Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary Information

Rotational Dynamics of the Organic Bridging Linkers in Metal-Organic Frameworks and Their Substituents Effects on Rotational Energy Barrier

Srimanta Pakhira[a]*

[a]Discipline of Physics, Indian Institute of Technology Indore (IIT), Simrol, Khandwa Road, Indore, 453552, MP, India. Telephone no.: +91-732-430-6830

*Corresponding author's Email: spakhira@iiti.ac.in or srimantacu@gmail.com

ORCID Srimanta Pakhira: 0000-0002-2488-300X.

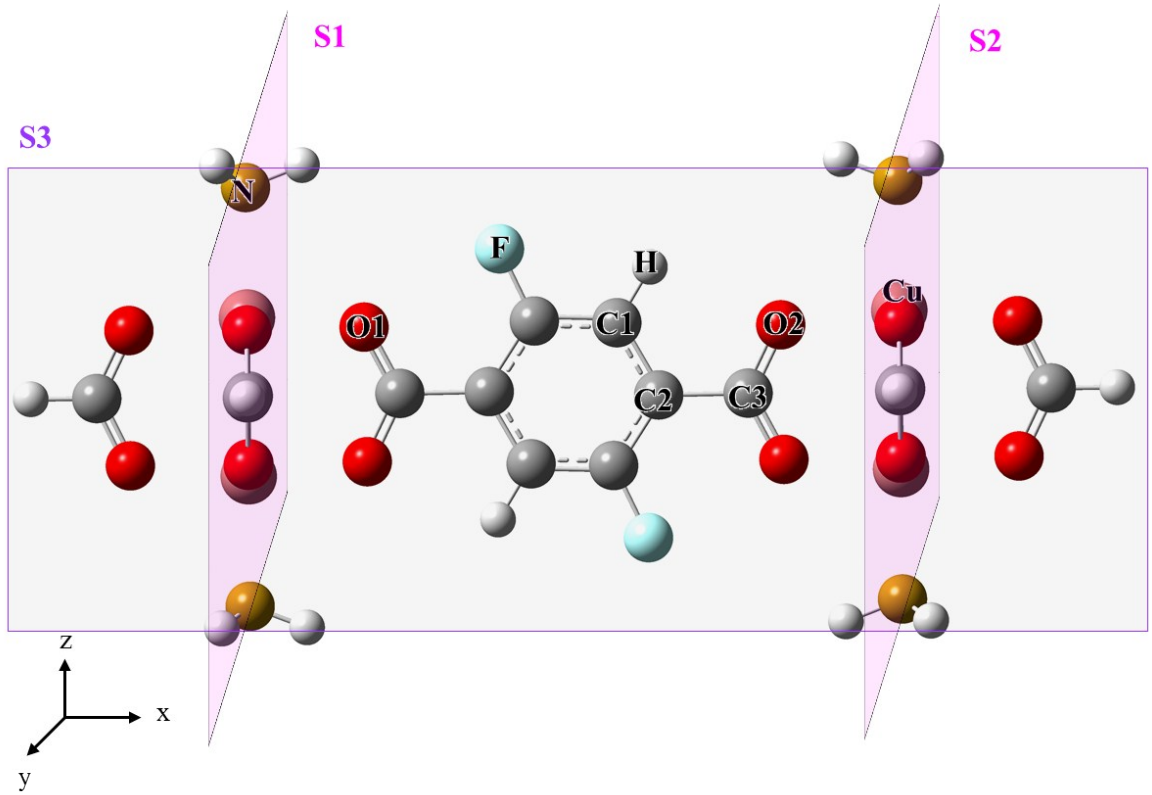

Figure S1. Optimized structure of the model $[Cu_4(DFBDC)(HCO_2)_6(NH_3)_4]$ MOF containing BFBDC linker (DFBDC = 2,5-difluro-1,4-benzenedicarboxylate) (Top View). The dihedral angle χ of the DFBDC organic bridging linker is represented by C1-C2-C3-O2. The atoms H, C, N, O, F and Cu were represented by the white, gray, light green, red, sky blue and black red colors respectively, and S1, S2 and S3 are the imaginary planes.

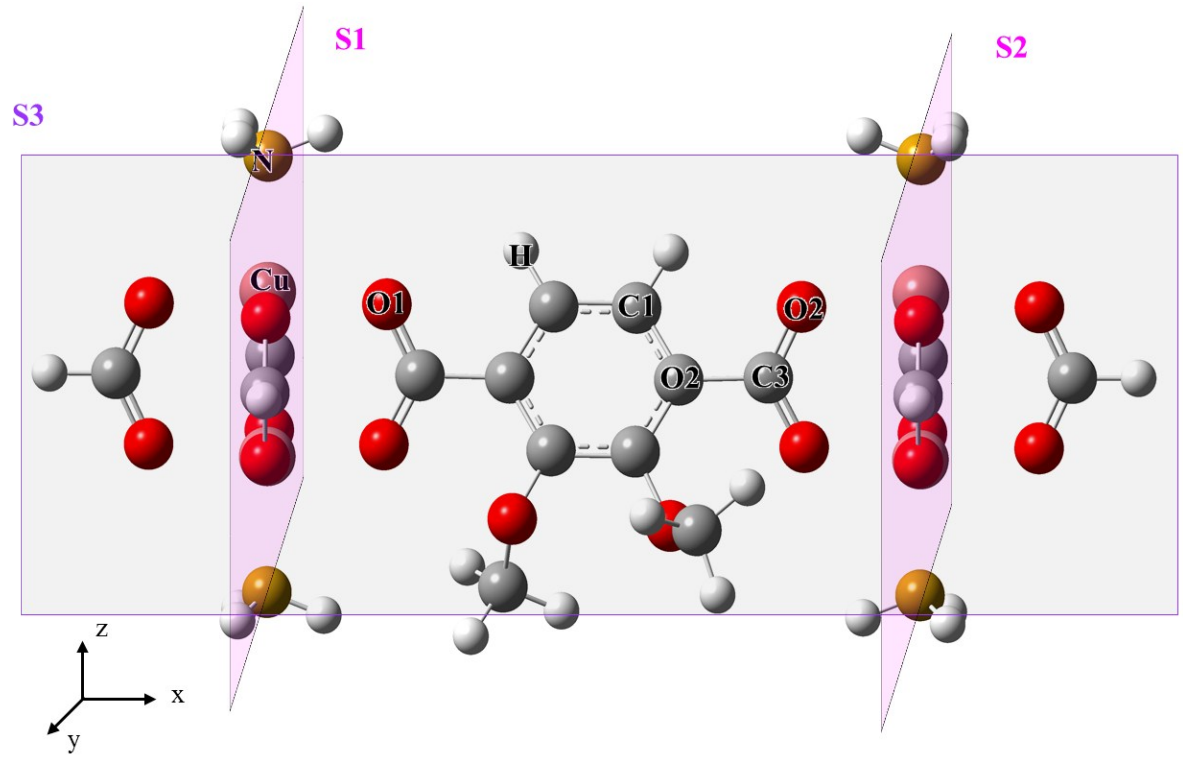

Figure S2. Optimized structure of the model $[Cu_4(DMBDC)(HCO_2)_6(NH_3)_4]$ MOF containing DMBDC linker (DMBDC = 2,3-dimethoxy-1,4-benzenedicarboxylate) (Top View).

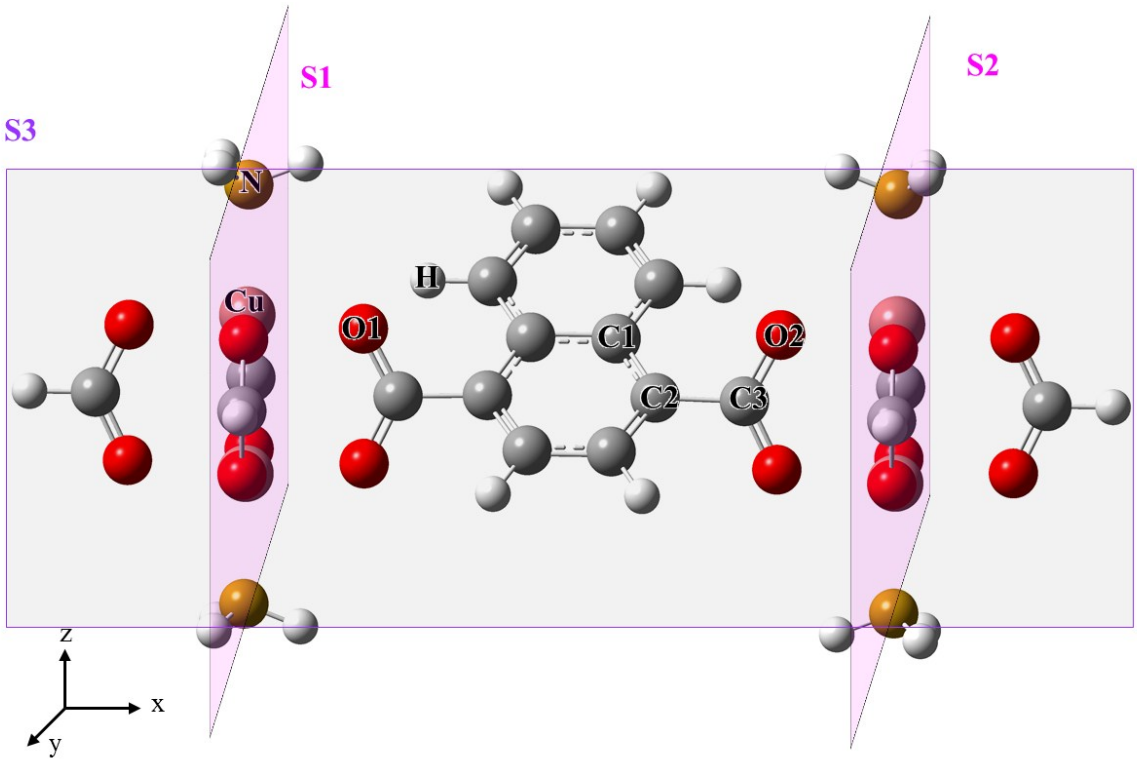

Figure S3. Optimized structure of the model $[Cu_4(NDC)(HCO_2)_6(NH_3)_4]$ MOF containing NDC (NDC = 1,4-naphthalenedicarboxylate) linker (Top View).

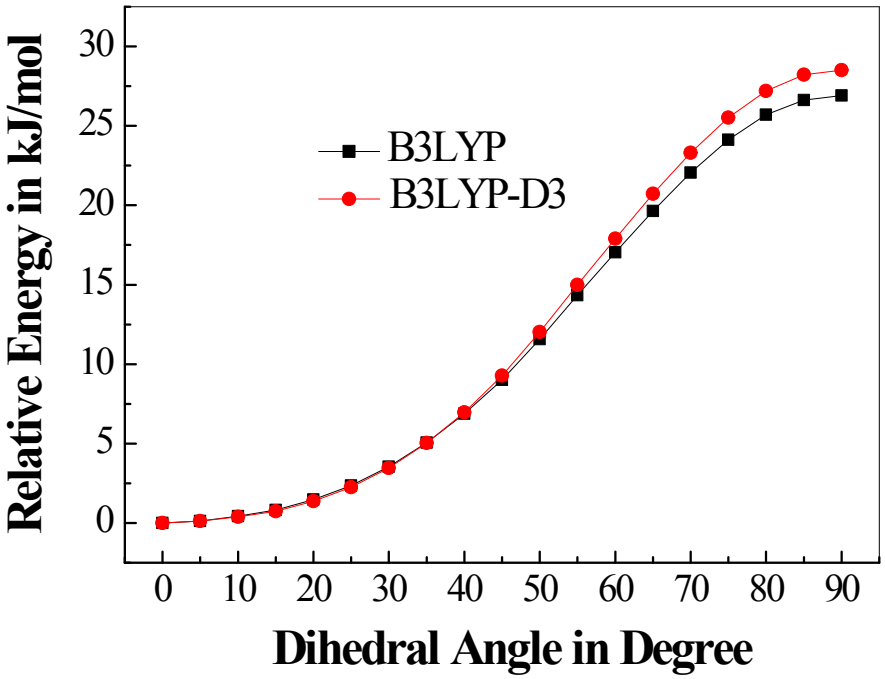

Figure S4. Potential energy curves (PECs) of the model $[Cu_4(DFBDC)(HCO_2)_6(NH_3)_4]$ MOF containing DFBDC.

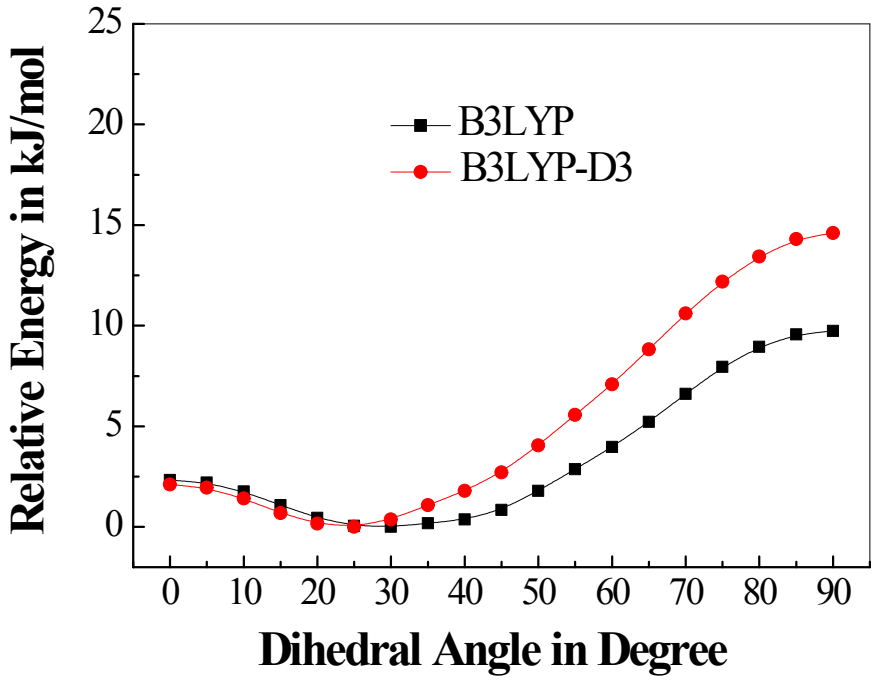

Figure S5. PECs of the model $[Cu_4(DMBDC)(HCO_2)_6(NH_3)_4]$ MOF containing DMBDC linker.

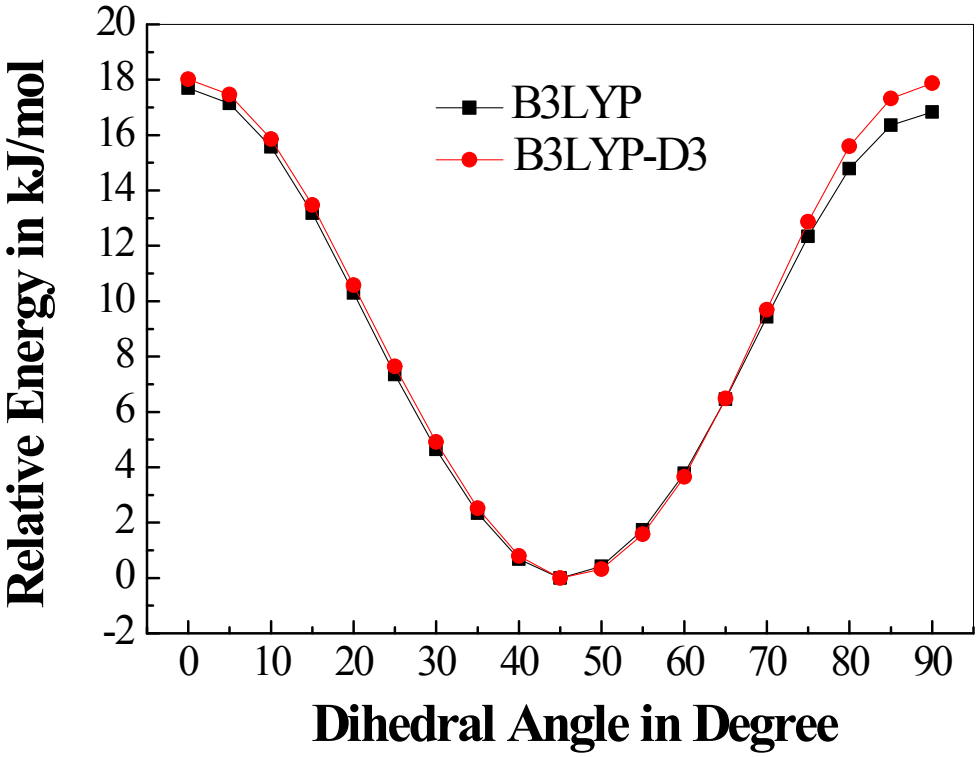

Figure S6. PECs of the model $[Cu_4(NDC)(HCO_2)_6(NH_3)_4]$ MOF containing NDC linker.

Force Field Parameters of the Model $[Cu_4(BDC)(HCO_2)_6(NH_3)_4]$ MOF with BDC Linker:

The force field parameters were computed by introducing DFT-D methods of the model $[Cu_2(X)_2DABCO]$ MOF considering BDC linker and Cu^{2+} followed by equation below:

$$V_{\mathrm{AMBER}} = \sum_{i}^{n_{\mathrm{bonds}}} b_i(r_i - r_{i,\mathrm{eq}})^2 + \sum_{i}^{n_{\mathrm{angles}}} a_i(\theta_i - \theta_{i,\mathrm{eq}})^2 + \sum_{i}^{n_{\mathrm{dihedrals}}} \sum_{n}^{n_{i,\max}} (V_{i,n}/2)[1 + \cos(n\phi_i - \gamma_{i,n})] + \sum_{i<j}^{n_{\mathrm{atoms}}}{}' \left(\frac{A_{ij}}{r_{ij}^{12}} - \frac{B_{ij}}{r_{ij}^{6}}\right) + \sum_{i<j}^{n_{\mathrm{atoms}}}{}' \frac{q_i q_j}{4\pi\varepsilon_0 r_{ij}},$$

Where V_{AMBER} is potential considered in the computation, and other notations have been followed of Assisted Model Building with Energy Refinement (AMBER) suite code such as:

The meanings of right hand side terms are:

- First term (summing over bonds): represents the energy between covalently bonded atoms. This harmonic (ideal spring) force is a good approximation near the equilibrium bond length, but becomes increasingly poor as atoms separate.
- Second term (summing over angles): represents the energy due to the geometry of electron orbitals involved in covalent bonding.
- Third term (summing over torsions): represents the energy for twisting a bond due to bond order (e.g., double bonds) and neighboring bonds or lone pairs of electrons. One bond may have more than one of these terms, such that the total torsional energy is expressed as a Fourier series.
- Fourth term (double summation over *i* and *j*): represents the non-bonded energy between all atom pairs, which can be decomposed into van der Waals (first term of summation) and electrostatic (second term of summation) energies.

DIHE					
o2-c -ca-ca	1	3.625	180.0	2.0	from ref. 1. *J. Am. Chem. Soc.* 134, ***2012***, 4207-4215.
o2-c -ca-ca	1	**1.055**	180.0	2.0	Developed here by MM fitting as shown in **Figure S7**.
MM stands for Molecular Mechanical Simulations.					

Reference 1: Grosch, J. S.; Paesani, F. *J. Am. Chem. Soc.* 134, ***2012***, 4207-4215.

In the above line, DIHE: o2-c-ca-ca represent the name of the rotational dihedral angle of the BDC linker, $V_{i,n}$ = 3.625 kcal/mol, d =180.0, and n=2.

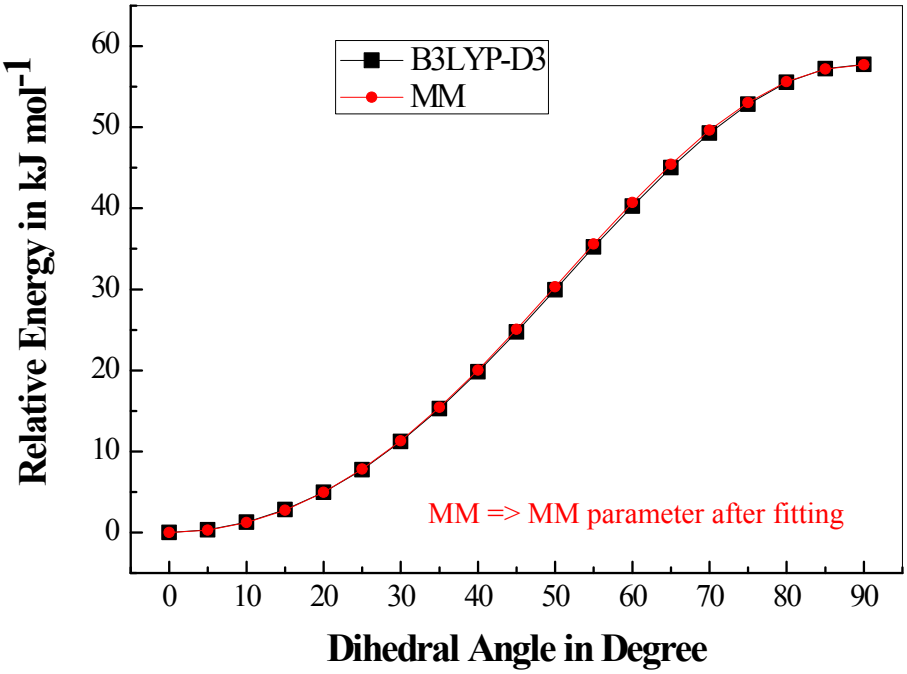

Figure S7: PECs of the model $[Cu_4(BDC)(HCO_2)_6(NH_3)_4]$ MOF containing BDC with fitted force filed parameters by MM simulations.

Optimized Geometry of the Model MOFs with various Linkers Computed at B3LYP-D3 method:

1. XYZ Co-ordinate of MOF with BDC Linker:

Cu	1.32902400	0.00000000	0.00000000
Cu	-1.32902400	0.00000000	0.00000000
Cu	1.32902400	0.00000000	10.92641400
Cu	-1.32902400	0.00000000	10.92641400
N	3.51339400	0.00000000	0.00000000
H	3.87936200	0.00000000	0.95338100
H	3.87936200	0.82565200	-0.47669000
H	3.87936200	-0.82565200	-0.47669000
N	-3.51339400	0.00000000	0.00000000
H	-3.87936200	0.00000000	0.95338100
H	-3.87936200	-0.82565200	-0.47669000
H	-3.87936200	0.82565200	-0.47669000
N	3.51339400	0.00000000	10.92641400
H	3.87936200	0.00000000	9.97303400
H	3.87936200	-0.82565200	11.40310400
H	3.87936200	0.82565200	11.40310400
N	-3.51339400	0.00000000	10.92641400
H	-3.87936200	0.00000000	9.97303400
H	-3.87936200	0.82565200	11.40310400
H	-3.87936200	-0.82565200	11.40310400
C	0.00000000	-2.54274700	0.00000000
O	1.13517000	-1.99025100	0.00000000
O	-1.13517000	-1.99025100	0.00000000
H	0.00000000	-3.65365100	0.00000000
C	0.00000000	2.54274700	0.00000000
O	1.13517000	1.99025100	0.00000000
O	-1.13517000	1.99025100	0.00000000
H	0.00000000	3.65365100	0.00000000
C	0.00000000	2.54274700	10.92641400
O	1.13517000	1.99025100	10.92641400
O	-1.13517000	1.99025100	10.92641400

H	0.00000000	3.65365100	10.92641400
C	0.00000000	-2.54274700	10.92641400
O	1.13517000	-1.99025100	10.92641400
O	-1.13517000	-1.99025100	10.92641400
H	0.00000000	-3.65365100	10.92641400
C	0.00000000	0.00000000	-2.53943500
O	1.13534600	0.00000000	-1.98729600
O	-1.13534600	0.00000000	-1.98729600
H	0.00000000	0.00000000	-3.65024600
C	0.00000000	0.00000000	13.46585000
O	1.13534600	0.00000000	12.91371100
O	-1.13534600	0.00000000	12.91371100
H	0.00000000	0.00000000	14.57666000
C	0.00000200	0.00000000	2.55836700
O	1.13052600	0.00000000	1.97926700
O	-1.13053200	0.00000000	1.97927600
C	-0.00000400	0.00000000	8.36743200
O	1.13037400	0.00000000	8.94715400
O	-1.13038700	0.00000000	8.94714900
C	-0.00000300	0.00000000	4.05957200
C	-0.00001100	0.00000000	6.86607000
C	1.21241500	0.00000000	4.76625400
C	-1.21242300	0.00000000	4.76625100
C	1.21240500	0.00000000	6.15930600
C	-1.21242500	0.00000000	6.15930500
H	2.14676200	0.00000000	4.20498200
H	-2.14676600	0.00000000	4.20497200
H	2.14679100	0.00000000	6.72056300
H	-2.14682000	0.00000000	6.72054600

2. XYZ Co-ordinate of MOF with DFBDC Linker:

Cu	1.33106300	0.00000000	0.00000000
Cu	-1.33106300	0.00000000	0.00000000
Cu	1.33106300	0.00000000	10.96867100
Cu	-1.33106300	0.00000000	10.96867100
N	3.51320400	0.00000000	0.00000000
H	3.87920200	0.00000000	0.95345500

H	3.87920200	0.82571600	-0.47672800
H	3.87920200	-0.82571600	-0.47672800
N	-3.51320400	0.00000000	0.00000000
H	-3.87920200	0.00000000	0.95345500
H	-3.87920200	-0.82571600	-0.47672800
H	-3.87920200	0.82571600	-0.47672800
N	3.51320400	0.00000000	10.96867100
H	3.87920200	0.00000000	10.01521600
H	3.87920200	-0.82571600	11.44539800
H	3.87920200	0.82571600	11.44539800
N	-3.51320400	0.00000000	10.96867100
H	-3.87920200	0.00000000	10.01521600
H	-3.87920200	0.82571600	11.44539800
H	-3.87920200	-0.82571600	11.44539800
C	0.00000000	-2.54183000	0.00000000
O	1.13521400	-1.98919500	0.00000000
O	-1.13521400	-1.98919500	0.00000000
H	0.00000000	-3.65275800	0.00000000
C	0.00000000	2.54183000	0.00000000
O	1.13521400	1.98919500	0.00000000
O	-1.13521400	1.98919500	0.00000000
H	0.00000000	3.65275800	0.00000000
C	0.00000000	2.54183000	10.96867100
O	1.13521400	1.98919500	10.96867100
O	-1.13521400	1.98919500	10.96867100
H	0.00000000	3.65275800	10.96867100
C	0.00000000	-2.54183000	10.96867100
O	1.13521400	-1.98919500	10.96867100
O	-1.13521400	-1.98919500	10.96867100
H	0.00000000	-3.65275800	10.96867100
C	0.00000000	0.00000000	-2.53945700
O	1.13533400	0.00000000	-1.98720000
O	-1.13533400	0.00000000	-1.98720000
H	0.00000000	0.00000000	-3.65030800
C	0.00000000	0.00000000	13.50812700
O	1.13533400	0.00000000	12.95587100
O	-1.13533400	0.00000000	12.95587100
H	0.00000000	0.00000000	14.61897800

C	0.03018900	0.00000000	2.55565800
O	1.14941200	0.00000000	1.96701200
O	-1.10983100	0.00000000	1.99618700
C	-0.02970700	0.00000000	8.41213600
O	1.11011900	0.00000000	8.97245200
O	-1.14873300	0.00000000	9.00133200
C	0.04440500	0.00000000	4.05954200
C	-0.04360300	0.00000000	6.90841400
C	1.22012400	0.00000000	4.83043100
C	-1.17548900	0.00000000	4.75004000
C	1.17632600	0.00000000	6.21805800
C	-1.21921800	0.00000000	6.13767900
F	2.43801000	0.00000000	4.25845700
H	-2.10539500	0.00000000	4.18383700
H	2.10637300	0.00000000	6.78408200
F	-2.43702600	0.00000000	6.70987900

3. XYZ Co-ordinate of MOF with DMBDC Linker:

Cu	1.32795700	0.00000000	0.00000000
Cu	-1.32795700	0.00000000	0.00000000
Cu	1.32795700	0.00000000	10.94459600
Cu	-1.32795700	0.00000000	10.94459600
N	3.51161900	0.00000000	0.00000000
H	3.87760900	0.00000000	0.95343600
H	3.87760900	0.82569900	-0.47671800
H	3.87760900	-0.82569900	-0.47671800
N	-3.51161900	0.00000000	0.00000000
H	-3.87760900	0.00000000	0.95343600
H	-3.87760900	-0.82569900	-0.47671800
H	-3.87760900	0.82569900	-0.47671800
N	3.51161900	0.00000000	10.94459600
H	3.87760900	0.00000000	9.99116100
H	3.87760900	-0.82569900	11.42131400
H	3.87760900	0.82569900	11.42131400

N	-3.51161900	0.00000000	10.94459600
H	-3.87760900	0.00000000	9.99116100
H	-3.87760900	0.82569900	11.42131400
H	-3.87760900	-0.82569900	11.42131400
C	0.00000000	-2.54476100	0.00000000
O	1.13515100	-1.99223900	0.00000000
O	-1.13515100	-1.99223900	0.00000000
H	0.00000000	-3.65580900	0.00000000
C	0.00000000	2.54476100	0.00000000
O	1.13515100	1.99223900	0.00000000
O	-1.13515100	1.99223900	0.00000000
H	0.00000000	3.65580900	0.00000000
C	0.00000000	2.54476100	10.94459600
O	1.13515100	1.99223900	10.94459600
O	-1.13515100	1.99223900	10.94459600
H	0.00000000	3.65580900	10.94459600
C	0.00000000	-2.54476100	10.94459600
O	1.13515100	-1.99223900	10.94459600
O	-1.13515100	-1.99223900	10.94459600
H	0.00000000	-3.65580900	10.94459600
C	0.00000000	0.00000000	-2.54049600
O	1.13537400	0.00000000	-1.98822800
O	-1.13537400	0.00000000	-1.98822800
H	0.00000000	0.00000000	-3.65146200
C	0.00000000	0.00000000	13.48509200
O	1.13537400	0.00000000	12.93282500
O	-1.13537400	0.00000000	12.93282500
H	0.00000000	0.00000000	14.59605800
C	-0.01931600	0.00000000	2.55244600
O	1.12451300	0.00000000	1.99909600
O	-1.13315300	0.00000000	1.94857200
C	-0.00985100	0.00000000	8.38939100
O	1.13207600	0.00000000	8.94726500
O	-1.12523500	0.00000000	8.99050800
C	-0.05964800	0.00000000	4.05396900
C	-0.04049400	0.00000000	6.88700400
C	1.03351400	0.51853800	4.77052100
C	-1.16145600	-0.50462200	4.77066900

C	1.04642000	0.51363500	6.16095500
C	-1.14831500	-0.50976900	6.18141700
H	1.87995200	0.90877300	4.20523200
O	-2.29811100	-0.98392800	4.17252000
H	1.89936200	0.90556800	6.71537000
O	-2.17861900	-1.15037100	6.81829200
C	-2.20762300	-2.33122100	3.70413000
H	-1.91239800	-3.00629700	4.52355500
H	-3.21581400	-2.60175400	3.35099300
H	-1.50462400	-2.40979100	2.85916700
C	-3.36223000	-0.36647700	6.98367300
H	-3.15295800	0.52484600	7.59693500
H	-4.08625900	-1.01074500	7.50811900
H	-3.78065600	-0.07132900	6.00789100

4. XYZ Co-ordinate of MOF with TFBDC Linker:

Cu	1.33431600	0.00000000	0.00000000
Cu	-1.33431600	0.00000000	0.00000000
Cu	1.33431600	0.00000000	10.93231700
Cu	-1.33431600	0.00000000	10.93231700
N	3.52691800	0.00000000	0.00000000
H	3.89285100	0.00000000	0.95328900
H	3.89285100	0.82557200	-0.47664400
H	3.89285100	-0.82557200	-0.47664400
N	-3.52691800	0.00000000	0.00000000
H	-3.89285100	0.00000000	0.95328900
H	-3.89285100	-0.82557200	-0.47664400
H	-3.89285100	0.82557200	-0.47664400
N	3.52691800	0.00000000	10.93231700
H	3.89285100	0.00000000	9.97902800
H	3.89285100	-0.82557200	11.40896100
H	3.89285100	0.82557200	11.40896100
N	-3.52691800	0.00000000	10.93231700
H	-3.89285100	0.00000000	9.97902800
H	-3.89285100	0.82557200	11.40896100
H	-3.89285100	-0.82557200	11.40896100

C	0.00000000	-2.53653900	0.00000000
O	1.13937600	-1.99876400	0.00000000
O	-1.13937600	-1.99876400	0.00000000
H	0.00000000	-3.64748800	0.00000000
C	0.00000000	2.53653900	0.00000000
O	1.13937600	1.99876400	0.00000000
O	-1.13937600	1.99876400	0.00000000
H	0.00000000	3.64748800	0.00000000
C	0.00000000	2.53653900	10.93231700
O	1.13937600	1.99876400	10.93231700
O	-1.13937600	1.99876400	10.93231700
H	0.00000000	3.64748800	10.93231700
C	0.00000000	-2.53653900	10.93231700
O	1.13937600	-1.99876400	10.93231700
O	-1.13937600	-1.99876400	10.93231700
H	0.00000000	-3.64748800	10.93231700
C	0.00000000	0.00000000	-2.53226700
O	1.13929900	0.00000000	-1.99476800
O	-1.13929900	0.00000000	-1.99476800
H	0.00000000	0.00000000	-3.64310500
C	0.00000000	0.00000000	13.46458400
O	1.13929900	0.00000000	12.92708500
O	-1.13929900	0.00000000	12.92708500
H	0.00000000	0.00000000	14.57542200
C	0.00000700	0.00000000	2.54179000
O	1.13558800	0.00000000	1.99256200
O	-1.13558500	0.00000000	1.99257400
C	0.00000300	0.00000000	8.39033700
O	1.13555800	0.00000000	8.93965800
O	-1.13556300	0.00000000	8.93964300
C	-0.00002700	0.00000000	4.04823400
C	-0.00002400	0.00000000	6.88398800
C	0.82351700	0.87051300	4.76914800
C	-0.82358800	-0.87049700	4.76914600
C	0.82351900	0.87050900	6.16314000
C	-0.82358000	-0.87049600	6.16314000
F	1.60979700	1.74871100	4.13093000
F	-1.60988500	-1.74868300	4.13093300

F	1.60971700	1.74871700	6.80137200
F	-1.60978900	-1.74869200	6.80137600

5. XYZ Co-ordinate of MOF with NDC Linker:

Cu	1.32925300	0.00000000	0.00000000
Cu	-1.32925300	0.00000000	0.00000000
Cu	1.32925300	0.00000000	10.93638500
Cu	-1.32925300	0.00000000	10.93638500
N	3.51287400	0.00000000	0.00000000
H	3.87886700	0.00000000	0.95344600
H	3.87886700	0.82570800	-0.47672300
H	3.87886700	-0.82570800	-0.47672300
N	-3.51287400	0.00000000	0.00000000
H	-3.87886700	0.00000000	0.95344600
H	-3.87886700	-0.82570800	-0.47672300
H	-3.87886700	0.82570800	-0.47672300
N	3.51287400	0.00000000	10.93638500
H	3.87886700	0.00000000	9.98294000
H	3.87886700	-0.82570800	11.41310800
H	3.87886700	0.82570800	11.41310800
N	-3.51287400	0.00000000	10.93638500
H	-3.87886700	0.00000000	9.98294000
H	-3.87886700	0.82570800	11.41310800
H	-3.87886700	-0.82570800	11.41310800
C	0.00000000	-2.54480700	0.00000000
O	1.13512600	-1.99200600	0.00000000
O	-1.13512600	-1.99200600	0.00000000
H	0.00000000	-3.65578100	0.00000000
C	0.00000000	2.54480700	0.00000000
O	1.13512600	1.99200600	0.00000000
O	-1.13512600	1.99200600	0.00000000
H	0.00000000	3.65578100	0.00000000
C	0.00000000	2.54480700	10.93638500
O	1.13512600	1.99200600	10.93638500
O	-1.13512600	1.99200600	10.93638500
H	0.00000000	3.65578100	10.93638500
C	0.00000000	-2.54480700	10.93638500

O	1.13512600	-1.99200600	10.93638500
O	-1.13512600	-1.99200600	10.93638500
H	0.00000000	-3.65578100	10.93638500
C	0.00000000	0.00000000	-2.53977600
O	1.13539600	0.00000000	-1.98751100
O	-1.13539600	0.00000000	-1.98751100
H	0.00000000	0.00000000	-3.65064700
C	0.00000000	0.00000000	13.47616200
O	1.13539600	0.00000000	12.92389600
O	-1.13539600	0.00000000	12.92389600
H	0.00000000	0.00000000	14.58703200
C	0.00589800	0.00000000	2.55391900
O	1.12652100	0.00000000	1.95664400
O	-1.13256500	0.00000000	1.99499500
C	0.00553100	0.00000000	8.38305800
O	1.12634400	0.00000000	8.97975100
O	-1.13307000	0.00000000	8.94110700
C	0.04224700	0.00000000	4.05603500
C	0.04208600	0.00000000	6.88087000
C	0.92562700	0.89759300	4.74961100
C	-0.77409100	-0.86322500	4.76184700
C	0.92557700	0.89761500	6.18764300
C	-0.77417200	-0.86324100	6.17500000
H	-1.43995800	-1.53176100	4.21372800
H	-1.44023000	-1.53154400	6.72313300
C	1.74838400	1.84545500	6.87021800
C	1.74831900	1.84565900	4.06715300
C	2.53455700	2.73787700	4.76166400
C	2.53464500	2.73771700	6.17581000
H	1.74345400	1.86742000	7.95721400
H	1.74314300	1.86808100	2.98017800
H	3.14915500	3.45713400	4.21508800
H	3.14942200	3.45675600	6.72247000

Vibrational Frequency Analysis:

(a) The vibrational modes and harmonic frequencies of the model MOF containing BDC linker.

Vibrational Modes Frequencies (cm^{-1})

1	1.9146
2	32.9121
3	49.0065
4	49.7701
5	54.9076
6	60.3082
7	66.2870
8	75.2869
9	118.0470
10	121.1001
11	149.0416
12	169.8780
13	209.9438
14	224.4611
15	227.4735
16	275.4106
17	301.6715
18	314.1149
19	326.6019
20	348.0385
21	371.8582
22	376.1638
23	386.2538
24	392.7503
25	482.4795
26	511.9815
27	515.3900
28	579.4796
29	644.7674
30	749.2860
31	772.7939
32	787.3507
33	868.2204
34	1005.3252
35	1042.3753
36	1045.2941
37	1116.9388
38	1119.4026

39	1170.0096
40	1366.5942
41	1370.6866
42	1372.8462
43	1375.9614
44	1380.8472
45	1448.1071
46	1567.2012
47	1611.7495
48	1632.2965
49	1634.7528
50	1636.4624
51	1705.4001
52	2999.3772
53	3001.9525
54	3206.9761
55	3460.4530
56	3460.5365
57	3589.5230
58	3590.5354

(b) The vibrational modes and harmonic frequencies of the model MOF containing DFBDC linker.

Vibrational Modes	Frequencies (cm^{-1})
1	3.3783
2	22.6156
3	42.4358
4	47.0193
5	54.3191
6	62.8118
7	64.6415
8	72.3761
9	117.0220
10	120.4465
11	149.2457
12	160.4245
13	193.1414
14	215.6550

15	226.5953
16	244.7659
17	274.6916
18	311.4176
19	320.5871
20	326.1424
21	352.9882
22	371.3575
23	376.8454
24	388.2369
25	410.1102
26	480.8292
27	509.5619
28	516.4852
29	525.0146
30	618.5938
31	722.4687
32	772.6331
33	785.9334
34	813.0693
35	914.5764
36	1043.3531
37	1045.9072
38	1119.8295
39	1122.3029
40	1226.1266
41	1369.4269
42	1371.3323
43	1373.4980
44	1377.3654
45	1396.7508
46	1522.1263
47	1595.4181
48	1611.2152
49	1632.1761
50	1636.1929
51	1637.4461
52	1712.3088

53	3000.5634
54	3003.4364
55	3459.6012
56	3459.9126
57	3588.4948
58	3589.3118

(c) The vibrational modes and harmonic frequencies of the model MOF containing DMBDC linker.

Vibrational Modes	Frequencies (cm^{-1})
1	7.7127
2	32.9492
3	42.6514
4	51.8669
5	58.2950
6	63.4552
7	67.5129
8	78.9103
9	115.7874
10	124.2364
11	147.0929
12	162.3490
13	173.7189
14	200.5901
15	215.0767
16	227.0117
17	244.9998
18	278.4616
19	310.3118
20	317.7934
21	325.5431
22	347.3406
23	370.5713
24	374.6728
25	386.8521
26	390.1334
27	475.4199
28	505.2338

29	513.3564
30	522.0079
31	604.4166
32	688.6223
33	772.3418
34	780.8822
35	799.2841
36	881.1792
37	997.3998
38	1044.6684
39	1046.5298
40	1116.1188
41	1119.5114
42	1171.8057
43	1225.4702
44	1329.7492
45	1370.5151
46	1372.7702
47	1375.6373
48	1380.4822
49	1441.6773
50	1463.1824
51	1476.9167
52	1570.3999
53	1611.6571
54	1632.1526
55	1633.0907
56	1636.4949
57	1704.9799
58	2997.7824
59	3000.3112
60	3012.6975
61	3102.7910
62	3224.2736
63	3460.2050
64	3589.1549
65	3589.9362
66	3590.2306

(d) The vibrational modes and harmonic frequencies of the model MOF containing TFBDC linker.

Vibrational Modes	Frequencies (cm^{-1})
1	8.7817
2	18.6142
3	31.0667
4	46.1061
5	49.8991
6	60.5201
7	69.5034
8	73.6036
9	108.1542
10	115.3211
11	131.0364
12	145.6506
13	156.3705
14	181.2445
15	206.1765
16	209.3355
17	228.1686
18	269.7781
19	292.2135
20	312.5602
21	339.1246
22	344.8675
23	356.3995
24	364.8792
25	407.6008
26	417.4667
27	441.4075
28	490.9623
29	496.7338
30	502.8308
31	522.1794
32	674.1766
33	769.5346
34	772.9293

35	789.7954
36	926.7824
37	1020.4194
38	1022.6127
39	1105.9376
40	1108.2471
41	1326.4343
42	1329.1452
43	1341.4249
44	1350.4234
45	1353.6191
46	1428.4373
47	1540.2635
48	1561.8914
49	1606.9590
50	1632.9483
51	1636.9913
52	1637.3088
53	3000.6878
54	3001.3427
55	3460.0818
56	3460.1009
57	3590.1798
58	3590.9893

(e) The vibrational modes and harmonic frequencies of the model MOF containing NDC linker.

Vibrational Modes	Frequencies (cm^{-1})
1	10.2180
2	31.1956
3	48.5214
4	52.8688
5	60.6010
6	65.1771
7	74.2034
8	77.0792
9	116.9288
10	130.5930

11	148.3225
12	167.5777
13	197.7477
14	221.2189
15	227.1890
16	245.4394
17	275.4246
18	310.7241
19	320.3260
20	327.0482
21	351.7287
22	371.3491
23	378.9831
24	388.4048
25	440.5469
26	480.0893
27	508.3451
28	515.5014
29	522.7197
30	598.0089
31	683.4265
32	772.1791
33	784.1376
34	796.8125
35	827.8368
36	902.9738
37	999.6505
38	1042.6182
39	1045.5274
40	1070.1920
41	1120.2474
42	1183.8430
43	1229.0121
44	1369.4542
45	1371.5086
46	1373.4397
47	1377.1917
48	1389.6332

49	1444.5078
50	1554.0686
51	1596.1906
52	1611.5891
53	1632.4551
54	1636.5914
55	1636.9833
56	1702.8567
57	2998.7868
58	3001.4482
59	3186.6548
60	3235.7082
61	3459.6803
62	3588.4536
63	3588.7014
64	3589.6549