Supporting Information

Reversible ammonia uptake at room temperature in a robust and tunable metal-organic framework

Jaechul Lee,[a‡] Younggyu Seo,[a‡] Dong Won Kang,[b] Seungjae Park,[a] Hyunyong Kim,[a] Jaheon Kim,[c] Kimoon Kim,[ade] Chang Seop Hong,*[b] Dae-Woon Lim,*[fg] Eunsung Lee*[ad]

[a] Department of Chemistry, Pohang University of Science and Technology (POSTECH), Pohang, 37673, Republic of Korea
[b] Department of Chemistry, Korea University, Seoul 02841, Republic of Korea
[c] Department of Chemistry, Soongsil University, Seoul 06978, Republic of Korea
[d] Division of Advanced Materials Science, Pohang University of Science and Technology, Pohang 37673, Republic of Korea
[e] Center for Self–assembly and Complexity, Institute for Basic Science (IBS), Pohang 37673, Republic of Korea
[f] Department of Chemistry, Graduate School of Science, Kyoto University, Kitashirakawa Oiwakecho, Sakyo-ku, Kyoto 606-8502, Japan
[g] Department of Chemistry and Medical Chemistry, Yonsei University, Wonju, 26493, Republic of Korea

Abstract: Ammonia is the second most-produced chemical in the world, but the effective removal of ammonia from atmosphere is also important because of its high toxicity and corrosiveness. Although metal-organic frameworks (MOFs) have emerged as a strong candidate for NH_3 adsorbents, most of MOFs suffer from a lack of stability and high regeneration temperatures. Here, we report the recyclable and tunable ammonia adsorption using a robust imidazolium-based MOF (**JCM-1**). **JCM-1** shows reversible NH_3 uptake which can be easily regenerated at room temperature without any structural deformation. Furthermore, we demonstrated the control of NH_3 adsorption affinity and uptake capacity of **JCM-1** by simple ion substitution in a post-synthetic manner. To understand the anion effect on NH_3 sorption in **JCM-1**, interaction energies of the frameworks toward NH_3 before and after ion substitution were simulated by density functional theory (DFT) calculations.

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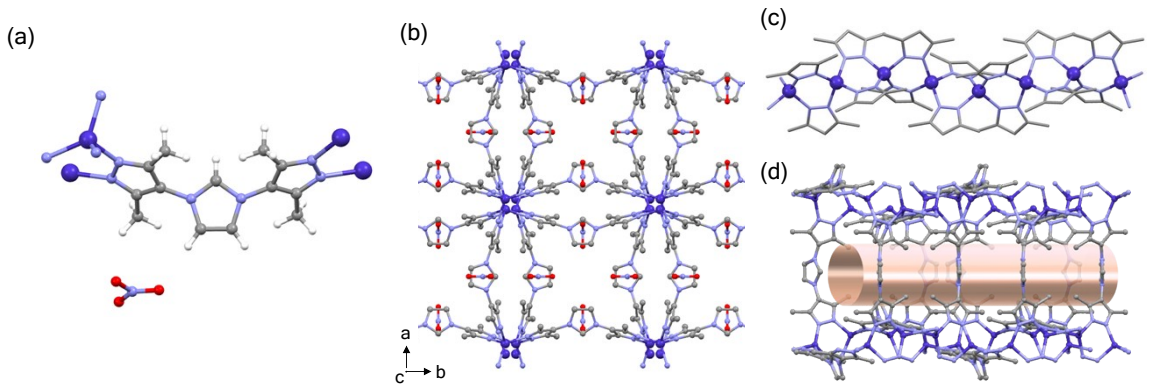


Crystal structure of JCM-1

Fig. S1 a) Repeating unit of **JCM-1** with Co^{II} nodes connected by the ligands b) The view of the crystal structure of **JCM-1** along the c axis. c) A perpendicular view of pyrazolate-bridged 4-fold helical $cobalt^{II}$ chain. d) imidazolium-aligned channel of **JCM-1 along** the c axis. Nitrate anions and hydrogen atoms are omitted for clarity in Fig S1c and d.

Single crystal structure of JCM-1(Cl^-)

In the crystal structure of **JCM-1(Cl^-)**, chloride anion was successfully assigned as below. Chloride looks to form weak hydrogen bonding interactions with three nearby protons from three imidazolium rings. (See supplementary crystal data for further details)

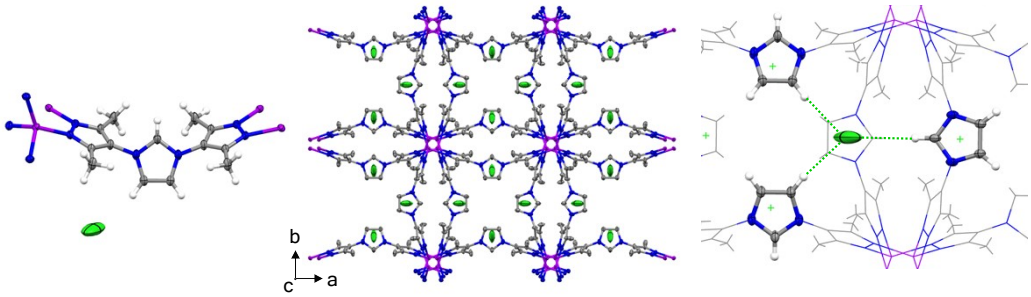


Fig. S2 Single crystal structure of **JCM-1(Cl^-)**.

Table S1.Crystal data and structure refinement for **JCM-1(Cl$^-$)**	
Identification code	I41amd_80
Empirical formula	C13H15ClCoN6
Formula weight	349.69
Temperature/K	173(2)
Crystal system	tetragonal
Space group	$I4_1/amd$
a/Å	23.354(3)
b/Å	23.354(3)
c/Å	13.117(3)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	7154(3)
Z	16
ρ_{calc}g/cm^3	1.299
μ/mm^{-1}	1.110
F(000)	2864.0
Crystal size/mm^3	0.02 × 0.01 × 0.005
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	3.562 to 52.742
Index ranges	-29 ≤ h ≤ 29, -29 ≤ k ≤ 29, -16 ≤ l ≤ 16
Reflections collected	27574
Independent reflections	1927 [R_{int} = 0.0742, R_{sigma} = 0.0256]
Data/restraints/parameters	1927/0/101
Goodness-of-fit on F^2	1.122
Final R indexes [I>=2σ (I)]	R_1 = 0.0716, wR_2 = 0.2286
Final R indexes [all data]	R_1 = 0.0806, wR_2 = 0.2377
Largest diff. peak/hole / e Å^{-3}	1.00/-0.86

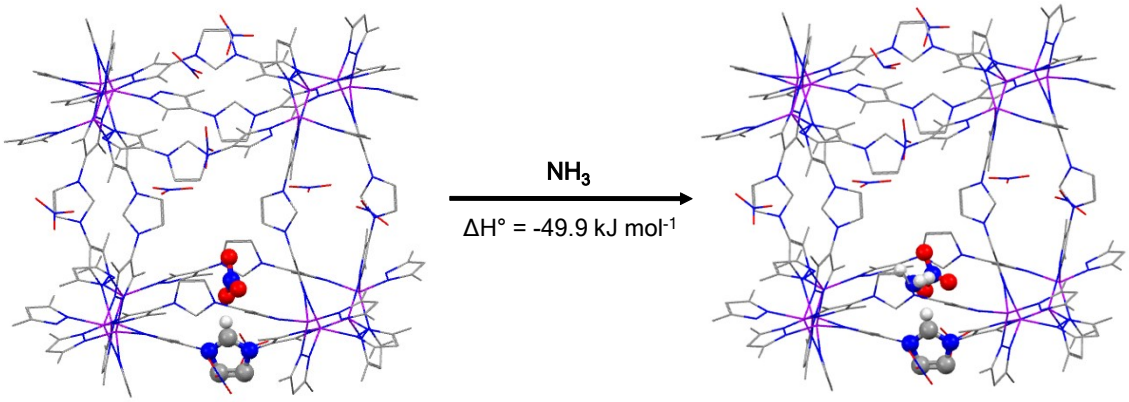
Isosteric heat of sorption

The fitting parameters of each sorption isotherm are summarized in Table S3. Overall fitting quality was still good as evidenced by R^2 values greater than 0.997.

	JCM-1	**JCM-1(Cl^-)**
a0	-6695.58285	-8747.36628
a1	335.34569	601.54978
a2	22.1313	-105.10037
a3	-13.60095	11.01191
a4	1.20E0	-4.17E-1
adj. R^2	0.9972027	0.9977129

Table S2. Fitted parameters by the dual-site Langmuir equation

DFT calculations



*- Standard interaction enthalpy of **JCM-1** with an NH_3 molecule*

Fig. S3 Standard enthalpy changes calculated on the model systems of **JCM-1**.

*- Standard interaction enthalpy of **JCM-1(Cl^-)** with an NH_3 molecule*

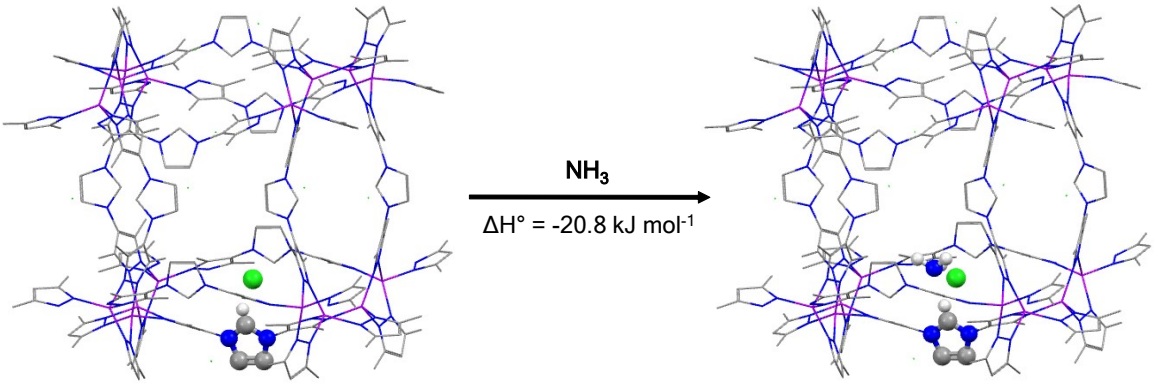


Fig. S4 Standard enthalpy changes calculated on the model systems **JCM-1(Cl^-)**.

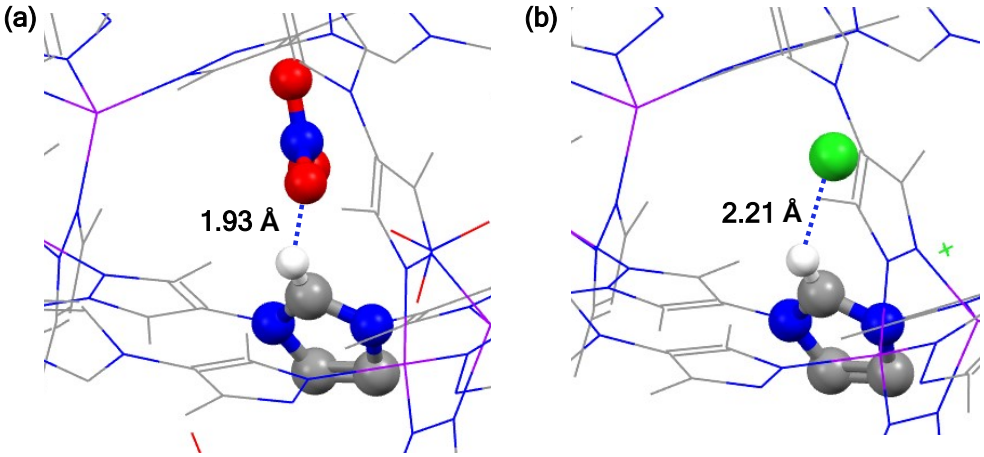
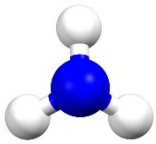


Fig. S5 Anion-imidazolium distance in the optimized structures of a) **JCM-1** and b) **JCM-1(Cl⁻)**.

- Coordinates of optimized structures

The following optimized geometries were displayed in Cartesian coordinates (atomic unit). E° represents the electronic energy of the optimized structure, and H° represents the sum of electronic and thermal enthalpies in Hartree unit.

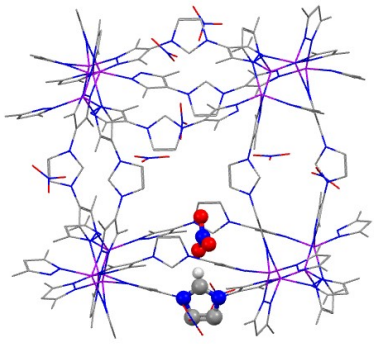
Coordinates of Optimized Structures of **NH_3** [H° = -56.519517]



Charge = 0; Multiplicity = 1;

N	-0.1097	-0.0055	0.2176
H	-0.7141	0.6574	-0.2635
H	0.7141	0.5236	0.4962
H	0.209	-0.6574	-0.4962

Coordinates of Optimized Structures of **JCM-1** [H° = -500.158804]



Charge = 0; Multiplicity = 1;

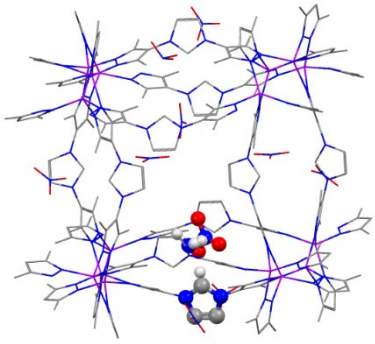
C	-6.9832	9.8599	-1.0375	C	-10.0755	5.8418	2.9737	C	-3.5635	7.6045	-0.2144
C	-4.6789	-3.5588	-3.5836	C	-9.4449	5.9973	4.3354	C	-3.6695	8.2309	1.1551
C	-4.3342	-2.8643	-2.4425	C	-10.0014	5.8262	5.5862	C	0.615	9.2796	-0.4467
C	-4.508	-3.7064	-1.3714	C	-9.0264	6.0877	6.5176	C	2.2826	6.4519	-3.0434
C	-4.2824	-3.4133	0.0924	C	-9.1404	6.0545	8.0227	C	2.9174	6.8209	-1.7253
C	-9.0769	3.1502	-10.0691	C	-0.0458	7.2041	-0.7609	C	2.3771	7.4905	-0.6469
C	-8.4462	3.3058	-8.7074	C	-0.7325	9.2843	-0.5508	C	3.3488	7.5802	0.3198
C	-9.0027	3.1346	-7.4566	C	-2.001	6.4669	-3.3744	C	-7.2041	9.407	0.3846
C	-8.0277	3.3962	-6.5252	C	-2.8282	6.8411	-2.1694	C	-3.5758	6.9	-8.5811
C	-8.1417	3.3629	-5.0201	C	-2.4555	7.5075	-1.0203	C	-7.4617	0.5154	1.6816

C	-9.3746	1.0481	0.7332
C	-7.3779	3.1337	3.7636
C	-7.3745	3.5874	2.3247
C	-7.7192	2.8928	1.1836
C	-7.5454	3.7348	0.1124
C	-7.7709	3.4417	-1.3514
C	-9.4003	-0.2757	1.0044
C	-7.4593	-1.0746	4.6258
C	-7.4837	-2.0571	3.4812
C	-7.8111	-1.8549	2.1563

C	-7.6768	-3.056	1.5037	C	8.6326	6.8904	-4.2257	Co	5.6305	-6.4155	-3.538	H	3.6179	-2.5392	0.7795
C	-7.9025	-3.3537	0.0408	C	10.2798	3.0823	-8.573	Co	5.3644	-6.5939	-0.1029	H	3.2314	-4.0439	0.9729
C	0.5366	3.0492	-8.4849	C	9.4485	3.2429	-7.3243	Co	5.9814	-5.9241	3.2248	H	1.9964	0.875	-1.7791
C	-0.1242	0.9738	-8.7991	C	9.805	3.0685	-6.0029	Co	5.7483	-4.3998	6.311	H	4.6772	1.3491	-5.8875
C	-1.7918	3.8015	-6.2025	C	8.7003	3.3374	-5.2322	H	-7.1421	6.6365	6.2019	H	4.9018	0.1976	-4.8465
C	-2.4266	3.4325	-7.5205	C	8.5815	3.3041	-3.7275	H	5.8879	3.3343	-8.6858	H	6.1223	1.0356	-5.3676
C	-1.8863	2.7629	-8.599	C	9.2812	5.7738	4.4698	H	-5.2823	6.7798	5.7338	H	3.7164	2.556	-0.2644
C	-2.858	2.6732	-9.5656	C	8.4498	5.9344	5.7185	H	4.1274	6.7468	6.4611	H	3.3877	4.0288	-0.6811
C	-2.7568	2.0468	-10.9356	C	8.8064	5.7601	7.0399	H	7.4595	-6.8014	-5.8928	H	4.8177	3.6662	-0.1534
C	1.2234	0.9691	-8.695	C	7.7016	6.0289	7.8106	H	5.6948	-6.6454	-6.641	H	6.7404	-10.0778	4.2521
C	2.4918	3.7865	-5.8714	C	7.5828	5.9957	9.3153	H	5.6991	-3.3888	9.2541	H	7.1304	-8.9284	3.2585
C	3.319	3.4123	-7.0764	C	-10.0524	-6.4384	2.1155	H	5.8921	6.5908	7.2093	H	5.6205	-9.2315	3.5502
C	2.9462	2.7459	-8.2255	C	-9.2252	-6.8126	0.9105	H	7.6629	3.7062	-8.0456	H	7.1181	-9.23	6.7817
C	4.0543	2.6489	-9.0314	C	-9.598	-7.4789	-0.2386	H	-7.3352	-3.3429	8.2466	H	3.149	-6.0727	5.1472
C	-7.3511	-9.1562	2.8586	C	-8.4898	-7.576	-1.0445	H	-6.7711	-6.7513	-6.9927	H	3.5788	-7.5793	5.1478
C	2.3204	6.1038	5.9664	C	-8.3838	-8.2024	-2.414	H	-6.5677	3.7562	-9.1455	H	2.0641	-7.1991	5.0408
C	1.9476	5.4374	4.8173	C	-9.263	-6.4646	-8.0993	H	-4.7182	3.3715	-9.5055	H	-1.6598	-9.3145	3.4624
C	3.0557	5.3404	4.0114	C	-8.6282	-6.0955	-6.7812	H	-4.9112	-6.6081	-7.4609	H	-1.366	-7.3814	-0.3436
C	3.1617	4.714	2.6419	C	-9.1684	-5.426	-5.7027	H	3.9241	-3.7608	8.6139	H	-2.257	-6.3154	-1.0735
C	-9.7891	7.1711	-0.6728	C	-8.1967	-5.3362	-4.7361	H	-5.4857	-3.7276	7.8865	H	-2.643	-7.8334	-1.1344
C	-8.9577	7.0104	-1.9216	C	-8.298	-4.7098	-3.3662	H	-6.0553	9.7617	-1.2634	H	-3.1227	-7.1809	4.6399
C	-9.3143	7.1848	-3.2429	C	-8.4776	-6.8715	7.3222	H	-7.5148	9.3229	-1.6292	H	-4.6386	-7.5504	4.5127
C	-8.2095	6.916	-4.0137	C	-7.7152	10.1046	1.4597	H	-7.2397	10.7818	-1.1229	H	-4.2032	-6.0469	4.579
C	-8.0907	6.9491	-5.5183	C	-7.714	9.2619	2.5443	H	-5.1092	-3.5221	0.5698	H	9.737	-6.0994	-7.3816
C	4.7272	-0.5198	-2.2203	C	-8.1598	9.5574	3.9563	H	-3.9706	-2.5126	0.193	H	11.0022	-6.2512	-6.4671
C	2.6876	-1.0385	-1.5774	C	-4.5917	-0.4871	-2.9405	H	-3.6291	-4.0198	0.4427	H	10.0666	-7.4844	-6.7261
C	5.1116	-3.1397	-4.2661	C	-2.6531	0.3041	-2.2634	H	-10.0035	2.9179	-9.9677	H	10.4888	-5.1667	-4.0549
C	4.8907	-3.5924	-2.844	C	-4.5941	1.103	-5.8848	H	-9.0034	3.9772	-10.5514	H	7.7752	-4.0653	-2.0934
C	4.3796	-2.8949	-1.769	C	-4.5697	2.0856	-4.7401	H	-8.6234	2.4566	-10.5531	H	8.1549	-5.4368	-1.4381
C	4.3809	-3.7376	-0.6843	C	-4.2423	1.8833	-3.4152	H	-9.8807	2.8865	-7.2764	H	9.2772	-4.4111	-1.8196
C	3.9351	-3.4421	0.7276	C	-4.3765	3.0845	-2.7627	H	-9.0321	3.1088	-4.7733	H	10.0036	-3.5597	6.5757
C	2.7132	0.2852	-1.8486	C	-4.1508	3.3823	-1.2998	H	-7.5173	2.7286	-4.6663	H	9.068	-4.7929	6.3167
C	5.1931	1.0687	-5.1283	C	-2.6787	-1.0196	-1.9921	H	-7.9471	4.2352	-4.6669	H	8.7383	-3.4078	5.6611
C	4.9999	2.052	-4.0004	C	-4.6755	-3.1053	-5.0226	H	-10.0021	6.6688	2.4913	H	9.4901	-2.4752	8.9879
C	4.4715	1.8527	-2.7417	C	3.2476	8.2066	1.6897	H	-11.0021	5.6094	3.0751	H	8.2786	-1.7196	11.2232
C	4.5122	3.0532	-2.0756	C	-5.0702	-9.8314	-0.2215	H	-9.6221	5.1481	2.4897	H	7.1563	-2.7453	11.6047
C	4.0666	3.3534	-0.6647	C	-4.8493	-9.3785	-1.6436	H	-10.8794	5.5782	5.7663	H	6.7765	-1.3738	10.9494
C	6.5021	-9.2048	3.9294	C	-4.3381	-10.076	-2.7186	H	-8.5159	5.4201	8.3765	H	5.9601	0.5291	3.0155
C	6.5265	-8.2223	5.074	C	-4.3394	-9.2334	-3.8033	H	-10.0308	5.8004	8.2695	H	9.5905	-0.9296	2.3473
C	6.8539	-8.4246	6.3989	C	-3.8936	-9.5288	-5.2152	H	-8.9458	6.9268	8.3759	H	6.6852	-0.2522	5.4148
C	6.7195	-7.2235	7.0514	C	-4.7022	9.1846	-4.1175	H	-0.0399	6.2816	-0.8792	H	5.4646	-1.0902	5.9359
C	-7.5443	-8.1729	3.9864	C	-4.5091	8.2014	-5.2454	H	-1.2855	10.0314	-0.5012	H	6.9097	-1.4037	6.4558
C	2.0934	-7.1734	2.3575	C	-3.9807	8.4006	-6.5042	H	-2.0281	5.515	-3.4974	H	7.8705	-2.6106	0.8326
C	3.0685	-6.9118	3.2889	C	-4.0215	7.2001	-7.1702	H	-1.0926	6.7482	-3.2386	H	8.1993	-4.0834	1.2493
C	2.9544	-6.945	4.794	C	4.1604	2.0224	-10.4009	H	-2.3579	6.9002	-4.153	H	6.7692	-3.7208	0.7217
C	-1.0799	-8.6682	3.1273	C	-0.4621	5.7407	4.5579	H	-2.8175	8.5884	1.4091	H	-8.3982	-9.1755	5.5823
C	-2.2644	-7.1426	-0.5861	C	-1.1229	3.6653	4.2437	H	-4.3196	8.9342	1.1352	H	5.1507	-9.4489	-5.0574
C	-3.0957	-6.9819	0.6626	C	-2.7904	6.493	6.8402	H	-3.9399	7.5626	1.7906	H	3.6705	-8.9512	-4.9303
C	-2.7391	-7.1563	1.984	C	-3.4252	6.124	5.5223	H	1.159	10.0228	-0.3123	H	4.012	-10.4583	-4.6806
C	-3.8439	-6.8875	2.7547	C	-2.885	5.4544	4.4438	H	2.7579	6.8821	-3.7576	H	4.8465	10.0232	-3.6839
C	-3.9627	-6.9207	4.2594	C	-3.8567	5.3647	3.4772	H	1.366	6.7396	-3.0484	H	5.9664	9.177	-2.9818
C	10.0938	-6.5326	-6.6031	C	-3.7554	4.7383	2.1072	H	2.3216	5.4997	-3.1612	H	4.4565	8.8739	-2.6902
C	9.2665	-6.1583	-5.3981	C	0.2247	3.6606	4.3478	H	-3.2257	7.6973	-8.9815	H	4.4688	9.1754	-6.2134
C	9.6394	-5.492	-4.249	C	1.4931	6.478	7.1714	H	-4.3268	6.5871	-9.0924	H	4.3629	7.6706	-8.3949
C	8.5313	-5.395	-3.4431	C	6.9452	-6.9257	8.5143	H	-2.8969	6.2245	-8.5648	H	3.9636	6.2005	-8.0346
C	8.4252	-4.7685	-2.0736	C	6.8701	9.8112	0.0333	H	-6.6071	0.5731	2.0441	H	5.4602	6.5527	-8.3359
C	9.0951	-3.8411	6.4397	C	6.8666	9.3576	1.4722	H	-10.0554	1.541	0.3332	H	9.2653	-5.5543	3.7294
C	8.268	-3.4668	7.6447	C	7.2114	10.0521	2.6134	H	-7.9904	3.6748	4.267	H	10.2209	-6.7942	3.6167
C	8.6407	-2.8005	8.7938	C	7.0376	9.2101	3.6845	H	-7.6509	2.2136	3.8083	H	8.8291	-6.9367	4.3258
C	7.5327	-2.7035	9.5997	C	7.2632	9.5032	5.1483	H	-6.495	3.2255	4.1295	H	10.0766	-7.8764	1.1537
C	7.4266	-2.077	10.9692	C	-0.318	-6.8651	2.1216	H	-8.0827	2.5411	-1.4519	H	9.2178	-8.6247	-1.2417
C	6.8597	0.4651	2.7886	C	0.2677	-8.6729	3.2314	H	-8.4243	4.0483	-1.7016	H	7.6892	-8.9598	-1.2021
C	8.8738	-0.3398	2.4169	C	2.0193	-7.1577	-0.255	H	-6.9442	3.5506	-1.8287	H	8.1746	-7.5913	-1.7906
C	6.3938	-1.1233	5.6966	C	2.6499	-7.0021	1.1067	H	-10.1018	-0.8604	0.8253	H	0.3203	-6.9066	-6.1379
C	6.587	-2.1066	4.5688	C	8.8993	0.9839	2.1457	H	-7.6977	-0.2016	4.303	H	1.7013	-3.6565	-7.95
C	7.1155	-1.9073	3.31	C	6.4753	3.0851	4.8344	H	-6.5777	-1.0479	5.005	H	1.4074	-5.5896	-4.144
C	7.0747	-3.1078	2.6439	C	6.6962	3.5379	3.4123	H	-8.0877	-1.351	5.2967	H	2.2985	-6.6556	-3.4141
C	7.5204	-3.4079	1.233	C	7.2074	2.8403	2.3373	H	-8.1813	-2.5543	-0.408	H	2.6844	-5.1375	-3.3533
C	-8.0727	-8.3722	5.2452	C	7.2061	3.683	1.2525	H	-8.5806	-4.0245	-0.0476	H	3.1641	-5.79	-9.1276
C	4.3238	-9.5577	-4.58	C	7.6519	3.3875	-0.1593	H	-7.0839	-3.6721	-0.349	H	4.2446	-6.9241	-9.0666
C	5.0849	9.1502	-3.361	C	4.7169	-9.8658	0.5349	H	0.5307	3.9717	-8.3666	H	4.68	-5.4205	-9.0003
C	5.0605	8.1678	-4.5057	C	4.7203	-9.4122	-0.904	H	-0.6681	0.2306	-8.9335	H	-0.7433	-3.6479	-8.1389
C	4.7331	8.3701	-5.8307	C	4.3755	-10.1067	-2.0451	H	-2.2671	3.3712	-5.4883	H	-2.4313	-5.1195	-3.7487
C	4.8674	7.1689	-6.4831	C	4.5494	-9.2647	-3.1163	H	-0.8752	3.5137	-6.1974	H	-1.0513	-5.581	-4.334
C	4.6417	6.8711	-7.946	C	1.3071	-3.1368	9.1413	H	-1.8309	4.7536	-6.0847	H	-2.0513	-6.6403	-3.7503
C	9.3043	-6.5064	3.6116	C	2.1385	-3.2975	7.8925	H	-3.407	1.348	-11.0162	H	-2.0226	-5.7718	-9.5284
C	8.6695	-6.8755	2.2936	C	1.7819	-3.1231	6.5712	H	-1.8783	1.6832	-11.0558	H	-3.5375	-5.3916	-9.6355
C	9.2098	-7.5451	1.2151	C	2.8867	-3.3919	5.8005	H	-2.9216	2.7166	-11.6047	H	-3.1076	-6.8982	-9.6349
C	8.2381	-7.6347	0.2485	C	3.0055	-3.3588	4.2958	H	1.7763	0.222	-8.7447	H	-0.6784	-4.2151	6.9049
C	8.3394	-8.2612	-1.1215	C	-1.2249	-1.6065	5.3238	H	2.8487	3.3532	-5.0929	H	0.7026	-0.9649	5.0928
C	0.3594	-6.1059	-6.6092	C	-2.9764	-3.1217	8.8102	H	1.5834	3.5051	-6.0073	H	-4.1063	-4.2067	3.4079
C	1.1214	-4.3028	-7.6149	C	-3.6072	-3.2773	7.4484	H	2.5189	4.7383	-5.7485	H	-3.0213	-3.0803	3.5144
C	2.3058	-5.8283	-3.9015	C	-3.0507	-3.1061	6.1977	H	-7.6424	-10.0272	3.1404	H	-4.5361	-2.7001	3.4073
C	3.1371	-5.989	-5.1503	C	-4.0257	-3.3676	5.2662	H	-6.4219	-9.1892	2.6193	H	10.4943	7.3355	0.7219
C	2.7806	-5.8146	-6.4716	C	-10.2616	-3.7731	4.9435	H	-7.8669	-8.8757	2.0994	H	9.4942	6.276	1.3056
C	3.8853	-6.0834	-7.2423	C	-9.6268	-3.4039	6.2616	H	2.3097	4.3565	2.3878	H	9.1142	7.7968	1.3072
C	4.0042	-6.0503	-8.747	C	-10.1671	-2.7343	7.34	H	3.8117	4.0107	2.6616	H	10.3715	7.3667	-1.9694
C	-0.2262	-4.298	-7.719	C	-9.1954	-2.6447	8.3067	H	3.4321	5.3823	2.0063	H	8.0081	7.5248	-4.5796
C	-1.9779	-5.8133	-4.2326	C	-9.2966	-2.0182	9.6766	H	-10.6874	7.4098	-0.9153	H	8.4379	6.0181	-4.579
C	-2.6085	-5.9688	-5.5944	Co	-6.9387	-4.3553	5.3304	H	-9.7963	6.3438	-0.1854	H	9.5229	7.1445	-4.4725
C	-2.052	-5.7977	-6.8451	Co	-6.7055	-5.8796	2.2441	H	-9.4104	7.8619	-0.1246	H	11.1782	2.8434	-8.3305
C	-3.027	-6.0592	-7.7765	Co	-6.4642	6.584	-0.3094	H	-10.1524	7.4389	-3.5557	H	10.2872	3.9095	-9.0604
C	-2.913	-6.026	-9.2816	Co	-6.7305	6.4055	3.1257	H	-8.9307	7.2094	-5.8989	H	9.9012	2.3914	-9.1213
C	-0.6392	-3.4143	6.4335	Co	-5.1147	4.3838	-6.5893	H	-7.4148	7.579	-5.7716	H	10.6432	2.8145	-5.6901
C	0.1227	-1.6112	5.4279	Co	-5.3479	5.908	-3.5031	H	-7.8501	6.0754	-5.8379	H	8.341	4.178	-3.4079
C	-8.032	-7.1716	5.9113	Co	-5.5891	-6.5555	-0.9496	H	5.6269	-0.5837	-2.4472	H	9.4215	3.044	-3.347
C	-3.9117	-3.3344	3.7612	Co	-5.3229	-6.377	-4.3847	H	1.95	-1.5264	-1.287	H	7.9056	2.6744	-3.4742
C	9.5677	7.1031	0.8233	Co	6.2226	6.5394	0.6712	H	4.8551	-2.2176	-4.3516	H	10.1795	5.5351	4.7123
C	8.937	6.9475	-0.5385	Co	5.6055	5.8695	-2.6565	H	4.58	-3.6767	-4.8579	H	9.2885	6.601	3.9824
C	9.4935	7.1187	-1.7892	Co	5.8387	4.3453	-5.7427	H	6.0396	-3.2378	-4.4921	H	8.9026	5.0829	3.9215
C	8.5186	6.8572	-2.7206	Co	5.9564	6.3609	4.1064	H	4.6779	-3.5565	1.3263	H	9.6445	5.506	7.3527

H	7.3423	6.8695	9.6349	H	1.85	6.0448	7.9499	N	-7.2755	-3.9774	2.4164	N	-3.9746	3.2772	-9.0838
H	8.4228	5.7355	9.6958	H	0.5847	6.1966	7.0355	N	-0.541	2.2808	-8.6673	N	-8.1426	6.3206	4.5229
H	6.9069	5.3659	9.5686	H	1.5203	7.4298	7.2943	N	1.624	2.2731	-8.5	N	5.1574	-4.8479	-2.41
H	-10.9608	-6.7197	1.9795	H	7.2241	-7.7252	8.9632	N	4.6439	3.6747	-7.1836	N	4.8832	-4.9313	-1.0913
H	-10.0253	-5.4865	2.2384	H	7.6233	-6.255	8.6028	N	5.0878	3.2454	-8.3834	N	3.9947	0.5972	-2.2484
H	-9.6955	-6.8716	2.894	H	6.1267	-6.6073	8.9041	N	-1.5396	4.9723	4.3755	N	5.3163	3.3661	-4.0929
H	-10.4473	-7.8042	-0.4328	H	7.1431	10.7313	-0.0113	N	-4.716	6.3956	5.2129	N	5.0555	3.9714	-2.9154
H	-9.2359	-8.5598	-2.6681	H	7.4825	9.2702	-0.47	N	0.6253	4.9647	4.5428	N	4.4504	-6.3215	-5.1356
H	-7.7338	-8.9056	-2.3943	H	5.9872	9.7194	-0.3325	N	3.6452	6.3663	5.8592	N	7.4979	-5.9914	-4.0911
H	-8.1136	-7.5342	-3.0495	H	7.5083	10.9327	2.6507	N	4.0891	5.9369	4.6594	N	4.9916	-8.0741	-2.6362
H	-9.2239	-7.4167	-8.2171	H	6.4364	9.3943	5.6257	N	3.9535	-1.5298	-1.8126	N	6.2373	-6.906	4.9348
H	-8.7876	-6.0342	-8.8135	H	7.5749	10.4038	5.2489	N	-7.2279	-6.8588	3.894	N	6.3183	-6.302	6.1387
H	-10.1795	-6.1768	-8.1043	H	7.9165	8.8966	5.4985	N	7.3788	-6.6038	1.9842	N	-3.9108	-6.2921	-5.7818
H	-10.0352	-5.0947	-5.6412	H	-0.2788	-6.0643	1.6502	N	4.2029	-6.5877	2.617	N	-4.1615	-6.3833	-7.1046
H	-7.6477	-4.0111	-3.2855	H	0.7846	-9.3231	3.6513	N	6.5314	-4.0259	3.4837	N	0.4762	-2.7476	6.1229
H	-8.1332	-5.3796	-2.697	H	1.0927	-7.39	-0.1536	N	6.5278	8.1043	1.8594	N	3.4517	-3.63	7.9072
H	-9.1764	-4.3463	-3.2459	H	2.0927	-6.3307	-0.7373	N	6.5954	8.0196	3.2045	N	-1.6888	-2.74	5.9556
H	-8.8278	-7.6688	7.7225	H	2.4728	-7.8514	-0.739	N	0.7316	-7.5395	2.5996	N	-4.9095	-3.6005	7.2609
H	-9.1565	-6.196	7.3058	H	9.637	1.4718	1.8553	N	3.9522	-6.6789	1.2942	N	-5.1601	-3.6917	5.9382
H	-7.7265	-6.5586	7.8334	H	6.7318	2.1631	4.9199	N	-1.4334	-7.5318	2.4323	N	7.1365	6.2669	5.7039
H	-8.008	10.9872	1.4514	H	5.5474	3.1832	5.0603	N	-4.409	-6.6494	0.648	N	7.384	6.5332	-2.0486
H	-8.4769	10.4602	4.0082	H	7.0069	3.6221	5.4262	N	-4.8594	-6.5559	1.9165	N	7.6347	6.6243	-0.726
H	-8.8634	8.9555	4.2016	H	7.9691	2.4847	-0.2112	N	5.0592	-8.1589	-1.2911	N	0.1295	2.9065	-3.0036
H	-7.4169	9.443	4.555	H	8.3555	3.9893	-0.4046	N	7.1216	-7.0307	0.7303	N	-4.321	1.1958	5.2959
H	-5.4463	-0.5448	-3.303	H	6.909	3.502	-0.7581	N	7.9417	-6.4209	-5.2909	N	-0.4973	-3.8199	2.2323
H	-1.9516	0.8889	-2.0842	H	4.4438	-10.7858	0.5796	N	4.9008	-6.4151	-6.4041	N	8.4594	-0.3753	-1.4763
H	-5.4757	1.0763	-6.2639	H	5.5997	-9.7739	0.9008	N	6.9431	-3.7293	7.7519	N	-0.4776	-9.1358	-3.3517
H	-4.3557	0.2302	-5.562	H	4.1044	-9.3248	1.0383	N	6.4993	-3.2999	8.9517	N	-0.9021	-7.1932	6.552
H	-3.9657	1.3795	-6.5556	H	4.0786	-10.9872	-2.0824	N	6.2707	-3.4207	4.6612	N	3.2062	1.1704	5.8783
H	-4.9695	3.7006	-0.91	H	0.4088	-2.898	8.8988	N	3.9021	-3.7236	6.6387	N	-8.3951	-0.439	-2.7535
H	-3.4729	4.0529	-1.2113	H	1.2999	-3.9641	9.6287	N	7.5922	-0.6518	2.8167	N	0.5958	6.9505	-6.8774
H	-3.8721	2.5827	-0.8509	H	1.6857	-2.446	9.6895	N	7.6334	1.4752	2.3809	N	-0.5311	9.1752	3.1281
H	-1.998	-1.5125	-1.5921	H	2.1654	-3.0985	3.9152	N	6.4296	4.7933	2.9783	O	0.1593	1.8546	-3.6724
H	-4.063	-3.6463	-5.5259	H	3.6813	-2.729	4.0425	N	6.7037	4.8768	1.6596	O	0.015	2.8555	-1.7631
H	-5.5584	-3.197	-5.3884	H	3.246	-4.2326	3.9762	N	5.3497	6.8515	-4.3665	O	0.1602	4.0103	-3.5798
H	-4.4024	-2.1852	-5.0672	H	-1.7419	-0.9563	4.9039	N	5.2687	6.2474	-5.5705	O	-4.3892	0.922	4.0813
H	3.4123	7.5368	2.3589	H	-3.43	-2.428	9.2941	N	1.4747	-5.4392	-6.9199	O	-5.3647	1.3505	5.96
H	2.3691	8.5701	1.81	H	-2.0499	-2.8894	8.7088	N	-0.6901	-5.4315	-7.0872	O	-3.2095	1.2854	5.8536
H	3.8979	8.9053	1.7704	H	-3.05	-3.9488	9.2925	N	-7.4886	-6.2535	5.0715	O	-0.3681	-2.5983	2.3442
H	-4.5386	-9.2944	0.3703	H	-11.1782	-3.4852	4.9385	N	7.6848	3.669	-6.0704	O	-0.9869	-4.3376	1.1767
H	-4.8137	-10.7533	-0.136	H	-10.2226	-4.7251	4.8257	N	6.6861	6.3605	6.9724	O	-0.1316	-4.6021	3.1806
H	-5.9981	-9.7332	0.0045	H	-9.7863	-3.3427	4.2293	N	8.1352	3.5754	-7.3389	O	9.4332	0.4032	-1.4767
H	-4.0452	-10.9587	-2.7103	H	-11.0339	-2.403	7.4015	N	-7.4564	-6.9795	-0.3965	O	7.5654	-0.2545	-0.616
H	-4.6365	-9.4145	-5.814	H	-10.1751	-1.6547	9.7969	N	-8.336	-3.6756	6.571	O	8.3604	-1.2498	-2.3596
H	-3.5765	-10.4317	-5.2671	H	-8.6463	-1.3196	9.7573	N	-7.0801	-5.9403	-5.2179	O	-1.0267	-10.0304	-2.6792
H	-3.19	-8.927	-5.4605	H	-9.1318	-2.6881	10.3458	N	-8.0788	-3.2487	7.8249	O	-0.4386	-9.2271	-4.5945
H	-4.411	10.0558	-4.3994	N	-6.9374	8.1516	0.8187	N	-7.9003	-6.5501	0.8033	O	0.1336	-8.214	-2.7773
H	-5.6314	9.2178	-3.8783	N	-7.8918	6.4117	5.8456	N	-7.3374	-6.3672	-6.4718	O	-0.3656	-8.299	6.7609
H	-4.1865	8.9041	-3.3583	N	-7.0355	4.8406	1.9375	N	-7.2115	8.0681	2.1374	O	-0.563	-6.5154	5.5625
H	-3.6552	9.2039	-6.8413	N	-4.9733	5.9687	3.959	N	-7.6444	6.678	-1.9069	O	-1.8527	-6.8179	7.2663
H	3.3083	1.665	-10.655	N	-1.1332	7.9802	-0.7458	N	-4.5969	7.008	-0.8624	O	2.0229	1.2673	6.2584
H	4.8104	1.3192	-10.3811	N	-4.153	6.5786	-2.0622	N	-7.1032	4.9253	0.5925	O	3.4587	0.898	4.6879
H	4.4306	2.6908	-11.0365	N	1.0318	7.9726	-0.5785	N	-3.8558	0.6247	-2.8552	O	4.1364	1.3175	6.6953
H	-0.4679	6.6632	4.6761	N	4.2082	6.5492	-1.4159	N	-4.8589	3.4019	-4.8794	O	-9.3813	-1.184	-2.5898
H	-1.6668	2.9221	4.1093	N	4.4654	6.9762	-0.162	N	-4.7779	4.0059	-3.6754	O	-7.6403	-0.1846	-1.7946
H	-3.2657	6.0628	7.5545	N	-4.8255	6.8872	-5.1529	N	-3.8969	-1.5022	-2.4194	O	-8.1418	0.0197	-3.8849
H	-1.8739	6.2053	6.8454	N	-7.194	6.5843	-3.1754	N	-5.0179	-4.8121	-3.1965	O	1.5001	7.8003	-6.9955
H	-2.8295	7.4451	6.9581	N	-5.116	-8.1231	-2.0776	N	-4.9501	-4.8968	-1.8514	O	-0.1128	6.6576	-7.8604
H	-2.877	4.3747	1.987	N	-4.8418	-8.0396	-3.3963	N	-3.7173	3.7041	-7.8299	O	0.3048	6.5078	-5.7494
H	-4.4057	4.0396	2.0266	N	-8.1564	1.5307	1.1605	N	-6.8933	3.7202	-7.1972	O	0.1189	10.2164	2.9096
H	-3.9202	5.4081	1.4381	N	-8.1975	-0.5963	1.5963	N	-4.5647	6.282	-6.3304	O	-0.2814	8.1393	2.4812
H	0.7776	2.9135	4.2981	N	-7.1945	-3.3734	3.6204	N	-7.144	3.6291	-8.5199	O	-1.497	9.1986	3.9164

Coordinates of Optimized Structures of NH_3@**JCM-1** [H° = -556.686229]



Charge = 0; Multiplicity = 1;

C	-6.9832	9.8599	-1.0375	C	-8.1417	3.3629	-5.0201	C	-2.8282	6.8411	-2.1694	C	-7.2041	9.407	0.3846
C	-4.6789	-3.5588	-3.5836	C	-10.0755	5.8418	2.9737	C	-2.4555	7.5075	-1.0203	C	-3.5758	6.9	-8.5811
C	-4.3342	-2.8643	-2.4425	C	-9.4449	5.9973	4.3354	C	-3.5635	7.6045	-0.2144	C	-7.4617	0.5154	1.6816
C	-4.508	-3.7064	-1.3714	C	-10.0014	5.8262	5.5862	C	-3.6695	8.2309	1.1551	C	-9.3746	1.0481	0.7332
C	-4.2824	-3.4133	0.0924	C	-9.0264	6.0877	6.5176	C	0.615	9.2796	-0.4467	C	-7.3779	3.1337	3.7636
C	-9.0769	3.1502	-10.0691	C	-9.1404	6.0545	8.0227	C	2.2826	6.4519	-3.0434	C	-7.3745	3.5874	2.3247
C	-8.4462	3.3058	-8.7074	C	-0.0458	7.2041	-0.7609	C	2.9174	6.8209	-1.7253	C	-7.7192	2.8928	1.1836
C	-9.0027	3.1346	-7.4566	C	-0.7325	9.2843	-0.5508	C	2.3771	7.4905	-0.6469	C	-7.5454	3.7348	0.1124
C	-8.0277	3.3962	-6.5252	C	-2.001	6.4669	-3.3744	C	3.3488	7.5802	0.3198	C	-7.7709	3.4417	-1.3514

C	-9.4003	-0.2757	1.0044	C	9.5677	7.1031	0.8233	Co	-6.7055	-5.8796	2.2441	H	4.8551	-2.2176	-4.3516
C	-7.4593	-1.0746	4.6258	C	8.937	6.9475	-0.5385	Co	-6.4642	6.584	-0.3094	H	4.58	-3.6767	-4.8579
C	-7.4837	-2.0571	3.4812	C	9.4935	7.1187	-1.7892	Co	-6.7305	6.4055	3.1257	H	6.0396	-3.2378	-4.4921
C	-7.8111	-1.8549	2.1563	C	8.5186	6.8572	-2.7206	Co	-5.1147	4.3838	-6.5893	H	4.6779	-3.5565	1.3263
C	-7.6768	-3.056	1.5037	C	8.6326	6.8904	-4.2257	Co	-5.3479	5.908	-3.5031	H	3.6179	-2.5392	0.7795
C	-7.9025	-3.3537	0.0408	C	10.2798	3.0823	-8.573	Co	-5.5891	-6.5555	-0.9496	H	3.2314	-4.0439	0.9729
C	0.5366	3.0492	-8.4849	C	9.4485	3.2429	-7.3243	Co	-5.3229	-6.377	-4.3847	H	1.9964	0.875	-1.7791
C	-0.1242	0.9738	-8.7991	C	9.805	3.0685	-6.0029	Co	6.2226	6.5394	0.6712	H	4.6772	1.3491	-5.8875
C	-1.7918	3.8015	-6.2025	C	8.7003	3.3374	-5.2322	H	-7.1421	6.6365	6.2019	H	4.9018	0.1976	-4.8465
C	-2.4266	3.4325	-7.5205	C	8.5815	3.3041	-3.7275	H	5.8879	3.3343	-8.6858	H	6.1223	1.0356	-5.3676
C	-1.8863	2.7629	-8.599	C	9.2812	5.7738	4.4698	H	-5.2823	6.7798	5.7338	H	3.7164	2.556	-0.2644
C	-2.858	2.6732	-9.5656	C	8.4498	5.9344	5.7185	H	4.1274	6.7468	6.4611	H	3.3877	4.0288	-0.6811
C	-2.7568	2.0468	-10.9356	C	8.8064	5.7601	7.0399	H	7.4595	-6.8014	-5.8928	H	4.8177	3.6662	-0.1534
C	1.2234	0.9691	-8.695	C	7.7016	6.0289	7.8106	H	5.6948	-6.6454	-6.641	H	6.7404	-10.0778	4.2521
C	2.4918	3.7865	-5.8714	C	7.5828	5.9957	9.3153	H	5.6991	-3.3888	9.2541	H	7.1304	-8.9284	3.2585
C	3.319	3.4123	-7.0764	C	-10.0524	-6.4384	2.1155	H	5.8921	6.5908	7.2093	H	5.6205	-9.2315	3.5502
C	2.9462	2.7459	-8.2255	C	-9.2252	-6.8126	0.9105	H	7.6629	3.7062	-8.0456	H	7.1181	-9.23	6.7817
C	4.0543	2.6489	-9.0314	C	-9.598	-7.4789	-0.2386	H	-7.3352	-3.3429	8.2466	H	3.149	-6.0727	5.1472
C	-7.3511	-9.1562	2.8586	C	-8.4898	-7.576	-1.0445	H	-6.7711	-6.7513	-6.9927	H	3.5788	-7.5793	5.1478
C	2.3204	6.1038	5.9664	C	-8.3838	-8.2024	-2.414	H	-6.5677	3.7562	-9.1455	H	2.0641	-7.1991	5.0408
C	1.9476	5.4374	4.8173	C	-9.263	-6.4646	-8.0993	H	-4.7182	3.3715	-9.5055	H	-1.6598	-9.3145	3.4624
C	3.0557	5.3404	4.0114	C	-8.6282	-6.0955	-6.7812	H	-4.9112	-6.6081	-7.4609	H	-1.366	-7.3814	-0.3436
C	3.1617	4.714	2.6419	C	-9.1684	-5.426	-5.7027	H	3.9241	-3.7608	8.6139	H	-2.257	-6.3154	-1.0735
C	-9.7891	7.1711	-0.6728	C	-8.1967	-5.3362	-4.7361	H	-5.4857	-3.7276	7.8865	H	-2.643	-7.8334	-1.1344
C	-8.9577	7.0104	-1.9216	C	-8.298	-4.7098	-3.3662	H	-6.0553	9.7617	-1.2634	H	-3.1227	-7.1809	4.6399
C	-9.3143	7.1848	-3.2429	C	-8.4776	-6.8715	7.3222	H	-7.5148	9.3229	-1.6292	H	-4.6386	-7.5504	4.5127
C	-8.2095	6.916	-4.0137	C	-7.7152	10.1046	1.4597	H	-7.2397	10.7818	-1.1229	H	-4.2032	-6.0469	4.579
C	-8.0907	6.9491	-5.5183	C	-7.714	9.2619	2.5443	H	-5.1092	-3.5221	0.5698	H	9.737	-6.0994	-7.3816
C	4.7272	-0.5198	-2.2203	C	-8.1598	9.5574	3.9563	H	-3.9706	-2.5126	0.193	H	11.0022	-6.2512	-6.4671
C	2.6876	-1.0385	-1.5774	C	-4.5917	-0.4871	-2.9405	H	-3.6291	-4.0198	0.4427	H	10.0666	-7.4844	-6.7261
C	5.1116	-3.1397	-4.2661	C	-2.6531	0.3041	-2.2634	H	-10.0035	2.9179	-9.9677	H	10.4888	-5.1667	-4.0549
C	4.8907	-3.5924	-2.844	C	-4.5941	1.103	-5.8848	H	-9.0034	3.9772	-10.5514	H	7.7752	-4.0653	-2.0934
C	4.3796	-2.8949	-1.769	C	-4.5697	2.0856	-4.7401	H	-8.6234	2.4566	-10.5531	H	8.1549	-5.4368	-1.4381
C	4.3809	-3.7376	-0.6843	C	-4.2423	1.8833	-3.4152	H	-9.8807	2.8865	-7.2764	H	9.2772	-4.4111	-1.8196
C	3.9351	-3.4421	0.7276	C	-4.3765	3.0845	-2.7627	H	-9.0321	3.1088	-4.7733	H	10.0036	-3.5597	6.5757
C	2.7132	0.2852	-1.8486	C	-4.1508	3.3823	-1.2998	H	-7.5173	2.7286	-4.6663	H	9.068	-4.7929	6.3167
C	5.1931	1.0687	-5.1283	C	-2.6787	-1.0196	-1.9921	H	-7.9471	4.2352	-4.6669	H	8.7383	-3.4078	5.6611
C	4.9999	2.052	-4.0004	C	-4.6755	-3.1053	-5.0226	H	-10.0021	6.6688	2.4913	H	9.4901	-2.4752	8.9879
C	4.4715	1.8527	-2.7417	C	3.2476	8.2066	1.6897	H	-11.0021	5.6094	3.0751	H	8.2786	-1.7196	11.2232
C	4.5122	3.0532	-2.0756	C	-5.0702	-9.8314	-0.2215	H	-9.6221	5.1481	2.4897	H	7.1563	-2.7453	11.6047
C	4.0666	3.3534	-0.6647	C	-4.8493	-9.3785	-1.6436	H	-10.8794	5.5782	5.7663	H	6.7765	-1.3738	10.9494
C	6.5021	-9.2048	3.9294	C	-4.3381	-10.076	-2.7186	H	-8.5159	5.4201	8.3765	H	5.9601	0.5291	3.0155
C	6.5265	-8.2223	5.074	C	-4.3394	-9.2334	-3.8033	H	-10.0308	5.8004	8.2695	H	9.5905	-0.9296	2.3473
C	6.8539	-8.4246	6.3989	C	-3.8936	-9.5288	-5.2152	H	-8.9458	6.9268	8.3759	H	6.6852	-0.2522	5.4148
C	6.7195	-7.2235	7.0514	C	-4.7022	9.1846	-4.1175	H	-0.0399	6.2816	-0.8792	H	5.4646	-1.0902	5.9359
C	-7.5443	-8.1729	3.9864	C	-4.5091	8.2014	-5.2454	H	-1.2855	10.0314	-0.5012	H	6.9097	-1.4037	6.4558
C	2.0934	-7.1734	2.3575	C	-3.9807	8.4006	-6.5042	H	-2.0281	5.515	-3.4974	H	7.8705	-2.6106	0.8326
C	3.0685	-6.9118	3.2889	C	-4.0215	7.2001	-7.1702	H	-1.0926	6.7482	-3.2386	H	8.1993	-4.0834	1.2493
C	2.9544	-6.945	4.794	C	4.1604	2.0224	-10.4009	H	-2.3579	6.9002	-4.153	H	6.7692	-3.7208	0.7217
C	-1.0799	-8.6682	3.1273	C	-0.4621	5.7407	4.5579	H	-2.8175	8.5884	1.4091	H	-8.3982	-9.1755	5.5823
C	-2.2644	-7.1426	-0.5861	C	-1.1229	3.6653	4.2437	H	-4.3196	8.9342	1.1352	H	5.1507	-9.4489	-5.0574
C	-3.0957	-6.9819	0.6626	C	-2.7904	6.493	6.8402	H	-3.9399	7.5626	1.7906	H	3.6705	-8.9512	-4.9303
C	-2.7391	-7.1563	1.984	C	-3.4252	6.124	5.5223	H	1.159	10.0228	-0.3123	H	4.012	-10.4583	-4.6806
C	-3.8439	-6.8875	2.7547	C	-2.885	5.4544	4.4438	H	2.7579	6.8821	-3.7576	H	4.8465	10.0232	-3.6839
C	-3.9627	-6.9207	4.2594	C	-3.8567	5.3647	3.4772	H	1.366	6.7396	-3.0484	H	5.9664	9.177	-2.9818
C	10.0938	-6.5326	-6.6031	C	-3.7554	4.7383	2.1072	H	2.3216	5.4997	-3.1612	H	4.4565	8.8739	-2.6902
C	9.2665	-6.1583	-5.3981	C	0.2247	3.6606	4.3478	H	-3.2257	7.6973	-8.9815	H	4.4688	9.1754	-6.2134
C	9.6394	-5.492	-4.249	C	1.4931	6.478	7.1714	H	-4.3268	6.5871	-9.0924	H	4.3629	7.6706	-8.3949
C	8.5313	-5.395	-3.4431	C	6.9452	-6.9257	8.5143	H	-2.8969	6.2245	-8.5648	H	3.9636	6.2005	-8.0346
C	8.4252	-4.7685	-2.0736	C	6.8701	9.8112	0.0333	H	-6.6071	0.5731	2.0441	H	5.4602	6.5527	-8.3359
C	9.0951	-3.8411	6.4397	C	6.8666	9.3576	1.4722	H	-10.0554	1.541	0.3332	H	9.2653	-5.5543	3.7294
C	8.268	-3.4668	7.6447	C	7.2114	10.0521	2.6134	H	-7.9904	3.6748	4.267	H	10.2209	-6.7942	3.6167
C	8.6407	-2.8005	8.7938	C	7.0376	9.2101	3.6845	H	-7.6509	2.2136	3.8083	H	8.8291	-6.9367	4.3258
C	7.5327	-2.7035	9.5997	C	7.2632	9.5032	5.1483	H	-6.495	3.2255	4.1295	H	10.0766	-7.8764	1.1537
C	7.4266	-2.077	10.9692	C	-0.318	-6.8651	2.1216	H	-8.0827	2.5411	-1.4519	H	9.2178	-8.6247	-1.2417
C	6.8597	0.4651	2.7886	C	0.2677	-8.6729	3.2314	H	-8.4243	4.0483	-1.7016	H	7.6892	-8.9598	-1.2021
C	8.8738	-0.3398	2.4169	C	2.0193	-7.1577	-0.255	H	-6.9442	3.5506	-1.8287	H	8.1746	-7.5913	-1.7906
C	6.3938	-1.1233	5.6966	C	2.6499	-7.0021	1.1067	H	-10.1018	-0.8604	0.8253	H	0.3203	-6.9066	-6.1379
C	6.587	-2.1066	4.5688	C	8.8993	0.9839	2.1457	H	-7.6977	-0.2016	4.303	H	1.7013	-3.6565	-7.95
C	7.1155	-1.9073	3.31	C	6.4753	3.0851	4.8344	H	-6.5777	-1.0479	5.005	H	1.4074	-5.5896	-4.144
C	7.0747	-3.1078	2.6439	C	6.6962	3.5379	3.4123	H	-8.0877	-1.351	5.2967	H	2.2985	-6.6556	-3.4141
C	7.5204	-3.4079	1.233	C	7.2074	2.8403	2.3373	H	-8.1813	-2.5543	-0.408	H	2.6844	-5.1375	-3.3533
C	-8.0727	-8.3722	5.2452	C	7.2061	3.683	1.2525	H	-8.5806	-4.0245	-0.0476	H	3.1641	-5.79	-9.1276
C	4.3238	-9.5577	-4.58	C	7.6519	3.3875	-0.1593	H	-7.0839	-3.6721	-0.349	H	4.2446	-6.9241	-9.0666
C	5.0849	9.1502	-3.361	C	4.7169	-9.8658	0.5349	H	0.5307	3.9717	-8.3666	H	4.68	-5.4205	-9.0003
C	5.0605	8.1678	-4.5057	C	4.7203	-9.4122	-0.904	H	-0.6681	0.2306	-8.9335	H	-0.7433	-3.6479	-8.1389
C	4.7331	8.3701	-5.8307	C	4.3755	-10.1067	-2.0451	H	-2.2671	3.3712	-5.4883	H	-2.4313	-5.1195	-3.7487
C	4.8674	7.1689	-6.4831	C	4.5494	-9.2647	-3.1163	H	-0.8752	3.5137	-6.1974	H	-1.0513	-5.581	-4.334
C	4.6417	6.8711	-7.946	C	1.3071	-3.1368	9.1413	H	-1.8309	4.7536	-6.0847	H	-2.0513	-6.6403	-3.7503
C	9.3043	-6.5064	3.6116	C	2.1385	-3.2975	7.8925	H	-3.407	1.348	-11.0162	H	-2.0226	-5.7718	-9.5284
C	8.6695	-6.8755	2.2936	C	1.7819	-3.1231	6.5712	H	-1.8783	1.6832	-11.0558	H	-3.5375	-5.3916	-9.6355
C	9.2098	-7.5451	1.2151	C	2.8867	-3.3919	5.8005	H	-2.9216	2.7166	-11.6047	H	-3.1076	-6.8982	-9.6349
C	8.2381	-7.6347	0.2485	C	3.0055	-3.3588	4.2958	H	1.7763	0.222	-8.7447	H	-0.6784	-4.2151	6.9049
C	8.3394	-8.2612	-1.1215	C	-1.2249	-1.6065	5.3238	H	2.8487	3.3532	-5.0929	H	0.7026	-0.9649	5.0928
C	0.3594	-6.1059	-6.6092	C	-2.9764	-3.1217	8.8102	H	1.5834	3.5051	-6.0073	H	-4.1063	-4.2067	3.4079
C	1.1214	-4.3028	-7.6149	C	-3.6072	-3.2773	7.4484	H	2.5189	4.7383	-5.7485	H	-3.0213	-3.0803	3.5144
C	2.3058	-5.8283	-3.9015	C	-3.0507	-3.1061	6.1977	H	-7.6424	-10.0272	3.1404	H	-4.5361	-2.7001	3.4073
C	3.1371	-5.989	-5.1503	C	-4.0257	-3.3676	5.2662	H	-6.4219	-9.1892	2.6193	H	10.4943	7.3355	0.7219
C	2.7806	-5.8146	-6.4716	C	-10.2616	-3.7731	4.9435	H	-7.8669	-8.8757	2.0994	H	9.4942	6.276	1.3056
C	3.8853	-6.0834	-7.2423	C	-9.6268	-3.4039	6.2616	H	2.3097	4.3565	2.3878	H	9.1142	7.7968	1.3072
C	4.0042	-6.0503	-8.747	C	-10.1671	-2.7343	7.34	H	3.8117	4.0107	2.6616	H	10.3715	7.3667	-1.9694
C	-0.2262	-4.298	-7.719	C	-9.1954	-2.6447	8.3067	H	3.4321	5.3823	2.0063	H	8.0081	7.5248	-4.5796
C	-1.9779	-5.8133	-4.2326	C	-9.2966	-2.0182	9.6766	H	-10.6874	7.4098	-0.9153	H	8.4379	6.0181	-4.579
C	-2.6085	-5.9688	-5.5944	Co	-6.9387	-4.3553	5.3304	H	-9.7963	6.3438	-0.1854	H	9.5229	7.1445	-4.4725
C	-2.052	-5.7977	-6.8451	Co	5.6055	5.8695	-2.6565	H	-9.4104	7.8619	-0.1246	H	11.1782	2.8434	-8.3305
C	-3.027	-6.0592	-7.7765	Co	5.8387	4.3453	-5.7427	H	-10.1524	7.4389	-3.5557	H	10.2872	3.9095	-9.0604
C	-2.913	-6.026	-9.2816	Co	5.9564	6.3609	4.1064	H	-8.9307	7.2094	-5.8989	H	9.9012	2.3914	-9.1213
C	-0.6392	-3.4143	6.4335	Co	5.6305	-6.4155	-3.538	H	-7.4148	7.579	-5.7716	H	10.6432	2.8145	-5.6901
C	0.1227	-1.6112	5.4279	Co	5.3644	-6.5939	-0.1029	H	-7.8501	6.0754	-5.8379	H	8.341	4.178	-3.4079
C	-8.032	-7.1716	5.9113	Co	5.9814	-5.9241	3.2248	H	5.6269	-0.5837	-2.4472	H	9.4215	3.044	-3.347
C	-3.9117	-3.3344	3.7612	Co	5.7483	-4.3998	6.311	H	1.95	-1.5264	-1.287	H	7.9056	2.6744	-3.4742

H	10.1795	5.5351	4.7123	H	-3.9202	5.4081	1.4381	N	-5.1601	-3.6917	5.9382
H	9.2885	6.601	3.9824	H	0.7776	2.9135	4.2981	N	7.1365	6.2669	5.7039
H	8.9026	5.0829	3.9215	H	1.85	6.0448	7.9499	N	7.384	6.5332	-2.0486
H	9.6445	5.506	7.3527	H	0.5847	6.1966	7.0355	N	7.6347	6.6243	-0.726
H	7.3423	6.8695	9.6349	H	1.5203	7.4298	7.2943	N	-6.9374	8.1516	0.8187
H	8.4228	5.7355	9.6958	H	7.2241	-7.7252	8.9632	N	-7.8918	6.4117	5.8456
H	6.9069	5.3659	9.5686	H	7.6233	-6.255	8.6028	N	-7.0355	4.8406	1.9375
H	-10.9608	-6.7197	1.9795	H	6.1267	-6.6073	8.9041	N	-4.9733	5.9687	3.959
H	-10.0253	-5.4865	2.2384	H	7.1431	10.7313	-0.0113	N	-1.1332	7.9802	-0.7458
H	-9.6955	-6.8716	2.894	H	7.4825	9.2702	-0.47	N	-4.153	6.5786	-2.0622
H	-10.4473	-7.8042	-0.4328	H	5.9872	9.7194	-0.3325	N	1.0318	7.9726	-0.5785
H	-9.2359	-8.5598	-2.6681	H	7.5083	10.9327	2.6507	N	4.2082	6.5492	-1.4159
H	-7.7338	-8.9056	-2.3943	H	6.4364	9.3943	5.6257	N	4.4654	6.9762	-0.162
H	-8.1136	-7.5342	-3.0495	H	7.5749	10.4038	5.2489	N	-4.8255	6.8872	-5.1529
H	-9.2239	-7.4167	-8.2171	H	7.9165	8.8966	5.4985	N	-7.194	6.5843	-3.1754
H	-8.7876	-6.0342	-8.8135	H	-0.2788	-6.0643	1.6502	N	-5.116	-8.1231	-2.0776
H	-10.1795	-6.1768	-8.1043	H	0.7846	-9.3231	3.6513	N	-4.8418	-8.0396	-3.3963
H	-10.0352	-5.0947	-5.6412	H	1.0927	-7.39	-0.1536	N	-8.1564	1.5307	1.1605
H	-7.6477	-4.0111	-3.2855	H	2.0927	-6.3307	-0.7373	N	-8.1975	-0.5963	1.5963
H	-8.1332	-5.3796	-2.697	H	2.4728	-7.8514	-0.739	N	-7.1945	-3.3734	3.6204
H	-9.1764	-4.3463	-3.2459	H	9.637	1.4718	1.8553	N	-7.2755	-3.9774	2.4164
H	-8.8278	-7.6688	7.7225	H	6.7318	2.1631	4.9199	N	-0.541	2.2808	-8.6673
H	-9.1565	-6.196	7.3058	H	5.5474	3.1832	5.0603	N	1.624	2.2731	-8.5
H	-7.7265	-6.5586	7.8334	H	7.0069	3.6221	5.4262	N	4.6439	3.6747	-7.1836
H	-8.008	10.9872	1.4514	H	7.9691	2.4847	-0.2112	N	5.0878	3.2454	-8.3834
H	-8.4769	10.4602	4.0082	H	8.3555	3.9893	-0.4046	N	-1.5396	4.9723	4.3755
H	-8.8634	8.9555	4.2016	H	6.909	3.502	-0.7581	N	-4.716	6.3956	5.2129
H	-7.4169	9.443	4.555	H	4.4438	-10.7858	0.5796	N	0.6253	4.9647	4.5428
H	-5.4463	-0.5448	-3.303	H	5.5997	-9.7739	0.9008	N	3.6452	6.3663	5.8592
H	-1.9516	0.8889	-2.0842	H	4.1044	-9.3248	1.0383	N	4.0891	5.9369	4.6594
H	-5.4757	1.0763	-6.2639	H	4.0786	-10.9872	-2.0824	N	3.9535	-1.5298	-1.8126
H	-4.3557	0.2302	-5.562	H	0.4088	-2.898	8.8988	N	-7.2279	-6.8588	3.894
H	-3.9657	1.3795	-6.5556	H	1.2999	-3.9641	9.6287	N	7.3788	-6.6038	1.9842
H	-4.9695	3.7006	-0.91	H	1.6857	-2.446	9.6895	N	4.2029	-6.5877	2.617
H	-3.4729	4.0529	-1.2113	H	2.1654	-3.0985	3.9152	N	6.5314	-4.0259	3.4837
H	-3.8721	2.5827	-0.8509	H	3.6813	-2.729	4.0425	N	6.5278	8.1043	1.8594
H	-1.998	-1.5125	-1.5921	H	3.246	-4.2326	3.9762	N	6.5954	8.0196	3.2045
H	-4.063	-3.6463	-5.5259	H	-1.7419	-0.9563	4.9039	N	0.7316	-7.5395	2.5996
H	-5.5584	-3.197	-5.3884	H	-3.43	-2.428	9.2941	N	3.9522	-6.6789	1.2942
H	-4.4024	-2.1852	-5.0672	H	-2.0499	-2.8894	8.7088	N	-1.4334	-7.5318	2.4323
H	3.4123	7.5368	2.3589	H	-3.05	-3.9488	9.2925	N	-4.409	-6.6494	0.648
H	2.3691	8.5701	1.81	H	-11.1782	-3.4852	4.9385	N	-4.8594	-6.5559	1.9165
H	3.8979	8.9053	1.7704	H	-10.2226	-4.7251	4.8257	N	5.0592	-8.1589	-1.2911
H	-4.5386	-9.2944	0.3703	H	-9.7863	-3.3427	4.2293	N	7.1216	-7.0307	0.7303
H	-4.8137	-10.7533	-0.136	H	-11.0339	-2.403	7.4015	N	7.9417	-6.4209	-5.2909
H	-5.9981	-9.7332	0.0045	H	-10.1751	-1.6547	9.7969	N	4.9008	-6.4151	-6.4041
H	-4.0452	-10.9587	-2.7103	H	-8.6463	-1.3196	9.7573	N	6.9431	-3.7293	7.7519
H	-4.6365	-9.4145	-5.814	H	-9.1318	-2.6881	10.3458	N	6.4993	-3.2999	8.9517
H	-3.5765	-10.4317	-5.2671	H	-0.3407	-4.4556	-1.625	N	6.2707	-3.4207	4.6612
H	-3.19	-8.927	-5.4605	H	-0.6176	-4.2248	-0.0277	N	3.9021	-3.7236	6.6387
H	-4.411	10.0558	-4.3994	H	0.8073	-3.8129	-0.6793	N	7.5922	-0.6518	2.8167
H	-5.6314	9.2178	-3.8783	N	5.3163	3.3661	-4.0929	N	7.6334	1.4752	2.3809
H	-4.1865	8.9041	-3.3583	N	5.0555	3.9714	-2.9154	N	6.4296	4.7933	2.9783
H	-3.6552	9.2039	-6.8413	N	4.4504	-6.3215	-5.1356	N	0.1291	2.9336	-3.0105
H	3.3083	1.665	-10.655	N	7.4979	-5.9914	-4.0911	N	6.7037	4.8768	1.6596
H	4.8104	1.3192	-10.3811	N	4.9916	-8.0741	-2.6362	N	-4.322	1.1897	5.2679
H	4.4306	2.6908	-11.0365	N	6.2373	-6.906	4.9348	N	-0.5276	-3.9186	2.5338
H	-0.4679	6.6632	4.6761	N	6.3183	-6.302	6.1387	N	8.4452	-0.3881	-1.4516
H	-1.6668	2.9221	4.1093	N	-3.9108	-6.2921	-5.7818	N	5.3497	6.8515	-4.3665
H	-3.2657	6.0628	7.5545	N	-4.1615	-6.3833	-7.1046	N	-0.4688	-9.0866	-3.3226
H	-1.8739	6.2053	6.8454	N	0.4762	-2.7476	6.1229	N	-1.073	-7.2514	6.6015
H	-2.8295	7.4451	6.9581	N	3.4517	-3.63	7.9072	N	5.2687	6.2474	-5.5705
H	-2.877	4.3747	1.987	N	-1.6888	-2.74	5.9556	N	3.2108	1.1633	5.8499
H	-4.4057	4.0396	2.0266	N	-4.9095	-3.6005	7.2609	N	-8.3844	-0.4177	-2.7343

N	0.7388	6.6367	-6.9091								
N	1.4747	-5.4392	-6.9199								
N	-0.5225	9.1736	3.1211								
N	0.0869	-4.5322	-0.7039								
N	-0.6901	-5.4315	-7.0872								
N	-7.4886	-6.2535	5.0715								
N	7.6848	3.669	-6.0704								
N	6.6861	6.3605	6.9724								
N	8.1352	3.5754	-7.3389								
N	-7.4564	-6.9795	-0.3965								
N	-8.336	-3.6756	6.571								
N	-7.0801	-5.9403	-5.2179								
N	-8.0788	-3.2487	7.8249								
N	-7.9003	-6.5501	0.8033								
N	-7.3374	-6.3672	-6.4718								
N	-7.2115	8.0681	2.1374								
N	-7.6444	6.678	-1.9069								
N	-4.5969	7.008	-0.8624								
N	-7.1032	4.9253	0.5925								
N	-3.8558	0.6247	-2.8552								
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N	-4.7779	4.0059	-3.6754								
N	-3.8969	-1.5022	-2.4194								
N	-5.0179	-4.8121	-3.1965								
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N	-3.7173	3.7041	-7.8299								
N	-6.8933	3.7202	-7.1972								
N	-4.5647	6.282	-6.3304								
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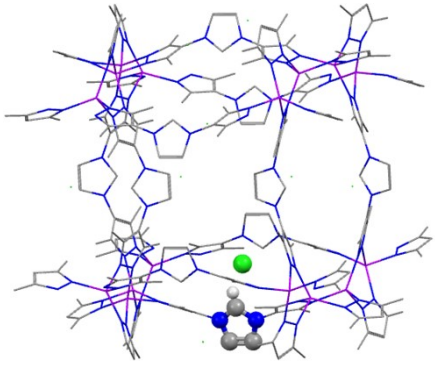
N	-8.1426	6.3206	4.5229								
N	5.1574	-4.8479	-2.41								
N	4.8832	-4.9313	-1.0913								
N	3.9947	0.5972	-2.2484								
O	0.1585	1.9152	-3.6544								
O	0.019	2.887	-1.8112								
O	0.1596	3.9995	-3.57								
O	-4.3946	0.9259	4.094								
O	-5.3272	1.3405	5.9152								
O	-3.2446	1.2753	5.801								
O	-0.1269	-2.7563	2.4015								
O	-1.4672	-4.3735	1.7949								
O	-0.0024	-4.7071	3.3837								
O	9.3756	0.3775	-1.4784								
O	7.5785	-0.2539	-0.6251								
O	8.3566	-1.2574	-2.2816								
O	-1.0156	-9.9382	-2.6684								
O	-0.4398	-9.1767	-4.524								
O	0.1302	-8.198	-2.772								
O	-0.855	-8.4316	6.7111								
O	-0.5401	-6.6228	5.7225								
O	-1.9276	-6.7339	7.2757								
O	2.065	1.2567	6.2112								
O	3.461	0.8996	4.7007								
O	4.1058	1.3074	6.644								
O	-9.3234	-1.1598	-2.5932								
O	-7.6523	-0.1894	-1.8047								
O	-8.1493	0.057	-3.8168								
O	1.4076	7.6361	-7.0007								
O	-0.1901	6.7704	-7.6666								
O	0.2786	6.6293	-5.7946								
O	0.1103	10.1773	2.9102								
O	-0.2837	8.1704	2.4977								
O	-1.4549	9.1996	3.8844								

Coordinates of Optimized Structures of **JCM-1(Cl$^-$)** [H° = -680.321789]



Charge = 0; Multiplicity = 1;

C	-1.7404	-3.9754	-8.7289	C	0.1631	-0.523	-3.2574	C	-6.0916	3.5992	0.2972	C	-11.7762	-5.5061	-0.4226
C	1.2073	-4.4233	-12.8488	C	1.2857	-1.7166	-7.0769	C	-4.634	3.9507	3.5165	C	-8.8285	-5.9539	-4.5425
C	7.4407	-8.2725	0.316	C	-0.8806	8.0713	10.0651	C	-4.9684	3.4109	-0.6318	C	-0.605	-4.0787	-11.0191
C	6.7363	-7.9405	1.446	C	-6.2802	-10.0771	-3.4462	C	-4.3134	2.0135	2.5449	C	0.6674	-4.3552	-11.453
C	8.0102	-7.1357	-0.1784	C	-5.1243	-9.4614	-3.8561	C	-7.9161	3.8587	3.4881	C	-0.6171	-4.1638	-9.6579
C	8.8732	-6.9699	-1.3563	C	-7.0595	-9.146	-2.8244	C	5.0006	0.7364	1.8177	Cl	-0.7784	-5.0081	1.2064
C	5.956	-8.8169	2.3774	C	-8.3779	-9.3129	-2.1968	C	-3.0899	3.8556	5.363	Cl	6.9951	0.9475	5.0543
C	4.9257	10.1193	0.6665	C	-3.932	-10.0369	-4.5573	C	-3.8012	4.1957	6.4863	Cl	-2.4512	-8.6457	2.902
C	4.342	9.5684	1.7797	C	2.0366	9.9183	6.3314	C	-1.7689	4.0891	5.6103	Cl	4.8989	-7.5511	-3.1789
C	5.7768	9.1963	0.1329	C	-8.7952	8.3147	-3.0957	C	-0.614	3.9043	4.7202	Cl	0.8317	0.1268	3.6408
C	6.6467	9.3124	-1.046	C	-7.5185	8.0475	-3.5224	C	-3.4471	2.1116	3.6097	Cl	1.4439	3.8888	-1.4227
C	3.3599	10.1678	2.7392	C	-9.2929	7.186	-2.513	C	-5.279	4.1575	6.7293	Cl	-3.4495	-0.2361	-7.7835
C	3.486	-1.9871	7.053	C	-10.6045	6.9694	-1.8865	C	3.9321	5.0447	-6.6477	Cl	-4.706	7.7436	3.2254
C	2.33	-2.6028	7.4628	C	-6.5281	8.9478	-4.1955	C	3.3459	-2.9995	2.7746	Cl	2.6522	8.8638	-2.8645
C	4.2653	-2.9182	6.4311	C	-0.1056	4.1408	11.8127	C	2.6597	5.3213	-6.214	Cl	-3.2777	-0.3388	-1.4101
C	2.9919	0.365	6.8911	C	0.4826	4.7011	10.7065	C	3.9442	5.1299	-8.0091	Co	1.2409	-5.3401	7.7074
C	5.5837	-2.7512	5.8036	C	-1.442	4.0203	11.5675	C	5.4019	5.4814	-4.7898	Co	1.4171	-5.0251	-7.557
C	4.8174	-0.1013	8.0089	C	-2.5004	3.4991	12.4441	C	5.0675	4.9415	-8.9381	Co	-2.6736	6.1595	-5.26
C	1.1378	-2.0273	8.1642	C	1.9151	5.07	10.4698	C	5.7224	3.5441	-5.7613	Co	-0.0456	5.6712	-7.3531
C	2.8374	2.7557	7.1435	C	9.9303	5.6715	3.5064	C	2.1198	5.3894	-4.8182	Co	-8.1259	4.4605	-1.8037
C	1.5607	3.0228	7.57	C	10.5185	6.2318	2.4002	C	6.946	5.3863	-2.9433	Co	-5.736	5.7141	-3.8636
C	3.3351	3.8843	6.5608	C	8.5938	5.5509	3.2612	C	3.3616	-0.1606	0.6739	Co	-0.2218	5.3562	7.9113
C	4.6467	4.1009	5.9342	C	7.5355	5.0298	4.1379	C	6.2346	5.7264	-1.82	Co	2.1681	6.6098	5.8514
C	4.631	1.262	8.0349	C	11.951	6.6007	2.1635	C	8.267	5.6198	-2.6959	Co	5.8245	-5.5084	2.8575
C	0.5703	2.1226	8.2432	C	-11.793	2.8164	-2.5524	C	9.4218	5.435	-3.5861	Co	8.2143	-4.2548	0.7975
C	7.8466	-6.4549	6.3197	C	-10.6438	3.4403	-2.969	C	6.5888	3.6423	-4.6965	Co	4.1236	6.9298	3.0945
C	6.5742	-6.1783	6.7536	C	-11.8206	2.8441	-1.1889	C	4.7569	5.6882	-1.5769	Co	6.7516	6.4415	1.0014
C	7.8587	-6.3697	4.9584	C	-12.8473	2.3266	-0.2733	C	5.8352	8.254	6.6	Co	-4.0352	-6.7241	-4.1007
C	8.982	-6.5581	4.0295	C	-10.1491	3.7029	-4.3584	C	4.686	7.6301	7.0166	Co	-0.9727	-6.2787	-5.497
C	6.0343	-6.1103	8.1492	C	-1.7571	4.347	-10.8587	C	5.8628	8.2262	5.2365	Co	3.8689	-5.8284	5.6143
C	-3.8408	-7.7793	-8.0454	C	-0.6079	4.9709	-11.2753	C	7.4223	-1.0212	0.4656	Co	-6.6632	-6.2358	-2.0075
C	-4.5522	-7.4392	-6.922	C	-1.7847	4.3748	-9.495	C	6.8895	8.7437	4.3211	H	-1.4684	-3.7617	-11.6764
C	-2.5198	-7.5458	-7.798	C	-2.8115	3.8573	-8.5796	C	4.1913	7.3675	8.4062	H	4.1756	-9.6693	5.3787
C	-1.3649	-7.7306	-8.6881	C	-0.1132	5.2335	-12.6647	C	-5.8522	6.9296	-7.765	H	0.5205	-7.7491	9.5902
C	-6.0299	-7.4774	-6.679	C	-2.8679	7.2147	-1.3153	C	-6.4404	6.3692	-6.6589	H	1.4314	10.3981	5.7611
C	-1.9377	-4.5701	5.2025	C	-2.1566	6.8746	-2.4386	C	-4.5158	7.0501	-7.5198	H	-1.5526	7.4113	9.8792
C	-2.5259	-5.1304	6.3086	C	-4.1889	6.9813	-1.5627	C	-3.4574	7.5712	-8.3965	H	5.7905	0.8352	2.2985
C	-0.6013	-4.4495	5.4477	C	-1.3238	7.1196	0.5312	C	-7.8729	6.0003	-6.422	H	2.8253	-0.7894	0.2472
C	-3.409	-5.0069	3.3458	C	-5.3438	7.1661	-0.6726	C	4.5066	3.0885	1.6558	H	7.8092	-0.4289	1.1147
C	0.4571	-3.9284	4.5709	C	-2.5107	8.9587	0.438	C	5.6625	3.7042	1.246	H	3.4469	-3.572	3.5388
C	-2.7588	-2.9216	3.5138	C	-0.6788	6.9128	-2.6817	C	3.0668	-9.0178	8.0423	H	2.4876	1.68	0.2943
C	-3.9584	-5.4993	6.5453	C	0.146	7.5563	2.3891	C	3.7273	4.0196	2.2777	H	7.3897	2.6382	1.1732
C	-4.9516	-4.9116	1.498	C	1.4183	7.2797	1.9553	C	2.4088	3.8527	2.9052	H	2.3564	4.4022	3.6908
C	-6.1008	-5.5355	1.9146	C	0.1338	7.4711	3.7505	C	3.1751	1.2027	0.6998	H	0.7344	-6.1529	0.0804
C	-4.924	-4.9394	0.1345	C	-0.9894	7.6595	4.6794	C	6.8548	3.1287	0.5447	H	1.1156	-9.7354	1.7115
C	-3.8973	-4.4218	-0.781	C	-1.6444	9.0569	1.5027	C	3.6506	-8.467	6.9291	H	3.3154	-5.5298	-0.0761
C	-3.6251	-3.0198	2.449	C	1.9583	7.2117	0.5596	C	2.1574	-7.1526	2.1089	H	1.0142	-7.0489	5.1373
C	-6.5955	-5.7981	3.304	C	-6.5096	1.6965	-4.3451	C	3.3066	-6.5287	1.6922	H	-0.4536	-9.9132	-0.2173
C	8.0982	-3.0394	-3.1038	C	-7.2141	2.0284	-3.2151	C	2.1298	-7.1248	3.4723	H	1.3664	-5.7507	-2.4718
C	7.5099	-3.5997	-1.9977	C	-5.9402	2.8332	-4.8395	C	0.6148	-7.0573	0.2611	H	-4.0531	-7.6232	-1.091
C	9.4346	-2.9188	-2.8586	C	-6.0171	-0.6559	-4.1818	C	1.103	-7.6423	4.3878	H	3.6513	-5.3338	10.7228
C	6.6268	-3.4762	-4.9605	C	-5.0771	2.999	-6.0175	C	0.8309	-9.0444	1.1577	H	-2.0647	-5.0374	12.1448
C	10.4929	-2.3977	-3.7353	C	-6.8718	-0.0415	-6.1033	C	3.8013	-6.2661	0.3027	H	13.6872	-3.8031	2.4165
C	7.277	-1.3909	-4.7925	C	-7.9944	1.152	-2.2838	C	2.2157	-8.0949	8.5759	H	7.9711	-3.5067	3.8386
C	6.0774	-3.9686	-1.761	C	5.1551	-1.6543	1.5654	C	-0.8565	-7.4941	-1.5955	H	-9.1009	-6.7789	-4.9511
C	0.5518	9.3739	8.3928	C	-5.861	-3.0463	-4.4355	C	-0.2683	-6.9338	-2.7018	H	-11.6987	-6.1292	0.3037
C	5.0843	-3.3809	-6.8083	C	-6.4448	-3.5972	-3.3224	C	-2.193	-7.6147	-1.8409	H	0.9349	-5.2482	-13.2574
C	3.935	-4.0048	-6.3917	C	-5.01	-3.9693	-4.9692	C	-3.2513	-8.1358	-0.9642	H	-1.6628	-4.5985	-8.0026
C	5.1118	-3.4087	-8.1718	C	-4.1401	-3.8532	-6.1481	C	-0.0354	-9.1426	0.093	H	6.5611	-9.2967	2.9477
C	6.1386	-2.8912	-9.0873	C	-6.6854	-1.4048	-6.1292	C	1.1642	-6.5649	-2.9385	H	9.5452	-6.3099	-1.1703
C	6.4107	-1.4891	-5.8573	C	-7.4269	-2.9978	-2.3628	C	1.3459	-8.211	9.7548	H	-12.59	1.4554	0.0373
C	3.4403	-4.2674	-5.0022	C	6.4318	-1.9214	1.1388	C	1.0466	-4.2849	11.6521	H	3.817	10.7707	3.3301
C	1.2563	9.0419	7.2628	C	2.0865	-8.8792	-6.2649	C	1.7579	-4.625	10.5288	H	7.4721	8.8505	-0.8814
C	-0.8477	2.4818	-4.9252	C	0.8098	-8.6121	-5.8383	C	-0.2744	-4.5183	11.4047	H	-2.6713	2.5795	12.2284
C	-0.2639	3.0326	-6.0383	C	2.5841	-7.7506	-6.8476	C	-1.4293	-4.3336	12.2949	H	2.202	0.2662	6.4103
C	-1.6988	3.4047	-4.3915	C	3.8958	-7.534	-7.4741	C	3.2357	-4.5868	10.2857	H	5.505	-0.5786	8.4146
C	-0.6917	0.0913	-5.1787	C	-0.1806	-9.5124	-5.1652	C	4.6327	-9.0664	5.9696	H	0.6028	-1.5368	7.5356
C	-2.5686	3.2886	-3.2126	C	-0.4285	9.5125	-5.9143	C	11.0824	-2.7542	3.3458	H	5.6361	-3.3008	5.018
C	-0.0233	0.8402	-3.2313	C	-1.5845	8.8968	-5.5046	C	11.7938	-3.0943	2.2225	H	5.1673	1.8908	8.4616
C	0.7182	2.4333	-6.9977	C	0.3508	8.5815	-6.5363	C	9.7614	-2.9877	3.0985	H	0.1834	1.5303	7.5941
C	-0.0176	8.2371	8.8872	C	1.6692	8.7484	-7.1639	C	8.6066	-2.8029	3.9886	H	4.5457	4.6734	5.1701
C	-0.1991	-2.261	-5.0156	C	4.6575	-2.7829	2.148	C	13.2715	-3.0561	1.9794	H	6.3067	-5.2853	8.5579
C	0.5053	-2.593	-6.1455	C	-2.7767	9.4723	-4.8034	C	-10.6408	-5.6093	-2.7128	H	8.9045	-5.935	3.3031
C	-0.7685	-3.3978	-4.5211	C	-6.1038	3.5141	1.6586	C	-9.3684	-5.8859	-3.1467	H	-6.4455	-6.7304	-7.116
C	-1.6316	-3.5636	-3.3432	C	-7.3761	3.7906	2.0923	C	-10.6529	-5.6945	-1.3516	H	-0.7295	-7.0268	-8.538

H	-3.5286	-5.9113	3.5264	H	-3.4218	-9.0554	-1.1803	H	-9.2138	3.9175	-4.33
H	-2.3406	-2.151	3.8242	H	-2.9703	-8.069	-0.0487	H	-2.5537	2.9861	-8.2694
H	-4.1606	-6.3135	6.0785	H	1.7332	-7.268	-2.6166	H	-3.6509	3.7971	-9.0413
H	1.2589	-4.441	4.6978	H	1.3112	-6.4396	-3.8789	H	-0.2456	4.4509	-13.2049
H	-3.9098	-2.3288	1.8954	H	-1.8415	-3.486	12.1124	H	0.8221	5.4482	-12.6361
H	-6.1096	-6.5344	3.6829	H	-1.136	-4.3567	13.2086	H	-5.756	8.0136	-0.8549
H	-3.8085	-5.0152	-1.5305	H	3.5967	-3.7693	10.6367	H	-5.0505	7.1429	0.2412
H	6.5073	-4.3807	-4.7799	H	3.4061	-4.6328	9.3421	H	-0.3178	7.7303	-2.3308
H	7.6952	-0.6203	-4.4821	H	8.1944	-1.9553	3.8061	H	-0.5084	6.8668	-3.6253
H	5.8753	-4.7828	-2.2278	H	8.8999	-2.826	4.9023	H	-0.9733	8.5556	5.0234
H	11.2947	-2.9103	-3.6085	H	13.6326	-2.2387	2.3304	H	-1.8166	7.5094	4.216
H	6.126	-0.7981	-6.4109	H	13.442	-3.1021	1.0358	H	1.6179	7.9496	0.0484
H	3.9262	-5.0037	-4.6233	H	-11.7601	-4.61	-0.0787	H	2.917	7.255	0.5849
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H	-1.005	0.0652	-6.0539	H	-9.1689	-5.2159	-5.0535	H	-4.6549	2.1623	-6.2252
H	0.1863	1.4192	-2.5343	H	-7.8698	-5.9106	-4.5173	H	-8.5164	0.528	-2.7935
H	0.2611	1.8303	-7.5888	H	-1.7242	-3.0793	-8.3849	H	-8.5776	1.6941	-1.7474
H	-3.394	3.7505	-3.3771	H	-2.5675	-4.1255	-9.1924	H	-4.5783	-4.242	-6.9086
H	0.5239	-1.0502	-2.5814	H	0.867	-3.6853	-13.3598	H	-3.959	-2.9266	-6.3222
H	0.6805	-1.2368	-7.6472	H	2.166	-4.38	-12.8235	H	-8.0998	-2.5182	-2.8516
H	-2.3036	-4.2236	-3.5292	H	8.3429	-6.6848	-2.104	H	-7.8405	-3.6962	-1.8502
H	-3.397	-10.5274	-3.9289	H	9.2955	-7.8067	-1.5641	H	4.4885	-7.1216	-6.8415
H	-8.4303	-8.7634	-1.4112	H	5.434	-9.441	1.8676	H	4.2609	-8.3772	-7.7522
H	-6.1412	9.54	-3.5464	H	5.3727	-8.2749	2.9137	H	0.2637	-10.0269	-4.4872
H	-10.5035	6.397	-1.1224	H	-12.9525	3.0204	0.6022	H	-0.8728	-8.9826	-4.7627
H	2.1173	5.8842	10.9365	H	6.2085	8.9236	-1.8065	H	2.3541	8.4868	-6.544
H	12.1531	7.4149	2.6303	H	6.8278	10.239	-1.2202	H	1.7932	9.6684	-7.4082
H	6.7337	5.5424	4.0111	H	2.687	10.6474	2.2505	H	-2.4834	10.0615	-4.1044
H	-10.6349	4.4391	-4.7373	H	2.9463	9.4694	3.2519	H	-3.2992	8.7616	-4.4245
H	-0.5991	5.9698	-13.0436	H	-3.4373	4.0987	12.2973	H	-4.9845	2.5147	-0.9757
H	-2.9003	4.4507	-7.8302	H	6.2686	-3.0128	6.4234	H	-4.1412	3.561	-0.1683
H	-0.9669	6.2879	0.3174	H	5.7077	-1.8312	5.5592	H	-7.5757	3.1207	3.9992
H	-3.1219	9.5999	0.1545	H	1.4311	-1.4381	8.8631	H	-8.8748	3.8154	3.4629
H	-0.2632	6.1659	-2.2447	H	0.6153	-2.738	8.5429	H	-0.2018	3.0567	4.9027
H	-5.9792	6.4622	-0.8225	H	5.2394	4.5134	6.5668	H	-0.9073	3.9274	3.8064
H	-1.5527	9.7777	2.0833	H	5.0118	3.2577	5.6562	H	-5.64	3.3401	6.3784
H	1.6859	6.3867	0.1509	H	1.0146	1.608	8.9211	H	-5.4494	4.2036	7.673
H	-0.9119	7.0364	5.4057	H	-0.1218	2.6523	8.6456	H	5.0514	4.0454	-9.282
H	-5.7037	-0.6297	-3.3067	H	8.9659	-7.4542	3.6854	H	5.8947	5.0916	-8.4746
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H	-7.3892	0.6722	-1.7135	H	6.3747	-6.8482	8.6604	H	1.1611	5.3461	-4.8434
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H	5.6308	2.8233	-6.3419	H	5.9304	-4.0939	-0.8206	H	7.5166	-9.1244	-0.0492
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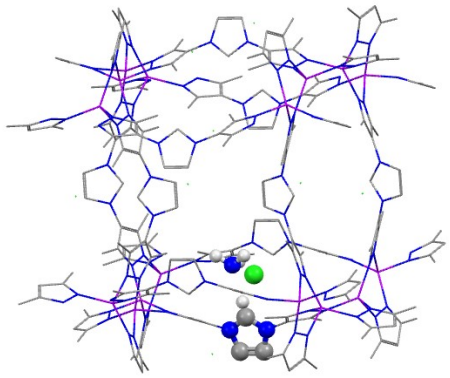
N	4.7421	7.5882	4.8482								
N	5.5835	4.9832	1.6013								
N	4.4166	5.1759	2.2403								
N	4.1933	1.71	1.4345								
N	3.968	-6.1395	2.7782								
N	6.8657	-6.6297	1.6288								
N	6.606	-6.0419	4.5885								
N	3.2505	-6.4868	3.8606								
N	1.1859	-7.7401	1.2378								
N	-1.224	-6.7279	-3.6033								
N	-2.396	-7.1267	-3.0795								
N	-0.1569	-7.8922	-0.4127								
N	5.8271	-5.9406	5.6794								
N	3.576	-4.0745	6.4685								
N	-0.3454	-4.9962	10.1476								
N	-1.5702	-5.3363	7.21								
N	9.6905	-3.4655	1.8414								
N	8.4656	-3.8056	-1.0962								
N	7.6498	-6.1395	0.6531								
N	-8.6213	-6.1236	-2.0726								
N	-9.4002	-6.0223	-0.9817								
N	1.4145	-4.5929	-10.3789								
N	0.6357	-4.4917	-9.288								

Coordinates of Optimized Structures of NH_3@**JCM-1(Cl$^-$)** [H° = -736.860321]



Charge = 0; Multiplicity = 1;

C	-1.7404	-3.9754	-8.7289	C	0.1631	-0.523	-3.2574	C	-6.0916	3.5992	0.2972	C	-11.7762	-5.5061	-0.4226
C	1.2073	-4.4233	-12.8488	C	1.2857	-1.7166	-7.0769	C	-4.634	3.9507	3.5165	C	-8.8285	-5.9539	-4.5425
C	7.4407	-8.2725	0.316	C	-0.8806	8.0713	10.0651	C	-4.9684	3.4109	-0.6318	C	-0.605	-4.0787	-11.0191
C	6.7363	-7.9405	1.446	C	-6.2802	-10.0771	-3.4462	C	-4.3134	2.0135	2.5449	C	0.6674	-4.3552	-11.453
C	8.0102	-7.1357	-0.1784	C	-5.1243	-9.4614	-3.8561	C	-7.9161	3.8587	3.4881	C	-0.6171	-4.1638	-9.6579
C	8.8732	-6.9699	-1.3563	C	-7.0595	-9.146	-2.8244	C	5.0006	0.7364	1.8177	Cl	-0.9435	-5.2168	1.3602
C	5.956	-8.8169	2.3774	C	-8.3779	-9.3129	-2.1968	C	-3.0899	3.8556	5.363	Cl	6.9889	0.9465	5.0561
C	4.9257	10.1193	0.6665	C	-3.932	-10.0369	-4.5573	C	-3.8012	4.1957	6.4863	Cl	-2.4495	-8.6448	2.9005
C	4.342	9.5684	1.7797	C	2.0366	9.9183	6.3314	C	-1.7689	4.0891	5.6103	Cl	4.8965	-7.5481	-3.1772
C	5.7768	9.1963	0.1329	C	-8.7952	8.3147	-3.0957	C	-0.614	3.9043	4.7202	Cl	0.8411	0.1177	3.6277
C	6.6467	9.3124	-1.046	C	-7.5185	8.0475	-3.5224	C	-3.4471	2.1116	3.6097	Cl	1.4443	3.8884	-1.4231
C	3.3599	10.1678	2.7392	C	-9.2929	7.186	-2.513	C	-5.279	4.1575	6.7293	Cl	-3.4525	-0.2368	-7.7776
C	3.486	-1.9871	7.053	C	-10.6045	6.9694	-1.8865	C	3.9321	5.0447	-6.6477	Cl	-4.7027	7.7419	3.2229
C	2.33	-2.6028	7.4628	C	-6.5281	8.9478	-4.1955	C	3.3459	-2.9995	2.7746	Cl	2.6513	8.8635	-2.8638
C	4.2653	-2.9182	6.4311	C	-0.1056	4.1408	11.8127	C	2.6597	5.3213	-6.214	Cl	-3.2615	-0.3478	-1.4157
C	2.9919	0.365	6.8911	C	0.4826	4.7011	10.7065	C	3.9442	5.1299	-8.0091	Co	1.2409	-5.3401	7.7074
C	5.5837	-2.7512	5.8036	C	-1.442	4.0203	11.5675	C	5.4019	5.4814	-4.7898	Co	1.4171	-5.0251	-7.557
C	4.8174	-0.1013	8.0089	C	-2.5004	3.4991	12.4441	C	5.0675	4.9415	-8.9381	Co	-2.6736	6.1595	-5.26
C	1.1378	-2.0273	8.1642	C	1.9151	5.07	10.4698	C	5.7224	3.5441	-5.7613	Co	-0.0456	5.6712	-7.3531
C	2.8374	2.7557	7.1435	C	9.9303	5.6715	3.5064	C	2.1198	5.3894	-4.8182	Co	-8.1259	4.4605	-1.8037
C	1.5607	3.0228	7.57	C	10.5185	6.2318	2.4002	C	6.946	5.3863	-2.9433	Co	-5.736	5.7141	-3.8636
C	3.3351	3.8843	6.5608	C	8.5938	5.5509	3.2612	C	3.3616	-0.1606	0.6739	Co	-0.2218	5.3562	7.9113
C	4.6467	4.1009	5.9342	C	7.5355	5.0298	4.1379	C	6.2346	5.7264	-1.82	Co	2.1681	6.6098	5.8514
C	4.631	1.262	8.0349	C	11.951	6.6007	2.1635	C	8.267	5.6198	-2.6959	Co	5.8245	-5.5084	2.8575
C	0.5703	2.1226	8.2432	C	-11.793	2.8164	-2.5524	C	9.4218	5.435	-3.5861	Co	8.2143	-4.2548	0.7975
C	7.8466	-6.4549	6.3197	C	-10.6438	3.4403	-2.969	C	6.5888	3.6423	-4.6965	Co	4.1236	6.9298	3.0945
C	6.5742	-6.1783	6.7536	C	-11.8206	2.8441	-1.1889	C	4.7569	5.6882	-1.5769	Co	6.7516	6.4415	1.0014
C	7.8587	-6.3697	4.9584	C	-12.8473	2.3266	-0.2733	C	5.8352	8.254	6.6	Co	-4.0352	-6.7241	-4.1007
C	8.982	-6.5581	4.0295	C	-10.1491	3.7029	-4.3584	C	4.686	7.6301	7.0166	Co	-0.9727	-6.2787	-5.497
C	6.0343	-6.1103	8.1492	C	-1.7571	4.347	-10.8587	C	5.8628	8.2262	5.2365	Co	3.8689	-5.8284	5.6143
C	-3.8408	-7.7793	-8.0454	C	-0.6079	4.9709	-11.2753	C	7.4223	-1.0212	0.4656	Co	-6.6632	-6.2358	-2.0075
C	-4.5522	-7.4392	-6.922	C	-1.7847	4.3748	-9.495	C	6.8895	8.7437	4.3211	H	3.2241	-9.8719	8.3751
C	-2.5198	-7.5458	-7.798	C	-2.8115	3.8573	-8.5796	C	4.1913	7.3675	8.4062	H	0.5205	-7.7491	9.5902
C	-1.3649	-7.7306	-8.6881	C	-0.1132	5.2335	-12.6647	C	-5.8522	6.9296	-7.765	H	1.7841	-7.8222	10.5154
C	-6.0299	-7.4774	-6.679	C	-2.8679	7.2147	-1.3153	C	-6.4404	6.3692	-6.6589	H	1.1647	-9.1375	9.929
C	-1.9377	-4.5701	5.2025	C	-2.1566	6.8746	-2.4386	C	-4.5158	7.0501	-7.5198	H	4.1756	-9.6693	5.3787
C	-2.5259	-5.1304	6.3086	C	-4.1889	6.9813	-1.5627	C	-3.4574	7.5712	-8.3965	H	5.3056	-9.546	6.4583
C	-0.6013	-4.4495	5.4477	C	-1.3238	7.1196	0.5312	C	-7.8729	6.0003	-6.422	H	5.0463	-8.368	5.4569
C	-3.409	-5.0069	3.3458	C	-5.3438	7.1661	-0.6726	C	4.5066	3.0885	1.6558	H	0.4758	10.2258	8.7581
C	0.4571	-3.9284	4.5709	C	-2.5107	8.9587	0.438	C	5.6625	3.7042	1.246	H	-1.5526	7.4113	9.8792
C	-2.7588	-2.9216	3.5138	C	-0.6788	6.9128	-2.6817	C	3.0668	-9.0178	8.0423	H	-0.3503	7.7862	10.8128
C	-3.9584	-5.4993	6.5453	C	0.146	7.5563	2.3891	C	3.7273	4.0196	2.2777	H	-1.3029	8.9081	10.2729
C	-4.9516	-4.9116	1.498	C	1.4183	7.2797	1.9553	C	2.4088	3.8527	2.9052	H	1.4314	10.3981	5.7611
C	-6.1008	-5.5355	1.9146	C	0.1338	7.4711	3.7505	C	3.1751	1.2027	0.6998	H	2.5586	10.5424	6.8412
C	-4.924	-4.9394	0.1345	C	-0.9894	7.6595	4.6794	C	6.8548	3.1287	0.5447	H	2.6198	9.3763	5.7951
C	-3.8973	-4.4218	-0.781	C	-1.6444	9.0569	1.5027	C	3.6506	-8.467	6.9291	H	5.7905	0.8352	2.2985
C	-3.6251	-3.0198	2.449	C	1.9583	7.2117	0.5596	C	2.1574	-7.1526	2.1089	H	3.4469	-3.572	3.5388
C	-6.5955	-5.7981	3.304	C	-6.5096	1.6965	-4.3451	C	3.3066	-6.5287	1.6922	H	2.7532	-3.412	2.142
C	8.0982	-3.0394	-3.1038	C	-7.2141	2.0284	-3.2151	C	2.1298	-7.1248	3.4723	H	2.9807	-2.1563	3.0526
C	7.5099	-3.5997	-1.9977	C	-5.9402	2.8332	-4.8395	C	0.6148	-7.0573	0.2611	H	2.8253	-0.7894	0.2472
C	9.4346	-2.9188	-2.8586	C	-6.0171	-0.6559	-4.1818	C	1.103	-7.6423	4.3878	H	7.8092	-0.4289	1.1147
C	6.6268	-3.4762	-4.9605	C	-5.0771	2.999	-6.0175	C	0.8309	-9.0444	1.1577	H	6.978	-0.5066	-0.2122
C	10.4929	-2.3977	-3.7353	C	-6.8718	-0.0415	-6.1033	C	3.8013	-6.2661	0.3027	H	8.1144	-1.5509	0.0632
C	7.277	-1.3909	-4.7925	C	-7.9944	1.152	-2.2838	C	2.2157	-8.0949	8.5759	H	2.3564	4.4022	3.6908
C	6.0774	-3.9686	-1.761	C	5.1551	-1.6543	1.5654	C	-0.8565	-7.4941	-1.5955	H	1.724	4.1142	2.2854
C	0.5518	9.3739	8.3928	C	-5.861	-3.0463	-4.4355	C	-0.2683	-6.9338	-2.7018	H	2.2848	2.9326	3.1496
C	5.0843	-3.3809	-6.8083	C	-6.4448	-3.5972	-3.3224	C	-2.193	-7.6147	-1.8409	H	2.4876	1.68	0.2943
C	3.935	-4.0048	-6.3917	C	-5.01	-3.9693	-4.9692	C	-3.2513	-8.1358	-0.9642	H	7.3897	2.6382	1.1732
C	5.1118	-3.4087	-8.1718	C	-4.1401	-3.8532	-6.1481	C	-0.0354	-9.1426	0.093	H	6.5614	2.5395	-0.1542
C	6.1386	-2.8912	-9.0873	C	-6.6854	-1.4048	-6.1292	C	1.1642	-6.5649	-2.9385	H	7.3773	3.8394	0.1659
C	6.4107	-1.4891	-5.8573	C	-7.4269	-2.9978	-2.3628	C	1.3459	-8.211	9.7548	H	0.7344	-6.1529	0.0805
C	3.4403	-4.2674	-5.0022	C	6.4318	-1.9214	1.1388	C	1.0466	-4.2849	11.6521	H	1.0142	-7.0489	5.1373
C	1.2563	9.0419	7.2628	C	2.0865	-8.8792	-6.2649	C	1.7579	-4.625	10.5288	H	1.3608	-8.5135	4.6981
C	-0.8477	2.4818	-4.9252	C	0.8098	-8.6121	-5.8383	C	-0.2744	-4.5183	11.4047	H	0.2636	-7.7025	3.9261
C	-0.2639	3.0326	-6.0383	C	2.5841	-7.7506	-6.8476	C	-1.4293	-4.3336	12.2949	H	1.1156	-9.7354	1.7115
C	-1.6988	3.4047	-4.3915	C	3.8958	-7.534	-7.4741	C	3.2357	-4.5868	10.2857	H	3.3154	-5.5298	-0.0761
C	-0.6917	0.0913	-5.1787	C	-0.1806	-9.5124	-5.1652	C	4.6327	-9.0664	5.9696	H	3.6689	-7.0487	-0.2374
C	-2.5686	3.2886	-3.2126	C	-0.4285	9.5125	-5.9143	C	11.0824	-2.7542	3.3458	H	4.7366	-6.0514	0.3312
C	-0.0233	0.8402	-3.2313	C	-1.5845	8.8968	-5.5046	C	11.7938	-3.0943	2.2225	H	-4.0531	-7.6232	-1.091
C	0.7182	2.4333	-6.9977	C	0.3508	8.5815	-6.5363	C	9.7614	-2.9877	3.0985	H	-3.4218	-9.0554	-1.1803
C	-0.0176	8.2371	8.8872	C	1.6692	8.7484	-7.1639	C	8.6066	-2.8029	3.9886	H	-2.9703	-8.069	-0.0487
C	-0.1991	-2.261	-5.0156	C	4.6575	-2.7829	2.148	C	13.2715	-3.0561	1.9794	H	-0.4536	-9.9132	-0.2173
C	0.5053	-2.593	-6.1455	C	-2.7767	9.4723	-4.8034	C	-10.6408	-5.6093	-2.7128	H	1.3664	-5.7507	-2.4718
C	-0.7685	-3.3978	-4.5211	C	-6.1038	3.5141	1.6586	C	-9.3684	-5.8859	-3.1467	H	1.7332	-7.268	-2.6166
C	-1.6316	-3.5636	-3.3432	C	-7.3761	3.7906	2.0923	C	-10.6529	-5.6945	-1.3516	H	1.3112	-6.4396	-3.8789

H	1.4032	-3.953	12.4443	H	10.6635	-1.4781	-3.5192	H	-4.6549	2.1623	-6.2252
H	-2.0647	-5.0374	12.1448	H	10.2119	-2.4645	-4.6508	H	-7.2327	0.4856	-6.7793
H	-1.8415	-3.486	12.1124	H	7.6952	-0.6203	-4.4821	H	-7.3892	0.6722	-1.7135
H	-1.136	-4.3567	13.2086	H	5.8753	-4.7828	-2.2278	H	-8.5164	0.528	-2.7935
H	3.6513	-5.3338	10.7228	H	5.5085	-3.2655	-2.0829	H	-8.5776	1.6941	-1.7474
H	3.5967	-3.7693	10.6367	H	5.9304	-4.0939	-0.8206	H	-3.3147	-4.3151	-5.9834
H	3.4061	-4.6328	9.3421	H	6.2274	-3.4846	-9.8368	H	-4.5783	-4.242	-6.9086
H	11.439	-2.4222	4.138	H	5.8808	-2.0201	-9.3976	H	-3.959	-2.9266	-6.3222
H	7.9711	-3.5067	3.8386	H	6.978	-2.831	-8.6255	H	-6.895	-1.9838	-6.8263
H	8.1944	-1.9553	3.8061	H	6.126	-0.7981	-6.4109	H	-6.9698	-2.3949	-1.7719
H	8.8999	-2.826	4.9023	H	3.9262	-5.0037	-4.6233	H	-8.0998	-2.5182	-2.8516
H	13.6872	-3.8031	2.4165	H	3.5728	-3.4848	-4.4621	H	-7.8405	-3.6962	-1.8502
H	13.6326	-2.2387	2.3304	H	2.5051	-4.4821	-5.0307	H	2.5346	-9.6889	-6.1727
H	13.442	-3.1021	1.0358	H	-1.005	0.0652	-6.0539	H	3.7947	-6.9616	-8.2383
H	-11.3683	-5.4001	-3.2531	H	-3.394	3.7505	-3.3771	H	4.4885	-7.1216	-6.8415
H	-11.6987	-6.1292	0.3037	H	-2.1304	3.6775	-2.4521	H	4.2609	-8.3772	-7.7522
H	-11.7601	-4.61	-0.0787	H	-2.7498	2.3621	-3.0385	H	-0.5675	-10.1046	-5.8142
H	-12.6034	-5.6562	-0.8861	H	0.1863	1.4192	-2.5343	H	0.2637	-10.0269	-4.4872
H	-9.1009	-6.7789	-4.9511	H	0.2611	1.8303	-7.5888	H	-0.8728	-8.9826	-4.7627
H	-9.1689	-5.2159	-5.0535	H	1.3911	1.9536	-6.5091	H	-0.2137	10.4087	-5.7897
H	-7.8698	-5.9106	-4.5173	H	1.1318	3.1316	-7.5105	H	1.7216	8.1988	-7.9493
H	-1.4684	-3.7617	-11.6764	H	-2.3036	-4.2236	-3.5292	H	2.3541	8.4868	-6.544
H	-1.6628	-4.5985	-8.0026	H	-1.1013	-3.8488	-2.5955	H	1.7932	9.6684	-7.4082
H	-1.7242	-3.0793	-8.3849	H	-2.0539	-2.7269	-3.1354	H	-3.3117	9.9629	-5.4318
H	-2.5675	-4.1255	-9.1924	H	0.5239	-1.0502	-2.5814	H	-2.4834	10.0615	-4.1044
H	0.9349	-5.2482	-13.2574	H	0.6805	-1.2368	-7.6472	H	-3.2992	8.7616	-4.4245
H	0.867	-3.6853	-13.3598	H	1.8076	-1.0925	-6.5672	H	-4.9909	4.7824	3.7303
H	2.166	-4.38	-12.8235	H	1.8689	-2.2586	-7.6132	H	-5.0459	4.0339	-1.3581
H	7.5166	-9.1244	-0.0492	H	-6.4949	-10.9734	-3.5706	H	-4.9845	2.5147	-0.9757
H	9.5452	-6.3099	-1.1703	H	-8.4303	-8.7634	-1.4112	H	-4.1412	3.561	-0.1683
H	8.3429	-6.6848	-2.104	H	-9.0628	-9.0514	-2.8165	H	-4.4051	1.2926	1.9644
H	9.2955	-7.8067	-1.5641	H	-8.502	-10.233	-1.9524	H	-7.6437	4.6836	3.8967
H	6.5611	-9.2967	2.9477	H	-3.397	-10.5274	-3.9289	H	-7.5757	3.1207	3.9992
H	5.434	-9.441	1.8676	H	-4.2254	-10.6261	-5.2563	H	-8.8748	3.8154	3.4629
H	5.3727	-8.2749	2.9137	H	-3.4095	-9.3262	-4.9362	H	0.0214	4.6082	4.8702
H	4.7684	10.9734	0.3338	H	-9.2432	9.1245	-3.1877	H	-0.2018	3.0567	4.9027
H	7.4721	8.8505	-0.8814	H	-10.5035	6.397	-1.1224	H	-0.9073	3.9274	3.8064
H	6.2085	8.9236	-1.8065	H	-11.1972	6.557	-2.5191	H	-2.8358	1.4705	3.8931
H	6.8278	10.239	-1.2202	H	-10.9696	7.8126	-1.6085	H	-5.6946	4.9045	6.2924
H	3.817	10.7707	3.3301	H	-6.1412	9.54	-3.5464	H	-5.64	3.3401	6.3784
H	2.687	10.6474	2.2505	H	-6.9724	9.4623	-4.8734	H	-5.4494	4.2036	7.673
H	2.9463	9.4694	3.2519	H	-5.836	8.4181	-4.598	H	5.0449	6.3131	-4.576
H	2.202	0.2662	6.4103	H	0.3311	3.8873	12.5938	H	4.99	5.5646	-9.6643
H	5.6361	-3.3008	5.018	H	-2.6713	2.5795	12.2284	H	5.0514	4.0454	-9.282
H	6.2686	-3.0128	6.4234	H	-3.4373	4.0987	12.2973	H	5.8947	5.0916	-8.4746
H	5.7077	-1.8312	5.5592	H	-2.2202	3.5667	13.3598	H	5.6308	2.8233	-6.3419
H	5.505	-0.5786	8.4146	H	2.1173	5.8842	10.9365	H	2.3922	6.2143	-4.4096
H	0.6028	-1.5368	7.5356	H	2.4841	4.3669	10.7917	H	2.4602	4.6514	-4.307
H	1.4311	-1.4381	8.8631	H	2.0622	5.1954	9.5295	H	1.1611	5.3461	-4.8434
H	0.6153	-2.738	8.5429	H	10.367	5.4181	4.2875	H	10.0573	6.1388	-3.436
H	4.5457	4.6734	5.1701	H	6.7337	5.5424	4.0111	H	9.834	4.5874	-3.4036
H	5.2394	4.5134	6.5668	H	7.365	4.1101	3.9217	H	9.1285	5.4581	-4.4998
H	5.0118	3.2577	5.6562	H	7.8165	5.0966	5.0534	H	7.2	3.0011	-4.4132
H	5.1673	1.8908	8.4616	H	12.1531	7.4149	2.6303	H	4.3412	6.4352	-2.0139
H	0.1834	1.5303	7.5941	H	12.52	5.8976	2.4854	H	4.3959	4.8707	-1.9279
H	1.0146	1.608	8.9211	H	12.098	6.726	1.2232	H	4.5864	5.7342	-0.6333
H	-0.1218	2.6523	8.6456	H	-12.4404	2.4401	-3.1038	H	6.4826	8.6303	7.1515
H	8.5741	-6.6641	6.86	H	-12.59	1.4554	0.0373	H	6.9783	8.1504	3.5715
H	8.9045	-5.935	3.3031	H	-12.9525	3.0204	0.6022	H	6.6317	9.6149	4.0107
H	8.9659	-7.4542	3.6854	H	-13.6872	2.2673	-0.7344	H	7.729	8.8039	4.7827
H	9.8092	-6.408	4.4928	H	-10.6349	4.4391	-4.7373	H	4.6772	6.6312	8.785
H	6.3067	-5.2853	8.5579	H	-10.2815	2.9203	-4.8986	H	4.3237	8.1501	8.9463
H	6.3747	-6.8482	8.6604	H	-9.2138	3.9175	-4.33	H	3.256	7.1528	8.3776
H	5.0756	-6.1536	8.124	H	-2.4045	3.9707	-11.4101	H	-6.2889	7.1831	-8.5459
H	-4.1974	-8.1112	-8.8375	H	-2.9003	4.4507	-7.8302	H	-2.6556	7.0586	-8.2696
H	-0.7295	-7.0268	-8.538	H	-2.5537	2.9861	-8.2694	H	-3.2869	8.4909	-8.1803
H	-0.9528	-8.5782	-8.5056	H	-3.6509	3.7971	-9.0413	H	-3.7385	7.5044	-9.312
H	-1.6583	-7.7075	-9.6019	H	-0.5991	5.9698	-13.0436	H	-8.0751	5.1861	-6.8889
H	-6.4455	-6.7304	-7.116	H	-0.2456	4.4509	-13.2049	H	-8.4419	6.7035	-6.7441
H	-6.3909	-8.2949	-7.0299	H	0.8221	5.4482	-12.6361	H	-8.0199	5.875	-5.4817
H	-6.2003	-7.4314	-5.7353	H	-0.9669	6.2879	0.3174	H	1.9779	-3.1827	-0.1587
H	-3.5286	-5.9113	3.5264	H	-5.9792	6.4622	-0.8225	H	0.9566	-3.2955	-1.4072
H	1.2589	-4.441	4.6978	H	-5.756	8.0136	-0.8549	H	0.5329	-3.923	0.0427
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H	-4.1606	-6.3135	6.0785	H	-0.3178	7.7303	-2.3308	N	2.4091	-3.8818	7.1075
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H	6.5073	-4.3807	-4.7799	H	-4.4051	3.659	-5.8315	N	-2.6373	-4.1719	4.0194
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N	2.2913	-7.0081	7.7842								
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N	6.3728	4.8596	-4.1439								
N	4.0246	7.241	5.9306								
N	4.7421	7.5882	4.8482								
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N	4.4166	5.1759	2.2403								
N	4.1933	1.71	1.4345								
N	3.968	-6.1395	2.7782								
N	6.8657	-6.6297	1.6288								
N	6.606	-6.0419	4.5885								
N	3.2505	-6.4868	3.8606								
N	1.1859	-7.7401	1.2378								
N	-1.224	-6.7279	-3.6033								
N	-2.396	-7.1267	-3.0795								
N	-0.1569	-7.8922	-0.4127								
N	1.3184	-3.8133	-0.6094								
N	5.8271	-5.9406	5.6794								
N	3.576	-4.0745	6.4685								
N	-0.3454	-4.9962	10.1476								
N	-1.5702	-5.3363	7.21								
N	9.6905	-3.4655	1.8414								
N	8.4656	-3.8056	-1.0962								
N	7.6498	-6.1395	0.6531								
N	-8.6213	-6.1236	-2.0726								
N	-9.4002	-6.0223	-0.9817								
N	1.4145	-4.5929	-10.3789								
N	0.6357	-4.4917	-9.288								

IR analysis

The ex-situ IR spectroscopic studies of NH_3 sorption in **JCM-1** and **JCM-1(Cl⁻)** were carried out in a glove box. The IR spectra of the MOFs before and after NH_3 adsorption were recorded at room temperature in attenuated total reflectance (ATR) mode on Bruker *ALPHA*. Black lines are spectra of the as-prepared samples and red lines are spectra of the NH_3-adsorbed samples. The peaks corresponding to imidazolium C-H stretching region (2900~3100 cm^{-1})[1] were blue-shifted and new peaks were appeared whilst other peaks from the framework remained intact. The broad peaks around 3200~3400 cm^{-1} in Figure S9a and S9b are NH_3 peaks adsorbed in the frameworks.

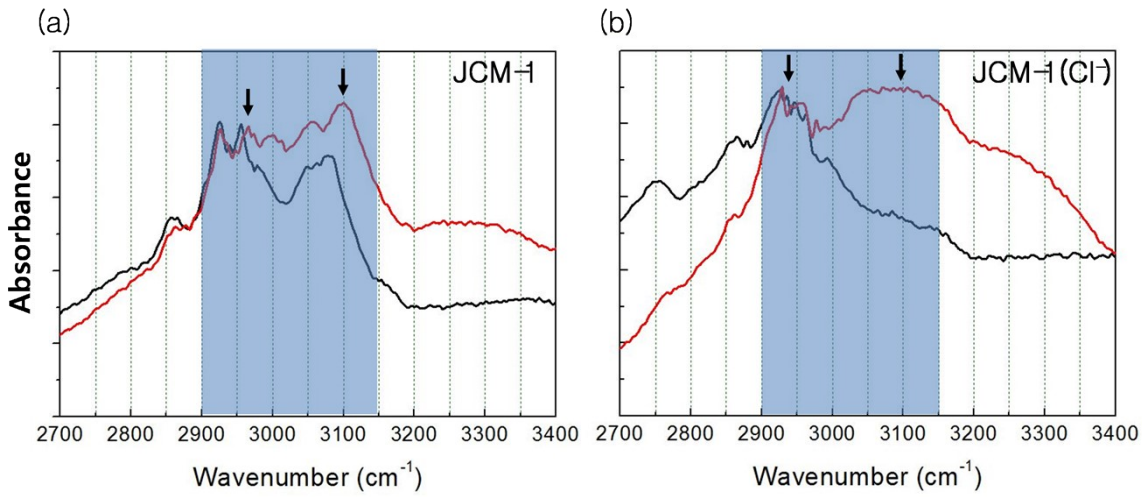

Fig. S6 IR spectra of a) **JCM-1** and b) **JCM-1(Cl⁻)** before (black line) and after (red line) NH_3 exposure. Broad peaks around 3200 ~ 3400 cm^{-1} are N-H stretch peaks of adsorbed NH_3 (black line: before exposure to NH_3, red line: after exposure to NH_3).

Breakthough experiments

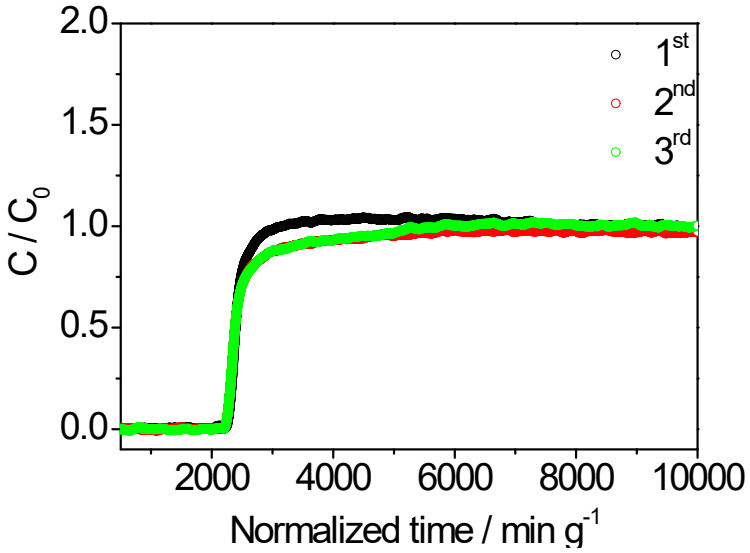

Fig. S7 Breakthrough curves of calculating ammonia breakthrough capacity in **JCM-1** at dry 1000 ppm (NH_3%: 0.1%). 1st = 0.307 mmol g^{-1} (activation - 120 °C 10 h under He flowing), 2nd = 0.385 mmol g^{-1} (activation - 25 °C 10 h under He flowing), 3rd = 0.409 mmol g^{-1} (activation - 25 °C 10 h under He flowing).

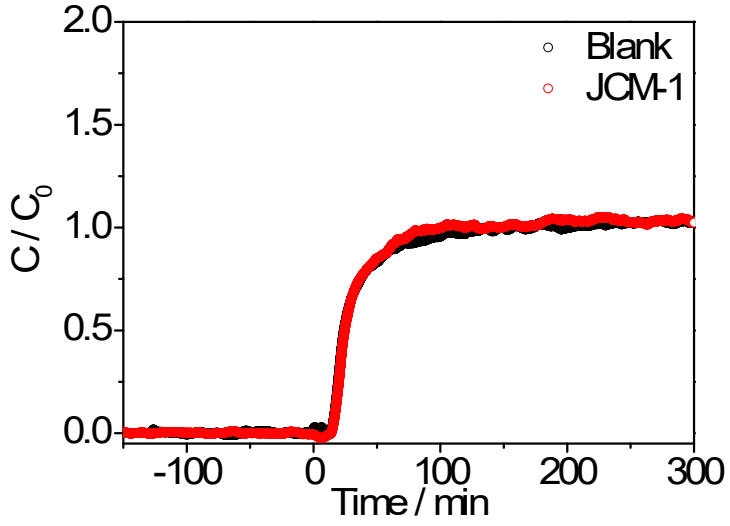

Fig. S8 Breakthrough curves of calculating ammonia breakthrough capacity in **JCM-1** at 80% RH and 1000 ppm (NH_3%: 0.1%). 1st = 0 mmol g^{-1} (activation - 120 °C 10 h under He flowing).

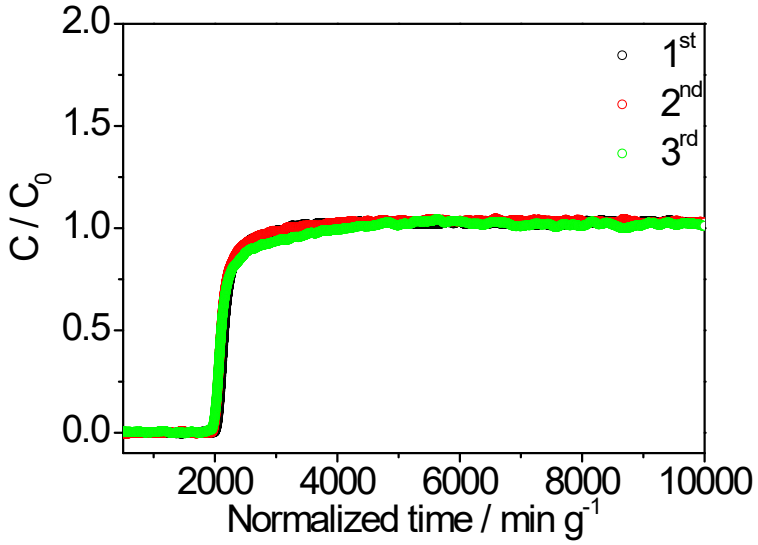

Fig. S9 Breakthrough curves of calculating ammonia breakthrough capacity in **JCM-1(Cl^-)** at dry 1000 ppm (NH_3%: 0.1%). 1st = 0.475 mmol g^{-1} (activation - 120 °C 10 h under He flowing), 2nd = 0.415 mmol g^{-1} (activation - 25 °C 10 h under He flowing), and 3rd = 0.485 mmol g^{-1} (activation - 25 °C 10 h under He flowing).

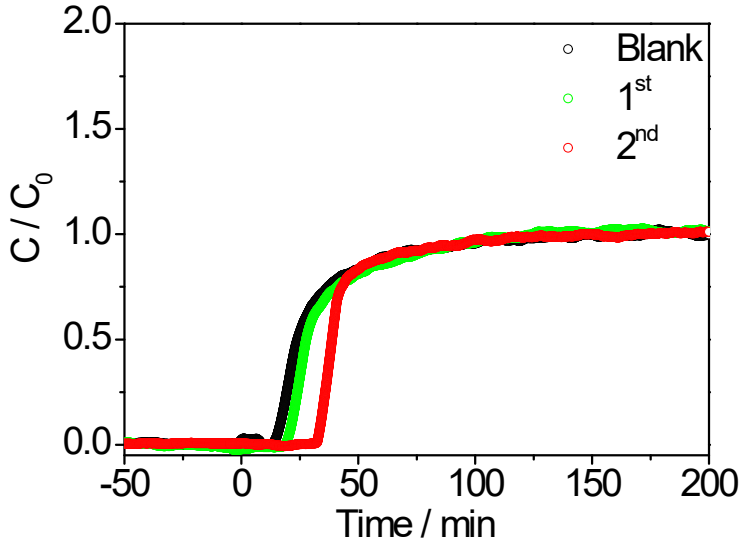

Fig. S10 Breakthrough curves of calculating ammonia breakthrough capacity in **JCM-1(Cl$^-$)** at 80% RH and 1000 ppm (NH_3%: 0.1%). 1st = 0.213 mmol g^{-1} (activation - 120 °C 10 h under He flowing) and 2nd = 0.318 mmol g^{-1} (activation - 25 °C 10 h under He flowing).

Table S3. The summary of the NH3 adsorption uptake amounts with various MOFs

Adsorbents	NH_3 uptake amounts (mmol g^{-1})	Uptake condition at 1 bar	Reference
JCM-1(Cl^-)	**11.7** **7.2**	**273 K** **298 K**	**This work**
JCM-1	**7.7** **5.7**	**273 K** **298 K**	**This work**
Mg-MOF-74	~16	298 K	[2]
Al-BTB	~6	298 K	[2]
MIL-53(Al)	4.28	298 K	[2]
ZIF-8	1.2	298 K	[2]
HKUST-1	12.1 ~6.0	301 K, 1.2 bar 313 K	[3] [4]
HKUST-1/GO	~5.4	313 K	[4]
MIL-100(Al)	8	298 K	[5]
NH_2-MIL-53	8	298 K	[5]
MIL-53	4.4	298 K	[5]
MIL-101(Cr)	10.0	298 K	[5]
DUT-6-$(OH)_2$	16.4	298 K	[6]
DUT-6	12	298 K	[6]
NU-300	8.28	298 K	[7]
Al-PMOF	7.67	298 K	[8]
Ga-PMOF	10.50	298 K	[8]
In-PMOF	9.41	298 K	[8]
NU-1401	8.41	298 K	[9]
Mg_2(dobpdc)	23.90	298 K	[10]
Ni_2(dobpdc)	20.82	298 K	[10]
Zn_2(dobpdc)	15.24	298 K	[10]
Co_2(dobpdc)	13.34	298 K	[10]
Mn_2(dobpdc)	13.26	298 K	[10]
CoHCC	21.9	298 K	[11]
CuHCF	20.2	298 K	[11]
PB	12.5	298 K	[11]
Co_2Cl_2BBTA	17.95	298 K	[12]
Cu_2Cl_2BBTA	19.79	298 K	[12]
Ni_2Cl_2BBTA	14.68	298 K	[12]
$[Zn_2(L1)_2(bpe)]$	17.8	273 K	[13]
$[Zn_2(L1)_2(bipy)]$	14.3	273 K	[13]
$Zn(NA)_2$	10.2	298 K	[14]
$Co(NA)_2$	17.5	298 K	[14]
$Cu(NA)_2$	13.4	298 K	[14]
$Cd(NA)_2$	6	298 K	[14]
Mn_2Cl_2BTDD	15.47	298 K	[15]
Co_2Cl_2BTDD	12	298 K	[15]
Ni_2Cl_2BTDD	12.02	298 K	[15]
UiO-66-NH_2	9.84	298 K	[15]
UiO-66-A	5.74	298 K	[16]
UiO-66-B	6.81	298 K	[16]
UiO-66-C	8.27	298 K	[16]
MOF-5	12.2	298 K, 1.06 bar	[17]
MOF-177	12.2	298 K, 1.06 bar	[17]
MOS-1	11.5	298 K	[18]
MOS-2	5.2	298 K	[18]
MOS-3	3.8	298 K	[18]
$Cu(INA)_2$	12.5	298 K	[19]
Co-2(INA)	~13	298 K	[19]
Ni-2(INA)	~13	298 K	[19]
Cd-2(INA)	~12	298 K	[19]

$Zn(INA)_2$	6	298 K	[20]
ELM-12	6.1	298 K	[21]
Fe-MIL-101-SO_3H	17.8	298 K	[22]
MFM-300(V^{IV})	17.3	298 K	[23]
MFM-300(Fe)	16.1	298 K	[23]
MFM-300(V^{III})	15.6	298 K	[23]
MFM-300(Cr)	14.0	298 K	[23]
$Ni_2(adc)_2(dabco)$	12.1	298 K	[24]
$Co_2(adc)_2(dabco)$	11.2	298 K	[24]
$Zn_2(adc)_2(dabco)$	8.3	298 K	[24]
$Cu_2(adc)_2(dabco)$	6.5	298 K	[24]
SION105-Eu	5.7	303 K	[25]
ECUT-36	3.6	298 K	[26]
MFM-300(Al)	15.7	298 K	[27]
MFM-303(Al)	9.9	273 K	[28]
UiO-67	8.40	298 K, 1.1 bar	[29]
UiO-bpydc	8.4	298 K	[29]
PFC-27	~4.7	298 K	[30]
PFC-27/CH_3COO^-	~8.5	298 K	[30]
PFC-27/CF_3COO^-	~8.8	298 K	[30]
PFC-27/$CFH_3SO_3^-$	10.4	298 K	[30]

References

[1] S. Cha, M. Ao, W. Sung, B. Moon, B. Ahlstrom, P. Johansson, Y. Ouchi, D. Kim, *Phys. Chem. Chem. Phys.* **2014**, *16*, 9591-9601.
[2] T. Kajiwara, M. Higuchi, D. Watanabe, H. Higashimura, T. Yamada, H. Kitagawa, *Chem. Eur. J.* **2014**, 20, 15611-15617.
[3] C. Petit, L. Huang, J. Jagiello, J. Kenvin, K. E. Gubbins, T. J. Bandosz, *Langmuir* **2011**, 27, 13043-13051.
[4] C. Petit, S. Wrabetz, T. J. Bandosz, *J. Mater. Chem.* **2012**, 22, 21443-21447.
[5] Y. Chen, F. Zhang, Y. Wang, C. Yang, J. Yang, J. Li, *Microporous Mesoporous Mater.* **2018**, 258, 170-177.
[6] I. Spanopoulos, P. Xydias, C. D. Malliakas, P. N. Trikalitis, *Inorg. Chem.* **2013**, 52, 855-862.
[7] Y. Chen, X. Zhang, K. Ma, Z. Chen, X. Wang, J. Knapp, S. Alayoglu, F. Wang, Q. Xia, Z. Li, T. Islamoglu, O. K. Farha, *ACS Appl. Nano Mater.* **2019**, 2, 6098-6102.
[8] S. Moribe, Z. Chen, S. Alayoglu, Z. H. Syed, T. Islamoglu, O. K. Farha, *ACS Mater. Lett.* **2019**, 1, 476-480.
[9] Y. Zhang, X. Zhang, Z. Chen, K. I. Otake, G. W. Peterson, Y. Chen, X. Wang, L. R. Redfern, S. Goswami, P. Li, T. Islamoglu, B. Wang, O. K. Farha, *ChemSusChem* **2020**, 13, 1710-1714.
[10] D. W. Kim, D. W. Kang, M. Kang, J.-H. Lee, J. H. Choe, Y. S. Chae, D. S. Choi, H. Yun and C. S. Hong, *Angew. Chem. Int. Ed.* **2020**, 59, 22531–22536.
[11] A. Takahashi, H. Tanaka, D. Parajuli, T. Nakamura, K. Minami, Y. Sugiyama, Y. Hakuta, S. Ohkoshi, T. Kawamoto, *J. Am. Chem. Soc.* **2016**, 138, 6376-6379.
[12] A. J. Rieth, M. Dinca, *J. Am. Chem. Soc.* **2018**, 140, 3461-3466.
[13] S. Glomb, D. Woschko, G. Makhloufi, C. Janiak, *ACS Appl. Mater. Interfaces* **2017**, 9, 37419-37434.
[14] Y. Chen, B. Shan, C. Yang, J. Yang, J. Li, B. Mu, *J. Mater. Chem. A* **2018**, 6, 9922-9929.
[15] A. J. Rieth, Y. Tulchinsky, M. Dinca, *J. Am. Chem. Soc.* **2016**, 138, 9401-9404.
[16] W. Morris, C. J. Doonan, O. M. Yaghi, *Inorg. Chem.* **2011**, 50, 6853-6855.
[17] D. Saha, S. Deng, J., *Colloid Interface Sci.* **2010**, 348, 615-620.
[18] Y. Chen, Y. Wang, C. Yang, S. Wang, J. Yang, J. Li, *ACS Sustain. Chem. Eng.* **2017**, 5, 5082-5089.
[19] Y. Chen, L. Li, J. Li, K. Ouyang, J. Yang, *J. Hazard. Mater.* **2016**, 306, 340−347.
[20] Y. Chen, C. Yang, X. Wang, J. Yang, K. Ouyang, J. Li, *J. Mater. Chem. A* **2016**, 4, 10345−10351.
[21] L. Li, Y. Wang, J. Yang, Y. Chen, J. Li, *ChemPlusChem* **2016**, 81, 222−228.
[22] J. F. Van Humbeck, T. M. McDonald, X. Jing, B. M. Wiers, G. Zhu, and J. R. Long, *J. Am. Chem. Soc.* **2014**, 136, 2432
[23] X. Han, W. Lu, Y. Chen, I. Silva, J. Li, L. Lin, W. Li, A. M. Sheveleva, H. G. W. Godfrey, Z. Lu, F. Tuna, E. J. L. Mcinnes, Y. Cheng, L. L. Daemen, L. J. M. McPherson, S. J. Teat, M. D. Frogley, S. Rudic, P. Manuel, A. J. Ramirez-cuesta, S. Yang and M. Schröder, *J. Am. Chem. Soc.* **2021**, 143, 3153– 3161.
[24] Z. Cao, K. N. Landström, F. Akhtar, *Catalysts* **2020**, 10, 1444−1454.
[25] T. N. Nguyen, I. M. Harreschou, J. H. Lee, K. C. Stylianou, D. W. Stephan, *Chem. Commun.* **2020**, 56, 9600.
[26] L. J. Sun, Y. L. Fan, M. J. Yin, H. P. Zhang, H. Feng, L. J. Guo, F. Luo, *Cryst. Growth Des.* **2020**, 20, 3605−3610.
[27] H. G. W. Godfrey, I. da Silva, L. Briggs, J. H. Carter, C. G. Morris, M. Savage, T. L. Easun, P. Manuel, C. A. Murray, C. C. Tang, M. D. Frogley, G. Cinque, S. Yang, M. Schröder, *Angew. Chem. Int. Ed.* **2018**, 57, 14778-14781.
[28] C. Marsh, X. Han, J. Li, Z. Lu, S. P. Argent, I. da Silva, Y. Cheng, L. L. Daemen, A. J. Ramirez-Cuesta, S. P. Thompson, A. J. Blake, S. Yang and M. Schröder, *J. Am. Chem. Soc.* **2021**, 143, 6586-6592.
[29] T. Yoskamtorn, P. Zhao, X.-P. Wu, K. Purchase, F. Orlandi, P. Manuel, J. Taylor, Y. Li, S. Day, L. Ye, C. C. Tang, Y. Zhao, S. C. E. Tsang, *J. Am. Chem. Soc.* **2021**, 143, 3205-3218.
[30] M. K. Matikolaei and E. Binaeian, *ACS Appl. Mater. Interfaces* **2021**, 13, 27159−27168.