

Supplementary Data 1. Optimized atomic coordinates of ZIF-8 (*I*-43*m*) after toluene adsorption.

Atom number	x	y	z
C1	0.58466	0.05763	0.26518
H2	0.5843	0.11635	0.23614
H3	0.6519	0.03982	0.5472
H4	0.76979	0.04979	0.53515
H5	0.65251	0.91587	0.47504
N6	0.64857	0.09351	0.37639
C7	0.79227	0.32019	0.7353
H8	0.8801	0.34897	0.76479
H9	0.49179	0.10525	0.45254
H10	0.51385	0.23499	0.4646
H11	0.44089	0.17876	0.52514
N12	0.71715	0.27271	0.62398
C13	0.208	0.94285	0.52807
H14	0.12021	0.88444	0.46892
H15	0.50786	0.96034	0.6125
H16	0.48555	0.94998	0.72017
H17	0.55973	0.08403	0.73733
N18	0.28327	0.90671	0.55532
C19	0.41377	0.67816	0.4703
H20	0.4145	0.64923	0.52924
H21	0.34908	0.89581	0.3881
H22	0.23008	0.76624	0.28061
H23	0.34656	0.82217	0.26255
N24	0.35095	0.72693	0.44387
C25	0.26463	0.58706	0.05701
H26	0.23518	0.58807	0.11563
H27	0.547	0.65171	0.03972
H28	0.53567	0.76993	0.0496
H29	0.47549	0.65257	0.91574
N30	0.37608	0.65025	0.09306
C31	0.73446	0.79171	0.32133
H32	0.76351	0.87961	0.35121
N33	0.62298	0.71588	0.27244
C34	0.52905	0.20818	0.9432
H35	0.47131	0.1201	0.88482
H36	0.61251	0.50831	0.96015
H37	0.71991	0.48541	0.94989
H38	0.73722	0.56004	0.08392
N39	0.55596	0.28343	0.90693
C40	0.46941	0.41235	0.67659
H41	0.52676	0.41129	0.6458
H42	0.388	0.34898	0.89502
H43	0.28008	0.22968	0.76602
H44	0.26247	0.34651	0.82182
N45	0.44223	0.349	0.7247
C46	0.05738	0.26541	0.58612
H47	0.1164	0.23655	0.5872

N48	0.09282	0.37667	0.64965
C49	0.32125	0.73441	0.79168
H50	0.35154	0.76344	0.87962
N51	0.2734	0.62314	0.71594
C52	0.94246	0.52912	0.20788
H53	0.88352	0.47139	0.11993
N54	0.90696	0.55699	0.28367
C55	0.67922	0.47129	0.4144
H56	0.64945	0.52943	0.41397
N57	0.72705	0.44353	0.35087
C58	0.05667	0.58533	0.26477
H59	0.11499	0.58453	0.23527
H60	0.03972	0.65201	0.54743
H61	0.04963	0.77004	0.53571
H62	0.91578	0.65269	0.4756
N63	0.09303	0.64872	0.37626
C64	0.3205	0.7917	0.73477
H65	0.34932	0.87955	0.76436
H66	0.10471	0.49139	0.45184
H67	0.23487	0.51418	0.46414
H68	0.17816	0.4403	0.52441
N69	0.27236	0.71656	0.6233
C70	0.94317	0.20805	0.5282
H71	0.88488	0.1202	0.46914
H72	0.95989	0.50764	0.61232
H73	0.94954	0.48531	0.71995
H74	0.08362	0.55962	0.73723
N75	0.90678	0.28311	0.5554
C76	0.67911	0.41432	0.47155
H77	0.64898	0.41389	0.52945
H78	0.89558	0.34855	0.38788
H79	0.7658	0.23	0.28041
H80	0.82205	0.34671	0.26277
N81	0.72687	0.35074	0.4441
C82	0.58619	0.26561	0.05743
H83	0.58754	0.23671	0.11647
N84	0.64906	0.37703	0.09301
C85	0.79193	0.73499	0.3221
H86	0.88004	0.7646	0.35282
H87	0.49149	0.45189	0.10454
H88	0.51437	0.4641	0.23476
H89	0.44008	0.52394	0.1778
N90	0.71664	0.62351	0.27378
C91	0.20774	0.52961	0.9428
H92	0.11982	0.47148	0.88402
N93	0.28349	0.55671	0.90703
C94	0.41249	0.46959	0.67705
H95	0.41163	0.52751	0.64703
N96	0.3495	0.44232	0.72552
C97	0.26516	0.05704	0.58611

H98	0.23593	0.11572	0.58677
N99	0.37648	0.09279	0.64972
C100	0.73497	0.32027	0.7922
H101	0.7641	0.34928	0.87998
N102	0.62368	0.27271	0.71661
C103	0.52775	0.9434	0.20803
H104	0.46902	0.88484	0.1202
N105	0.55586	0.90743	0.28341
C106	0.4699	0.67741	0.41221
H107	0.52732	0.64682	0.41077
N108	0.44257	0.72601	0.34941
C109	0.62875	0.00054	0.38423
C110	0.67832	0.00115	0.49073
C111	0.61615	0.24477	0.61584
C112	0.51041	0.18839	0.50943
C113	0.38417	-0.00037	0.62874
C114	0.49	-0.00115	0.67758
C115	0.37068	0.75495	0.37084
C116	0.32155	0.81262	0.32268
C117	0.38426	0.62951	0.00018
C118	0.49094	0.67844	0.00097
C119	0.61547	0.61513	0.24462
C120	0.50976	0.50842	0.18763
C121	0.62847	0.38457	-0.00022
C122	0.67737	0.49025	-0.00121
C123	0.36985	0.36951	0.75345
C124	0.32226	0.32115	0.81187
C125	-0.00049	0.38412	0.62871
C126	-0.00152	0.48982	0.67742
C127	0.24471	0.61559	0.61511
C128	0.18776	0.50973	0.50852
C129	0.00023	0.6292	0.38448
C130	0.00103	0.67855	0.49113
C131	0.75499	0.37071	0.37123
C132	0.8124	0.32147	0.32274
Zn133	0.74997	0.25024	0.50016
Zn134	0.24996	0.74985	0.49971
Zn135	0.50004	0.75022	0.24968
Zn136	0.50006	0.25011	0.75002
Zn137	0.25	0.49985	0.74995
Zn138	0.7498	0.49989	0.25032
C139	0.28617	0.30904	0.32835
C140	0.33677	0.32506	0.26567
C141	0.36541	0.24836	0.21681
C142	0.34153	0.15495	0.23001
C143	0.29037	0.13921	0.29223
C144	0.26235	0.2163	0.34297
H145	0.26369	0.36919	0.36614
H146	0.3535	0.39784	0.25525
H147	0.40556	0.26093	0.16828

H148	0.3632	0.09414	0.19186
H149	0.27204	0.06568	0.30169
C150	0.20919	0.20053	0.41191
H151	0.18736	0.26508	0.44012
H152	0.26597	0.2049	0.48655
H153	0.13309	0.11863	0.36469
