

## checkCIF/PLATON report

Structure factors have been supplied for datablock(s) mo\_17mv\_db12\_mosn17nco\_0a,  
mo\_17mv\_db13\_mose5ns17\_0a, mo\_Mos17Co4N\_0m\_a, mo\_MosECo174\_0m\_a,  
mo\_MosMCoNN\_0m\_a

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: mo\_Mos17Co4N\_0m\_a

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Bond precision:	C-C = 0.0033 A	Wavelength=0.71073
Cell:	a=17.330(2)      b=10.0232(13)      c=18.8315(17)	alpha=90      beta=113.688(4)      gamma=90
Temperature:	294 K	
	Calculated	Reported
Volume	2995.5(6)	2995.6(6)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C32 H30 Co N O4 Sn	C32 H30 Co N O4 Sn
Sum formula	C32 H30 Co N O4 Sn	C32 H30 Co N O4 Sn
Mr	670.21	670.19
Dx, g cm <sup>-3</sup>	1.486	1.486
Z	4	4
Mu (mm <sup>-1</sup> )	1.423	1.423
F000	1352.0	1352.0
F000'	1351.24	
h,k,lmax	22,12,24	22,12,24
Nref	6682	6669
Tmin,Tmax	0.684,0.821	0.569,0.629
Tmin'	0.582	

Correction method= # Reported T Limits: Tmin=0.569 Tmax=0.629  
AbsCorr = MULTI-SCAN

Data completeness= 0.998

Theta(max)= 27.205

R(reflections)= 0.0221( 5785)

wR2(reflections)= 0.0538( 6669)

S = 1.065

Npar= 366

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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 G**

PLAT012_ALERT_1_G	No	_shelx_res_checksum Found in CIF .....	Please Check
PLAT168_ALERT_4_G	The CIF-Embedded .res File Contains EXYZ Records		1 Report
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records		1 Report
PLAT230_ALERT_2_G	Hirshfeld Test Diff for O1	--C1 .	5.0 s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Co1	--C1 .	8.8 s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Co1	--C2 .	8.7 s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Co1	--C3 .	9.1 s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Co1	--C4 .	6.9 s.u.
PLAT301_ALERT_3_G	Main Residue Disorder .....	(Resd 1 )	5% Note
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).		1 Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600		12 Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.		6 Info

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

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

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## Datablock: mo\_MosECo174\_0m\_a

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Bond precision: C-C = 0.0065 A

Wavelength=0.71073

Cell: a=11.1220(8) b=13.0137(9) c=20.5020(16)  
alpha=102.525(2) beta=100.985(2) gamma=102.511(2)

Temperature: 294 K

	Calculated	Reported
Volume	2738.8(4)	2738.8(3)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C28 H23 Co O4 S Sn	C28 H23 Co O4 S Sn
Sum formula	C28 H23 Co O4 S Sn	C28 H23 Co O4 S Sn
Mr	633.16	633.14
Dx,g cm-3	1.536	1.536
Z	4	4
Mu (mm-1)	1.624	1.624
F000	1264.0	1264.0
F000'	1263.70	
h,k,lmax	13,16,25	13,16,25
Nref	11248	11224
Tmin,Tmax	0.825,0.881	0.616,0.714
Tmin'	0.456	

Correction method= # Reported T Limits: Tmin=0.616 Tmax=0.714  
AbsCorr = MULTI-SCAN

Data completeness= 0.998                      Theta(max)= 26.411

R(reflections)= 0.0309( 8324)              wR2(reflections)= 0.0709( 11224)

S = 1.048                                      Npar= 696

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	3.5	Ratio
PLAT220_ALERT_2_C	NonSolvent	Resd 2	C	Ueq(max)/Ueq(min) Range	3.1	Ratio
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of		C43	Check
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of		C7	Check
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of		C13	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of		C41	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of		C5	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of		C11	Check
PLAT331_ALERT_2_C	Small Aver	Phenyl	C-C Dist	C41 --C46	.	1.37 Ang.
PLAT331_ALERT_2_C	Small Aver	Phenyl	C-C Dist	C53A --C58A	.	1.36 Ang.
PLAT331_ALERT_2_C	Small Aver	Phenyl	C-C Dist	C53B --C58B	.	1.37 Ang.
PLAT331_ALERT_2_C	Small Aver	Phenyl	C-C Dist	C11 --C16	.	1.36 Ang.
PLAT331_ALERT_2_C	Small Aver	Phenyl	C-C Dist	C23 --C28	.	1.37 Ang.
PLAT910_ALERT_3_C	Missing # of FCF	Reflection(s)	Below Theta(Min).		6	Note

### Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle	Restraints on AtSite	34	Note
PLAT012_ALERT_1_G	No	_shelx_res_checksum Found in CIF	.....	Please Check
PLAT154_ALERT_1_G	The s.u.'s on the Cell	Angles are Equal ..(Note)	0.002	Degree
PLAT168_ALERT_4_G	The CIF-Embedded .res	File Contains EXYZ Records	3	Report

PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records	14	Report
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	12	Report
PLAT173_ALERT_4_G	The CIF-Embedded .res File Contains DANG Records	10	Report
PLAT174_ALERT_4_G	The CIF-Embedded .res File Contains FLAT Records	5	Report
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Co31 --C32 .	7.3	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Co31 --C33 .	7.5	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Co1 --C2 .	7.5	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Co1 --C3 .	6.5	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Co1 --C4 .	5.4	s.u.
PLAT301_ALERT_3_G	Main Residue Disorder .....(Resd 1 )	40%	Note
PLAT410_ALERT_2_G	Short Intra H...H Contact H42 ..H54B .	2.13	Ang.
	x,y,z =	1_555	Check
PLAT411_ALERT_2_G	Short Inter H...H Contact H43 ..H55B .	1.82	Ang.
	2-x,1-y,1-z =	2_766	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C13 ..C38A	2.93	Ang.
	1+x,y,z =	1_655	Check
PLAT721_ALERT_1_G	Bond Calc 0.96000, Rep 0.97000 Dev...	0.01	Ang.
	C39A -H39D 1.555 1.555 .....	# 104	Check
PLAT721_ALERT_1_G	Bond Calc 0.97000, Rep 0.96000 Dev...	0.01	Ang.
	C40A -H40D 1.555 1.555 .....	# 106	Check
PLAT860_ALERT_3_G	Number of Least-Squares Restraints .....	74	Note
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .		Please Do !
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	21	Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	4	Info

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

5 **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  
3 **ALERT type 3** Indicator that the structure quality may be low  
6 **ALERT type 4** Improvement, methodology, query or suggestion  
0 **ALERT type 5** Informative message, check

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## Datablock: mo\_MosMCoNN\_0m\_a

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Bond precision: C-C = 0.0039 A

Wavelength=0.71073

Cell: a=11.4488(10) b=12.1620(12) c=12.7391(12)  
alpha=81.979(3) beta=67.923(3) gamma=84.949(3)

Temperature: 150 K

	Calculated	Reported
Volume	1626.4(3)	1626.4(3)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C34 H36 Co N3 O3 Sn	?
Sum formula	C34 H36 Co N3 O3 Sn	C11.33 H12 Co0.33 I0 N O S0 Sn0.33
Mr	712.30	237.43
Dx,g cm-3	1.454	1.454
Z	2	6
Mu (mm-1)	1.315	1.315
F000	724.0	724.0
F000'	723.61	
h,k,lmax	13,14,14	13,14,14
Nref	5551	5543
Tmin,Tmax	0.611,0.905	0.265,1.000
Tmin'	0.561	

Correction method= # Reported T Limits: Tmin=0.265 Tmax=1.000  
AbsCorr = MULTI-SCAN

Data completeness= 0.999

Theta(max)= 24.712

R(reflections)= 0.0218( 5116)

wR2(reflections)= 0.0530( 5543)

S = 1.060

Npar= 387

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

THETM01\_ALERT\_3\_C The value of sine(theta\_max)/wavelength is less than 0.590

Calculated sin(theta\_max)/wavelength = 0.5882

PLAT041\_ALERT\_1\_C Calc. and Reported SumFormula Strings Differ Please Check

PLAT232\_ALERT\_2\_C Hirshfeld Test Diff (M-X) Co1 --C22 . 5.7 s.u.

PLAT241\_ALERT\_2\_C High 'MainMol' Ueq as Compared to Neighbors of C12 Check

PLAT910\_ALERT\_3\_C Missing # of FCF Reflection(s) Below Theta(Min). 6 Note

PLAT911\_ALERT\_3\_C Missing FCF Refl Between Thmin & STh/L= 0.588 2 Report



#### Alert level G

CELLZ01\_ALERT\_1\_G Difference between formula and atom\_site contents detected.

CELLZ01\_ALERT\_1\_G ALERT: Large difference may be due to a

symmetry error - see SYMMG tests

From the CIF: \_cell\_formula\_units\_Z 6

From the CIF: \_chemical\_formula\_sum C11.33 H12 Co0.33 I0 N O S0 Sn0.33

TEST: Compare cell contents of formula and atom\_site data

atom	Z*formula	cif sites	diff
C	67.98	68.00	-0.02
H	72.00	72.00	0.00

Co	1.98	2.00	-0.02	
I	6.00	0.00	6.00	
N	6.00	6.00	0.00	
O	6.00	6.00	0.00	
S	6.00	0.00	6.00	
Sn	1.98	2.00	-0.02	

PLAT045\_ALERT\_1\_G Calculated and Reported Z Differ by a Factor ... 0.33 Check  
 PLAT154\_ALERT\_1\_G The s.u.'s on the Cell Angles are Equal ..(Note) 0.003 Degree  
 PLAT230\_ALERT\_2\_G Hirshfeld Test Diff for O1 --C1 . 5.9 s.u.  
 PLAT232\_ALERT\_2\_G Hirshfeld Test Diff (M-X) Co1 --C1 . 10.1 s.u.  
 PLAT232\_ALERT\_2\_G Hirshfeld Test Diff (M-X) Co1 --C2 . 7.1 s.u.  
 PLAT232\_ALERT\_2\_G Hirshfeld Test Diff (M-X) Co1 --C3 . 8.3 s.u.  
 PLAT380\_ALERT\_4\_G Incorrectly? Oriented X(sp2)-Methyl Moiety ..... C29 Check  
 PLAT883\_ALERT\_1\_G No Info/Value for \_atom\_sites\_solution\_primary . Please Do !  
 PLAT909\_ALERT\_3\_G Percentage of I>2sig(I) Data at Theta(Max) Still 84% Note  
 PLAT913\_ALERT\_3\_G Missing # of Very Strong Reflections in FCF .... 2 Note  
 PLAT933\_ALERT\_2\_G Number of OMIT Records in Embedded .res File ... 1 Note  
 PLAT978\_ALERT\_2\_G Number C-C Bonds with Positive Residual Density. 5 Info

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

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## Datablock: mo\_17mv\_db12\_mosn17nco\_0a

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Bond precision: C-C = 0.0088 A

Wavelength=0.71073

Cell: a=11.4801(6) b=17.7989(9) c=24.9466(13)  
 alpha=83.494(2) beta=82.941(2) gamma=89.901(2)  
 Temperature: 173 K

	Calculated	Reported
Volume	5025.8(5)	5025.8(5)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C32.90 H32.12 Co N2.11 O3 Sn, 2(C32 H31 Co N2 O3 Sn), C6 H14, C	3.03(C32 H31 Co N2 O3 Sn), C H Cl3, C6 H14
Sum formula	C103.90 H109.12 Cl3 Co3 N6.11 O9 Sn3	C103.88 H109.10 Cl3 Co3 N6.11 O9 Sn3
Mr	2226.68	2226.39
Dx, g cm <sup>-3</sup>	1.471	1.471
Z	2	2
Mu (mm <sup>-1</sup> )	1.356	1.356
F000	2258.6	2258.0
F000'	2258.29	
h,k,lmax	14,22,31	14,22,31
Nref	20577	20545
Tmin,Tmax	0.741,0.876	0.727,0.910
Tmin'	0.604	

Correction method= # Reported T Limits: Tmin=0.727 Tmax=0.910  
AbsCorr = INTEGRATION

Data completeness= 0.998                      Theta(max)= 26.372


R(reflections)= 0.0490( 17683)              wR2(reflections)= 0.1259( 20545)

S = 1.043                                      Npar= 1199

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 B**

PLAT242\_ALERT\_2\_B Low              'MainMol' Ueq as Compared to Neighbors of                      N2 Check

**Author Response: There is a large amount of disorder in the structure (especially in re**

PLAT910\_ALERT\_3\_B Missing # of FCF Reflection(s) Below Theta(Min).                      15 Note

**Author Response: These reflections were probably affected by unexpected deviations in their intensities for symmetry equivalent measurements and omitted during initial data reduction.**

PLAT971\_ALERT\_2\_B Check Calcd Resid. Dens.    0.21A    From N5                      2.89 eA-3

**Author Response: The residual density peak could not be modelled as any chemically sens**

PLAT971\_ALERT\_2\_B Check Calcd Resid. Dens. 0.16A From C11 2.51 eA-3

**Author Response: The residual density peak could not be modelled as any chemically sens**

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**Alert level C**

PLAT041_ALERT_1_C	Calc. and Reported SumFormula	Strings Differ	Please Check
PLAT077_ALERT_4_C	Unitcell Contains Non-integer Number of Atoms ..		Please Check
PLAT220_ALERT_2_C	NonSolvent Resd 1 C	Ueq(max)/Ueq(min) Range	5.0 Ratio
PLAT221_ALERT_2_C	Solv./Anion Resd 2 C	Ueq(max)/Ueq(min) Range	7.6 Ratio
PLAT222_ALERT_3_C	NonSolvent Resd 1 H	Uiso(max)/Uiso(min) Range	4.4 Ratio
PLAT223_ALERT_4_C	Solv./Anion Resd 2 H	Ueq(max)/Ueq(min) Range	7.6 Ratio
PLAT230_ALERT_2_C	Hirshfeld Test Diff for N5	--C86	5.7 s.u.
PLAT230_ALERT_2_C	Hirshfeld Test Diff for N5	--C88	6.3 s.u.
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	N5	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C29	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C30	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C86	Check

**Author Response: There is a large amount of disorder in the structure (especially in re**

PLAT242\_ALERT\_2\_C Low 'MainMol' Ueq as Compared to Neighbors of C25 Check

**Author Response: There is a large amount of disorder in the structure (especially in re**

PLAT243_ALERT_4_C	High 'Solvent' Ueq as Compared to Neighbors of	C98	Check
PLAT243_ALERT_4_C	High 'Solvent' Ueq as Compared to Neighbors of	C101	Check
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of	C99	Check
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of	C103	Check
PLAT250_ALERT_2_C	Large U3/U1 Ratio for Average U(i,j) Tensor ....	2.5	Note
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including	C97	0.128 Check
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including	C11	0.291 Check
PLAT334_ALERT_2_C	Small Aver. Benzene C-C Dist	C25 -C30	1.37 Ang.
PLAT336_ALERT_2_C	Long Bond Distance for .....	C103 -C13	1.930 Ang.
PLAT342_ALERT_3_C	Low Bond Precision on C-C Bonds .....		0.00878 Ang.
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance .....		2.655 Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.600	18 Report
PLAT918_ALERT_3_C	Reflection(s) with I(obs) much Smaller I(calc) .		3 Check
PLAT971_ALERT_2_C	Check Calcd Resid. Dens. 0.21A From C13		1.79 eA-3

**Author Response: The residual density peak could not be modelled as any chemically sens**

PLAT972_ALERT_2_C	Check Calcd Resid. Dens. 0.08A From N2	-1.67 eA-3
PLAT972_ALERT_2_C	Check Calcd Resid. Dens. 0.63A From C11	-1.62 eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on H96I	-0.33 eA-3

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**Alert level G**



FORMU01\_ALERT\_1\_G There is a discrepancy between the atom counts in the  
 \_chemical\_formula\_sum and \_chemical\_formula\_moiety. This is  
 usually due to the moiety formula being in the wrong format.  
 Atom count from \_chemical\_formula\_sum: C103.88 H109.1 Cl3 Co3 N6.11  
 Atom count from \_chemical\_formula\_moiety:C103.96 H108.93 Cl3 Co3.03 N6

FORMU01\_ALERT\_2\_G There is a discrepancy between the atom counts in the  
 \_chemical\_formula\_sum and the formula from the \_atom\_site\* data.  
 Atom count from \_chemical\_formula\_sum:C103.88 H109.1 Cl3 Co3 N6.11 O9  
 Atom count from the \_atom\_site data: C103.8959 H109.12 Cl3 Co3 N6.112

CELLZ01\_ALERT\_1\_G Difference between formula and atom\_site contents detected.  
 CELLZ01\_ALERT\_1\_G ALERT: check formula stoichiometry or atom site occupancies.  
 From the CIF: \_cell\_formula\_units\_Z 2  
 From the CIF: \_chemical\_formula\_sum C103.88 H109.10 Cl3 Co3 N6.11 O9 S  
 TEST: Compare cell contents of formula and atom\_site data

atom	Z*formula	cif sites	diff
C	207.76	207.79	-0.03
H	218.20	218.24	-0.04
Cl	6.00	6.00	0.00
Co	6.00	6.00	0.00
N	12.22	12.22	0.00
O	18.00	18.00	0.00
Sn	6.00	6.00	0.00

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	25	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	18	Report
PLAT042_ALERT_1_G	Calc. and Reported MoietyFormula Strings Differ		Please Check
PLAT068_ALERT_1_G	Reported F000 Differs from Calcd (or Missing)...		Please Check
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	20.71	Why ?
PLAT154_ALERT_1_G	The s.u.'s on the Cell Angles are Equal ..(Note)	0.002	Degree
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records	3	Report
PLAT175_ALERT_4_G	The CIF-Embedded .res File Contains SAME Records	1	Report
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains SADI Records	3	Report
PLAT177_ALERT_4_G	The CIF-Embedded .res File Contains DELU Records	2	Report
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records	2	Report
PLAT187_ALERT_4_G	The CIF-Embedded .res File Contains RIGU Records	3	Report
PLAT301_ALERT_3_G	Main Residue Disorder .....(Resd 1 )	25%	Note
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in ..... (Resd 1 )	72.13	Check
PLAT411_ALERT_2_G	Short Inter H...H Contact H26 ..H90B .	1.96	Ang.
	x,y,z =	1_555	Check
PLAT413_ALERT_2_G	Short Inter XH3 .. XHn H31A ..H96F .	2.04	Ang.
	2-x,1-y,1-z =	2_766	Check
PLAT413_ALERT_2_G	Short Inter XH3 .. XHn H32C ..H95H .	1.60	Ang.
	1-x,1-y,1-z =	2_666	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact Cl1 ..C8	3.08	Ang.
	x,y,z =	1_555	Check
PLAT802_ALERT_4_G	CIF Input Record(s) with more than 80 Characters	2	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints .....	263	Note
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .		Please Do !
PLAT913_ALERT_3_G	Missing # of Very Strong Reflections in FCF ....	1	Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...	21	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity .....	4.9	Low
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	1	Info

---

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

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

31 ALERT type 2 Indicator that the structure model may be wrong or deficient  
10 ALERT type 3 Indicator that the structure quality may be low  
14 ALERT type 4 Improvement, methodology, query or suggestion  
0 ALERT type 5 Informative message, check

---

## Datablock: mo\_17mv\_db13\_mose5ns17\_0a

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Bond precision: C-C = 0.0032 A                      Wavelength=0.71073  
Cell:                      a=12.0248(4)              b=12.6795(4)              c=17.7219(6)  
                            alpha=90                      beta=102.947(2)              gamma=90  
Temperature:              173 K

	Calculated	Reported
Volume	2633.34(15)	2633.34(15)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C28 H24 Co N O3 S Sn	C28 H24 Co N O3 S Sn
Sum formula	C28 H24 Co N O3 S Sn	C28 H24 Co N O3 S Sn
Mr	632.18	632.16
Dx,g cm-3	1.595	1.595
Z	4	4
Mu (mm-1)	1.687	1.687
F000	1264.0	1264.0
F000'	1263.66	
h,k,lmax	15,16,23	15,16,23
Nref	6353	6345
Tmin,Tmax	0.679,0.819	0.744,0.846
Tmin'	0.641	

Correction method= # Reported T Limits: Tmin=0.744 Tmax=0.846  
AbsCorr = INTEGRATION

Data completeness= 0.999                      Theta(max)= 27.999

R(reflections)= 0.0239( 5413)              wR2(reflections)= 0.0582( 6345)

S = 1.120                      Npar= 355

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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

PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min).	8 Note
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) .	1 Check
PLAT934_ALERT_3_C Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers ..	1 Check

---

## ● 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 Uij Restrained non-H Atoms ...	9	Report
PLAT175_ALERT_4_G	The CIF-Embedded .res File Contains SAME Records	1	Report
PLAT177_ALERT_4_G	The CIF-Embedded .res File Contains DELU Records	2	Report
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records	2	Report
PLAT230_ALERT_2_G	Hirshfeld Test Diff for O3 --C3 .	5.3	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Co1 --C1 .	9.0	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Co1 --C2 .	8.5	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Co1 --C3 .	9.2	s.u.
PLAT301_ALERT_3_G	Main Residue Disorder .....(Resd 1 )	11%	Note
PLAT860_ALERT_3_G	Number of Least-Squares Restraints .....	80	Note
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .		Please Do !
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	4	Info

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

1 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  
5 ALERT type 3 Indicator that the structure quality may be low  
3 ALERT type 4 Improvement, methodology, query or suggestion  
0 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.

PLATON version of 05/12/2020; check.def file version of 05/12/2020

Datablock mo\_Mos17Co4N\_0m\_a - ellipsoid plot

