

Supplementary Data 2. Optimized atomic coordinates of ZIF-8 (*Cm*) after toluene adsorption.

Atom number	x	y	z
C1	0.51878	0.5752	0.69853
N2	0.54068	0.63277	0.75184
C3	0.45756	0.76274	0.9738
N4	0.42269	0.6892	0.93924
C5	0.27548	0.2184	0.29018
N6	0.3558	0.26286	0.31415
C7	0.70806	0.40092	0.08624
N8	0.59883	0.3326	0.12345
C9	0.64964	0.24673	0.8214
N10	0.70811	0.35793	0.74503
C11	0.91772	0.71017	0.62221
N12	0.88352	0.60105	0.68807
C13	0.37222	0.61981	0.34906
N14	0.26963	0.56838	0.36061
C15	0.04297	0.45554	0.24845
N16	0.0798	0.41871	0.31939
C17	0.76943	0.03027	0.56745
N18	0.69711	0.06723	0.59958
C19	0.67482	0.3673	0.40591
N20	0.65794	0.26171	0.45484
C21	0.39647	0.92912	0.30585
N22	0.32224	0.89527	0.41282
C23	0.19122	0.66054	0.76565
N24	0.26626	0.71699	0.65371
Zn25	0.47908	0.72707	0.78151
Zn26	0.48316	0.23517	0.28454
Zn27	0.7376	0.22504	0.53432
C28	0.3484	0.59038	0.03242
C29	0.29215	0.48696	0.03299
C30	0.74532	0.36606	0.64435
C31	0.81198	0.47237	0.53853
C32	0.9761	0.59584	0.67286
C33	0.97702	0.49248	0.72725
C34	0.20543	0.59333	0.42569
C35	0.08906	0.55882	0.45572
C36	0.9886	0.33792	0.41751
C37	0.99076	0.27398	0.51717
H38	0.46423	0.57833	0.66573
H39	0.51924	0.84848	0.91492
H40	0.26565	0.15054	0.27466
H41	0.73659	0.40476	0.14377
H42	0.61131	0.21703	0.90941
H43	0.85892	0.7369	0.61862
H44	0.44094	0.61552	0.29888
H45	0.10008	0.52194	0.16369
H46	0.85604	0.08732	0.5078
H47	0.72442	0.43092	0.41595

H48	0.40081	0.87001	0.27998
H49	0.10386	0.62824	0.79595
H50	0.31571	0.5038	0.94827
H51	0.20212	0.44815	0.08147
H52	0.31416	0.42648	0.07055
H53	0.75981	0.50345	0.51793
H54	0.85817	0.46275	0.47077
H55	0.87015	0.53526	0.54438
H56	0.91352	0.42405	0.73199
H57	0.95964	0.46893	0.81242
H58	0.05778	0.50222	0.6808
H59	0.07557	0.55262	0.3894
H60	0.06792	0.61827	0.47053
H61	0.03143	0.47792	0.5313
H62	0.01042	0.21029	0.51156
H63	0.91061	0.23349	0.59174
H64	0.05433	0.32776	0.52593
H65	0.67192	0.59754	0.89395
H66	0.36351	0.43495	0.41189
C67	0.57498	0.51842	0.69881
N68	0.63254	0.54025	0.75213
C69	0.7639	0.45581	0.973
N70	0.69001	0.42188	0.93852
C71	0.21877	0.27467	0.29058
N72	0.26319	0.3548	0.3148
C73	0.40303	0.70671	0.08703
N74	0.33389	0.5977	0.12423
C75	0.24764	0.65663	0.8219
N76	0.35848	0.71058	0.74566
C77	0.71115	0.9176	0.62169
N78	0.6021	0.88335	0.68791
C79	0.62152	0.3721	0.34683
N80	0.56953	0.2693	0.35893
C81	0.45633	0.04184	0.24842
N82	0.41953	0.07919	0.31879
C83	0.03037	0.76858	0.56837
N84	0.06736	0.69627	0.60047
C85	0.36736	0.67277	0.40846
N86	0.26185	0.65624	0.45717
C87	0.93025	0.39589	0.30538
N88	0.89584	0.3217	0.41255
C89	0.65283	0.1903	0.76512
N90	0.71331	0.26571	0.65301
Zn91	0.72699	0.47843	0.78112
Zn92	0.23569	0.48226	0.28565
Zn93	0.22534	0.73737	0.53525
C94	0.59119	0.34782	0.03172
C95	0.48747	0.2922	0.03254
C96	0.36642	0.74609	0.64508
C97	0.47236	0.80944	0.53931

C98	0.59682	0.97595	0.67238
C99	0.49334	0.97668	0.72665
C100	0.59467	0.20515	0.42381
C101	0.55967	0.08857	0.45436
C102	0.33869	0.98838	0.41716
C103	0.27578	0.99145	0.51663
H104	0.57774	0.46348	0.66639
H105	0.84971	0.51718	0.91407
H106	0.15056	0.26457	0.27561
H107	0.40766	0.73504	0.14454
H108	0.21832	0.6207	0.90977
H109	0.73792	0.85884	0.61805
H110	0.6174	0.44085	0.29644
H111	0.52284	0.0986	0.16364
H112	0.08741	0.85528	0.50905
H113	0.43095	0.7221	0.4187
H114	0.87149	0.40045	0.27905
H115	0.61773	0.10271	0.79555
H116	0.50388	0.31612	0.94789
H117	0.44842	0.20211	0.08076
H118	0.42734	0.31432	0.07063
H119	0.50193	0.75537	0.52128
H120	0.46302	0.85441	0.47075
H121	0.5364	0.86859	0.5432
H122	0.42546	0.91435	0.72962
H123	0.46856	0.95736	0.81248
H124	0.5037	0.05798	0.68103
H125	0.55197	0.07437	0.38891
H126	0.6196	0.06756	0.46809
H127	0.47941	0.03131	0.53078
H128	0.21516	0.01578	0.50946
H129	0.23217	0.91042	0.59097
H130	0.33112	0.05228	0.52698
H131	0.59732	0.67028	0.89528
H132	0.43772	0.36357	0.4098
C133	0.60973	0.60959	0.78296
C134	0.65539	0.65512	0.84258
C135	0.34494	0.34423	0.32917
C136	0.41191	0.41118	0.36102
H137	0.7333	0.7338	0.78506
H138	0.48626	0.48652	0.28819
C139	0.18068	0.33111	0.64355
C140	0.18749	0.25031	0.61915
C141	0.25481	0.20968	0.63983
C142	0.31514	0.25094	0.68472
C143	0.30792	0.33187	0.70915
C144	0.24039	0.37291	0.68928
H145	0.12798	0.36286	0.6273
H146	0.14106	0.2197	0.58269
H147	0.26053	0.14671	0.62029

H148	0.368	0.21981	0.70131
H149	0.35512	0.36387	0.74455
C150	0.23079	0.45897	0.71644
H151	0.14479	0.43036	0.77355
H152	0.259	0.53461	0.64191
H153	0.27872	0.48049	0.75564
