Geometries of models used in our work (https://doi.org/10.1016/j.isci.2020.101757). Geometries were optimized using M062X/aug-cc-pVTZ level of theory using Gaussian09, Revision C.01. First column denotes atom number, second column denotes atomic number of the atom, last three columns correspond to *x*, *y*, *z* Cartesian coordinate.

Ammonia

1	7	-0.000002	-0.000002	-0.112423
2	1	0.251556	0.905894	0.262324
3	1	-0.910314	-0.235095	0.262319
4	1	0.658775	-0.670782	0.262320

Ammonium ion

1	7	-0.000001	0.000000	-0.000001
2	1	0.328751	0.816292	-0.523741
3	1	-1.007192	-0.115518	-0.144778
4	1	0.188113	0.135962	0.997410
5	1	0.490336	-0.836735	-0.328887

Ammonia-ammonia dimer

1	7	1.680783	-0.000307	-0.104356
2	1	2.110135	0.811149	0.322046
3	1	0.701310	-0.000142	0.168565
4	1	2.110423	-0.810184	0.324759
5	7	-1.565971	-0.000424	0.041347
6	1	-2.314527	-0.051133	0.721015
7	1	-1.721903	0.837857	-0.505057
8	1	-1.689121	-0.782430	-0.590267

Ammonia-water dimer

1	7	-1.382357	-0.022980	0.000100
2	1	-1.810235	-0.293226	0.876847
3	1	-1.580150	0.960409	-0.140359
4	1	-1.852597	-0.532440	-0.737460
5	1	1.949736	-0.764875	0.000775
6	8	1.547748	0.104743	-0.000125
7	1	0 .587759	-0.046951	0.000495

Ammonia-solvated

1	7	-0.121904	0.427803	-0.132670
2	1	0.392918	0.707997	0.702362
3	1	-0.450060	1.303008	-0.545980
4	1	-0.959877	-0.044732	0.214715
5	1	1.263180	-2.400201	-0.410351
6	8	0.816165	-2.643806	0.423623
7	1	1.078990	-1.943224	1.051572
8	8	1.968051	2.318140	-1.747755

9	1	1.455862	2.807571	-1.065460
10	1	2.592350	1.758348	-1.249955
11	8	1.515435	-1.028129	-1.670250
12	1	0.828840	-0.474643	-1.149531
13	1	1.374333	-0.766139	-2.598103
14	8	-1.668694	-2.330295	-0.560371
15	1	-1.997508	-3.200305	-0.825647
16	1	-0.776348	-2.483101	-0.146480
17	1	-1.775947	-0.958301	-1.881282
18	8	-1.978340	-0.140650	-2.378500
19	1	-1.130431	0.180564	-2.749178
20	1	-2.685521	0.987001	-1.308678
21	8	-3.039407	1.504843	-0.537786
22	1	-3.733209	2.082381	-0.882779
23	1	-2.281207	0.749023	2.199382
24	8	-1.938428	1.664959	2.214376
25	1	-2.113336	1.974228	1.307036
26	1	1.207493	1.208344	2.575140
27	8	0.727755	2.055221	2.568980
28	1	-0.235706	1.847458	2.634016
29	1	2.582061	-0.833240	2.612465
30	8	2.037441	-0.445877	1.912392
31	1	2.657669	-0.169224	1.196604
32	1	2.842842	-0.340031	-0.980276
33	8	3.400367	0.234059	-0.377894
34	1	4.330989	0.051639	-0.565898
35	1	-2.711997	-1.423958	0.719122
36	8	-3.064219	-0.671013	1.229365
37	1	-3.410316	-0.044074	0.567017
38	1	1.002929	1.444399	-2.806091
39	8	0.476600	0.831453	-3.392452
40	1	0.441272	1.242331	-4.266560
41	1	0.653849	2.985593	1.136585
42	8	0.453201	3.403633	0.259616
43	1	0.396813	4.355768	0.413270