

Supporting Information

**Exemplary Role of Nanoconfinement on the Proton Transfer from Acids to
Ammonia**

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Supporting Information

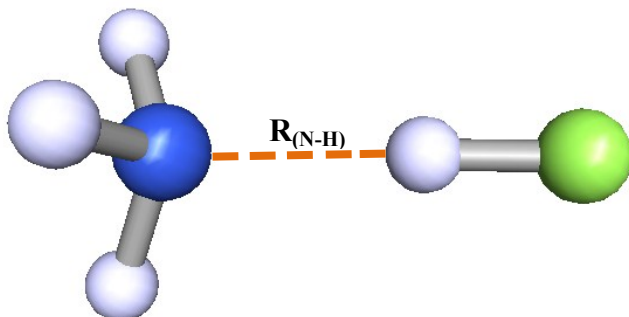


Figure SI-1: Optimized structure of $\text{NH}_3 \cdots \text{HX}$ complex at B3LYP/TZVP level. $R_{(\text{N-H})}$ value in $\text{NH}_3 \cdots \text{HX}$ is 1.637, 1.652, 1.584 and 1.547 Å for the complex comprising X = F, Cl, Br and I, respectively.



Table SI-1: Variation in X—H distance in NH₃...HX Complex on micro-solvating with water molecules. X = F, Cl, Br and I.

No. of water molecule	F-H Dist. (Å)	Cl-H Dist. (Å)	Br-H Dist. (Å)	I-H Dist. (Å)
0	0.968	1.361	1.538	1.761
1	0.995	1.476	1.953	2.238
2	1.022	1.864	2.077	2.343
3	1.060	2.006	2.198	2.439
4	1.424	2.044	---	---
5	1.534	---	---	---

Table SI-2: NBO Charge on each atom of NH₃...HF complex.

Cavity Size (Å)	q(N)	q(H1)	q(H2)	q(H3)	q(F)	q(H4)	q(NH4)	q(Total) on NH ₃ HF
∞	-1.05	0.38	0.38	0.38	-0.62	0.54	0.62	0.00
12.2	-1.04	0.38	0.38	0.38	-0.64	0.54	0.64	0.00
8.7	-1.04	0.38	0.38	0.38	-0.65	0.54	0.64	-0.01
8.2	-1.03	0.38	0.38	0.38	-0.67	0.53	0.64	-0.02
7.1	-1.05	0.43	0.40	0.40	-0.72	0.49	0.66	-0.06
6.1	-1.21	0.45	0.47	0.50	-0.77	0.48	0.70	-0.08
5.2	-1.82	0.67	0.67	0.67	-0.87	0.65	0.84	-0.03
5.2	-2.07	0.70	0.71	0.71	-0.48	0.71	0.77	0.28

Table SI-3: NBO Charge on each atom of NH₃...HCl complex.

Cavity Size (Å)	q _(N)	q _(H1)	q _(H2)	q _(H3)	q _(Cl)	q _(H4)	q _(NH4)	q(Total) on NH ₃ HCl
∞	-1.02	0.38	0.38	0.38	-0.41	0.29	0.41	0.00
12.2	-0.99	0.39	0.38	0.39	-0.49	0.31	0.48	-0.01
8.7	-0.91	0.42	0.42	0.42	-0.76	0.41	0.76	-0.01
8.2	-0.92	0.42	0.42	0.42	-0.74	0.37	0.71	-0.03
7.1	-1.17	0.50	0.50	0.52	-0.89	0.50	0.83	-0.06
6.1	-1.63	0.62	0.62	0.64	-0.10	0.61	0.87	0.77
5.2	-1.93	0.74	0.69	0.61	0.07	0.65	0.76	0.83
5.2	-1.77	0.71	0.71	0.64	0.28	0.71	1.00	1.28

Table SI-4: NBO Charge on each atom of NH₃...HBr complex.

Cavity Size (Å)	q _(N)	q _(H1)	q _(H2)	q _(H3)	q _(Br)	q _(H4)	q _(NH4)	q(Total) on NH ₃ HBr
∞	-0.99	0.38	0.38	0.38	-0.40	0.25	0.40	0.00
12.2	-0.92	0.43	0.43	0.42	-0.77	0.40	0.76	-0.01
8.7	-0.91	0.42	0.42	0.43	-0.78	0.40	0.77	-0.01
8.2	-0.95	0.46	0.43	0.43	-0.83	0.41	0.78	-0.05
7.1	-1.32	0.53	0.53	0.53	-0.82	0.53	0.80	-0.02
6.1	-1.57	0.69	0.66	0.66*	0.32	0.68	1.12	1.44
5.2	-2.01	0.67	0.74	0.63	0.38	0.69	0.72	1.10
5.2	-2.00	0.70	0.71	0.64*	1.32	0.69	0.74	2.06

Table SI-5: NBO Charge on each atom of NH₃...HI complex.

Cavity Size (Å)	q(N)	q(H1)	q(H2)	q(H3)	q(I)	q(H4)	q(NH4)	q(Total) on NH ₃ HI
∞	-0.98	0.39	0.39	0.39	-0.37	0.18	0.37	0.00
12.2	-0.91	0.45	0.45	0.43	-0.87	0.45	0.86	-0.01
8.7	-0.93	0.43	0.44	0.44	-0.78	0.40	0.78	0.00
8.2	-1.03	0.49	0.46	0.47	-0.86	0.47	0.86	0.00
7.1	-1.54	0.56	0.59	0.58	-0.44	0.59	0.77	0.33
6.1	-1.80	0.67	0.70	0.64*	0.53	0.69	0.90	1.43
5.2	-2.10	0.68	0.70	0.63	1.33	0.67	0.58	1.91
5.2	-2.22	0.65	0.67	0.67*	3.58	0.63	0.40	3.98

XYZ files of optimized NH₃...HX complexes in nanocavities of different sizes.

1. NH₃-HF@C₁₈₀

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N  2.4320803  0.2715430 -2.0362311
H  2.4947899  0.1929240 -3.0429887
H  3.0298580  1.0323839 -1.7400884
H  1.4770589  0.5155596 -1.8016975
F  2.9087881 -1.9507250 -0.8060927
H  2.7869259 -1.1065179 -1.2973346
C  1.6797299  1.7723172  4.8055214
C  1.5653142  3.0217656  4.0783207
C -0.6762601  1.9139992  5.3945316
C  0.5023914  1.1695465  5.3955600
C -0.7884075  3.1426985  4.6792568
C  0.2746972  3.6642329  3.9436991
C  2.8428146  0.9301841  4.6163028
C  2.6139581  3.4226888  3.1640292
C  0.3957154 -0.2599510  5.5999804

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2. NH₃-HF@C₉₆

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H	1.5309642	-1.7364460	-2.4302518
H	-0.0074036	-2.2258067	-2.2426457
H	1.2125376	-3.2403199	-1.8657730
F	0.3511360	-1.5133486	0.5609425

H	0.6319060	-1.7893481	-0.3449777
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C	-2.5351784	-2.6451264	-1.2197765
C	-1.9029075	-3.9666193	-1.2701055
C	-1.3752457	-4.4187643	-2.4916572
C	-1.7529338	-0.6069080	2.4016471
C	-2.1269727	0.1563344	1.2539438
C	-2.5320121	-0.4634606	0.0636106
C	-1.8608523	-1.9790202	2.3803184
C	-2.3425273	-2.6363514	1.2068595
C	-2.6421798	-1.9240626	0.0382985
C	0.7859646	1.8799606	2.3672435
C	-0.6174570	0.0057070	3.0335341
C	-0.4534295	1.2800223	2.3924381
C	0.2742206	-4.8152466	2.2507240
C	1.4782432	-4.3545327	2.8847350
C	1.5918749	-3.0361918	3.3941171
C	-0.8589902	-4.0356862	2.2995187
C	-0.8323783	-2.7767535	2.9889358
C	0.3820602	-2.2112814	3.4518024

C	0.4949111	-0.7524368	3.4753187
C	1.8157521	-0.1186519	3.4439213
C	1.9046078	1.2184834	2.9791783
C	-1.3719165	-4.5601985	-0.0563489
C	-0.1668290	-5.3914860	-0.1079595
C	0.6025683	-5.5279050	1.0579399
C	-1.7062516	-3.9377440	1.1558484

3. NH₃-HF@C₈₀

86

N	-2.6426210	0.3811101	-0.5851333
H	-3.4203875	0.5028438	-1.2229497
H	-2.1023417	-0.4161871	-0.9012046
H	-2.0536264	1.2023485	-0.6553594
F	-3.4518426	0.0411276	1.7620568
H	-3.1292904	0.1777622	0.8254188
C	-0.0263027	2.8016178	1.5883401
C	-0.4571796	3.3899682	0.3548535
C	-0.0418485	2.7759809	-0.8697881
C	-1.6888240	4.0973696	0.3551521
C	-0.8728037	2.8307293	2.7685668
C	-3.1819020	2.8899023	3.5514202
C	-2.1500432	3.4514521	2.7391311
C	-2.5300748	4.1381315	1.5384583
C	-2.5291749	4.1047839	-0.7948092
C	-2.1552010	3.4089698	-2.0076842
C	-0.8755531	2.7956121	-2.0477891
C	-3.1975766	2.8226723	-2.7714098
C	-3.8792147	4.1329684	-0.3383438
C	-5.9889791	2.9025930	-0.2999347
C	-4.9067644	3.4617207	-1.0526204
C	-4.5570416	2.8442418	-2.2949749
C	-4.5405087	2.9131153	3.1217175
C	-4.8976009	3.4974386	1.8693621
C	-3.8723638	4.1597721	1.1126974
C	-5.9766135	2.9172455	1.1522771
C	-2.9974335	1.5958787	-3.4909295
C	-1.7363545	0.9228909	-3.4632386
C	-0.6697213	1.5591932	-2.7561480
C	-1.7578009	-0.5057366	-3.4692964
C	-4.2372523	0.8652074	-3.4663680
C	-5.3117300	-1.1719620	-2.6247493
C	-4.2464855	-0.5519172	-3.3842424
C	-2.9989020	-1.2279690	-3.4309863

C	-6.6168674	1.7089424	-0.7135172
C	-6.1927421	1.0257004	-1.8995588
C	-5.1953700	1.6443121	-2.7182199
C	-6.2654518	-0.3926523	-1.9072594
C	-0.7797620	-1.2722542	-2.7429422
C	0.2222296	-0.6287903	-1.9699031
C	0.2938981	0.7880597	-2.0203267
C	0.6361749	-1.2721219	-0.7406052
C	-1.4295016	-2.4626693	-2.2478435
C	-2.0990709	-3.7035179	-0.2326044
C	-1.0752548	-3.0436593	-0.9886451
C	0.0012693	-2.4586284	-0.2712263
C	-5.0990996	-2.3717965	-1.8869729
C	-3.8234414	-2.9950848	-1.8561350
C	-2.7896365	-2.4326823	-2.6702761
C	-3.4437819	-3.6820164	-0.6586508
C	1.0264482	-0.5152404	0.4021451
C	1.0033864	0.9045557	0.3812890
C	0.6744428	1.5449051	-0.8549643
C	0.6905915	1.5868270	1.6014530
C	0.6425778	-1.2518256	1.5928553
C	-0.7816751	-1.1836930	3.5930572
C	0.2168467	-0.5669625	2.7806319
C	0.2938062	0.8510936	2.7893518
C	-2.0933701	-3.6775706	1.2192140
C	-1.0675984	-3.0054936	1.9357611
C	0.0149493	-2.4434624	1.1802848
C	-1.4164704	-2.3893088	3.1757394
C	-1.7425588	-0.4049465	4.3337089
C	-1.7310164	1.0083740	4.2586907
C	-0.6617272	1.6299441	3.5029980
C	-2.9744955	1.6847775	4.3134934
C	-2.9782100	-1.1371947	4.3696038
C	-5.3014136	-1.0996577	3.6373297
C	-4.2410740	-0.4674282	4.3570335
C	-4.2157782	0.9614691	4.3528842
C	-3.4428810	-3.6466372	1.6736787
C	-5.0890520	-2.3282105	2.9215355
C	-3.8161500	-2.9467302	2.8863932
C	-2.7764952	-2.3655954	3.6524146
C	-5.9460292	-2.3419053	-0.7080350
C	-5.9243201	-2.3133038	1.7476984
C	-5.5135045	-2.9305018	0.5275748
C	-4.2843244	-3.6421426	0.5256229
C	-7.0013581	0.9733420	0.4787142

C	-6.6478942	-1.0854164	1.7355556
C	-6.9767861	-0.4464364	0.5022030
C	-6.6614851	-1.1290834	-0.7204167
C	-5.1865485	1.7227622	3.6146546
C	-6.2669880	-0.3298449	2.9021413
C	-6.1906861	1.0837007	2.8480849
C	-6.6082564	1.7293003	1.6195379

4. NH₃-HF@C₆₀

66

N	-0.7134146	2.3084680	1.8688589
H	-1.4446369	1.9214694	2.4148397
H	-0.4592708	3.2182749	2.2112345
H	0.1017724	1.7208454	1.8903791
F	-0.3283078	2.9040033	-0.1887485
H	-0.7983037	2.5426793	0.6519901
C	-0.0195005	2.1566428	4.6218218
C	0.0383573	0.7662600	4.1700427
C	1.2926542	0.5905176	3.4366417
C	2.0050661	1.8581098	3.4389180
C	1.1989109	2.8206775	4.1672030
C	-3.2168426	3.1802554	3.3651375
C	-2.4597901	2.1973533	4.1422889
C	-1.2415503	2.8592447	4.6227031
C	-1.2685069	4.2412215	4.1425181
C	-2.4815834	4.4319589	3.3674392
C	-2.2873499	-0.4648858	1.7340840
C	-1.0709168	-0.6760973	2.4927704
C	-1.1313134	0.1298391	3.7093468
C	-2.4079869	0.8549062	3.6970179
C	-3.1128224	0.4777845	2.4669121
C	1.3771029	-0.1582568	-0.0895535
C	2.0974407	0.2220313	1.1064947
C	1.3383523	-0.2025927	2.2777246
C	0.1341838	-0.8451169	1.7985712
C	0.1664579	-0.8169926	0.3439994
C	2.7264604	3.6531289	0.3961188
C	2.6910142	3.6353484	1.8505065
C	2.7244652	2.2622690	2.3020682
C	2.7807974	1.4319421	1.1172604
C	2.7816799	2.2864554	-0.0601977
C	-0.0898791	5.7204760	2.5215888
C	-0.0901393	4.8754063	3.7109322
C	1.1659657	4.1509533	3.7253815

C	1.9235544	4.5600875	2.5498878
C	1.1521033	5.5289434	1.8043706
C	-3.0851022	3.2271902	-1.2990305
C	-2.2900624	2.2715429	-2.0452353
C	-1.0798272	2.9384051	-2.5280833
C	-1.1340499	4.3274573	-2.0587613
C	-2.3746863	4.4891006	-1.3014685
C	-3.8377751	1.4308610	1.7371956
C	-3.7935904	1.4542499	0.2809582
C	-3.8211868	2.8259044	-0.1715267
C	-3.8781673	3.6534599	1.0125436
C	-3.8871797	2.8011215	2.1930163
C	-1.0015527	-0.6165143	-0.3818606
C	-1.0018143	0.2332128	-1.5637129
C	-2.2533023	0.9510744	-1.5845912
C	-3.0159166	0.5380450	-0.4150135
C	-2.2450373	-0.4314061	0.3310705
C	2.1057936	1.9169137	-1.2280371
C	1.3576145	2.8958786	-2.0159806
C	0.1436107	2.2359065	-2.5066760
C	0.1675526	0.8612383	-2.0045366
C	1.3761327	0.6666759	-1.2270986
C	1.1807228	5.5400511	0.3996672
C	-0.0284054	5.7573928	-0.3661297
C	0.0340173	4.9588480	-1.5892186
C	1.3023841	4.2289939	-1.5669935
C	1.9958090	4.5949279	-0.3330646
C	-2.4684423	5.2422300	2.2204025
C	-3.1845360	4.8556416	1.0230978
C	-2.4221407	5.2734306	-0.1431350
C	-1.2260345	5.9217013	0.3334449
C	-1.2580247	5.9025471	1.7890110

5. NH₃-HF@C₅₀

56

N	-0.0805946	2.0354354	-2.8223294
H	-0.7158626	1.3526464	-3.1726905
H	0.8155690	1.6073448	-2.8118241
H	-0.0792976	2.8514036	-3.3637087
F	-0.3313355	1.1168360	-1.0259093
H	-0.3267791	1.9694394	-1.7047949
C	-0.2673245	4.6734328	-0.9982812
C	-0.5398102	3.8977443	0.1352971
C	0.5338254	3.1533064	0.7627624

C	-1.1566761	4.6951540	-2.1445907
C	-1.7305551	3.0796626	0.2248938
C	-2.5493104	3.0342467	-0.9166209
C	-2.2716119	3.8475398	-2.1073711
C	-1.3845849	1.8529792	0.9715908
C	0.0575730	1.9368710	1.2622370
C	-1.9036166	0.6235365	0.5471972
C	-2.7858200	0.5849873	-0.6347136
C	-3.0837840	1.7641578	-1.3544933
C	-0.9721258	-0.5279645	0.4228937
C	0.5055839	-0.3557693	0.4674752
C	1.0156333	0.8780179	0.8913787
C	2.0734033	1.5345690	0.0961163
C	2.5713272	0.9554878	-1.0850940
C	1.0423385	-0.9705111	-0.7627093
C	2.0419502	-0.3190537	-1.5236645
C	2.0569953	3.7257555	-1.0779451
C	2.6387515	3.1467883	-2.2729358
C	1.7819468	2.9519939	0.0553089
C	2.8755466	1.7617810	-2.2779952
C	2.5406722	0.9897733	-3.4698048
C	2.0346021	3.8118064	-3.4376129
C	1.7118459	3.0815574	-4.5936510
C	1.9775211	1.6335301	-4.6176072
C	0.9373611	-0.8785728	-3.6590262
C	2.0108796	-0.2868080	-2.9875154
C	1.0792526	4.6945841	-1.5177149
C	1.0617721	4.7702523	-2.9162576
C	0.3870975	3.3084002	-5.2152137
C	-0.6840247	4.0664641	-4.5252964
C	-0.3325068	4.7867768	-3.3629803
C	-0.1320250	2.0673864	-5.6188770
C	-1.0997131	-0.3979945	-4.6958340
C	0.3364030	-0.2097274	-4.8091234
C	0.8313264	1.0123236	-5.2825709
C	-0.0830810	-1.5413938	-1.4835338
C	-1.3626222	-1.1446708	-3.5408276
C	-0.1233123	-1.4911260	-2.8797273
C	-3.1310949	1.8014225	-2.8162595
C	-2.8440199	0.6415257	-3.5426379
C	-2.4569844	-0.5543814	-2.8046356
C	-2.4265539	-0.5917271	-1.4058941
C	-1.3009903	-1.2403971	-0.7320598
C	-1.5435181	1.9727694	-5.2209359
C	-1.8855543	3.2022123	-4.4982067

C	-2.6413014	3.0908635	-3.2934919
C	-2.0125239	0.7340638	-4.7452120

6. NH₃-HF@C₄₈

54

N	3.9583124	6.0729481	-1.8576547
H	4.9596585	6.0516268	-1.9063789
H	3.5904776	6.8600230	-1.3896198
H	3.4444473	6.0823691	-2.6968814
F	1.8247345	6.1262088	-1.8334408
H	3.5599413	5.3070638	-1.3798374
C	6.9091739	4.8216758	-3.0257474
C	6.0443800	3.8748061	-2.5371762
C	4.7149719	3.7636717	-2.9830750
C	1.9641573	3.8643310	-2.9602695
C	2.6171369	4.7651100	-3.9102295
C	6.3399907	5.9533356	-3.7714690
C	4.8217939	8.2648604	-3.1344292
C	4.1717942	7.2799819	-4.0131002
C	4.9395844	5.9720986	-4.2008044
C	4.1107643	4.7191250	-3.9242789
C	2.6616575	3.4649200	-1.7482307
C	4.0052960	3.4061083	-1.7507534
C	-0.1817734	5.0723783	-0.5731176
C	1.9665007	3.9334673	-0.5547637
C	0.6320400	4.0531584	-0.9965072
C	-0.1894221	4.9905483	-3.0145767
C	0.6305095	4.0063356	-2.5246196
C	1.8519892	6.0470768	-4.1496642
C	0.4276710	6.0937461	-3.7654547
C	2.6773956	7.3054922	-3.9973843
C	6.0503455	3.9228076	-1.0150930
C	6.9148000	4.9044694	-0.6029046
C	4.7279075	3.8291614	-0.5436857
C	1.8704271	6.2019483	0.4617828
C	0.4402327	6.2235557	0.0978379
C	2.6296865	4.9083045	0.3181561
C	4.1246706	4.8626451	0.3265530
C	4.9496065	6.1298276	0.4949752
C	6.3493052	6.0823950	0.0662594
C	7.6376739	5.3155276	-1.8321645
C	7.6704113	6.6585460	-1.8773451
C	6.9691941	7.1846536	-0.6795595
C	6.1512629	8.1755258	-1.1581514

C	4.8353579	8.3627290	-0.6962949
C	2.6896921	7.4465716	0.2339857
C	4.1856589	7.4219800	0.2425007
C	2.0721056	8.3898993	-0.7049620
C	6.1455510	8.1220982	-2.6803039
C	6.9639588	7.1048589	-3.1026852
C	2.7865806	8.7426283	-1.9261722
C	4.1314666	8.7349848	-1.9301946
C	-0.1276298	7.3552174	-0.6502392
C	0.7327488	8.3040997	-1.1397531
C	-0.8888189	5.5193228	-1.8085893
C	-0.8573453	6.8606051	-1.8537697
C	2.0691443	8.2976088	-3.1096403
C	0.7306504	8.2487114	-2.6676293
C	-0.1357159	7.2734004	-3.0913241

7. NH₃-HF@C₃₆

42

N	-0.5698048	-1.6315195	-1.5148215
H	0.0620848	-2.2201005	-1.0546301
H	-0.3496300	-1.5171801	-2.4565762
H	-1.4517159	-2.0454805	-1.4447285
F	-1.0902485	-1.8878290	0.2632838
H	-0.6089424	-0.7793544	-1.0351774
C	1.3098791	-3.0354373	-2.4754933
C	1.1830061	-3.0806455	0.4006802
C	1.8159062	-1.9345782	-0.2796698
C	1.8928766	-1.9098051	-1.7474138
C	0.5829406	-2.4683179	-3.6376912
C	-0.7372475	-3.0439599	-3.6352182
C	-1.9017275	-2.2104689	-3.6325082
C	0.7368695	-1.0170538	-3.6197854
C	-0.4547472	-0.1742389	-3.6125690
C	-1.7584192	-0.7854837	-3.6102805
C	0.7881214	0.3360619	-0.2545269
C	0.8448662	0.4045519	-1.7213529
C	1.5555203	-0.6599712	-2.4470611
C	1.3938210	-0.7651768	0.4340550
C	-3.1784688	-1.4086921	-1.7777149
C	-2.7858428	-2.6226703	-2.4926010
C	-3.2543116	-1.4497774	-0.3063140
C	-2.5463365	-0.2677845	-2.4522188
C	-2.1289735	-3.7329322	-1.8041246
C	-0.8594026	-3.9985636	-2.4945375

C	-2.1967484	-3.7893205	-0.3326017
C	-2.9315916	-2.7201701	0.3420764
C	-0.9386398	-4.0874114	0.4161871
C	0.3656940	-4.0044663	-0.3208266
C	0.3994437	-3.9807069	-1.7856920
C	-1.9106324	-2.2703286	1.3820990
C	-0.8199938	-3.3178580	1.6508647
C	0.4494312	-2.6214644	1.6160319
C	-1.9745951	-0.7648332	1.6790183
C	-1.6959534	0.6529192	-1.7337989
C	-1.7237952	0.6161330	-0.2690876
C	-2.6415563	-0.3222109	0.4587690
C	-0.3906017	0.7247701	-2.4335052
C	-0.4840606	0.6055041	0.4417465
C	-0.6136488	-0.2706137	1.6422740
C	0.5209239	-1.1729768	1.6098931

8. $\text{NH}_3\text{-HCl@C}_{180}$

186

N	-1.7856235	2.2972295	0.7776934
H	-1.1697226	2.0873216	-0.0000537
H	-1.6416165	3.2611478	1.0487981
H	-2.7422304	2.1834211	0.4692350
Cl	-1.1393225	0.5531863	3.0599815
H	-1.4844455	1.3997340	1.9705272
C	4.4552609	-3.2634022	3.7373671
C	5.4157616	-2.2765224	3.2872441
C	3.8408657	-1.8064967	5.5839049
C	3.5898854	-2.9687188	4.8583335
C	4.7852922	-0.8356374	5.1410456
C	5.5067216	-0.9991379	3.9605092
C	4.0743401	-4.3512996	2.8627047
C	5.9914781	-2.3814776	1.9644335
C	2.2865377	-3.5798169	4.9975432
C	4.7899626	-4.5116936	1.6780668
C	2.8070553	-1.1251160	6.2895790
C	5.7346733	-3.5407808	1.2354097
C	4.3354327	0.4451192	5.5741329
C	5.9587493	0.1932593	3.2776344
C	2.7813964	-4.9929867	2.9603723
C	1.9517443	-4.6617903	4.0981371
C	3.1128790	0.2660486	6.2835465
C	6.4538872	-1.2184735	1.2386210
C	6.5231352	0.0367361	1.9548131

C	1.2362575	-2.8847582	5.7125816
C	1.4922614	-1.5837529	6.2868677
C	5.5022559	1.4955344	3.7189637
C	4.5949536	1.6000173	4.8402729
C	4.2081846	-5.1172132	0.5268820
C	5.7364138	-3.5463247	-0.1898565
C	0.6357559	-5.1184441	4.0962484
C	2.1901984	-5.6093691	1.7903483
C	6.4562929	-1.2245407	-0.2103188
C	6.7763354	1.1912352	1.2172779
C	4.7928375	-4.5207137	-0.6274774
C	2.1122889	1.2345880	6.2759935
C	2.8943281	-5.5810755	0.5268205
C	-0.1432470	-3.2735021	5.5272692
C	5.9960328	-2.3934171	-0.9277885
C	0.4376783	-0.6123219	6.4765966
C	-0.3962421	-4.4346568	4.8019802
C	5.6126193	2.6359928	2.8361936
C	3.6685719	2.7023759	4.9725540
C	0.0543087	-5.7252773	2.9454671
C	6.3275579	2.4721373	1.6516976
C	0.7717531	-5.8925774	1.7629092
C	0.7476088	0.7986510	6.4718886
C	2.4248997	2.5177805	5.6910931
C	6.7780286	1.1851423	-0.2076277
C	6.5278355	0.0245887	-0.9365389
C	-1.2307970	-2.3362100	5.7019572
C	-0.9251617	-1.0475786	6.2776638
C	4.0815571	-4.3710789	-1.8161368
C	2.1941683	-5.6195916	-0.7387526
C	3.8176508	3.8181212	4.0651157
C	4.7089276	3.7621258	2.9272328
C	5.4241336	-2.2996957	-2.2531093
C	-1.6149771	-4.6191823	4.0888993
C	-1.3371991	-5.4168901	2.9413932
C	6.0522432	3.2577810	0.4950586
C	2.7890532	-5.0134666	-1.9124246
C	0.0260805	-5.9381774	0.5239550
C	4.4651522	-3.2905246	-2.6984028
C	6.3305037	2.4623559	-0.6541293
C	-0.3068236	1.7653294	6.2694405
C	1.3349821	3.4475274	5.5002199
C	5.9675269	0.1702611	-2.2623915
C	0.7755422	-5.9029299	-0.7131379
C	-1.9266681	-0.0800480	6.2807432

C	5.5174715	-1.0278867	-2.9367424
C	-2.4676696	-2.5234700	4.9798801
C	2.8148159	4.7846994	4.0579692
C	-2.6126115	-3.6476671	4.0826913
C	4.4304140	4.5615724	1.7516422
C	-0.0450239	3.0566302	5.6817051
C	-1.6224683	1.3107501	6.2793504
C	1.5918620	4.6017169	4.7661695
C	5.0557579	4.2312774	0.4896325
C	-2.0518940	-5.2688351	1.7552896
C	-1.3887944	-5.6259772	0.5203831
C	5.6204808	2.6167915	-1.8428028
C	1.9629312	-4.6926216	-3.0559784
C	5.5129987	1.4689989	-2.7164105
C	3.6037558	-3.0054771	-3.8252886
C	0.0619150	-5.7476132	-1.8997464
C	-3.1484285	-0.2647310	5.5739543
C	-3.3921839	-1.4219736	4.8395900
C	4.8011696	-0.8746516	-4.1218609
C	2.5403223	5.5697190	2.9015494
C	-3.4977250	-3.6020892	2.9423765
C	3.2611835	5.4124955	1.7199042
C	0.6470020	-5.1502672	-3.0537847
C	-3.2182631	-4.4142228	1.7762636
C	2.3009682	-3.6190835	-3.9651063
C	-2.6565248	1.9872217	5.5701176
C	3.8583463	-1.8494391	-4.5600553
C	-1.0914205	3.7399787	4.9563121
C	4.4344965	4.5507023	-0.7770537
C	0.5613998	5.2713951	4.0479364
C	-2.0483847	-5.2808679	-0.7200217
C	4.7173437	3.7419716	-1.9457265
C	-1.3298947	-5.4406897	-1.9028817
C	-3.6006825	1.0131485	5.1341319
C	4.6101181	1.5640253	-3.8423911
C	4.3536382	0.4024599	-4.5676589
C	1.1471426	5.8699184	2.8959952
C	-2.3946292	3.1334049	4.8248286
C	-4.2888509	-1.3281117	3.7131591
C	-0.7523483	4.8097121	4.0478812
C	-4.3969259	-2.4753736	2.8402226
C	2.6016368	5.7563773	0.4799523
C	3.2653723	5.4025324	-0.7554600
C	-3.8408246	-4.0959024	0.5104263
C	-0.3830153	-4.4746177	-3.7701201

C	2.8279350	-1.1746848	-5.2768465
C	1.2535730	-2.9329401	-4.6941972
C	-3.2166874	-4.4279902	-0.7518167
C	3.8305786	3.7895337	-3.0877711
C	-1.6047385	-4.6545086	-3.0592089
C	3.6853465	2.6667496	-3.9884141
C	-4.3021099	1.1637297	3.9410493
C	3.1344829	0.2172384	-5.2816063
C	0.4346032	6.0250932	1.7108967
C	-4.7415022	-0.0320001	3.2625673
C	-0.1273811	-3.3228980	-4.5108862
C	1.5134166	-1.6365039	-5.2807516
C	-5.1112955	-2.3248311	1.6551738
C	-3.2508442	3.4185664	3.6967939
C	1.1854783	6.0640087	0.4768659
C	-1.5802458	5.1352087	2.9087930
C	-4.8368424	-3.1222715	0.5063083
C	2.5498171	5.5521497	-1.9413216
C	2.8286547	4.7576731	-3.0910988
C	-4.2054941	2.4310344	3.2533154
C	-3.4965766	-3.6300455	-1.9280735
C	-2.6068394	-3.6870110	-3.0670374
C	-0.9842559	5.7422862	1.7369578
C	-2.8790178	4.5059381	2.8191293
C	2.1358039	1.1882456	-5.2916417
C	2.4457874	2.4780520	-4.7145588
C	-5.2961207	0.1121650	1.9376042
C	-5.5521183	-1.0467731	1.2096943
C	-1.2160537	-2.3893716	-4.6997337
C	0.4599742	-0.6665905	-5.4864914
C	0.4399838	6.0173207	-0.7595072
C	-5.1109628	-2.3370953	-0.6501544
C	1.1573357	5.8549357	-1.9426713
C	-2.4580477	-2.5720809	-3.9761688
C	-4.3986612	-2.5033560	-1.8357936
C	1.6090904	4.5708795	-3.8037756
C	0.7721076	0.7486073	-5.4921578
C	-4.7831938	2.5327815	1.9323072
C	1.3566074	3.4125956	-4.5354765
C	-1.6877284	5.7124347	0.4756987
C	-0.9047980	-1.1039725	-5.2863204
C	-3.6008060	4.6704777	1.6356683
C	-5.5523509	-1.0543017	-0.2142455
C	-5.2281819	1.3606462	1.2132719
C	-0.9778876	5.7314110	-0.7842756

C	0.5764437	5.2482884	-3.0930502
C	-4.5437874	3.6947257	1.1976596
C	-3.0077762	5.2591984	0.4786206
C	-3.3825940	-1.4678425	-3.8411508
C	-4.2872739	-1.3632692	-2.7178170
C	-0.2818187	1.7196574	-5.2965590
C	-0.0232276	3.0197135	-4.7183511
C	-5.2989869	0.0983234	-0.9509892
C	-5.2286385	1.3530031	-0.2342001
C	-1.9040431	-0.1329533	-5.2880961
C	-0.7376202	4.7873086	-3.0919738
C	-1.5659207	5.1131354	-1.9513708
C	-4.7397712	-0.0603893	-2.2736682
C	-3.1247587	-0.3122090	-4.5751822
C	-4.5338684	3.6828415	-0.2297834
C	-1.5966148	1.2586817	-5.2925467
C	-3.5796809	4.6434466	-0.6701147
C	-1.0718282	3.7091261	-3.9942058
C	-4.7779193	2.5180984	-0.9590805
C	-2.8569556	4.4738834	-1.8499397
C	-4.2880079	1.1306689	-2.9541791
C	-3.5709185	0.9679079	-4.1372511
C	-2.3730096	3.0973143	-3.8511499
C	-2.6268222	1.9382284	-4.5800700
C	-4.1955569	2.4062988	-2.2778826
C	-3.2345195	3.3893464	-2.7261892

9. NH₃-HCl@C₉₆

102

N	0.5922945	0.5576529	-1.3862060
H	-0.3334265	0.9801911	-1.4554336
H	0.7140045	-0.0847738	-2.1673205
H	1.2976054	1.2907277	-1.4595984
Cl	0.9282894	-1.2365634	0.8442121
H	0.7128201	-0.0761615	-0.4301999
C	0.6287341	3.9060075	0.3156798
C	-0.8073079	3.6072757	0.3121947
C	1.3391999	3.7681935	1.5194008
C	-1.4094445	3.1963002	1.5127331
C	-2.5632772	2.2430467	-0.8936512
C	-1.4704217	3.2240951	-0.9228820
C	-0.7493535	3.3943942	-2.1192289
C	-2.8346427	1.5133072	-2.0619960
C	-2.0263286	1.6531335	-3.2330653

C	-1.0040752	2.5779615	-3.2652154
C	-2.9951156	1.6536162	0.3640329
C	-3.4554813	0.2602006	0.4094493
C	-2.4949105	2.2323489	1.5395330
C	-3.3673231	-0.4352727	1.6255994
C	0.6717392	3.6896710	-2.1158438
C	1.3954511	3.8196705	-0.9160530
C	2.7893336	3.3561271	-0.8810643
C	1.2360659	3.0440509	-3.2605278
C	2.5427780	2.6041544	-3.2233196
C	3.3344180	2.7964639	-2.0477820
C	0.2366386	2.2376122	-3.9072641
C	3.4143707	2.9860636	0.3793944
C	2.7191572	3.3168178	1.5522229
C	2.8839406	2.5574592	2.7511152
C	4.3913972	1.8915083	0.4282282
C	4.5825361	1.2176524	1.6446522
C	3.7971219	1.5278419	2.7968633
C	4.0660571	0.8945875	-3.1403552
C	4.3037999	1.7170755	-1.9991861
C	4.7412841	1.1691285	-0.7822557
C	4.3467051	-0.4525162	-3.0873182
C	4.8747972	-1.0305839	-1.8908480
C	5.0421589	-0.2675099	-0.7254117
C	2.8899406	1.3503598	-3.8298475
C	1.9039317	0.4522719	-4.3159696
C	0.5117779	0.9187353	-4.3643843
C	3.8273455	-2.0181728	2.9252705
C	3.4701896	0.3159659	3.4950752
C	4.2615961	-0.7130330	2.8815212
C	4.9862907	-0.9807849	0.5399644
C	4.8815373	-0.2022272	1.7014095
C	3.9934482	-2.8632641	1.7871059
C	4.5239592	-2.3723775	0.5856038
C	2.5959894	-2.3393325	3.5890844
C	1.7069658	-1.3306816	4.0370258
C	2.1639267	0.0599152	3.9807571
C	1.1909425	1.1528694	3.9266299
C	1.6124422	2.4012129	3.4009939
C	0.7090334	3.2723110	2.7015065
C	-0.2420539	0.8546068	3.9231156
C	-1.1237818	1.8323831	3.3945059
C	-0.6389273	2.9919529	2.6982657
C	2.1253301	-3.5473416	2.9698840
C	0.2737921	-1.6289606	4.0339996

C	-0.6989446	-0.5356549	3.9741208
C	0.7779848	-3.8281640	2.9672449
C	-0.1378376	-2.9083627	3.5836735
C	2.3394924	-4.3290851	0.6383088
C	2.9165643	-3.8351097	1.8163106
C	0.1724522	-4.4068946	1.8103240
C	0.9040717	-4.6283228	0.6351922
C	3.0267517	-4.0277667	-0.6062557
C	4.4242687	-2.4107125	-1.8464884
C	4.1211260	-3.0498666	-0.6335714
C	2.3272125	-4.2774989	-1.7959311
C	-2.3490294	1.4692332	2.7384760
C	-2.7758038	0.1609635	2.7811674
C	-1.9962814	-0.8208926	3.4817483
C	-1.2024887	-3.9443269	1.7754610
C	-1.3918996	-3.1037953	2.9133010
C	-2.3093313	-2.0793741	2.8654258
C	-1.8788360	-3.7035583	0.5708081
C	-2.8566033	-2.6115582	0.5213718
C	-3.0754612	-1.8566817	1.6820536
C	0.3640334	-4.0071285	-2.9951796
C	0.9060410	-4.5732355	-1.7994552
C	0.1593616	-4.6243082	-0.6129842
C	-0.9429287	-3.5770338	-3.0255992
C	-1.7607067	-3.6963639	-1.8606949
C	-1.2340393	-4.1630968	-0.6459174
C	3.6318952	-2.6260527	-3.0150204
C	1.3752444	-3.2420212	-3.6679371
C	2.6046030	-3.5414779	-2.9898407
C	-2.7439988	-0.5212240	-3.1567300
C	-1.8431465	0.3659521	-3.8409738
C	-0.5790962	-0.0640466	-4.3217588
C	-2.4646538	-1.8684429	-3.1034759
C	-1.2746581	-2.3681113	-3.7291759
C	-0.2789373	-1.4986579	-4.2490051
C	1.1096551	-1.9577718	-4.2134471
C	2.2002354	-0.9831865	-4.2429900
C	3.4572771	-1.3843837	-3.7179125
C	-3.1865447	-1.9786327	-0.7449059
C	-3.4834663	-0.5411143	-0.8020030
C	-3.2950606	0.1368875	-2.0173515
C	-2.7236586	-2.6105357	-1.9088312

10. NH₃-HCl@C₈₀

86

N	-2.1961858	-0.3366271	1.4780902
H	-1.7298984	-1.2269643	1.5928982
H	-3.1940892	-0.4353031	1.6111439
H	-1.8188918	0.3508322	2.1168412
Cl	-1.7487373	0.5197648	-1.0345066
H	-2.0144468	0.0193973	0.4345791
C	-3.6611287	3.6230029	1.2902301
C	-2.9763070	3.2315133	2.4846598
C	-3.5390588	2.1919281	3.2961254
C	-1.5717015	3.3943739	2.5086184
C	-2.9387985	4.0645926	0.1053068
C	-0.8550755	3.8646812	-1.1391629
C	-1.5262122	4.1296028	0.0947311
C	-0.8494256	3.8431290	1.3281813
C	-0.7472712	2.4900150	3.2361486
C	-1.3054444	1.3884495	4.0045776
C	-2.7234972	1.2877361	4.0720991
C	-0.5500278	0.1839115	4.0674185
C	0.4675077	2.3590410	2.5040206
C	1.8806833	0.8091807	1.2781926
C	1.1649221	1.1294045	2.4761445
C	0.6601586	0.0603266	3.2878924
C	0.4140374	3.2210442	-1.1420992
C	1.0272082	2.8330518	0.0893022
C	0.4004732	3.2088098	1.3258488
C	1.8075263	1.6541202	0.0953378
C	-1.1959613	-1.1076856	4.1035878
C	-2.6318263	-1.2226534	4.0910654
C	-3.3860779	0.0042968	4.1105492
C	-3.1926574	-2.3241826	3.3522892
C	-0.3672239	-2.0186334	3.3491216
C	-0.2576459	-3.4005331	1.3186132
C	-0.9360752	-3.0551402	2.5578663
C	-2.3484826	-3.2266256	2.6031134
C	1.9915290	-0.5228647	0.8447102
C	1.3902829	-1.5857190	1.5923695
C	0.7712762	-1.2839001	2.8499969
C	0.8869116	-2.6863437	0.8616856
C	-4.4216265	-2.1743642	2.6076090
C	-5.1173731	-0.9331358	2.5676538
C	-4.6143108	0.1367622	3.3601655
C	-5.7994266	-0.5869058	1.3305088

C	-4.3219347	-2.9739605	1.4091681
C	-4.3135122	-2.9633511	-1.0585526
C	-4.9393169	-2.5880724	0.1737239
C	-5.7193543	-1.4088040	0.1703846
C	-0.9723227	-3.8193776	0.1604583
C	-2.3848873	-3.8849920	0.1683683
C	-3.0568623	-3.6157391	1.4061539
C	-3.0606400	-3.5990142	-1.0608358
C	-5.8992228	0.7594462	0.8761914
C	-5.3046373	1.8139077	1.6067900
C	-4.6926482	1.4904923	2.8622485
C	-4.8027497	2.9271729	0.8592070
C	-5.9032333	0.7655430	-0.5781998
C	-4.6869919	1.5308980	-2.5847080
C	-5.3001970	1.8307719	-1.3291075
C	-4.7986300	2.9306648	-0.5962895
C	-4.3791507	-2.1135561	-2.2382212
C	-5.0748543	-0.8830498	-2.2123797
C	-5.7926729	-0.5632191	-1.0106129
C	-4.5751902	0.1824291	-3.0237426
C	-3.5428675	2.2609584	-3.0740162
C	-2.9732519	3.2926852	-2.2862534
C	-3.6522582	3.6401368	-1.0489416
C	-1.5664342	3.4651095	-2.3289821
C	-2.7142540	1.3473688	-3.8226470
C	-0.5307078	0.2387350	-3.8284186
C	-1.2818317	1.4636714	-3.8146973
C	-0.7239068	2.5598356	-3.0724020
C	-3.1629637	-2.2429300	-2.9640519
C	-1.1917513	-1.0433973	-3.7967479
C	-2.6047122	-1.1407219	-3.7298989
C	-3.3598578	0.0576377	-3.7921149
C	-0.2491411	-3.3782266	-1.0227113
C	-0.3717108	-1.9518321	-3.0327313
C	-0.9348105	-2.9848730	-2.2211137
C	-2.3391619	-3.1495643	-2.2429580
C	1.9875965	-0.5152618	-0.6108391
C	0.7851880	-1.2479125	-2.5969103
C	1.3925733	-1.5678249	-1.3435837
C	0.8897977	-2.6839363	-0.5927089
C	0.5068440	2.4126099	-2.3334650
C	0.6990141	0.1075261	-3.0842674
C	1.1983803	1.1751404	-2.2959551
C	1.8821478	0.8297595	-1.0607377

11. NH₃-HCl@C₆₀

66

N	-1.0280256	0.1539261	0.9681693
H	-0.2644668	-0.1645075	1.5463946
H	-1.9081172	-0.1038092	1.3100710
H	-0.9030645	1.1521393	0.8884957
H	-0.8337289	-0.2127432	0.0478194
Cl	1.0073147	0.7307369	0.1724119
C	2.7670299	0.4872845	2.8305773
C	2.3716365	1.8766444	2.8239727
C	1.0929937	1.9652631	3.5190192
C	0.6879007	0.6522633	3.9619332
C	1.7244600	-0.2557037	3.5313599
C	3.4921652	-0.0699495	-0.6503522
C	3.7201515	0.7638346	0.5397029
C	3.4228363	-0.0604553	1.7171956
C	3.0149194	-1.3829183	1.2700129
C	3.0581384	-1.3921301	-0.1836631
C	1.6402446	3.6099216	-0.2037326
C	1.6046194	3.5893066	1.2501765
C	2.6445701	2.6803214	1.7060669
C	3.3331504	2.1267661	0.5341960
C	2.7046491	2.7085418	-0.6615866
C	-1.9149984	3.0271087	1.9401294
C	-1.2918744	2.4492486	3.1044508
C	0.1120597	2.8456319	3.0917448
C	0.3754392	3.6662719	1.9337165
C	-0.8771647	3.7643451	1.2201053
C	-2.3748518	-0.9920349	2.9112718
C	-1.0680140	-1.0680371	3.5901919
C	-0.6684777	0.2668759	3.9964248
C	-1.6994292	1.1883549	3.5647197
C	-2.7751784	0.4367272	2.8996958
C	0.9933409	-2.8264068	1.2446746
C	2.0081127	-2.0880490	1.9578617
C	1.3529393	-1.5251153	3.1164437
C	-0.0531074	-1.9275139	3.1328455
C	-0.2751927	-2.7343457	1.9592747
C	-0.5507453	0.2744528	-2.9051969
C	-1.5765644	1.1837019	-2.4531389
C	-2.6098719	0.4423588	-1.7378207
C	-2.2258696	-0.9468196	-1.7401011
C	-0.9511128	-1.0377098	-2.4510767
C	2.4847129	1.9050870	-1.8079547

C	1.1981607	1.9939105	-2.5085966
C	0.8039730	0.6592653	-2.9317031
C	1.8397035	-0.2664261	-2.5008506
C	2.8866503	0.4899590	-1.8028900
C	-0.8473912	3.7618404	-0.1657763
C	-1.8549593	3.0031902	-0.8683874
C	-1.2038044	2.4498707	-2.0321502
C	0.1938665	2.8641982	-2.0568403
C	0.4177947	3.6844215	-0.8889690
C	-3.3912122	1.0028229	1.7441229
C	-3.6137366	0.1605508	0.5435148
C	-3.2729693	0.9841638	-0.6264853
C	-2.8690317	2.3026609	-0.1822896
C	-2.9274421	2.3191832	1.2676746
C	-1.5017645	-2.6639273	1.2821238
C	-1.4667499	-2.6453495	-0.1659746
C	-2.5150265	-1.7518886	-0.6236144
C	-3.2321013	-1.2142431	0.5470120
C	-2.5925707	-1.7961739	1.7528234
C	2.0578086	-2.1010634	-0.8667336
C	1.4404567	-1.5310875	-2.0419116
C	0.0324737	-1.9135444	-2.0189480
C	-0.2338767	-2.7145076	-0.8476722
C	1.0197899	-2.8229638	-0.1404977

12. NH₃-HCl@C₅₀

56

N	0.1422962	-0.8646306	0.0087366
H	1.0078040	-0.3492519	0.0174515
H	-0.3905245	-0.6844513	-0.8282583
H	0.3603106	-1.8449458	0.0239157
Cl	-0.2635512	1.2196338	-0.0246161
H	-0.4186089	-0.6639029	0.8223425
C	-2.3311067	2.1546458	1.2556454
C	-1.1443126	2.9158208	1.3122635
C	-0.5562999	3.1392562	-0.0522579
C	-2.3524836	0.8953722	2.0220706
C	0.0488463	2.5672471	2.0982152
C	-0.0003077	1.3099472	2.7887982
C	-1.2083325	0.4843437	2.7567545
C	1.2686498	2.8865873	1.2666611
C	0.8754981	3.3929289	-0.0343513
C	2.3486349	1.9612268	1.2642182
C	2.2920809	0.7157379	2.0382140

C	1.1382360	0.3890031	2.7588242
C	2.9705487	1.6275067	0.0188187
C	2.3857866	1.9294365	-1.2524256
C	1.3066054	2.8540997	-1.3100867
C	0.1117486	2.5136775	-2.1691999
C	0.0826061	1.2392749	-2.8291538
C	2.3516015	0.6647215	-1.9959953
C	1.2195599	0.3197026	-2.7422181
C	-2.2923432	2.1214099	-1.3869700
C	-2.2914145	0.8432327	-2.1216033
C	-1.1040354	2.8812622	-1.4276134
C	-1.1261191	0.4142898	-2.8116544
C	-0.7211639	-1.0062642	-2.7638593
C	-2.9897954	-0.1284237	-1.2988028
C	-2.6149384	-1.4892601	-1.2677683
C	-1.4686440	-1.9678345	-2.0441430
C	1.4074141	-2.0886257	-2.0090089
C	0.7400503	-1.0704414	-2.7369227
C	-2.9244201	1.8718039	-0.0712611
C	-3.3423835	0.5215269	-0.0603483
C	-2.6026962	-2.1817272	-0.0153844
C	-2.6516655	-1.4579495	1.2182668
C	-3.0267286	-0.0968953	1.2039407
C	-1.5042052	-3.0947349	0.0124417
C	1.3009743	-3.2702552	0.0560476
C	0.6266068	-3.0957035	-1.2309421
C	-0.7974092	-3.0264173	-1.2557208
C	3.0151318	-0.3661336	-1.1948697
C	2.4683006	-2.4102794	0.0623858
C	2.5674383	-1.7158467	-1.1980310
C	0.6586988	-1.0010304	2.7747987
C	1.3469089	-2.0370528	2.0928946
C	2.5305511	-1.6842903	1.3073376
C	2.9785895	-0.3348322	1.2832981
C	3.3746845	0.2452757	0.0422149
C	-0.8352180	-2.9942345	1.2987009
C	-1.5289629	-1.9164531	2.0400478
C	-0.8027756	-0.9368417	2.7570986
C	0.5889138	-3.0636647	1.3176708

13. NH₃-HCl@C₄₈

54

N	-0.9216778	0.8920439	-0.0093049
H	-1.8709128	0.7834840	0.2320912

H	-0.4237380	1.2969036	0.7334371
H	-0.4972250	0.0417766	-0.2736418
Cl	1.4823144	0.9266761	-0.1306484
H	-0.8221209	1.5588469	-0.7315183
C	-3.3337722	-0.2752126	1.1161321
C	-2.4834628	-1.3051453	0.7146080
C	-1.1701078	-1.3967369	1.1975082
C	1.6119351	-1.3796187	1.2443300
C	0.9227055	-0.3595562	2.0489200
C	-2.7819025	0.8978728	1.8556167
C	-1.2093644	3.2174684	1.1501573
C	-0.5824729	2.2424143	2.0909075
C	-1.3773048	0.9152554	2.3301900
C	-0.5610857	-0.3740450	2.0860722
C	0.9256089	-1.8720673	0.0390873
C	-0.4105588	-1.8560023	0.0091345
C	3.8858959	-0.2474626	-1.0718653
C	1.6881366	-1.4612668	-1.1547211
C	3.0045837	-1.2702409	-0.6603017
C	3.7777166	-0.2107988	1.2976107
C	2.9572152	-1.2511349	0.8417314
C	1.7108405	0.9480732	2.2299530
C	3.1454865	0.9570664	1.9525159
C	0.9029700	2.2459288	2.0392023
C	-2.4454816	-1.3315986	-0.8165795
C	-3.2628707	-0.3037372	-1.2863393
C	-1.1159488	-1.4541359	-1.2350034
C	1.7938520	0.9041145	-1.9921656
C	3.3176646	0.9215346	-1.7453186
C	1.0190315	-0.4733463	-2.0233273
C	-0.4471905	-0.4518676	-2.1253094
C	-1.2418043	0.8601891	-2.4051367
C	-2.6555002	0.8515926	-2.0094736
C	-3.9843221	0.1798328	-0.1174479
C	-3.9978985	1.5538888	-0.1318648
C	-3.2750926	2.0161699	-1.3076933
C	-2.4776357	3.0699434	-0.8632113
C	-1.1518962	3.2198691	-1.2863161
C	1.0007782	2.2659735	-2.0518515
C	-0.4641309	2.2198213	-2.1744866
C	1.6483967	3.2867250	-1.2049147
C	-2.5164466	3.0775839	0.6663743
C	-3.3501722	2.0454737	1.0877161
C	0.8747352	3.6993550	-0.0170869
C	-0.4582064	3.6606378	-0.0462049

C	3.8643535	2.1094829	-1.0997852
C	2.9655440	3.1284799	-0.7060647
C	4.5241050	0.2556828	0.1456940
C	4.5104033	1.6416554	0.1303390
C	1.5724455	3.2548794	1.1980830
C	2.9190670	3.1397560	0.7941548
C	3.7572010	2.1210440	1.2704129

14. NH₃-HCl@C₃₆

42

N	-0.6315059	-1.7082789	-1.6348170
H	0.0791445	-2.4067777	-1.7090443
H	-0.3636974	-2.1903716	-3.0166902
H	-1.5394705	-1.9783378	-1.9137182
Cl	-0.7422885	-1.6048446	-0.1051231
H	-0.3707146	-0.8035227	-1.9108146
C	1.3439954	-3.0390020	-2.4382322
C	1.2132140	-3.0626818	0.4884080
C	1.8348947	-1.9181761	-0.1587222
C	1.8887108	-1.8741098	-1.6400778
C	0.6510174	-2.4654735	-3.6263294
C	-0.7791331	-3.1138500	-3.6664841
C	-1.9838924	-2.2104725	-3.6463632
C	0.7375165	-0.9667147	-3.5325351
C	-0.4670351	-0.1679233	-3.5196701
C	-1.7920490	-0.7820654	-3.5506407
C	0.7740176	0.3943498	-0.0685332
C	0.8139323	0.4341403	-1.5565555
C	1.5327055	-0.6360540	-2.3090491
C	1.4536175	-0.6983540	0.6018312
C	-3.2084649	-1.4006580	-1.7049392
C	-2.8330088	-2.6339865	-2.4821164
C	-3.2455272	-1.4460476	-0.2188313
C	-2.5711368	-0.2725468	-2.3553776
C	-2.1452219	-3.7269762	-1.7896150
C	-0.8683559	-4.0367087	-2.5049863
C	-2.1774072	-3.7497269	-0.3091689
C	-2.9098218	-2.6953857	0.4478070
C	-0.9394314	-4.0279787	0.3931775
C	0.3624940	-3.9880326	-0.2708952
C	0.4115981	-3.9904513	-1.7675553
C	-2.0847929	-2.3348295	1.6542566
C	-0.8881298	-3.1485067	1.6345620
C	0.4343204	-2.5592251	1.6957402

C	-1.9547508	-0.8746654	1.7021980
C	-1.7157021	0.6404069	-1.5906787
C	-1.7635079	0.6299111	-0.1042287
C	-2.6992175	-0.2956506	0.5651147
C	-0.4159522	0.7350636	-2.2848401
C	-0.4960027	0.7200442	0.6559249
C	-0.6135314	-0.2539530	1.7569210
C	0.5723195	-1.1210178	1.7451440

15. NH₃-HBr@C₁₈₀

186

N	2.4195882	0.5485998	-1.9864534
H	2.7568245	0.4400925	-2.9416855
H	3.0397524	1.1851084	-1.4876071
H	1.4834419	0.9488281	-2.0129420
Br	2.3330228	-2.1375237	-0.4873336
H	2.4075522	-0.4549191	-1.4558607
C	1.6857172	1.7654560	4.8003049
C	1.5717779	3.0149103	4.0736814
C	-0.6695928	1.9087685	5.3914038
C	0.5085738	1.1636251	5.3914490
C	-0.7814343	3.1369490	4.6753445
C	0.2816909	3.6579761	3.9395275
C	2.8477014	0.9222524	4.6099952
C	2.6202019	3.4141830	3.1586517
C	0.4016473	-0.2654860	5.5966042
C	3.9069091	1.4345273	3.8630559
C	-1.9520108	1.2857612	5.4009083
C	3.7934242	2.6613716	3.1472456
C	-2.1330675	3.2717576	4.2412219
C	-0.0343674	4.5111446	2.8133825
C	2.7898806	-0.5117746	4.7958369
C	1.5911411	-1.0641241	5.3896067
C	-2.8561409	2.1277624	4.6895419
C	2.3549167	4.2617960	2.0163371
C	1.0488415	4.8794116	1.9255858
C	-0.9021209	-0.8990880	5.6067699
C	-2.0943705	-0.1008171	5.4110588
C	-1.4093222	4.6495122	2.3724475
C	-2.4633231	3.9328344	3.0594211
C	4.7989837	0.5859347	3.1441428
C	4.6147160	2.5688856	1.9861205
C	1.4488817	-2.4499090	5.3859390
C	3.6962209	-1.3723661	4.0622434

C	3.1949852	4.1689993	0.8374920
C	0.7206492	5.5294088	0.7369771
C	5.2353591	1.2861859	1.9841077
C	-3.9309122	1.6097496	3.9689625
C	4.6573353	-0.7995131	3.1464476
C	-1.0115532	-2.3294572	5.4111896
C	4.2939016	3.2302372	0.8040652
C	-3.3023274	-0.6577887	4.8380112
C	0.1668900	-3.0737033	5.3984232
C	-1.6951927	5.1574029	1.0468162
C	-3.6853987	3.5426841	2.3887842
C	2.3435253	-3.2950958	4.6667377
C	-0.6309468	5.6674929	0.3043177
C	3.4042669	-2.7807242	3.9250144
C	-4.2224165	0.1991639	4.1155972
C	-4.4207027	2.3789593	2.8441932
C	1.5465384	5.4351694	-0.4207249
C	2.7261724	4.6925126	-0.4253933
C	-2.1957150	-2.9347716	4.8388784
C	-3.3607871	-2.0936665	4.6594971
C	5.5493430	0.6219020	0.8005739
C	5.1598871	-1.5325945	2.0050390
C	-3.9238928	4.0739604	1.0633084
C	-2.9016739	4.7937520	0.3328323
C	4.7859959	2.6658320	-0.4356672
C	0.2704634	-4.3056497	4.6881034
C	1.6160767	-4.4409854	4.2357678
C	-0.6400320	5.6612105	-1.1213992
C	5.6091019	-0.8208575	0.8306303
C	3.8797602	-3.5527810	2.7980204
C	5.4127680	1.3566530	-0.4372038
C	0.7059454	5.5159900	-1.5683502
C	-5.1976202	-0.3824212	3.2174031
C	-5.3919164	1.7510223	1.9726496
C	3.1820113	4.1556891	-1.6906896
C	4.8425455	-2.9376546	1.9132738
C	-4.4289008	-2.6127424	3.9291493
C	4.2956501	3.2304946	-1.6746716
C	-2.0903632	-4.1874134	4.1162179
C	-4.9908395	3.5480483	0.3364346
C	-0.8015638	-4.8298785	3.9687292
C	-2.9112714	4.7893525	-1.1177046
C	-5.7149373	0.3433395	2.0764456
C	-5.3326977	-1.7698255	3.2183301
C	-5.7148914	2.4045446	0.7847217

C	-1.7134524	5.1469857	-1.8475540
C	1.9292947	-5.1003116	3.0497421
C	3.1404650	-4.7125010	2.3594960
C	1.0198129	4.8543269	-2.7534277
C	5.7420552	-1.5153031	-0.4280355
C	2.3243475	4.2336964	-2.8545408
C	5.5523477	0.6200074	-1.6745956
C	5.1677322	-3.6031963	0.7344249
C	-4.3255451	-3.8450338	3.2192938
C	-3.1503839	-4.5947860	3.2175613
C	4.6131695	2.5646452	-2.8620878
C	-4.9992926	3.5433398	-1.0893908
C	-0.4994636	-5.6876790	2.8429244
C	-3.9418055	4.0653074	-1.8320296
C	5.6147370	-2.9019130	-0.4229866
C	0.8684702	-5.8219811	2.3835170
C	5.5993239	-0.8261604	-1.6902352
C	-5.7880808	-2.4812301	2.0695093
C	5.2423570	1.2830321	-2.8644622
C	-6.1782248	-0.3802985	0.9082116
C	-1.4432164	4.6283995	-3.1715058
C	-6.1708968	1.6930474	-0.3638824
C	3.3677559	-5.2504208	1.0382039
C	-0.0730591	4.4825288	-3.6243514
C	4.4371687	-4.7464868	0.3020117
C	-5.1656799	-3.7640670	2.0703989
C	2.5788995	3.3785579	-3.9916242
C	3.7627139	2.6391954	-4.0029242
C	-5.7281037	2.3968771	-1.5222459
C	-6.1225344	-1.8268408	0.8851666
C	-2.8991667	-5.4506297	2.0767390
C	-6.3171346	0.3068417	-0.3588862
C	-1.5927301	-6.0655993	1.9733114
C	-3.7196944	3.5252234	-3.1568951
C	-2.5050216	3.9095788	-3.8435836
C	1.1400780	-6.3343110	1.0594778
C	5.1602004	-3.6139360	-1.5708944
C	4.7883074	0.5700199	-4.0145036
C	5.1390912	-1.5478449	-2.8537825
C	2.3358681	-5.9714077	0.3295035
C	0.2297117	3.6210271	-4.7452388
C	4.4327479	-4.7544866	-1.1220952
C	1.5173615	2.9744182	-4.8862908
C	-4.8565862	-4.4309305	0.8858530
C	3.8731918	1.4116428	-4.7196836

C	-5.4207905	1.7362577	-2.7104997
C	-3.7540131	-5.3687988	0.9088006
C	4.8225977	-2.9543832	-2.7495725
C	4.6324769	-0.8197799	-3.9963212
C	-1.2766293	-6.7222407	0.7857425
C	-5.9939644	-2.5679900	-0.3519508
C	-4.4600405	2.3586732	-3.5971967
C	-6.1934130	-0.3881860	-1.6234206
C	0.0699622	-6.8567007	0.3371630
C	-2.1885144	3.2418934	-5.0256938
C	-0.8408320	3.1002837	-5.4694545
C	-5.3598106	-3.8724214	-0.3516878
C	2.3288105	-5.9777724	-1.1145610
C	3.3545175	-5.2643583	-1.8409920
C	-5.7447251	0.3281108	-2.8017605
C	-6.1371350	-1.8347502	-1.5922166
C	2.7928137	0.8889910	-5.4362846
C	1.6233986	1.7243291	-5.6088772
C	-3.2989499	-5.9028516	-0.3577298
C	-2.1173620	-6.6420934	-0.3625238
C	3.8470023	-3.5752264	-3.6142695
C	3.6466854	-1.3992789	-4.8823306
C	-3.9832001	1.5825051	-4.7231926
C	0.0618156	-6.8609930	-1.0873260
C	-2.9169061	2.0960019	-5.4598372
C	3.1117371	-4.7333635	-3.1611815
C	1.1239578	-6.3447553	-1.8262623
C	-0.7373897	1.8685144	-6.1792558
C	2.7277593	-0.5446215	-5.6067005
C	-4.8710828	-4.4385846	-1.5918011
C	0.4398309	1.1222690	-6.1856806
C	-5.2410599	-0.4049497	-3.9442077
C	3.3538948	-2.8071279	-4.7333502
C	-5.8175263	-2.4969016	-2.7764641
C	-1.2898603	-6.7287272	-1.5202704
C	-3.7687362	-5.3767489	-1.6221590
C	-4.2765966	0.1707217	-4.8576371
C	-2.0208223	1.2482841	-6.1750541
C	-5.1950807	-3.7797446	-2.7768524
C	-5.3754886	-1.7924812	-3.9347186
C	1.8904237	-5.1226052	-3.8319095
C	0.8366760	-5.8404445	-3.1493637
C	1.5210574	-1.1002551	-6.1821074
C	0.3300729	-0.3052195	-6.3829397
C	-1.6202117	-6.0807469	-2.7085128

C	-2.9278417	-5.4664423	-2.7997764
C	2.2832308	-3.3249890	-5.4586257
C	-2.1639572	-0.1383702	-6.1753495
C	-3.3655692	-0.6914539	-5.5859095
C	-0.5368926	-5.7085764	-3.5930255
C	1.5624745	-4.4704806	-5.0176501
C	-4.3680800	-3.8678693	-3.9347259
C	1.3794400	-2.4847537	-6.1706342
C	-4.4800760	-2.6399575	-4.6508371
C	-0.9742804	-0.9382377	-6.3781779
C	-3.1929379	-4.6179536	-3.9425745
C	-3.4215021	-2.1260648	-5.3982098
C	-0.8524227	-4.8576536	-4.7204115
C	0.2114585	-4.3383360	-5.4554630
C	-1.0807977	-2.3668044	-6.1738994
C	0.0984996	-3.1101266	-6.1697588
C	-2.1435972	-4.2163598	-4.8564510
C	-2.2586389	-2.9685675	-5.5857458

16. NH₃-HBr@C₉₆

102

N	0.8158122	-2.5207126	-1.8009852
H	1.4679849	-3.0128640	-2.4072959
H	0.0941030	-2.0653299	-2.3543973
H	0.3811913	-3.1868727	-1.1685305
Br	2.1321345	-0.7412444	0.2028141
H	1.3440089	-1.7923778	-1.1541814
C	5.4279816	-3.2234144	-1.4623169
C	4.6018570	-4.4376876	-1.4717274
C	5.5046294	-2.4629752	-2.6371483
C	3.9286196	-4.7894550	-2.6538104
C	2.7440293	-5.6064587	-0.2111779
C	4.0648140	-4.9635613	-0.2311265
C	4.5590358	-4.4031401	0.9571966
C	2.0397964	-5.6407900	1.0004020
C	2.5426372	-4.9922202	2.1717299
C	3.7776287	-4.3848692	2.1519083
C	1.9602660	-5.7233747	-1.4325455
C	0.4926253	-5.6410199	-1.3993175
C	2.6192894	-5.4187017	-2.6330824
C	-0.1911233	-5.2567550	-2.5716038
C	5.3781754	-3.2047516	0.9668757
C	5.7116799	-2.5322201	-0.2153400
C	5.8206793	-1.0697751	-0.1813272

C	5.0641058	-2.4893661	2.1612752
C	5.1666745	-1.1167614	2.1958728
C	5.5853273	-0.4042199	1.0313358
C	3.9742577	-3.1365281	2.8351098
C	5.6455448	-0.2994184	-1.3980563
C	5.6186088	-1.0158907	-2.6065848
C	4.9117636	-0.5238194	-3.7453990
C	5.0142998	1.0248155	-1.3449000
C	4.3996208	1.5087533	-2.5092225
C	4.3134677	0.7139292	-3.6957235
C	4.1881675	0.9514533	2.2858255
C	4.9711625	0.9105474	1.0886928
C	4.5668750	1.5819329	-0.0763897
C	3.0478506	1.7244363	2.3352112
C	2.6498404	2.4834739	1.1894928
C	3.3519299	2.4049779	-0.0236934
C	4.1908567	-0.3446540	2.9121436
C	3.0080406	-0.9376067	3.4260659
C	2.8936389	-2.3992649	3.3772828
C	1.0512018	2.0964105	-3.5767117
C	3.0312399	0.9012136	-4.3129518
C	2.4230578	1.9972644	-3.6133572
C	2.5944571	2.6659856	-1.2392389
C	3.2003360	2.3227356	-2.4569423
C	0.4028623	2.5235674	-2.3784925
C	1.1303628	2.7642371	-1.2007487
C	0.2495592	1.0996280	-4.2355989
C	0.8120861	-0.0864627	-4.7749339
C	2.2700091	-0.1884525	-4.8150249
C	2.9028238	-1.5054631	-4.8663085
C	4.2426430	-1.6101133	-4.4101030
C	4.7393745	-2.8068658	-3.7953444
C	2.0780456	-2.7205292	-4.8823219
C	2.6716062	-3.9286971	-4.4313660
C	3.9659657	-3.9473863	-3.8035959
C	-1.0068632	1.0925191	-3.5441485
C	-0.0135230	-1.3010169	-4.7910161
C	0.6138170	-2.6260791	-4.8535574
C	-1.7815376	-0.0470989	-3.5518791
C	-1.3262980	-1.2158621	-4.2565871
C	-1.5080439	1.4827024	-1.1591276
C	-0.9006187	1.8835986	-2.3574587
C	-2.4801179	-0.4406014	-2.3730028
C	-2.3314213	0.2664042	-1.1682622
C	-0.8961732	1.9512783	0.0735720

C	1.2007951	2.5695646	1.2226741
C	0.4237394	2.5916625	0.0543328
C	-1.3263875	1.3447147	1.2601807
C	1.9018930	-4.9555433	-3.7806419
C	0.5225044	-4.8739906	-3.7531152
C	-0.1259362	-3.7472966	-4.3731939
C	-2.5820752	-1.8891465	-2.4053818
C	-1.9572531	-2.3368623	-3.6117047
C	-1.3727510	-3.5878994	-3.6700530
C	-2.5514408	-2.6624491	-1.2349271
C	-1.9341632	-3.9960732	-1.2931286
C	-1.3955681	-4.4401620	-2.5190521
C	-1.7627317	-0.6258777	2.3947755
C	-2.1384833	0.1414339	1.2505687
C	-2.5478224	-0.4770460	0.0583794
C	-1.8711947	-1.9978725	2.3649619
C	-2.3584756	-2.6569882	1.1929442
C	-2.6579005	-1.9414742	0.0253983
C	0.7632425	1.8701085	2.3880608
C	-0.6349660	-0.0091629	3.0367253
C	-0.4752320	1.2688266	2.4033564
C	0.2629169	-4.8258531	2.2341762
C	1.4629458	-4.3594443	2.8735731
C	1.5769933	-3.0414919	3.3887794
C	-0.8742774	-4.0539603	2.2839307
C	-0.8443368	-2.7936742	2.9744846
C	0.3675682	-2.2207582	3.4416705
C	0.4792535	-0.7608435	3.4825062
C	1.7969176	-0.1160328	3.4786300
C	1.8815517	1.2217990	3.0125438
C	-1.3992443	-4.5909656	-0.0753666
C	-0.1829485	-5.4153221	-0.1287312
C	0.5936256	-5.5343013	1.0385652
C	-1.7253730	-3.9613594	1.1403042

17. NH₃-HBr@C₈₀

86

N	-2.9201415	0.4468716	-1.0625954
H	-3.5108524	0.4626173	-1.8780503
H	-2.1928490	-0.2563036	-1.1415310
H	-2.4861996	1.3507233	-0.9051824
Br	-3.0288204	0.0802146	1.6117433
H	-3.4441906	0.2232309	-0.1698743
C	-0.0425715	2.7715433	1.6452560

C	-0.4598398	3.3564140	0.4046116
C	-0.0511759	2.7487014	-0.8259270
C	-1.6835223	4.0600605	0.3966124
C	-0.8754561	2.8100270	2.8350053
C	-3.1659699	2.8822993	3.6307720
C	-2.1429053	3.4284363	2.8020997
C	-2.5177273	4.0998737	1.5771092
C	-2.5170226	4.0768805	-0.7718431
C	-2.1463490	3.4011386	-2.0033675
C	-0.8754262	2.7753809	-2.0211796
C	-3.1825746	2.8378484	-2.8147550
C	-3.8553345	4.1010837	-0.3177333
C	-5.9400418	2.8791417	-0.2848203
C	-4.8723405	3.4368414	-1.0464193
C	-4.5308855	2.8376709	-2.3136008
C	-4.5178472	2.8934375	3.1753721
C	-4.8647581	3.4686579	1.9076739
C	-3.8506219	4.1230316	1.1456755
C	-5.9351222	2.8951317	1.1785653
C	-2.9825110	1.6205006	-3.5802247
C	-1.7200225	0.9264017	-3.5164076
C	-0.6688958	1.5470792	-2.7403548
C	-1.7404105	-0.5133275	-3.5150367
C	-4.2389998	0.8773696	-3.5520352
C	-5.2909046	-1.1676673	-2.6412839
C	-4.2463971	-0.5589313	-3.4560156
C	-2.9907075	-1.2442617	-3.4844312
C	-6.5689225	1.6959445	-0.7032603
C	-6.1581861	1.0272469	-1.9109064
C	-5.1845690	1.6506435	-2.7611655
C	-6.2325624	-0.3838923	-1.9102346
C	-0.7837122	-1.2693447	-2.7303088
C	0.2050422	-0.6342907	-1.9277930
C	0.2794753	0.7763343	-1.9834455
C	0.6171931	-1.2759559	-0.6922442
C	-1.4397850	-2.4426781	-2.2208474
C	-2.1013191	-3.6757341	-0.1904999
C	-1.0879270	-3.0243755	-0.9496237
C	-0.0177347	-2.4491518	-0.2229312
C	-5.0773370	-2.3624454	-1.8818161
C	-3.8105417	-2.9827846	-1.8443698
C	-2.7874102	-2.4303392	-2.6756136
C	-3.4367703	-3.6563517	-0.6256963
C	0.9981422	-0.5214729	0.4622422
C	0.9802967	0.8904782	0.4387468

C	0.6553696	1.5275297	-0.8068608
C	0.6685396	1.5589448	1.6620728
C	0.6182559	-1.2528151	1.6554581
C	-0.7708013	-1.1989553	3.7032523
C	0.2082712	-0.5798825	2.8662036
C	0.2866244	0.8309334	2.8655013
C	-2.0970180	-3.6591098	1.2741274
C	-1.0786758	-2.9935335	2.0037555
C	-0.0073924	-2.4350033	1.2405507
C	-1.4177656	-2.3969913	3.2647389
C	-1.7229968	-0.4228659	4.4683249
C	-1.7138940	1.0018141	4.3843875
C	-0.6621204	1.6125648	3.5861077
C	-2.9622163	1.6879590	4.4216924
C	-2.9715140	-1.1594078	4.4956414
C	-5.2889308	-1.1014140	3.6896923
C	-4.2321581	-0.4749381	4.4502242
C	-4.2113289	0.9592603	4.4479994
C	-3.4337797	-3.6284710	1.7226862
C	-5.0778608	-2.3280091	2.9721025
C	-3.8074319	-2.9474649	2.9515456
C	-2.7719047	-2.3854078	3.7518145
C	-5.9087309	-2.3220774	-0.6928419
C	-5.9018353	-2.3030279	1.7797178
C	-5.4910003	-2.9078971	0.5533469
C	-4.2689396	-3.6130041	0.5576681
C	-6.9493756	0.9666145	0.4920529
C	-6.6149484	-1.0805190	1.7618384
C	-6.9326428	-0.4450918	0.5193277
C	-6.6181499	-1.1125168	-0.7089358
C	-5.1715173	1.7167853	3.6771981
C	-6.2431392	-0.3294695	2.9403062
C	-6.1606290	1.0795631	2.8845204
C	-6.5652066	1.7204317	1.6434471

18. NH₃-HBr@C₆₀

66

N	-0.8025763	2.1383747	2.2666132
H	-0.9951949	1.8306159	3.1698755
H	-0.6556705	3.1343362	2.2176260
H	0.0263375	1.7160142	1.8786814
Br	-0.3453722	2.8675976	0.1262760
H	-1.5462223	1.9358876	1.6169302
C	-0.0168112	2.1494337	4.6895680

C	0.0414302	0.7295734	4.2272827
C	1.2843106	0.5896111	3.4347534
C	1.9825192	1.8641336	3.4114060
C	1.1872283	2.8190194	4.1587696
C	-3.2064625	3.1820882	3.3364068
C	-2.4945182	2.1938814	4.1707609
C	-1.2593435	2.8662953	4.6751946
C	-1.2706525	4.2428693	4.1302703
C	-2.4680799	4.4301484	3.3281719
C	-2.2808476	-0.4415979	1.7074384
C	-1.0763931	-0.6701802	2.4817053
C	-1.1495951	0.0920480	3.7439507
C	-2.4475333	0.8311560	3.7250690
C	-3.1175041	0.4848323	2.4511111
C	1.3888494	-0.1365208	-0.1354047
C	2.0875264	0.2513380	1.0700444
C	1.3249782	-0.1725692	2.2488363
C	0.1267611	-0.8097196	1.7673524
C	0.1719497	-0.7783706	0.3052742
C	2.7614459	3.6786422	0.3435572
C	2.6860225	3.6435174	1.8026336
C	2.6965907	2.2744049	2.2624974
C	2.7747167	1.4550280	1.0754487
C	2.8162383	2.3061567	-0.1130069
C	-0.0811871	5.7140284	2.4655756
C	-0.0947742	4.8633853	3.6601380
C	1.1501541	4.1390360	3.6748893
C	1.9140783	4.5591205	2.4996359
C	1.1659018	5.5446006	1.7530526
C	-3.0849044	3.2608852	-1.3797330
C	-2.2831146	2.2975079	-2.1257374
C	-1.0573391	2.9647932	-2.5905805
C	-1.1116700	4.3637033	-2.1251494
C	-2.3700379	4.5327515	-1.3823168
C	-3.8155495	1.4490741	1.6950083
C	-3.7662608	1.4825338	0.2296864
C	-3.8026005	2.8515573	-0.2341152
C	-3.8449525	3.6687920	0.9566438
C	-3.8581882	2.8161549	2.1453919
C	-0.9873478	-0.5787221	-0.4274452
C	-0.9835813	0.2492016	-1.6317627
C	-2.2385900	0.9708323	-1.6564387
C	-2.9889786	0.5702174	-0.4667087
C	-2.2233420	-0.3886853	0.2960833
C	2.1549239	1.9274737	-1.2964132

C	1.3989945	2.9181752	-2.0773977
C	0.1751481	2.2552396	-2.5666270
C	0.1998403	0.8681297	-2.0783667
C	1.4141520	0.6708750	-1.2943437
C	1.2214283	5.5941096	0.3424720
C	0.0064463	5.8203891	-0.4322141
C	0.0679086	5.0033111	-1.6538170
C	1.3458359	4.2667275	-1.6289157
C	2.0484464	4.6439498	-0.3931948
C	-2.4400659	5.2347811	2.1661154
C	-3.1525997	4.8691568	0.9636769
C	-2.4061558	5.3144865	-0.2113866
C	-1.2056728	5.9657867	0.2685719
C	-1.2394468	5.9082887	1.7294354

19. NH₃-HBr@C₅₀

56

N	-0.0966761	1.9693456	-2.9242068
H	-0.8172199	1.5867513	-3.5238125
H	0.8212407	1.6621657	-3.2313009
H	0.4776806	2.9157655	-4.1544605
Br	-0.2905563	1.2919085	-1.3388786
H	-0.1833584	2.9700836	-2.7778556
C	-0.2630741	4.6584394	-0.9068190
C	-0.5328264	3.8984419	0.2602247
C	0.5485537	3.1771218	0.8668383
C	-1.1650182	4.6445197	-2.0491224
C	-1.7418464	3.0597282	0.3311577
C	-2.5871436	2.9950057	-0.8041753
C	-2.3005955	3.7997445	-2.0125352
C	-1.3628525	1.8149345	1.0439253
C	0.0546515	1.9007841	1.3319525
C	-1.8822596	0.5567008	0.5961421
C	-2.8102048	0.5051082	-0.5695832
C	-3.1283361	1.7024764	-1.2587556
C	-0.9636329	-0.5542077	0.4641115
C	0.4760869	-0.3868212	0.5027507
C	0.9994503	0.8675243	0.9522103
C	2.0843011	1.5258896	0.1839186
C	2.5725406	0.9277532	-1.0047825
C	1.0328189	-1.0355683	-0.7178827
C	2.0412990	-0.3691299	-1.4594906
C	2.0377938	3.7341460	-0.9952044
C	2.6029766	3.1367422	-2.1929580

C	1.7851653	2.9685742	0.1708096
C	2.8433536	1.7432633	-2.2105024
C	2.5106199	0.9732994	-3.4042270
C	2.0315982	3.8273844	-3.3579801
C	1.7568420	3.0896340	-4.5599983
C	1.9767211	1.6250299	-4.5974530
C	0.9145255	-0.9066486	-3.6258771
C	1.9883050	-0.3143713	-2.9401727
C	1.0718267	4.7000425	-1.4232262
C	1.0490675	4.7692012	-2.8514988
C	0.3590725	3.3283882	-5.1949673
C	-0.7443289	4.0750085	-4.4619426
C	-0.3517739	4.7616778	-3.2757086
C	-0.1614197	2.0338150	-5.6302739
C	-1.1025904	-0.4135807	-4.6653415
C	0.3102094	-0.2321687	-4.7844263
C	0.8132484	1.0100476	-5.2835419
C	-0.1107689	-1.6260087	-1.4448924
C	-1.3814343	-1.2139555	-3.5039283
C	-0.1531439	-1.5552878	-2.8639769
C	-3.1495582	1.7473564	-2.7400736
C	-2.8418293	0.5921450	-3.4801844
C	-2.4611099	-0.6317869	-2.7754977
C	-2.4448541	-0.6922196	-1.3541361
C	-1.3143038	-1.3155408	-0.7221490
C	-1.5498125	1.9564501	-5.1885018
C	-1.9090963	3.1852514	-4.4366294
C	-2.6680032	3.0493818	-3.2029660
C	-2.0100584	0.6969960	-4.6951727

20. NH₃-HBr@C₄₈

54

N	0.0171966	-1.2935900	-1.4311967
H	-0.6992696	-1.0290657	-0.8020984
H	0.8662860	-0.8816386	-1.1458761
H	0.0930957	-2.2722052	-1.4938911
Br	0.0504597	1.1743336	-1.4565154
H	-0.2616986	-0.9188762	-2.2896726
C	-1.2136704	-3.4839526	-2.5970040
C	-2.2240214	-2.6203452	-2.1562118
C	-2.3185013	-1.3044647	-2.6213878
C	-2.3080621	1.4934409	-2.6498690
C	-1.3047748	0.7826308	-3.4964163
C	-0.0449688	-2.9515209	-3.3684368
C	2.2990295	-1.4151319	-2.6722053

C	1.3110740	-0.7668359	-3.5749261
C	-0.0181128	-1.5393984	-3.8265269
C	-1.3347459	-0.6992099	-3.5687498
C	-2.7476232	0.7876397	-1.4280101
C	-2.7254514	-0.5471664	-1.4119167
C	-1.0397003	3.6702864	-0.3015005
C	-2.2836051	1.5292177	-0.2346633
C	-2.1065455	2.8465122	-0.7052807
C	-1.0679658	3.6347595	-2.6777052
C	-2.1231475	2.8236530	-2.2230506
C	0.0413595	1.5508345	-3.6466454
C	0.0793779	3.0128999	-3.3641197
C	1.3493464	0.7131455	-3.5122217
C	-2.2133549	-2.6036022	-0.6234936
C	-1.1857458	-3.4476295	-0.1921833
C	-2.3053397	-1.2731365	-0.1812039
C	0.0954079	1.6139855	0.6955990
C	0.1246777	3.0716096	0.3741650
C	-1.2565786	0.8427918	0.6023339
C	-1.2797957	-0.6379910	0.7148792
C	0.0386728	-1.4599900	0.9384085
C	0.0030819	-2.8805291	0.5224207
C	-0.7426395	-4.1578898	-1.3901165
C	0.6368705	-4.1914191	-1.4052401
C	1.1442037	-3.5073990	-0.2164407
C	2.2021853	-2.7131593	-0.6734995
C	2.3509989	-1.3866651	-0.2362116
C	1.4084094	0.7753826	0.5694556
C	1.3660676	-0.7048909	0.6673051
C	2.4420610	1.4174056	-0.2900028
C	2.1757202	-2.7315919	-2.2090444
C	1.1161408	-3.5471093	-2.6276702
C	2.8474098	0.6580310	-1.4912154
C	2.7744978	-0.6768443	-1.4739683
C	1.3015118	3.6174225	-0.3291184
C	2.3153452	2.7426671	-0.7563859
C	-0.5564141	4.3397355	-1.5066833
C	0.8229588	4.3091783	-1.5228372
C	2.4054040	1.3804402	-2.7006712
C	2.2949319	2.7190789	-2.2740264
C	1.2716931	3.5803327	-2.7048145

21. NH₃-HBr@C₃₆

42

N	-0.6399522	-1.6683827	-1.6979390
H	0.2541777	-2.1588058	-1.7592217
H	-0.3849171	-2.2197999	-3.0060824
H	-1.5205922	-2.1490268	-1.9482685
Br	-0.7767545	-1.6836761	-0.0498752
H	-0.6504467	-0.6970749	-1.9066924
C	1.3269008	-3.0553254	-2.4067648
C	1.2407896	-3.1628186	0.5321116
C	1.7804219	-2.0102682	-0.1618962
C	1.8824832	-1.9252323	-1.6229689
C	0.6560648	-2.4756919	-3.6170086
C	-0.7695603	-3.1231155	-3.6667559
C	-1.9975819	-2.2143301	-3.6552429
C	0.7629293	-0.9818763	-3.5254421
C	-0.4835097	-0.1379596	-3.5384597
C	-1.7844625	-0.7392258	-3.5695124
C	0.6609295	0.3607012	-0.0996661
C	0.7650975	0.4187601	-1.5828187
C	1.5077900	-0.6583858	-2.3212628
C	1.3002852	-0.7967304	0.5933176
C	-3.2028464	-1.3268225	-1.7278071
C	-2.8029690	-2.6084189	-2.5014386
C	-3.2173117	-1.3193315	-0.2701716
C	-2.5689423	-0.2138399	-2.3781928
C	-2.1071059	-3.7498416	-1.7914852
C	-0.8549804	-4.0435927	-2.4905453
C	-2.0820482	-3.7941110	-0.3188316
C	-2.6630425	-2.5767215	0.3823138
C	-0.9139411	-4.1436314	0.4522380
C	0.3970825	-4.0939933	-0.2560074
C	0.4202003	-4.0408737	-1.7225787
C	-2.0504740	-2.3206161	1.7028284
C	-0.8448649	-3.2321507	1.6863891
C	0.4672557	-2.6453653	1.7384538
C	-1.9404094	-0.8355305	1.7379644
C	-1.7588512	0.7462330	-1.6002112
C	-1.8058376	0.7357000	-0.1393818
C	-2.7049619	-0.2274851	0.5396028
C	-0.4268530	0.7650886	-2.3223892
C	-0.5240013	0.7423451	0.6519113
C	-0.6240405	-0.2224617	1.7972654
C	0.5825990	-1.1457565	1.7949749

22. NH₃-HI@C₁₈₀

186

N	2.2572441	0.6211002	-2.3272990
H	2.4197892	0.0171011	-3.1353828
H	3.1684793	0.8593103	-1.9317596
H	1.7777340	1.4775399	-2.6224909
I	2.1678315	-2.0817639	-0.4096617
H	1.7888961	0.0002298	-1.6016560
C	1.6841931	1.7600029	4.8127950
C	1.5711791	3.0099484	4.0875672
C	-0.6716747	1.9029953	5.4020217
C	0.5064923	1.1579433	5.4023963
C	-0.7827985	3.1315018	4.6865139
C	0.2811100	3.6530538	3.9524076
C	2.8460556	0.9167001	4.6219544
C	2.6205995	3.4095251	3.1740901
C	0.3994715	-0.2712092	5.6057164
C	3.9064343	1.4291611	3.8774871
C	-1.9540118	1.2798459	5.4095575
C	3.7937255	2.6565542	3.1628324
C	-2.1339479	3.2663515	4.2507400
C	-0.0340133	4.5068599	2.8264808
C	2.7879978	-0.5171165	4.8059427
C	1.5890447	-1.0693950	5.3982224
C	-2.8574008	2.1220958	4.6975670
C	2.3557805	4.2571863	2.0318803
C	1.0499716	4.8752509	1.9399066
C	-0.9040517	-0.9048569	5.6145128
C	-2.0962014	-0.1066837	5.4183806
C	-1.4084387	4.6454085	2.3839315
C	-2.4631268	3.9282600	3.0691860
C	4.7989586	0.5807718	3.1588341
C	4.6151905	2.5633838	2.0018582
C	1.4472417	-2.4547791	5.3937000
C	3.6947721	-1.3769442	4.0723997
C	3.1949087	4.1620076	0.8533943
C	0.7229562	5.5264464	0.7515381
C	5.2361709	1.2812443	1.9997443
C	-3.9313555	1.6044995	3.9755340
C	4.6572008	-0.8042057	3.1588940
C	-1.0130902	-2.3349319	5.4177691
C	4.2921194	3.2220265	0.8193395
C	-3.3035438	-0.6633555	4.8437571
C	0.1655167	-3.0786619	5.4050667

C	-1.6929160	5.1539304	1.0582549
C	-3.6843695	3.5383905	2.3970069
C	2.3424603	-3.2988254	4.6744103
C	-0.6280695	5.6647913	0.3173142
C	3.4038129	-2.7845910	3.9342100
C	-4.2229261	0.1938747	4.1209772
C	-4.4199654	2.3743383	2.8507721
C	1.5491223	5.4300031	-0.4055986
C	2.7263133	4.6844390	-0.4092264
C	-2.1966198	-2.9399757	4.8441584
C	-3.3616802	-2.0990636	4.6642642
C	5.5525406	0.6172188	0.8169134
C	5.1638608	-1.5369162	2.0193126
C	-3.9215426	4.0703527	1.0716224
C	-2.8986727	4.7905987	0.3427285
C	4.7796941	2.6542277	-0.4193516
C	0.2700757	-4.3095564	4.6936346
C	1.6158462	-4.4441072	4.2422512
C	-0.6357283	5.6582841	-1.1084203
C	5.6152104	-0.8247860	0.8466857
C	3.8822207	-3.5566051	2.8089586
C	5.4126516	1.3508818	-0.4202431
C	0.7102722	5.5120154	-1.5540759
C	-5.1970403	-0.3872225	3.2213692
C	-5.3901515	1.7468451	1.9777183
C	3.1810143	4.1458885	-1.6737065
C	4.8477447	-2.9421831	1.9269884
C	-4.4290555	-2.6178600	3.9326634
C	4.2880663	3.2152972	-1.6567178
C	-2.0902384	-4.1916940	4.1205562
C	-4.9877574	3.5449363	0.3432916
C	-0.8010680	-4.8330741	3.9731911
C	-2.9069486	4.7871507	-1.1077298
C	-5.7131240	0.3390949	2.0802719
C	-5.3320371	-1.7745847	3.2213001
C	-5.7122415	2.4011406	0.7900239
C	-1.7084608	5.1450757	-1.8360290
C	1.9309227	-5.1020606	3.0565594
C	3.1438720	-4.7155291	2.3693402
C	1.0251055	4.8518428	-2.7395586
C	5.7502566	-1.5183183	-0.4121050
C	2.3294259	4.2307396	-2.8406581
C	5.5606097	0.6170755	-1.6583758
C	5.1772803	-3.6087499	0.7494776
C	-4.3247573	-3.8496265	3.2220975

C	-3.1492599	-4.5987333	3.2208214
C	4.6197202	2.5643815	-2.8473182
C	-4.9945839	3.5410214	-1.0824813
C	-0.4973229	-5.6893594	2.8473478
C	-3.9364754	4.0636495	-1.8236180
C	5.6227974	-2.9049855	-0.4074224
C	0.8709144	-5.8224687	2.3892633
C	5.6104870	-0.8287228	-1.6750384
C	-5.7859968	-2.4852729	2.0714838
C	5.2513523	1.2824410	-2.8501501
C	-6.1751010	-0.3838407	0.9111387
C	-1.4369549	4.6274564	-3.1598281
C	-6.1668338	1.6902811	-0.3595283
C	3.3735235	-5.2530928	1.0488284
C	-0.0662184	4.4814848	-3.6112720
C	4.4459309	-4.7512494	0.3150216
C	-5.1635319	-3.7680411	2.0722910
C	2.5923843	3.3853148	-3.9845478
C	3.7765712	2.6433336	-3.9939101
C	-5.7227125	2.3947526	-1.5169350
C	-6.1193236	-1.8302666	0.8872242
C	-2.8965152	-5.4534632	2.0796902
C	-6.3126796	0.3040630	-0.3556400
C	-1.5894979	-6.0670831	1.9769356
C	-3.7129010	3.5243153	-3.1484436
C	-2.4974526	3.9088771	-3.8333001
C	1.1442375	-6.3334960	1.0660131
C	5.1668790	-3.6141075	-1.5563398
C	4.7966081	0.5720910	-4.0008745
C	5.1497460	-1.5474565	-2.8398336
C	2.3411186	-5.9711210	0.3384480
C	0.2386016	3.6198445	-4.7308028
C	4.4403832	-4.7556646	-1.1092794
C	1.5277652	2.9747191	-4.8728733
C	-4.8530308	-4.4340379	0.8876690
C	3.8873147	1.4150769	-4.7092676
C	-5.4141845	1.7349834	-2.7053299
C	-3.7502615	-5.3715071	0.9112119
C	4.8300427	-2.9528945	-2.7347149
C	4.6430092	-0.8170782	-3.9816393
C	-1.2718440	-6.7230213	0.7898640
C	-5.9892832	-2.5705979	-0.3501772
C	-4.4524889	2.3580248	-3.5904543
C	-6.1875131	-0.3901020	-1.6205054
C	0.0751849	-6.8560764	0.3428697

C	-2.1790577	3.2418707	-5.0152224
C	-0.8306817	3.0997275	-5.4560633
C	-5.3549788	-3.8748305	-0.3500204
C	2.3349488	-5.9757817	-1.1045720
C	3.3610949	-5.2622326	-1.8289360
C	-5.7377671	0.3269758	-2.7978689
C	-6.1310960	-1.8366630	-1.5901708
C	2.8098105	0.8945759	-5.4311925
C	1.6361817	1.7252340	-5.5968486
C	-3.2934462	-5.9043845	-0.3550410
C	-2.1114900	-6.6428198	-0.3589378
C	3.8554363	-3.5725147	-3.6001518
C	3.6584446	-1.3970163	-4.8694317
C	-3.9739432	1.5826500	-4.7162508
C	0.0685896	-6.8590237	-1.0810371
C	-2.9067349	2.0966426	-5.4512840
C	3.1195395	-4.7299964	-3.1482322
C	1.1312367	-6.3415670	-1.8175177
C	-0.7257698	1.8685318	-6.1658724
C	2.7412537	-0.5406071	-5.5983192
C	-4.8646726	-4.4399778	-1.5899586
C	0.4517543	1.1231514	-6.1724762
C	-5.2326340	-0.4052387	-3.9401385
C	3.3639547	-2.8042550	-4.7192398
C	-5.8102733	-2.4980389	-2.7745012
C	-1.2824300	-6.7274889	-1.5154575
C	-3.7619594	-5.3776511	-1.6195599
C	-4.2670505	0.1709711	-4.8519272
C	-2.0091568	1.2491503	-6.1647425
C	-5.1877327	-3.7807809	-2.7750312
C	-5.3667721	-1.7927478	-3.9316752
C	1.8991939	-5.1180821	-3.8198593
C	0.8452263	-5.8364505	-3.1397118
C	1.5330541	-1.0969505	-6.1709682
C	0.3419405	-0.3031587	-6.3714069
C	-1.6116521	-6.0787479	-2.7031238
C	-2.9195615	-5.4659160	-2.7959380
C	2.2938169	-3.3210292	-5.4452278
C	-2.1525027	-0.1372461	-6.1665121
C	-3.3551037	-0.6906632	-5.5795903
C	-0.5274146	-5.7051240	-3.5851679
C	1.5729534	-4.4664347	-5.0058856
C	-4.3591705	-3.8678596	-3.9318657
C	1.3911926	-2.4809808	-6.1584354
C	-4.4704496	-2.6395673	-4.6472988

C	-0.9625970	-0.9363319	-6.3684906
C	-3.1837027	-4.6172480	-3.9385537
C	-3.4111582	-2.1251065	-5.3932258
C	-0.8417209	-4.8541240	-4.7121010
C	0.2229660	-4.3344198	-5.4452781
C	-1.0692715	-2.3645891	-6.1656040
C	0.1105674	-3.1067613	-6.1596286
C	-2.1331171	-4.2143210	-4.8503330
C	-2.2478488	-2.9669084	-5.5796818

23. NH₃-HI@C₉₆

102

N	0.8920986	-2.4137793	-2.1089360
H	1.3448396	-1.6946929	-2.6729724
H	-0.1088536	-2.3909917	-2.2711914
H	1.2825749	-3.3208715	-2.3401607
I	2.0270719	-0.8589925	0.2562523
H	1.1210697	-2.1438236	-1.0965863
C	5.4111273	-3.2361820	-1.4424133
C	4.5834475	-4.4475599	-1.4509452
C	5.4900591	-2.4841409	-2.6205854
C	3.9099871	-4.8046816	-2.6338375
C	2.7318320	-5.6053422	-0.1863162
C	4.0503837	-4.9648363	-0.2069534
C	4.5456076	-4.3997735	0.9801378
C	2.0304948	-5.6305602	1.0263497
C	2.5346403	-4.9794622	2.1968123
C	3.7687828	-4.3749759	2.1765679
C	1.9475900	-5.7262859	-1.4089679
C	0.4844092	-5.6260444	-1.3752342
C	2.6030068	-5.4368553	-2.6161383
C	-0.2027676	-5.2598543	-2.5540160
C	5.3653002	-3.2043517	0.9877114
C	5.6985632	-2.5400990	-0.1974005
C	5.8119075	-1.0798328	-0.1646808
C	5.0584076	-2.4857241	2.1833983
C	5.1678557	-1.1138824	2.2198663
C	5.5829046	-0.4093562	1.0487604
C	3.9709747	-3.1282060	2.8635168
C	5.6362639	-0.3175547	-1.3850742
C	5.6053180	-1.0389933	-2.5917255
C	4.8955028	-0.5523798	-3.7303932
C	5.0095950	1.0076076	-1.3344015
C	4.3967212	1.4879605	-2.5010803

C	4.3035690	0.6862009	-3.6836218
C	4.1986069	0.9582891	2.3096624
C	4.9733291	0.9064948	1.1046055
C	4.5679560	1.5711900	-0.0652927
C	3.0592579	1.7356753	2.3585694
C	2.6592547	2.4843943	1.2033139
C	3.3565919	2.3970123	-0.0137596
C	4.2043507	-0.3341918	2.9495553
C	3.0213797	-0.9217035	3.4787435
C	2.8986337	-2.3873876	3.4186377
C	1.0513143	2.0690846	-3.5667811
C	3.0216794	0.8691911	-4.2989641
C	2.4209965	1.9701644	-3.6036520
C	2.5988628	2.6514020	-1.2319218
C	3.2011925	2.3035384	-2.4502934
C	0.4069102	2.5055471	-2.3703312
C	1.1362643	2.7511557	-1.1935313
C	0.2478425	1.0723633	-4.2241588
C	0.8004656	-0.1168799	-4.7714291
C	2.2575339	-0.2205935	-4.8040716
C	2.8855997	-1.5389198	-4.8606952
C	4.2238029	-1.6385261	-4.3934204
C	4.7220176	-2.8311451	-3.7775545
C	2.0589734	-2.7570185	-4.8987476
C	2.6543418	-3.9567305	-4.4251174
C	3.9459272	-3.9689793	-3.7872922
C	-1.0063002	1.0746638	-3.5337856
C	-0.0329933	-1.3301985	-4.8083411
C	0.5876900	-2.6645515	-4.8900180
C	-1.7822147	-0.0630988	-3.5427757
C	-1.3372665	-1.2345243	-4.2534232
C	-1.4986850	1.4746356	-1.1483947
C	-0.8967923	1.8706488	-2.3491178
C	-2.4789636	-0.4483689	-2.3611557
C	-2.3240907	0.2616835	-1.1566138
C	-0.8839391	1.9478224	0.0826440
C	1.2111190	2.5720650	1.2354363
C	0.4344390	2.5869405	0.0642553
C	-1.3110819	1.3477424	1.2716968
C	1.8844721	-4.9818205	-3.7714240
C	0.5008701	-4.9024499	-3.7535598
C	-0.1556280	-3.7855618	-4.3974328
C	-2.5901517	-1.8952250	-2.3943484
C	-1.9726573	-2.3511782	-3.6062039
C	-1.3947685	-3.6090309	-3.6721171

C	-2.5520302	-2.6584632	-1.2168672
C	-1.9250709	-3.9840751	-1.2723787
C	-1.4027371	-4.4421731	-2.5027776
C	-1.7507429	-0.6120279	2.4119894
C	-2.1250559	0.1484832	1.2641953
C	-2.5391688	-0.4724073	0.0737401
C	-1.8630150	-1.9817505	2.3841064
C	-2.3530809	-2.6425932	1.2131714
C	-2.6547164	-1.9333708	0.0433852
C	0.7751287	1.8814394	2.4074666
C	-0.6252205	0.0055117	3.0596252
C	-0.4623758	1.2782340	2.4184668
C	0.2604896	-4.8090689	2.2602717
C	1.4596712	-4.3425940	2.9002380
C	1.5785383	-3.0265418	3.4220701
C	-0.8732115	-4.0358099	2.3086591
C	-0.8385599	-2.7753909	2.9979516
C	0.3715959	-2.2034202	3.4736905
C	0.4856681	-0.7418628	3.5219594
C	1.8072747	-0.0934331	3.5310630
C	1.8928127	1.2427614	3.0488722
C	-1.3929513	-4.5710342	-0.0531769
C	-0.1841103	-5.3946821	-0.1048209
C	0.5873717	-5.5201091	1.0642155
C	-1.7228059	-3.9455312	1.1628174

24. NH₃-HI@C₈₀

86

N	-3.5019070	0.2407350	-1.1200375
H	-3.8086069	0.3939695	-2.0651539
H	-2.8749002	-0.5588188	-1.0724260
H	-3.0057439	1.0647843	-0.7794455
I	-2.6187550	0.2536649	1.4262717
H	-4.2983067	0.0704585	-0.5095161
C	0.0052905	2.7909739	1.7319190
C	-0.4229710	3.3591628	0.4874426
C	-0.0189141	2.7435964	-0.7392776
C	-1.6491515	4.0592094	0.4624048
C	-0.8104190	2.8504708	2.9185695
C	-3.1204563	2.9110535	3.6575662
C	-2.0871540	3.4644287	2.8629681
C	-2.4736075	4.1059168	1.6150533
C	-2.4980124	4.0607326	-0.7266939
C	-2.1420216	3.3594413	-1.9214313

C	-0.8740643	2.7416205	-1.9239170
C	-3.1779628	2.8004659	-2.7576805
C	-3.8303202	4.0992825	-0.2983998
C	-5.9142228	2.8823091	-0.3054764
C	-4.8541285	3.4359185	-1.0507394
C	-4.5314482	2.8378421	-2.3229268
C	-4.4786235	2.9109569	3.1719047
C	-4.8334751	3.4787140	1.9047880
C	-3.8210209	4.1188667	1.1598878
C	-5.9094668	2.9042821	1.1541210
C	-2.9800397	1.6067554	-3.5488147
C	-1.7338879	0.9131753	-3.4188690
C	-0.6716339	1.5331106	-2.6369491
C	-1.7461015	-0.5055762	-3.4515434
C	-4.2531302	0.8838356	-3.6175832
C	-5.3171739	-1.1851627	-2.7522704
C	-4.2719973	-0.5800576	-3.5576065
C	-2.9843172	-1.2537095	-3.5089579
C	-6.5577381	1.6960765	-0.7492025
C	-6.1958236	1.0384105	-2.0000802
C	-5.2148056	1.6689603	-2.8342615
C	-6.2694605	-0.3823010	-2.0084744
C	-0.7917495	-1.2505774	-2.6519195
C	0.2112646	-0.6246420	-1.8420957
C	0.2878040	0.7798571	-1.8916726
C	0.6428263	-1.2636437	-0.6320748
C	-1.4201939	-2.4295116	-2.1958491
C	-2.0664820	-3.6522623	-0.1859042
C	-1.0564438	-3.0081467	-0.9278179
C	0.0174755	-2.4345881	-0.1823541
C	-5.0704044	-2.3655038	-1.9538512
C	-3.7960368	-2.9793528	-1.8875251
C	-2.7730700	-2.4383962	-2.7031349
C	-3.4125855	-3.6313893	-0.6449666
C	1.0457192	-0.5066631	0.5426218
C	1.0296032	0.9029015	0.5289377
C	0.6900254	1.5385140	-0.7212476
C	0.7391367	1.5716254	1.7568438
C	0.6743479	-1.2327831	1.7151316
C	-0.6889388	-1.1931566	3.7717396
C	0.3014541	-0.5661320	2.9569271
C	0.3882319	0.8531471	2.9642428
C	-2.0580441	-3.6428719	1.2719340
C	-1.0272412	-2.9808975	2.0257874
C	0.0331220	-2.4217334	1.2791369

C	-1.3556918	-2.3829021	3.2878122
C	-1.6568502	-0.4106439	4.5163144
C	-1.6410001	1.0253755	4.4421058
C	-0.5834275	1.6442174	3.6829919
C	-2.9156110	1.7035498	4.4235747
C	-2.9160062	-1.1301886	4.4844300
C	-5.2265225	-1.0727260	3.6141496
C	-4.1646139	-0.4451431	4.3912821
C	-4.1607112	0.9744588	4.4221268
C	-3.3882155	-3.6041900	1.6998088
C	-5.0192947	-2.2818266	2.9051159
C	-3.7498046	-2.9032064	2.8996687
C	-2.7159973	-2.3426123	3.7219338
C	-5.8734777	-2.3032673	-0.7601633
C	-5.8638317	-2.2734466	1.7105652
C	-5.4558347	-2.8848906	0.4883516
C	-4.2347739	-3.5899815	0.5109831
C	-6.9299015	0.9768097	0.4286408
C	-6.5763548	-1.0674367	1.6917990
C	-6.9061387	-0.4308477	0.4464946
C	-6.6039304	-1.0927882	-0.7866445
C	-5.1158339	1.7290091	3.6370534
C	-6.1773672	-0.3106984	2.8663720
C	-6.1037276	1.0961059	2.8220095
C	-6.5312893	1.7343973	1.6018966

25. NH₃-HI@C₆₀

66

N	-0.8235283	2.1087096	2.3555766
H	-1.0163990	1.8001404	3.2649967
H	-0.7858222	3.1181791	2.3356957
H	0.0662805	1.7394954	2.0493666
I	-0.3564300	2.8451118	0.1897158
H	-1.5461703	1.7940294	1.7231372
C	-0.0126059	2.1487487	4.7041096
C	0.0453544	0.7192558	4.2412273
C	1.2822697	0.5916197	3.4306092
C	1.9807999	1.8652262	3.4050538
C	1.1885196	2.8179615	4.1560055
C	-3.2056269	3.1843247	3.3358032
C	-2.5044210	2.1940468	4.1833246
C	-1.2617796	2.8699148	4.6933950
C	-1.2691464	4.2417838	4.1265953
C	-2.4651661	4.4300598	3.3234846

C	-2.2792222	-0.4374516	1.7035682
C	-1.0778914	-0.6693715	2.4792047
C	-1.1522069	0.0805532	3.7531466
C	-2.4591816	0.8230015	3.7374136
C	-3.1154902	0.4874498	2.4491664
C	1.4020742	-0.1495755	-0.1571730
C	2.0889996	0.2531058	1.0505611
C	1.3190704	-0.1634015	2.2339644
C	0.1262150	-0.7967579	1.7551783
C	0.1769973	-0.7742952	0.2877332
C	2.7770376	3.6840503	0.3268488
C	2.6911302	3.6465400	1.7892020
C	2.6940996	2.2765913	2.2495099
C	2.7786013	1.4570871	1.0613962
C	2.8312084	2.3089958	-0.1307006
C	-0.0722121	5.7196373	2.4492948
C	-0.0906664	4.8584474	3.6427486
C	1.1476445	4.1371505	3.6572082
C	1.9184980	4.5665833	2.4830545
C	1.1814018	5.5665305	1.7438571
C	-3.1044380	3.2729505	-1.4120807
C	-2.2994507	2.3039510	-2.1524403
C	-1.0619245	2.9650389	-2.5947923
C	-1.1152716	4.3669231	-2.1277776
C	-2.3850965	4.5453832	-1.4066414
C	-3.8049137	1.4589351	1.6847878
C	-3.7655417	1.4925219	0.2136857
C	-3.8197501	2.8599383	-0.2543916
C	-3.8435107	3.6742864	0.9396127
C	-3.8468072	2.8190652	2.1334114
C	-0.9866012	-0.5750336	-0.4412253
C	-0.9851754	0.2471076	-1.6541200
C	-2.2421946	0.9703739	-1.6784646
C	-2.9884593	0.5754246	-0.4796931
C	-2.2199948	-0.3799497	0.2870125
C	2.1731792	1.9175037	-1.3221114
C	1.4035883	2.9149706	-2.0809343
C	0.1761269	2.2513886	-2.5709301
C	0.2112144	0.8566233	-2.1055967
C	1.4327762	0.6574767	-1.3279861
C	1.2417224	5.6242244	0.3240800
C	0.0197193	5.8461766	-0.4460331
C	0.0703253	5.0087630	-1.6543723
C	1.3509967	4.2700002	-1.6300251
C	2.0674084	4.6655854	-0.4079791

C	-2.4334955	5.2348818	2.1550753
C	-3.1494257	4.8755182	0.9519193
C	-2.4071660	5.3299716	-0.2271664
C	-1.2042533	5.9820822	0.2533058
C	-1.2347957	5.9141323	1.7173970

26. NH₃-HI@C₅₀

56

N	-0.0625457	2.0329819	-3.1058136
H	-0.7537577	1.6804282	-3.7440998
H	0.8530195	1.7539606	-3.3989536
H	-0.1272614	3.0301087	-2.9839745
I	-0.3598458	1.2378902	-1.4345241
H	0.5554810	2.4690013	-0.9627495
C	-0.2811890	4.6983381	-0.9777879
C	-0.5709966	3.9511861	0.1999738
C	0.5186437	3.2253099	0.8328034
C	-1.1712333	4.6541466	-2.1432514
C	-1.7743227	3.1047420	0.2525770
C	-2.6225911	3.0244039	-0.8978634
C	-2.3055635	3.8139168	-2.1108420
C	-1.3952032	1.8603263	0.9687924
C	0.0278105	1.9534899	1.2901254
C	-1.9276748	0.5900802	0.5557157
C	-2.8560447	0.5224818	-0.6108015
C	-3.1678231	1.7288842	-1.3344398
C	-0.9879946	-0.5343578	0.4455279
C	0.4681132	-0.3643743	0.4855896
C	0.9814738	0.9131965	0.9086521
C	2.0938637	1.5585025	0.1708200
C	2.5820609	0.9444909	-1.0284927
C	1.0431719	-1.0357667	-0.7127370
C	2.0639062	-0.3608855	-1.4698525
C	2.0358049	3.7782126	-1.0435029
C	2.5945481	3.1497648	-2.2470826
C	1.7814769	3.0082664	0.1387757
C	2.8435680	1.7603711	-2.2405446
C	2.5163511	0.9757103	-3.4420847
C	2.0014086	3.8102070	-3.4282461
C	1.6946068	3.0745201	-4.6152550
C	1.9821556	1.6090305	-4.6316261
C	0.9335488	-0.9236375	-3.6340412
C	2.0080186	-0.3219147	-2.9520291
C	1.0631324	4.7352690	-1.4798296

C	1.0330941	4.7482289	-2.9202119
C	0.3890293	3.2892063	-5.2348892
C	-0.6797678	4.0191151	-4.5572553
C	-0.3381289	4.7450244	-3.3663250
C	-0.1315579	2.0071760	-5.6689262
C	-1.0872321	-0.4484815	-4.6880231
C	0.3294180	-0.2617935	-4.8045086
C	0.8309496	0.9697323	-5.3236745
C	-0.1038801	-1.6265389	-1.4410515
C	-1.3732265	-1.2392257	-3.5193229
C	-0.1424746	-1.5699108	-2.8654289
C	-3.1574877	1.7434213	-2.8200192
C	-2.8399514	0.5738696	-3.5385100
C	-2.4657787	-0.6477727	-2.8063844
C	-2.4647371	-0.6835436	-1.3795430
C	-1.3270276	-1.3080800	-0.7240869
C	-1.5327430	1.9143122	-5.2671024
C	-1.8885257	3.1538620	-4.5272789
C	-2.6521034	3.0407260	-3.3092993
C	-1.9957227	0.6591226	-4.7501149

27. NH₃-HI@C₄₈

54

N	-1.4354526	-0.0487798	0.0167694
H	-1.1473568	0.7324805	0.5535647
H	-2.4163186	-0.1012326	-0.0187038
H	-1.1045654	0.0660409	-0.8962403
I	1.0969658	0.0121585	0.0077845
H	-1.0609901	-0.8715657	0.4179581
C	3.6017599	1.2447528	1.2026684
C	2.7525464	2.2839257	0.7713939
C	1.4167590	2.3908113	1.2101453
C	-1.4023450	2.2813449	1.2191112
C	-0.7452093	1.2980589	2.1505125
C	3.0456690	0.0596538	1.9014277
C	1.5232325	-2.3466826	1.2260205
C	0.8105963	-1.3094100	2.0664529
C	1.6006285	0.0280064	2.2675514
C	0.7535842	1.3263658	2.0589957
C	-0.6649429	2.7058506	-0.0101538
C	0.6696955	2.8070038	-0.0035089
C	-3.5278360	1.0625647	-1.2214013
C	-1.3877194	2.2513505	-1.2293757
C	-2.7095898	2.1186517	-0.7812418

C	-3.5375002	1.0741200	1.1858875
C	-2.7216718	2.1350278	0.7508333
C	-1.5078117	-0.0470206	2.3740068
C	-2.9305047	-0.0814073	1.9325363
C	-0.6873314	-1.3481918	2.1516935
C	2.7582207	2.2776673	-0.7575363
C	3.6109091	1.2371448	-1.1756196
C	1.4246557	2.3794798	-1.2063982
C	-1.5015812	-0.0632014	-2.4108773
C	-2.9314206	-0.0933094	-1.9699789
C	-0.7293423	1.2866827	-2.1567270
C	0.7672471	1.3132171	-2.0557194
C	1.6174023	0.0141616	-2.2503271
C	3.0597579	0.0474483	-1.8720611
C	4.3123507	0.7716411	0.0179979
C	4.3441893	-0.6072507	0.0224288
C	3.6634739	-1.1110394	-1.1678417
C	2.8584901	-2.1856207	-0.7426385
C	1.5305269	-2.3492152	-1.1892013
C	-0.6719384	-1.3611889	-2.1376619
C	0.8235814	-1.3187630	-2.0416477
C	-1.2845588	-2.3528959	-1.2132044
C	2.8533369	-2.1821944	0.7864931
C	3.6548798	-1.1037174	1.2099681
C	-0.5417487	-2.7704339	0.0084229
C	0.7967188	-2.8044937	0.0159033
C	-3.4775498	-1.2695398	-1.2148261
C	-2.6132829	-2.2850911	-0.7680217
C	-4.2057682	0.5789059	-0.0174873
C	-4.1759929	-0.8085178	-0.0130473
C	-1.2987880	-2.3700520	1.2330015
C	-2.6241564	-2.2925356	0.7644631
C	-3.4868106	-1.2666573	1.1935378

28. NH₃-HI@C₃₆

42

N	-0.6548028	-1.6416789	-1.6399810
H	0.2456477	-2.1611015	-1.6446559
H	-0.4196760	-2.1844762	-2.9088734
H	-1.5636213	-2.1127751	-1.8281864
I	-0.7452112	-1.6431000	0.2181609
H	-0.5867319	-0.6492341	-1.8966769
C	1.3170241	-3.0290641	-2.4218732
C	1.2070299	-3.0946700	0.5103525

C	1.8501548	-1.9469804	-0.1942915
C	1.9123798	-1.8965264	-1.6398503
C	0.6305546	-2.4512748	-3.5940318
C	-0.7760608	-3.0855904	-3.6401294
C	-1.9877961	-2.2013418	-3.6447984
C	0.7516971	-0.9642219	-3.5266859
C	-0.4642029	-0.1270915	-3.5356347
C	-1.8119765	-0.7392048	-3.5745161
C	0.8002720	0.3829889	-0.1660005
C	0.8554557	0.4448136	-1.6048064
C	1.5419996	-0.6363801	-2.3457769
C	1.4319656	-0.7473963	0.5715203
C	-3.2265171	-1.3871390	-1.7581817
C	-2.8200352	-2.6178802	-2.5182143
C	-3.2456513	-1.4426604	-0.3177135
C	-2.5813647	-0.2387623	-2.4389083
C	-2.1491790	-3.7597682	-1.7955825
C	-0.8740316	-4.0251544	-2.4916973
C	-2.1771505	-3.7778467	-0.3481666
C	-2.8641179	-2.6947721	0.4111703
C	-0.9413446	-4.0620212	0.4237730
C	0.3561877	-4.0150701	-0.2881245
C	0.3974610	-3.9994663	-1.7414944
C	-2.1699242	-2.4049054	1.7037167
C	-0.8934881	-3.3021933	1.6984360
C	0.5220862	-2.6656624	1.7548156
C	-2.0231951	-0.8442545	1.7619083
C	-1.7367207	0.7019858	-1.6652070
C	-1.7619240	0.6475547	-0.2239932
C	-2.6379395	-0.3389300	0.4793280
C	-0.4057949	0.7561298	-2.3649670
C	-0.4828785	0.6349676	0.5586240
C	-0.5894008	-0.1948028	1.8140334
C	0.6745704	-1.1144850	1.8076322