MOFseq

fjh_v1-3c_B_Ch_v2-4c_Cu_1_Ch_v3-4c_Cu_1_Ch_2-1B_2F_Ch[Cu][Cu].[O-]C(=O)c1cc(F)c(cc1F)c1cc(cc(c1)c1cc(F)c(cc1F)C(=O)[O-])c1cc(F)c(cc1F)C(=O)[O-]

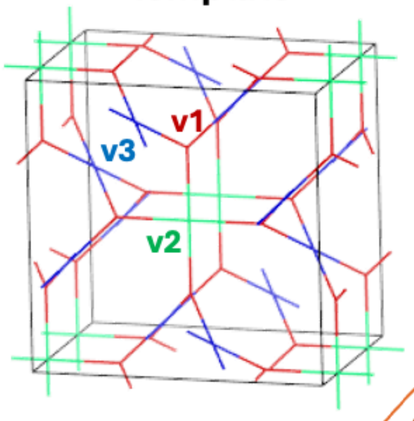
Local Strings — **Global Strings**

SMILES

[Cu][Cu] Atomic symbols indicate elements in building block $= \alpha$

[O-]C(=O)c1cc(F)c(cc1F)c1cc(cc(c1)c1cc(F)c(cc1F)C(=O)[O-])c1cc(F)c(cc1F)C(=O)[O-] Sequence of atomic symbols and special characters indicate connectivity patterns $= \beta$

Topological template

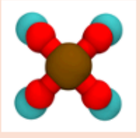


fjh_v1-A_v2-B_v3-C_2-D

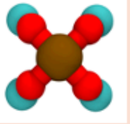
v_n: vertix of type n

number of times edge repeats

coordination_metal_version_END



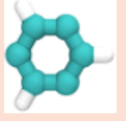
C = *4c_Cu_1_Ch*



B = *4c_Cu_1_Ch*

Inorganic NBB

coordination_spacername_END



A = *3c_B_Ch*

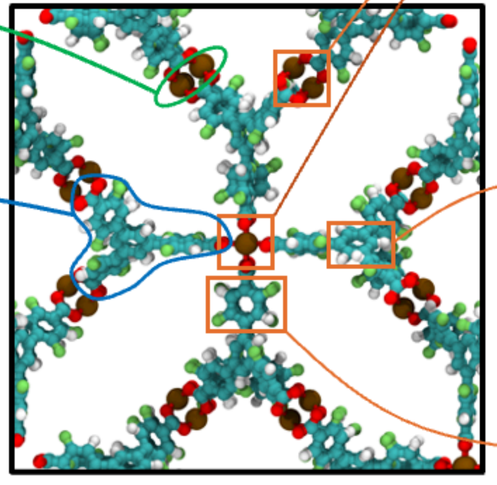
Organic NBB

#spacername_functionalization_END

D = *1B_2F_Ch*

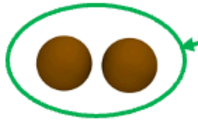
Organic EBB

MOF unit cell

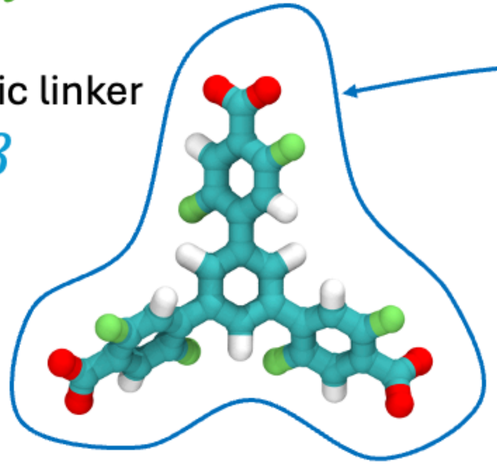


number of times spacer or functionalization repeats

Metal node α



Organic linker β



building blocks for MOF chemical synthesis

building blocks for MOF computer generation