checkCIF (basic structural check) running

Checking for embedded fcf data in CIF ...
Found embedded fcf data in CIF. Extracting fcf data from uploaded CIF, please wait . . . . . .

checkCIF/PLATON (basic structural check)

Structure factors have been supplied for datablock(s) Pd4Si3CNtBu4

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.
Please wait while processing ....

CIF dictionary
Interpreting this report

Structure factor report

Datablock: Pd4Si3CNtBu4

Bond precision: C-C = 0.0075 A Wavelength=0.71075
Cell: a=10.8179(6) b=22.0783(12) c=22.8654(12)
alpha=90 beta=92.1391(12) gamma=90
Temperature: 193 K

	Calculated	Reported
Volume	5457.4(5)	5457.4(5)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	2(C38 H78 N4 Pd4 Si3), C7	C38 H78 N4 Pd4 Si3
Sum formula	C83 H156 N8 Pd8 Si6	C38 H78 N4 Pd4 Si3
Mr	2285.91	1100.92
Dx,g cm-3	1.391	1.340
Z	2	4
Mu (mm-1)	1.391	1.389
F000	2324.0	2240.0
F000'	2309.46	
h,k,lmax	14,28,29	14,28,29
Nref	12544	12489
Tmin,Tmax	0.846,0.895	0.784,0.895
Tmin'	0.812	

Correction method= # Reported T Limits: Tmin=0.784
Tmax=0.895 AbsCorr = MULTI-SCAN
Data completeness= 0.996 Theta(max)= 27.520
R(reflections)= 0.0516(11907) wR2(reflections)= 0.1518(12489)
S = 1.101 Npar= 470

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

PLAT043_ALERT_1_B	Calculated and Reported Mol. Weight Differ by ..	84.07	Check
PLAT910_ALERT_3_B	Missing # of FCF Reflection(s) Below Theta(Min).	18	Note
PLAT934_ALERT_3_B	Number of (Iobs-Icalc)/SigmaW > 10 Outliers	5	Check
PLAT973_ALERT_2_B	Check Calcd Positive Residual Density on Pd4	1.90	eA-3
PLAT973_ALERT_2_B	Check Calcd Positive Residual Density on Pd3	1.89	eA-3

Alert level C

CHEMW03_ALERT_2_C The ratio of given/expected molecular weight as
calculated from the _atom_site* data lies outside
the range 0.99 <> 1.01
From the CIF: _cell_formula_units_Z 4
From the CIF: _chemical_formula_weight 1100.92
TEST: Calculate formula weight from _atom_site_*

atom	mass	num	sum
C	12.01	41.50	498.46
H	1.01	78.00	78.62
N	14.01	4.00	56.03
Pd	106.42	4.00	425.68
Si	28.09	3.00	84.26

Calculated formula weight 1143.05

PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ Please Check
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)... Please Check
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density .... 2.84 Report
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C7 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C17 Check
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ..... 2.984 Check
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L= 0.600 6 Report
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) . 6 Check
PLAT971_ALERT_2_C Check Calcd Residual Density 0.67A From C40 2.36 eA-3
And 7 other PLAT971 Alerts

PLAT971_ALERT_2_C Check Calcd Residual Density 0.82A From C42 2.10 eA-3
PLAT971_ALERT_2_C Check Calcd Residual Density 0.82A From C44 2.10 eA-3
PLAT971_ALERT_2_C Check Calcd Residual Density 0.62A From C40 2.06 eA-3
PLAT971_ALERT_2_C Check Calcd Residual Density 0.48A From C44 1.83 eA-3
PLAT971_ALERT_2_C Check Calcd Residual Density 0.85A From C42 1.77 eA-3
PLAT971_ALERT_2_C Check Calcd Residual Density 0.79A From C45 1.63 eA-3
PLAT971_ALERT_2_C Check Calcd Residual Density 0.76A From C45 1.56 eA-3

PLAT973_ALERT_2_C Check Calcd Positive Residual Density on Pd1 1.41 eA-3
PLAT973_ALERT_2_C Check Calcd Positive Residual Density on Pd2 1.32 eA-3

Alert level G

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:C38 H78 N4 Pd4 Si3
Atom count from the _atom_site data: C41.5 H78 N4 Pd4 Si3
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 4
From the CIF: _chemical_formula_sum C38 H78 N4 Pd4 Si3
TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
C	152.00	166.00	-14.00
H	312.00	312.00	0.00
N	16.00	16.00	0.00
Pd	16.00	16.00	0.00
Si	12.00	12.00	0.00

CHEMS02_ALERT_1_G Please check that you have entered the correct
_publ_requested_category classification of your compound;
FI or CI or EI for inorganic; FM or CM or EM for metal-organic;
FO or CO or EO for organic.
From the CIF: _publ_requested_category CHOOSE FI FM FO CI CM CO or
From the CIF: _chemical_formula_sum:C38 H78 N4 Pd4 Si3
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ Please Check
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ... 0.50 Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 13.00 Why ?
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Pd2 -- Si1 .. 5.2 s.u.
PLAT300_ALERT_4_G Atom Site Occupancy of C39 is Constrained at 0.5 Check
And 6 other PLAT300 Alerts

PLAT300_ALERT_4_G Atom Site Occupancy of C40 is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C41 is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C42 is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C43 is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C44 is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C45 is Constrained at 0.5 Check

PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 2).. 100% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms (3.50) in Resd. # 2 Check
PLAT882_ALERT_1_G Missing datum for _diffrn_reflns_av_unetI/netI . Please Check
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 31 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF .... 1 Note

PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 2 Info

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

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

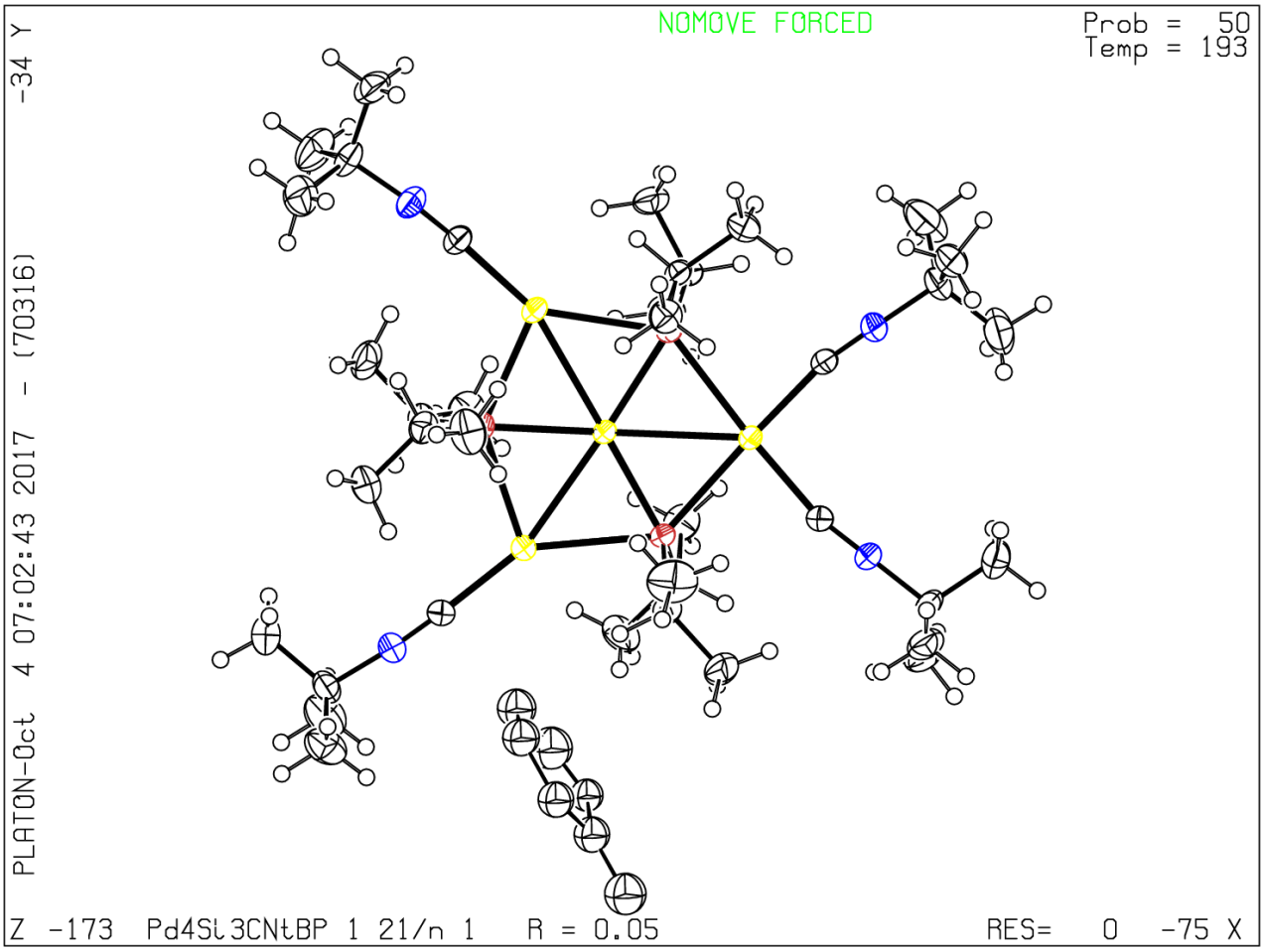
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section 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.

PLATON version of 13/08/2017; check.def file version of 27/07/2017

Datablock Pd4Si3CNtBu4 - ellipsoid plot



Download CIF editor (publCIF) from the IUCr
Download CIF editor (enCIFer) from the CCDC
Test a new CIF entry

checkCIF (basic structural check) running

Checking for embedded fcf data in CIF ...
Found embedded fcf data in CIF. Extracting fcf data from uploaded CIF, please wait . . . .

checkCIF/PLATON (basic structural check)

Structure factors have been supplied for datablock(s) Pd4Si3NHCiPr3

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.
Please wait while processing ....

CIF dictionary
Interpreting this report

Structure factor report

Datablock: Pd4Si3NHCiPr3

Bond precision: C-C = 0.0068 A Wavelength=0.71075
Cell: a=14.505(3) b=15.339(4) c=15.655(4)
alpha=89.593(12) beta=63.724(6) gamma=81.301(11)
Temperature: 193 K

	Calculated	Reported
Volume	3080.2(13)	3080.2(13)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C51 H100 N6 Pd4 Si3	C51 H100 N6 Pd4 Si3
Sum formula	C51 H100 N6 Pd4 Si3	C51 H100 N6 Pd4 Si3
Mr	1307.25	1307.25
Dx,g cm-3	1.410	1.409
Z	2	2
Mu (mm-1)	1.243	1.243
F000	1348.0	1348.0
F000'	1340.77	
h,k,lmax	18,19,20	18,19,20
Nref	14145	14053
Tmin,Tmax	0.928,0.940	0.863,0.940
Tmin'	0.883	

Correction method= # Reported T Limits: Tmin=0.863
Tmax=0.940 AbsCorr = MULTI-SCAN
Data completeness= 0.993 Theta(max)= 27.495
R(reflections)= 0.0439(11359) wR2(reflections)= 0.1016(14053)
S = 1.076 Npar= 577

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

PLAT412_ALERT_2_B Short Intra XH3 .. XHn H5B .. H10C .. 1.79 Ang.
PLAT412_ALERT_2_B Short Intra XH3 .. XHn H8A .. H11C .. 1.77 Ang.
PLAT910_ALERT_3_B Missing # of FCF Reflection(s) Below Theta(Min). 22 Note

Alert level C

PLAT230_ALERT_2_C Hirshfeld Test Diff for C46 -- C48 .. 5.2 s.u.
PLAT412_ALERT_2_C Short Intra XH3 .. XHn H16B .. H21C .. 1.89 Ang.

```
PLAT412_ALERT_2_C Short Intra XH3 .. XHn     H31B   ..  H33C    ..       1.82 Ang.
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ......      5.205 Check
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L=  0.600         20 Report
PLAT977_ALERT_2_C Check the Negative Difference Density on    H10B      -0.32 eA-3
And 10 other PLAT977 Alerts

PLAT977_ALERT_2_C Check the Negative Difference Density on    H11A      -0.33 eA-3
PLAT977_ALERT_2_C Check the Negative Difference Density on    H11B      -0.53 eA-3
PLAT977_ALERT_2_C Check the Negative Difference Density on    H11C      -0.38 eA-3
PLAT977_ALERT_2_C Check the Negative Difference Density on    H21A      -0.48 eA-3
PLAT977_ALERT_2_C Check the Negative Difference Density on    H21B      -0.32 eA-3
PLAT977_ALERT_2_C Check the Negative Difference Density on    H21C      -0.38 eA-3
PLAT977_ALERT_2_C Check the Negative Difference Density on    H22A      -0.36 eA-3
PLAT977_ALERT_2_C Check the Negative Difference Density on    H32B      -0.36 eA-3
PLAT977_ALERT_2_C Check the Negative Difference Density on    H32C      -0.43 eA-3
PLAT977_ALERT_2_C Check the Negative Difference Density on    H33B      -0.33 eA-3

PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density.          0 Info
```

Alert level G

```
CHEMS02_ALERT_1_G  Please check that you have entered the correct
           _publ_requested_category classification of your compound;
           FI or CI or EI for inorganic; FM or CM or EM for metal-organic;
           FO or CO or EO for organic.
           From the CIF: _publ_requested_category   CHOOSE FI FM FO CI CM CO or
           From the CIF: _chemical_formula_sum:C51 H100 N6 Pd4 Si3
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Pd1    --  Si1     ..        7.4 s.u.
And 3 other PLAT232 Alerts

PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Pd1    --  Si3     ..        5.5 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Pd2    --  Si1     ..        6.6 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Pd3    --  Si2     ..        8.2 s.u.

PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for        C46 Check
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for        C49 Check
PLAT367_ALERT_2_G Long?   C(sp?)-C(sp?) Bond  C46    -   C47    ..       1.52 Ang.
And 3 other PLAT367 Alerts

PLAT367_ALERT_2_G Long?   C(sp?)-C(sp?) Bond  C46    -   C48    ..       1.54 Ang.
PLAT367_ALERT_2_G Long?   C(sp?)-C(sp?) Bond  C49    -   C50    ..       1.53 Ang.
PLAT367_ALERT_2_G Long?   C(sp?)-C(sp?) Bond  C49    -   C51    ..       1.52 Ang.

PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C32 Check
PLAT882_ALERT_1_G Missing datum for _diffrn_reflns_av_unetI/netI .     Please Check
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600         51 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....          2 Note
```

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

  2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 27 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
  2 ALERT type 4 Improvement, methodology, query or suggestion
  0 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

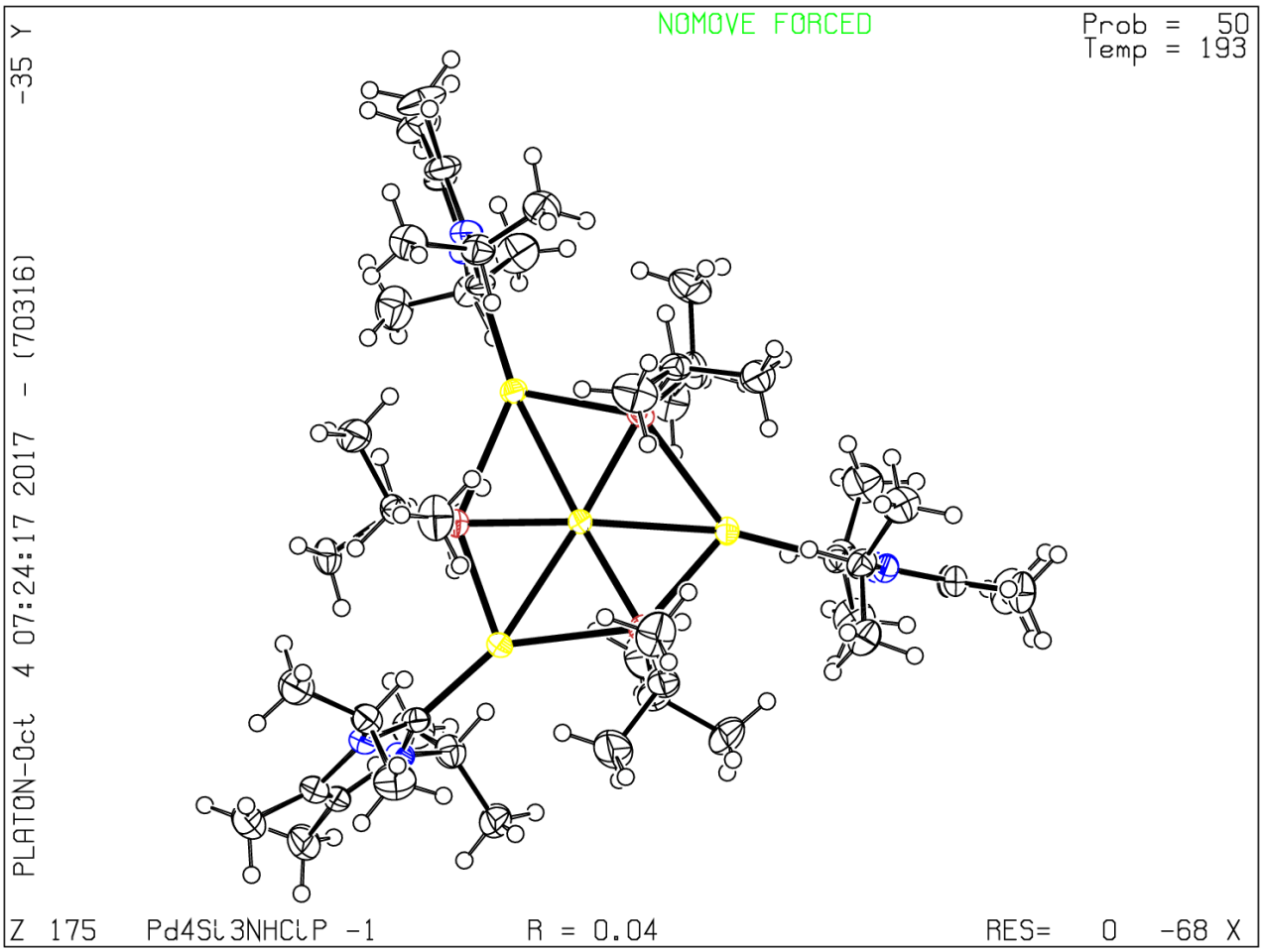
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section 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.

PLATON version of 13/08/2017; check.def file version of 27/07/2017

Datablock Pd4Si3NHCiPr3 - ellipsoid plot



Download CIF editor (publCIF) from the IUCr
Download CIF editor (enCIFer) from the CCDC
Test a new CIF entry

checkCIF (basic structural check) running

Checking for embedded fcf data in CIF ...
Found embedded fcf data in CIF. Extracting fcf data from uploaded CIF, please wait . . . .

checkCIF/PLATON (basic structural check)

Structure factors have been supplied for datablock(s) Pd4Si3POR3

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
Please wait while processing .... Interpreting this report

Structure factor report

Datablock: Pd4Si3POR3

Bond precision: C-C = 0.0059 A Wavelength=0.71075
Cell: a=11.2891(18) b=12.711(2) c=19.549(3)
alpha=81.516(6) beta=85.854(6) gamma=64.096(5)
Temperature: 103 K

	Calculated	Reported
Volume	2495.6(7)	2495.6(7)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	2(C36 H75 O9 P3 Pd3 Si3), C5	C36 H75 O9 P3 Pd3 Si3
Sum formula	C77 H150 O18 P6 Pd6 Si6	C36 H75 O9 P3 Pd3 Si3
Mr	2356.74	1148.36
Dx,g cm-3	1.568	1.528
Z	1	2
Mu (mm-1)	1.284	0.000
F000	1206.0	1176.0
F000'	1201.48	
h,k,lmax	14,16,25	14,16,25
Nref	11479	11457
Tmin,Tmax		0.834,1.000
Tmin'		

Correction method= # Reported T Limits: Tmin=0.834
Tmax=1.000 AbsCorr = MULTI-SCAN
Data completeness= 0.998 Theta(max)= 27.485
R(reflections)= 0.0370(9364) wR2(reflections)= 0.0830(11457)
S = 1.023 Npar= 507

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

PLAT043_ALERT_1_B Calculated and Reported Mol. Weight Differ by .. 60.02 Check
PLAT910_ALERT_3_B Missing # of FCF Reflection(s) Below Theta(Min). 13 Note

Alert level C

CHEMW03_ALERT_2_C The ratio of given/expected molecular weight as
calculated from the _atom_site* data lies outside
the range 0.99 <> 1.01

```
           From the CIF: _cell_formula_units_Z                   2
           From the CIF: _chemical_formula_weight          1148.36
           TEST: Calculate formula weight from _atom_site_*
           atom     mass    num     sum
           C        12.01   38.50  462.42
           H         1.01   75.00   75.60
           O        16.00    9.00  143.99
           Pd      106.42    3.00  319.26
           Si       28.09    3.00   84.26
           P        30.97    3.00   92.92
           Calculated formula weight             1178.45
PLAT041_ALERT_1_C Calc. and Reported SumFormula    Strings  Differ     Please Check
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....       2.47 Report
PLAT220_ALERT_2_C Non-Solvent Resd 1   C   Ueq(max)/Ueq(min) Range       3.2 Ratio
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ......     3.516 Check
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L=  0.600         9 Report
PLAT971_ALERT_2_C Check Calcd Residual Density  0.44A From     C37       2.02 eA-3
PLAT971_ALERT_2_C Check Calcd Residual Density  0.47A From     C37       1.77 eA-3
PLAT977_ALERT_2_C Check the Negative Difference Density on    H30C      -0.34 eA-3
```

Alert level G

```
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:C36 H75 O9 P3 Pd3 Si3
           Atom count from the _atom_site data:  C38.5 H75 O9 P3 Pd3 Si3
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    2
           From the CIF: _chemical_formula_sum  C36 H75 O9 P3 Pd3 Si3
           TEST: Compare cell contents of formula and atom_site data

           atom    Z*formula  cif sites diff
           C         72.00     77.00   -5.00
           H        150.00    150.00    0.00
           O         18.00     18.00    0.00
           P          6.00      6.00    0.00
           Pd         6.00      6.00    0.00
           Si         6.00      6.00    0.00
CHEMS02_ALERT_1_G  Please check that you have entered the correct
           _publ_requested_category classification of your compound;
           FI or CI or EI for inorganic; FM or CM or EM for metal-organic;
           FO or CO or EO for organic.
           From the CIF: _publ_requested_category   CHOOSE FI FM FO CI CM CO or
           From the CIF: _chemical_formula_sum:C36 H75 O9 P3 Pd3 Si3
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ     Please Check
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...       0.50 Check
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Pd1    --  P1      ..        8.8 s.u.
And 8 other PLAT232 Alerts

PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Pd1    --  Si1     ..        8.2 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Pd1    --  Si3     ..        6.6 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Pd2    --  P2      ..        7.6 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Pd2    --  Si1     ..        8.2 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Pd2    --  Si2     ..       10.0 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Pd3    --  P3      ..       11.0 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Pd3    --  Si2     ..        8.6 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Pd3    --  Si3     ..        7.4 s.u.

PLAT300_ALERT_4_G Atom Site Occupancy of C37     is Constrained at        0.5 Check
And 4 other PLAT300 Alerts

PLAT300_ALERT_4_G Atom Site Occupancy of C38     is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C39     is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C40     is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C41     is Constrained at        0.5 Check

PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  2)..       100% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms (   2.50) in Resd. #         2 Check
PLAT395_ALERT_2_G Deviating  X-O-Y  Angle from 120 Deg for  O1          117.3 Degree
And 8 other PLAT395 Alerts

PLAT395_ALERT_2_G Deviating  X-O-Y  Angle from 120 Deg for  O2          117.0 Degree
PLAT395_ALERT_2_G Deviating  X-O-Y  Angle from 120 Deg for  O3          115.3 Degree
PLAT395_ALERT_2_G Deviating  X-O-Y  Angle from 120 Deg for  O4          117.1 Degree
PLAT395_ALERT_2_G Deviating  X-O-Y  Angle from 120 Deg for  O5          116.5 Degree
PLAT395_ALERT_2_G Deviating  X-O-Y  Angle from 120 Deg for  O6          116.7 Degree
PLAT395_ALERT_2_G Deviating  X-O-Y  Angle from 120 Deg for  O7          116.5 Degree
```

```
PLAT395_ALERT_2_G Deviating  X-O-Y  Angle from 120 Deg for  O8          116.5 Degree
PLAT395_ALERT_2_G Deviating  X-O-Y  Angle from 120 Deg for  O9          115.8 Degree

PLAT432_ALERT_2_G Short Inter X...Y Contact  C37    ..  C41     ..       1.73 Ang.
And 10 other PLAT432 Alerts

PLAT432_ALERT_2_G Short Inter X...Y Contact  C37    ..  C40     ..       2.60 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  C38    ..  C41     ..       2.31 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  C38    ..  C39     ..       2.41 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  C38    ..  C40     ..       2.51 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  C38    ..  C38     ..       3.03 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  C39    ..  C41     ..       1.31 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  C39    ..  C40     ..       1.67 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  C39    ..  C39     ..       2.12 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  C40    ..  C40     ..       2.36 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  C40    ..  C41     ..       2.62 Ang.

PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #        101 Do !
            C40 -C38 -C39 -C41    99.00  8.00   1.555   1.555   1.555   2.577
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #        102 Do !
            C37 -C38 -C39 -C41   -84.00  8.00   1.555   1.555   1.555   2.577
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C37    --  C41     .       1.73 Ang.
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C41    --  C37     .       1.73 Ang.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        292 Check
              C39  -C37  -C38     1.555   1.555   1.555             38.20 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        301 Check
              C38  -C39  -C40     1.555   1.555   1.555             43.20 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        306 Check
              C41  -C39  -C40     2.577   1.555   2.577             41.50 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        309 Check
              C38  -C40  -C39     1.555   1.555   1.555             41.90 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        316 Check
              C39  -C41  -C37     2.577   1.555   2.577             44.80 Deg.
PLAT882_ALERT_1_G Missing datum for _diffrn_reflns_av_unetI/netI .     Please Check
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 ...         22 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          3 Info
PLAT981_ALERT_1_G No non-zero f" Anomalous Scattering Values Found     Please Check
PLAT986_ALERT_1_G No non-zero f' Anomalous Scattering Values Found     Please Check
```

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

 10 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 40 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
 14 ALERT type 4 Improvement, methodology, query or suggestion
  0 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

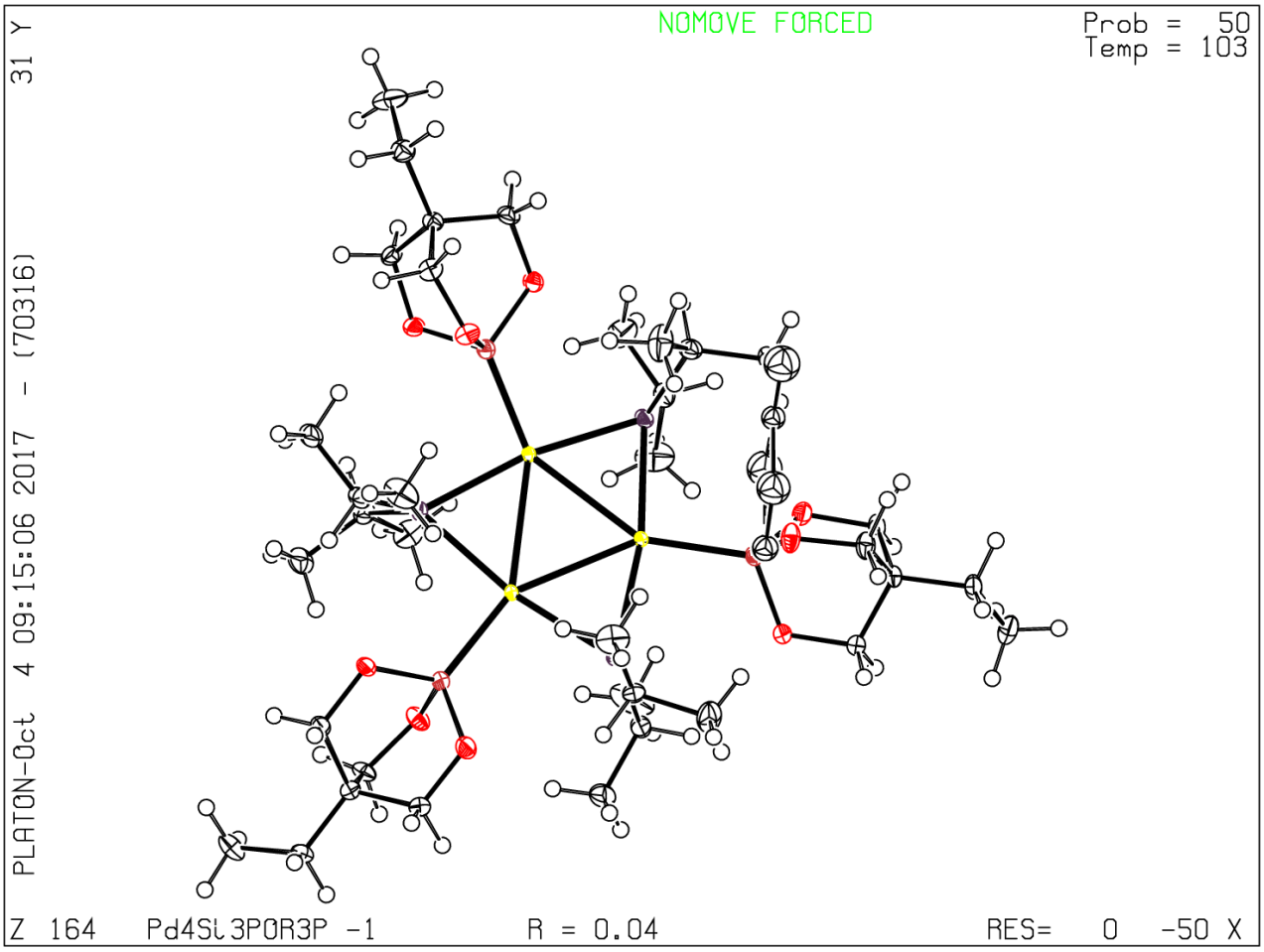
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section 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.

PLATON version of 13/08/2017; check.def file version of 27/07/2017

Datablock Pd4Si3POR3 - ellipsoid plot



Download CIF editor (publCIF) from the IUCr
Download CIF editor (enCIFer) from the CCDC
Test a new CIF entry