

checkCIF/PLATON report

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No syntax errors found. CIF dictionary Interpreting this report

Datablock: 71220am

Bond precision: C-C = 0.0040 Å

Wavelength=0.71073

Cell: a=12.3957(15) b=13.1933(16) c=14.4155(18)
 alpha=111.293(2) beta=106.666(2) gamma=94.493(2)
Temperature: 173 K

	Calculated	Reported
Volume	2059.9(4)	2059.9(4)
Space group	P -1	P-1
Hall group	-P 1	?
Moiety formula	C15 H12 N6 O3 S3, C H2 Cl2 ?	
Sum formula	C16 H14 Cl2 N6 O3 S3	C16 H14 Cl2 N6 O3 S3
Mr	505.41	505.41
Dx, g cm-3	1.630	1.630
Z	4	4
Mu (mm-1)	0.652	0.652
F000	1032.0	1032.0
F000'	1034.98	
h, k, lmax	15, 15, 17	15, 15, 17
Nref	7656	7495
Tmin, Tmax	0.855, 0.937	0.828, 0.938
Tmin'	0.822	

Correction method= # Reported T Limits: Tmin=0.828 Tmax=0.938
AbsCorr = MULTI-SCAN

Data completeness= 0.979

Theta(max)= 25.500

R(reflections)= 0.0421(6118)

wR2(reflections)= 0.1117(7495)

S = 1.021

Npar= 547

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 C

PLAT029_ALERT_3_C	_diffn_measured_fraction_theta_full	value Low	0.979	Why?
PLAT230_ALERT_2_C	Hirshfeld Test Diff for	S2 --C14	5.3	s.u.
PLAT244_ALERT_4_C	Low	'Solvent' Ueq as Compared to Neighbors of	C31	Check
PLAT244_ALERT_4_C	Low	'Solvent' Ueq as Compared to Neighbors of	C32	Check

● Alert level G

PLAT005_ALERT_5_G	No Embedded Refinement Details Found	in the CIF	Please Do !
PLAT066_ALERT_1_G	Predicted and Reported Tmin&Tmax Range	Identical	? Check
PLAT154_ALERT_1_G	The s.u.'s on the Cell Angles are Equal	..(Note)	0.002 Degree
PLAT398_ALERT_2_G	Deviating	C-O-C Angle From 120 for 01	102.4 Degree
PLAT398_ALERT_2_G	Deviating	C-O-C Angle From 120 for 02	102.4 Degree
PLAT398_ALERT_2_G	Deviating	C-O-C Angle From 120 for 03	102.0 Degree
PLAT398_ALERT_2_G	Deviating	C-O-C Angle From 120 for 04	102.4 Degree
PLAT398_ALERT_2_G	Deviating	C-O-C Angle From 120 for 05	102.1 Degree
PLAT398_ALERT_2_G	Deviating	C-O-C Angle From 120 for 06	102.2 Degree
PLAT899_ALERT_4_G	SHELXL97	is Deprecated and Succeeded by SHELXL	2018 Note

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- 2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
7 ALERT type 2 Indicator that the structure model may be wrong or deficient
1 ALERT type 3 Indicator that the structure quality may be low
3 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check
-
-

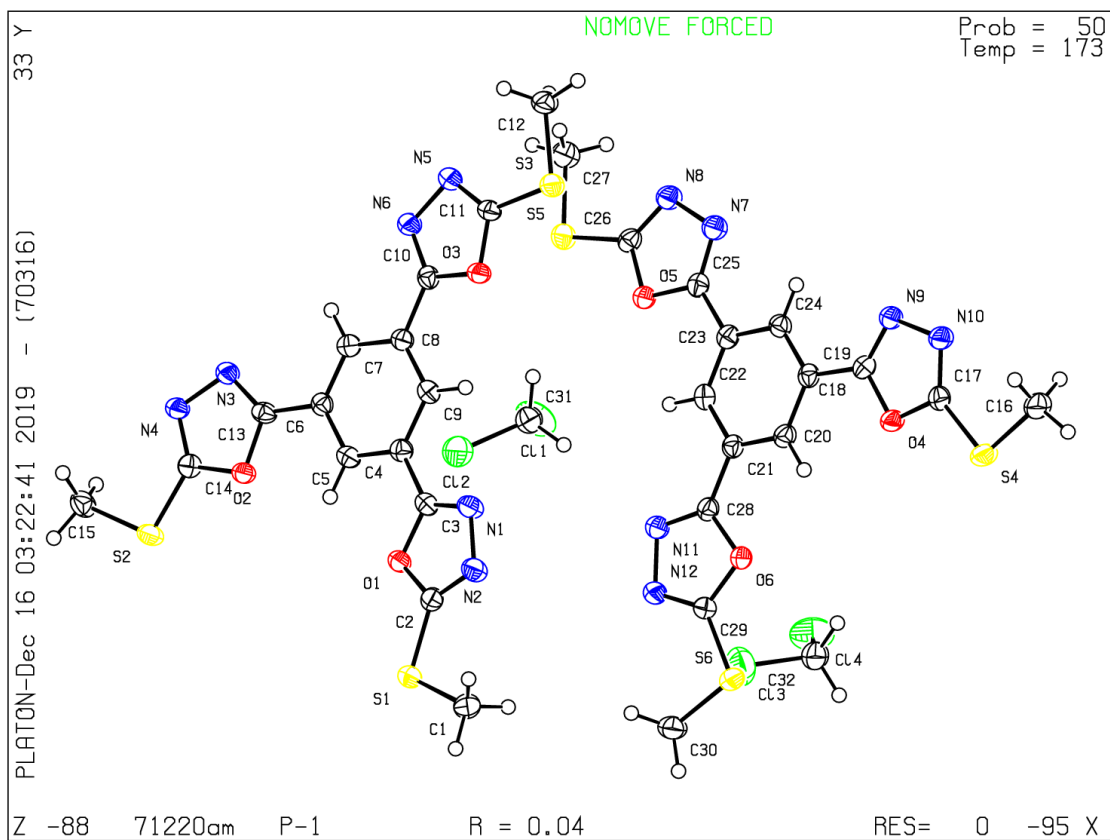
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No syntax errors found.

[CIF dictionary](#)

[Interpreting this report](#)

Datablock: 71205d

Bond precision: C-C = 0.0070 Å

Wavelength=0.71073

Cell: a=29.635(2)

b=29.635(2)

c=15.200(2)

alpha=90

beta=90

gamma=90

Temperature: 173 K

	Calculated	Reported
Volume	13349(3)	13350(2)
Space group	I 41/a	I4(1)/a
Hall group	-I 4ad	?
Moiety formula	C16 H14 Ag2 F3 N6 O7 S4, C ? F3 O3 S, C H2 Cl2	?
Sum formula	C18 H16 Ag2 Cl2 F6 N6 O10 S5	C18 H16 Ag2 Cl2 F6 N6 O10 S5
Mr	1037.31	1037.31
Dx, g cm ⁻³	2.065	2.064
Z	16	16
Mu (mm ⁻¹)	1.739	1.738
F000	8128.0	8128.0
F000'	8118.11	
h, k, lmax	35, 35, 18	35, 35, 18
Nref	5899	5907
Tmin, Tmax	0.812, 0.870	0.723, 0.873
Tmin'	0.706	

Correction method= # Reported T Limits: Tmin=0.723 Tmax=0.873

AbsCorr = MULTI-SCAN

Data completeness= 1.001

Theta(max)= 25.030

R(reflections)= 0.0493(5034)

wR2(reflections)= 0.1100(5907)

S = 1.098

Npar= 474

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 C

PLAT220_ALERT_2_C	NonSolvent Resd 1 C Ueq(max) / Ueq(min) Range	4.0 Ratio
PLAT220_ALERT_2_C	NonSolvent Resd 1 0 Ueq(max) / Ueq(min) Range	4.3 Ratio
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	S4 Check
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of	S5 Check
PLAT250_ALERT_2_C	Large U3/U1 Ratio for Average U(i,j) Tensor	2.3 Note
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including Cl1'	0.103 Check

● Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	6 Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	2 Report
PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	3 Info
PLAT005_ALERT_5_G	No Embedded Refinement Details Found in the CIF	Please Do !
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	2 Report
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	7.81 Why ?
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of	C16 Check
PLAT244_ALERT_4_G	Low 'Solvent' Ueq as Compared to Neighbors of	C17 Check
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 3)	100% Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 4)	100% Note
PLAT398_ALERT_2_G	Deviating C-O-C Angle From 120 for O1	103.6 Degree
PLAT398_ALERT_2_G	Deviating C-O-C Angle From 120 for O2	103.2 Degree
PLAT398_ALERT_2_G	Deviating C-O-C Angle From 120 for O3	103.2 Degree
PLAT432_ALERT_2_G	Short Inter X...Y Contact Cl2' ..C8	3.19 Ang.
	3/2-x,2-y,1/2+z =	2_675 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact O10 ..C9	2.97 Ang.
	-1/4+y,5/4-x,1/4-z =	15_565 Check
PLAT434_ALERT_2_G	Short Inter HL..HL Contact F6 ..F6	2.74 Ang.
	3/2-x,3/2-y,1/2-z =	13_665 Check
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	16 Note
PLAT899_ALERT_4_G	SHELXL97 is Deprecated and Succeeded by SHELXL	2018 Note

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3 ALERT type 5 Informative message, check

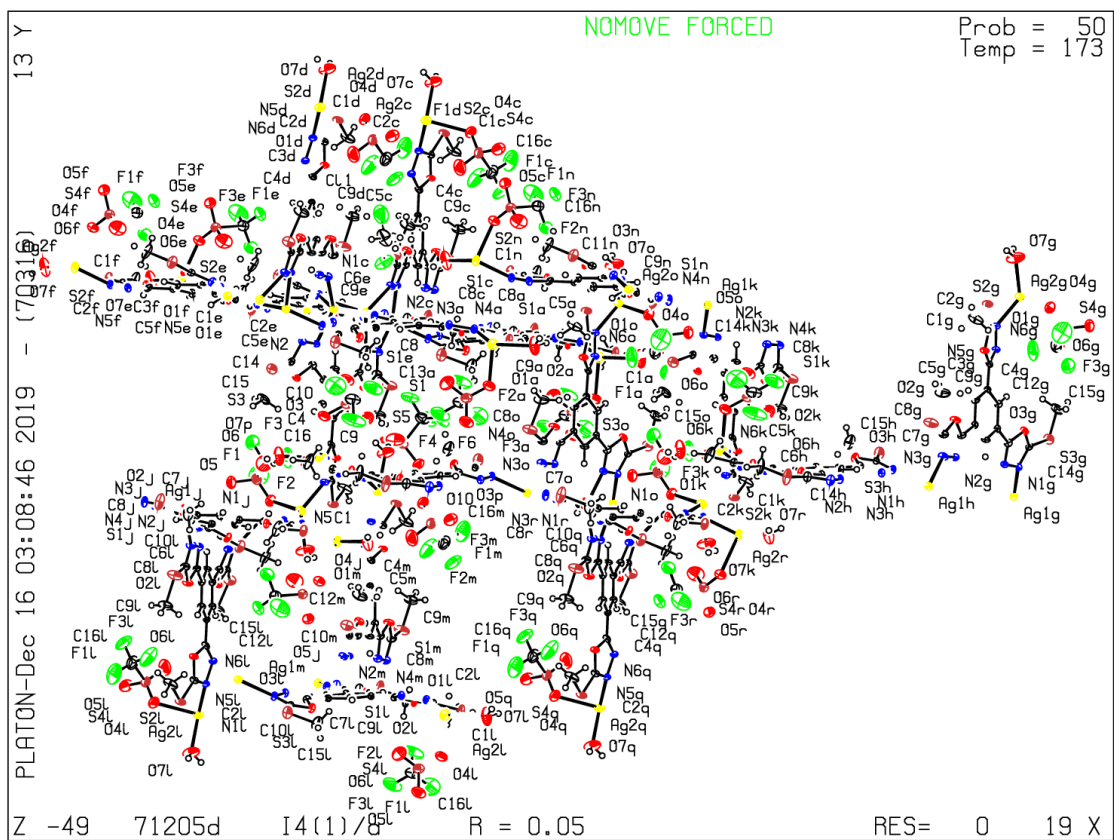
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[CIF dictionary](#)

[Interpreting this report](#)

Datablock: 80108b

Bond precision: C-C = 0.0131 Å

Wavelength=0.71073

Cell: a=23.442(3)

b=49.277(8)

c=22.284(3)

alpha=90

beta=90

gamma=90

Temperature: 298 K

	Calculated	Reported
Volume	25741(6)	25741(6)
Space group	F d d 2	Fdd2
Hall group	F 2 -2d	?
Moiety formula	C60 H52 Ag5 N24 O14 S12, 5(F6 Sb), 5(C4 H8 O)	?
Sum formula	C80 H92 Ag5 F30 N24 O19 S12 Sb5	C80 H92 Ag5 F30 N24 O19 S12 Sb5
Mr	3796.65	3796.60
Dx, g cm ⁻³	1.959	1.959
Z	8	8
Mu (mm ⁻¹)	2.079	2.079
F000	14752.0	14752.0
F000'	14712.15	
h, k, lmax	27, 58, 26	27, 58, 26
Nref	11398[5859]	11022
Tmin, Tmax	0.741, 0.796	0.435, 0.804
Tmin'	0.369	

Correction method= # Reported T Limits: Tmin=0.435 Tmax=0.804

AbsCorr = MULTI-SCAN

Data completeness= 1.88/0.97

Theta(max)= 25.040

R(reflections)= 0.0452(10079)

wR2(reflections)= 0.1150(11022)

S = 1.029

Npar= 740

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test-name_ALERT_alert-type_alert-level.

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● Alert level C

PLAT090_ALERT_3_C	Poor Data / Parameter Ratio (Zmax > 18)	7.92	Note
PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density	2.50	Report
PLAT165_ALERT_3_C	Nr. of Status R Flagged Non-Hydrogen Atoms	1	Note
PLAT202_ALERT_3_C	Isotropic non-H Atoms in Anion/Solvent	13	Check
	08 C35 C36 C37 C38 09		etc.
PLAT220_ALERT_2_C	NonSolvent Resd 1 C Ueq(max) / Ueq(min) Range	3.1	Ratio
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	S2	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C14	Check
PLAT243_ALERT_4_C	High 'Solvent' Ueq as Compared to Neighbors of	C35	Check
PLAT243_ALERT_4_C	High 'Solvent' Ueq as Compared to Neighbors of	C37	Check
PLAT243_ALERT_4_C	High 'Solvent' Ueq as Compared to Neighbors of	C40	Check
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of	Sb1	Check
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of	Sb2	Check
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of	Sb3	Check
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of	08	Check
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of	C36	Check
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of	C38	Check
PLAT250_ALERT_2_C	Large U3/U1 Ratio for Average U(i,j) Tensor	2.6	Note
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including Sb1	0.111	Check
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including Sb2	0.127	Check
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including Sb3	0.171	Check
PLAT314_ALERT_2_C	Small Angle for H2O: Metal-07 -H7B .	92.73	Degree
PLAT342_ALERT_3_C	Low Bond Precision on C-C Bonds	0.01313	Ang.
PLAT601_ALERT_2_C	Structure Contains Solvent Accessible VOIDS of .	67	Ang**3

● Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	18	Note
PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	3	Info
PLAT005_ALERT_5_G	No Embedded Refinement Details Found in the CIF	Please	Do !
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	2	Report
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	40.38	Why ?
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 7)	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 8)	100%	Note
PLAT398_ALERT_2_G	Deviating C-O-C Angle From 120 for 01	103.0	Degree
PLAT398_ALERT_2_G	Deviating C-O-C Angle From 120 for 02	103.3	Degree
PLAT398_ALERT_2_G	Deviating C-O-C Angle From 120 for 03	103.2	Degree
PLAT398_ALERT_2_G	Deviating C-O-C Angle From 120 for 04	103.3	Degree
PLAT398_ALERT_2_G	Deviating C-O-C Angle From 120 for 05	103.6	Degree
PLAT398_ALERT_2_G	Deviating C-O-C Angle From 120 for 06	102.8	Degree
PLAT432_ALERT_2_G	Short Inter X...Y Contact F12 ..C28	2.95	Ang.
	5/4-x,1/4+y,1/4+z =	4_655	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact 010 ..C13	2.91	Ang.
	3/2-x,3/2-y,z =	14_665	Check
PLAT794_ALERT_5_G	Tentative Bond Valency for Sb1 (V) .	5.25	Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Sb2 (V) .	4.94	Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Sb3 (V) .	5.62	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	19	Note
PLAT899_ALERT_4_G	SHELXL97 is Deprecated and Succeeded by SHELXL	2018	Note

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PLATON version of 11/12/2019; check.def file version of 11/12/2019

