1/2-z =			4_555 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C007 ..C007	.		2.55 Ang.
	1-y,1+x-y,1/2-z =			5_665 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C007 ..C007	.		2.55 Ang.
	-x+y,1-x,1/2-z =			6_565 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C6 ..C000	.		2.60 Ang.
	x,y,z =			1_555 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C8 ..C000	.		2.98 Ang.
	x,y,z =			1_555 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C10 ..C00Q	.		2.87 Ang.
	x,y,z =			1_555 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C00J ..C00J	.		2.55 Ang.
	x,y,1/2-z =			4_555 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C000 ..C97	.		1.78 Ang.
	x,y,z =			1_555 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C000 ..C36	.		1.89 Ang.
	x,y,z =			1_555 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C000 ..C47	.		2.73 Ang.
	x,y,z =			1_555 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C00Q ..C78	.		1.82 Ang.
	x,y,z =			1_555 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C00Q ..C105	.		2.62 Ang.

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                                x,y,z =      1_555 Check
PLAT606_ALERT_4_G Solvent Accessible VOID(S) in Crystal Structure      ! Info
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels .....      23 Note
      C001      C002      C003      O005      C006      C007      C008      C00A
      C00D      C00H      C00P      C00K      C00B      C00C      C00E      C00J
      C00O      C009      C00Q      N01N      C01Z      C00F      C019
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C001      --C00B      1.72 Ang.
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C000      --C97      1.78 Ang.
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C000      --C36      1.89 Ang.
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C00Q      --C78      1.82 Ang.
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters      2 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .....      11 Note
PLAT868_ALERT_4_G ALERTS Due to the Use of _smtbx_masks Suppressed      ! Info
PLAT908_ALERT_2_G Max. Perc. Data with I > 2*s(I) per Res.Shell .      63.81% Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....      2 Note
      0 0 2, 0 1 2,
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value .....      10.397 Note
      Predicted wR2: Based on SigI*2 3.40 or SHELX Weight 26.56
PLAT994_ALERT_1_G SHELXL .ins Contains no or MERG 0 Instruction ..      ! Note

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

 6 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
72 ALERT type 2 Indicator that the structure model may be wrong or deficient
 9 ALERT type 3 Indicator that the structure quality may be low
11 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. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```

# start Validation Reply Form
_vrf_PLAT082_saber_cof-612_f_2
;
PROBLEM: High R1 Value .....      0.11 Report
RESPONSE: ...
;
_vrf_PLAT084_saber_cof-612_f_2
;
PROBLEM: High wR2 Value (i.e. > 0.25) .....      0.35 Report
RESPONSE: ...
;
_vrf_PLAT214_saber_cof-612_f_2
;

```

PROBLEM: Atom C9 (Anion/Solvent) ADP max/min Ratio 4.8 prolat
RESPONSE: ...
;
_vrf_PLAT767_saber_cof-612_f_2
;
PROBLEM: INS Embedded LIST 6 Instruction Should be LIST 4 Please Check
RESPONSE: ...
;
_vrf_PLAT905_saber_cof-612_f_2
;
PROBLEM: Negative K value in the Analysis of Variance ... -3.887 Report
RESPONSE: ...
;
_vrf_PLAT910_saber_cof-612_f_2
;
PROBLEM: Missing FCF Reflection(s) Below Theta(Min) [Deg]= 3.55 Note
RESPONSE: ...
;
end Validation Reply Form

PLATON version of 15/01/2026; check.def file version of 02/01/2026

duplicate check

No duplication found

