

Supplementary Data 3. Optimized atomic coordinates of ZIF-8 (*R3m*) after toluene adsorption.

Atom number	x	y	z
C1	0.92854	0.41519	0.71069
N2	0.89795	0.33296	0.61056
H3	0.86814	0.42525	0.73214
H4	0.92515	0.19386	0.46702
C5	0.78493	0.25676	0.31317
N6	0.72923	0.27657	0.3692
H7	0.81946	0.20348	0.31774
H8	0.57831	0.324	0.39834
C9	0.04024	0.76916	0.47267
N10	0.08063	0.70651	0.42666
H11	0.09416	0.85016	0.54275
H12	0.01116	0.46909	0.31158
C13	0.37254	0.66806	0.61174
N14	0.26896	0.65489	0.56227
H15	0.43831	0.71719	0.60356
H16	0.07429	0.62115	0.54733
H17	0.26021	0.06978	0.55057
Zn18	0.741	0.2363	0.48843
C19	0.99212	0.34277	0.61149
C20	-0.00027	0.27327	0.51945
C21	0.71052	0.92868	0.41494
N22	0.6104	0.89812	0.33273
H23	0.73197	0.86825	0.42493
H24	0.46692	0.92535	0.19366
C25	0.3125	0.78391	0.25588
N26	0.36901	0.72875	0.27624
H27	0.31691	0.81814	0.20234
H28	0.39844	0.57811	0.32489
C29	0.47271	0.04004	0.76927
N30	0.42662	0.08039	0.70664
H31	0.5427	0.09398	0.85034
H32	0.3113	0.01049	0.46895
C33	0.61251	0.37311	0.66908
N34	0.56315	0.26951	0.65589
H35	0.60453	0.43891	0.71849
H36	0.54828	0.07501	0.62207
H37	0.55044	0.26039	0.07013
Zn38	0.48845	0.74101	0.23624
C39	0.61136	0.99234	0.34262
C40	0.51942	0	0.273
C41	0.41483	0.71038	0.92845
N42	0.3327	0.61021	0.89792
H43	0.42475	0.73184	0.86802
H44	0.1937	0.46676	0.92547
C45	0.25636	0.31304	0.78412
N46	0.27608	0.36884	0.72822
H47	0.20307	0.31773	0.8186

H48	0.32253	0.39614	0.57595
C49	0.76908	0.47263	0.04017
N50	0.70645	0.42668	0.08059
H51	0.85012	0.54266	0.09407
H52	0.46909	0.31196	0.0113
C53	0.6691	0.61269	0.37309
N54	0.65582	0.56318	0.26948
H55	0.71841	0.60466	0.43889
H56	0.62187	0.54817	0.07484
H57	0.0702	0.55056	0.26032
Zn58	0.23596	0.48829	0.74088
C59	0.34261	0.61124	0.99218
C60	0.27317	0.5193	-0.00003
C61	0.41507	0.9284	0.71053
N62	0.33284	0.89781	0.61038
H63	0.42515	0.86799	0.73195
H64	0.19359	0.92504	0.46702
C65	0.25589	0.78384	0.31237
N66	0.27626	0.72863	0.36884
H67	0.2023	0.81801	0.31672
H68	0.32537	0.57881	0.39905
C69	0.76921	0.04031	0.47273
N70	0.70657	0.08069	0.42672
H71	0.85023	0.09423	0.54279
H72	0.46897	0.0109	0.31139
C73	0.6689	0.37316	0.61261
N74	0.65574	0.26958	0.56315
H75	0.71814	0.43896	0.60453
H76	0.62208	0.07504	0.54829
H77	0.06991	0.26056	0.55047
Zn78	0.23618	0.74086	0.48817
C79	0.34261	0.99202	0.61138
C80	0.27296	-0.00034	0.51945
C81	0.92861	0.71048	0.41484
N82	0.89807	0.61035	0.33262
H83	0.86818	0.73191	0.42482
H84	0.92548	0.46681	0.19368
C85	0.78478	0.31326	0.25658
N86	0.72901	0.36918	0.27643
H87	0.81911	0.31787	0.20315
H88	0.57694	0.39679	0.32359
C89	0.04018	0.47288	0.76939
N90	0.0805	0.42679	0.70671
H91	0.09413	0.54293	0.85041
H92	0.01053	0.31167	0.46903
C93	0.37256	0.6119	0.66844
N94	0.26903	0.56272	0.65543
H95	0.43839	0.60405	0.71796
H96	0.07434	0.54746	0.62125
H97	0.26066	0.55041	0.07027

Zn98	0.74093	0.48846	0.23624
C99	0.99228	0.61131	0.34254
C100	0.00007	0.51938	0.27307
C101	0.71033	0.41486	0.92854
N102	0.61015	0.33274	0.89802
H103	0.73176	0.42481	0.8681
H104	0.46648	0.19393	0.92545
C105	0.31299	0.25658	0.78428
N106	0.3689	0.27627	0.72845
H107	0.31773	0.20345	0.81896
H108	0.39721	0.32296	0.57683
C109	0.47258	0.76914	0.04009
N110	0.42662	0.70651	0.0805
H111	0.54257	0.8502	0.09399
H112	0.31175	0.46895	0.01072
C113	0.61276	0.66919	0.37312
N114	0.56329	0.65596	0.26953
H115	0.60476	0.71853	0.43893
H116	0.54805	0.62192	0.07487
H117	0.55052	0.07007	0.26017
Zn118	0.4883	0.23601	0.74094
C119	0.61117	0.34267	0.99227
C120	0.51924	0.27326	0.0001
C121	0.69617	0.34419	0.34418
C122	0.62929	0.38324	0.38333
H123	0.68006	0.46089	0.46038
C124	0.20883	0.59125	0.59129
C125	0.09248	0.55867	0.55869
H126	0.03677	0.4813	0.48141
C127	0.34434	0.6961	0.34422
C128	0.38446	0.63027	0.38427
H129	0.46194	0.68185	0.46149
C130	0.59184	0.20937	0.59188
C131	0.55944	0.09305	0.55944
H132	0.48214	0.03706	0.48213
C133	0.34374	0.34377	0.69527
C134	0.38244	0.38242	0.6279
H135	0.45956	0.45999	0.67818
C136	0.59184	0.59187	0.20931
C137	0.55928	0.55933	0.09295
H138	0.48199	0.48201	0.03703
C139	0.21313	0.34744	0.21469
C140	0.27455	0.32881	0.16464
C141	0.33019	0.27292	0.18824
C142	0.32352	0.2356	0.26173
C143	0.26206	0.25473	0.31178
C144	0.20651	0.31127	0.28945
H145	0.16991	0.39143	0.19619
H146	0.27944	0.35835	0.10723
H147	0.37861	0.25855	0.14946

H148	0.36672	0.19176	0.28054
H149	0.25711	0.22585	0.36967
C150	0.14213	0.33399	0.34492
H151	0.05707	0.30225	0.28484
H152	0.17659	0.42229	0.39621
H153	0.14156	0.29636	0.39728
