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: Compound1

```
Bond precision:  C-C = 0.0204 A          Wavelength=1.54183

Cell:            a=20.2893(5)     b=20.2893(5)     c=15.0224(4)
                 alpha=90         beta=90          gamma=90
Temperature:     298 K
```

	Calculated	Reported
Volume	6184.1(3)	6184.1(3)
Space group	I 41/a	I 41/a
Hall group	-I 4ad	-I 4ad
Moiety formula	C112 Fe4 N48 Nb2 O16, 4(O)	?
Sum formula	C112 Fe4 N48 Nb2 O20	C56 Fe2 N24 Nb O10
Mr	2746.82	1373.35
Dx,g cm-3	1.475	1.480
Z	2	4
Mu (mm-1)	5.855	0.000
F000	2708.0	2708.0
F000’	2706.84	
h,k,lmax	15,15,11	15,15,11
Nref	664	662
Tmin,Tmax		
Tmin’		

```
Correction method= Not given

Data completeness= 0.997          Theta(max)= 35.000

R(reflections)=                   wR2(reflections)=

S =                       Npar=
```

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

```
POWD004_ALERT_1_B No 'Bragg' R factor has been given. Please supply a value
             for _refine_ls_R_factor_all [R(F)], refine_ls_R_Fsqd_factor
             [R(F^2)] or _refine_ls_R_I_factor [R(I)].
PLAT242_ALERT_2_B Low    'MainMol' Ueq as Compared to Neighbors of        Nb1 Check
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) .......         O1 Check
PLAT342_ALERT_3_B Low Bond Precision on  C-C Bonds ...............     0.0204 Ang.
```

Alert level C

```
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of         C1 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of         C2 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        Fe1 Check
```

Alert level G

```
PLAT040_ALERT_1_G No H-atoms in this Carbon Containing Compound ..     Please Check
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...       0.50 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms ( 113.75) in Resd. #          1 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms (   0.50) in Resd. #          2 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  O1     ..  C6      ..       2.40 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  O1     ..  C6      ..       2.40 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  O1     ..  C8      ..       2.97 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  O1     ..  C8      ..       2.97 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  N5     ..  C14     ..       2.80 Ang.
PLAT794_ALERT_5_G Tentative Bond Valency for Fe1     (II)    .....       1.93 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............         68 Note
PLAT982_ALERT_1_G The  C-f'=     0.017 Deviates from the  IT-value      0.018 Check
PLAT982_ALERT_1_G The Fe-f'=    -1.187 Deviates from the  IT-value     -1.134 Check
PLAT982_ALERT_1_G The  N-f'=     0.029 Deviates from the  IT-value      0.031 Check
PLAT982_ALERT_1_G The Nb-f'=    -0.246 Deviates from the  IT-value     -0.112 Check
PLAT982_ALERT_1_G The  O-f'=     0.046 Deviates from the  IT-value      0.049 Check
PLAT983_ALERT_1_G The Fe-f"=     3.202 Deviates from the  IT-Value      3.197 Check
PLAT983_ALERT_1_G The Nb-f"=     2.485 Deviates from the  IT-Value      2.483 Check
```

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

  10 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  10 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
   1 ALERT type 5 Informative message, check
```

Datablock: Compound2

```
Bond precision:  C-C = 0.0196 A          Wavelength=1.54183

Cell:            a=20.2683(5)     b=20.2683(5)     c=15.0156(5)
                 alpha=90         beta=90          gamma=90
Temperature:     298 K
```

	Calculated	Reported
Volume	6168.5(4)	6168.5(3)
Space group	I 41/a	I 41/a
Hall group	-I 4ad	-I 4ad
Moiety formula	C224 Co0.64 Fe7.36 N96 Nb4 O32, 8(O)	?
Sum formula	C224 Co0.64 Fe7.36 N96 Nb4 O40	C56 Co0.16 Fe1.84 N24 Nb O10
Mr	5495.61	1373.84
Dx,g cm-3	1.479	1.480
Z	1	4
Mu (mm-1)	5.906	0.000
F000	2708.6	2708.6
F000’	2706.69	
h,k,lmax	15,15,11	15,15,11
Nref	663	662
Tmin,Tmax		
Tmin’		

Correction method= Not given

Data completeness= 0.998 Theta(max)= 35.000

R(reflections)= wR2(reflections)=

S = Npar=

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

POWD004_ALERT_1_B No ’Bragg’ R factor has been given. Please supply a value for _refine_ls_R_factor_all [R(F)], refine_ls_R_Fsqd_factor [R(F^2)] or _refine_ls_R_I_factor [R(I)].
PLAT242_ALERT_2_B Low ’MainMol’ Ueq as Compared to Neighbors of Nb1 Check
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) ..... O1 Check

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Alert level C

PLAT077_ALERT_4_C Unitcell contains non-integer number of atoms .. Please Check
PLAT241_ALERT_2_C High ’MainMol’ Ueq as Compared to Neighbors of C1 Check
PLAT241_ALERT_2_C High ’MainMol’ Ueq as Compared to Neighbors of C2 Check
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.0196 Ang.

Alert level G

PLAT040_ALERT_1_G No H-atoms in this Carbon Containing Compound .. Please Check
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ... 0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Fe1 is Constrained at 0.92 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Co1 is Constrained at 0.08 Check
PLAT301_ALERT_3_G Main Residue Disorder .....(Resd 1).. 3% Note

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PLAT304_ALERT_4_G Non-Integer Number of Atoms ( 113.75) in Resd. #          1 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms (   0.50) in Resd. #          2 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  O1     ..  C6      ..       2.40 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  O1     ..  C6      ..       2.40 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  O1     ..  C8      ..       2.99 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  O1     ..  C8      ..       2.99 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  O2     ..  C6      ..       2.96 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  N5     ..  C14     ..       2.77 Ang.
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        65 Note
PLAT982_ALERT_1_G The  C-f'=     0.017 Deviates from the  IT-value      0.018 Check
PLAT982_ALERT_1_G The Co-f'=    -2.436 Deviates from the  IT-value     -2.365 Check
PLAT982_ALERT_1_G The Fe-f'=    -1.187 Deviates from the  IT-value     -1.134 Check
PLAT982_ALERT_1_G The  N-f'=     0.029 Deviates from the  IT-value      0.031 Check
PLAT982_ALERT_1_G The Nb-f'=    -0.246 Deviates from the  IT-value     -0.112 Check
PLAT982_ALERT_1_G The  O-f'=     0.046 Deviates from the  IT-value      0.049 Check
PLAT983_ALERT_1_G The Co-f"=     3.620 Deviates from the  IT-Value      3.614 Check
PLAT983_ALERT_1_G The Fe-f"=     3.202 Deviates from the  IT-Value      3.197 Check
PLAT983_ALERT_1_G The Nb-f"=     2.485 Deviates from the  IT-Value      2.483 Check
```

```
   0 ALERT level A = Most likely a serious problem - resolve or explain
   3 ALERT level B = A potentially serious problem, consider carefully
   4 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

  12 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  10 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
   5 ALERT type 4 Improvement, methodology, query or suggestion
   0 ALERT type 5 Informative message, check
```

Datablock: Compound3

```
Bond precision:  C-C = 0.0189 A          Wavelength=1.54183

Cell:            a=20.2572(6)     b=20.2572(6)     c=15.0154(6)
                 alpha=90         beta=90          gamma=90
Temperature:     298 K
```

	Calculated	Reported
Volume	6161.6(4)	6161.6(3)
Space group	I 41/a	I 41/a
Hall group	-I 4ad	-I 4ad
Moiety formula	C224 Co2.32 Fe5.68 N96 Nb4 O32, 8(O)	?
Sum formula	C224 Co2.32 Fe5.68 N96 Nb4 O40	C56 Co0.58 Fe1.42 N24 Nb O10
Mr	5500.79	1375.14
Dx,g cm-3	1.482	1.480
Z	1	4
Mu (mm-1)	6.005	0.000
F000	2710.3	2710.3
F000’	2706.31	
h,k,lmax	15,15,11	15,15,11
Nref	663	661
Tmin,Tmax		
Tmin’		

Correction method= Not given

Data completeness= 0.997 Theta(max)= 35.000

R(reflections)= wR2(reflections)=

S = Npar=

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

POWD004_ALERT_1_B No ’Bragg’ R factor has been given. Please supply a value for _refine_ls_R_factor_all [R(F)], refine_ls_R_Fsqd_factor [R(F^2)] or _refine_ls_R_I_factor [R(I)].
PLAT242_ALERT_2_B Low ’MainMol’ Ueq as Compared to Neighbors of Nb1 Check
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) ..... O1 Check

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Alert level C

PLAT077_ALERT_4_C Unitcell contains non-integer number of atoms .. Please Check
PLAT241_ALERT_2_C High ’MainMol’ Ueq as Compared to Neighbors of N1 Check
PLAT241_ALERT_2_C High ’MainMol’ Ueq as Compared to Neighbors of C1 Check
PLAT241_ALERT_2_C High ’MainMol’ Ueq as Compared to Neighbors of C2 Check
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.0189 Ang.

Alert level G

PLAT040_ALERT_1_G No H-atoms in this Carbon Containing Compound .. Please Check
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ... 0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Fe1 is Constrained at 0.71 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Co1 is Constrained at 0.29 Check

```
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1)..         3% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms ( 113.75) in Resd. #          1 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms (   0.50) in Resd. #          2 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  O1     ..  C6      ..       2.40 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  O1     ..  C6      ..       2.40 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  O1     ..  C8      ..       3.00 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  O1     ..  C8      ..       3.00 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  N5     ..  C14     ..       2.78 Ang.
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        59 Note
PLAT982_ALERT_1_G The  C-f'=     0.017 Deviates from the  IT-value      0.018 Check
PLAT982_ALERT_1_G The Co-f'=    -2.436 Deviates from the  IT-value     -2.365 Check
PLAT982_ALERT_1_G The Fe-f'=    -1.187 Deviates from the  IT-value     -1.134 Check
PLAT982_ALERT_1_G The  N-f'=     0.029 Deviates from the  IT-value      0.031 Check
PLAT982_ALERT_1_G The Nb-f'=    -0.246 Deviates from the  IT-value     -0.112 Check
PLAT982_ALERT_1_G The  O-f'=     0.046 Deviates from the  IT-value      0.049 Check
PLAT983_ALERT_1_G The Co-f"=     3.620 Deviates from the  IT-Value      3.614 Check
PLAT983_ALERT_1_G The Fe-f"=     3.202 Deviates from the  IT-Value      3.197 Check
PLAT983_ALERT_1_G The Nb-f"=     2.485 Deviates from the  IT-Value      2.483 Check
```

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

  12 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  10 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
   5 ALERT type 4 Improvement, methodology, query or suggestion
   0 ALERT type 5 Informative message, check
```

Datablock: Compound4

```
Bond precision:  C-C = 0.0199 A          Wavelength=1.54183

Cell:            a=20.2453(8)     b=20.2453(8)     c=15.0151(8)
                 alpha=90         beta=90          gamma=90
Temperature:     298 K
```

	Calculated	Reported
Volume	6154.3(6)	6154.2(5)
Space group	I 41/a	I 41/a
Hall group	-I 4ad	-I 4ad
Moiety formula	C112 Co2 Fe2 N48 Nb2 O16, 4(O)	?
Sum formula	C112 Co2 Fe2 N48 Nb2 O20	C56 Co1 Fe1 N24 Nb O10
Mr	2752.98	1376.44
Dx,g cm-3	1.486	1.490
Z	2	4
Mu (mm-1)	6.105	0.000
F000	2712.0	2712.0
F000'	2705.93	
h,k,lmax	15,15,11	15,15,11
Nref	663	661
Tmin,Tmax		
Tmin'		

Correction method= Not given

Data completeness= 0.997 Theta(max)= 35.000

R(reflections)= wR2(reflections)=

S = Npar=

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

POWD004_ALERT_1_B No 'Bragg' R factor has been given. Please supply a value for _refine_ls_R_factor_all [R(F)], refine_ls_R_Fsqd_factor [R(F^2)] or _refine_ls_R_I_factor [R(I)].
PLAT242_ALERT_2_B Low 'MainMol' Ueq as Compared to Neighbors of Nb1 Check
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) ..... O1 Check

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Alert level C

PLAT076_ALERT_1_C Occupancy 0.500 less than 1.0 for Sp.pos . FE1
PLAT076_ALERT_1_C Occupancy 0.500 less than 1.0 for Sp.pos . CO1
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C1 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C2 Check
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.0199 Ang.

Alert level G

PLAT040_ALERT_1_G No H-atoms in this Carbon Containing Compound .. Please Check
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ... 0.50 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Co1 is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Fe1 is Constrained at 0.5 Check
PLAT301_ALERT_3_G Main Residue Disorder .....(Resd 1).. 2% Note

```
PLAT304_ALERT_4_G Non-Integer Number of Atoms ( 113.75) in Resd. #          1 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms (   0.50) in Resd. #          2 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  O1     ..  C6      ..       2.38 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  O1     ..  C6      ..       2.38 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  O1     ..  C8      ..       3.01 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  O1     ..  C8      ..       3.01 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  O2     ..  C6      ..       2.94 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  N5     ..  C14     ..       2.79 Ang.
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        59 Note
PLAT982_ALERT_1_G The  C-f'=     0.017 Deviates from the  IT-value      0.018 Check
PLAT982_ALERT_1_G The Co-f'=    -2.436 Deviates from the  IT-value     -2.365 Check
PLAT982_ALERT_1_G The Fe-f'=    -1.187 Deviates from the  IT-value     -1.134 Check
PLAT982_ALERT_1_G The  N-f'=     0.029 Deviates from the  IT-value      0.031 Check
PLAT982_ALERT_1_G The Nb-f'=    -0.246 Deviates from the  IT-value     -0.112 Check
PLAT982_ALERT_1_G The  O-f'=     0.046 Deviates from the  IT-value      0.049 Check
PLAT983_ALERT_1_G The Co-f"=     3.620 Deviates from the  IT-Value      3.614 Check
PLAT983_ALERT_1_G The Fe-f"=     3.202 Deviates from the  IT-Value      3.197 Check
PLAT983_ALERT_1_G The Nb-f"=     2.485 Deviates from the  IT-Value      2.483 Check
```

```
   0 ALERT level A = Most likely a serious problem - resolve or explain
   3 ALERT level B = A potentially serious problem, consider carefully
   5 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

  14 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  10 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
   4 ALERT type 4 Improvement, methodology, query or suggestion
   0 ALERT type 5 Informative message, check
```

Datablock: Compound5

```
Bond precision:  C-C = 0.0206 A          Wavelength=1.54183

Cell:            a=20.2238(11)    b=20.2238(11)    c=15.0065(13)
                 alpha=90         beta=90          gamma=90
Temperature:     298 K
```

	Calculated	Reported
Volume	6137.7(9)	6137.7(7)
Space group	I 41/a	I 41/a
Hall group	-I 4ad	-I 4ad
Moiety formula	C224 Co6.32 Fe1.68 N96 Nb4 O32, 8(O)	?
Sum formula	C224 Co6.32 Fe1.68 N96 Nb4 O40	C56 Co1.58 Fe0.42 N24 Nb O10
Mr	5513.11	1378.23
Dx,g cm-3	1.492	1.490
Z	1	4
Mu (mm-1)	6.250	0.000
F000	2714.3	2714.3
F000’	2705.40	
h,k,lmax	15,15,11	14,14,11
Nref	660	658
Tmin,Tmax		
Tmin’		

Correction method= Not given

Data completeness= 0.997 Theta(max)= 35.000

R(reflections)= wR2(reflections)=

S = Npar=

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

POWD004_ALERT_1_B No ’Bragg’ R factor has been given. Please supply a value for _refine_ls_R_factor_all [R(F)], refine_ls_R_Fsqd_factor [R(F^2)] or _refine_ls_R_I_factor [R(I)].
PLAT242_ALERT_2_B Low ’MainMol’ Ueq as Compared to Neighbors of Nb1 Check
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) ..... O1 Check
PLAT342_ALERT_3_B Low Bond Precision on C-C Bonds ..... 0.0206 Ang.

Alert level C

PLAT077_ALERT_4_C Unitcell contains non-integer number of atoms .. Please Check
PLAT241_ALERT_2_C High ’MainMol’ Ueq as Compared to Neighbors of C1 Check
PLAT241_ALERT_2_C High ’MainMol’ Ueq as Compared to Neighbors of C2 Check

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Alert level G

PLAT040_ALERT_1_G No H-atoms in this Carbon Containing Compound .. Please Check
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ... 0.25 Check
PLAT152_ALERT_1_G The Supplied and Calc. Volume s.u. Differ by ... 2 Units
PLAT300_ALERT_4_G Atom Site Occupancy of Co1 is Constrained at 0.79 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Fe1 is Constrained at 0.21 Check

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PLAT301_ALERT_3_G Main Residue  Disorder .............(Resd  1)..         3% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms ( 113.75) in Resd. #          1 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms (   0.50) in Resd. #          2 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  O1     ..  C6      ..       2.32 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  O1     ..  C6      ..       2.32 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  O1     ..  C8      ..       2.99 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  O1     ..  C8      ..       2.99 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  O2     ..  C6      ..       2.89 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  N5     ..  C14     ..       2.80 Ang.
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        59 Note
PLAT982_ALERT_1_G The  C-f'=     0.017 Deviates from the  IT-value      0.018 Check
PLAT982_ALERT_1_G The Co-f'=    -2.436 Deviates from the  IT-value     -2.365 Check
PLAT982_ALERT_1_G The Fe-f'=    -1.187 Deviates from the  IT-value     -1.134 Check
PLAT982_ALERT_1_G The  N-f'=     0.029 Deviates from the  IT-value      0.031 Check
PLAT982_ALERT_1_G The Nb-f'=    -0.246 Deviates from the  IT-value     -0.112 Check
PLAT982_ALERT_1_G The  O-f'=     0.046 Deviates from the  IT-value      0.049 Check
PLAT983_ALERT_1_G The Co-f"=     3.620 Deviates from the  IT-Value      3.614 Check
PLAT983_ALERT_1_G The Fe-f"=     3.202 Deviates from the  IT-Value      3.197 Check
PLAT983_ALERT_1_G The Nb-f"=     2.485 Deviates from the  IT-Value      2.483 Check
```

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

  13 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  10 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
   5 ALERT type 4 Improvement, methodology, query or suggestion
   0 ALERT type 5 Informative message, check
```

Datablock: Compound6

```
Bond precision:  C-C = 0.0207 A          Wavelength=1.54183

Cell:            a=20.2105(11)    b=20.2105(11)    c=15.0066(13)
                 alpha=90         beta=90          gamma=90
Temperature:     298 K
```

	Calculated	Reported
Volume	6129.7(9)	6129.7(7)
Space group	I 41/a	I 41/a
Hall group	-I 4ad	-I 4ad
Moiety formula	C112 Co4 N48 Nb2 O16, 4(O)	?
Sum formula	C112 Co4 N48 Nb2 O20	C56 Co2 N24 Nb O10
Mr	2759.14	1379.53
Dx,g cm-3	1.495	1.490
Z	2	4
Mu (mm-1)	6.351	0.000
F000	2716.0	2716.0
F000’	2705.02	
h,k,lmax	15,15,11	14,14,11
Nref	658	658
Tmin,Tmax		
Tmin’		

Correction method= Not given

Data completeness= 1.000 Theta(max)= 35.000

R(reflections)= wR2(reflections)=

S = Npar=

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

POWD004_ALERT_1_B No ’Bragg’ R factor has been given. Please supply a value for _refine_ls_R_factor_all [R(F)], refine_ls_R_Fsqd_factor [R(F^2)] or _refine_ls_R_I_factor [R(I)].
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) ..... O1 Check
PLAT342_ALERT_3_B Low Bond Precision on C-C Bonds ..... 0.0207 Ang.

Alert level C

PLAT241_ALERT_2_C High ’MainMol’ Ueq as Compared to Neighbors of C1 Check
PLAT241_ALERT_2_C High ’MainMol’ Ueq as Compared to Neighbors of C2 Check
PLAT242_ALERT_2_C Low ’MainMol’ Ueq as Compared to Neighbors of Nb1 Check

---

Alert level G

PLAT040_ALERT_1_G No H-atoms in this Carbon Containing Compound .. Please Check
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ... 0.50 Check
PLAT152_ALERT_1_G The Supplied and Calc. Volume s.u. Differ by ... 2 Units
PLAT304_ALERT_4_G Non-Integer Number of Atoms (113.75) in Resd. # 1 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms (0.50) in Resd. # 2 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact O1 .. C6 .. 2.35 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact O1 .. C6 .. 2.35 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact O1 .. C8 .. 3.02 Ang.

```
PLAT432_ALERT_2_G Short Inter X...Y Contact  O1     ..  C8      ..       3.02 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  O2     ..  C6      ..       2.89 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  N5     ..  C14     ..       2.77 Ang.
PLAT794_ALERT_5_G Tentative Bond Valency for Co1     (III)   .....       1.89 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............         59 Note
PLAT982_ALERT_1_G The  C-f'=     0.017 Deviates from the  IT-value      0.018 Check
PLAT982_ALERT_1_G The Co-f'=    -2.436 Deviates from the  IT-value     -2.365 Check
PLAT982_ALERT_1_G The  N-f'=     0.029 Deviates from the  IT-value      0.031 Check
PLAT982_ALERT_1_G The Nb-f'=    -0.246 Deviates from the  IT-value     -0.112 Check
PLAT982_ALERT_1_G The  O-f'=     0.046 Deviates from the  IT-value      0.049 Check
PLAT983_ALERT_1_G The Co-f"=     3.620 Deviates from the  IT-Value      3.614 Check
PLAT983_ALERT_1_G The Nb-f"=     2.485 Deviates from the  IT-Value      2.483 Check
```

---

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

11 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
10 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
1 ALERT type 5 Informative message, check

---

checkCIF publication errors

Alert level G

```
PUBL017_ALERT_1_G The _publ_section_references section is missing or
           empty.
```

---

0 **ALERT level A** = Data missing that is essential or data in wrong format
1 **ALERT level G** = General alerts. Data that may be required is missing

---

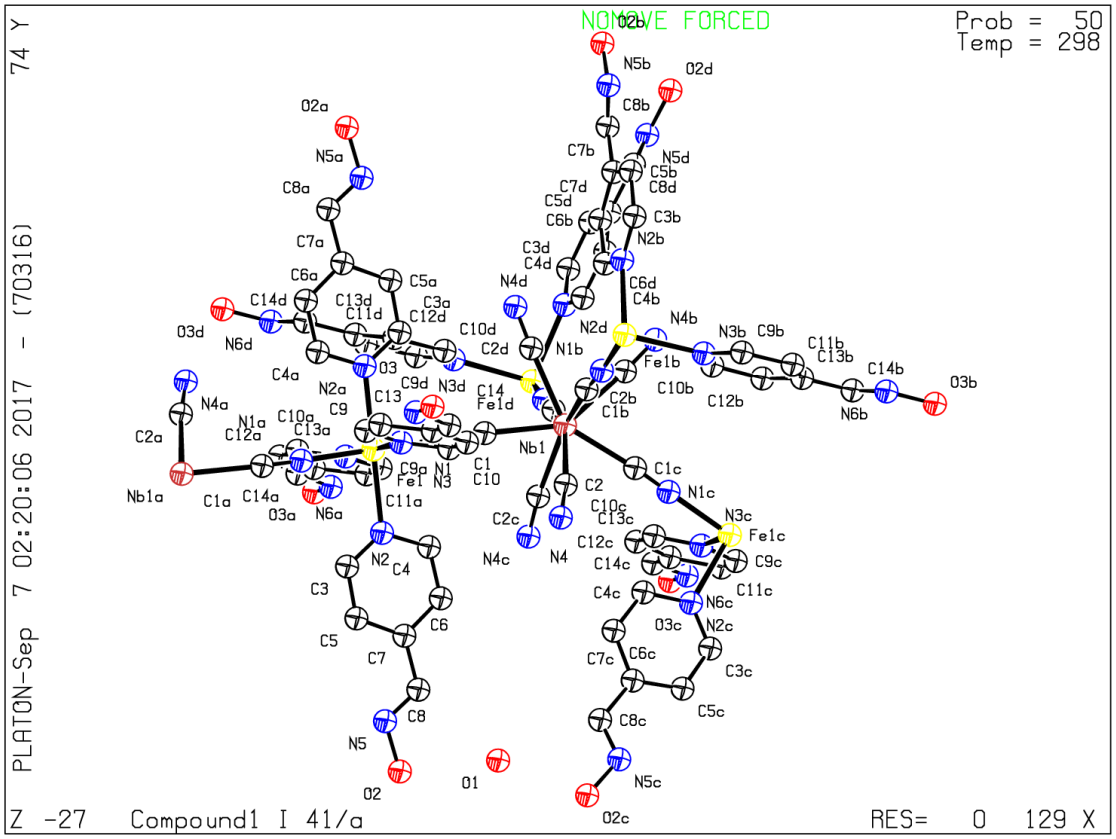
Publication of your CIF

You should 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 nature of your study may justify the reported deviations from journal submission requirements and the more serious of these should 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.

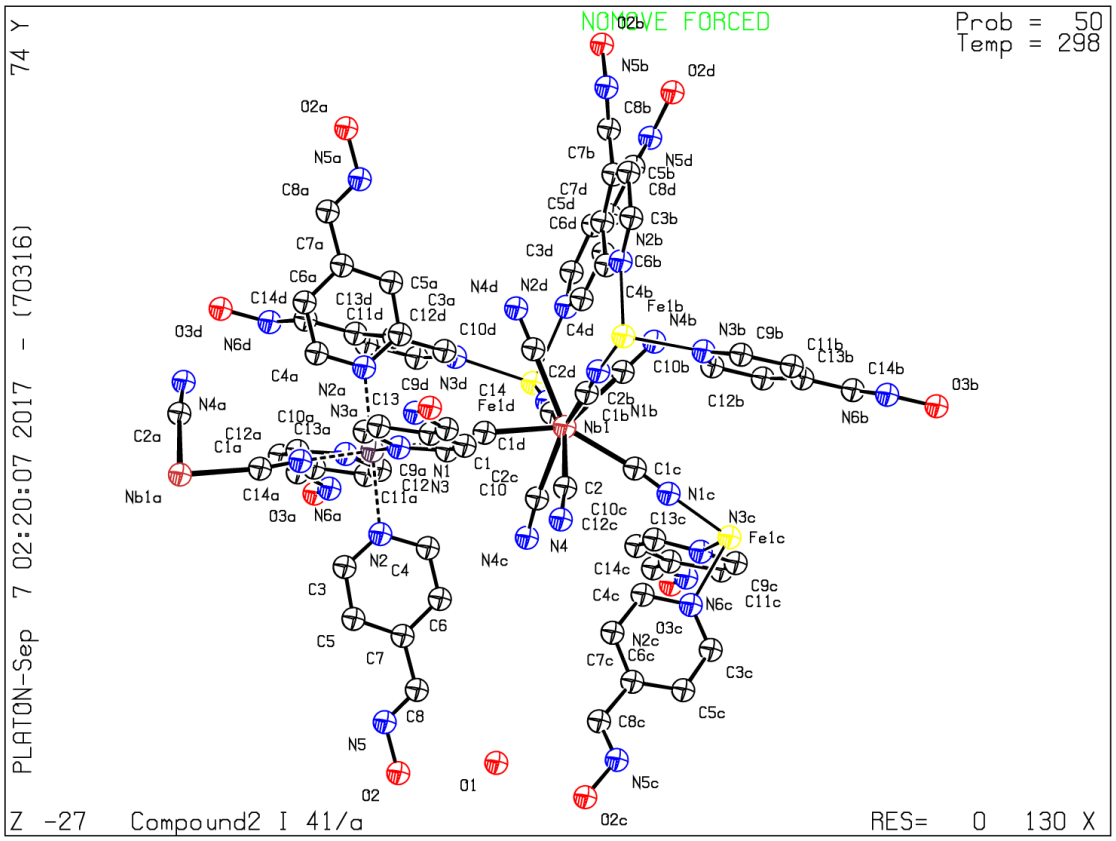
If you wish to submit your CIF for publication in Acta Crystallographica Section C or E, you should upload your CIF via the web. If you wish to submit your CIF for publication in IUCrData you should upload your CIF via the web. If your CIF is to form part of a submission to another IUCr journal, you will be asked, either during electronic submission or by the Co-editor handling your paper, to upload your CIF via our web site.

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

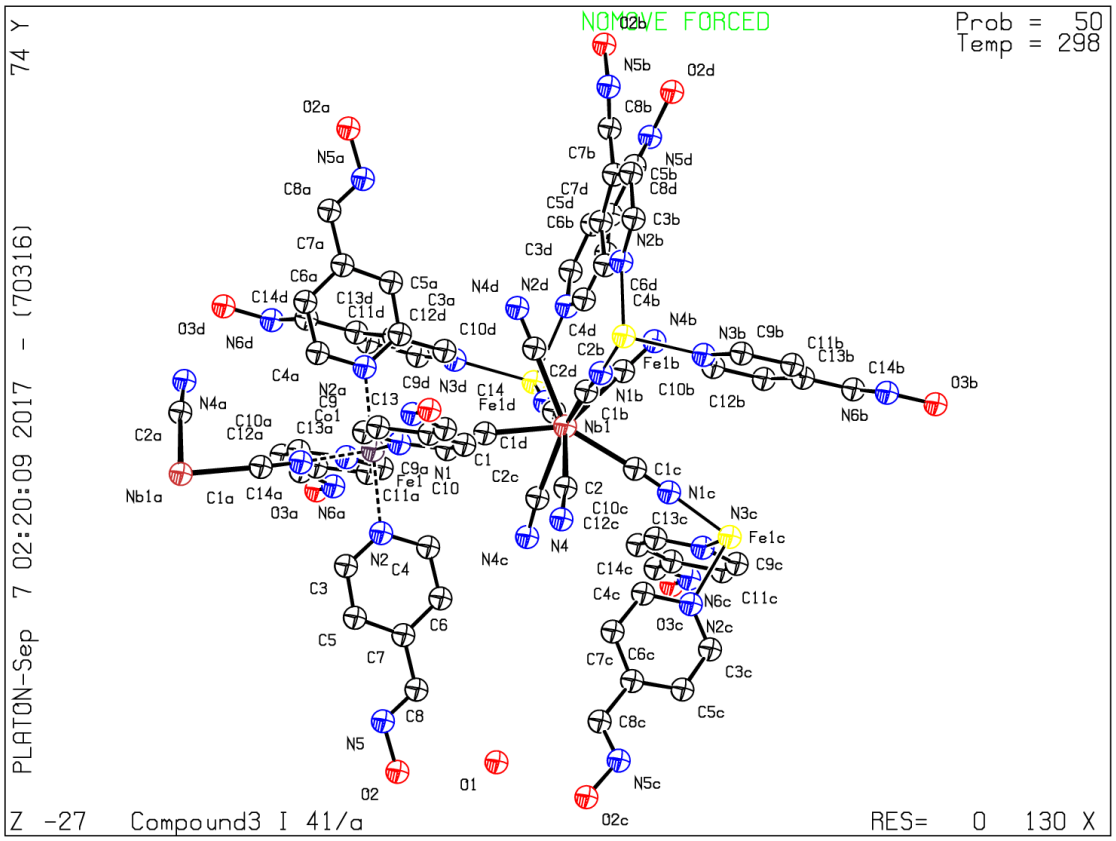
Datablock Compound1 - ellipsoid plot



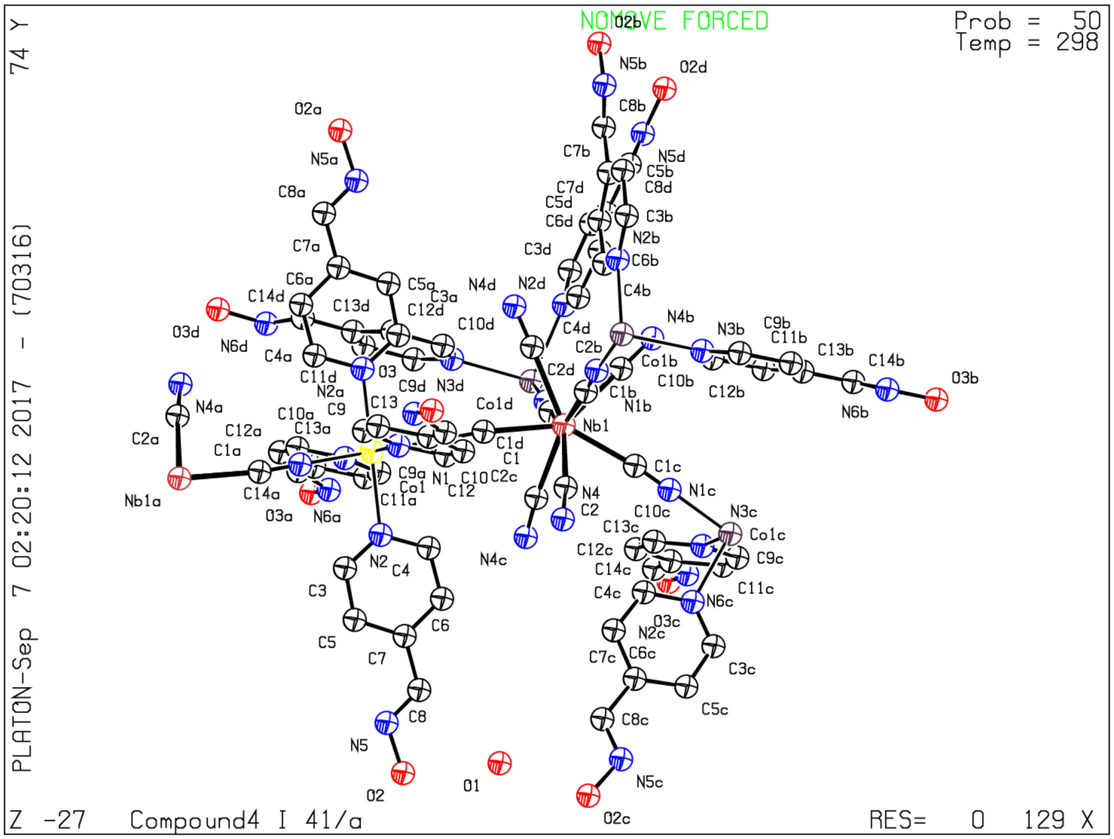
Datablock Compound2 - ellipsoid plot



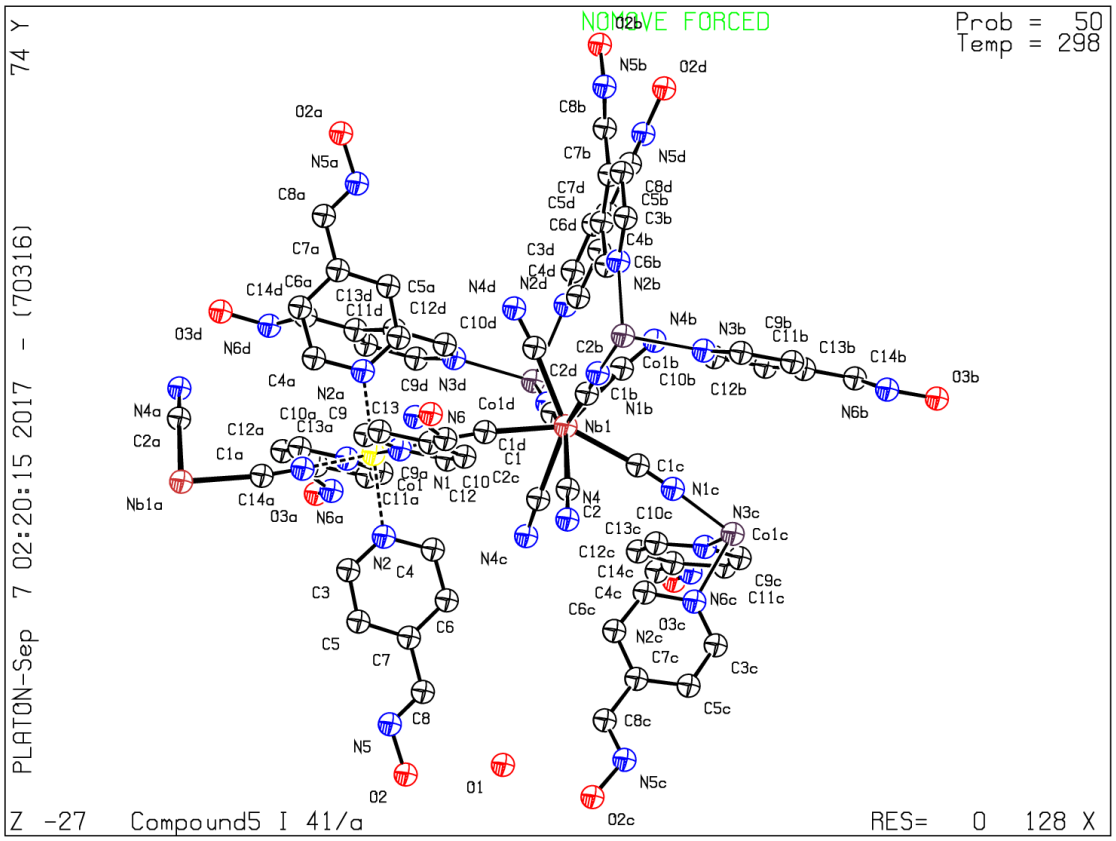
Datablock Compound3 - ellipsoid plot



Datablock Compound4 - ellipsoid plot



Datablock Compound5 - ellipsoid plot



Datablock Compound6 - ellipsoid plot