SUPPORTING INFORMATION

Versatile Single-Ion Electrolyte with Grotthuss-like Li Conduction Mechanism for Dendrite-Free Li-Metal Batteries

Shouyi Yuan[1], Junwei Lucas Bao[2], Jishi Wei[1], Yongyao Xia[1], Donald G. Truhlar[2] and Yonggang Wang[1]**

[1] Department of Chemistry and Shanghai Key Laboratory of Molecular Catalysis and Innovative Materials, Institution of New Energy, Collaborative Innovation Center of Chemistry for Energy Materials, Fudan University, Shanghai, 200433, China

E-mail: ygwang@fudan.edu.cn.

[2] Department of Chemistry, Chemical Theory Center and Supercomputing Institute, University of Minnesota, 207 pleasant street SE, Minneapolis, State of Minnesota, MS 55455-0431, USA

E-mail: truhlar@umn.edu

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Computational Details:

Periodic electronic structure calculations were carried out using the *VASP* code.[S1] We used a unit cell that contains 6 Cu, 24 C, 6 H and 18 O atoms for optimizing the bulk structure of Cu-MOF-74. The optimization was performed at the spin-polarized density-functional theory (DFT) level with periodic boundary conditions by using the Perdew−Burke−Ernzerhof[S2] (PBE) exchange-correlation functional with D3-BJ functions[S3] for dispersion corrections. All degrees of freedom, including atomic positions, cell shape and cell volume, were fully relaxed. Spin-polarized calculations were performed with the projector augmented wave method,[S4] in which a planewave cutoff energy of 700 eV is adopted, and the precision ("PREC") for integration was set to "accurate", and the Brillouin zone was integrated based on a set of Γ-point centered 9×9×9 Monkhorst−Pack[S5] *k* points.

Cluster calculations are performed with *Gaussian 16* code[S6] to investigate the free energy of activation for Li ions hopping (a) between the two oxygen sites on Cu-MOF 74 in the large pore and (b) between the two perchlorate fragments that are added to Cu-MOF 74 in the large pore. The cluster model is shown in **Figure S5**; it is cleaved from the periodic-DFT optimized bulk structure and has the formula $C_{181}H_{87}Cu_{24}O_{94}$. Considering the computational cost for this large cluster, we optimized the geometries of all of the stationary points with the semiempirical PM7 [S7] method; all of the atoms except those shown explicitly in **Figure 3** were fixed at their corresponding positions in the bulk MOF structure during geometry optimization. PM7 is suitable for describing noncovalent interactions (with an error about 0.03 eV[S7] and should be sufficient for computing qualitatively correct free energies of activation. The natures of the stationary points were confirmed by normal mode analysis; the first-order saddle point (i.e., transition state structure) has only one imaginary frequency, and the local minimum has none (its frequencies are all real numbers). All of the harmonic frequencies are scaled by a factor of 1.078[S8] to approximately correct for vibrational anharmonicity and the systematic error in computing the harmonic frequencies, and they are used for computing the Gibbs free energies at 298 K. Our final reported Gibbs free energies are based on self-consistent reaction field (SCRF) calculations in diethyl ether solvent, in which the solvation free energies are obtained via single-point calculations with the SMD solvation model. [S9]

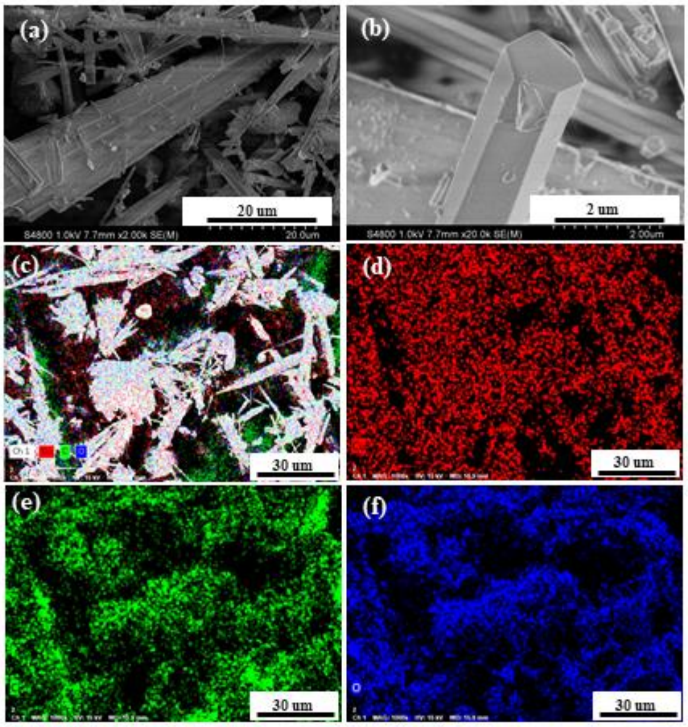

Figure S1. SEM images and element mapping of Cu-MOF-74: a,b) SEM images of Cu-MOF-74; c-f) EDS mapping of Cu-MOF-74.

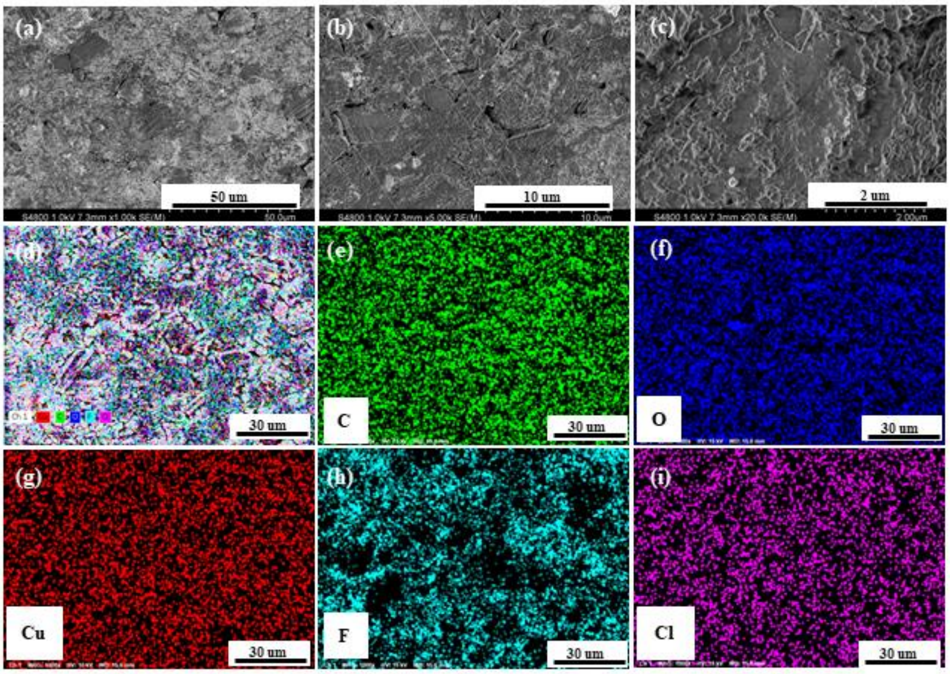

Figure S2. SEM images and element mapping of the electrolyte: a-c) SEM images of the single ion pellet; d-i) elemental mapping of the single ion electrolyte.

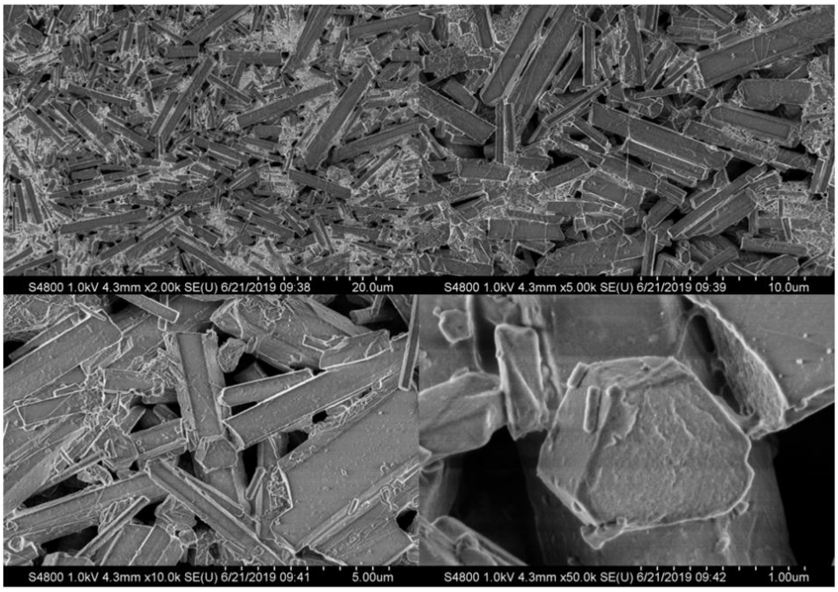

Figure S3. SEM images of the Single-ion electrolyte after cycling.

Figure S3 shows the SEM images of the single-ion electrolyte after cycling for 20 times. It can be observed that the morphology of the single-ion electrolyte after cycling remains unchanged.

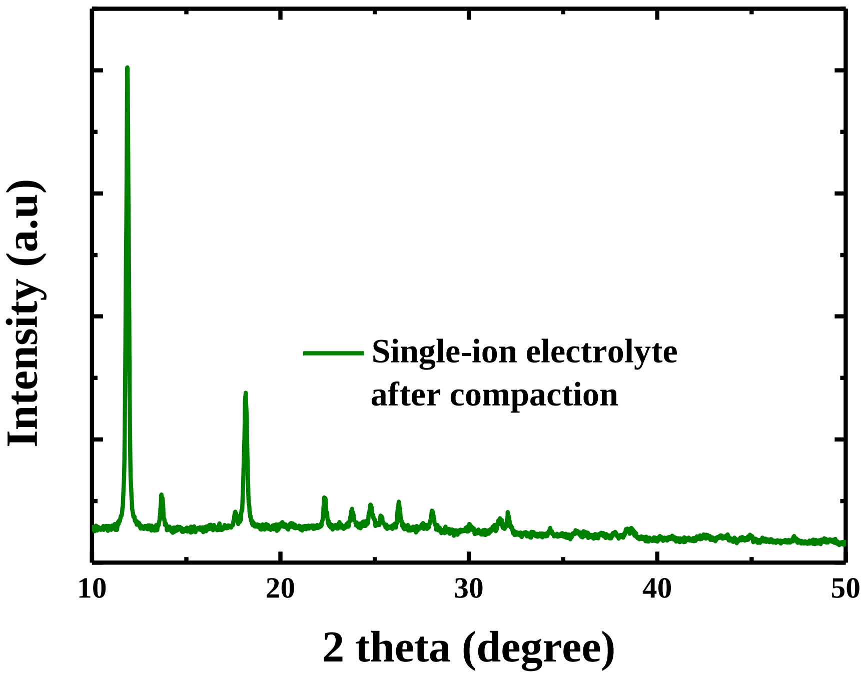

Figure S4. X-ray diffraction pattern of the single-ion electrolyte after compaction.

Figure S4 shows the XRD pattern of the single-ion electrolyte after compaction. Compared with the pristine MOF electrolyte, the XRD pattern remains unchanged, indicating the structural stability of the Cu MOF-74 after compaction.

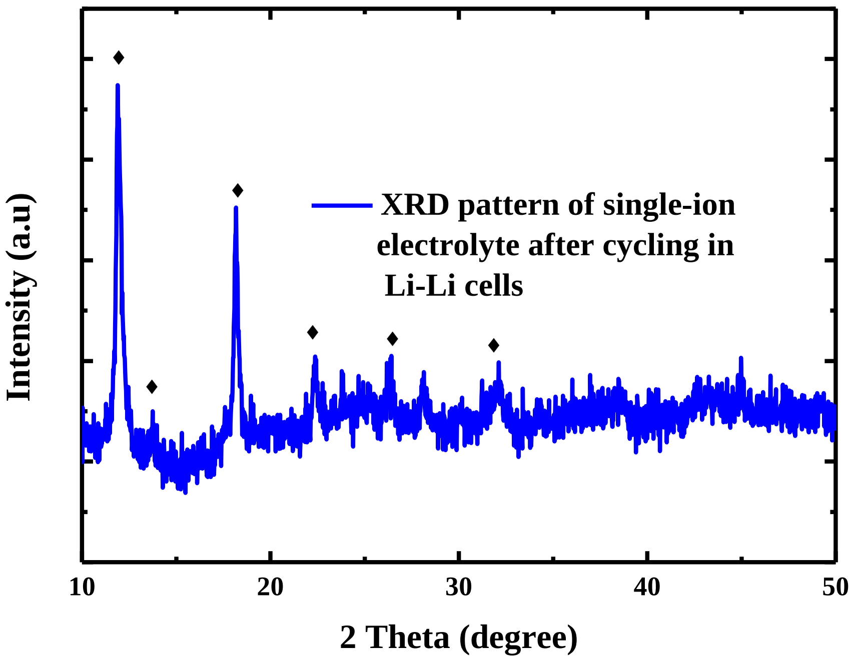

Figure S5. X-ray diffraction pattern of the single-ion electrolyte after cycling in Li-Li symmetric cells.

Figure S5 shows the XRD pattern of the single-ion electrolyte, which is retracted from the Li-Li symmetric cells. It can be identified in the Figure S5 that after cycling in Li-Li symmetric cell, the XRD pattern of single-ion electrolyte remains unchanged, indicating the structural stability of the single-ion electrolyte in the batteries.

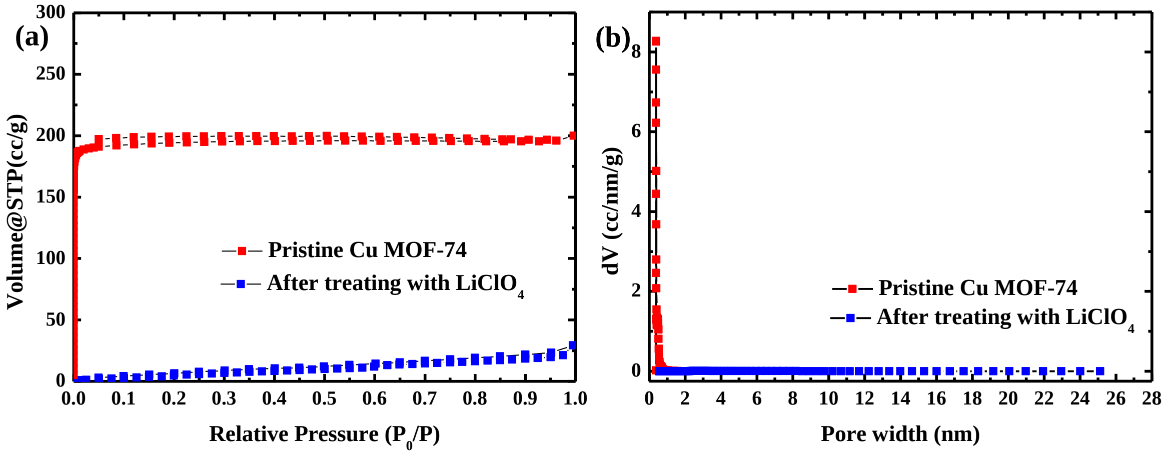

Figure S6. (a) N_2 adsorption and desorption isotherm of Pristine Cu MOF-74 and after treating with $LiClO_4$; (b) BJH Pore distribution of Cu MOF-74 and after treating with $LiClO_4$.

Figure S6a shows the N_2 adsorption and desorption isotherms of Pristine Cu MOF-74 and Cu MOF-74 after treating with $LiClO_4$. The pristine Cu MOF-74 exhibits a type-I adsorption-desorption isotherm, indicating the presence of micropores in the pristine Cu MOF-74. In addition, a high specific area of 630 m^2/g is obtained for the pristine Cu MOF-74. However, after treating with $LiClO_4$ solutions, the adsorption-desorption isotherm become type-III, indicating that the pore is clogged by $LiClO_4$ nanoparticles. In addition, the specific are sharply decrease from 630 m^2/g to 35 m^2/g. The result suggests that treating with $LiClO_4$, most of the micropore in the Cu MOF-74 was clogged. The BJH pore distribution of pristine Cu MOF-74 before and after treating with $LiClO_4$ is also given in **Figure S6b**. The result also confirms that the micropore of Cu MOF-74 was clogged after treating with $LiClO_4$.

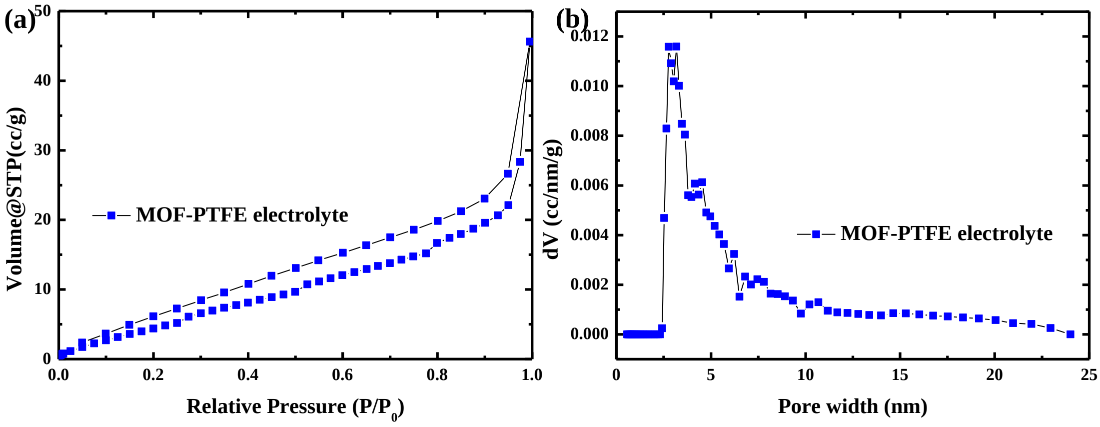

Figure S7. N_2 adsorption and desorption isotherm of Pristine Cu MOF-74 PTFE pellet after densification.

Figure S7a shows the N_2 adsorption desorption isotherm of the MOF-PTFE electrolyte after compaction. The electrolyte exhibits a H3 type adsorption and desorption isotherm with a specific area of $27 m^2 g^{-1}$, suggesting that some stacked pores still exsits even after compaction. Futhermore, the pore distribution of the MOF-PTFE electrolyte (**Figure S7b**) also confirm the existance of the stacked pore in the MOF-PTFE electrolyte. As shown in the **Figure S7b**, the pore width of the stacked pore is around 2.5nm. In addition, no micropores are observed in the MOF-PTFE electrolyte, indicating that the $LiClO_4$ are inside the micropores of the Cu MOF-74.

No.	*Electrolyte Type*	*Anionic Center*	*Ion Conductivity*	*Ref.*
1	Blend polymer	$-CO_2^-$	10^{-7}(25 °C)	S11
2	Random copolymer	$-CO_2^-$	10^{-7}(25 °C)	S12
3	Block copolymer	$-CO_2^-$	10^{-7}(25 °C)	S13
4	Blend polymer	$-(CF_2)_3CO_2^-$	10^{-8}(25 °C)	S14
5	Blend polymer	$-SO_3^-$	10^{-7}(25 °C)	S15
6	Random polymer	$-SO_3^-$	10^{-7}(25 °C)	S16
7	Grafted copolymer	$-SO_3^-$	10^{-8}(25 °C)	S17
8	Random polymer	$-CF(CF_3)SO_3^-$	10^{-7}(25 °C)	S18
9	Blend polymer	$-C_6H_5SO_3^-$	10^{-8}(25°C)	S19
10	Random polymer	$-C_6H_5SO_3^-$	10^{-7}(30 °C)	S20
11	Blend polymer	$-COCF_2SO_2N^-$	10^{-6}(100 °C)	S21
12	Blend polymer	$SO_2N^{(-)}SO_2CF_3$	10^{-9}(25°C)	S22
13	Homopolymer	$OB^{(-)}(O)(C_2O_4)$	10^{-6}(25 °C)	S23
14	**Metal organic framework**	$\mathbf{ClO_4^-}$	**10^{-3} (without drying)** **10^{-5}(after drying)**	**This work**

Table S1. Comparison of the ion conductivity of polymer electrolyte

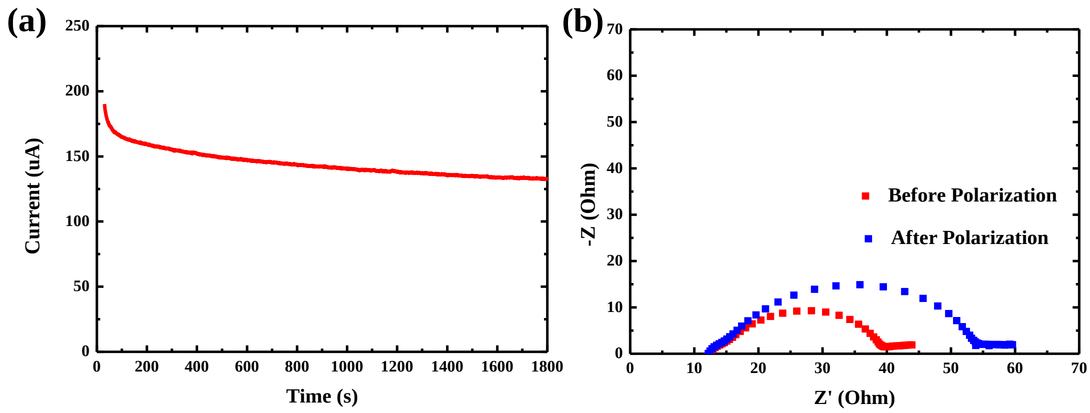

Figure S8. Li^+ transference number measurement. (a) $I(t)$-t plot of single-ion electrolyte with a voltage fluctuation of 10 mV. (b) The EIS spectrum of Li||Li symmetric cells before and after polarization.

The lithium ion transference number (t_{Li+}) was measured by combining an AC impedance measurement and a potentiostatic polarization measurement using Li||electrolyte||Li cells according to the previous report[S10]. First, an AC impedance test (10^6 to 1 Hz, 20 mV amplitude) was performed to obtain the initial resistance (R_0). The symmetric cell was then subjected to a constant DC voltage (V, 10 mV), during which the initial current (I_0) was monitored until reaching the steady-state current (I_{ss}). Another AC impedance test was then conducted to obtain the steady state resistance (R_{ss}). The Li ion transference number was calculated by the Evans-Vincent-Bruce equation:

$$t_+ = \frac{I_{ss}(\Delta V - I_0 R_0)}{I_0(\Delta V - I_{ss} R_{ss})}$$

where t_+ is the Li ion transference number, I_{ss} is the equilibrium current, I_0 is the initial current, R_0 is the initial impedance, R_{ss} is the impedance after reaching the equilibrium current, and ΔV is the applied voltage fluctuation (10 mV).

As shown in **Figure S3a**, the initial current (I_0) is 0.19 mA, and after stabilizing for 1800 s, an equilibrium current (I_{ss}) of 135 mA is obtained. **Figure S3b** shows the EIS spectra before and after polarization. The cell shows an initial impedance(R_0) of 28 Ω before polarization, and after reaching an equilibrium current, the impedance increases to 44 Ω. Thus, the calculated Li transference number is 0.82.

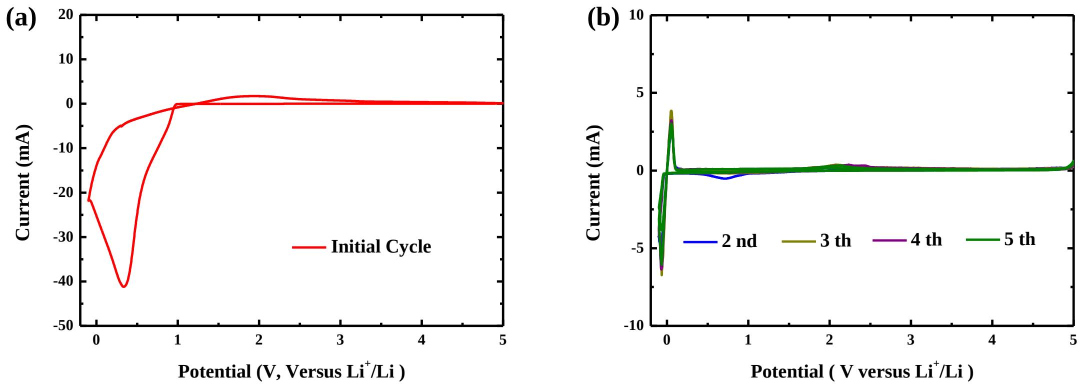

Figure S9. Cyclic voltammetry (CV) profiles of the electrolyte scanning from –0.2 V to 5 V at a scan rate of 1 mV s^{-1}.

The CV was carried out with a scan rate of 1 mV cm^{-2} from –0.2 V to 5.0 V to probe the electrochemical window of the single-ion electrolyte. A peak below 1 V is observed in the initial cycle due to the formation of the solid electrolyte interphase (SEI) layer (**Figure S3a**). After the initial cycle, the peak disappears (**Figure S3b**). Except for a small peak at 2.02 V, which is ascribed to the reversible lithiation process in the electrolyte, no other significant current is observed from 2.1 to 4.9 V. Therefore, the electrochemical window for the electrolyte is from 2.1 V to 4.9 V, which makes it appropriate for use with most cathode materials.

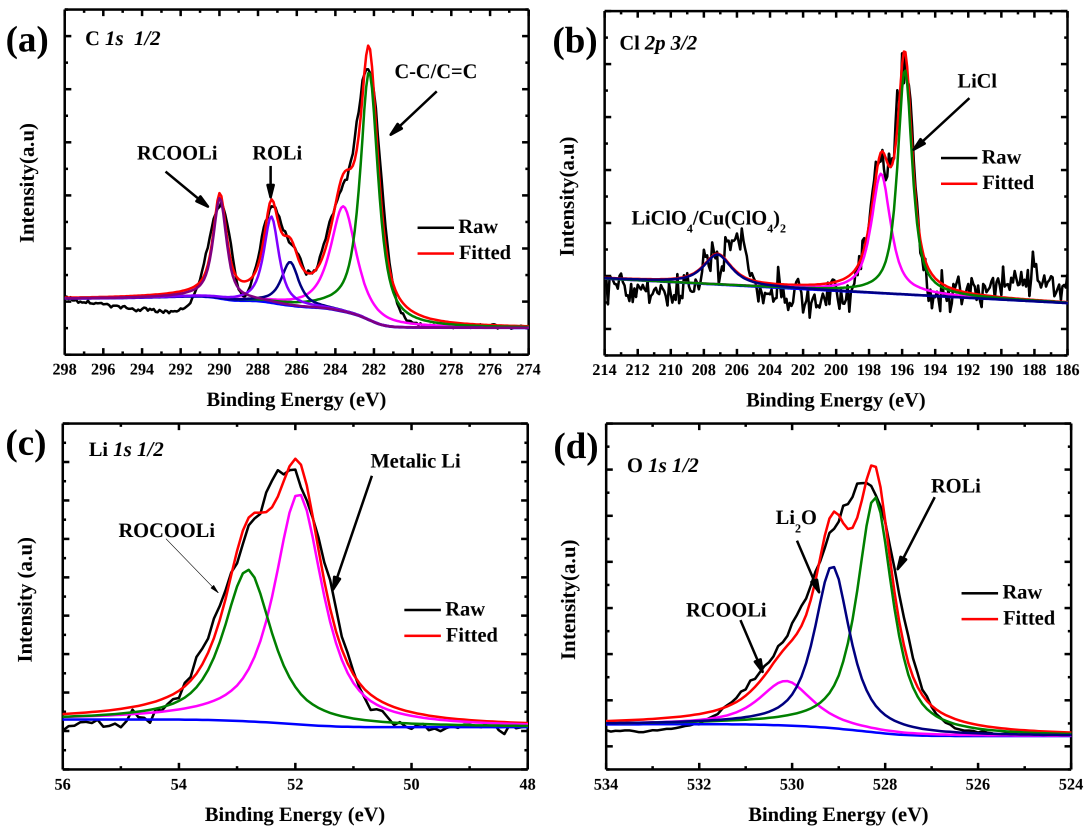

Figure S10. X-ray photoelectron spectroscopy of the Li metal retracted from the Li||Li symmetric cells: a) C *1s 1/2* XPS spectrum; b) Cl *2p 3/2* XPS spectrum; c) Li *1s 1/2* XPS spectrum; d) O *1s 1/2* XPS spectrum.

Figure S10 shows the XPS spectrum of the Li metal cycled in Li||Li symmetric cell. Prior to XPS measurement, the Li metal was washed several times with pure DME to remove any impurity on the surface. As shown in **Figure S10a**, the C *1s 1/2* XPS spectrum exhibits three main peaks, which are attributed to C-C/C=C groups(~284.0eV), ROLi groups (~287.0eV) and RCOOLi(~292.0eV) respectively. In addition, two peaks at ~195.0eV and ~197.0 eV are observed in Cl *1s 1/2* spectrum (**Figure S10b**), which is attributed to LiCl on the surface of Li metal. The LiCl mainly arises from the reduction of ClO_4^- on the surface of Li metal. In addition two weak peaks corresponding to the residual $LiClO_4$ and $Cu(ClO_4)_2$ are observed at ~ 208.0eV and ~206.0eV. As shown in **Figure 10c**, the Li *1s 1/2* spectrum of the Li metal can be fitted by two peaks corresponding to the metallic Li (~51.8eV) and ROCOOLi (~53.2eV). Finally, the O *1s 1/2* are fitted by three peaks corresponding to RCOOLi (~531.2eV), Li_2O(~529.0 eV) and ROLi(528.2 eV). Since the solvent in the Li||Li symmetric cell is DOL/DME, which is stable against Li metal, those functional groups corresponding to carboxyl groups and hydroxyl groups on the surface of Li metals come from the Cu MOF-74 matrix. Above all, the MOF backbones of the single-ion electrolyte participate in the formation of SEI layers on the Li metal.

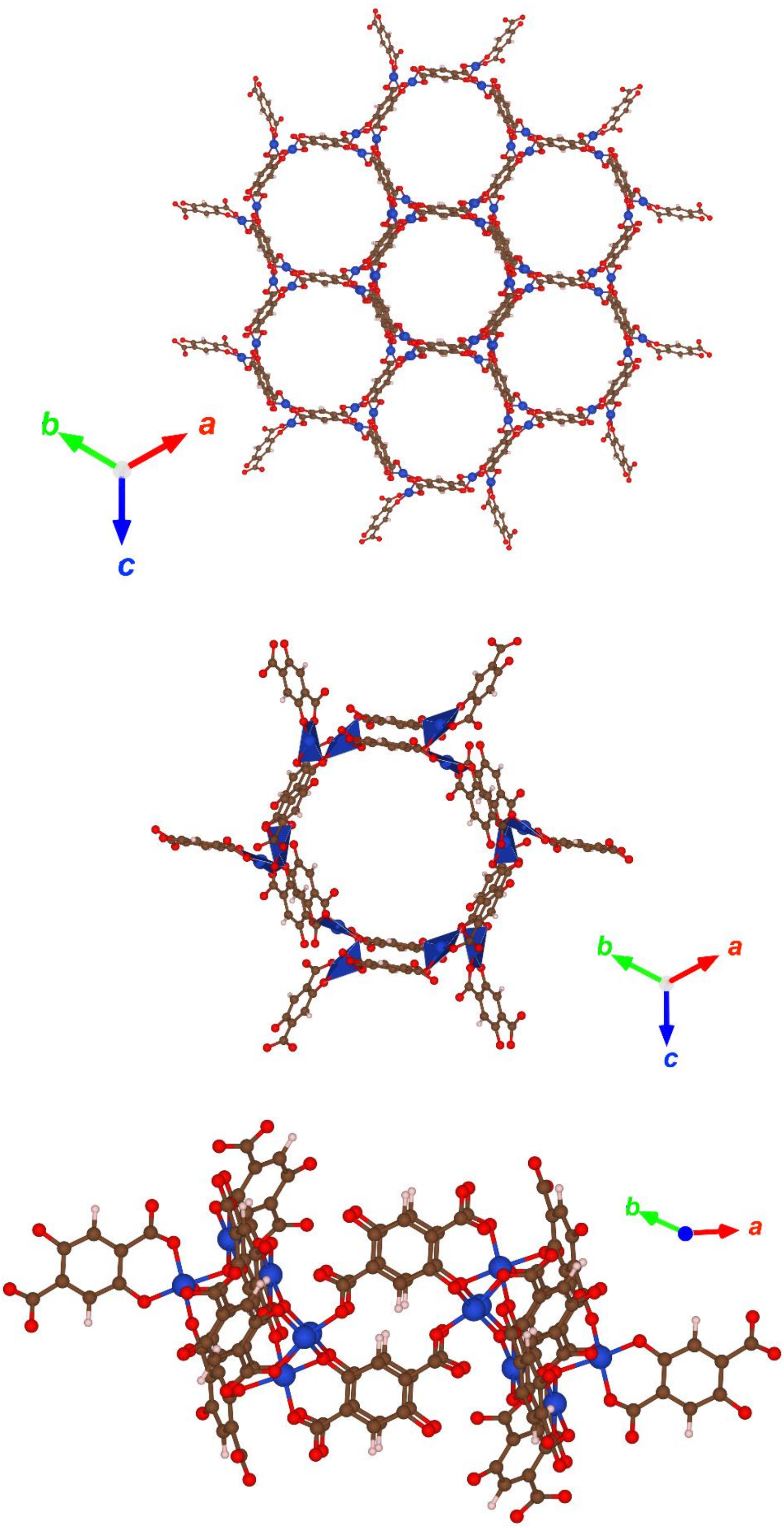

Figure S11. Optimized structure of Cu-MOF-74: (Top panel) overview of the crystalline structure; (Bottom panels) unit cell. (Cu: blue; O: red; C: brown; H: white). The three crystallographic basis vectors are denoted as ***a***, ***b***, and ***c***.

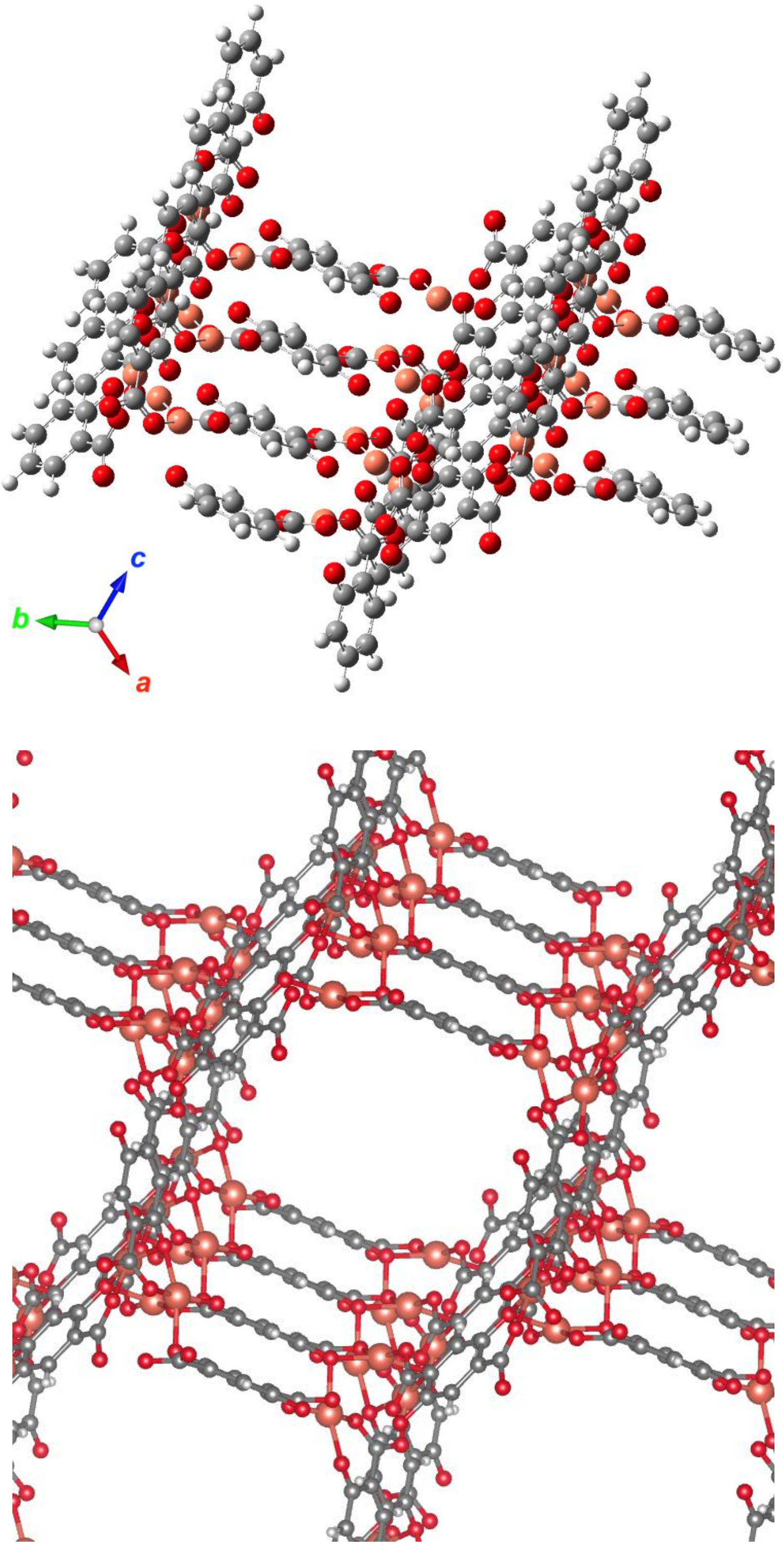

Figure S12. The structure of the cluster model (top) carved from the bulk MOF structure (bottom). (Color code: Cu orange, O red, C grey, and H white).

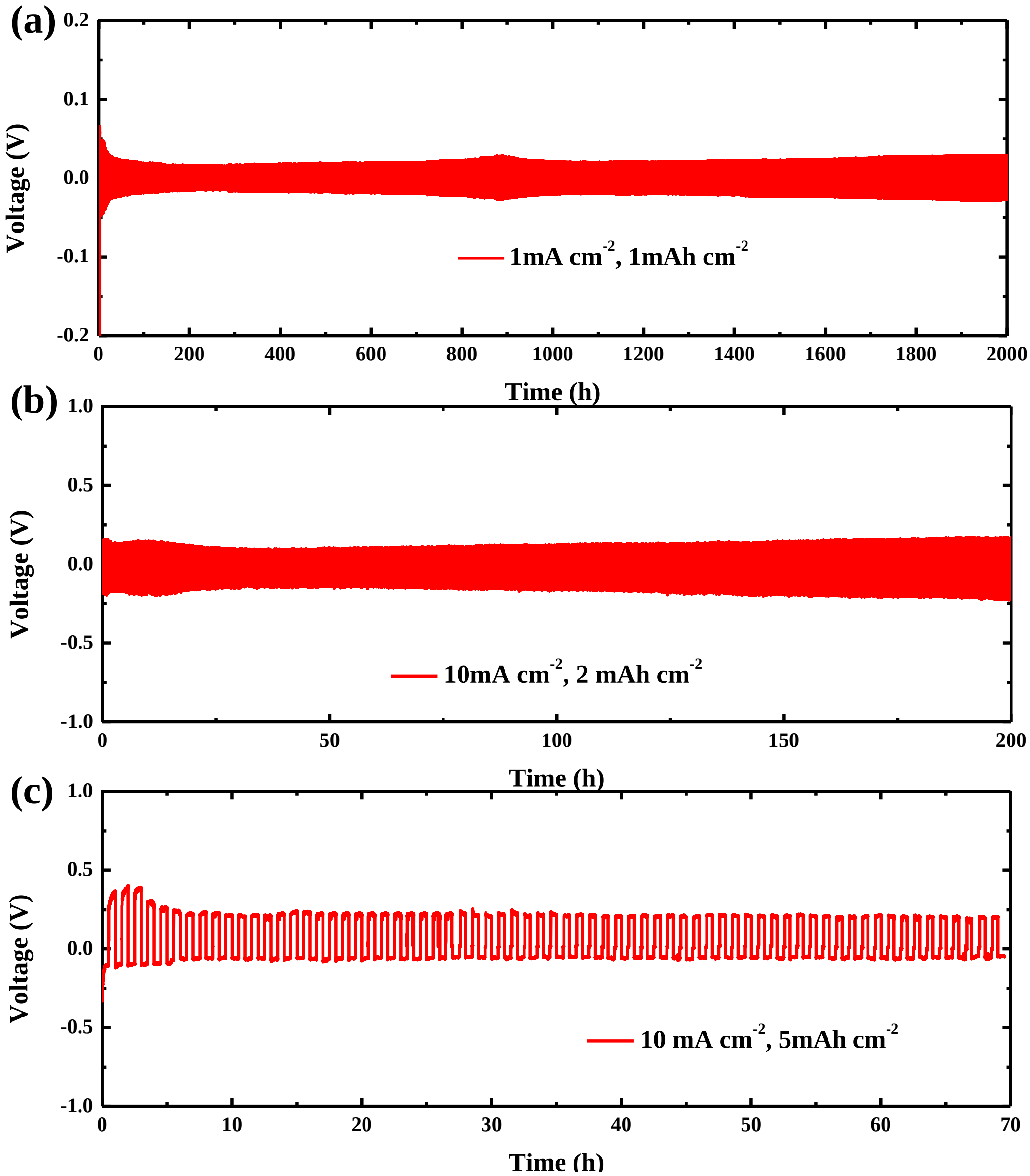

Figure S13. Li||Li symmetric cells with single-ion electrolyte at higher current density.

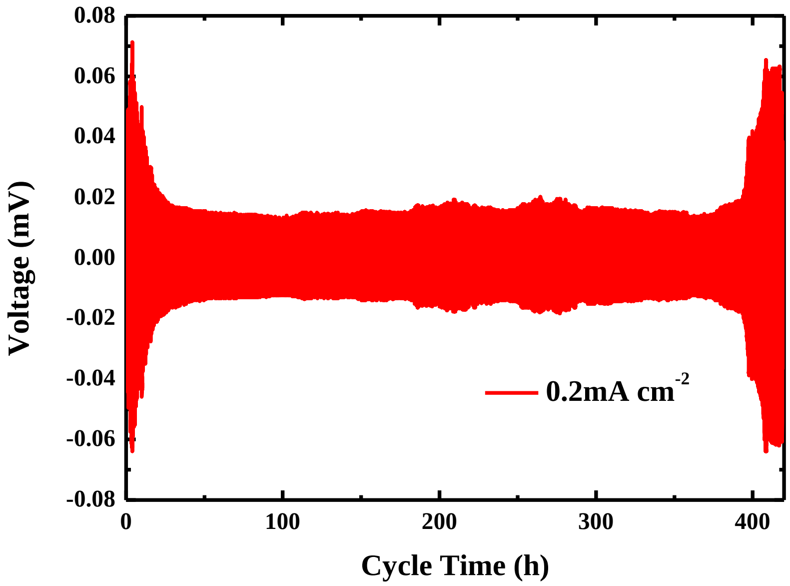

Figure S14. Voltage profile of Li||Li symmetric cells in the liquid electrolyte

No.	***Material***	***Current density***	***Capacity***	***Cycle life***	***Ref.***
1	PAN@LAGP	2 mA cm^{-2}	1 mAh cm^{-2}	1000 h	S24
2	CTAC Addictive[a]	4 mA cm^{-2}	2 mAh cm^{-2}	100 h	S25
3	Al_2O_3 Skeleton	8 mA cm^{-2}	1 mAh cm^{-2}	60 h	S26
4	Ag Graphene	5 mA cm^{-2}	1 mAh cm^{-2}	120 h	S27
5	$LiPS_4$ SEI layer	0.5 mA cm^{-2}	1 mAh cm^{-2}	2000 h	S28
6	InF_3 added electrolyte	1mA cm^{-2}	-	1000h	S29
7	3D flowable interphase	0.5mA cm^{-2}	0.5mAh cm^{-2}	900 h	S30
8	PEM additives	0.065mA cm^{-2}	-	1960 h	S31
9	Cu-CuO-Ni anode	0.5mA cm^{-2}	0.5mAh cm^{-2}	550 h	S32
10	Polymer Electrolyte	0.5mA cm^{-2}	-	300 h	34
		0.2mA cm^{-2}	**0.066 mAh cm^{-2}**	**2000 h**	**Present**
11	**Single ion electrolyte**	**1mA cm^{-2}**	**1 mAh cm^{-2}**	**2000 h**	**Present**
		10mA cm^{-2}	**2 mAh cm^{-2}**	**200 h**	**Present**
		10 mA cm^{-2}	**5 mAh cm^{-2}**	**70 h**	**Present**

Table S2. Comparisons of the performance of Li||Li symmetric cells

[a] hexadecyl trimethylammonium chloride

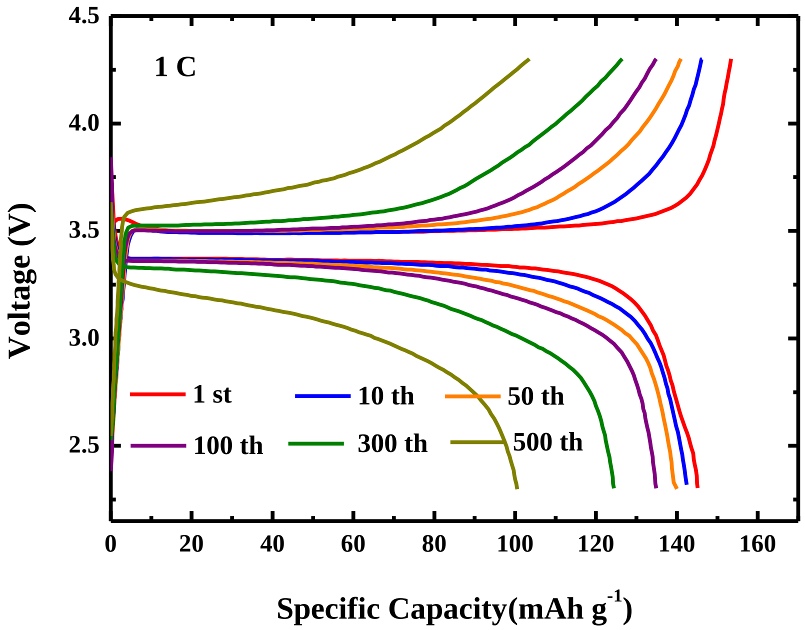

Figure S15. Voltage profiles of Li||$LiFePO_4$ Full cell in the liquid electrolyte at the current rate of 1C.

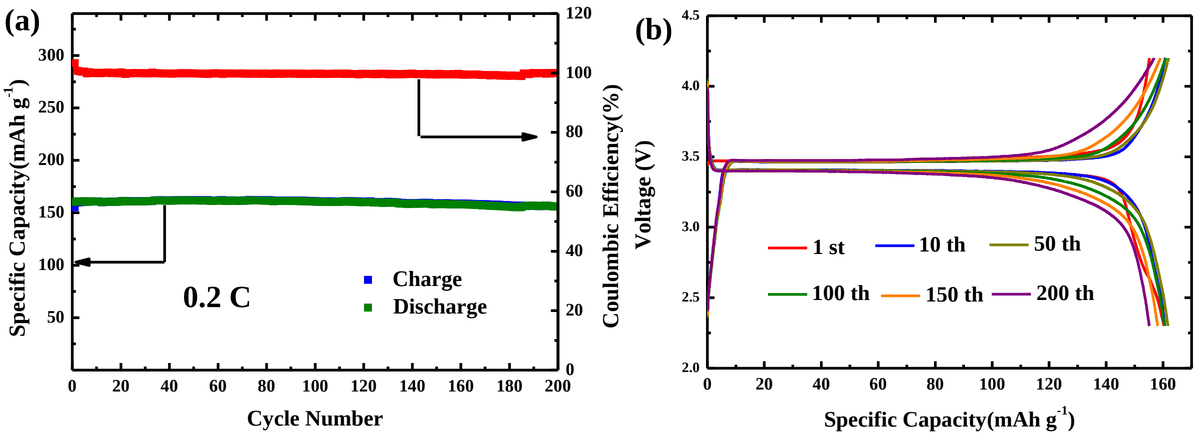

Figure S16. Cycle performance and Voltage profile of Li||$LiFePO_4$ full cell at 0.2C with single ion electrolyte: a) Cycle performance; b) Corresponding voltages profiles.

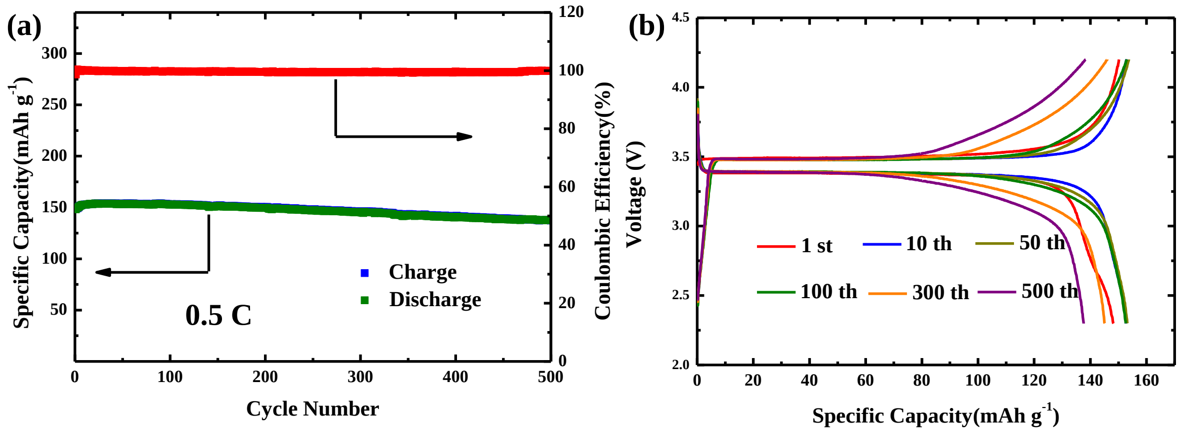

Figure S17. Cycle performance and Voltage profile of Li||$LiFePO_4$ full cell at 0.5C with single ion electrolyte: a) Cycle performance; b) Corresponding voltages profiles.

No.	***Material***	***Rate***	***Cycle life***	***Capacity retention***	***Ref.***
1	Li@3DCP	10 C, 90 mAh g^{-1}	1000	43.7%	S33
2	GPE	0.5 C, 140mAh g^{-1}	700	95.7%	S34
3	Li@3D porous Cu	1 C, 135 mAh g^{-1}	250	98%	S35
4	CNF interlayer	1 C, 140 mAh g^{-1}	800	80%	S36
5	Ionic Liquid	3 C, 10 mAh g^{-1}	1000	95%	S37
6	polymer electrolyte	1 C, 100 mAh g^{-1}	200	75%	S38
7	Dual crosslinked polymer electrolyte	2.5 C, 40 mAh g^{-1}	300	95%	S39
8	Li-rich Li_3AlF_6 Solid Electrolyte addictive	1 C, 80 mAh g^{-1}	110	80%	S40
9	Carbon Fiber	2 C, 100.9 mAh g^{-1}	500	90%	S41
10	Garnet solid electrolyte	0.05 C, 140 mAhg^{-1}	50	100%	S42
11	Ag@CF@Li composite	1 C, 140 mAh g^{-1}	400	60%	S43
12	Polymer Electrolyte	3 C 80 mAh g^{-1}	1000	-	34
13	**Single-ion electrolyte**	**5 C, 113 mAh g^{-1}**	**2000**	**75%**	**Present**

Table S3. Comparison of the performance of Li||$LiFePO_4$ full cell.

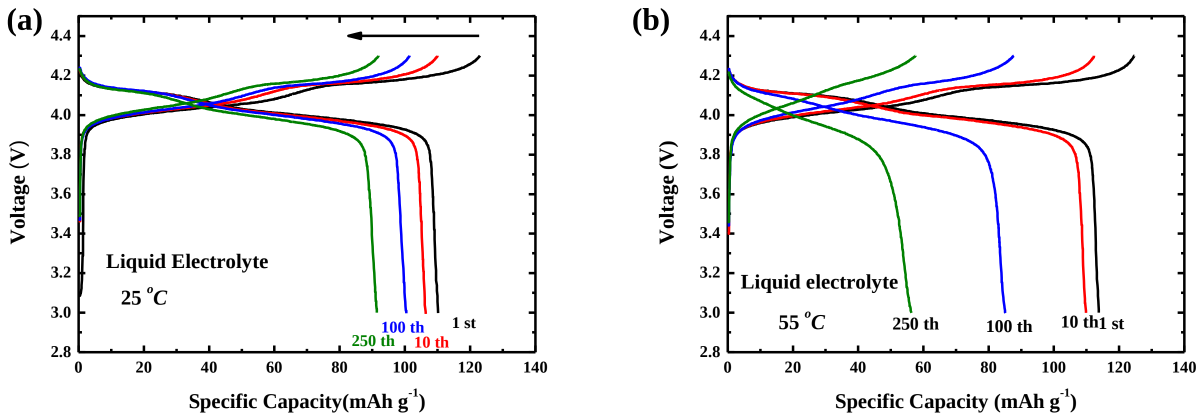

Figure S18. Voltage profiles of Li||$LiMn_2O_4$ full cells in liquid electrolyte at current rate of 1C under different temperature: a) 25 ºC; b) 55 ºC.

Table S4. Cartesian coordinates (Å) of the computed structures.

PBE-D3BJ optimized Cu-MOF-74

Lattice vectors:

15.2022259181068247	-0.0534076907396519	-0.2040355900782999
-7.1262469271205262	13.4260808018563598	-0.2026163510540593
-7.1265975943115523	-11.8002178112848153	6.4077490189541022

Direct (Cartesian) coordinates of atoms in the cell:

C	H	O	Cu
24	6	18	6

0.0332687727743497	0.1328199922418096	0.5601256363674794
0.0973412794676834	0.6321287071074475	0.1827762725446185
0.1328082428382339	0.5600760817332684	0.0332781518267908
0.1827850005492695	0.0973513753920224	0.6321047990294199
0.2142975321966007	0.7872713461023746	0.3842298773864681
0.2102104140797413	0.2227670952829874	0.6852409107695409
0.2227519830264914	0.6852229454378093	0.2102159605773401
0.2127017439151726	0.6157239533747254	0.7856855037990248
0.3147542352079497	0.7897692069365071	0.7772269820057335
0.3842389451931213	0.2143007880058905	0.7872184051225183
0.3678768830601663	0.8172170157129414	0.9026711678158175
0.4399144998592886	0.9667431764232701	0.8671822031469482
0.5600868239398866	0.0332582908519627	0.1328190163464363
0.6321220687942066	0.1827823421899808	0.0973284973071889
0.6157610271913226	0.7856993279323659	0.2127812657073541
0.6852453834840945	0.2102301529858274	0.2227726853790228
0.7872992261915672	0.3842767578845927	0.2143157122492718
0.7772489870802199	0.3147777658214449	0.7897852554709993
0.7897892046123240	0.7772322646393185	0.3147587566151870
0.7857024401878646	0.2127287698359030	0.6157697934433901
0.8172146181428314	0.9026479845303120	0.3678948683553294
0.8671927272685342	0.4399246295260142	0.9667230642214846
0.9026583392243679	0.3678706528148017	0.8172233948401519
0.9667308459177087	0.8671793676804752	0.4398740310172839
0.1688611687079737	0.6251763601597515	0.6021752456330036
0.3748297656133945	0.3978584266758044	0.8311656270857866
0.3978246062728318	0.8311373743487150	0.3748372253006004
0.6021763638339578	0.1688633369105604	0.6251639907476750
0.6251698530786568	0.6021409332464945	0.1688340402989909
0.8311388036764987	0.3748237557785190	0.3978244251968687
0.1359003781986814	0.7971217551936587	0.3866015497917399
0.0798963005590442	0.2711080429615951	0.6342790979175962
0.0805934280449136	0.4411214355192767	0.5989622087095955

0.2711204620066537	0.6342234893441675	0.0799463195559957
0.2028494658866860	0.6133483845321508	0.8641079770044180
0.3866010963640338	0.1358606649057114	0.7970362135834781
0.3657460402223814	0.9200743061545622	0.7288547033737551
0.4010602601985304	0.9194020540829955	0.5588701574854469
0.4411175492401195	0.5989203306987837	0.0806478053555577
0.5588820694519318	0.4010790292235152	0.9193518620292056
0.5989393584935210	0.0805973058393177	0.4411295098993164
0.6342539321621193	0.0799258097836585	0.2711449674561670
0.6133998737427203	0.8641400463535782	0.2029650024648186
0.7971505064978006	0.3866517314061553	0.1358916938254827
0.7288795103778257	0.3657766265941172	0.9200533512738909
0.9194061906471873	0.5588779244030578	0.4010374586751324
0.9201033181330213	0.7288913169606683	0.3657205694671671
0.8640992404933699	0.2028776047285904	0.6133981175930233
0.1394049175913913	0.8298112892856762	0.5659953752270592
0.1701808868206140	0.4339476242439780	0.8606383134306984
0.4339553782802228	0.8605827774717927	0.1701947605339211
0.5660442404118355	0.1394165824505347	0.8298049068508635
0.8298187318714444	0.5660517356783281	0.1393613539540791
0.8605950547931095	0.1701888266525872	0.4340042956028914

Carved cluster for Cu-MOF-74

C	-6.18932900	-7.80304600	-8.70672200
C	9.01436000	-7.80304600	-8.70672200
C	-5.32609700	-6.36172900	-2.65986000
C	9.87759200	-6.36172900	-2.65986000
C	-4.46286600	-4.92041300	3.38700300
C	-13.25992400	-8.55892000	-4.94163900
C	1.94376700	-8.55892000	-4.94163900
C	-12.39669200	-7.11760400	1.10522300
C	2.80699700	-7.11760400	1.10522300
C	-11.13210800	-7.73629200	-5.84563400
C	4.07158200	-7.73629200	-5.84563400
C	-10.26887600	-6.29497600	0.20122800
C	4.93481300	-6.29497600	0.20122800
C	-4.17794400	-9.13956300	-8.27147500
C	11.02574500	-9.13956300	-8.27147500
C	-3.31471300	-7.69824600	-2.22461200
C	11.88897700	-7.69824600	-2.22461200
C	-2.45148100	-6.25693000	3.82225100
C	1.16504600	-8.88932800	-3.72347700
C	2.02827600	-7.44801100	2.32338500
C	-5.04121800	-8.09412000	-7.95016800
C	10.16247200	-8.09412000	-7.95016800
C	-4.17798600	-6.65280300	-1.90330500
C	11.02570200	-6.65280300	-1.90330500
C	-3.31475500	-5.21148600	4.14355800
C	-11.93065900	-8.17549100	-4.77571600
C	3.27303100	-8.17549100	-4.77571600
C	-11.06742800	-6.73417400	1.27114700
C	4.13626200	-6.73417400	1.27114700
C	-8.54107700	-4.02842600	-7.34279300
C	6.66261300	-4.02842600	-7.34279300
C	-7.67784500	-2.58711000	-1.29593000
C	7.52584400	-2.58711000	-1.29593000
C	-6.81461400	-1.14579300	4.75093200
C	-8.17675600	-1.59428300	-7.39394000
C	7.02693400	-1.59428300	-7.39394000
C	-0.14351800	-13.55726100	-1.34707800
C	-7.31352400	-0.15296600	-1.34707800
C	7.89016500	-0.15296600	-1.34707800

C	0.71971200	-12.11594500	4.69978500
C	-6.45029300	1.28835000	4.69978500
C	-3.06586300	-9.42755900	-7.33352400
C	-2.20263200	-7.98624200	-1.28666100
C	-1.33940100	-6.54492600	4.76020100
C	-8.46538700	-2.72705100	-6.63539700
C	6.73830200	-2.72705100	-6.63539700
C	-0.43215000	-14.69002900	-0.58853400
C	-7.60215600	-1.28573400	-0.58853400
C	7.60153300	-1.28573400	-0.58853400
C	0.43108000	-13.24871300	5.45832800
C	-6.73892500	0.15558200	5.45832800
C	-8.18778200	-0.29820500	-6.84999400
C	7.01590800	-0.29820500	-6.84999400
C	-0.15454500	-12.26118300	-0.80313100
C	-7.32455100	1.14311200	-0.80313100
C	7.87913800	1.14311200	-0.80313100
C	0.70868600	-10.81986600	5.24373100
C	-6.46131900	2.58442900	5.24373100
C	5.59808800	-4.02574000	-11.29058600
C	-1.57236500	-15.98871900	-5.24372400
C	-8.74236900	-2.58442400	-5.24372400
C	6.46131900	-2.58442400	-5.24372400
C	-0.70913300	-14.54740200	0.80313800
C	-7.87913800	-1.14310700	0.80313800
C	7.32455100	-1.14310700	0.80313800
C	5.87568500	-1.59690300	-11.50519300
C	-1.29476800	-13.55988200	-5.45833100
C	-8.46477200	-0.15558700	-5.45833100
C	6.73891600	-0.15558700	-5.45833100
C	-0.43153700	-12.11856600	0.58853200
C	-7.60154200	1.28573000	0.58853200
C	7.60214700	1.28573000	0.58853200
C	-6.69428300	-6.85936500	-4.76020300
C	8.50940800	-6.85936500	-4.76020300
C	-5.83105100	-5.41804800	1.28665900
C	9.37263900	-5.41804800	1.28665900
C	5.58706300	-2.72967100	-10.74665000
C	-1.58339000	-14.69265000	-4.69978700
C	-8.75339300	-1.28835500	-4.69978700
C	6.45029400	-1.28835500	-4.69978700
C	-0.72015800	-13.25133300	1.34707600
C	-7.89016300	0.15296200	1.34707600
C	7.31352600	0.15296200	1.34707600
C	-1.21907000	-12.25850700	-4.75092500
C	-0.35583800	-10.81719000	1.29593800
C	2.17051400	-8.11144300	-7.31800200
C	-12.16994300	-6.67012600	-1.27114000
C	3.03374500	-6.67012600	-1.27114000
C	-11.30671300	-5.22881000	4.77572300
C	3.89697600	-5.22881000	4.77572300
C	-4.71892800	-8.19281200	-4.14355900
C	10.48476200	-8.19281200	-4.14355900
C	-3.85569700	-6.75149600	1.90330300
C	11.34799200	-6.75149600	1.90330300
C	4.27849900	-7.39759500	-8.37025000
C	-10.06195800	-5.95627800	-2.32338700
C	5.14173000	-5.95627800	-2.32338700
C	-9.19872800	-4.51496200	3.72347500
C	6.00496100	-4.51496200	3.72347500
C	-5.58220200	-7.14737000	-3.82225300
C	9.62148900	-7.14737000	-3.82225300
C	-4.71897000	-5.70605400	2.22461000
C	10.48471900	-5.70605400	2.22461000
C	1.37196200	-8.55064100	-6.24808400
C	-12.96849400	-7.10932400	-0.20122100
C	2.23519300	-7.10932400	-0.20122100
C	-12.10526400	-5.66800800	5.84564200
C	3.09842500	-5.66800800	5.84564200
C	3.49977900	-7.72801200	-7.15208800
C	-10.84067800	-6.28669500	-1.10522500
C	4.36301000	-6.28669500	-1.10522500
C	-9.97744800	-4.84537800	4.94163800
C	5.22624100	-4.84537800	4.94163800
C	-3.57081700	-8.48388700	-3.38700500
C	11.63287400	-8.48388700	-3.38700500
C	-2.70758500	-7.04257000	2.65985800

C	12.49610300	-7.04257000	2.65985800
H	-7.95953700	-1.70639400	-8.45245500
H	7.24415300	-1.70639400	-8.45245500
H	0.07370000	-13.66937300	-2.40559200
H	-7.09630600	-0.26507700	-2.40559200
H	8.10738400	-0.26507700	-2.40559200
H	0.93693100	-12.22805600	3.64127100
H	-6.23307500	1.17623900	3.64127100
H	-4.84014800	-7.49283700	-7.06778100
H	10.36354200	-7.49283700	-7.06778100
H	-3.97691700	-6.05152100	-1.02091800
H	11.22677200	-6.05152100	-1.02091800
H	-3.11368500	-4.61020400	5.02594400
H	-11.49552500	-8.18897100	-3.78027300
H	3.70816400	-8.18897100	-3.78027300
H	-10.63229400	-6.74765400	2.26658900
H	4.57139500	-6.74765400	2.26658900
H	1.73538000	-8.09796200	-8.31344400
H	-12.60507700	-6.65664600	-2.26658200
H	2.59861100	-6.65664600	-2.26658200
H	-11.74184600	-5.21532900	3.78028100
H	3.46184200	-5.21532900	3.78028100
H	-4.91999700	-8.79409500	-5.02594700
H	10.28369300	-8.79409500	-5.02594700
H	-4.05676500	-7.35277800	1.02091600
H	11.14692400	-7.35277800	1.02091600
H	5.36984300	-2.61755000	-9.68813500
H	-1.80061000	-14.58052800	-3.64127300
H	-8.97061300	-1.17623400	-3.64127300
H	6.23307500	-1.17623400	-3.64127300
H	-0.93737800	-13.13921200	2.40559000
H	-8.10738300	0.26508300	2.40559000
H	7.09630600	0.26508300	2.40559000
O	-0.11451300	-8.78566200	-3.70913600
O	0.74871700	-7.34434600	2.33772600
O	-7.00365800	-6.83648800	-8.25832700
O	8.20003100	-6.83648800	-8.25832700
O	-6.14042700	-5.39517100	-2.21146400
O	9.06326300	-5.39517100	-2.21146400
O	-5.27719500	-3.95385500	3.83539800
O	-7.95881800	-4.13508300	-8.47188300
O	7.24487200	-4.13508300	-8.47188300
O	-7.09558700	-2.69376600	-2.42502000
O	8.10810300	-2.69376600	-2.42502000
O	-6.23235600	-1.25245000	3.62184200
O	-9.89552100	-7.30069000	-5.56343800
O	5.30816900	-7.30069000	-5.56343800
O	-9.03229000	-5.85937300	0.48342400
O	6.17140000	-5.85937300	0.48342400
O	-9.23615800	-4.99843600	-6.86858300
O	5.96753100	-4.99843600	-6.86858300
O	-8.37292800	-3.55711900	-0.82172100
O	6.83076100	-3.55711900	-0.82172100
O	-7.50969600	-2.11580300	5.22514200
O	-2.53793200	-10.59644400	-7.27415700
O	-1.67470000	-9.15512800	-1.22729400
O	-0.81146900	-7.71381100	4.81956900
O	0.04430800	-11.23193700	-1.63957800
O	0.90753800	-9.79062100	4.40728400
O	1.80490000	-9.20742600	-2.66745200
O	2.66813100	-7.76611000	3.37941100
O	-7.06284500	-7.78229500	-5.55919600
O	8.14084500	-7.78229500	-5.55919600
O	-6.19961300	-6.34097800	0.48766600
O	9.00407600	-6.34097800	0.48766600
O	-2.69730200	-8.50463900	-6.53453100
O	-1.83407000	-7.06332200	-0.48766800
O	-0.97083900	-5.62200500	5.55919500
O	3.63864400	-7.07950600	-9.42627500
O	-10.70181300	-5.63818900	-3.37941300
O	4.50187500	-5.63818900	-3.37941300
O	-9.83858200	-4.19687300	2.66744900
O	5.36510700	-4.19687300	2.66744900
O	5.39923600	-5.05498500	-10.45414900
O	-8.94122100	-3.61366900	-4.40728600
O	6.26246700	-3.61366900	-4.40728600
O	-8.07799100	-2.17235200	1.63957600

O	7.12569800	-2.17235200	1.63957600
O	-7.22221500	-5.69049000	-4.81956100
O	7.98147500	-5.69049000	-4.81956100
O	-6.35898400	-4.24917300	1.22730100
O	8.84470600	-4.24917300	1.22730100
O	-0.52398800	-11.28848700	-5.22514400
O	0.33924400	-9.84717100	0.82171800
O	0.13537500	-8.98623400	-6.53028900
O	0.99860700	-7.54491700	-0.48342600
O	1.86183800	-6.10360100	5.56343700
O	-1.80132900	-12.15184900	-3.62184400
O	-0.93809700	-10.71053200	2.42501800
O	-2.75648800	-9.45044500	-3.83540100
O	-1.89325600	-8.00912900	2.21146200
O	5.55805800	-7.50127000	-8.38459100
O	-8.78239900	-6.05995400	-2.33772800
O	6.42128900	-6.05995400	-2.33772800
O	-7.91916800	-4.61863700	3.70913400
O	7.28452000	-4.61863700	3.70913400
Cu	-1.58195100	-10.49356700	-2.62436600
Cu	-0.71872000	-9.05225000	3.42249600
Cu	-8.42165800	-7.36166900	-6.88956400
Cu	6.78203200	-7.36166900	-6.88956400
Cu	-7.55842700	-5.92035200	-0.84270100
Cu	7.64526200	-5.92035200	-0.84270100
Cu	-6.69519600	-4.47903600	5.20416200
Cu	-9.68994900	-5.34614300	-5.01771800
Cu	5.51374100	-5.34614300	-5.01771800
Cu	-8.82671700	-3.90482600	1.02914400
Cu	6.37697100	-3.90482600	1.02914400
Cu	-0.07019700	-10.94079000	-7.07600900
Cu	0.79303400	-9.49947400	-1.02914600
Cu	1.65626600	-8.05815700	5.01771600
Cu	-1.33848800	-8.92526400	-5.20416400
Cu	-0.47525600	-7.48394700	0.84269900
Cu	7.02549500	-5.79335600	-9.46936000
Cu	-7.31496200	-4.35203900	-3.42249800
Cu	7.88872600	-4.35203900	-3.42249800
Cu	-6.45173200	-2.91072300	2.62436400
Cu	8.75195700	-2.91072300	2.62436400
C	-6.44543100	-8.58868500	-9.86911600
C	8.75825700	-8.58868500	-9.86911600
C	-13.83172400	-8.55064100	-6.24808400
C	-11.70390800	-7.72801200	-7.15208800
C	-4.43404600	-9.92520100	-9.43386700
C	10.76964200	-9.92520100	-9.43386700
C	0.15409800	-13.10608600	6.85000100
C	-7.01590700	0.29821000	6.85000100
C	0.43169500	-10.67724900	6.63539500
C	-6.73831100	2.72704600	6.63539500
C	5.87507200	-4.16836500	-12.68225900
C	-1.29538200	-16.13134400	-6.63539700
C	6.15267700	-1.73951900	-12.89685500
C	-1.01777600	-13.70249700	-6.84999400
C	10.74082200	-4.92041300	3.38700300
C	-11.53346100	-5.67628700	7.15208600
C	3.67022800	-5.67628700	7.15208600
C	-9.40564500	-4.85365900	6.24809100
C	5.79804300	-4.85365900	6.24809100
C	12.75220700	-6.25693000	3.82225100
O	-9.64562900	-7.50127000	-8.38459100
O	-8.16905800	-4.41805600	6.53028700
O	-5.33638200	-4.89966200	6.53452900
O	-0.81892300	-12.67325200	-7.68644100
O	0.94166900	-10.64874100	-8.71431400
O	1.20247500	-8.40585400	6.86858100
O	7.11824400	-7.13180400	-10.86642400
O	9.92649300	-3.95385500	3.83539800
O	8.97133300	-1.25245000	3.62184200
C	-7.55751100	-8.30067900	-10.80706600
C	-5.58215700	-9.63412700	-10.19042200
C	7.64617600	-8.30067900	-10.80706600
C	9.62153100	-9.63412700	-10.19042200
C	-13.03317300	-8.11144300	-7.31800200
C	-10.92518800	-7.39759500	-8.37025000
O	-3.61971700	-10.89176000	-9.88226300
C	0.14307300	-11.81001700	7.39393900

C	-7.02693200	1.59427900	7.39393900
O	-7.21476000	-0.73103500	7.68643900
C	0.50739300	-9.37587400	7.34280000
C	5.79938300	-5.46974100	-13.38965400
C	6.16370300	-3.03559800	-13.44080200
C	-1.00675000	-14.99857600	-7.39394000
C	11.88893300	-5.21148600	4.14355800
C	-10.20419600	-5.29285800	7.31800900
C	4.99949200	-5.29285800	7.31800900
C	2.89150700	-6.00669500	8.37024800
O	7.03463000	-4.41805600	6.53028700
C	-4.96781900	-3.97673100	7.33352200
C	0.30181500	-10.33064300	-9.77034000
C	8.38907400	-1.14579300	4.75093200
O	-7.92607400	-9.22361000	-11.60605900
O	-8.08544300	-7.13180400	-10.86642400
H	-5.78322600	-10.23541000	-11.07280900
O	7.27761400	-9.22361000	-11.60605900
H	9.42046200	-10.23541000	-11.07280900
H	-13.46830700	-8.09796200	-8.31344400
O	-11.56504200	-7.07950600	-9.42627500
H	-0.07414700	-11.69789500	8.45245300
H	-7.24415200	1.70640000	8.45245300
O	-0.07486600	-9.26921600	8.47188100
O	6.38164100	-5.57639800	-14.51874400
O	5.10430000	-6.43975100	-12.91544500
H	6.38092200	-3.14770800	-14.49931600
H	-0.78953100	-15.11068700	-8.45245500
H	12.09000300	-4.61020400	5.02594400
H	-9.76906300	-5.30633800	8.31345200
H	5.43462500	-5.30633800	8.31345200
O	1.61194800	-5.90302900	8.38458900
O	3.53136100	-6.32479300	9.42627300
C	-9.32800200	-1.59690300	-11.50519300
O	-5.49575200	-2.80785700	7.27416400
C	-3.85573900	-4.26473700	8.27147200
C	1.08053500	-10.00023500	-10.98850300
O	-0.97774500	-10.22697600	-9.75599900
O	7.69399200	-2.11580300	5.22514200
C	8.46476400	0.15558200	5.45832800
C	-9.05101100	-1.73951900	-12.89685500
C	-9.61662300	-2.72967100	-10.74665000
C	-2.99246500	-5.31017900	7.95016600
C	-3.59963500	-3.47909600	9.43386600
C	0.50873300	-9.99195600	-12.29494500
C	2.40980000	-9.61680600	-10.82257800
C	8.75339500	1.28835000	4.69978500
C	8.18778200	0.29821000	6.85000100
C	-9.03998500	-3.03559800	-13.44080200
C	-9.60559800	-4.02574000	-11.29058600
H	-9.83384300	-2.61755000	-9.68813500
H	-3.19353400	-5.91146200	7.06777900
C	-1.84435400	-5.60125400	8.70672000
C	-2.45152400	-3.77017000	10.19042000
C	1.30728400	-9.55275700	-13.36486400
C	3.20835100	-9.17760700	-11.89249700
H	2.84493300	-9.63028500	-9.82713600
H	8.97061300	1.17623900	3.64127100
C	8.74236900	2.58442900	5.24373100
C	8.17675700	1.59427900	7.39393900
O	7.98892900	-0.73103500	7.68643900
H	-8.82276600	-3.14770800	-14.49931600
C	-9.32861700	-4.16836500	-12.68225900
O	-9.80445100	-5.05498500	-10.45414900
O	-1.03002500	-6.56781100	8.25832500
C	-1.58825000	-4.81561300	9.86911400
H	-2.25045400	-3.16888800	11.07280700
H	0.87215100	-9.53927700	-14.36030600
C	2.63654900	-9.16932700	-13.19895000
O	4.44493800	-8.74200400	-11.61030100
C	8.46537800	2.72704600	6.63539500
H	7.95953700	1.70640000	8.45245300
C	-9.40430500	-5.46974100	-13.38965400
C	-0.47616900	-5.10360900	10.80706400
O	-8.82204700	-5.57639800	-14.51874400
O	-10.09938800	-6.43975100	-12.91544500
O	0.05176200	-6.27249400	10.86643100

O	-0.10760800	-4.18068800	11.60605700
Cu	4.65050900	-6.78745700	-11.06458100
Cu	0.38797500	-6.04263100	6.88956200
Cu	-8.17819200	-5.79335600	-9.46936000
H	13.59887362	-6.46822706	4.44145144
H	13.15931027	-7.83132097	2.37188574
H	12.73564395	-7.90954186	-1.60541160
H	12.29608133	-9.27263784	-3.67497747
H	11.87241118	-9.35086074	-7.65227418
H	11.43284974	-10.71395138	-9.72183979
H	-1.30905592	-17.09864182	-7.09261462
H	-1.76631263	-16.84415499	-4.63093237
H	-0.44582372	-15.65732732	-1.04575057
H	-0.90308108	-15.40283770	1.41592989
H	0.41740535	-14.21601108	5.00111096
H	-0.03984925	-13.96152177	7.46279306
H	-14.84023026	-8.86979286	-6.40919642
H	-13.84584243	-8.85660901	-4.09725707
H	-13.97700078	-7.42847475	-0.36233235
H	-12.98260951	-7.41529511	1.94960483
H	-13.11377068	-5.98715926	5.68453103
H	-12.11937833	-5.97397654	7.99646851
H	8.47903693	3.69434420	7.09261227
H	8.93632256	3.43986729	4.63094445
H	7.61580566	2.25302831	1.04574904
H	8.07309124	1.99855041	-1.41591748
H	6.75257467	0.81171130	-5.00111395
H	7.20986254	0.55723308	-7.46278053
H	5.88934360	-0.62960514	-11.04797501
H	6.34663156	-0.88408039	-13.50964078
H	-8.85705714	-0.88408035	-13.50964095
H	-9.31434342	-0.62960513	-11.04797502
H	-7.99382885	0.55723315	-7.46278087
H	-8.45111263	0.81171125	-5.00111385
H	-7.13059776	1.99855041	-1.41591748
H	-7.58788334	2.25302831	1.04574904
H	-6.26736475	3.43986725	4.63094462
H	-6.72465279	3.69434426	7.09261216
H	3.22246514	-8.87163829	-14.04333363
H	-0.49977344	-10.31110791	-12.45605618
H	-4.26284238	-2.69034522	9.72183854

Li in Cu-MOF cluster

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.971147	6.730897	0.466353
2	6	0	-9.221398	7.310550	0.414210
3	6	0	4.873069	0.561345	0.122919
4	6	0	-10.319477	1.140997	0.070776
5	6	0	3.774992	-5.608209	-0.220513
6	6	0	12.895598	2.894033	1.905435
7	6	0	-2.297019	3.473674	1.853300
8	6	0	11.797520	-3.275520	1.562002
9	6	0	-3.395021	-2.695840	1.509884
10	6	0	10.800992	3.717390	0.927563
11	6	0	-4.391555	4.297043	0.875421
12	6	0	9.702914	-2.452163	0.584131
13	6	0	-5.489632	-1.872510	0.531988
14	6	0	3.949223	6.617831	1.852138
15	6	0	-11.243328	7.197493	1.799997
16	6	0	2.851118	0.448322	1.508633
17	6	0	-12.341407	1.027939	1.456563
18	6	0	1.753145	-5.721333	1.165306
19	6	0	-1.564102	2.305358	2.398327
20	6	0	-2.662226	-3.864460	2.054762
21	6	0	4.796023	6.082673	0.883662
22	6	0	-10.396517	6.662321	0.831528
23	6	0	3.697955	-0.086888	0.540242
24	6	0	-11.494593	0.492767	0.488094
25	6	0	2.599876	-6.256442	0.196807

26	6	0	11.559669	2.713229	1.553162
27	6	0	-3.632876	3.292880	1.501013
28	6	0	10.461592	-3.456325	1.209728
29	6	0	-4.730955	-2.876673	1.157587
30	6	0	8.256249	4.627386	-2.996642
31	6	0	-6.936298	5.207039	-3.048784
32	6	0	7.158170	-1.542167	-3.340074
33	6	0	-8.034375	-0.962514	-3.392217
34	6	0	6.060093	-7.711720	-3.683508
35	6	0	7.885812	4.257719	-5.402161
36	6	0	-7.306734	4.837372	-5.454303
37	6	0	-0.331132	0.750633	7.419402
38	6	0	6.787734	-1.911834	-5.745594
39	6	0	-8.404812	-1.332181	-5.797737
40	6	0	-1.429208	-5.418921	7.075970
41	6	0	5.689657	-8.081387	-6.089027
42	6	0	2.803088	5.789449	2.298908
43	6	0	1.704981	-0.380340	1.955442
44	6	0	0.606825	-6.549584	1.611881
45	6	0	8.149189	3.702776	-4.151349
46	6	0	-7.043357	4.282429	-4.203492
47	6	0	-0.067754	0.195689	8.670214
48	6	0	7.051112	-2.466778	-4.494782
49	6	0	-8.141434	-1.887125	-4.546925
50	6	0	-1.165830	-5.973864	8.326781
51	6	0	5.953035	-8.636330	-4.838215
52	6	0	7.871655	3.491459	-6.580491
53	6	0	-7.320892	4.071112	-6.632633
54	6	0	-0.345298	-0.015624	6.241076
55	6	0	6.773578	-2.678095	-6.923924
56	6	0	-8.418968	-2.098442	-6.976067
57	6	0	-1.443397	-6.185183	5.897643
58	6	0	5.675499	-8.847648	-7.267358
59	6	0	-5.722047	9.047639	-3.751408
60	6	0	1.253557	4.960900	9.122299
61	6	0	8.372420	2.298434	-4.042698
62	6	0	-6.820124	2.878086	-4.094840
63	6	0	0.155478	-1.208653	8.778865
64	6	0	7.274343	-3.871119	-4.386131
65	6	0	-7.918203	-3.291466	-4.438274
66	6	0	-5.999573	8.836333	-6.180542
67	6	0	0.976017	4.749575	6.693181
68	6	0	8.094895	2.087127	-6.471832
69	6	0	-7.097650	2.666780	-6.523975
70	6	0	-0.122046	-1.419960	6.349732
71	6	0	6.996818	-4.082426	-6.815266
72	6	0	-8.195727	-3.502774	-6.867408
73	6	0	6.322034	2.663038	0.242924
74	6	0	-8.870513	3.242691	0.190781
75	6	0	5.223956	-3.506515	-0.100510
76	6	0	-9.968591	-2.926862	-0.152653
77	6	0	-5.736205	8.281390	-4.929731
78	6	0	1.239391	4.194649	7.943977
79	6	0	8.358261	1.532184	-5.221021
80	6	0	-6.834283	2.111837	-5.273163
81	6	0	0.141320	-1.974904	7.600542
82	6	0	7.260185	-4.637370	-5.564454
83	6	0	-7.932361	-4.057717	-5.616597
84	6	0	0.868976	3.825053	5.538491
85	6	0	-0.229098	-2.344574	5.195015
86	6	0	-2.434446	5.739138	0.988649
87	6	0	11.660008	-1.010073	0.697365
88	6	0	-3.532516	-0.430449	0.645151
89	6	0	10.561932	-7.179627	0.353933
90	6	0	-4.633409	-6.597881	0.332447
91	6	0	4.329171	2.369719	1.658144
92	6	0	-10.863365	2.949354	1.606001
93	6	0	3.231098	-3.799848	1.314701
94	6	0	-11.961442	-3.220199	1.262569
95	6	0	-4.503225	6.726891	0.091466
96	6	0	9.591243	-0.022316	-0.199824
97	6	0	-5.601302	0.557337	-0.251967
98	6	0	8.493166	-6.191869	-0.543257
99	6	0	-6.702148	-5.610173	-0.564856
100	6	0	5.175993	1.834531	0.689675
101	6	0	-10.016554	2.414183	0.637533
102	6	0	4.077915	-4.335023	0.346243

103	6	0	-11.114630	-3.755370	0.294101
104	6	0	-1.675707	4.734921	1.614205
105	6	0	12.418685	-2.014236	1.322963
106	6	0	-2.773787	-1.434522	1.270888
107	6	0	11.320609	-8.183789	0.979530
108	6	0	-3.874582	-7.602097	0.957903
109	6	0	-3.770391	5.558339	0.636388
110	6	0	10.324079	-1.190871	0.345089
111	6	0	-4.868465	-0.611219	0.292943
112	6	0	9.226003	-7.360424	0.001655
113	6	0	-5.969317	-6.778722	-0.019927
114	6	0	3.154024	1.721334	2.075500
115	6	0	-12.038484	2.301125	2.023320
116	6	0	2.055989	-4.448140	1.732032
117	6	0	-13.136559	-3.868429	1.679887
118	1	0	7.709494	5.326767	-5.481254
119	1	0	-7.483053	5.906420	-5.533396
120	1	0	-0.507449	1.819680	7.340310
121	1	0	6.611416	-0.842787	-5.824687
122	1	0	-8.581130	-0.263134	-5.876830
123	1	0	-1.605526	-4.349874	6.996877
124	1	0	5.513339	-7.012341	-6.168120
125	1	0	4.559406	5.115559	0.448601
126	1	0	-10.633140	5.695212	0.396458
127	1	0	3.461329	-1.053995	0.105168
128	1	0	-11.731217	-0.474342	0.053026
129	1	0	2.363251	-7.223548	-0.238266
130	1	0	11.086947	1.753452	1.742355
131	1	0	-4.105598	2.333105	1.690213
132	1	0	9.988870	-4.416100	1.398922
133	1	0	-5.203675	-3.836448	1.346779
134	1	0	-1.961737	6.698906	0.799460
135	1	0	12.132729	-0.050298	0.508172
136	1	0	-3.059823	0.529362	0.456050
137	1	0	11.034652	-6.219852	0.164738
138	1	0	-4.160654	-5.638164	0.143118
139	1	0	4.565804	3.336811	2.093214
140	1	0	-10.626743	3.916464	2.041071
141	1	0	3.467732	-2.832748	1.749790
142	1	0	-11.724820	-2.253089	1.697638
143	1	0	-5.559886	7.212341	-4.850647
144	1	0	1.415718	3.125601	8.023058
145	1	0	8.534581	0.463135	-5.141937
146	1	0	-6.657964	1.042788	-5.194080
147	1	0	0.317640	-3.043952	7.679626
148	1	0	7.436505	-5.706419	-5.485371
149	1	0	-7.756041	-5.126766	-5.537513
150	8	0	-0.303258	2.189746	2.356752
151	8	0	-1.422034	-4.118630	1.839475
152	8	0	6.764475	6.086693	-0.402011
153	8	0	-8.428071	6.666346	-0.454154
154	8	0	5.666398	-0.082861	-0.745444
155	8	0	-9.526149	0.496792	-0.797587
156	8	0	4.568320	-6.252414	-1.088877
157	8	0	7.717830	5.778772	-3.094932
158	8	0	-7.474717	6.358425	-3.147075
159	8	0	6.619752	-0.390781	-3.438366
160	8	0	-8.572794	0.188871	-3.490508
161	8	0	5.521675	-6.560334	-3.781799
162	8	0	9.553061	3.409427	0.544995
163	8	0	-5.639486	3.989080	0.492852
164	8	0	8.454984	-2.760126	0.201561
165	8	0	-6.737563	-2.180473	0.149418
166	8	0	8.936061	4.307508	-1.955265
167	8	0	-6.256485	4.887161	-2.007408
168	8	0	7.837985	-1.862045	-2.298699
169	8	0	-7.354561	-1.282392	-2.350841
170	8	0	6.739906	-8.031598	-2.642131
171	8	0	2.277397	5.959386	3.457833
172	8	0	1.179331	-0.210109	3.114398
173	8	0	0.081341	-6.379745	2.771018
174	8	0	-0.515615	0.630943	5.078507
175	8	0	-1.613718	-5.538301	4.734872
176	8	0	-2.242646	1.347820	2.897112
177	8	0	-3.340769	-4.821680	2.553740
178	8	0	6.723948	3.599093	1.009926
179	8	0	-8.468598	4.178746	0.957784

180	8	0	5.625870	-2.570460	0.666493
181	8	0	-9.566676	-1.990807	0.614350
182	8	0	2.401191	4.960334	1.438772
183	8	0	1.305900	-1.311022	1.217852
184	8	0	0.040298	-7.268830	0.780991
185	8	0	-3.824665	7.684137	-0.407553
186	8	0	10.269802	0.934931	-0.698844
187	8	0	-4.922743	1.514584	-0.750986
188	8	0	9.171725	-5.234621	-1.042276
189	8	0	-6.023590	-4.652926	-1.063875
190	8	0	-5.551708	8.401078	-2.588885
191	8	0	8.542759	1.651872	-2.880175
192	8	0	-6.649785	2.231525	-2.932318
193	8	0	7.444683	-4.517681	-3.223609
194	8	0	-7.747862	-3.938028	-3.275752
195	8	0	6.847841	2.492940	-0.915998
196	8	0	-8.344706	3.072593	-0.968140
197	8	0	5.749764	-3.676613	-1.259431
198	8	0	-9.442783	-3.096960	-1.311574
199	8	0	0.215492	4.148537	4.487149
200	8	0	-0.908948	-2.024697	4.153640
201	8	0	-0.493522	5.005431	2.090636
202	8	0	-1.537489	-1.254925	1.622066
203	8	0	-2.721884	-7.301086	1.319782
204	8	0	1.407353	2.673596	5.636737
205	8	0	0.309280	-3.495969	5.293329
206	8	0	2.308603	2.286741	2.874512
207	8	0	1.131689	-3.865633	2.477251
208	8	0	-5.780944	6.808254	0.186536
209	8	0	8.313523	0.059048	-0.104754
210	8	0	-6.879022	0.638700	-0.156896
211	8	0	7.215446	-6.110505	-0.448187
212	8	0	-7.979868	-5.528810	-0.469786
213	29	0	1.144487	1.405706	4.182034
214	29	0	0.046402	-4.763700	3.838674
215	29	0	8.131047	4.780400	0.363581
216	29	0	-7.061499	5.360053	0.311439
217	29	0	7.032970	-1.389153	0.020148
218	29	0	-8.159575	-0.809501	-0.031995
219	29	0	5.934893	-7.558707	-0.323285
220	29	0	9.320143	2.532319	-1.281684
221	29	0	-5.872404	3.111972	-1.333826
222	29	0	8.222065	-3.637234	-1.625118
223	29	0	-6.970480	-3.057581	-1.677260
224	29	0	-0.194901	5.919700	3.823441
225	29	0	-1.292974	-0.249555	3.480166
226	29	0	-2.391064	-6.419690	3.136948
227	29	0	0.955445	3.704809	1.825304
228	29	0	-0.042502	-2.582599	1.666479
229	29	0	-7.211794	7.626391	-1.692396
230	29	0	6.882673	0.877185	-1.983687
231	29	0	-8.309871	1.456838	-2.035830
232	29	0	5.784597	-5.292368	-2.327120
233	29	0	-9.407948	-4.712715	-2.379262
234	6	0	6.274069	8.004084	1.033107
235	6	0	-8.918476	8.583737	0.980965
236	6	0	13.516761	4.155318	1.666396
237	6	0	11.422155	4.978683	0.688522
238	6	0	4.252144	7.891020	2.418900
239	6	0	-10.940406	8.470677	2.366751
240	6	0	-0.942599	-7.378206	8.435433
241	6	0	6.176266	-10.040673	-4.729565
242	6	0	-1.220125	-7.589514	6.006298
243	6	0	5.898741	-10.251980	-7.158698
244	6	0	-5.945281	10.451981	-3.860061
245	6	0	1.030324	6.365242	9.013646
246	6	0	-6.222815	10.240663	-6.289202
247	6	0	0.752792	6.153930	6.584504
248	6	0	-11.417553	-5.028556	-0.272656
249	6	0	10.699443	-9.445073	1.218569
250	6	0	-4.496040	-8.863530	1.196698
251	6	0	8.604837	-8.621717	0.240697
252	6	0	-6.590477	-8.040021	0.219098
253	6	0	-13.439483	-5.141615	1.113131
254	8	0	9.411599	6.228601	0.238679
255	8	0	7.356906	-8.929679	-0.141873
256	8	0	4.527793	-8.740014	0.323060

257	8	0	0.582452	6.800609	5.421915
258	8	0	-1.144584	7.517463	3.240711
259	8	0	-2.006997	-8.194250	3.810192
260	8	0	-7.246628	9.242146	-0.624710
261	8	0	-10.624225	-5.672761	-1.141020
262	8	0	-9.670870	-5.980681	-3.833941
263	6	0	7.420108	8.832591	0.586354
264	6	0	5.427256	8.539254	2.001575
265	6	0	-7.772435	9.412244	0.534211
266	6	0	-9.765288	9.118907	1.949433
267	6	0	12.758084	5.159479	1.040799
268	6	0	10.689319	6.147238	0.143609
269	8	0	3.458811	8.535230	3.287258
270	6	0	-0.956757	-8.144457	7.257110
271	6	0	6.162108	-10.806924	-5.907888
272	8	0	6.346606	-10.687235	-3.567042
273	6	0	-1.327196	-8.514132	4.851594
274	6	0	-5.838222	11.376591	-2.705352
275	6	0	-6.208657	11.006925	-5.110871
276	6	0	0.766947	6.920185	7.762834
277	6	0	-12.592671	-5.676787	0.144661
278	6	0	9.363514	-9.625878	0.866296
279	6	0	-5.831784	-9.044198	0.844646
280	6	0	-3.762844	-10.031444	1.742123
281	8	0	-7.838408	-8.347984	-0.163471
282	6	0	4.125878	-9.676069	-0.443944
283	6	0	-0.466033	8.474691	2.741645
284	6	0	-9.132451	-7.132067	-3.735650
285	8	0	7.822023	9.768646	1.353358
286	8	0	7.945915	8.662493	-0.572567
287	1	0	5.663879	9.506364	2.436645
288	8	0	-7.370521	10.348299	1.301215
289	1	0	-9.528666	10.086017	2.384503
290	1	0	13.230805	6.119254	0.851604
291	8	0	11.367877	7.104484	-0.355410
292	1	0	-0.780437	-9.213506	7.336192
293	1	0	6.338427	-11.875972	-5.828804
294	8	0	-0.788773	-9.665510	4.949881
295	8	0	-6.376640	12.527977	-2.803643
296	8	0	-5.158408	11.056714	-1.663976
297	1	0	-6.384976	12.075971	-5.189966
298	1	0	0.590628	7.989233	7.683741
299	1	0	-12.829294	-6.643895	-0.290408
300	1	0	8.890793	-10.585654	1.055489
301	1	0	-6.304520	-10.003958	1.033890
302	8	0	-2.485772	-10.005238	1.676778
303	8	0	-4.441535	-10.989243	2.240857
304	6	0	9.192971	8.256680	-6.128400
305	8	0	4.651686	-9.846166	-1.602864
306	6	0	2.979827	-10.504565	0.002794
307	6	0	-1.198871	9.643240	2.196723
308	8	0	0.811686	8.393321	2.646566
309	8	0	-8.452638	-7.451945	-2.694274
310	6	0	-9.239511	-8.056678	-4.890358
311	6	0	8.969730	9.661010	-6.237060
312	6	0	9.456337	7.701737	-4.877588
313	6	0	2.132995	-9.969346	0.971283
314	6	0	2.676915	-11.777763	-0.563947
315	6	0	-0.577707	10.904522	1.957686
316	6	0	-2.534800	9.462434	1.844451
317	6	0	-9.502888	-7.501734	-6.141169
318	6	0	-9.016280	-9.461020	-4.781707
319	6	0	8.983887	10.427272	-5.058729
320	6	0	9.470495	8.467986	-3.699265
321	1	0	9.632657	6.632688	-4.798505
322	1	0	2.369655	-9.002302	1.406358
323	6	0	0.957714	-10.617794	1.388550
324	6	0	1.501823	-12.426014	-0.146594
325	8	0	3.470242	-12.421968	-1.432311
326	6	0	-1.336384	11.908685	1.332087
327	6	0	-3.293477	10.466596	1.218852
328	1	0	-3.007521	8.502659	2.033643
329	1	0	-9.679205	-6.432688	-6.220262
330	6	0	-9.517045	-8.267995	-7.319500
331	6	0	-9.030438	-10.227271	-5.960030
332	8	0	-8.845940	-10.107582	-3.619185
333	1	0	8.807569	11.496318	-5.137823

334	6	0	9.247265	9.872328	-3.807918
335	8	0	9.640836	7.821426	-2.536743
336	8	0	0.291303	-10.114522	2.288096
337	6	0	0.655031	-11.890810	0.821789
338	1	0	1.265174	-13.393101	-0.581698
339	1	0	-0.863663	12.868460	1.142893
340	6	0	-2.672313	11.727889	0.979811
341	8	0	-4.541408	10.158634	0.836282
342	6	0	-9.293805	-9.672327	-7.210841
343	1	0	-8.854118	-11.296320	-5.880947
344	6	0	9.354323	10.796938	-2.653210
345	8	0	8.815905	11.948324	-2.751501
346	8	0	10.034137	10.477061	-1.611833
347	29	0	-4.774326	9.281525	-0.990396
348	29	0	-1.578171	-10.210183	3.131546
349	29	0	7.980750	7.046738	-1.640253
350	1	0	-14.308413	-5.680503	1.428502
351	1	0	-13.785601	-3.419413	2.402402
352	1	0	-13.210338	0.489051	1.771933
353	1	0	-12.687526	2.750141	2.745836
354	1	0	-12.112259	6.658604	2.115369
355	1	0	-11.589448	8.919694	3.089266
356	1	0	1.064731	6.986685	9.884004
357	1	0	1.426927	4.503447	10.073918
358	1	0	-0.033347	0.817131	9.540574
359	1	0	0.328849	-1.666106	9.730484
360	1	0	-1.131422	-5.352421	9.197141
361	1	0	-0.769229	-7.835660	9.387052
362	1	0	14.531763	4.332165	1.955179
363	1	0	13.449913	2.094515	2.350863
364	1	0	13.433687	-1.837390	1.611745
365	1	0	12.351834	-4.075037	2.007432
366	1	0	12.335611	-8.006944	1.268313
367	1	0	11.253757	-10.244592	1.663997
368	1	0	-9.328197	-10.293771	-8.081200
369	1	0	-9.690422	-7.810547	-8.271121
370	1	0	-8.230119	-4.124217	-7.737768
371	1	0	-8.592344	-1.640994	-7.927687
372	1	0	-7.132042	2.045337	-7.394334
373	1	0	-7.494269	4.528560	-7.584254
374	1	0	-6.033965	8.214889	-7.050901
375	1	0	-6.396192	10.698110	-7.240823
376	1	0	8.796353	10.118458	-7.188681
377	1	0	9.158579	7.635236	-6.998759
378	1	0	7.698279	3.948907	-7.532111
379	1	0	8.060502	1.465684	-7.342192
380	1	0	6.600202	-2.220647	-7.875545
381	1	0	6.962426	-4.703870	-7.685625
382	1	0	5.502122	-8.390200	-8.218978
383	1	0	5.864350	-10.873423	-8.029058
384	3	0	-1.426090	-6.031812	0.451740
385	1	0	-3.226625	12.527408	0.534383
386	1	0	0.437296	11.081369	2.246469
387	1	0	-0.213942	-12.429714	1.137217

Li in Cu-MOF cluster (transition state structure)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.950173	-6.740735	0.462515
2	6	0	9.243841	-7.280863	0.414207
3	6	0	-4.868078	-0.568520	0.116211
4	6	0	10.325937	-1.108647	0.067902
5	6	0	-3.785984	5.603697	-0.230092
6	6	0	-12.884925	-2.921182	1.898039
7	6	0	2.309172	-3.461294	1.849743
8	6	0	-11.802830	3.251034	1.551735
9	6	0	3.391204	2.710868	1.503448
10	6	0	-10.787954	-3.739578	0.921072
11	6	0	4.406062	-4.279706	0.872765
12	6	0	-9.705859	2.432638	0.574770
13	6	0	5.488156	1.892510	0.526462

14	6	0	-3.928874	-6.621704	1.848711
15	6	0	11.265145	-7.161841	1.800407
16	6	0	-2.846763	-0.449516	1.502311
17	6	0	12.347241	-0.989624	1.454103
18	6	0	-1.764761	5.722790	1.156152
19	6	0	1.573057	-2.294631	2.393981
20	6	0	2.655233	3.877867	2.047546
21	6	0	-4.776838	-6.089243	0.879770
22	6	0	10.417171	-6.629366	0.831470
23	6	0	-3.694749	0.082978	0.533473
24	6	0	11.499264	-0.457149	0.485166
25	6	0	-2.612664	6.255204	0.187183
26	6	0	-11.549389	-2.737079	1.545985
27	6	0	3.644626	-3.277206	1.497673
28	6	0	-10.467295	3.435138	1.199681
29	6	0	4.726715	2.895018	1.151353
30	6	0	-8.239931	-4.644932	-3.002078
31	6	0	6.954085	-5.185060	-3.050385
32	6	0	-7.157835	1.527284	-3.348380
33	6	0	8.036179	0.987156	-3.396689
34	6	0	-6.075741	7.699500	-3.694685
35	6	0	-7.869894	-4.275520	-5.407698
36	6	0	7.324122	-4.815648	-5.456005
37	6	0	0.334888	-0.740567	7.414001
38	6	0	-6.787799	1.896696	-5.754001
39	6	0	8.406217	1.356568	-5.802309
40	6	0	1.416981	5.431650	7.067699
41	6	0	-5.705705	8.068912	-6.100304
42	6	0	-2.784998	-5.790101	2.295336
43	6	0	-1.702693	0.382562	1.948987
44	6	0	-0.620671	6.554217	1.602572
45	6	0	-8.135007	-3.720631	-4.157228
46	6	0	7.059008	-4.260759	-4.205537
47	6	0	0.069773	-0.185677	8.664471
48	6	0	-7.052914	2.451586	-4.503532
49	6	0	8.141102	1.911458	-4.551840
50	6	0	1.151866	5.986539	8.318167
51	6	0	-5.970820	8.623801	-4.849835
52	6	0	-7.857455	-3.509822	-6.586412
53	6	0	7.336561	-4.049950	-6.634720
54	6	0	0.347339	0.025125	6.235293
55	6	0	-6.775361	2.662395	-6.932716
56	6	0	8.418654	2.122267	-6.981024
57	6	0	1.429466	6.197350	5.888989
58	6	0	-5.693265	8.834611	-7.279020
59	6	0	5.750001	-9.029163	-3.751346
60	6	0	-1.239235	-4.954082	9.118662
61	6	0	-8.361919	-2.316820	-4.049341
62	6	0	6.832095	-2.856947	-4.097648
63	6	0	-0.157139	1.218134	8.772358
64	6	0	-7.279825	3.855396	-4.395644
65	6	0	7.914190	3.315268	-4.443953
66	6	0	6.027545	-8.818365	-6.180522
67	6	0	-0.961677	-4.743265	6.689502
68	6	0	-8.084375	-2.106021	-6.478517
69	6	0	7.109639	-2.646149	-6.526825
70	6	0	0.120403	1.428933	6.343183
71	6	0	-7.002281	4.066195	-6.824821
72	6	0	8.191733	3.526068	-6.873129
73	6	0	-6.311595	-2.673917	0.236943
74	6	0	8.882421	-3.214045	0.188635
75	6	0	-5.229500	3.498300	-0.109361
76	6	0	9.964516	2.958171	-0.157670
77	6	0	5.762440	-8.263477	-4.930054
78	6	0	-1.226788	-4.188393	7.939955
79	6	0	-8.349478	-1.551133	-5.228049
80	6	0	6.844535	-2.091261	-5.276356
81	6	0	-0.144700	1.983823	7.593650
82	6	0	-7.267385	4.621084	-5.574352
83	6	0	7.926630	4.080956	-5.622660
84	6	0	-0.856769	-3.819050	5.534369
85	6	0	0.225306	2.353238	5.188014
86	6	0	2.452686	-5.726832	0.986264
87	6	0	-11.659219	0.985516	0.688278
88	6	0	3.534771	0.445436	0.639863
89	6	0	-10.577126	7.157733	0.341976
90	6	0	4.619711	6.615528	0.324372

91	6	0	-4.319835	-2.374694	1.652480
92	6	0	10.874171	-2.914805	1.604170
93	6	0	-3.237744	3.797553	1.306138
94	6	0	11.956265	3.257411	1.257868
95	6	0	4.524241	-6.709652	0.090067
96	6	0	-9.587679	0.002694	-0.207928
97	6	0	5.606335	-0.537435	-0.256236
98	6	0	-8.505586	6.174910	-0.554231
99	6	0	6.691196	5.632761	-0.571994
100	6	0	-5.167822	-1.842201	0.683544
101	6	0	10.026197	-2.382330	0.635234
102	6	0	-4.085732	4.330021	0.337250
103	6	0	11.108290	3.789886	0.288932
104	6	0	1.691196	-4.724278	1.611141
105	6	0	-12.420654	1.988017	1.313191
106	6	0	2.773164	1.447777	1.265049
107	6	0	-11.338561	8.160233	0.966887
108	6	0	3.858169	7.618081	0.949255
109	6	0	3.788240	-5.542735	0.634225
110	6	0	-10.323682	1.169613	0.336222
111	6	0	4.870326	0.629491	0.287896
112	6	0	-9.241590	7.341829	-0.010082
113	6	0	5.955201	6.799670	-0.027816
114	6	0	-3.146472	-1.723036	2.069792
115	6	0	12.047501	-2.263308	2.021435
116	6	0	-2.064431	4.448952	1.723418
117	6	0	13.129593	3.908909	1.675131
118	1	0	-7.690775	-5.344145	-5.486208
119	1	0	7.503241	-5.884273	-5.534515
120	1	0	0.514006	-1.809191	7.335492
121	1	0	-6.608680	0.828072	-5.832511
122	1	0	8.585335	0.287944	-5.880819
123	1	0	1.596100	4.363026	6.989189
124	1	0	-5.526586	7.000289	-6.178814
125	1	0	-4.542637	-5.121736	0.444273
126	1	0	10.651378	-5.661864	0.395965
127	1	0	-3.460543	1.050481	0.097970
128	1	0	11.733472	0.510353	0.049663
129	1	0	-2.378448	7.222697	-0.248334
130	1	0	-11.079211	-1.775979	1.734802
131	1	0	4.114803	-2.316107	1.686495
132	1	0	-9.997117	4.396236	1.388499
133	1	0	5.196897	3.856109	1.340191
134	1	0	1.982523	-6.687925	0.797456
135	1	0	-12.129396	0.024418	0.499462
136	1	0	3.064632	-0.515724	0.451194
137	1	0	-11.047302	6.196635	0.153157
138	1	0	4.149468	5.654498	0.135363
139	1	0	-4.554049	-3.342181	2.087980
140	1	0	10.639965	-3.882307	2.039675
141	1	0	-3.471964	2.830045	1.741691
142	1	0	11.722059	2.289909	1.693372
143	1	0	5.583320	-7.194850	-4.851553
144	1	0	-1.405915	-3.119768	8.018454
145	1	0	-8.528599	-0.482506	-5.149548
146	1	0	6.665415	-1.022634	-5.197856
147	1	0	-0.323821	3.052448	7.672151
148	1	0	-7.446506	5.689711	-5.495852
149	1	0	7.747509	5.149583	-5.544159
150	8	0	0.309177	-2.180921	2.359264
151	8	0	1.391507	3.956083	1.967756
152	8	0	-6.744971	-6.099038	-0.406360
153	8	0	8.449044	-6.639166	-0.454669
154	8	0	-5.662878	0.073179	-0.752664
155	8	0	9.531139	-0.466949	-0.800972
156	8	0	-4.580783	6.245395	-1.098967
157	8	0	-7.698493	-5.794962	-3.099659
158	8	0	7.495523	-6.335091	-3.147967
159	8	0	-6.616399	0.377254	-3.445963
160	8	0	8.577617	-0.162874	-3.494271
161	8	0	-5.534305	6.549470	-3.792267
162	8	0	-9.540739	-3.428561	0.538639
163	8	0	5.653277	-3.968689	0.490331
164	8	0	-8.458645	2.743655	0.192335
165	8	0	6.735371	2.203527	0.144026
166	8	0	-8.920817	-4.326298	-1.961022
167	8	0	6.273198	-4.866426	-2.009330

168	8	0	-7.838724	1.845918	-2.307326
169	8	0	7.355291	1.305790	-2.355633
170	8	0	-6.756629	8.018134	-2.653628
171	8	0	-2.259146	-5.958101	3.454464
172	8	0	-1.177110	0.213992	3.108172
173	8	0	-0.095066	6.386340	2.761917
174	8	0	0.519590	-0.621600	5.073067
175	8	0	1.601709	5.550372	4.726548
176	8	0	2.249005	-1.335070	2.892473
177	8	0	3.331157	4.837050	2.546381
178	8	0	-6.711251	-3.610626	1.004325
179	8	0	8.482764	-4.150754	0.956018
180	8	0	-5.629156	2.561590	0.658022
181	8	0	9.564859	2.021462	0.609714
182	8	0	-2.386935	-4.956781	1.436858
183	8	0	-1.249041	1.277611	1.192337
184	8	0	-0.197435	7.417636	0.856410
185	8	0	3.848292	-7.668913	-0.408625
186	8	0	-10.263627	-0.956569	-0.706621
187	8	0	4.930387	-1.496697	-0.754928
188	8	0	-9.181533	5.215646	-1.052923
189	8	0	6.015249	4.673499	-1.070686
190	8	0	5.577707	-8.382460	-2.589191
191	8	0	-8.534213	-1.670116	-2.887186
192	8	0	6.659801	-2.210244	-2.935494
193	8	0	-7.452120	4.502100	-3.233490
194	8	0	7.741894	3.961972	-3.281798
195	8	0	-6.837571	-2.505774	-0.922188
196	8	0	8.356445	-3.045903	-0.970495
197	8	0	-5.755478	3.666442	-1.268491
198	8	0	9.438539	3.126313	-1.316799
199	8	0	-0.199868	-4.135390	4.484628
200	8	0	0.906262	2.034607	4.146975
201	8	0	0.510589	-4.998772	2.096227
202	8	0	1.487325	1.302683	1.462088
203	8	0	2.721933	7.350400	1.342241
204	8	0	-1.398165	-2.668955	5.631904
205	8	0	-0.316079	3.503278	5.285628
206	8	0	-2.298553	-2.267988	2.880723
207	8	0	-1.256005	3.915136	2.643318
208	8	0	5.802145	-6.787640	0.185476
209	8	0	-8.309774	-0.075296	-0.112519
210	8	0	6.884240	-0.615423	-0.160826
211	8	0	-7.227680	6.096920	-0.458822
212	8	0	7.969101	5.554773	-0.476585
213	29	0	-1.138276	-1.401108	4.176624
214	29	0	-0.056165	4.770855	3.830410
215	29	0	-8.115119	-4.795919	0.358251
216	29	0	7.078897	-5.336047	0.309944
217	29	0	-7.033025	1.376297	0.011948
218	29	0	8.160990	0.836170	-0.036360
219	29	0	-5.950931	7.548514	-0.334355
220	29	0	-9.309677	-2.551774	-1.288430
221	29	0	5.884339	-3.091902	-1.336737
222	29	0	-8.227582	3.620442	-1.634734
223	29	0	6.966432	3.080314	-1.683041
224	29	0	0.212959	-5.911787	3.820632
225	29	0	1.295082	0.260186	3.474454
226	29	0	2.376810	6.432823	3.128510
227	29	0	-0.923825	-3.717713	1.787957
228	29	0	-0.195501	2.461399	2.216123
229	29	0	7.235560	-7.603000	-1.692707
230	29	0	-6.876359	-0.890656	-1.990703
231	29	0	8.317654	-1.430784	-2.039012
232	29	0	-5.794266	5.281560	-2.337007
233	29	0	9.399748	4.741432	-2.385314
234	6	0	-6.249912	-8.014419	1.029843
235	6	0	8.944102	-8.554547	0.981536
236	6	0	-13.502747	-4.184200	1.659494
237	6	0	-11.405775	-5.002604	0.682526
238	6	0	-4.228613	-7.895391	2.416049
239	6	0	10.965406	-8.435523	2.367736
240	6	0	0.924955	7.390350	8.426056
241	6	0	-6.197731	10.027613	-4.741949
242	6	0	1.202500	7.601150	5.996879
243	6	0	-5.920188	10.238412	-7.171124
244	6	0	5.976915	-10.432974	-3.859235

245	6	0	-1.012322	-6.357893	9.010773
246	6	0	6.254467	-10.222164	-6.288418
247	6	0	-0.734768	-6.147089	6.581590
248	6	0	11.408030	5.063569	-0.278400
249	6	0	-10.720736	9.423250	1.205432
250	6	0	4.476160	8.881479	1.186810
251	6	0	-8.623765	8.604855	0.228466
252	6	0	6.573016	8.062707	0.210703
253	6	0	13.429334	5.182593	1.107801
254	8	0	-9.391867	-6.247512	0.233785
255	8	0	-7.376550	8.915871	-0.153969
256	8	0	-4.547062	8.733807	0.311719
257	8	0	-0.562481	-6.793910	5.419366
258	8	0	1.166929	-7.507371	3.238929
259	8	0	1.988690	8.204645	3.800121
260	8	0	7.274350	-9.218119	-0.624195
261	8	0	10.613232	5.705267	-1.147275
262	8	0	9.659710	6.009341	-3.840574
263	6	0	-7.393686	-8.846133	0.583243
264	6	0	-5.401936	-8.546892	1.998780
265	6	0	7.800326	-9.386261	0.534935
266	6	0	9.792077	-9.087021	1.950473
267	6	0	-12.741312	-5.186699	1.034583
268	6	0	-10.669772	-6.169523	0.138376
269	8	0	-3.433810	-8.537094	3.284919
270	6	0	0.937394	8.156039	7.247348
271	6	0	-6.185291	10.793301	-5.920656
272	8	0	-6.370026	10.674317	-3.579793
273	6	0	1.306816	8.525308	4.841590
274	6	0	5.871992	-11.357275	-2.704083
275	6	0	6.242028	-10.987864	-5.109703
276	6	0	-0.747208	-6.912782	7.760304
277	6	0	12.581359	5.715068	0.138863
278	6	0	-9.385200	9.607354	0.853379
279	6	0	5.811554	9.065233	0.835529
280	6	0	3.738836	10.048758	1.732240
281	8	0	7.820231	8.373724	-0.171731
282	6	0	-4.147405	9.670517	-0.455666
283	6	0	0.490991	-8.466613	2.740189
284	6	0	9.118272	7.159372	-3.742992
285	8	0	-7.793343	-9.782842	1.350628
286	8	0	-7.919662	-8.677990	-0.575886
287	1	0	-5.636143	-9.514395	2.434285
288	8	0	7.400670	-10.322970	1.302319
289	1	0	9.557871	-10.054523	2.385977
290	1	0	-13.211488	-6.147797	0.845764
291	8	0	-11.345719	-7.128785	-0.360316
292	1	0	0.758273	9.224665	7.325847
293	1	0	-6.364411	11.861927	-5.842155
294	8	0	0.766543	9.677690	4.939725
295	8	0	6.413429	-12.507306	-2.801665
296	8	0	5.191104	-11.038642	-1.663028
297	1	0	6.421148	-12.056487	-5.188215
298	1	0	-0.568088	-7.981407	7.681794
299	1	0	12.815566	6.682569	-0.296641
300	1	0	-8.915023	10.568453	1.042196
301	1	0	6.281757	10.026305	1.024433
302	8	0	2.462478	10.042492	1.649999
303	8	0	4.416112	11.006972	2.230943
304	6	0	-9.166468	-8.278237	-6.132215
305	8	0	-4.673383	9.838658	-1.614794
306	6	0	-3.003747	10.502336	-0.008904
307	6	0	1.226996	-9.633527	2.196032
308	8	0	-0.786913	-8.388618	2.644773
309	8	0	8.437385	7.478006	-2.701936
310	6	0	9.223196	8.083674	-4.898143
311	6	0	-8.939547	-9.682036	-6.240111
312	6	0	-9.431571	-7.723349	-4.881746
313	6	0	-2.155771	9.969969	0.959863
314	6	0	-2.703890	11.775914	-0.576396
315	6	0	0.609174	-10.896542	1.957489
316	6	0	2.562533	-9.449422	1.843979
317	6	0	9.488309	7.528784	-6.148611
318	6	0	8.996284	9.487485	-4.790256
319	6	0	-8.951985	-10.447736	-5.061395
320	6	0	-9.444011	-8.489035	-3.703038
321	1	0	-9.610692	-6.654722	-4.803245

322	1	0	-2.389786	9.002187	1.395269
323	6	0	-0.980967	10.620170	1.376623
324	6	0	-1.530715	12.427539	-0.158927
325	8	0	-3.498688	12.417612	-1.445271
326	6	0	1.370609	-11.899043	1.332576
327	6	0	3.323968	-10.451922	1.219066
328	1	0	3.032709	-8.488324	2.032795
329	1	0	9.667427	6.460161	-6.227122
330	6	0	9.500748	8.294483	-7.327327
331	6	0	9.008724	10.253173	-5.968964
332	8	0	8.823989	10.134189	-3.628101
333	1	0	-8.772867	-11.516359	-5.139907
334	6	0	-9.217100	-9.892846	-3.810927
335	8	0	-9.616307	-7.842333	-2.540883
336	8	0	-0.336358	10.139718	2.302075
337	6	0	-0.682813	11.895046	0.809929
338	1	0	-1.296355	13.394913	-0.594636
339	1	0	0.900432	-12.860141	1.143758
340	6	0	2.706145	-11.714949	0.980520
341	8	0	4.571182	-10.140906	0.836631
342	6	0	9.273828	9.698284	-7.219432
343	1	0	8.829603	11.321800	-5.890463
344	6	0	-9.322022	-10.817147	-2.655776
345	8	0	-8.780585	-11.967177	-2.753358
346	8	0	-10.002910	-10.498514	-1.614719
347	29	0	4.802245	-9.264118	-0.990437
348	29	0	1.557434	10.209573	3.098834
349	29	0	-7.958453	-7.062872	-1.644399
350	1	0	14.296785	5.723900	1.423101
351	1	0	13.779632	3.461950	2.398025
352	1	0	13.214693	-0.448317	1.769403
353	1	0	12.697540	-2.710267	2.744329
354	1	0	12.132597	-6.620533	2.115709
355	1	0	11.615445	-8.882483	3.090630
356	1	0	-1.045315	-6.978983	9.881438
357	1	0	-1.414018	-4.496600	10.070009
358	1	0	0.036780	-0.806766	9.535137
359	1	0	-0.331924	1.675616	9.723705
360	1	0	1.118872	5.365449	9.188834
361	1	0	0.750171	7.847833	9.377402
362	1	0	-14.517353	-4.363543	1.948130
363	1	0	-13.441424	-2.122884	2.342932
364	1	0	-13.435260	1.808675	1.601826
365	1	0	-12.359328	4.049331	1.996631
366	1	0	-12.353167	7.980892	1.255523
367	1	0	-11.277234	10.221549	1.650326
368	1	0	9.306806	10.319375	-8.090098
369	1	0	9.675538	7.837006	-8.278676
370	1	0	8.224711	4.147158	-7.743795
371	1	0	8.593443	1.664790	-7.932372
372	1	0	7.142617	-2.025059	-7.397491
373	1	0	7.511351	-4.507427	-7.586068
374	1	0	6.060523	-8.197274	-7.051188
375	1	0	6.429258	-10.679640	-7.239767
376	1	0	-8.764757	-10.139513	-7.191460
377	1	0	-9.133490	-7.657146	-7.002881
378	1	0	-7.682666	-3.967299	-7.537760
379	1	0	-8.051396	-1.484931	-7.349184
380	1	0	-6.600572	2.204918	-7.884064
381	1	0	-6.969303	4.687286	-7.695487
382	1	0	-5.518475	8.377134	-8.230368
383	1	0	-5.887210	10.859502	-8.041790
384	3	0	1.121943	2.452758	-0.066182
385	1	0	3.262641	-12.513247	0.535626
386	1	0	-0.405433	-11.075885	2.246125
387	1	0	0.184956	12.436171	1.124986

$LiClO_4$ in Cu-MOF cluster

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.363449	-6.339244	0.561922

2	6	0	8.759468	-7.902730	0.490294
3	6	0	-4.868801	-0.257422	0.155280
4	6	0	10.254147	-1.820979	0.083660
5	6	0	-3.374089	5.824256	-0.251348
6	6	0	-13.021441	-2.047752	1.974259
7	6	0	2.101532	-3.611271	1.902714
8	6	0	-11.526762	4.033998	1.567625
9	6	0	3.596187	2.470477	1.496069
10	6	0	-10.986836	-3.014686	1.001149
11	6	0	4.136080	-4.578170	0.929523
12	6	0	-9.492157	3.067064	0.594515
13	6	0	5.630758	1.503580	0.522889
14	6	0	-4.335207	-6.343910	1.943125
15	6	0	10.787662	-7.907336	1.871524
16	6	0	-2.840662	-0.262365	1.536430
17	6	0	12.282341	-1.825585	1.464890
18	6	0	-1.345845	5.819616	1.129813
19	6	0	1.447307	-2.392497	2.436910
20	6	0	2.941766	3.689474	2.030492
21	6	0	-5.147858	-5.764453	0.970834
22	6	0	9.975073	-7.327950	0.899187
23	6	0	-3.653042	0.317424	0.564371
24	6	0	11.469750	-1.246199	0.492553
25	6	0	-2.158494	6.399043	0.157555
26	6	0	-11.677420	-1.957373	1.617984
27	6	0	3.445487	-3.520848	1.546329
28	6	0	-10.182742	4.124378	1.211350
29	6	0	4.940167	2.560902	1.139701
30	6	0	-8.515440	-4.126185	-2.918032
31	6	0	6.607476	-5.689670	-2.989658
32	6	0	-7.020761	1.955566	-3.324665
33	6	0	8.102154	0.392082	-3.396291
34	6	0	-5.526083	8.037316	-3.731300
35	6	0	-8.127375	-3.804947	-5.327722
36	6	0	6.995541	-5.368431	-5.399348
37	6	0	0.329031	-0.711970	7.444631
38	6	0	-6.632696	2.276803	-5.734357
39	6	0	8.490219	0.713319	-5.805983
40	6	0	1.823708	5.369782	7.037997
41	6	0	-5.138018	8.358555	-6.140991
42	6	0	-3.136805	-5.587054	2.379505
43	6	0	-1.642294	0.494986	1.973002
44	6	0	-0.147524	6.576551	1.566500
45	6	0	-8.351364	-3.221843	-4.082059
46	6	0	6.771551	-4.785327	-4.153684
47	6	0	0.105042	-0.128865	8.690295
48	6	0	-6.856686	2.859908	-4.488693
49	6	0	8.266229	1.296424	-4.560319
50	6	0	1.599719	5.952886	8.283660
51	6	0	-5.362008	8.941659	-4.895327
52	6	0	-8.066318	-3.052826	-6.513641
53	6	0	7.056597	-4.616310	-6.585266
54	6	0	0.390084	0.040151	6.258712
55	6	0	-6.571640	3.028926	-6.920275
56	6	0	8.551274	1.465442	-6.991901
57	6	0	1.884763	6.121906	5.852075
58	6	0	-5.076961	9.110675	-7.326910
59	6	0	5.145343	-9.450221	-3.652009
60	6	0	-1.521169	-4.793760	9.191971
61	6	0	-8.482893	-1.804987	-3.987017
62	6	0	6.640021	-3.368471	-4.058643
63	6	0	-0.026489	1.287991	8.785336
64	6	0	-6.988215	4.276764	-4.393651
65	6	0	8.134700	2.713280	-4.465277
66	6	0	5.430379	-9.281214	-6.083584
67	6	0	-1.236133	-4.624753	6.760396
68	6	0	-8.197857	-1.635980	-6.418592
69	6	0	6.925057	-3.199464	-6.490218
70	6	0	0.258545	1.456998	6.353762
71	6	0	-6.703180	4.445772	-6.825226
72	6	0	8.419735	2.882288	-6.896852
73	6	0	-6.450569	-2.259588	0.298607
74	6	0	8.672348	-3.823072	0.226981
75	6	0	-4.955890	3.822162	-0.108028
76	6	0	10.167026	2.258678	-0.179654
77	6	0	5.206399	-8.698111	-4.837920
78	6	0	-1.460112	-4.041649	8.006060

79	6	0	-8.421836	-1.052876	-5.172928
80	6	0	6.701077	-2.616360	-5.244554
81	6	0	0.034567	2.040102	7.599425
82	6	0	-6.927158	5.028876	-5.579562
83	6	0	8.195756	3.465391	-5.651188
84	6	0	-1.072061	-3.720408	5.596363
85	6	0	0.422631	2.361353	5.189734
86	6	0	2.089876	-5.889191	1.060248
87	6	0	-11.538301	1.756019	0.725347
88	6	0	3.584620	0.192524	0.653748
89	6	0	-10.043623	7.837771	0.318714
90	6	0	5.079265	6.274255	0.247111
91	6	0	-4.439690	-2.082084	1.707596
92	6	0	10.683272	-3.645614	1.635897
93	6	0	-2.944966	3.999628	1.300880
94	6	0	12.177949	2.436136	1.229264
95	6	0	4.088289	-7.017730	0.169602
96	6	0	-9.539947	0.627505	-0.165407
97	6	0	5.582967	-0.935979	-0.237032
98	6	0	-8.045270	6.709256	-0.572040
99	6	0	7.077645	5.145772	-0.643666
100	6	0	-5.252256	-1.502722	0.735220
101	6	0	9.870682	-3.066229	0.663561
102	6	0	-3.757556	4.579007	0.328555
103	6	0	11.365360	3.015522	0.256928
104	6	0	1.399263	-4.831864	1.677364
105	6	0	-12.228885	2.813333	1.342182
106	6	0	2.893956	1.249907	1.270393
107	6	0	-10.734208	8.895085	0.935548
108	6	0	4.388725	7.331698	0.863988
109	6	0	3.433954	-5.798842	0.704074
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335	8	0	0.435676	10.063831	2.135954
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356	1	0	11.690403	-7.422821	2.180074
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398	8	0	-1.005322	0.189643	-1.286656
399	3	0	-2.787276	-0.225521	-1.794980

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