

checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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: k18c6cr5

Bond precision: C-C = 0.0072 A

Wavelength=0.71073

Cell: a=11.6269(2) b=21.5546(4) c=21.8560(4)
 alpha=95.633(2) beta=89.892(1) gamma=90.377(2)
Temperature: 100 K

	Calculated	Reported
Volume	5450.83(17)	5450.83(17)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C22 H44 Cr N4 Si4, C20 H40 K O8	C22 H44 Cr N4 Si4, C20 H40 K O8
Sum formula	C42 H84 Cr K N4 O8 Si4	C42 H84 Cr K N4 O8 Si4
Mr	976.59	976.59
Dx, g cm-3	1.190	1.190
Z	4	4
Mu (mm-1)	0.422	0.422
F000	2108.0	2108.0
F000'	2112.07	
h, k, lmax	14, 27, 27	14, 27, 27
Nref	23810	23726
Tmin, Tmax	0.863, 0.918	0.624, 0.848
Tmin'	0.863	

Correction method= # Reported T Limits: Tmin=0.624 Tmax=0.848
AbsCorr = NUMERICAL

Data completeness= 0.996

Theta(max)= 27.000

R(reflections)= 0.0563(20467)

wR2(reflections)= 0.1502(23726)

S = 1.075

Npar= 1112

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**

PLAT155_ALERT_4_C	The Triclinic Unitcell is NOT Reduced	Please Do !
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	001V Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	0013 Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C03B Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	0017 Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C03A Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	Si2A Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	Si2B Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	K003 Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	K005 Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C02T Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	K006 Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C01M Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C03C Check
PLAT341_ALERT_3_C	Low Bond Precision on C-C Bonds	0.00721 Ang.
PLAT360_ALERT_2_C	Short C(sp3)-C(sp3) Bond C03A - C03C .	1.43 Ang.

 **Alert level G**

PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	12.47 Why ?
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	139 Note
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #	2 Note
	C22 H44 Cr N4 Si4	
PLAT794_ALERT_5_G	Tentative Bond Valency for Cr1A (II) .	1.93 Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Cr1B (II) .	1.92 Info
PLAT870_ALERT_4_G	ALERTS Related to Twinning Effects Suppressed ..	! Info

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

- 0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
15 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
4 ALERT type 4 Improvement, methodology, query or suggestion
2 ALERT type 5 Informative message, check
-
-

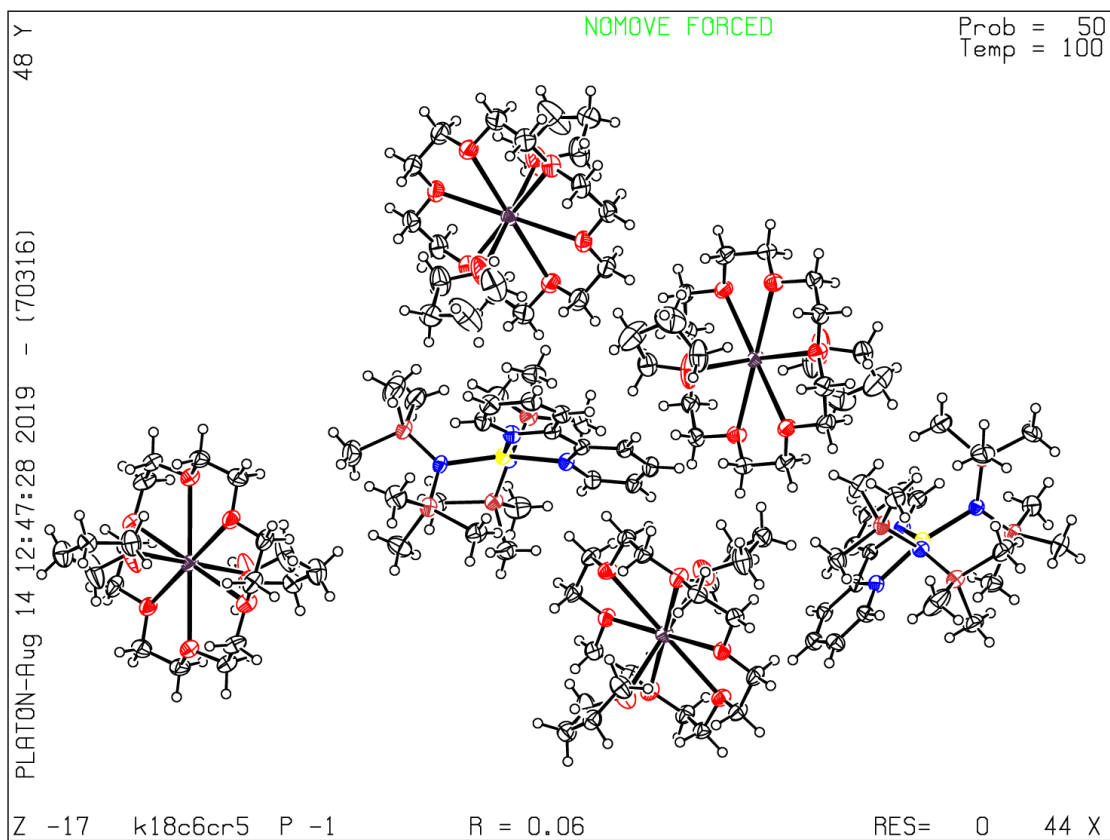
It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious 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.



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No syntax errors found. CIF dictionary Interpreting this report

Datablock: k18c6mn6

Bond precision:	C-C = 0.0085 A	Wavelength=0.71073
Cell:	a=34.8403 (17)	b=18.4715 (11) c=14.5302 (8)
	alpha=90	beta=96.555 (4) gamma=90
Temperature:	150 K	
	Calculated	Reported
Volume	9289.8 (9)	9289.8 (9)
Space group	C 2	C 1 2 1
Hall group	C 2y	C 2y
Moiety formula	C12 H24 K O6, C22 H44 Mn N4 Si4	0.25(C124 H248 K3 Mn4 N16 O18 Si16), 0.25(C12 H24 K O6)
Sum formula	C34 H68 K Mn N4 O6 Si4	C34 H68 K Mn N4 O6 Si4
Mr	835.32	835.32
Dx, g cm ⁻³	1.194	1.194
Z	8	8
Mu (mm ⁻¹)	0.518	0.518
F000	3584.0	3584.0
F000'	3591.94	
h, k, lmax	45, 24, 18	45, 24, 18
Nref	21359 [11012]	21354
Tmin, Tmax	0.894, 0.964	0.789, 0.976
Tmin'	0.869	

Correction method= # Reported T Limits: Tmin=0.789 Tmax=0.976
AbsCorr = NUMERICAL

Data completeness= 1.94/1.00 Theta (max)= 27.499

R(reflections)= 0.0368 (16849) wR2(reflections)= 0.0786 (21354)

S = 0.911 Npar= 1270

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

PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density	3.90	Report
PLAT215_ALERT_3_C	Disordered C19# has ADP max/min Ratio	3.5	Note
PLAT215_ALERT_3_C	Disordered C20# has ADP max/min Ratio	3.8	Note
PLAT220_ALERT_2_C	Non-Solvent Resd 4 C Ueq(max)/Ueq(min) Range	3.3	Ratio
PLAT230_ALERT_2_C	Hirshfeld Test Diff for O00N --C01W .	5.5	s.u.
PLAT234_ALERT_4_C	Large Hirshfeld Difference Si2B --C2 .	0.18	Ang.
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C3B	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C8B	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C022	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	K005	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	Si1B	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	Si2B	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	Si3B	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	Si1A	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	Si3A	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	Si4A	Check
PLAT341_ALERT_3_C	Low Bond Precision on C-C Bonds	0.00854	Ang.



Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	54	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	54	Report
PLAT033_ALERT_4_G	Flack x Value Deviates > 3.0 * sigma from Zero .	0.086	Note
PLAT042_ALERT_1_G	Calc. and Reported MoietyFormula Strings Differ	Please	Check
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records	2	Report
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	1	Report
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains SADI Records	2	Report
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records	1	Report
PLAT186_ALERT_4_G	The CIF-Embedded .res File Contains ISOR Records	1	Report
PLAT187_ALERT_4_G	The CIF-Embedded .res File Contains RIGU Records	1	Report
PLAT300_ALERT_4_G	Atom Site Occupancy of O1_1 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of O2_1 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of O3_1 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of O4_1 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of O5_1 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of O6_1 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C1_1 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C2_1 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C3_1 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C4_1 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C5_1 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C6_1 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C7_1 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C8_1 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C9_1 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C10_1 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C11_1 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C12_1 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H1A_1 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H1B_1 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H2A_1 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H2B_1 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H3A_1 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H3B_1 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H4A_1 Constrained at	0.5	Check

PLAT300_ALERT_4_G	Atom Site Occupancy of H4B_1	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H5A_1	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H5B_1	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H6A_1	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H6B_1	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H7A_1	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H7B_1	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H8A_1	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H8B_1	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H9A_1	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H9B_1	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H10A_1	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H10B_1	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H11A_1	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H11B_1	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H12A_1	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H12B_1	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C21B	Constrained at	0.8	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C22B	Constrained at	0.8	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C23B	Constrained at	0.8	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C2	Constrained at	0.2	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C3	Constrained at	0.2	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C9	Constrained at	0.2	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H21A	Constrained at	0.8	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H21B	Constrained at	0.8	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H21C	Constrained at	0.8	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H22A	Constrained at	0.8	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H22B	Constrained at	0.8	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H22C	Constrained at	0.8	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H23A	Constrained at	0.8	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H23B	Constrained at	0.8	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H23C	Constrained at	0.8	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H2A	Constrained at	0.2	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H2C	Constrained at	0.2	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H2D	Constrained at	0.2	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H3A	Constrained at	0.2	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H3C	Constrained at	0.2	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H3D	Constrained at	0.2	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H9A	Constrained at	0.2	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H9C	Constrained at	0.2	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H9D	Constrained at	0.2	Check
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)		95%	Note
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 2)		95%	Note
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 3)		10%	Note
PLAT412_ALERT_2_G	Short Intra XH3 .. XHn H19B ..H9D .		1.90	Ang.
	x,y,z =	1_555		Check
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels		179	Note
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF . #		246	Check
	O3_1 -C5_1 -K005 1.555 1.555 1.555		44.40	Deg.
PLAT789_ALERT_4_G	Atoms with Negative _atom_site_disorder_group #		126	Check
PLAT794_ALERT_5_G	Tentative Bond Valency for Mn0A (II) .		1.98	Info
PLAT811_ALERT_5_G	No ADDSYM Analysis: Too Many Excluded Atoms			! Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints		1546	Note
PLAT870_ALERT_4_G	ALERTS Related to Twinning Effects Suppressed ..			! Info

0 **ALERT level A** = Most likely a serious problem - resolve or explain
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1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

16 ALERT type 2 Indicator that the structure model may be wrong or deficient
7 ALERT type 3 Indicator that the structure quality may be low
78 ALERT type 4 Improvement, methodology, query or suggestion
2 ALERT type 5 Informative message, check

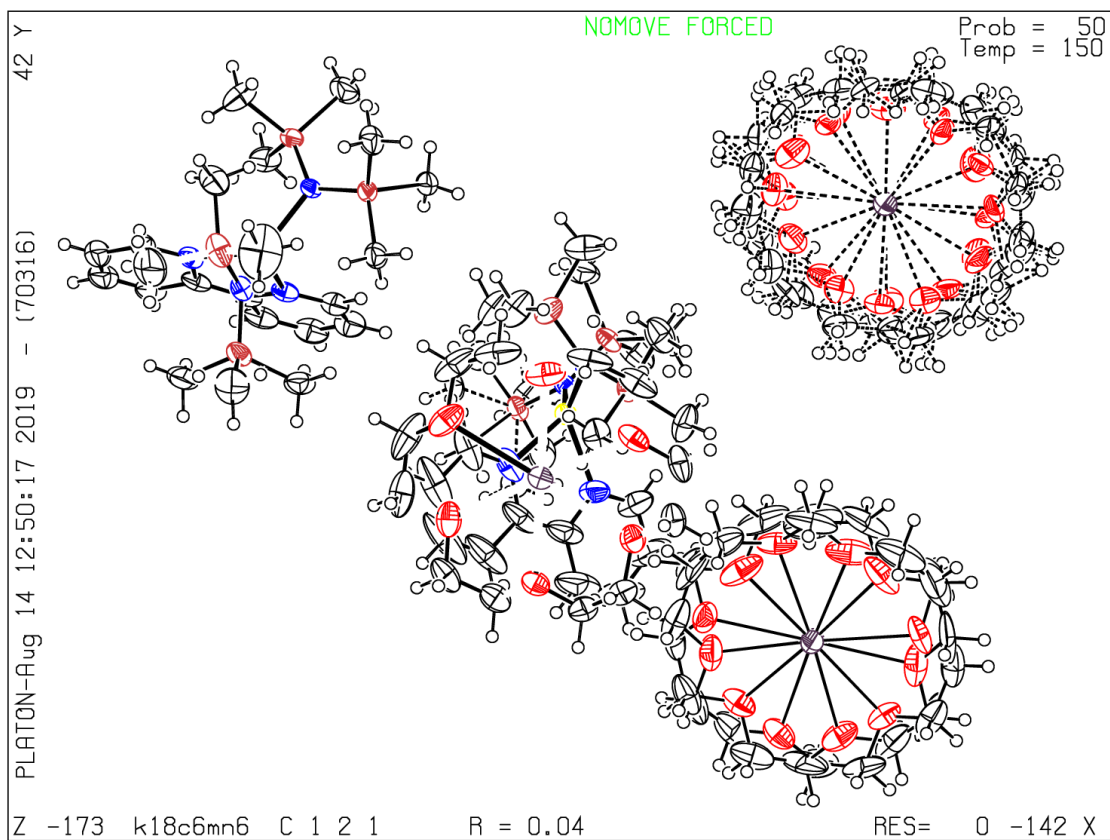
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No syntax errors found. CIF dictionary Interpreting this report

Datablock: k18c6fe7

Bond precision: C-C = 0.0020 A

Wavelength=0.71073

Cell: a=10.8613(5) b=13.2627(6) c=19.8669(9)
 alpha=77.597(1) beta=80.062(2) gamma=83.452(2)
Temperature: 100 K

	Calculated	Reported
Volume	2744.3(2)	2744.3(2)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C20 H40 K O8, C22 H44 Fe N4 Si4	C22 H44 Fe N4 Si4, 2(C10 H20 K0.5 O4)
Sum formula	C42 H84 Fe K N4 O8 Si4	C42 H84 Fe K N4 O8 Si4
Mr	980.44	980.44
Dx, g cm-3	1.186	1.187
Z	2	2
Mu (mm-1)	0.485	0.485
F000	1058.0	1058.0
F000'	1060.08	
h, k, lmax	14, 17, 25	14, 17, 25
Nref	12672	12642
Tmin, Tmax	0.903, 0.948	0.900, 0.950
Tmin'	0.903	

Correction method= # Reported T Limits: Tmin=0.900 Tmax=0.950
AbsCorr = MULTISCAN

Data completeness= 0.998

Theta(max)= 27.562

R(reflections)= 0.0280(10773)

wR2(reflections)= 0.0675(12642)

S = 1.060

Npar= 648

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

PLAT213_ALERT_2_C	Atom C3S	has ADP max/min Ratio	3.4	oblate
PLAT230_ALERT_2_C	Hirshfeld Test Diff for	Si3 --C31 .	5.4	s.u.
PLAT230_ALERT_2_C	Hirshfeld Test Diff for	Si3 --C33 .	5.9	s.u.



Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	20	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	20	Report
PLAT042_ALERT_1_G	Calc. and Reported MoietyFormula Strings Differ	Please	Check
PLAT066_ALERT_1_G	Predicted and Reported Tmin&Tmax Range Identical	?	Check
PLAT175_ALERT_4_G	The CIF-Embedded .res File Contains SAME Records	2	Report
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records	2	Report
PLAT186_ALERT_4_G	The CIF-Embedded .res File Contains ISOR Records	2	Report
PLAT187_ALERT_4_G	The CIF-Embedded .res File Contains RIGU Records	2	Report
PLAT230_ALERT_2_G	Hirshfeld Test Diff for	C2SA --C3SA .	7.0 s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Fe1 --N2 .	6.6 s.u.
PLAT301_ALERT_3_G	Main Residue Disorder	(Resd 1)	34% Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2)		34% Note
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	71	Note
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF . #	339	Check
	O1S -C2S -K2	1.555 1.555 1.555	44.20 Deg.
PLAT794_ALERT_5_G	Tentative Bond Valency for Fe1 (II)	.	1.90 Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	560	Note
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .		Please Do !
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...	2	Note

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 7 ALERT type 4 Improvement, methodology, query or suggestion
 1 ALERT type 5 Informative message, check

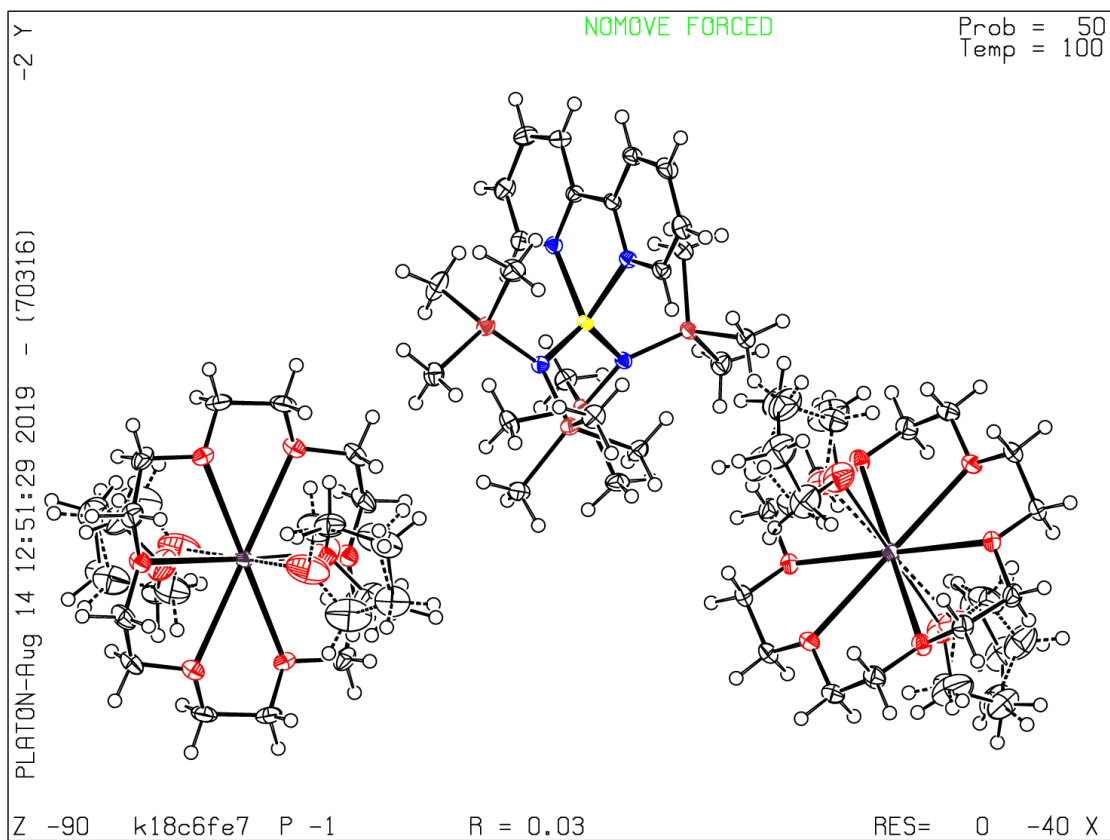
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checkCIF/PLATON report

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No syntax errors found. CIF dictionary Interpreting this report

Datablock: k18c6co8

Bond precision: C-C = 0.0034 Å

Wavelength=0.71073

Cell: a=10.8097(5) b=13.2648(6) c=19.9051(10)
 alpha=77.712(2) beta=80.199(2) gamma=83.606(2)
Temperature: 100 K

	Calculated	Reported
Volume	2739.7(2)	2739.7(2)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C20 H40 K O8, C22 H44 Co N4 Si4	C22 H44 Co N4 Si4, 2(C10 H20 K0.5 O4)
Sum formula	C42 H84 Co K N4 O8 Si4	C42 H84 Co K N4 O8 Si4
Mr	983.52	983.52
Dx, g cm ⁻³	1.192	1.192
Z	2	2
Mu (mm ⁻¹)	0.524	0.524
F000	1060.0	1060.0
F000'	1062.08	
h, k, lmax	14, 17, 25	14, 17, 25
Nref	12595	12549
Tmin, Tmax	0.916, 0.964	0.704, 0.746
Tmin'	0.886	

Correction method= # Reported T Limits: Tmin=0.704 Tmax=0.746
AbsCorr = MULTISCAN

Data completeness= 0.996

Theta(max)= 27.529

R(reflections)= 0.0420(9015)

wR2(reflections)= 0.0830(12549)

S = 1.017

Npar= 584

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	Non-Solvent	Resd 3	C	Ueq(max)/Ueq(min)	Range	3.6	Ratio
PLAT230_ALERT_2_C	Hirshfeld Test	Diff for	Si21	--C212	.	5.2	s.u.
PLAT230_ALERT_2_C	Hirshfeld Test	Diff for	Si22	--C222	.	5.2	s.u.
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to	Neighbors of		O300	Check
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to	Neighbors of		C303	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to	Neighbors of		K2	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to	Neighbors of		C304	Check

 **Alert level G**

PLAT003_ALERT_2_G	Number of Uiso or Uij	Restrained non-H Atoms ...	8	Report
PLAT042_ALERT_1_G	Calc. and Reported	MoietyFormula Strings Differ		Please Check
PLAT154_ALERT_1_G	The s.u.'s on the	Cell Angles are Equal ..(Note)	0.002	Degree
PLAT187_ALERT_4_G	The CIF-Embedded	.res File Contains RIGU Records	1	Report
PLAT301_ALERT_3_G	Main Residue	Disorder(Resd 1)	21%	Note
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard	Labels	20	Note
PLAT860_ALERT_3_G	Number of Least-Squares	Restraints	57	Note
PLAT883_ALERT_1_G	No Info/Value for	_atom_sites_solution_primary .		Please Do !

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0 **ALERT level B** = A potentially serious problem, consider carefully
7 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
8 **ALERT level G** = General information/check it is not something unexpected

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

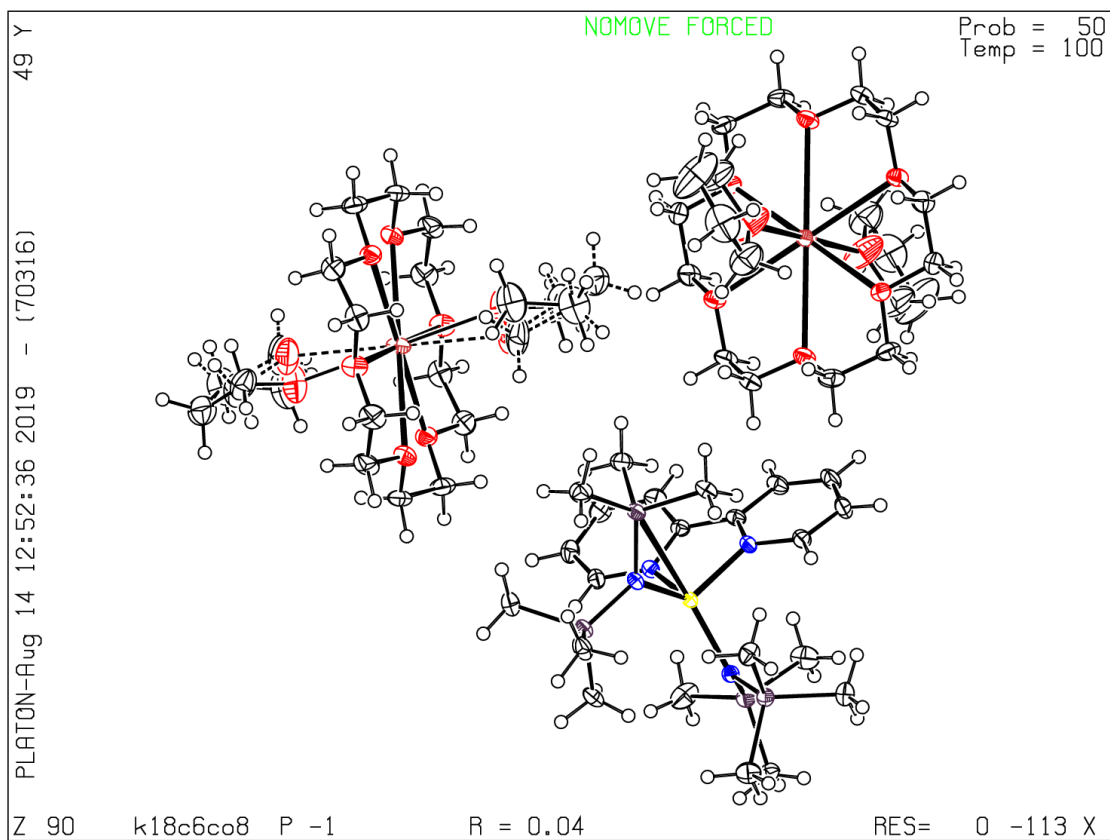
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No syntax errors found. CIF dictionary Interpreting this report

Datablock: co4

Bond precision: C-C = 0.0051 A Wavelength=0.71073

Cell: a=18.7674 (9) b=18.1030 (8) c=17.5930 (7)
 alpha=90 beta=90 gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	5977.2 (5)	5977.2 (5)
Space group	P c a 21	P c a 21
Hall group	P 2c -2ac	P 2c -2ac
Moiety formula	C22 H44 Co N4 Si4	C22 H44 Co N4 Si4
Sum formula	C22 H44 Co N4 Si4	C22 H44 Co N4 Si4
Mr	535.90	535.90
Dx, g cm ⁻³	1.191	1.191
Z	8	8
Mu (mm ⁻¹)	0.751	0.751
F000	2296.0	2296.0
F000'	2301.71	
h, k, lmax	23, 22, 21	23, 22, 21
Nref	11744 [6081]	10939
Tmin, Tmax	0.835, 0.861	0.829, 0.935
Tmin'	0.792	

Correction method= # Reported T Limits: Tmin=0.829 Tmax=0.935
AbsCorr = NUMERICAL

Data completeness= 1.80/0.93 Theta(max)= 25.999

R(reflections)= 0.0280 (10341) wR2(reflections)= 0.0679 (10939)

S = 1.014 Npar= 588

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

STRVA01_ALERT_4_C Flack test results are ambiguous.
From the CIF: `_refine_ls_abs_structure_Flack` 0.495
From the CIF: `_refine_ls_abs_structure_Flack_su` 0.010

Alert level G

PLAT164_ALERT_4_G Nr. of Refined C-H H-Atoms in Heavy-Atom Struct. 1 Note
PLAT870_ALERT_4_G ALERTS Related to Twinning Effects Suppressed .. ! Info

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 - 0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 - 0 ALERT type 2 Indicator that the structure model may be wrong or deficient
 - 0 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
-
-

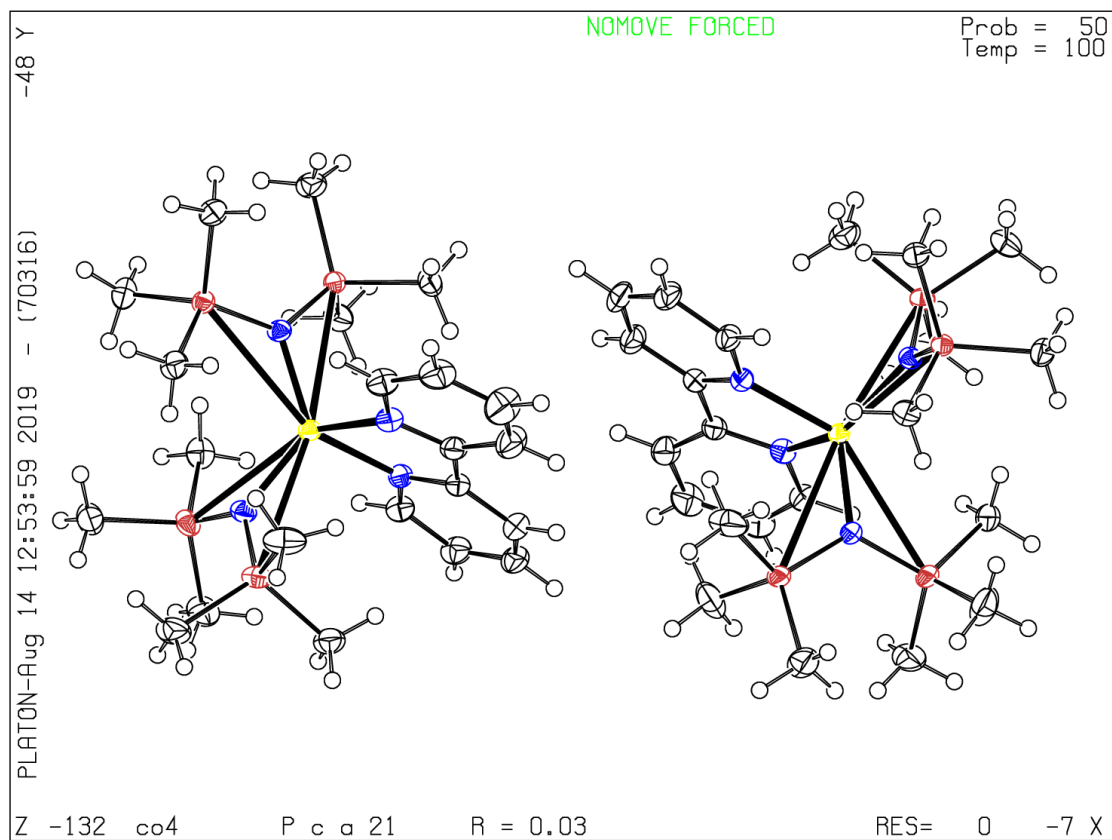
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No syntax errors found. CIF dictionary Interpreting this report

Datablock: zn9

Bond precision: C-C = 0.0072 Å Wavelength=0.71073

Cell: a=18.8806(12) b=18.0560(13) c=17.6133(17)
 alpha=90 beta=90 gamma=90

Temperature: 100 K

	Calculated	Reported
Volume	6004.5(8)	6004.5(8)
Space group	P c a 21	P c a 21
Hall group	P 2c -2ac	P 2c -2ac
Moiety formula	C22 H44 N4 Si4 Zn	2(C22 H44 N4 Si4 Zn)
Sum formula	C22 H44 N4 Si4 Zn	C44 H88 N8 Si8 Zn2
Mr	542.36	1084.68
Dx, g cm ⁻³	1.200	1.200
Z	8	4
Mu (mm ⁻¹)	0.994	0.994
F000	2320.0	2320.0
F000'	2325.18	
h, k, lmax	23, 22, 21	23, 22, 21
Nref	11796[6108]	11789
Tmin, Tmax		0.873, 0.874
Tmin'		

Correction method= # Reported T Limits: Tmin=0.873 Tmax=0.874
AbsCorr = SPHERE

Data completeness= 1.93/1.00 Theta(max)= 25.998

R(reflections)= 0.0340(9936) wR2(reflections)= 0.0718(11789)

S = 0.969 Npar= 584

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

PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density 2.70 Report
 PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds 0.00722 Ang.



Alert level G

PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ Please Check
 PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ... 2.00 Check
 PLAT794_ALERT_5_G Tentative Bond Valency for Zn1 (II) . 1.69 Info
 PLAT794_ALERT_5_G Tentative Bond Valency for Zn2 (II) . 1.67 Info
 PLAT870_ALERT_4_G ALERTS Related to Twinning Effects Suppressed .. ! Info

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

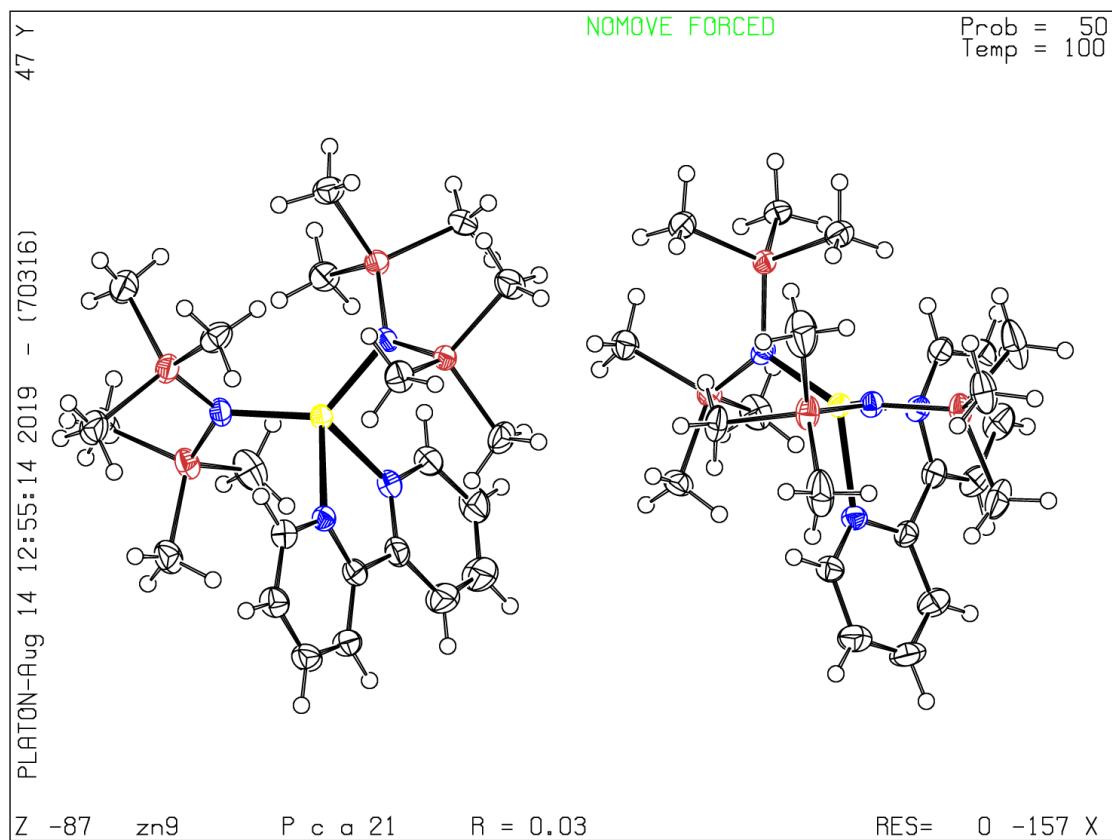
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No syntax errors found. CIF dictionary Interpreting this report

Datablock: k18c6zn10

Bond precision: Si- C = 0.0135 A Wavelength=0.71073

Cell: a=12.1899(7) b=18.4365(10) c=22.8273(13)
 alpha=90 beta=95.423(2) gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	5107.2(5)	5107.2(5)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C22 H44 N4 Si4 Zn, C16 H34 K O7	C22 H44 N4 Si4 Zn, C16 H34 K O7
Sum formula	C38 H78 K N4 O7 Si4 Zn	C38 H78 K N4 O7 Si4 Zn
Mr	919.90	919.87
Dx, g cm-3	1.196	1.196
Z	4	4
Mu (mm-1)	0.700	0.700
F000	1980.0	1980.0
F000'	1983.82	
h, k, lmax	14, 21, 27	14, 21, 27
Nref	8993	8987
Tmin, Tmax	0.732, 0.900	0.665, 0.745
Tmin'	0.702	

Correction method= # Reported T Limits: Tmin=0.665 Tmax=0.745
AbsCorr = MULTII-SCAN

Data completeness= 0.999 Theta(max)= 24.999

R(reflections)= 0.1281(7347) wR2(reflections)= 0.2596(8987)

S = 1.086 Npar= 693

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

PLAT082_ALERT_2_C	High R1 Value	0.13	Report
PLAT084_ALERT_3_C	High wR2 Value (i.e. > 0.25)	0.26	Report
PLAT220_ALERT_2_C	Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range	3.9	Ratio
PLAT222_ALERT_3_C	Non-Solv. Resd 1 H Uiso(max)/Uiso(min) Range	4.9	Ratio
PLAT230_ALERT_2_C	Hirshfeld Test Diff for Si1 --C21 .	6.8	s.u.
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of Si1	Check	
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of K1	Check	



Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	91	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	79	Report
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	100.83	Why ?
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records	20	Report
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	1	Report
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains SADI Records	70	Report
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records	9	Report
PLAT186_ALERT_4_G	The CIF-Embedded .res File Contains ISOR Records	11	Report
PLAT187_ALERT_4_G	The CIF-Embedded .res File Contains RIGU Records	9	Report
PLAT230_ALERT_2_G	Hirshfeld Test Diff for Si3A --N4 .	6.0	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Zn1 --N1A .	6.0	s.u.
PLAT300_ALERT_4_G	Atom Site Occupancy of Si3 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Si3A Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Si6 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Si6A Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of N1 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of N1A Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of N2 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of N2A Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C1 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C1A Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C2 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C2A Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C3 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C3A Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C4 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C4A Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C5 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C5A Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C6 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C6A Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C7 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C7A Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C8 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C8A Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C9 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C9A Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C10 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C10A Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C19 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C20 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C23 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C23A Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C24 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C24A Constrained at	0.5	Check

[illegible]

[illegible]

[illegible]

PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF . #	204	Check
K1	-C34 -H34A 1.555 1.555 1.555	31.20	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF . #	319	Check
O3	-C62 -K1 1.555 1.555 1.555	41.60	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF . #	365	Check
O13	-C40 -K1 1.555 1.555 1.555	41.20	Deg.
PLAT789_ALERT_4_G	Atoms with Negative _atom_site_disorder_group #	26	Check
PLAT811_ALERT_5_G	No ADDSYM Analysis: Too Many Excluded Atoms		! Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	1954	Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...	1	Note

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 7 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
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0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 13 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
 225 ALERT type 4 Improvement, methodology, query or suggestion
 1 ALERT type 5 Informative message, check

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