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Electronic Supplementary Information

# Complexation of 1,1'-Bis(diphenylphosphino)ferrocene Dioxide ($dppfO_2$) with *3d* Metals and Revisit of its Coordination to Pd(II)

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**Suffix** CheckCIF/Platon report of **1** and the metal centers are fitted as Co, Ni, Cu and Zn using the same diffraction data as that of **1**. ..... 16

**Table S1** Selected bond distances (Å) and angles (°) for **2−12**

| | | | |
|---|---|---|---|
| **2** | | | |
| Ni(1)-O(4) | 1.977(4) | Ni(1)-O(2) | 2.012(4) |
| Ni(1)-O(3) | 2.020(4) | Ni(1)-O(1) | 2.033(4) |
| Ni(1)-Cl(1) | 2.3336(17) | Ni(1)-Cl(2) | 2.3525(16) |
| O(4)-Ni(1)-O(2) | 179.12(16) | O(4)-Ni(1)-O(3) | 91.19(16) |
| O(2)-Ni(1)-O(3) | 89.65(16) | O(4)-Ni(1)-O(1) | 87.04(16) |
| O(2)-Ni(1)-O(1) | 92.12(16) | O(3)-Ni(1)-O(1) | 177.98(16) |
| O(4)-Ni(1)-Cl(1) | 92.55(13) | O(2)-Ni(1)-Cl(1) | 87.70(12) |
| O(3)-Ni(1)-Cl(1) | 90.20(13) | O(1)-Ni(1)-Cl(1) | 90.84(12) |
| O(4)-Ni(1)-Cl(2) | 91.80(13) | O(2)-Ni(1)-Cl(2) | 87.97(12) |
| O(3)-Ni(1)-Cl(2) | 88.60(13) | O(1)-Ni(1)-Cl(2) | 90.50(12) |
| Cl(1)-Ni(1)-Cl(2) | 175.51(7) | | |
| **3** | | | |
| Cr(1)-O(1) | 1.960(2) | Cr(1)-O(2) | 1.971(2) |
| Cr(1)-O(3) | 1.967(2) | Cr(1)-O(4) | 1.963(2) |
| Cr(1)-Cl(1) | 2.3303(9) | Cr(1)-Cl(2) | 2.3399(8) |
| **4** | | | |
| Fe(1)-O(1) | 1.998(3) | Fe(1)-O(3) | 2.000(4) |
| Fe(1)-O(4) | 2.002(3) | Fe(1)-O(2) | 2.015(3) |
| Fe(1)-Cl(2) | 2.3316(14) | Fe(1)-Cl(1) | 2.3596(14) |
| O(1)-Fe(1)-O(3) | 178.06(15) | O(1)-Fe(1)-O(4) | 88.21(15) |
| O(3)-Fe(1)-O(4) | 93.11(15) | O(1)-Fe(1)-O(2) | 90.43(15) |
| O(3)-Fe(1)-O(2) | 88.28(15) | O(4)-Fe(1)-O(2) | 178.22(15) |
| O(1)-Fe(1)-Cl(2) | 91.56(11) | O(3)-Fe(1)-Cl(2) | 89.90(11) |
| O(4)-Fe(1)-Cl(2) | 88.44(11) | O(2)-Fe(1)-Cl(2) | 90.45(11) |
| O(1)-Fe(1)-Cl(1) | 89.04(11) | O(3)-Fe(1)-Cl(1) | 89.53(11) |
| O(4)-Fe(1)-Cl(1) | 90.18(11) | O(2)-Fe(1)-Cl(1) | 90.95(11) |
| Cl(2)-Fe(1)-Cl(1) | 178.48(6) | | |
| **5** | | | |

| | | | |
|---|---|---|---|
| Fe(1)-O(3) | 2.000(3) | Fe(1)-O(1) | 2.005(3) |
| Fe(1)-O(4) | 2.015(3) | Fe(1)-O(2) | 2.033(3) |
| Fe(1)-Cl(1) | 2.3433(11) | Fe(1)-Cl(2) | 2.3495(10) |
| O(3)-Fe(1)-O(1) | 177.99(11) | O(3)-Fe(1)-O(4) | 91.92(11) |
| O(1)-Fe(1)-O(4) | 87.61(11) | O(3)-Fe(1)-O(2) | 88.35(11) |
| O(1)-Fe(1)-O(2) | 92.20(11) | O(4)-Fe(1)-O(2) | 177.84(11) |
| O(3)-Fe(1)-Cl(1) | 90.13(8) | O(1)-Fe(1)-Cl(1) | 91.82(8) |
| O(4)-Fe(1)-Cl(1) | 89.88(8) | O(2)-Fe(1)-Cl(1) | 87.97(8) |
| O(3)-Fe(1)-Cl(2) | 88.15(8) | O(1)-Fe(1)-Cl(2) | 89.91(8) |
| O(4)-Fe(1)-Cl(2) | 91.94(8) | O(2)-Fe(1)-Cl(2) | 90.21(8) |
| Cl(1)-Fe(1)-Cl(2) | 177.53(4) | | |

**6**

| | | | |
|---|---|---|---|
| Fe(1)-O(2) | 2.017(5) | Fe(1)-O(1) | 2.053(5) |
| Fe(1)-I(1) | 2.777(2) | | |
| O(2)-Fe(1)-O(2)#1 | 159.3(3) | O(2)-Fe(1)-O(1)#1 | 90.48(19) |
| O(2)-Fe(1)-O(1) | 85.95(19) | O(1)#1-Fe(1)-O(1) | 160.0(3) |
| O(2)-Fe(1)-I(1) | 100.33(16) | O(1)-Fe(1)-I(1) | 99.99(14) |

Symmetry codes: #1: $-x + 2, y, -z + 1/2$; #2: $-x + 1/2, -y + 3/2, -z$.

**7**

| | | | |
|---|---|---|---|
| Cu(1)-O(1) | 2.006(5) | Cu(1)-O(2) | 2.017(6) |
| Cu(1)-Cl(1) | 2.347(2) | | |
| O(1)#1-Cu(1)-O(1) | 87.9(3) | O(1)-Cu(1)-O(2)#1 | 178.6(2) |
| O(1)-Cu(1)-O(2) | 91.6(2) | O(2)#1-Cu(1)-O(2) | 88.9(3) |
| O(1)-Cu(1)-Cl(1)#1 | 90.09(17) | O(2)-Cu(1)-Cl(1)#1 | 89.81(18) |
| O(1)-Cu(1)-Cl(1) | 88.86(17) | O(2)-Cu(1)-Cl(1) | 91.23(18) |
| Cl(1)#1-Cu(1)-Cl(1) | 178.55(13) | | |

Symmetry code: #1: $-x + 1, y, -z + 3/2$.

**8**

| | | | |
|---|---|---|---|
| Mn(1)-O(2) | 2.0172(18) | Mn(1)-O(1) | 2.0324(19) |
| Mn(1)-Cl(2) | 2.3052(11) | Mn(1)-Cl(1) | 2.3341(9) |
| O(2)-Mn(1)-O(1) | 104.60(7) | O(2)-Mn(1)-Cl(2) | 105.82(6) |
| O(1)-Mn(1)-Cl(2) | 111.70(5) | O(2)-Mn(1)-Cl(1) | 103.77(6) |

| | | | |
|---|---|---|---|
| O(1)-Mn(1)-Cl(1) | 102.13(5) | Cl(2)-Mn(1)-Cl(1) | 126.74(4) |
| **9** | | | |
| Co(1)-O(1) | 1.9753(16) | Co(1)-O(2) | 1.9859(18) |
| Co(1)-Cl(1) | 2.2370(8) | Co(1)-Cl(2) | 2.2489(8) |
| O(1)-Co(1)-O(2) | 99.11(7) | O(1)-Co(1)-Cl(1) | 105.30(6) |
| O(2)-Co(1)-Cl(1) | 119.36(6) | O(1)-Co(1)-Cl(2) | 113.21(6) |
| O(2)-Co(1)-Cl(2) | 108.70(6) | Cl(1)-Co(1)-Cl(2) | 110.70(3) |
| **10** | | | |
| Co(1)-O(1) | 1.959(3) | Co(1)-O(2) | 1.972(3) |
| Co(1)-Br(1) | 2.3695(8) | Co(1)-Br(2) | 2.3770(8) |
| O(1)-Co(1)-O(2) | 107.51(14) | O(1)-Co(1)-Br(1) | 113.27(11) |
| O(2)-Co(1)-Br(1) | 107.17(10) | O(1)-Co(1)-Br(2) | 99.95(12) |
| O(2)-Co(1)-Br(2) | 111.13(11) | Br(1)-Co(1)-Br(2) | 117.40(3) |
| **11** | | | |
| Co(1)-O(1) | 1.940(4) | Co(1)-O(2) | 1.950(4) |
| Co(1)-I(1) | 2.5624(8) | Co(1)-I(2) | 2.5722(8) |
| O(1)-Co(1)-O(2) | 108.04(18) | O(1)-Co(1)-I(1) | 112.86(14) |
| O(2)-Co(1)-I(1) | 106.94(12) | O(1)-Co(1)-I(2) | 99.48(14) |
| O(2)-Co(1)-I(2) | 111.57(13) | I(1)-Co(1)-I(2) | 117.61(3) |
| **12** | | | |
| Zn(1)-O(1) | 1.971(3) | Zn(1)-O(2) | 1.985(3) |
| Zn(1)-Cl(2) | 2.2005(16) | Zn(1)-Cl(1) | 2.2122(14) |
| O(1)-Zn(1)-O(2) | 102.07(15) | O(1)-Zn(1)-Cl(2) | 107.33(12) |
| O(2)-Zn(1)-Cl(2) | 108.56(12) | O(1)-Zn(1)-Cl(1) | 107.94(11) |
| O(2)-Zn(1)-Cl(1) | 109.23(11) | Cl(2)-Zn(1)-Cl(1) | 120.19(7) |

**Figure S1** Ortep view of the structures of **3−5**, **8**, and **10−12**.

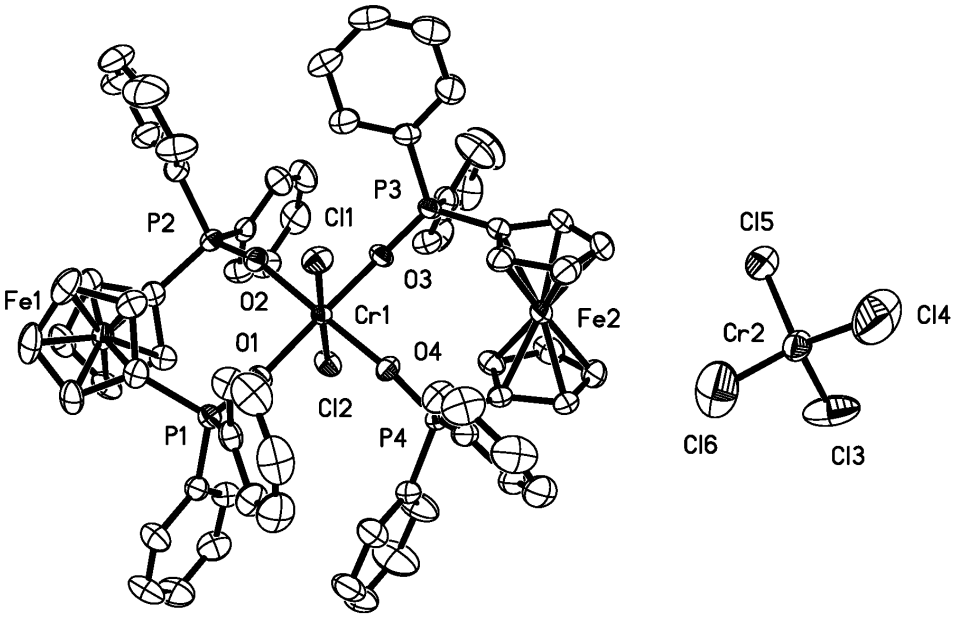



**Figure S1a** Structure of **3** wtih all hydrogen atoms and disordered MeOH molecules were omitted for clarity.

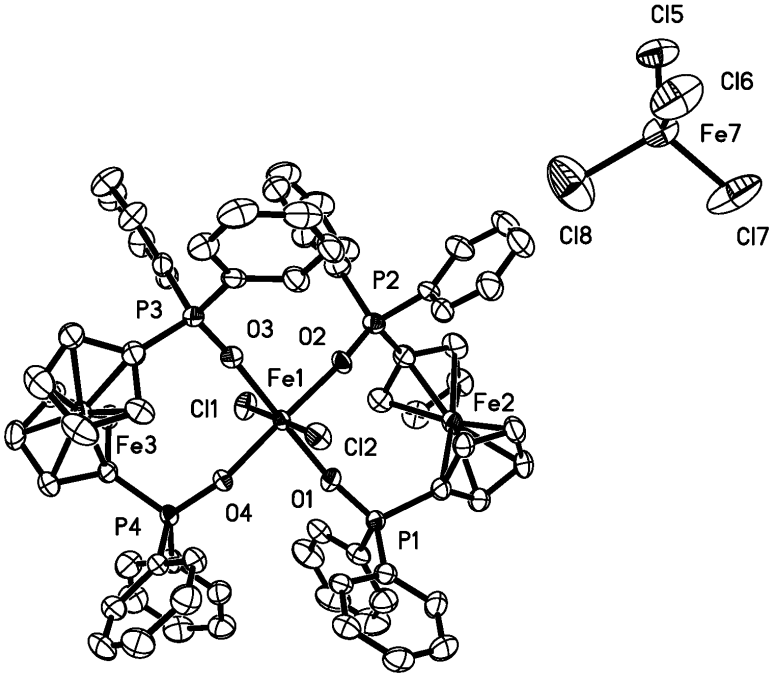



**Figure S1b** Structure of **4** with only one $[FeCl_2(dppfO_2)_2][FeCl_4]$ asymmetric unit being shown. The other unit, solvents, disodered moieties and hydrogen atoms were omitted for clarity.

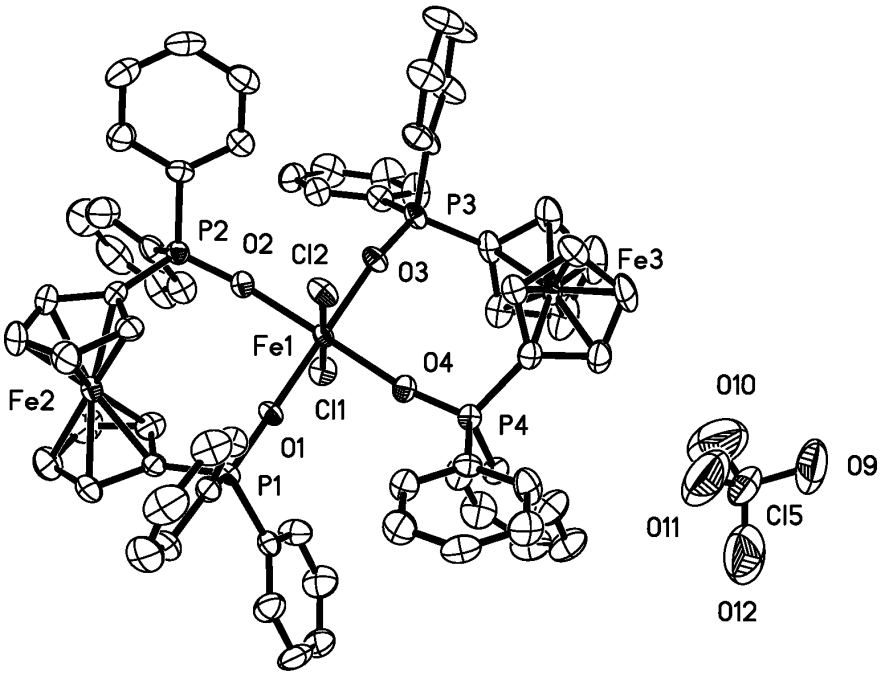



**Figure S1c** Structure of **5** with only one $[FeCl_2(dppfO_2)_2][ClO_4]$ asymmetric unit being shown. The other unit, solvents, and hydrogen atoms were omitted for clarity.

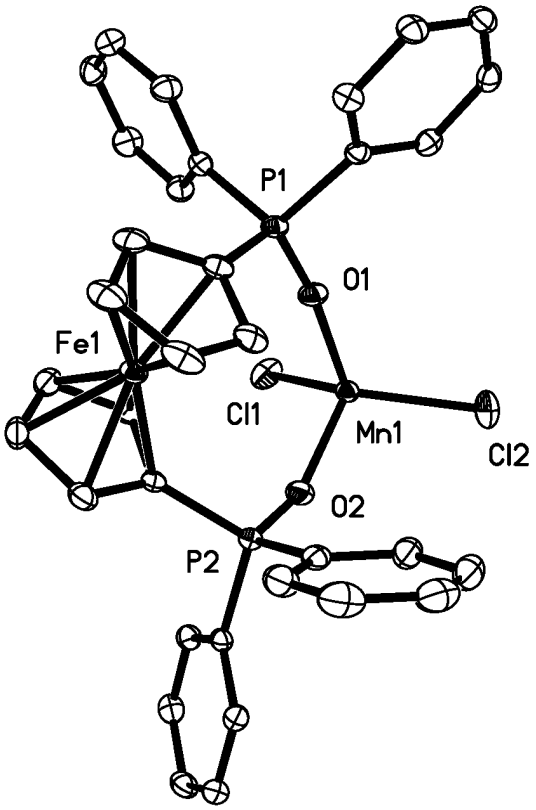



**Figure S1d** Structure of **8**. All hydrogen atoms were omitted for clarity.

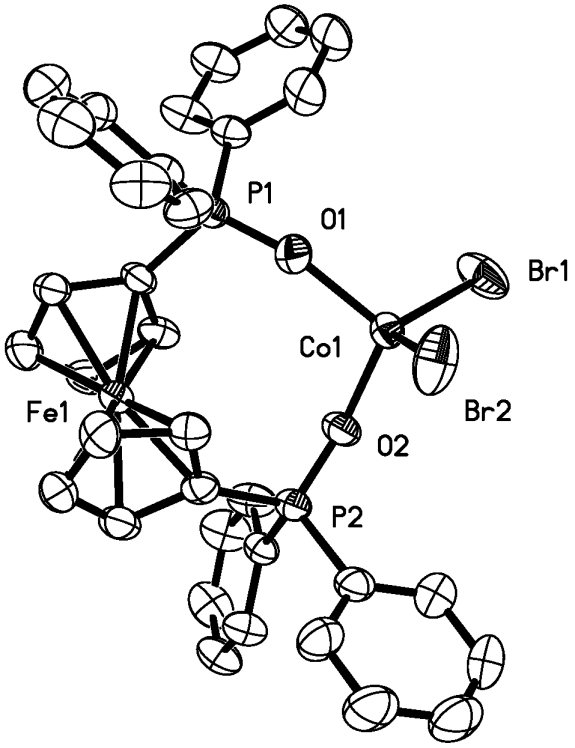



**Figure S1e** Structure of **10**. All hydrogen atoms were omitted for clarity.

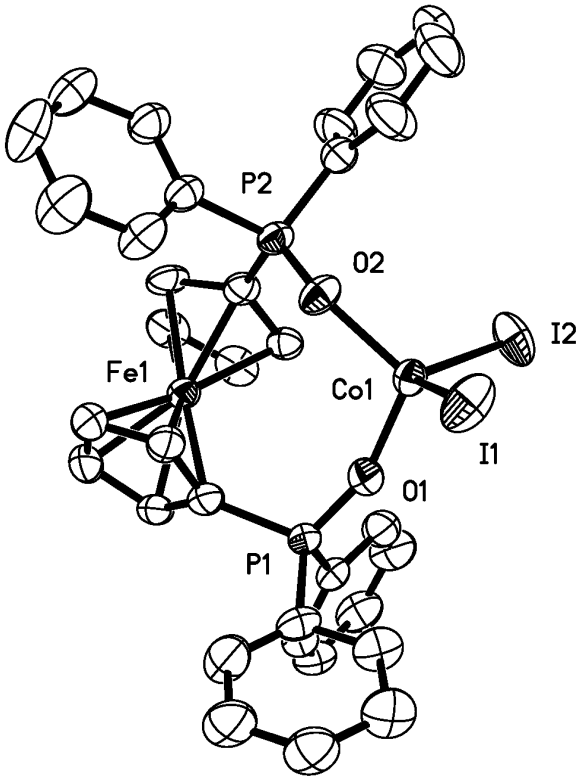



**Figure S1f** Structure of **11**. All hydrogen atoms were omitted for clarity.

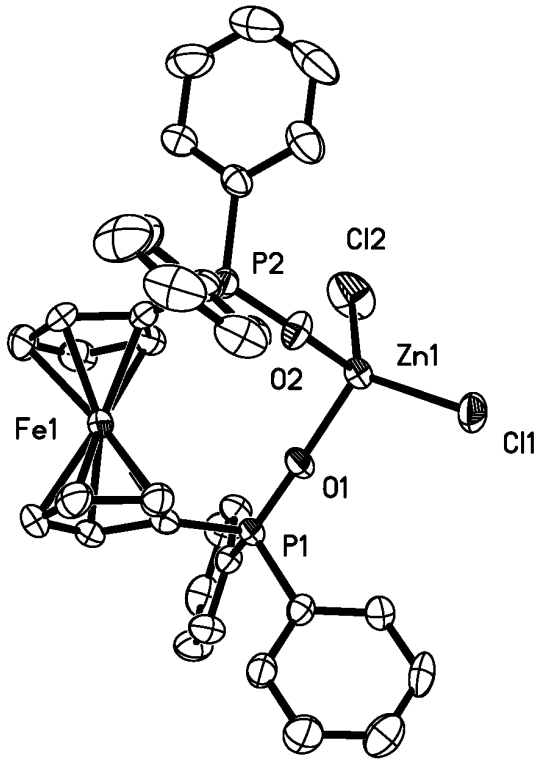
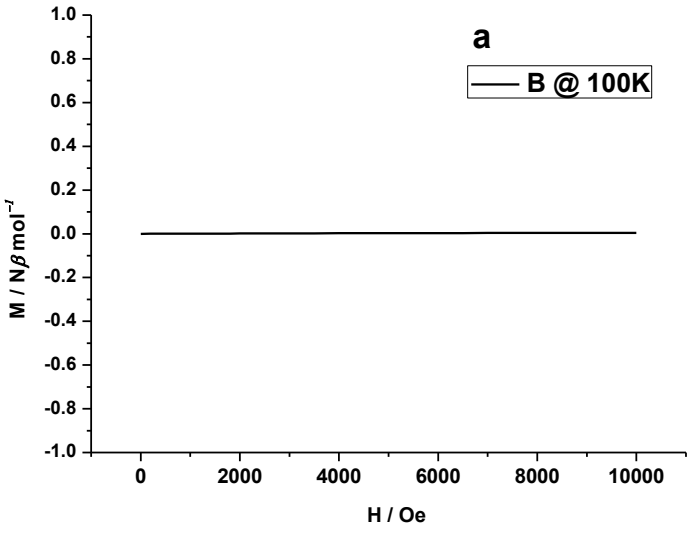
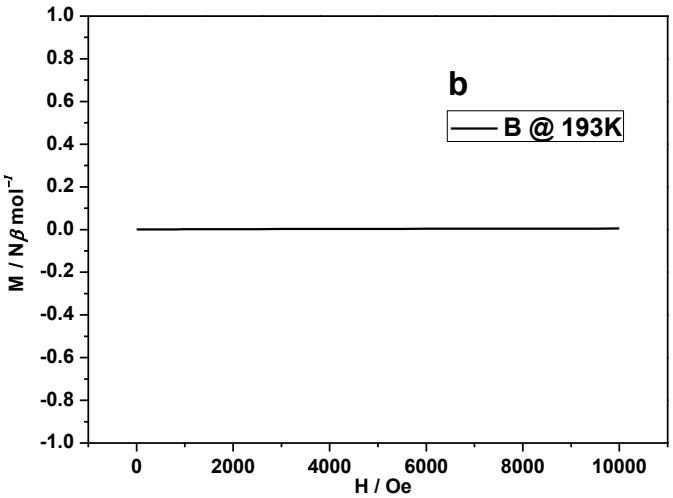
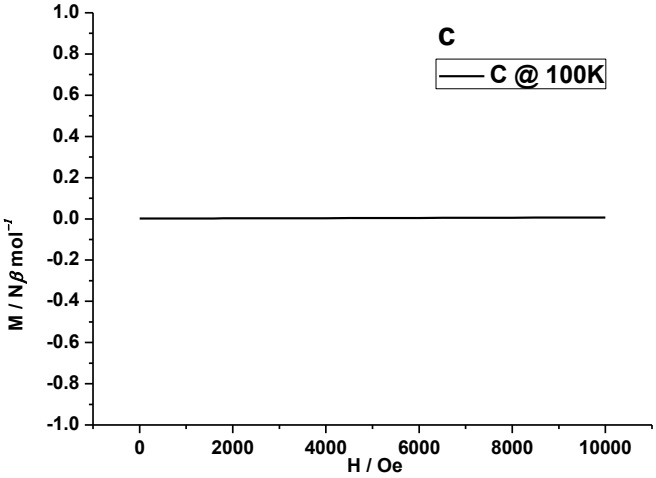



**Figure S1g** Structure of **12**. The disordered solvent molecules and all hydrogen atoms were omitted for clarity.

**Figure S2** Field dependence of the magnetization for **B** and **C**, a) **B** at 100 K, b) **B** at 193K, c) **C** at 100 K, and d) **C** at 193 K.




b
B @ 193K
M / Nβ mol⁻¹
H / Oe
1.0
0.8
0.6
0.4
0.2
0.0
-0.2
-0.4
-0.6
-0.8
-1.0
0
2000
4000
6000
8000
10000


c
C @ 100K
M / Nβ mol⁻¹
H / Oe
1.0
0.8
0.6
0.4
0.2
0.0
-0.2
-0.4
-0.6
-0.8
-1.0
0
2000
4000
6000
8000
10000

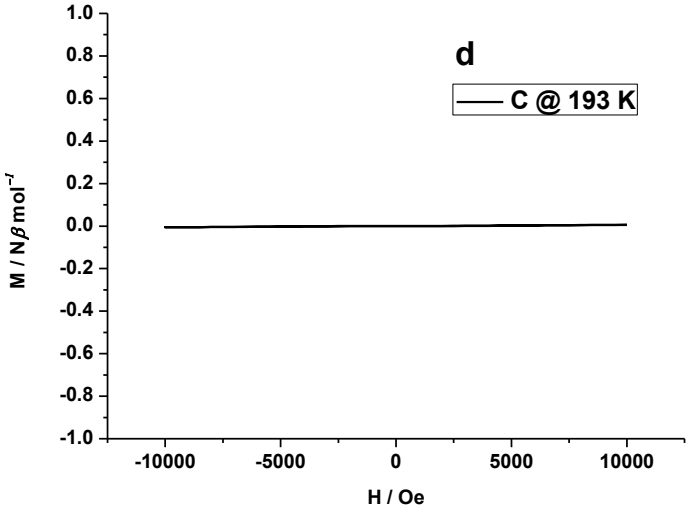

d
C @ 193 K
M / Nβ mol⁻¹
H / Oe
1.0
0.8
0.6
0.4
0.2
0.0
-0.2
-0.4
-0.6
-0.8
-1.0
-10000
-5000
0
5000
10000

**Figure S3** $^1$H VT NMR spectra for the *in situ* reaction mixture $PdCl_2(MeCN)_2$ and $dppfO_2$ in $CD_2Cl_2$.

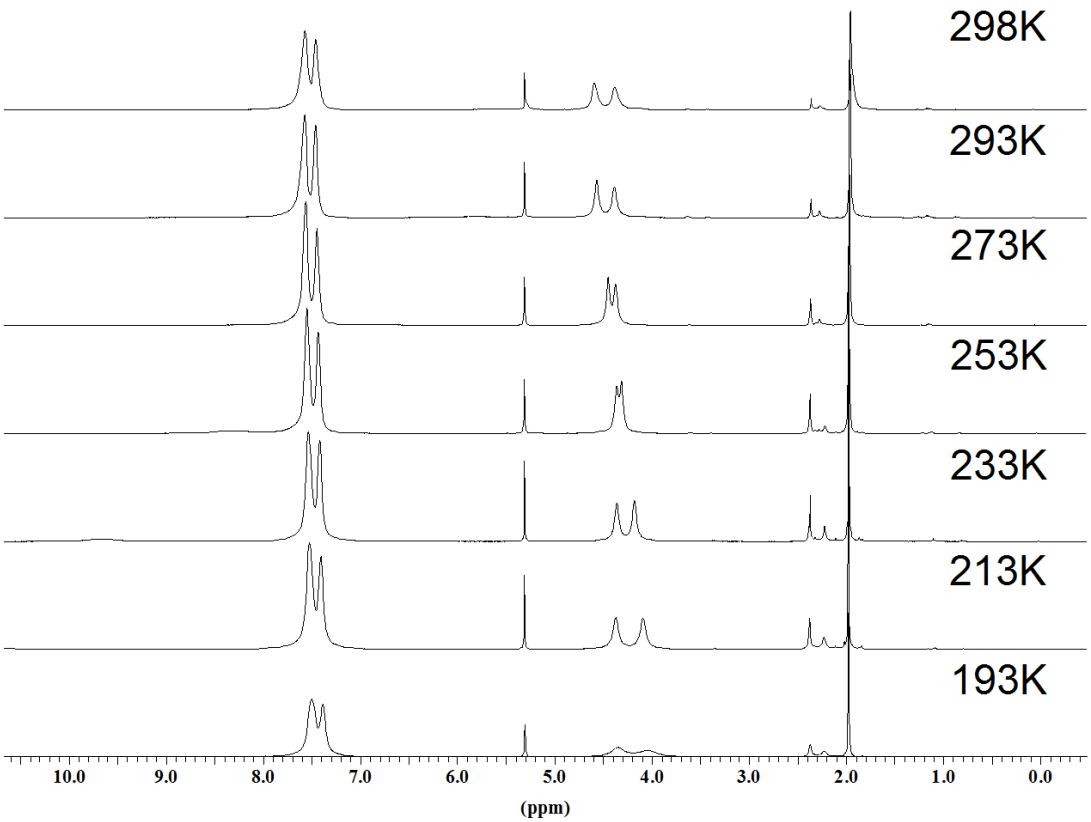
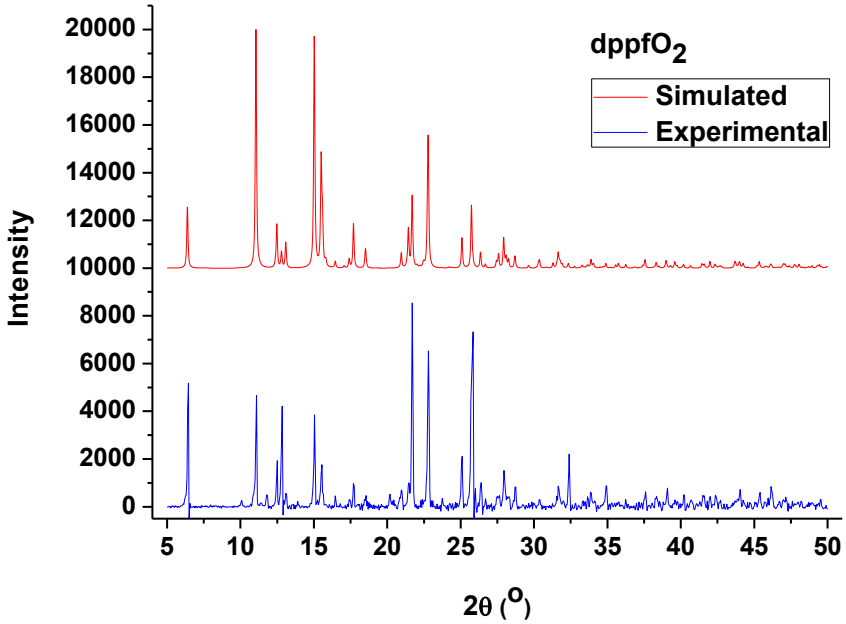
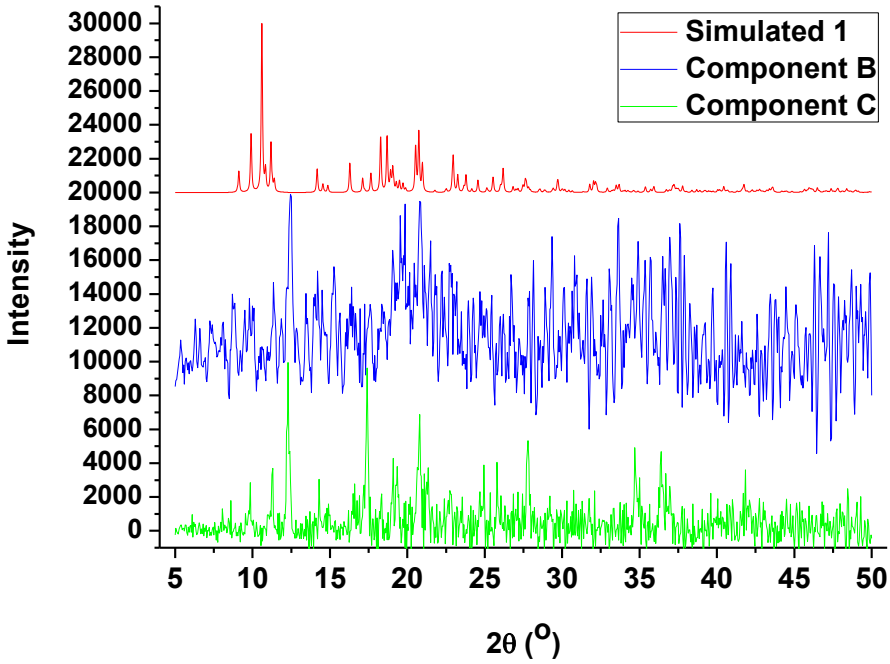
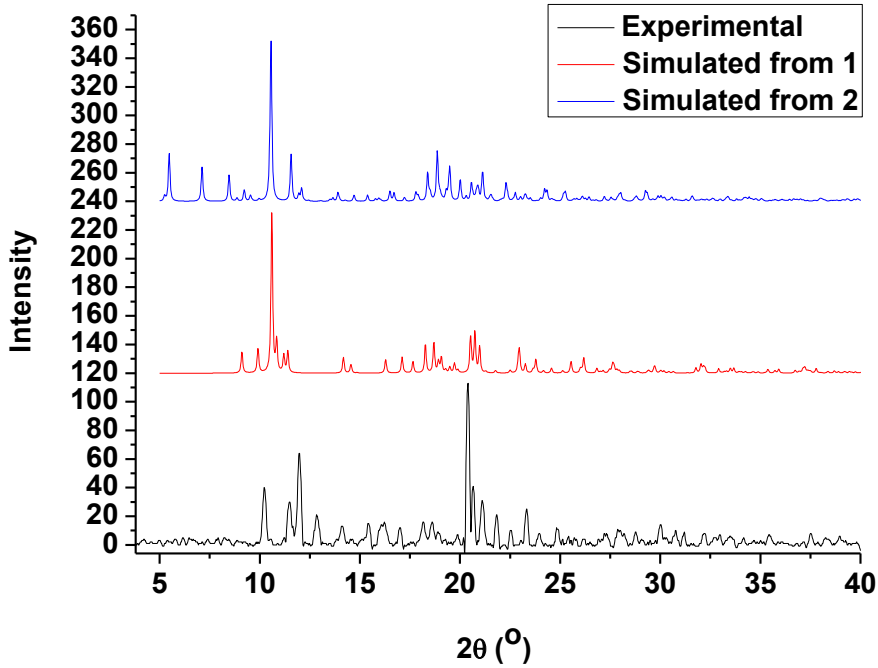
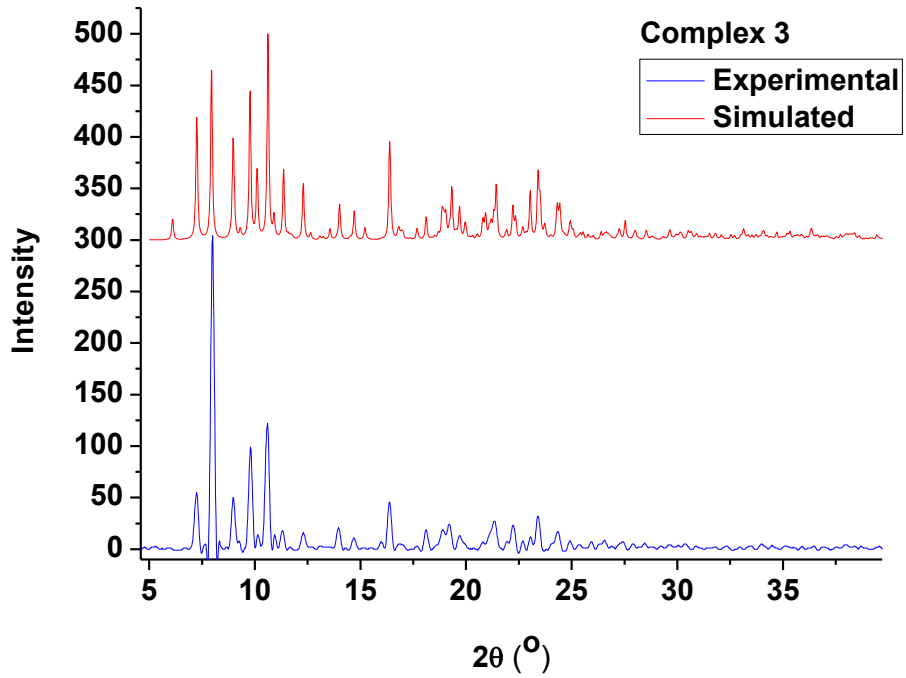


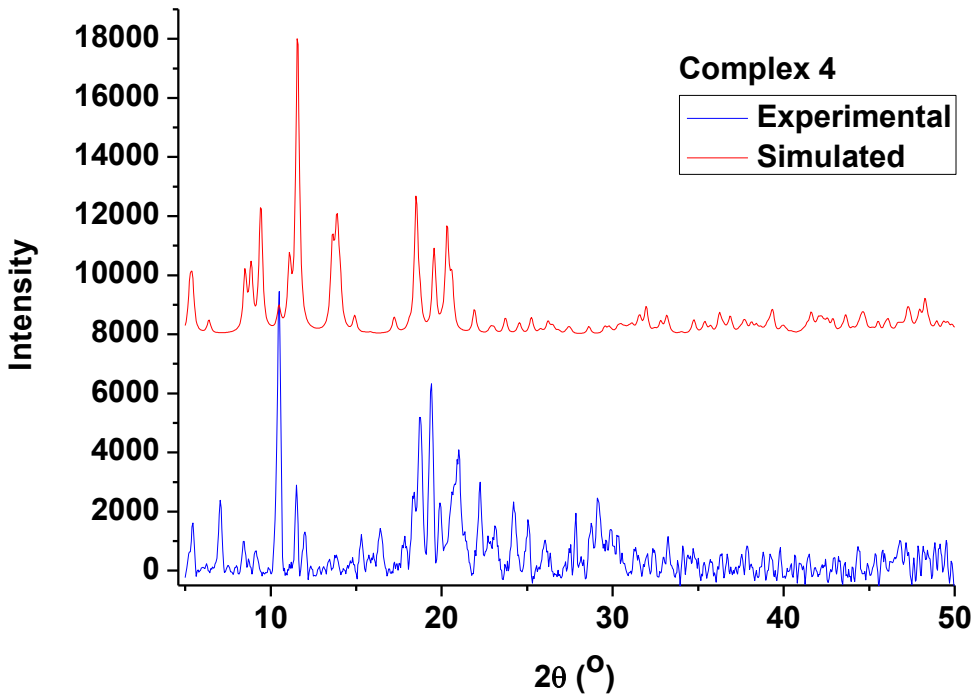

**Figure S4** Comparison of experimental powder X-ray diffraction pattern and those simulated from single crystal diffraction data.

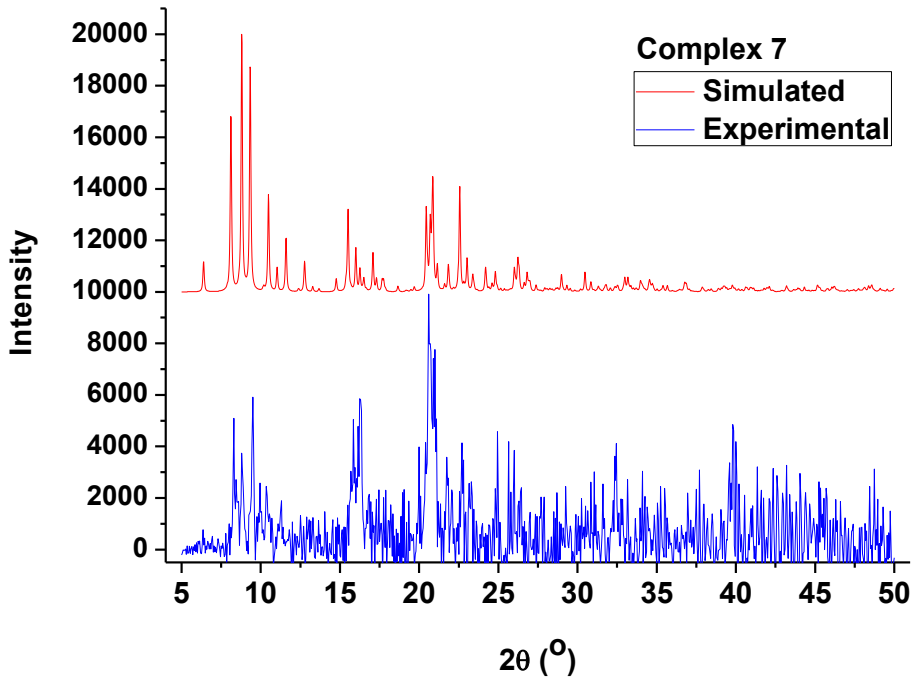


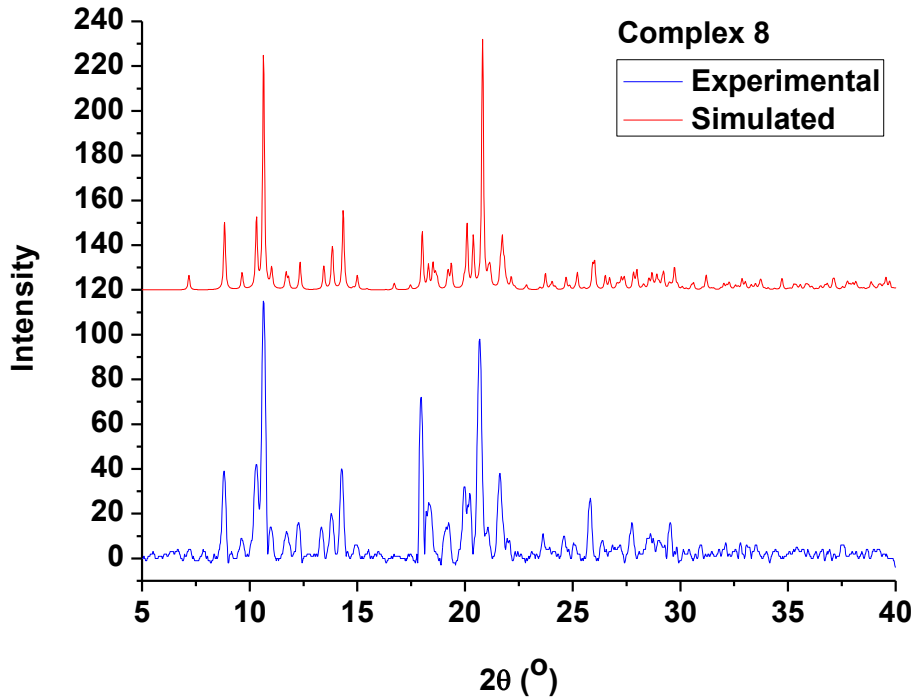

Simulated 1
Component B
Component C
Intensity
2θ (O)

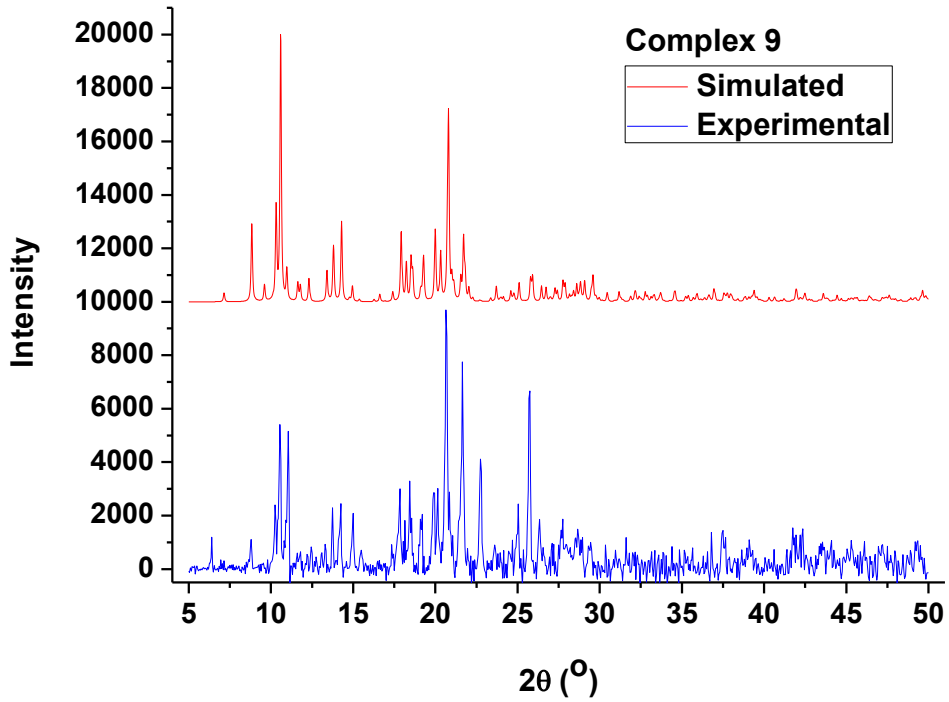

Experimental
Simulated from 1
Simulated from 2
Intensity
2θ (O)

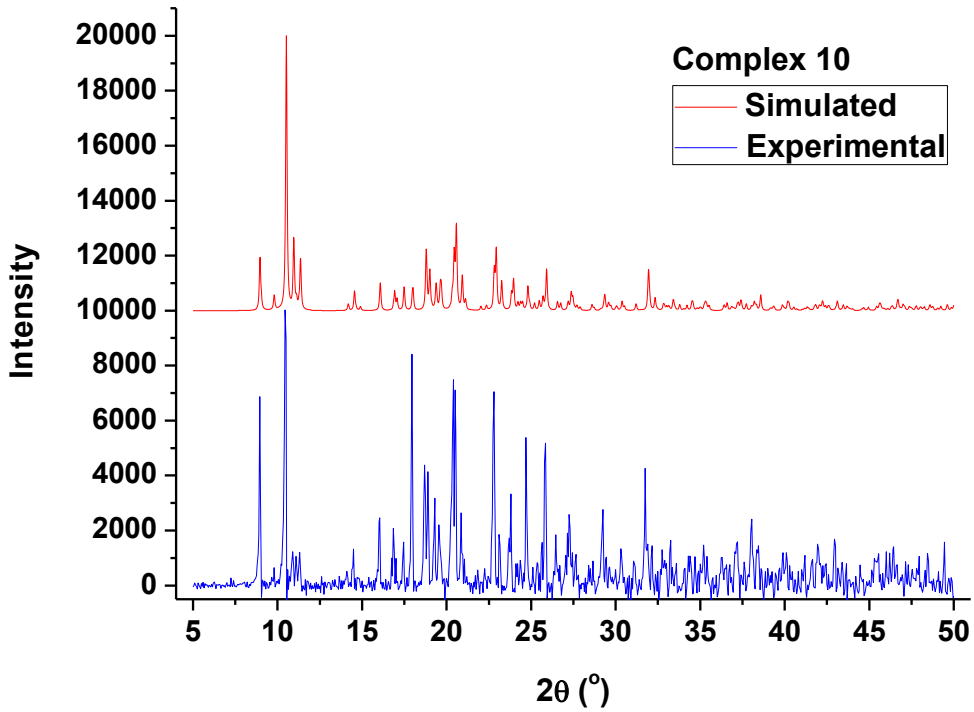

Complex 3
Experimental
Simulated
Intensity
500
450
400
350
300
250
200
150
100
50
0
5
10
15
20
25
30
35
2θ (O)

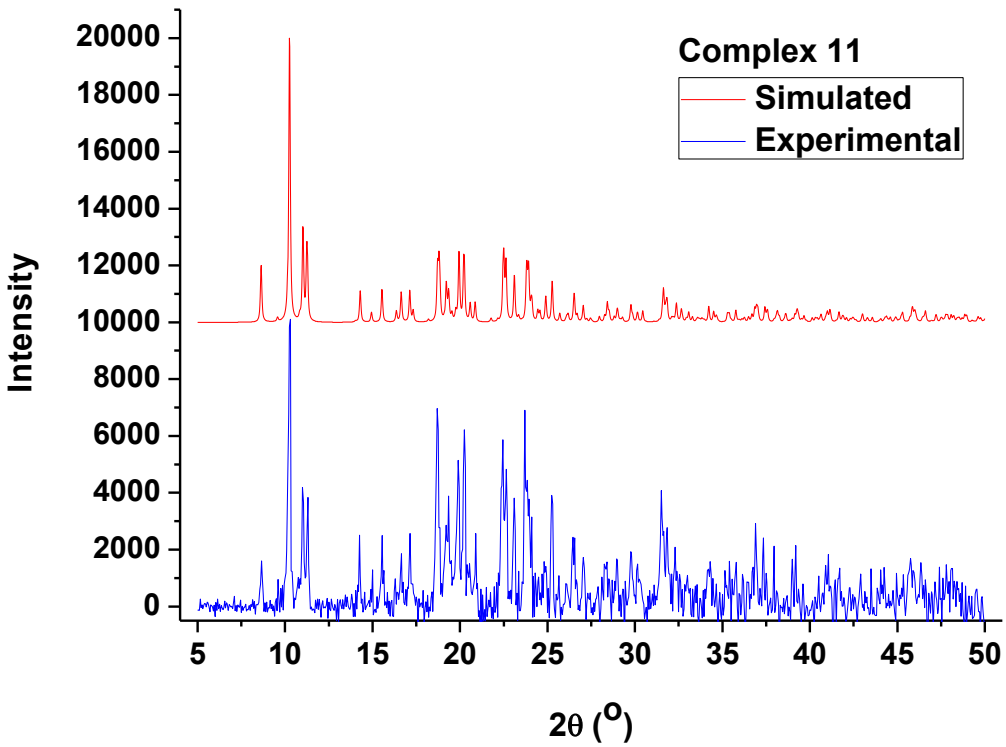

Complex 4
Experimental
Simulated
Intensity
18000
16000
14000
12000
10000
8000
6000
4000
2000
0
10
20
30
40
50
2θ (O)

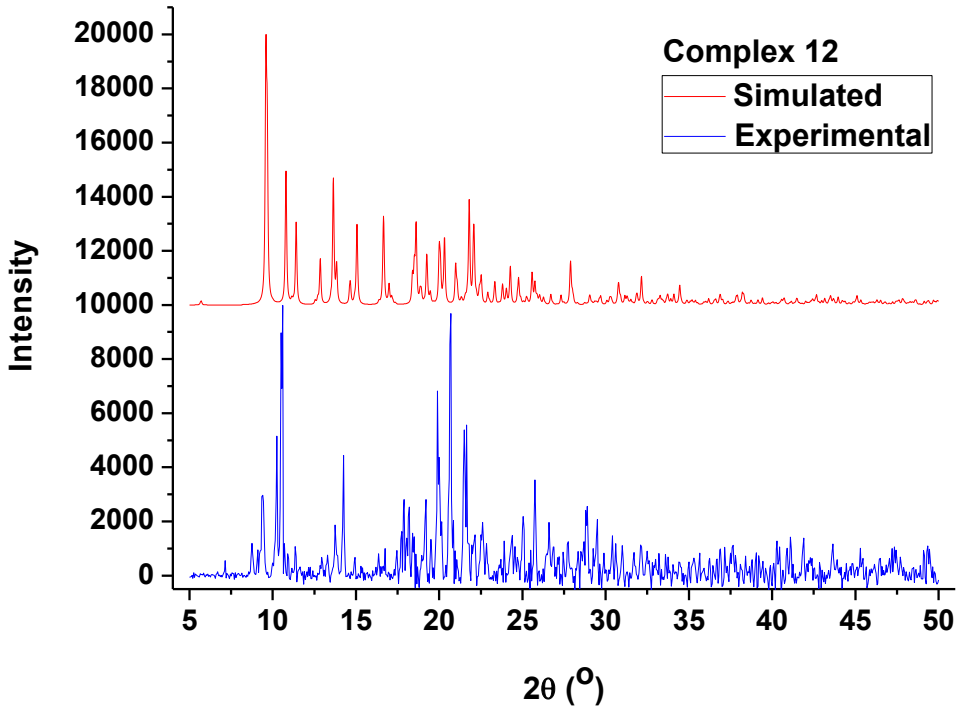

Complex 7
Simulated
Experimental
Intensity
20000
18000
16000
14000
12000
10000
8000
6000
4000
2000
0
5
10
15
20
25
30
35
40
45
50
2θ (O)


Complex 8
Experimental
Simulated
Intensity
240
220
200
180
160
140
120
100
80
60
40
20
0
5
10
15
20
25
30
35
40
2θ (O)


Complex 9
Simulated
Experimental
Intensity
20000
18000
16000
14000
12000
10000
8000
6000
4000
2000
0
5
10
15
20
25
30
35
40
45
50
2θ (°)


Complex 10
Simulated
Experimental
Intensity
20000
18000
16000
14000
12000
10000
8000
6000
4000
2000
0
5
10
15
20
25
30
35
40
45
50
2θ (°)


Complex 11
Simulated
Experimental
Intensity
20000
18000
16000
14000
12000
10000
8000
6000
4000
2000
0
5
10
15
20
25
30
35
40
45
50
2θ (O)


Complex 12
Simulated
Experimental
Intensity
20000
18000
16000
14000
12000
10000
8000
6000
4000
2000
0
5
10
15
20
25
30
35
40
45
50
2θ (O)

**Suffix** CheckCIF/Platon report of **1** and the metal centers are fitted as Co, Ni, Cu and Zn using the same diffraction data as that of **1**.

**Datablock: Pd**

---

Bond precision: C-C = 0.0195 A Wavelength=0.71073

Cell: a=10.0444(2) b=19.4070(3) c=16.3157(1)

alpha=90 beta=91.340(2) gamma=90

Temperature: 293 K

| | Calculated | Reported |
|---|---|---|
| Volume | 3179.58(8) | 3179.58(8) |
| Space group | C c | Cc |
| Hall group | C -2yc | ? |
| Moiety formula | C34 H28 Cl2 Fe O2 P2 Pd | ? |
| Sum formula | C34 H28 Cl2 Fe O2 P2 Pd | C34 H28 Cl2 Fe O2 P2 Pd |
| Mr | 763.65 | 763.65 |
| Dx,g cm-3 | 1.595 | 1.595 |
| Z | 4 | 4 |
| Mu (mm-1) | 1.321 | 1.321 |
| F000 | 1536.0 | 1536.0 |
| F000' | 1535.80 | |
| h,k,lmax | 11,22,19 | 11,23,19 |
| Nref | 2792[ 5573] | 4010 |
| Tmin,Tmax | 0.752,0.842 | 0.719,0.825 |
| Tmin' | 0.647 | |

Correction method= 'S

Data completeness= 1.44/0.72 Theta(max)= 25.000

R(reflections)= 0.0679( 3799) wR2(reflections)= 0.2169( 4010)

S = 1.061 Npar= 344

---

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 A**

DIFF003_ALERT_1_A _diffrn_measurement_device_type is missing

Diffractometer make and type. Replaces _diffrn_measurement_type.

DIFF019_ALERT_1_A _diffrn_standards_number is missing

Number of standards used in measurement.

DIFF020_ALERT_1_A _diffrn_standards_interval_count and

_diffrn_standards_interval_time are missing. Number of measurements

between standards or time (min) between standards.

DIFF022_ALERT_1_A _diffrn_standards_decay_% is missing

Percentage decrease in standards intensity.

ABSTY01_ALERT_1_A The absorption correction should be one of the following

* none
* analytical
* integration
* numerical
* gaussian
* empirical
* psi-scan
* multi-scan
* refdelf
* sphere
* cylinder

PLAT761_ALERT_1_A CIF Contains no X-H Bonds ..... ?

PLAT762_ALERT_1_A CIF Contains no X-Y-H or H-Y-H Angles ..... ?

---

**Alert level B**

PLAT052_ALERT_1_B Info on Absorption Correction Method Missing ... ?

PLAT093_ALERT_1_B No su's on H-atoms, but refinement reported as . mixed

PLAT201_ALERT_2_B Isotropic non-H Atoms in Main Residue(s) ..... 6

---

**Alert level C**

PLAT048_ALERT_1_C MoietyFormula Not Given ..... ?

PLAT057_ALERT_3_C Correction for Absorption Required RT(exp) ... 1.12

PLAT125_ALERT_4_C No '_symmetry_space_group_name_Hall' Given ..... ?

PLAT143_ALERT_4_C su on c - Axis Small or Missing (x 100000) ..... 10 Ang.

PLAT220_ALERT_2_C Large Non-Solvent C Ueq(max)/Ueq(min) ... 3.22 Ratio

PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X) Pd1 -- O1 .. 6.75 su

PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X) Pd1 -- O2 .. 7.25 su

PLAT234_ALERT_4_C Large Hirshfeld Difference C8 -- C9 .. 0.16 Ang.

PLAT234_ALERT_4_C Large Hirshfeld Difference C20 -- C21 .. 0.17 Ang.

PLAT234_ALERT_4_C Large Hirshfeld Difference C26 -- C27 .. 0.19 Ang.

PLAT234_ALERT_4_C Large Hirshfeld Difference C30 -- C31 .. 0.22 Ang.

PLAT234_ALERT_4_C Large Hirshfeld Difference C32 -- C33 .. 0.16 Ang.

PLAT241_ALERT_2_C Check High Ueq as Compared to Neighbors for C9

PLAT241_ALERT_2_C Check High Ueq as Compared to Neighbors for C21

PLAT241_ALERT_2_C Check High Ueq as Compared to Neighbors for C26

PLAT330_ALERT_2_C Large Average Phenyl C-C Dist. C17 -C22 1.41 Ang.

PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds (x 1000) Ang .. 20

---

**Datablock: Co**

---

Bond precision: C-C = 0.0112 A Wavelength=0.71073

Cell: a=10.0444(2) b=19.4070(3) c=16.3157(1)

alpha=90 beta=91.3400 gamma=90

Temperature: 293 K

| | Calculated | Reported |
|---|---|---|
| Volume | 3179.58(8) | 3179.58(8) |
| Space group | C c | Cc |
| Hall group | C -2yc | ? |
| Moiety formula | C34 H28 Cl2 Co Fe O2 P2 | ? |
| Sum formula | C34 H28 Cl2 Co Fe O2 P2 | C34 H28 Cl2 Co Fe O2 P2 |
| Mr | 716.18 | 716.18 |
| Dx,g cm-3 | 1.496 | 1.496 |
| Z | 4 | 4 |
| Mu (mm-1) | 1.277 | 1.277 |

| | | |
|---|---|---|
| F000 | 1460.0 | 1460.0 |
| F000' | 1465.15 | |
| h,k,lmax | 11,22,19 | 11,23,19 |
| Nref | 2792[ 5573] | 4010 |
| Tmin,Tmax | | |
| Tmin' | | |

Correction method= Not given

Data completeness= 1.44/0.72 Theta(max)= 25.000

R(reflections)= 0.0391( 3799) wR2(reflections)= 0.1172( 4010)

S = 1.130 Npar= 344

---

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 A**

EXPT005_ALERT_1_A _exptl_crystal_description is missing

Crystal habit description.

The following tests will not be performed.

CRYSR_01

EXPT009_ALERT_1_A No crystal dimensions have been given.

The following tests will not be performed.

CRYSS_01,CRYSS_02

EXPT108_ALERT_1_A The magnitudes of the crystal dimensions do not

match the min, mid and max definitions

EXPT010_ALERT_1_A _exptl_crystal_colour (_pd_char_colour for powder) is missing

Crystal colour.

The following tests will not be performed.

CRYSC_01

DENSX01_ALERT_1_A The ratio of the calculated to measured crystal density

lies outside the range 0.80 <> 1.20

Calculated density = 1.496

Measured density = 0.000

PLAT053_ALERT_1_A Minimum Crystal Dimension Missing (or Error) ... ?

PLAT054_ALERT_1_A Medium Crystal Dimension Missing (or Error) ... ?

PLAT055_ALERT_1_A Maximum Crystal Dimension Missing (or Error) ... ?

PLAT761_ALERT_1_A CIF Contains no X-H Bonds ..... ?

PLAT762_ALERT_1_A CIF Contains no X-Y-H or H-Y-H Angles ..... ?

---

**Alert level B**

PLAT093_ALERT_1_B No su's on H-atoms, but refinement reported as . mixed

PLAT201_ALERT_2_B Isotropic non-H Atoms in Main Residue(s) ..... 6

---

**Alert level C**

PLAT048_ALERT_1_C MoietyFormula Not Given ..... ?

PLAT125_ALERT_4_C No '_symmetry_space_group_name_Hall' Given ..... ?

PLAT143_ALERT_4_C su on c - Axis Small or Missing (x 100000) ..... 10 Ang.

PLAT145_ALERT_4_C su on beta Small or Missing (x 10000) ..... 0 Deg.

PLAT230_ALERT_2_C Hirshfeld Test Diff for C25 -- C26 .. 5.27 su

PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X) Co1 -- O2 .. 6.50 su

PLAT234_ALERT_4_C Large Hirshfeld Difference C24 -- C25 .. 0.17 Ang.

PLAT241_ALERT_2_C Check High Ueq as Compared to Neighbors for O1

PLAT241_ALERT_2_C Check High Ueq as Compared to Neighbors for C25

PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for Co1

PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for C23

PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds (x 1000) Ang .. 11

---

**Datablock: Ni**

---

Bond precision: C-C = 0.0106 A Wavelength=0.71073

Cell: a=10.0444(2) b=19.4070(3) c=16.3157(1)

alpha=90 beta=91.3400 gamma=90

Temperature: 293 K

| | Calculated | Reported |
|---|---|---|
| Volume | 3179.58(8) | 3179.58(8) |
| Space group | C c | Cc |
| Hall group | C -2yc | ? |

| | | |
|---|---|---|
| Moiety formula | C34 H28 Cl2 Fe Ni O2 P2 | ? |
| Sum formula | C34 H28 Cl2 Fe Ni O2 P2 | C34 H28 Cl2 Fe Ni O2 P2 |
| Mr | 715.94 | 715.96 |
| Dx,g cm-3 | 1.496 | 1.496 |
| Z | 4 | 4 |
| Mu (mm-1) | 1.347 | 1.347 |
| F000 | 1464.0 | 1464.0 |
| F000' | 1469.11 | |
| h,k,lmax | 11,22,19 | 11,23,19 |
| Nref | 2792[ 5573] | 4010 |
| Tmin,Tmax | | |
| Tmin' | | |

Correction method= Not given

Data completeness= 1.44/0.72 Theta(max)= 25.000

R(reflections)= 0.0354( 3799) wR2(reflections)= 0.1067( 4010)

S = 1.151 Npar= 344

---

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 A**

EXPT005_ALERT_1_A _exptl_crystal_description is missing

Crystal habit description.

The following tests will not be performed.

CRYSR_01

EXPT009_ALERT_1_A No crystal dimensions have been given.

The following tests will not be performed.

CRYSS_01,CRYSS_02

EXPT108_ALERT_1_A The magnitudes of the crystal dimensions do not

match the min, mid and max definitions

EXPT010_ALERT_1_A _exptl_crystal_colour (_pd_char_colour for powder) is missing

Crystal colour.

The following tests will not be performed.

CRYSC_01

ABSTY01_ALERT_1_A The absorption correction should be one of the following

* none
* analytical
* integration
* numerical
* gaussian
* empirical
* psi-scan
* multi-scan
* refdelf
* sphere
* cylinder

DENSX01_ALERT_1_A The ratio of the calculated to measured crystal density

lies outside the range 0.80 <> 1.20

Calculated density = 1.496

Measured density = 0.000

PLAT053_ALERT_1_A Minimum Crystal Dimension Missing (or Error) ... ?

PLAT054_ALERT_1_A Medium Crystal Dimension Missing (or Error) ... ?

PLAT055_ALERT_1_A Maximum Crystal Dimension Missing (or Error) ... ?

PLAT761_ALERT_1_A CIF Contains no X-H Bonds ..... ?

PLAT762_ALERT_1_A CIF Contains no X-Y-H or H-Y-H Angles ..... ?

---

**Alert level B**

PLAT052_ALERT_1_B Info on Absorption Correction Method Missing ... ?

PLAT093_ALERT_1_B No su's on H-atoms, but refinement reported as . mixed

PLAT201_ALERT_2_B Isotropic non-H Atoms in Main Residue(s) ..... 6

---

**Alert level C**

ABSTY02_ALERT_1_C An _exptl_absorpt_correction_type has been given without

a literature citation. This should be contained in the

_exptl_absorpt_process_details field.

Absorption correction given as Not Given

PLAT048_ALERT_1_C MoietyFormula Not Given ..... ?

PLAT125_ALERT_4_C No '_symmetry_space_group_name_Hall' Given ..... ?

PLAT143_ALERT_4_C su on c - Axis Small or Missing (x 100000) ..... 10 Ang.

PLAT145_ALERT_4_C su on beta Small or Missing (x 10000) ..... 0 Deg.

PLAT234_ALERT_4_C Large Hirshfeld Difference C24 -- C25 .. 0.16 Ang.

PLAT234_ALERT_4_C Large Hirshfeld Difference C25 -- C26 .. 0.22 Ang.

PLAT241_ALERT_2_C Check High Ueq as Compared to Neighbors for O1

PLAT241_ALERT_2_C Check High Ueq as Compared to Neighbors for C25

PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for Ni1

PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for C23

PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds (x 1000) Ang .. 11

---

**Datablock: Cu**

---

Bond precision: C-C = 0.0095 A Wavelength=0.71073

Cell: a=10.0444(2) b=19.4070(3) c=16.3157(1)

alpha=90 beta=91.3400 gamma=90

Temperature: 293 K

| | Calculated | Reported |
|---|---|---|
| Volume | 3179.58(8) | 3179.58(8) |
| Space group | C c | Cc |
| Hall group | C -2yc | ? |
| Moiety formula | C34 H28 Cl2 Cu Fe O2 P2 | ? |
| Sum formula | C34 H28 Cl2 Cu Fe O2 P2 | C34 H28 Cl2 Cu Fe O2 P2 |
| Mr | 720.80 | 720.79 |
| Dx,g cm-3 | 1.506 | 1.506 |
| Z | 4 | 4 |
| Mu (mm-1) | 1.424 | 1.424 |
| F000 | 1468.0 | 1468.0 |
| F000' | 1473.03 | |
| h,k,lmax | 11,22,19 | 11,23,19 |
| Nref | 2792[ 5573] | 4010 |
| Tmin,Tmax | | |
| Tmin' | | |

Correction method= Not given

Data completeness= 1.44/0.72 Theta(max)= 25.000

R(reflections)= 0.0330( 3799) wR2(reflections)= 0.1002( 4010)

S = 1.170 Npar= 344

---

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 A**

EXPT005_ALERT_1_A _exptl_crystal_description is missing

Crystal habit description.

The following tests will not be performed.

CRYSR_01

EXPT009_ALERT_1_A No crystal dimensions have been given.

The following tests will not be performed.

CRYSS_01,CRYSS_02

EXPT108_ALERT_1_A The magnitudes of the crystal dimensions do not

match the min, mid and max definitions

EXPT010_ALERT_1_A _exptl_crystal_colour (_pd_char_colour for powder) is missing

Crystal colour.

The following tests will not be performed.

CRYSC_01

DENSX01_ALERT_1_A The ratio of the calculated to measured crystal density

lies outside the range 0.80 <> 1.20

Calculated density = 1.506

Measured density = 0.000

PLAT053_ALERT_1_A Minimum Crystal Dimension Missing (or Error) ... ?

PLAT054_ALERT_1_A Medium Crystal Dimension Missing (or Error) ... ?

PLAT055_ALERT_1_A Maximum Crystal Dimension Missing (or Error) ... ?

PLAT761_ALERT_1_A CIF Contains no X-H Bonds ..... ?

PLAT762_ALERT_1_A CIF Contains no X-Y-H or H-Y-H Angles ..... ?

---

**Alert level B**

PLAT093_ALERT_1_B No su's on H-atoms, but refinement reported as . mixed

PLAT201_ALERT_2_B Isotropic non-H Atoms in Main Residue(s) ..... 6

---

**Alert level C**

PLAT048_ALERT_1_C MoietyFormula Not Given ..... ?

PLAT125_ALERT_4_C No '_symmetry_space_group_name_Hall' Given ..... ?

PLAT143_ALERT_4_C su on c - Axis Small or Missing (x 100000) ..... 10 Ang.

PLAT145_ALERT_4_C su on beta Small or Missing (x 10000) ..... 0 Deg.

PLAT234_ALERT_4_C Large Hirshfeld Difference C25 -- C26 .. 0.18 Ang.

PLAT241_ALERT_2_C Check High Ueq as Compared to Neighbors for O1

PLAT241_ALERT_2_C Check High Ueq as Compared to Neighbors for C25

PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for Cu1

PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for C23

PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds (x 1000) Ang .. 9

---

**Datablock: Zn**

---

Bond precision: C-C = 0.0095 A Wavelength=0.71073

Cell: a=10.0444(2) b=19.4070(3) c=16.3157(1)

alpha=90 beta=91.3400 gamma=90

Temperature: 293 K

| | Calculated | Reported |
|---|---|---|
| Volume | 3179.58(8) | 3179.58(8) |
| Space group | C c | ? |
| Hall group | C -2yc | ? |
| Moiety formula | C34 H28 Cl2 Fe O2 P2 Zn | ? |
| Sum formula | C34 H28 Cl2 Fe O2 P2 Zn | C34 H28 Cl2 Fe O2 P2 Zn |
| Mr | 722.64 | 722.62 |
| Dx,g cm-3 | 1.510 | 1.510 |
| Z | 4 | 4 |
| Mu (mm-1) | 1.510 | 1.510 |
| F000 | 1472.0 | 1472.0 |
| F000' | 1476.89 | |

| | | |
|---|---|---|
| h,k,lmax | 11,22,19 | 11,23,19 |
| Nref | 2792[ 5573] | 4010 |
| Tmin,Tmax | | |
| Tmin' | | |

Correction method= Not given

Data completeness= 1.44/0.72 Theta(max)= 25.000

R(reflections)= 0.0331( 3799) wR2(reflections)= 0.1000( 4010)

S = 1.180 Npar= 344

---

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 A**

SYMM001_ALERT_1_A _symmetry_cell_setting is missing

The cell setting should be one of the following

* triclinic
* monoclinic
* orthorhombic
* tetragonal
* rhombohedral
* trigonal
* hexagonal
* cubic

The following tests will not be performed.

SYMMS_01,SYMMS_02

SYMM003_ALERT_1_A _symmetry_space_group_name_H-M is missing

Space-group symbol, including unique axis.

The following tests will not be performed.

CELLZ_01,CHEMW_03,REFLT_03,SYMMG_01,SYMMG_02

CELL003_ALERT_1_A _cell_measurement_reflns_used is missing

Number of reflections used to measure unit cell.

CELL004_ALERT_1_A _cell_measurement_theta_min is missing

Minimum theta of reflections used to measure unit cell.

The following tests will not be performed.

CELLT_01

CELL005_ALERT_1_A _cell_measurement_theta_max is missing

Maximum theta of reflections used to measure unit cell.

The following tests will not be performed.

CELLT_01

EXPT005_ALERT_1_A _exptl_crystal_description is missing

Crystal habit description.

The following tests will not be performed.

CRYSR_01

EXPT009_ALERT_1_A No crystal dimensions have been given.

The following tests will not be performed.

CRYSS_01,CRYSS_02

EXPT108_ALERT_1_A The magnitudes of the crystal dimensions do not

match the min, mid and max definitions

EXPT010_ALERT_1_A _exptl_crystal_colour (_pd_char_colour for powder) is missing

Crystal colour.

The following tests will not be performed.

CRYSC_01

DIFF003_ALERT_1_A _diffrn_measurement_device_type is missing

Diffractometer make and type. Replaces _diffrn_measurement_type.

DIFF005_ALERT_1_A _diffrn_measurement_method is missing

Mode of intensity measurement and scan.

DIFF019_ALERT_1_A _diffrn_standards_number is missing

Number of standards used in measurement.

DIFF020_ALERT_1_A _diffrn_standards_interval_count and

_diffrn_standards_interval_time are missing. Number of measurements

between standards or time (min) between standards.

DIFF022_ALERT_1_A _diffrn_standards_decay_% is missing

Percentage decrease in standards intensity.

ABSTY01_ALERT_1_A The absorption correction should be one of the following

* none
* analytical
* integration
* numerical
* gaussian
* empirical

* psi-scan
* multi-scan
* refdelf
* sphere
* cylinder

PLAT053_ALERT_1_A Minimum Crystal Dimension Missing (or Error) ... ?

PLAT054_ALERT_1_A Medium Crystal Dimension Missing (or Error) ... ?

PLAT055_ALERT_1_A Maximum Crystal Dimension Missing (or Error) ... ?

PLAT122_ALERT_1_A No _symmetry_space_group_name_H-M Given ..... ?

PLAT761_ALERT_1_A CIF Contains no X-H Bonds ..... ?

PLAT762_ALERT_1_A CIF Contains no X-Y-H or H-Y-H Angles ..... ?

---

**Alert level B**

PLAT052_ALERT_1_B Info on Absorption Correction Method Missing ... ?

PLAT093_ALERT_1_B No su's on H-atoms, but refinement reported as . mixed

PLAT201_ALERT_2_B Isotropic non-H Atoms in Main Residue(s) ..... 6

---

**Alert level C**

ABSTY02_ALERT_1_C An _exptl_absorpt_correction_type has been given without
a literature citation. This should be contained in the
_exptl_absorpt_process_details field.
Absorption correction given as Not Given

PLAT048_ALERT_1_C MoietyFormula Not Given ..... ?

PLAT125_ALERT_4_C No '_symmetry_space_group_name_Hall' Given ..... ?

PLAT143_ALERT_4_C su on c - Axis Small or Missing (x 100000) ..... 10 Ang.

PLAT145_ALERT_4_C su on beta Small or Missing (x 10000) ..... 0 Deg.

PLAT234_ALERT_4_C Large Hirshfeld Difference C25 -- C26 .. 0.18 Ang.

PLAT241_ALERT_2_C Check High Ueq as Compared to Neighbors for O1

PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for Zn1

PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for C23

PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds (x 1000) Ang .. 9