Supplementary Information

Design Principles for High H_2 Storage Using Chelation of Abundant Transition Metals in Covalent Organic Frameworks for 0-700 bar at 298K

Yohanes Pramudya[1,2], Jose L. Mendoza-Cortes[1,2]

[1] Department of Chemical and Biomedical Engineering, College of Engineering, Florida State University and Florida A&M, Tallahassee, FL 32310

[2] Scientific Computing Department, Materials Science and Engineering Program, High Performance Material Institute, Condensed Matter Theory-National High Magnetic Field Laboratory, Florida State University, Tallahassee FL, 32310, USA.

E-mail: jmendozacortes@fsu.edu

Contents

List of Figures

1 Force Fields (FF) Fitting

The force fields fitting using Morse potential is performed using the optimized/relaxed geometry from molecular Quantum Mechanics in DFT level using hybrid B3LYP-D3 in Amsterdam Density Functional (ADF) 2016. General Utilities Lattice Program (GULP) is used to get the force fields parameter of the transition metals (Co(II), Cu(II), Fe(II), Mn(II), and Ni(II)) chelated in the ligands studied: (E)-N'-benzylidene-benzohydrazide (**BBH**), (E)-2- ((phenylimino) methyl) phenol (**PIP**), (E)-N-(pyridin-2-ylmethylene) aniline (**PIA**), 2,2'-bipyridine (**BPY**), and phenanthroline (**PHEN**) (shown in Figure S1).

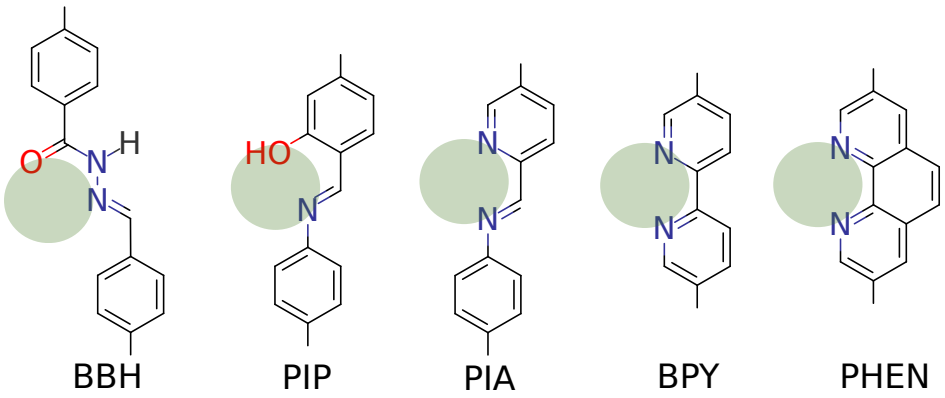

Figure S1: Linkers are used for the force fields fitting parameters where the chelation sites are shown in green circles.

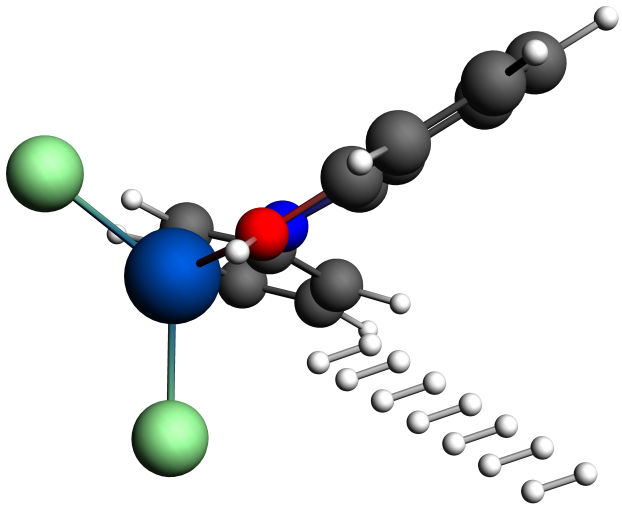

Figure S2: Chelated Tm in linkers used for the force field fitting parameters between Tm and molecule H_2. Multiple H_2 molecules represents the different distances between Tm and H_2

The scan of the H_2 binding enthalpy ΔH°_{bind} to ligands for different distances is presented in Figure S2. We only used the fitting for one molecule H_2 interact with Tm in the ligands to get the fitting parameters between Tm and H_2 molecules.

2 Geometries of the Ligand Molecules

Some of the optimized geometries of the chelated Tm in ligands are presented in Figure S3. The shape of the geometry depends on the the coordination number, ionization states, and spins of the transition metals.

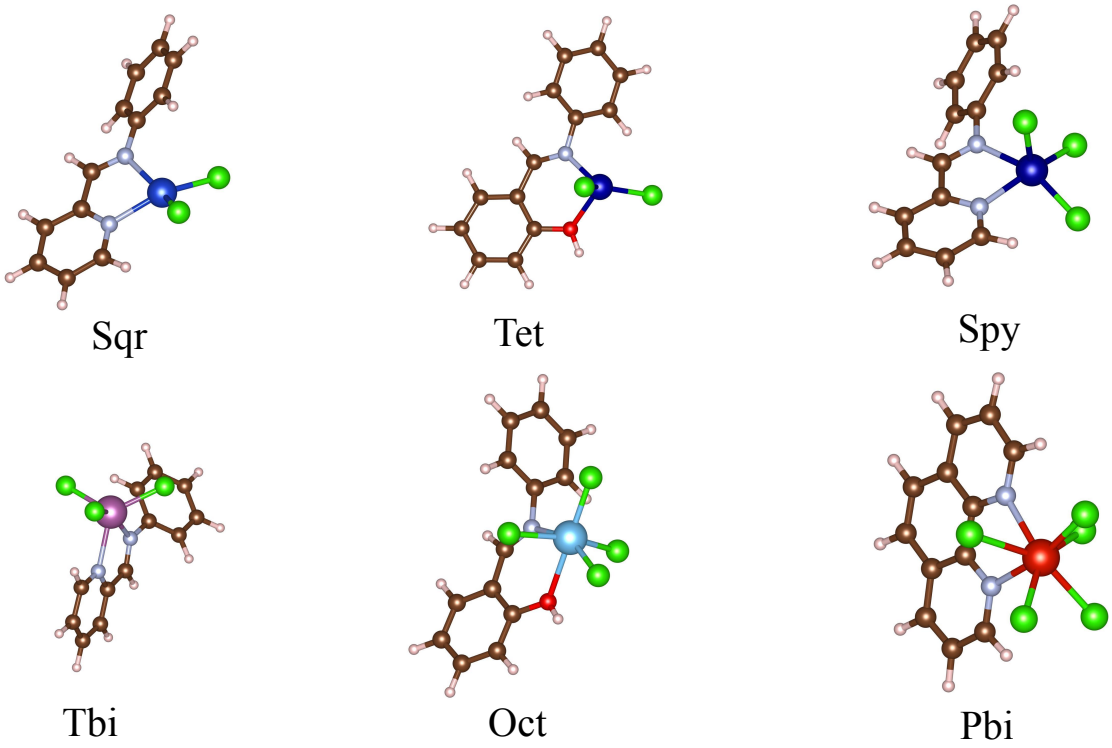

Figure S3: Different geometries of the transition metals Tm chelated by the ligands depend on the number of coordinations, ionization states, and spins. Square (Sqr) geometry is representated by $CuCl_2$ in **PIA**, tetrahedral (Tet) by $CoCl_2$ in **PIP**, square pyramidal (Spy) by $CrCl_3$ in **PIA**, trigonal bipyramidal (Tbi) by $ScCl_3$ in **PIA**, octahedral by $TiCl_4$ in **PIP**, and pentagonal bipyramidal (Pbi) by VCl_5 in **PHEN**.

3 Theoretical Method for Surface Area and Pore Volume

The surface area and pore volume were estimated using accessible solvent algorithm. The algorithm consists of placing a solvent molecule (probe) through the pore and then backtracking the surface and pore volume from this placement. For the surface area and pore volume, Connolly algorithm was tested. The Connolly algorithm consists of a ball rolling through a van der Waals surface, and getting the pore and surface area from backtracking it (Figure S4). The solvent radius of 1.71 Å was used and the illustration is shown in Figure S5. The solid areas are the surface and accessible volume of the COFs.

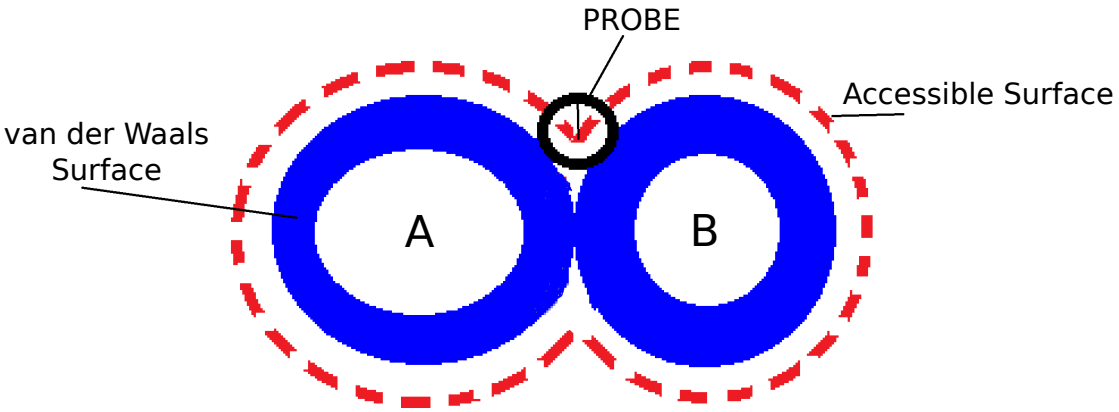

Figure S4: A solvent/probe (black circle) is rolled through the van der Waals Surface of molecule A and B to get the accessible surface.

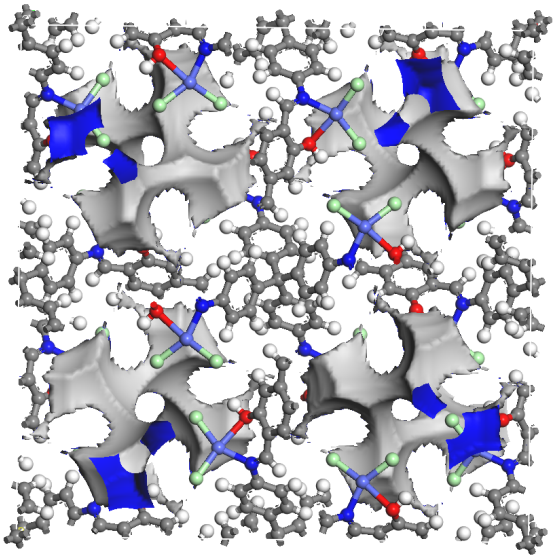

Figure S5: Accessible surface area and pore volume of COF-301-$CoCl_2$

4 Gravimetric Uptake Plots

For each framework, the total gravimetric uptakes (weight %) are presented in Figure S6.

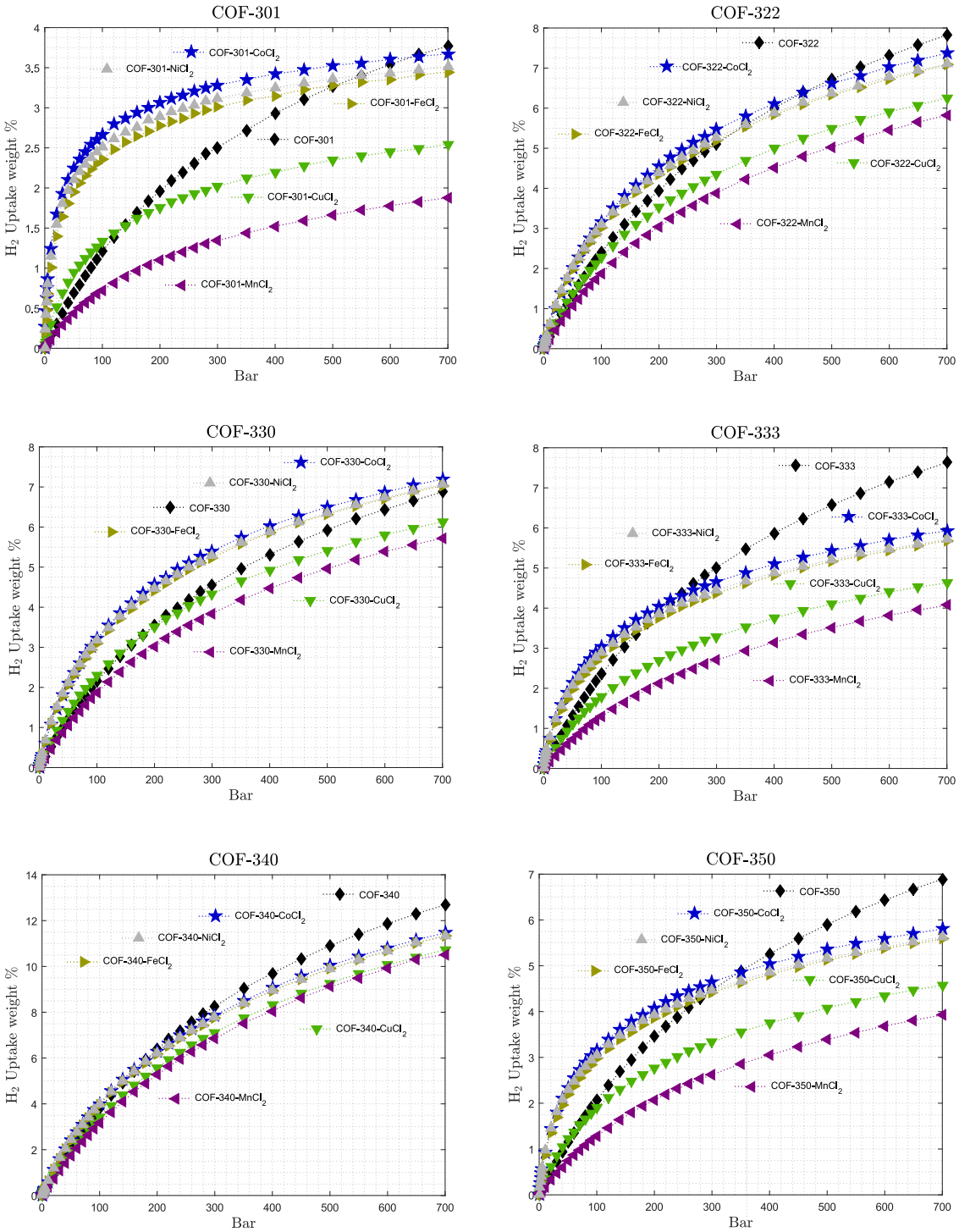

Figure S6: Total gravimetric density of H_2 uptake (% weight) from GCMC results in the range of 0-700 bar and 298 K.

5 Adsorption Isotherm Plots

For each framework, the isosteric heat Q_{st} values are represented in one plot and scaled to the maximum of each plot. The values of Q_{st} which contain first row transition metal have similar trend except in COF-301. In COF-301-$TmCl_2$, the Q_{st} does not drop significantly above 10 bar. In other COFs, the values drop between 30% - 50%. Ni(II), Co (II), and Fe (II) have very similar values coincide with the trend in the uptake followed by Cu(II) and Mn(II).

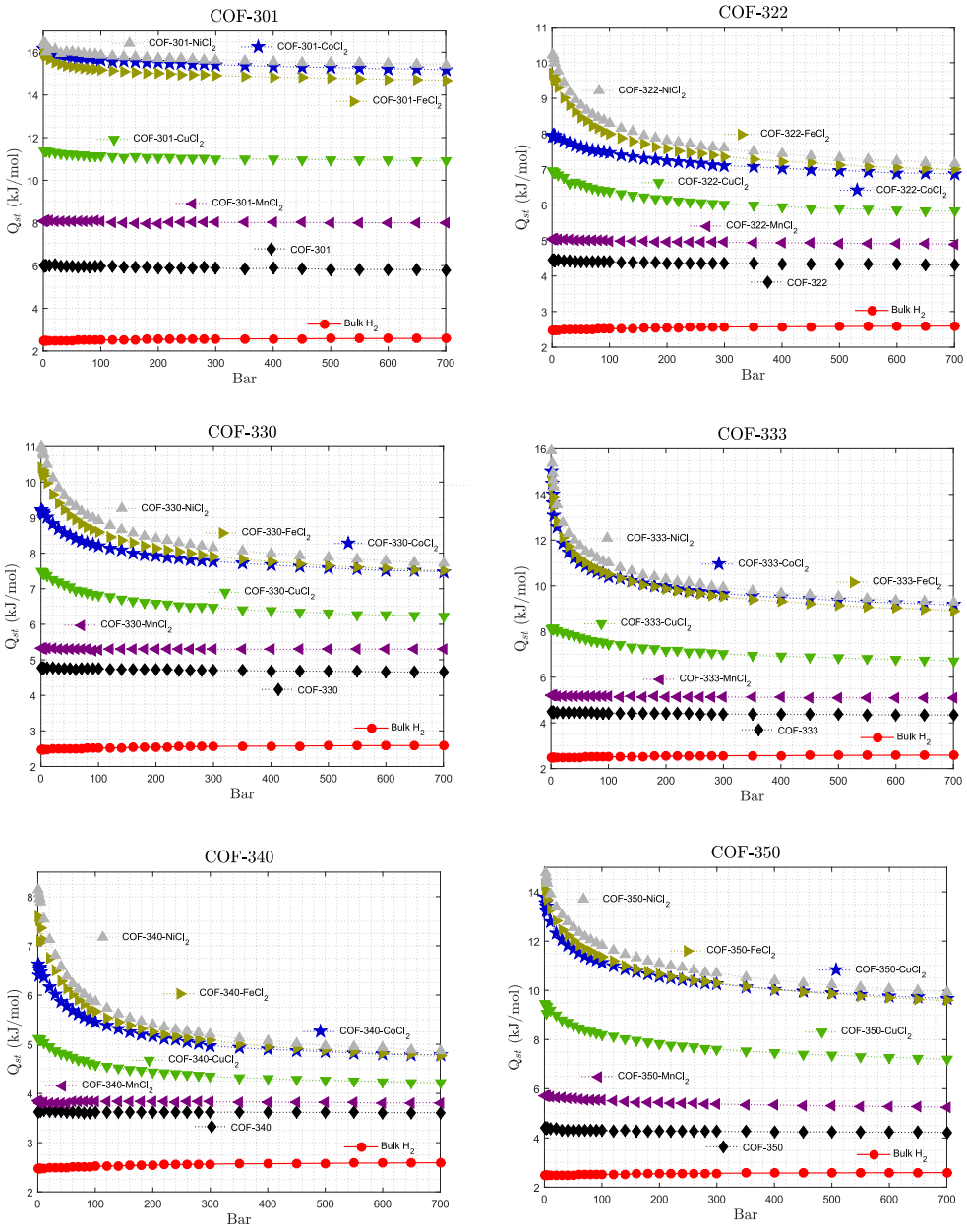

Figure S7: Isosteric heat of H_2 uptake from GCMC results in the range of 0-700 bar and 298 K.

6 Geometries of COFs

Some of the relaxed periodic structures of the frameworks are presented which were obtained from periodic Quantum Mechanics(QM) calculation using VASP. For the metalated version, one example of the geometry is shown.

6.1 COF-300

```
data_COF-300

_symmetry_space_group_name_H-M    'I41/A'
_symmetry_Int_Tables_number       88
_symmetry_cell_setting            tetragonal
loop_
_symmetry_equiv_pos_as_xyz
x,y,z
-x+1/2,-y+1/2,z+1/2
-y,x+1/2,z+1/4
y+1/2,-x,z+3/4
-x,-y+1/2,-z+1/4
x+1/2,y,-z+3/4
y,-x,-z
-y+1/2,x+1/2,-z+1/2
x+1/2,y+1/2,z+1/2
-x,-y,z
-y+1/2,x,z+3/4
y,-x+1/2,z+1/4
-x+1/2,-y,-z+3/4
x,y+1/2,-z+1/4
y+1/2,-x+1/2,-z+1/2
-y,x,-z
_cell_length_a                    28.2626
_cell_length_b                    28.2626
_cell_length_c                    8.8931
_cell_angle_alpha                 90.0000
_cell_angle_beta                  90.0000
_cell_angle_gamma                 90.0000
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
_atom_site_adp_type
_atom_site_occupancy
H1     H     0.44070  -0.54626   0.18384   0.01267  Uiso   1.00
H9     H     0.45941  -0.58793  -0.06631   0.01267  Uiso   1.00
H17    H     0.89872  -0.10599   0.23538   0.01267  Uiso   1.00
H25    H     0.99202  -0.12731   0.09402   0.01267  Uiso   1.00
H33    H     0.44197  -0.18666  -0.43932   0.01267  Uiso   1.00
H41    H     0.89412  -0.45826   0.13199   0.01267  Uiso   1.00
H49    H     0.57840  -0.22750  -0.26593   0.01267  Uiso   1.00
C1     C     1.04427  -0.23804   0.06307   0.01267  Uiso   1.00
C9     C     0.90939   0.01321   0.18530   0.01267  Uiso   1.00
C17    C     0.44184  -0.47697  -0.20206   0.01267  Uiso   1.00
```

```
C25    C     0.44528  -0.55974  -0.13677   0.01267  Uiso   1.00
C33    C     0.91208  -0.07002   0.25152   0.01267  Uiso   1.00
C41    C     0.89336  -0.03365   0.16112   0.01267  Uiso   1.00
C49    C     0.46009  -0.51313  -0.11023   0.01267  Uiso   1.00
C57    C     1.01134  -0.20242   0.09968   0.01267  Uiso   1.00
C65    C     0.51641  -0.15401  -0.29609   0.01267  Uiso   1.00
C73    C     0.53276  -0.28518  -0.33720   0.01267  Uiso   1.00
N1     N     0.85456  -0.54267   0.18077   0.01267  Uiso   1.00
C81    C     0.50000  -0.50000   0.00000   0.01267  Uiso   1.00
```

6.2 COF-320

```
data_COF-320

_symmetry_space_group_name_H-M    'I41/A'
_symmetry_Int_Tables_number       88
_symmetry_cell_setting            tetragonal
loop_
_symmetry_equiv_pos_as_xyz
x,y,z
-x+1/2,-y+1/2,z+1/2
-y,x+1/2,z+1/4
y+1/2,-x,z+3/4
-x,-y+1/2,-z+1/4
x+1/2,y,-z+3/4
y,-x,-z
-y+1/2,x+1/2,-z+1/2
x+1/2,y+1/2,z+1/2
-x,-y,z
-y+1/2,x,z+3/4
y,-x+1/2,z+1/4
-x+1/2,-y,-z+3/4
x,y+1/2,-z+1/4
y+1/2,-x+1/2,-z+1/2
-y,x,-z
_cell_length_a                    34.9863
_cell_length_b                    34.9863
_cell_length_c                    12.1462
_cell_angle_alpha                 90.0000
_cell_angle_beta                  90.0000
_cell_angle_gamma                 90.0000
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
_atom_site_adp_type
_atom_site_occupancy
H1     H    -0.44437  -0.52593  -0.36502   0.01267  Uiso   1.00
H9     H    -0.56145  -0.54859  -0.45099   0.01267  Uiso   1.00
H17    H    -0.44529  -0.57819  -0.23038   0.01267  Uiso   1.00
H25    H    -0.56278  -0.60159  -0.31509   0.01267  Uiso   1.00
H33    H    -0.16135  -0.56630  -0.22098   0.01267  Uiso   1.00
H41    H    -0.11498  -0.54075  -0.34789   0.01267  Uiso   1.00
H49    H    -0.23505  -0.44554  -0.22948   0.01267  Uiso   1.00
H57    H    -0.17781  -0.45227  -0.34574   0.01267  Uiso   1.00
H65    H    -0.21814  -0.56016  -0.10594   0.01267  Uiso   1.00
```

```
C1     C    -0.47101  -0.57229  -0.27810   0.01267  Uiso   1.00
C9     C    -0.50222  -0.53428  -0.42076   0.01267  Uiso   1.00
C17    C    -0.53584  -0.55512  -0.40354   0.01267  Uiso   1.00
C25    C    -0.53684  -0.58473  -0.32678   0.01267  Uiso   1.00
C33    C    -0.47024  -0.54294  -0.35498   0.01267  Uiso   1.00
C41    C    -0.50471  -0.59395  -0.26287   0.01267  Uiso   1.00
C49    C    -0.17775  -0.53968  -0.22300   0.01267  Uiso   1.00
C57    C    -0.16575  -0.51000  -0.29313   0.01267  Uiso   1.00
C65    C    -0.13249  -0.51506  -0.36400   0.01267  Uiso   1.00
C73    C    -0.18722  -0.47586  -0.29327   0.01267  Uiso   1.00
C81    C    -0.21026  -0.53604  -0.15793   0.01267  Uiso   1.00
C89    C    -0.23244  -0.50230  -0.15878   0.01267  Uiso   1.00
C97    C    -0.21947  -0.47245  -0.22757   0.01267  Uiso   1.00
N1     N    -0.00915  -0.12467  -0.69051   0.01267  Uiso   1.00
C105   C    -0.50000  -0.50000  -0.50000   0.01267  Uiso   1.00
```

6.3 COF-322

```
data_COF-322

_symmetry_space_group_name_H-M    'I41'
_symmetry_Int_Tables_number       80
_symmetry_cell_setting            tetragonal
loop_
_symmetry_equiv_pos_as_xyz
x,y,z
-x+1/2,-y+1/2,z+1/2
-y,x+1/2,z+1/4
y+1/2,-x,z+3/4
x+1/2,y+1/2,z+1/2
-x,-y,z
-y+1/2,x,z+3/4
y,-x+1/2,z+1/4
_cell_length_a                    36.2836
_cell_length_b                    36.2836
_cell_length_c                    11.7221
_cell_angle_alpha                 90.0000
_cell_angle_beta                  90.0000
_cell_angle_gamma                 90.0000
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
_atom_site_adp_type
_atom_site_occupancy
C1     C     0.26525   0.50620   0.29648   0.01267  Uiso   1.00
C5     C     0.20493   0.54450   0.22629   0.01267  Uiso   1.00
C9     C    -0.02898   0.57180   0.39912   0.01267  Uiso   1.00
C13    C     0.47113   0.04612  -0.03297   0.01267  Uiso   1.00
C17    C     0.50076   0.03437   0.02699   0.01267  Uiso   1.00
C21    C     0.53060   0.05302  -0.00509   0.01267  Uiso   1.00
C25    C     0.00033   0.59315   0.36853   0.01267  Uiso   1.00
C29    C     0.53141   0.07921  -0.07371   0.01267  Uiso   1.00
C33    C     0.02458   0.68899   0.15313   0.01267  Uiso   1.00
```

```
C37    C    -0.01595   0.63919   0.24523   0.01267  Uiso   1.00
C41    C     0.52317   0.33482   0.33838   0.01267  Uiso   1.00
C45    C     0.52336   0.36926   0.25234   0.01267  Uiso   1.00
C49    C     0.49469   0.31037   0.34386   0.01267  Uiso   1.00
C53    C     0.50412   0.40878   0.11427   0.01267  Uiso   1.00
C57    C     0.47205   0.44509  -0.01846   0.01267  Uiso   1.00
C61    C     0.53052   0.45658   0.01148   0.01267  Uiso   1.00
C65    C     0.22479   0.51468   0.21654   0.01267  Uiso   1.00
C69    C     0.53208   0.43160   0.08208   0.01267  Uiso   1.00
C73    C     0.28360   0.53250   0.34865   0.01267  Uiso   1.00
C77    C    -0.01007   0.67481   0.16653   0.01267  Uiso   1.00
C81    C     0.54797   0.32281   0.41596   0.01267  Uiso   1.00
C85    C     0.47265   0.41928   0.05237   0.01267  Uiso   1.00
C89    C     0.50023   0.46574  -0.05017   0.01267  Uiso   1.00
C93    C    -0.03227   0.69732   0.10604   0.01267  Uiso   1.00
N1     N     0.27477   0.47042   0.29814   0.01267  Uiso   1.00
N5     N     0.00383   0.62708   0.28763   0.01267  Uiso   1.00
N9     N     0.50327   0.37604   0.20040   0.01267  Uiso   1.00
N13    N     0.21723   0.48665   0.14482   0.01267  Uiso   1.00
H1     H     0.27315   0.56741   0.34058   0.01267  Uiso   1.00
H5     H     0.21320   0.57028   0.29985   0.01267  Uiso   1.00
H9     H     0.05041   0.67001   0.20616   0.01267  Uiso   1.00
H13    H     0.46667   0.31959   0.26803   0.01267  Uiso   1.00
H17    H    -0.05998   0.58200   0.34670   0.01267  Uiso   1.00
H21    H     0.06237   0.59704   0.40251   0.01267  Uiso   1.00
H25    H     0.56258   0.04312   0.03949   0.01267  Uiso   1.00
H29    H    -0.06957   0.68632   0.11024   0.01267  Uiso   1.00
H33    H    -0.05285   0.63289   0.23499   0.01267  Uiso   1.00
H37    H     0.07813   0.84348  -0.07525   0.01267  Uiso   1.00
H41    H     0.55693   0.38431   0.27458   0.01267  Uiso   1.00
H45    H     0.44300   0.39942   0.07546   0.01267  Uiso   1.00
H49    H     0.43955   0.45214  -0.06613   0.01267  Uiso   1.00
H53    H     0.06066  -0.02378   0.49317   0.01267  Uiso   1.00
H57    H     0.43984   0.02815  -0.01527   0.01267  Uiso   1.00
H61    H     0.56360   0.42424   0.13568   0.01267  Uiso   1.00
C97    C     0.50000   0.00000   0.11318   0.01267  Uiso   1.00
```

6.4 COF-330

```
data_COF330

_symmetry_space_group_name_H-M    'I41'
_symmetry_Int_Tables_number       80
_symmetry_cell_setting            tetragonal
loop_
_symmetry_equiv_pos_as_xyz
x,y,z
-x+1/2,-y+1/2,z+1/2
-y,x+1/2,z+1/4
y+1/2,-x,z+3/4
x+1/2,y+1/2,z+1/2
-x,-y,z
-y+1/2,x,z+3/4
y,-x+1/2,z+1/4
_cell_length_a                    33.1193
_cell_length_b                    33.1193
_cell_length_c                    12.7065
```

```
_cell_angle_alpha                 90.0000
_cell_angle_beta                  90.0000
_cell_angle_gamma                 90.0000
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
_atom_site_adp_type
_atom_site_occupancy
H1     H    -0.08171   0.05750  -0.62941   0.01267  Uiso   1.00
H5     H    -0.52620  -0.44134  -0.00087   0.01267  Uiso   1.00
H9     H    -0.05426  -0.06453  -0.41172   0.01267  Uiso   1.00
H13    H    -0.10919  -0.06545  -0.54084   0.01267  Uiso   1.00
H17    H    -0.10567   0.02907  -0.77902   0.01267  Uiso   1.00
H21    H     0.36746  -0.46125  -0.45242   0.01267  Uiso   1.00
H25    H    -0.35603  -0.03368  -0.02799   0.01267  Uiso   1.00
H29    H    -0.38996  -0.02879  -0.20372   0.01267  Uiso   1.00
H33    H    -0.38923   0.06413  -0.44959   0.01267  Uiso   1.00
H37    H     0.05501  -0.43645  -0.08074   0.01267  Uiso   1.00
H41    H    -0.47439  -0.05849  -0.48513   0.01267  Uiso   1.00
H45    H    -0.41939  -0.05690  -0.35401   0.01267  Uiso   1.00
H49    H    -0.20967  -0.01972  -0.72129   0.01267  Uiso   1.00
H53    H    -0.29303   0.02236  -0.28957   0.01267  Uiso   1.00
H57    H    -0.22041   0.04439  -0.25420   0.01267  Uiso   1.00
H61    H    -0.16259   0.05016  -0.13298   0.01267  Uiso   1.00
H65    H    -0.40137  -0.28981  -0.18336   0.01267  Uiso   1.00
H69    H    -0.39764  -0.27954  -0.06365   0.01267  Uiso   1.00
H73    H    -0.53651  -0.29533  -0.01276   0.01267  Uiso   1.00
H77    H    -0.51668  -0.33794  -0.01833   0.01267  Uiso   1.00
C1     C    -0.48422   0.26020  -0.39137   0.01267  Uiso   1.00
C5     C    -0.49885   0.26356  -0.28631   0.01267  Uiso   1.00
C9     C    -0.07567   0.03043  -0.58246   0.01267  Uiso   1.00
C13    C    -0.04465   0.03141  -0.50897   0.01267  Uiso   1.00
C17    C    -0.03664  -0.00232  -0.44422   0.01267  Uiso   1.00
C21    C    -0.06009  -0.03726  -0.45747   0.01267  Uiso   1.00
C25    C    -0.09145  -0.03801  -0.53065   0.01267  Uiso   1.00
C29    C    -0.09994  -0.00440  -0.59523   0.01267  Uiso   1.00
C33    C     0.29621  -0.50759  -0.30031   0.01267  Uiso   1.00
C37    C    -0.13209   0.01123  -0.75436   0.01267  Uiso   1.00
C41    C    -0.16573   0.00946  -0.82807   0.01267  Uiso   1.00
C45    C     0.33888  -0.47503  -0.42933   0.01267  Uiso   1.00
C49    C    -0.32932  -0.01950  -0.06327   0.01267  Uiso   1.00
C53    C    -0.32906  -0.00556  -0.16841   0.01267  Uiso   1.00
C57    C    -0.36509  -0.00977  -0.23323   0.01267  Uiso   1.00
C61    C    -0.29372   0.01201  -0.20770   0.01267  Uiso   1.00
C65    C    -0.40070   0.00477  -0.39012   0.01267  Uiso   1.00
C69    C    -0.40878   0.03781  -0.45695   0.01267  Uiso   1.00
C73    C    -0.43985   0.03711  -0.53070   0.01267  Uiso   1.00
C77    C     0.03638  -0.49771  -0.04249   0.01267  Uiso   1.00
C81    C    -0.45588  -0.03120  -0.47632   0.01267  Uiso   1.00
C85    C    -0.42525  -0.02993  -0.40165   0.01267  Uiso   1.00
C89    C    -0.47758   0.19324  -0.25101   0.01267  Uiso   1.00
C93    C     0.00471  -0.27003  -0.71578   0.01267  Uiso   1.00
C97    C    -0.22271   0.03350  -0.17410   0.01267  Uiso   1.00
C101   C    -0.19075   0.03682  -0.10701   0.01267  Uiso   1.00
N1     N    -0.01653  -0.20229  -0.74980   0.01267  Uiso   1.00
```

```
N5     N    -0.00917  -0.26527  -0.61618   0.01267  Uiso   1.00
N9     N    -0.13224  -0.00755  -0.66567   0.01267  Uiso   1.00
N13    N    -0.36789   0.00876  -0.32227   0.01267  Uiso   1.00
Zn1    Zn   -0.46528  -0.29690  -0.08155   0.01267  Uiso   1.00
Cl1    Cl   -0.46306  -0.28192   0.09303   0.01267  Uiso   1.00
Cl5    Cl   -0.43813  -0.36066  -0.09398   0.01267  Uiso   1.00
O1     O    -0.53329  -0.31879  -0.05902   0.01267  Uiso   1.00
O5     O    -0.40608  -0.26815  -0.13199   0.01267  Uiso   1.00
C105   C     0.00000  -0.50000  -0.11878   0.01267  Uiso   1.00
```

6.5 COF-333

```
data_COF-333

_symmetry_space_group_name_H-M    'I41/A'
_symmetry_Int_Tables_number       88
_symmetry_cell_setting            tetragonal
loop_
_symmetry_equiv_pos_as_xyz
x,y,z
-x+1/2,-y+1/2,z+1/2
-y,x+1/2,z+1/4
y+1/2,-x,z+3/4
-x,-y+1/2,-z+1/4
x+1/2,y,-z+3/4
y,-x,-z
-y+1/2,x+1/2,-z+1/2
x+1/2,y+1/2,z+1/2
-x,-y,z
-y+1/2,x,z+3/4
y,-x+1/2,z+1/4
-x+1/2,-y,-z+3/4
x,y+1/2,-z+1/4
y+1/2,-x+1/2,-z+1/2
-y,x,-z
_cell_length_a                    34.7108
_cell_length_b                    34.7108
_cell_length_c                    12.1061
_cell_angle_alpha                 90.0000
_cell_angle_beta                  90.0000
_cell_angle_gamma                 90.0000
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
_atom_site_adp_type
_atom_site_occupancy
C1     C     0.76754   0.00276  -0.09156   0.01267  Uiso   1.00
C9     C     0.78953   0.03687  -0.09370   0.01267  Uiso   1.00
C17    C     0.78159  -0.02670  -0.02094   0.01267  Uiso   1.00
C25    C     0.45698  -0.47001  -0.14554   0.01267  Uiso   1.00
C33    C     0.42744  -0.47084  -0.22270   0.01267  Uiso   1.00
C41    C     0.46563  -0.50226  -0.07958   0.01267  Uiso   1.00
C49    C     0.44475  -0.53614  -0.09636   0.01267  Uiso   1.00
```

```
C57    C     0.41499  -0.53727  -0.17332   0.01267  Uiso   1.00
C65    C     0.40565  -0.50494  -0.23761   0.01267  Uiso   1.00
C73    C     0.83276   0.00920   0.04140   0.01267  Uiso   1.00
C81    C     0.86636   0.01390   0.11342   0.01267  Uiso   1.00
C89    C     0.82215   0.04001  -0.02777   0.01267  Uiso   1.00
H1     H     0.78154   0.06111  -0.14609   0.01267  Uiso   1.00
H9     H     0.42144  -0.44491  -0.27092   0.01267  Uiso   1.00
H17    H     0.39791  -0.56329  -0.18552   0.01267  Uiso   1.00
H25    H     0.88379   0.03989   0.09608   0.01267  Uiso   1.00
H33    H     0.47411  -0.44397  -0.13503   0.01267  Uiso   1.00
H41    H     0.76682  -0.05447  -0.01653   0.01267  Uiso   1.00
H49    H     0.45141  -0.56176  -0.04838   0.01267  Uiso   1.00
H57    H     0.83957   0.06632  -0.02766   0.01267  Uiso   1.00
N1     N     0.81250  -0.02407   0.04311   0.01267  Uiso   1.00
N9     N     0.87449  -0.01016   0.19076   0.01267  Uiso   1.00
C97    C     0.50000  -0.50000  -0.00000   0.01267  Uiso   1.00
```

6.6 COF-340

```
data_COF-340

_symmetry_space_group_name_H-M    'I41'
_symmetry_Int_Tables_number       80
_symmetry_cell_setting            tetragonal
loop_
_symmetry_equiv_pos_as_xyz
x,y,z
-x+1/2,-y+1/2,z+1/2
-y,x+1/2,z+1/4
y+1/2,-x,z+3/4
x+1/2,y+1/2,z+1/2
-x,-y,z
-y+1/2,x,z+3/4
y,-x+1/2,z+1/4
_cell_length_a                    48.1247
_cell_length_b                    48.1247
_cell_length_c                    16.1129
_cell_angle_alpha                 90.0000
_cell_angle_beta                  90.0000
_cell_angle_gamma                 90.0000
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
_atom_site_adp_type
_atom_site_occupancy
H1     H    -0.55852   0.32736  -0.42795   0.01267  Uiso   1.00
H5     H    -0.04779   0.04201  -0.58096   0.01267  Uiso   1.00
H9     H    -0.51287  -0.45923   0.03055   0.01267  Uiso   1.00
H13    H    -0.04140  -0.04004  -0.39368   0.01267  Uiso   1.00
H17    H    -0.07691  -0.03886  -0.50607   0.01267  Uiso   1.00
H21    H    -0.08383   0.03980  -0.65820   0.01267  Uiso   1.00
H25    H    -0.11365   0.05674  -0.76784   0.01267  Uiso   1.00
H29    H    -0.37025  -0.06258  -0.26305   0.01267  Uiso   1.00
H33    H    -0.40400  -0.04299  -0.35667   0.01267  Uiso   1.00
```

H37	H	-0.41982	0.03890	-0.48468	0.01267	Uiso	1.00
H41	H	0.04011	-0.45905	-0.08214	0.01267	Uiso	1.00
H45	H	-0.48494	-0.04057	-0.50317	0.01267	Uiso	1.00
H49	H	-0.44539	-0.04279	-0.40635	0.01267	Uiso	1.00
H53	H	0.04894	-0.34902	-0.62236	0.01267	Uiso	1.00
H57	H	-0.03807	-0.34725	-0.56007	0.01267	Uiso	1.00
H61	H	-0.47269	-0.20035	-0.07574	0.01267	Uiso	1.00
H65	H	-0.52776	-0.16136	-0.25220	0.01267	Uiso	1.00
H69	H	-0.53846	-0.18604	-0.38025	0.01267	Uiso	1.00
H73	H	-0.03394	-0.72836	0.03109	0.01267	Uiso	1.00
H77	H	-0.46073	-0.30940	-0.30401	0.01267	Uiso	1.00
H81	H	-0.01514	-0.77504	0.00922	0.01267	Uiso	1.00
H85	H	-0.47154	0.32195	-0.48882	0.01267	Uiso	1.00
H89	H	-0.11567	-0.03010	-0.70332	0.01267	Uiso	1.00
H93	H	-0.36497	0.02428	-0.32542	0.01267	Uiso	1.00
C1	C	0.00093	-0.32253	-0.65604	0.01267	Uiso	1.00
C5	C	-0.49149	0.33250	-0.49513	0.01267	Uiso	1.00
C9	C	-0.51476	0.32165	-0.45290	0.01267	Uiso	1.00
C13	C	-0.54024	0.33582	-0.45911	0.01267	Uiso	1.00
C17	C	-0.04711	0.02416	-0.53919	0.01267	Uiso	1.00
C21	C	-0.02740	0.02353	-0.47629	0.01267	Uiso	1.00
C25	C	-0.02492	0.00064	-0.42205	0.01267	Uiso	1.00
C29	C	-0.04305	-0.02177	-0.43332	0.01267	Uiso	1.00
C33	C	-0.06289	-0.02132	-0.49649	0.01267	Uiso	1.00
C37	C	-0.06530	0.00141	-0.55075	0.01267	Uiso	1.00
C41	C	-0.12373	-0.01308	-0.74102	0.01267	Uiso	1.00
C45	C	-0.09216	0.01842	-0.66281	0.01267	Uiso	1.00
C49	C	-0.11261	0.01369	-0.72812	0.01267	Uiso	1.00
C53	C	-0.12210	0.03588	-0.77745	0.01267	Uiso	1.00
C57	C	-0.35975	-0.04249	-0.25736	0.01267	Uiso	1.00
C61	C	-0.37034	-0.01926	-0.30005	0.01267	Uiso	1.00
C65	C	-0.39509	-0.02184	-0.35204	0.01267	Uiso	1.00
C69	C	-0.35639	0.00639	-0.29268	0.01267	Uiso	1.00
C73	C	-0.42878	-0.00221	-0.44133	0.01267	Uiso	1.00
C77	C	-0.43407	0.02136	-0.49035	0.01267	Uiso	1.00
C81	C	0.04353	-0.47772	-0.04522	0.01267	Uiso	1.00
C85	C	0.02545	-0.50037	-0.05313	0.01267	Uiso	1.00
C89	C	-0.47014	-0.02342	-0.50080	0.01267	Uiso	1.00
C93	C	-0.44778	-0.02461	-0.44628	0.01267	Uiso	1.00
C97	C	0.03155	-0.35716	-0.58630	0.01267	Uiso	1.00
C101	C	0.00502	-0.34548	-0.59751	0.01267	Uiso	1.00
C105	C	-0.01729	-0.35566	-0.54971	0.01267	Uiso	1.00
C109	C	-0.48351	-0.20035	-0.13557	0.01267	Uiso	1.00
C113	C	-0.49382	-0.22388	-0.25577	0.01267	Uiso	1.00
C117	C	-0.51134	-0.20177	-0.28361	0.01267	Uiso	1.00
C121	C	-0.51454	-0.17851	-0.23184	0.01267	Uiso	1.00
C125	C	-0.52548	-0.20354	-0.36144	0.01267	Uiso	1.00
C129	C	-0.52302	-0.22667	-0.40979	0.01267	Uiso	1.00
C133	C	-0.50628	-0.24965	-0.38355	0.01267	Uiso	1.00
C137	C	-0.49125	-0.24854	-0.30710	0.01267	Uiso	1.00
C141	C	-0.47349	-0.29232	-0.32795	0.01267	Uiso	1.00
C145	C	-0.48766	-0.29587	-0.40475	0.01267	Uiso	1.00
C149	C	-0.50410	-0.27391	-0.43164	0.01267	Uiso	1.00
N1	N	-0.08511	-0.00145	-0.61357	0.01267	Uiso	1.00
N5	N	-0.40525	-0.00066	-0.39042	0.01267	Uiso	1.00
N9	N	-0.48002	-0.22259	-0.18257	0.01267	Uiso	1.00
N13	N	-0.47512	-0.26989	-0.28084	0.01267	Uiso	1.00
C153	C	0.00000	-0.50000	-0.11137	0.01267	Uiso	1.00

6.7 COF-350

```
data_COF-350

_symmetry_space_group_name_H-M    'I41'
_symmetry_Int_Tables_number       80
_symmetry_cell_setting            tetragonal
loop_
_symmetry_equiv_pos_as_xyz
x,y,z
-x+1/2,-y+1/2,z+1/2
-y,x+1/2,z+1/4
y+1/2,-x,z+3/4
x+1/2,y+1/2,z+1/2
-x,-y,z
-y+1/2,x,z+3/4
y,-x+1/2,z+1/4
_cell_length_a                    32.7572
_cell_length_b                    32.7572
_cell_length_c                    12.8057
_cell_angle_alpha                 90.0000
_cell_angle_beta                  90.0000
_cell_angle_gamma                 90.0000
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
_atom_site_adp_type
_atom_site_occupancy
H1     H     0.43121   0.88548   0.48906   0.01267  Uiso   1.00
H5     H     0.93663   0.44131   0.11597   0.01267  Uiso   1.00
H9     H     0.55167   0.97773   0.47881   0.01267  Uiso   1.00
H13    H     0.54584   0.92241   0.35007   0.01267  Uiso   1.00
H17    H     0.44968   0.58704   0.64512   0.01267  Uiso   1.00
H21    H     0.44831   0.52472   0.53918   0.01267  Uiso   1.00
H25    H     0.06399   0.05692   0.90092   0.01267  Uiso   1.00
H29    H     0.56578   0.61975   0.50670   0.01267  Uiso   1.00
H33    H     0.38786   0.77299   0.80589   0.01267  Uiso   1.00
H37    H     0.88711   0.32369   0.44821   0.01267  Uiso   1.00
H41    H     0.34629   0.03719   0.92983   0.01267  Uiso   1.00
H45    H     0.79503   0.50808   0.51913   0.01267  Uiso   1.00
H49    H     0.78325   0.49526   0.69292   0.01267  Uiso   1.00
H53    H     0.73157   0.49618   0.83045   0.01267  Uiso   1.00
H57    H     0.47838   0.80643   0.21624   0.01267  Uiso   1.00
H61    H     0.83750   0.99701   0.60449   0.01267  Uiso   1.00
O1     O     0.92155   0.36762   0.58733   0.01267  Uiso   1.00
O5     O     0.41240   0.70350   0.72238   0.01267  Uiso   1.00
C1     C     0.24280   0.55688   0.60985   0.01267  Uiso   1.00
C5     C     0.24135   0.52724   0.69040   0.01267  Uiso   1.00
C9     C     0.45768   0.90570   0.48592   0.01267  Uiso   1.00
C13    C     0.46113   0.93717   0.55937   0.01267  Uiso   1.00
C17    C     0.49528   0.96295   0.55968   0.01267  Uiso   1.00
C21    C     0.52562   0.95701   0.48301   0.01267  Uiso   1.00
C25    C     0.52235   0.92582   0.40996   0.01267  Uiso   1.00
C29    C     0.48810   0.89992   0.41043   0.01267  Uiso   1.00
C33    C     0.94170   0.33436   0.60023   0.01267  Uiso   1.00
```

```
C37    C     0.44429   0.71464   0.77160   0.01267  Uiso   1.00
C41    C     0.50652   0.60955   0.57819   0.01267  Uiso   1.00
C45    C     0.47386   0.58176   0.58820   0.01267  Uiso   1.00
C49    C     0.47337   0.54633   0.52864   0.01267  Uiso   1.00
C53    C     0.00451   0.03772   0.95608   0.01267  Uiso   1.00
C57    C     0.53844   0.56392   0.45235   0.01267  Uiso   1.00
C61    C     0.53952   0.59927   0.51295   0.01267  Uiso   1.00
C65    C     0.30097   0.55834   0.77393   0.01267  Uiso   1.00
C69    C     0.27006   0.52786   0.77147   0.01267  Uiso   1.00
C73    C     0.48581   0.86562   0.33660   0.01267  Uiso   1.00
C77    C     0.50826   0.64619   0.64136   0.01267  Uiso   1.00
C81    C     0.41144   0.77191   0.86601   0.01267  Uiso   1.00
C85    C     0.91079   0.30032   0.44691   0.01267  Uiso   1.00
N1     N     0.46489   0.86733   0.24998   0.01267  Uiso   1.00
N5     N     0.46450   0.83244   0.18851   0.01267  Uiso   1.00
N9     N     0.48017   0.69939   0.73573   0.01267  Uiso   1.00
N13    N     0.47617   0.66886   0.66106   0.01267  Uiso   1.00
C89    C    -0.00000   0.00000   0.88471   0.01267  Uiso   1.00
```

6.8 Metalated COF-301 example: COF-301-CoCl2

```
data_COF-301-CoCl2

_symmetry_space_group_name_H-M    'I41/A'
_symmetry_Int_Tables_number       88
_symmetry_cell_setting            tetragonal
loop_
_symmetry_equiv_pos_as_xyz
x,y,z
-x+1/2,-y+1/2,z+1/2
-y,x+1/2,z+1/4
y+1/2,-x,z+3/4
-x,-y+1/2,-z+1/4
x+1/2,y,-z+3/4
y,-x,-z
-y+1/2,x+1/2,-z+1/2
x+1/2,y+1/2,z+1/2
-x,-y,z
-y+1/2,x,z+3/4
y,-x+1/2,z+1/4
-x+1/2,-y,-z+3/4
x,y+1/2,-z+1/4
y+1/2,-x+1/2,-z+1/2
-y,x,-z
_cell_length_a                    28.8135
_cell_length_b                    28.8135
_cell_length_c                    8.7546
_cell_angle_alpha                 90.0000
_cell_angle_beta                  90.0000
_cell_angle_gamma                 90.0000
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
_atom_site_adp_type
_atom_site_occupancy
```

```
C1     C     0.48064   0.71291   0.20660   0.01267  Uiso   1.00
C9     C     0.51126   0.70385   0.08480   0.01267  Uiso   1.00
C17    C     0.51679   0.65676   0.03478   0.01267  Uiso   1.00
C25    C     0.03045   0.24208   0.50362   0.01267  Uiso   1.00
C33    C     0.53600   0.60408  -0.16033   0.01267  Uiso   1.00
C41    C     0.07034   1.08616   0.24324   0.01267  Uiso   1.00
C49    C     0.05937   1.05393   0.13066   0.01267  Uiso   1.00
C57    C     0.01371   1.03862   0.11197   0.01267  Uiso   1.00
C65    C    -0.02045   1.05556   0.21282   0.01267  Uiso   1.00
C73    C     0.49000   0.58799  -0.17586   0.01267  Uiso   1.00
N1     N     0.54672   0.64281  -0.06850   0.01267  Uiso   1.00
H1     H     0.46567   0.68413   0.27097   0.01267  Uiso   1.00
H9     H     0.49043   0.63249   0.07586   0.01267  Uiso   1.00
H17    H     0.10597   1.09770   0.25731   0.01267  Uiso   1.00
H25    H     0.08668   1.04116   0.05536   0.01267  Uiso   1.00
H33    H    -0.05620   1.04333   0.20215   0.01267  Uiso   1.00
H41    H     0.46191   0.60166  -0.10552   0.01267  Uiso   1.00
H49    H     0.75671   0.41743   0.13414   0.01267  Uiso   1.00
O1     O     0.05881   0.23242   0.38283   0.01267  Uiso   1.00
Co1    Co    0.67275   0.38835   0.07326   0.01267  Uiso   1.00
Cl1    Cl    0.11352   0.84642   0.50175   0.01267  Uiso   1.00
Cl9    Cl    0.73064   0.34314   0.11815   0.01267  Uiso   1.00
C81    C     0.50000   0.50000   0.50000   0.01267  Uiso   1.00
```

6.9 Metalated COF-322 example: COF-322-PdCl2

```
data_COF-322-PdCl2

_symmetry_space_group_name_H-M    'I41'
_symmetry_Int_Tables_number       80
_symmetry_cell_setting            tetragonal
loop_
_symmetry_equiv_pos_as_xyz
x,y,z
-x+1/2,-y+1/2,z+1/2
-y,x+1/2,z+1/4
y+1/2,-x,z+3/4
x+1/2,y+1/2,z+1/2
-x,-y,z
-y+1/2,x,z+3/4
y,-x+1/2,z+1/4
_cell_length_a                    35.7733
_cell_length_b                    35.7733
_cell_length_c                    11.4329
_cell_angle_alpha                 90.0000
_cell_angle_beta                  90.0000
_cell_angle_gamma                 90.0000
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
_atom_site_adp_type
_atom_site_occupancy
H1     H     0.06205  -0.07571   0.63437   0.01267  Uiso   1.00
H5     H    -0.44146  -0.52489  -0.00885   0.01267  Uiso   1.00
H9     H    -0.05810  -0.04801   0.43251   0.01267  Uiso   1.00
```

```
H13    H    -0.05472  -0.09963   0.57637   0.01267  Uiso   1.00
H17    H     0.05360  -0.11627   0.77200   0.01267  Uiso   1.00
H21    H    -0.42349   0.34328   0.42336   0.01267  Uiso   1.00
H25    H    -0.06617  -0.31152   0.10656   0.01267  Uiso   1.00
H29    H    -0.04963  -0.36670   0.23763   0.01267  Uiso   1.00
H33    H     0.05988  -0.40384   0.40187   0.01267  Uiso   1.00
H37    H     0.06002  -0.45669   0.54168   0.01267  Uiso   1.00
H41    H    -0.05815  -0.47062   0.48653   0.01267  Uiso   1.00
H45    H    -0.05859  -0.41818   0.34831   0.01267  Uiso   1.00
H49    H    -0.03234  -0.18169   0.77516   0.01267  Uiso   1.00
H53    H     0.04933  -0.33059   0.20625   0.01267  Uiso   1.00
H57    H     0.21380  -0.43048   0.29738   0.01267  Uiso   1.00
H61    H     0.27285  -0.43410   0.34137   0.01267  Uiso   1.00
C1     C     0.28196  -0.46303   0.34974   0.01267  Uiso   1.00
C5     C     0.26179  -0.49134   0.29266   0.01267  Uiso   1.00
C9     C     0.03550  -0.07023   0.59029   0.01267  Uiso   1.00
C13    C     0.03368  -0.04154   0.50865   0.01267  Uiso   1.00
C17    C     0.00039  -0.03341   0.44790   0.01267  Uiso   1.00
C21    C    -0.03164  -0.05405   0.47526   0.01267  Uiso   1.00
C25    C    -0.03005  -0.08299   0.55641   0.01267  Uiso   1.00
C29    C     0.00337  -0.09193   0.61509   0.01267  Uiso   1.00
C33    C    -0.50873   0.31228   0.33299   0.01267  Uiso   1.00
C37    C     0.02726  -0.13207   0.76238   0.01267  Uiso   1.00
C41    C    -0.47650   0.33487   0.33646   0.01267  Uiso   1.00
C45    C    -0.44795   0.32531   0.41539   0.01267  Uiso   1.00
C49    C    -0.03642  -0.30446   0.10742   0.01267  Uiso   1.00
C53    C    -0.00950  -0.32527   0.16868   0.01267  Uiso   1.00
C57    C    -0.01996  -0.35830   0.23739   0.01267  Uiso   1.00
C61    C     0.02816  -0.31379   0.16208   0.01267  Uiso   1.00
C65    C     0.00107  -0.40629   0.36740   0.01267  Uiso   1.00
C69    C     0.03406  -0.41857   0.42257   0.01267  Uiso   1.00
C73    C     0.03391  -0.44806   0.50119   0.01267  Uiso   1.00
C77    C     0.00048  -0.46641   0.52891   0.01267  Uiso   1.00
C81    C    -0.03225  -0.45554   0.46988   0.01267  Uiso   1.00
C85    C    -0.03241  -0.42589   0.39126   0.01267  Uiso   1.00
C89    C     0.20642  -0.45201   0.23391   0.01267  Uiso   1.00
C93    C    -0.27188   0.01554   0.72507   0.01267  Uiso   1.00
N1     N     0.27393  -0.52757   0.29459   0.01267  Uiso   1.00
N5     N    -0.28224  -0.01301   0.65147   0.01267  Uiso   1.00
N9     N     0.00108  -0.12251   0.69095   0.01267  Uiso   1.00
N13    N     0.00595  -0.37537   0.29464   0.01267  Uiso   1.00
Pd1    Pd   -0.56184   0.25362   0.43032   0.01267  Uiso   1.00
Cl1    Cl   -0.59254   0.28315   0.28397   0.01267  Uiso   1.00
Cl5    Cl   -0.11409  -0.27600  -0.00644   0.01267  Uiso   1.00
C97    C    -0.50000  -0.00000   0.11288   0.01267  Uiso   1.00
```

6.10 Metalated COF-330 example: COF-330-PdCl2

```
data_COF-330-PdCl2

_symmetry_space_group_name_H-M    'I41'
_symmetry_Int_Tables_number       80
_symmetry_cell_setting            tetragonal
loop_
_symmetry_equiv_pos_as_xyz
x,y,z
-x+1/2,-y+1/2,z+1/2
-y,x+1/2,z+1/4
y+1/2,-x,z+3/4
```

```
x+1/2,y+1/2,z+1/2
-x,-y,z
-y+1/2,x,z+3/4
y,-x+1/2,z+1/4
_cell_length_a                    32.8160
_cell_length_b                    32.8160
_cell_length_c                    12.7769
_cell_angle_alpha                 90.0000
_cell_angle_beta                  90.0000
_cell_angle_gamma                 90.0000
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
_atom_site_adp_type
_atom_site_occupancy
H1     H    -0.08180   0.05663  -0.62814   0.01267  Uiso   1.00
H5     H    -0.52626  -0.44167  -0.00365   0.01267  Uiso   1.00
H9     H    -0.05431  -0.06485  -0.41470   0.01267  Uiso   1.00
H13    H    -0.10958  -0.06567  -0.54003   0.01267  Uiso   1.00
H17    H    -0.10649   0.02977  -0.77876   0.01267  Uiso   1.00
H21    H     0.36583  -0.46214  -0.45244   0.01267  Uiso   1.00
H25    H    -0.35924  -0.03293  -0.02910   0.01267  Uiso   1.00
H29    H    -0.39120  -0.02996  -0.20437   0.01267  Uiso   1.00
H33    H    -0.38919   0.06468  -0.45020   0.01267  Uiso   1.00
H37    H     0.05556  -0.43595  -0.07494   0.01267  Uiso   1.00
H41    H    -0.47426  -0.05819  -0.48166   0.01267  Uiso   1.00
H45    H    -0.41946  -0.05596  -0.35423   0.01267  Uiso   1.00
H49    H    -0.20823  -0.02046  -0.72170   0.01267  Uiso   1.00
H53    H    -0.29264   0.02130  -0.27993   0.01267  Uiso   1.00
H57    H    -0.22128   0.04335  -0.24791   0.01267  Uiso   1.00
H61    H    -0.16332   0.04938  -0.12795   0.01267  Uiso   1.00
C1     C    -0.48502   0.26076  -0.38532   0.01267  Uiso   1.00
C5     C    -0.49897   0.26386  -0.28294   0.01267  Uiso   1.00
C9     C    -0.07606   0.03008  -0.58152   0.01267  Uiso   1.00
C13    C    -0.04473   0.03125  -0.50876   0.01267  Uiso   1.00
C17    C    -0.03695  -0.00191  -0.44258   0.01267  Uiso   1.00
C21    C    -0.06061  -0.03725  -0.45678   0.01267  Uiso   1.00
C25    C    -0.09202  -0.03825  -0.52977   0.01267  Uiso   1.00
C29    C    -0.09987  -0.00487  -0.59299   0.01267  Uiso   1.00
C33    C     0.29550  -0.50818  -0.29866   0.01267  Uiso   1.00
C37    C    -0.13258   0.01211  -0.75510   0.01267  Uiso   1.00
C41    C    -0.16707   0.00911  -0.82768   0.01267  Uiso   1.00
C45    C     0.33736  -0.47554  -0.42850   0.01267  Uiso   1.00
C49    C    -0.33161  -0.02011  -0.05962   0.01267  Uiso   1.00
C53    C    -0.33031  -0.00671  -0.16304   0.01267  Uiso   1.00
C57    C    -0.36616  -0.01143  -0.23074   0.01267  Uiso   1.00
C61    C    -0.29437   0.01095  -0.20049   0.01267  Uiso   1.00
C65    C    -0.40071   0.00497  -0.39227   0.01267  Uiso   1.00
C69    C    -0.40769   0.03780  -0.45787   0.01267  Uiso   1.00
C73    C    -0.43895   0.03680  -0.53094   0.01267  Uiso   1.00
C77    C     0.03692  -0.49823  -0.04387   0.01267  Uiso   1.00
C81    C    -0.45573  -0.03119  -0.47654   0.01267  Uiso   1.00
C85    C    -0.42485  -0.02976  -0.40235   0.01267  Uiso   1.00
C89    C    -0.47807   0.19478  -0.24871   0.01267  Uiso   1.00
C93    C     0.00465  -0.26858  -0.71543   0.01267  Uiso   1.00
```

```
C97    C    -0.22428   0.03248  -0.16918   0.01267  Uiso   1.00
C101   C    -0.19134   0.03594  -0.10098   0.01267  Uiso   1.00
N1     N    -0.01626  -0.20165  -0.74771   0.01267  Uiso   1.00
N5     N    -0.00914  -0.26411  -0.61753   0.01267  Uiso   1.00
N9     N    -0.13228  -0.00714  -0.66734   0.01267  Uiso   1.00
N13    N    -0.36820   0.00764  -0.31863   0.01267  Uiso   1.00
Pd1    Pd   -0.47133  -0.28940  -0.10684   0.01267  Uiso   1.00
Cl1    Cl   -0.46273  -0.28554   0.06154   0.01267  Uiso   1.00
Cl5    Cl   -0.44172  -0.34871  -0.08824   0.01267  Uiso   1.00
C105   C    -0.00000  -0.50000  -0.11829   0.01267  Uiso   1.00
```

6.11 Metalated COF-333 example: COF-333-CoCl2

```
data_COF-333-\ce{CoCl2tetra}

_symmetry_space_group_name_H-M    'I41/A'
_symmetry_Int_Tables_number       88
_symmetry_cell_setting            tetragonal
loop_
_symmetry_equiv_pos_as_xyz
x,y,z
-x+1/2,-y+1/2,z+1/2
-y,x+1/2,z+1/4
y+1/2,-x,z+3/4
-x,-y+1/2,-z+1/4
x+1/2,y,-z+3/4
y,-x,-z
-y+1/2,x+1/2,-z+1/2
x+1/2,y+1/2,z+1/2
-x,-y,z
-y+1/2,x,z+3/4
y,-x+1/2,z+1/4
-x+1/2,-y,-z+3/4
x,y+1/2,-z+1/4
y+1/2,-x+1/2,-z+1/2
-y,x,-z
_cell_length_a                    35.3908
_cell_length_b                    35.3908
_cell_length_c                    11.9080
_cell_angle_alpha                 90.0000
_cell_angle_beta                  90.0000
_cell_angle_gamma                 90.0000
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
_atom_site_adp_type
_atom_site_occupancy
H1     H     0.55932   0.07629  -0.02508   0.01267  Uiso   1.00
H9     H     0.44182   0.05275   0.19666   0.01267  Uiso   1.00
H17    H     0.55699   0.02321   0.10779   0.01267  Uiso   1.00
H25    H     0.55306   0.14327  -0.04799   0.01267  Uiso   1.00
H33    H     0.44093   0.09989   0.04111   0.01267  Uiso   1.00
H41    H     0.79115   0.07239   0.11276   0.01267  Uiso   1.00
H49    H     0.73892   0.05707  -0.01544   0.01267  Uiso   1.00
```

```
H57    H     0.30289   0.45773   0.37751   0.01267  Uiso   1.00
C1     C     0.53328   0.07123   0.02287   0.01267  Uiso   1.00
C9     C     0.53212   0.04156   0.10098   0.01267  Uiso   1.00
C17    C     0.49969   0.03425   0.16751   0.01267  Uiso   1.00
C25    C     0.46692   0.08383   0.06001   0.01267  Uiso   1.00
C33    C     0.50027   0.09229  -0.00063   0.01267  Uiso   1.00
C41    C     0.46737   0.05658   0.14601   0.01267  Uiso   1.00
C49    C     0.52743   0.14487  -0.10076   0.01267  Uiso   1.00
C57    C     0.79303   0.04732   0.05853   0.01267  Uiso   1.00
C65    C     0.82500   0.02325   0.06719   0.01267  Uiso   1.00
C73    C     0.76353   0.03837  -0.01461   0.01267  Uiso   1.00
C81    C     0.26507   0.50542   0.41499   0.01267  Uiso   1.00
C89    C     0.29841   0.48332   0.42769   0.01267  Uiso   1.00
N1     N     0.49875   0.12132  -0.08420   0.01267  Uiso   1.00
N9     N     0.32672   0.49137   0.49989   0.01267  Uiso   1.00
Co1    Co    0.87373  -0.04068   0.04648   0.01267  Uiso   1.00
Cl1    Cl    0.36400   0.39966   0.59378   0.01267  Uiso   1.00
Cl9    Cl    0.42439   0.46486   0.44016   0.01267  Uiso   1.00
C97    C     0.50000   0.00000   0.25000   0.01267  Uiso   1.00
```

6.12 Metalated COF-340 example: COF-340-PdCl2

```
data_COF340-PdCl2_c5

_symmetry_space_group_name_H-M    'I41'
_symmetry_Int_Tables_number       80
_symmetry_cell_setting            tetragonal
loop_
_symmetry_equiv_pos_as_xyz
x,y,z
-x+1/2,-y+1/2,z+1/2
-y,x+1/2,z+1/4
y+1/2,-x,z+3/4
x+1/2,y+1/2,z+1/2
-x,-y,z
-y+1/2,x,z+3/4
y,-x+1/2,z+1/4
_cell_length_a                    48.0168
_cell_length_b                    48.0168
_cell_length_c                    16.0856
_cell_angle_alpha                 90.0000
_cell_angle_beta                  90.0000
_cell_angle_gamma                 90.0000
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
_atom_site_adp_type
_atom_site_occupancy
H1     H     0.32756  -0.55908   0.42717   0.01267  Uiso   1.00
H5     H     0.04196  -0.04779   0.58117   0.01267  Uiso   1.00
H9     H    -0.45905  -0.51291  -0.02968   0.01267  Uiso   1.00
H13    H    -0.04020  -0.04150   0.39354   0.01267  Uiso   1.00
H17    H    -0.03894  -0.07693   0.50609   0.01267  Uiso   1.00
H21    H     0.03987  -0.08384   0.65816   0.01267  Uiso   1.00
H25    H     0.05653  -0.11382   0.76860   0.01267  Uiso   1.00
```

H29	H	-0.06274	-0.37017	0.26313	0.01267	Uiso	1.00
H33	H	-0.04318	-0.40397	0.35698	0.01267	Uiso	1.00
H37	H	0.03892	-0.41977	0.48457	0.01267	Uiso	1.00
H41	H	-0.45892	0.04018	0.08212	0.01267	Uiso	1.00
H45	H	-0.04081	-0.48489	0.50262	0.01267	Uiso	1.00
H49	H	-0.04279	-0.44535	0.40629	0.01267	Uiso	1.00
H53	H	-0.34880	0.04893	0.62231	0.01267	Uiso	1.00
H57	H	-0.34704	-0.03852	0.55908	0.01267	Uiso	1.00
H61	H	-0.20228	-0.47192	0.07635	0.01267	Uiso	1.00
H65	H	-0.16094	-0.52756	0.25044	0.01267	Uiso	1.00
H69	H	-0.18578	-0.53900	0.38245	0.01267	Uiso	1.00
H73	H	-0.72814	-0.03441	-0.02907	0.01267	Uiso	1.00
H77	H	-0.30826	-0.46000	0.29848	0.01267	Uiso	1.00
H81	H	-0.77576	-0.01465	-0.00883	0.01267	Uiso	1.00
H85	H	0.32187	-0.47158	0.48815	0.01267	Uiso	1.00
H89	H	-0.03024	-0.11570	0.70365	0.01267	Uiso	1.00
H93	H	0.02411	-0.36461	0.32490	0.01267	Uiso	1.00
C1	C	-0.32191	0.00069	0.65543	0.01267	Uiso	1.00
C5	C	0.33236	-0.49169	0.49389	0.01267	Uiso	1.00
C9	C	0.32174	-0.51511	0.45130	0.01267	Uiso	1.00
C13	C	0.33580	-0.54065	0.45819	0.01267	Uiso	1.00
C17	C	0.02410	-0.04711	0.53936	0.01267	Uiso	1.00
C21	C	0.02352	-0.02739	0.47628	0.01267	Uiso	1.00
C25	C	0.00059	-0.02496	0.42183	0.01267	Uiso	1.00
C29	C	-0.02186	-0.04316	0.43300	0.01267	Uiso	1.00
C33	C	-0.02140	-0.06298	0.49634	0.01267	Uiso	1.00
C37	C	0.00133	-0.06532	0.55059	0.01267	Uiso	1.00
C41	C	-0.01323	-0.12380	0.74122	0.01267	Uiso	1.00
C45	C	0.01848	-0.09217	0.66319	0.01267	Uiso	1.00
C49	C	0.01358	-0.11275	0.72848	0.01267	Uiso	1.00
C53	C	0.03572	-0.12239	0.77776	0.01267	Uiso	1.00
C57	C	-0.04275	-0.35962	0.25708	0.01267	Uiso	1.00
C61	C	-0.01948	-0.37017	0.29964	0.01267	Uiso	1.00
C65	C	-0.02206	-0.39502	0.35174	0.01267	Uiso	1.00
C69	C	0.00617	-0.35621	0.29203	0.01267	Uiso	1.00
C73	C	-0.00217	-0.42881	0.44116	0.01267	Uiso	1.00
C77	C	0.02141	-0.43401	0.49022	0.01267	Uiso	1.00
C81	C	-0.47761	0.04359	0.04525	0.01267	Uiso	1.00
C85	C	-0.50030	0.02544	0.05322	0.01267	Uiso	1.00
C89	C	-0.02341	-0.47022	0.50071	0.01267	Uiso	1.00
C93	C	-0.02456	-0.44782	0.44596	0.01267	Uiso	1.00
C97	C	-0.35676	0.03139	0.58633	0.01267	Uiso	1.00
C101	C	-0.34503	0.00475	0.59676	0.01267	Uiso	1.00
C105	C	-0.35533	-0.01761	0.54929	0.01267	Uiso	1.00
C109	C	-0.20104	-0.48343	0.13493	0.01267	Uiso	1.00
C113	C	-0.22362	-0.49472	0.25894	0.01267	Uiso	1.00
C117	C	-0.20134	-0.51192	0.28499	0.01267	Uiso	1.00
C121	C	-0.17847	-0.51459	0.23137	0.01267	Uiso	1.00
C125	C	-0.20329	-0.52600	0.36305	0.01267	Uiso	1.00
C129	C	-0.22651	-0.52352	0.41150	0.01267	Uiso	1.00
C133	C	-0.24947	-0.50670	0.38550	0.01267	Uiso	1.00
C137	C	-0.24771	-0.49209	0.30932	0.01267	Uiso	1.00
C141	C	-0.29219	-0.47323	0.32606	0.01267	Uiso	1.00
C145	C	-0.29585	-0.48736	0.40273	0.01267	Uiso	1.00
C149	C	-0.27409	-0.50393	0.43162	0.01267	Uiso	1.00
N1	N	-0.00145	-0.08510	0.61393	0.01267	Uiso	1.00
N5	N	-0.00078	-0.40520	0.38988	0.01267	Uiso	1.00
N9	N	-0.22311	-0.48067	0.18497	0.01267	Uiso	1.00
N13	N	-0.26887	-0.47556	0.28104	0.01267	Uiso	1.00

```
Pd1    Pd   -0.25896  -0.45826   0.16783   0.01267  Uiso   1.00
Cl1    Cl   -0.24462  -0.44214   0.04162   0.01267  Uiso   1.00
Cl5    Cl   -0.29989  -0.43447   0.16034   0.01267  Uiso   1.00
C153   C    -0.50000  -0.00000   0.11140   0.01267  Uiso   1.00
```

6.13 Metalated COF-350 example: COF-350-PdCl2

```
data_COF-350-PdCl2-

_symmetry_space_group_name_H-M    'I41'
_symmetry_Int_Tables_number       80
_symmetry_cell_setting            tetragonal
loop_
_symmetry_equiv_pos_as_xyz
x,y,z
-x+1/2,-y+1/2,z+1/2
-y,x+1/2,z+1/4
y+1/2,-x,z+3/4
x+1/2,y+1/2,z+1/2
-x,-y,z
-y+1/2,x,z+3/4
y,-x+1/2,z+1/4
_cell_length_a                    32.6204
_cell_length_b                    32.6204
_cell_length_c                    12.7518
_cell_angle_alpha                 90.0000
_cell_angle_beta                  90.0000
_cell_angle_gamma                 90.0000
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
_atom_site_adp_type
_atom_site_occupancy
H1     H    -0.11051   0.06226  -0.54660   0.01267  Uiso   1.00
H5     H    -0.55707  -0.43682   0.08920   0.01267  Uiso   1.00
H9     H    -0.02262  -0.06003  -0.49500   0.01267  Uiso   1.00
H13    H    -0.07715  -0.06211  -0.62756   0.01267  Uiso   1.00
H17    H    -0.40945   0.05584  -0.36544   0.01267  Uiso   1.00
H21    H    -0.46892   0.05965  -0.48617   0.01267  Uiso   1.00
H25    H     0.04888  -0.56668  -0.07092   0.01267  Uiso   1.00
H29    H    -0.39297  -0.07145  -0.44701   0.01267  Uiso   1.00
H33    H    -0.21286   0.08905  -0.22320   0.01267  Uiso   1.00
H37    H     0.33887  -0.40943  -0.57717   0.01267  Uiso   1.00
H41    H    -0.46411  -0.36108  -0.52100   0.01267  Uiso   1.00
H45    H    -0.49201  -0.30813  -0.44278   0.01267  Uiso   1.00
H49    H    -0.51596  -0.29286  -0.28066   0.01267  Uiso   1.00
H53    H    -0.51732  -0.24212  -0.13633   0.01267  Uiso   1.00
H57    H     0.31794  -0.50030  -0.31737   0.01267  Uiso   1.00
H61    H    -0.02432  -0.34533  -0.42398   0.01267  Uiso   1.00
O1     O     0.36480  -0.42158  -0.40538   0.01267  Uiso   1.00
O5     O    -0.28132   0.07677  -0.29670   0.01267  Uiso   1.00
C1     C    -0.45118   0.25373  -0.38975   0.01267  Uiso   1.00
C5     C    -0.47067   0.26264  -0.29382   0.01267  Uiso   1.00
C9     C    -0.09243   0.03472  -0.53255   0.01267  Uiso   1.00
```

C13	C	-0.06179	0.03526	-0.45621	0.01267	Uiso	1.00
C17	C	-0.03680	0.00100	-0.44050	0.01267	Uiso	1.00
C21	C	-0.04312	-0.03399	-0.50321	0.01267	Uiso	1.00
C25	C	-0.07431	-0.03532	-0.57665	0.01267	Uiso	1.00
C29	C	-0.09921	-0.00068	-0.59214	0.01267	Uiso	1.00
C33	C	0.33695	-0.44834	-0.39978	0.01267	Uiso	1.00
C37	C	-0.28121	0.04776	-0.23149	0.01267	Uiso	1.00
C41	C	-0.39733	-0.00800	-0.39887	0.01267	Uiso	1.00
C45	C	-0.41872	0.02911	-0.41087	0.01267	Uiso	1.00
C49	C	-0.45161	0.03118	-0.47957	0.01267	Uiso	1.00
C53	C	0.03702	-0.50280	-0.04072	0.01267	Uiso	1.00
C57	C	-0.44211	-0.03992	-0.52568	0.01267	Uiso	1.00
C61	C	-0.40990	-0.04271	-0.45472	0.01267	Uiso	1.00
C65	C	-0.44904	0.19653	-0.22713	0.01267	Uiso	1.00
C69	C	0.03035	-0.26595	-0.71253	0.01267	Uiso	1.00
C73	C	-0.12982	-0.00130	-0.67549	0.01267	Uiso	1.00
C77	C	-0.36248	-0.01056	-0.32813	0.01267	Uiso	1.00
C81	C	-0.21762	0.07198	-0.15094	0.01267	Uiso	1.00
C85	C	0.31078	-0.42709	-0.57031	0.01267	Uiso	1.00
N1	N	-0.12834	0.02399	-0.75388	0.01267	Uiso	1.00
N5	N	-0.16061	0.02212	-0.82510	0.01267	Uiso	1.00
N9	N	-0.30475	0.01413	-0.24852	0.01267	Uiso	1.00
N13	N	-0.33324	0.01635	-0.32947	0.01267	Uiso	1.00
Pd1	Pd	-0.56704	-0.08632	-0.05740	0.01267	Uiso	1.00
Pd5	Pd	-0.18328	-0.56372	0.07282	0.01267	Uiso	1.00
Cl1	Cl	-0.54736	-0.02902	0.02683	0.01267	Uiso	1.00
Cl5	Cl	-0.61792	-0.04986	-0.13122	0.01267	Uiso	1.00
Cl9	Cl	-0.54096	-0.34544	0.17182	0.01267	Uiso	1.00
Cl13	Cl	0.11862	-0.20736	-0.26158	0.01267	Uiso	1.00
C89	C	0.00000	-0.50000	-0.11482	0.01267	Uiso	1.00