Supporting Information

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SI Text

Calculations on Models Systems. To test the feasibility of using the G3MP2 and G3 methods in the study of proton-bound homodimers, the analogous calculations were performed on the model complexes of ammonia, methylamine, dimethyl amine, and trimethyl amine and compared with known experimental values (1). Using geometry optimizations performed at the B3LYP/6–31++G(d,p) level of theory, the energy calculations were performed by using the B3LYP/6–31++G(d,p), G3(MP2), and G3 methods. The calculated proton affinities for this family of molecules are shown in Table S1 and agree with the experimentally determined values (2). Having demonstrated the validity of these computational methods in accurately calculating the proton affinity of the model compounds, the enthalpy of the hydrogen bond formed between the protonated amine and water ($[B{\cdot\cdot}H{\cdot\cdot}OH_2]^+$) and between the protonated amine and a second amine molecule ($[B{\cdot\cdot}H{\cdot\cdot}B]^+$) were calculated. The calculated hydrogen bond enthalpies agree well with known values (1, 2) for both the $[B{\cdot\cdot}H{\cdot\cdot}OH_2]^+$ and $[B{\cdot\cdot}H{\cdot\cdot}B]^+$ complexes (Table S6). As is expected based on published analysis of the accuracy of B3LYP calculations, the deviation of the B3LYP energies from experimentally determined values increases (3) as the number of bonds in the molecule increases. In comparison, the G3MP2 and G3 energies were in good agreement with experimentally determined values for each compound investigated.

1. Mautner M (2005) The ionic hydrogen bond. *Chem Rev* 105:213–284.
2. Meot-Ner (Mautner) ML, Lia SG (2001) Binding energies between ions and molecules, and the thermochemistry of cluster ions. *NIST Chemistry Webbook*, eds Linstrom PJ, Mallard WG (NIST Standard Reference Database Number 69; National Institute of Standards and Technology, Gaithersburg, MD) accessible at http://webbook.nist.gov.
3. Redfern PC, Zapol P, Curtiss LA, Raghavachari K (2000) Assessment of Gaussian-3 and density functional theories for enthalpies of formation of C_1-C_{16} alkanes. *J Phys Chem A* 104:5850–5854.

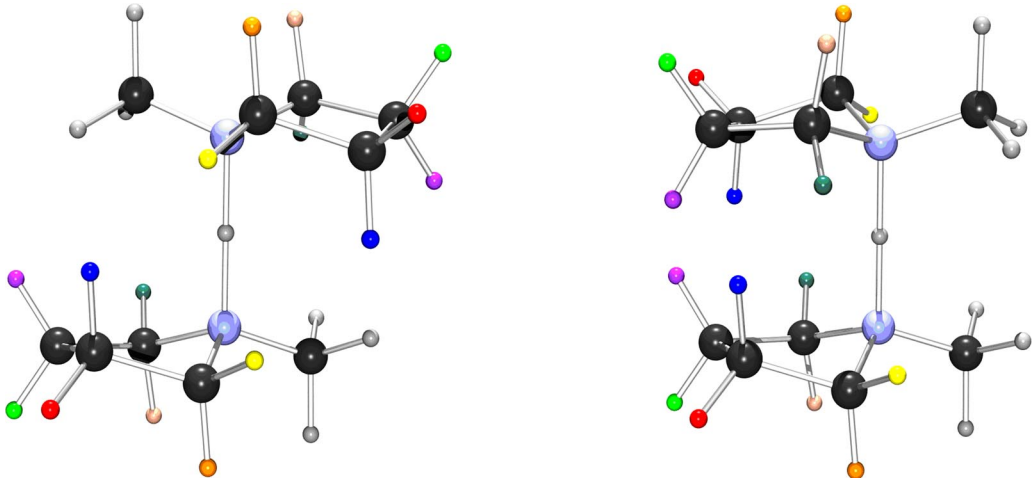

Fig. S1. Symmetry of encapsulated homodimers. Two conformations of the proton-bound homodimer of *N*-methylpyrrolidine. The C_{2v} (*Left*) and C_{2h} (*Right*) conformation of the proton-bound homodimer of *N*-methylpyrrolidine. The hydrogens are color-coded to show equivalent hydrogens upon encapsulation in **1**.

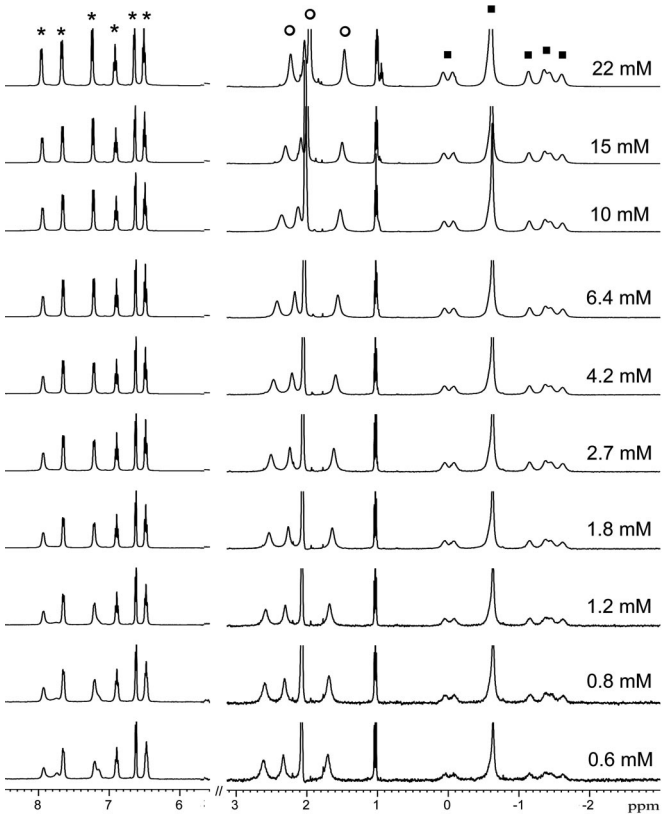

Fig. S2. Dilution ^{1}H NMR experiments of *N*-methylpyrrolidine and **1**. The resonances corresponding to the assembly (*), external *N*-methylpyrrolidine (○), and encapsulated *N*-methylpyrrolidine (■) are labeled for clarity. The guest region of the spectra (3 to −3 ppm) has been enlarged 4 times for clarity.

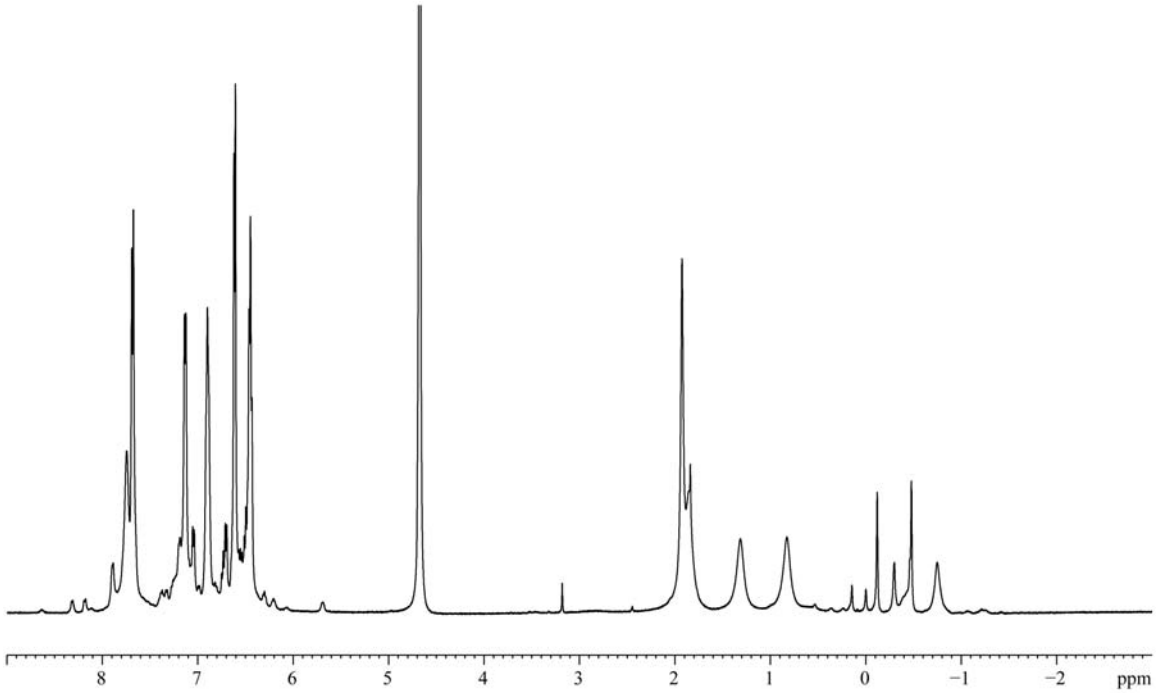

Fig. S3. ^{1}H NMR spectrum of 2 equivalents of *N*-methylaziridine in **1**.

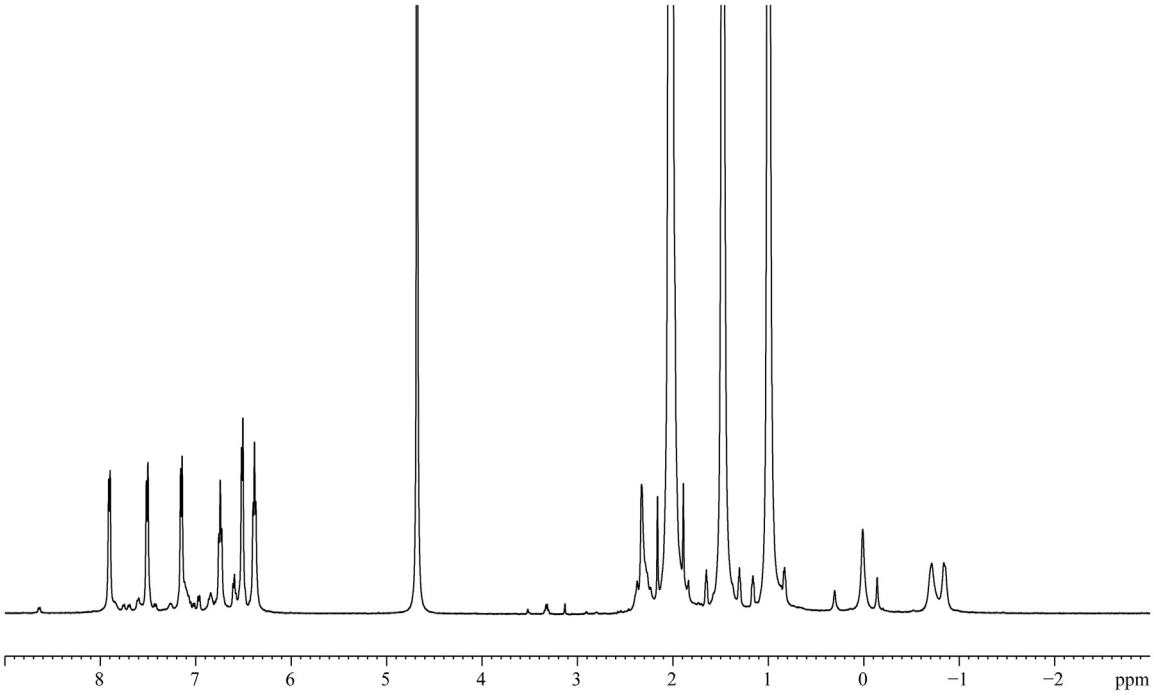

Fig. S4. ^{1}H NMR spectrum of 3 equivalents of *N*-methylaziridine in **1**.

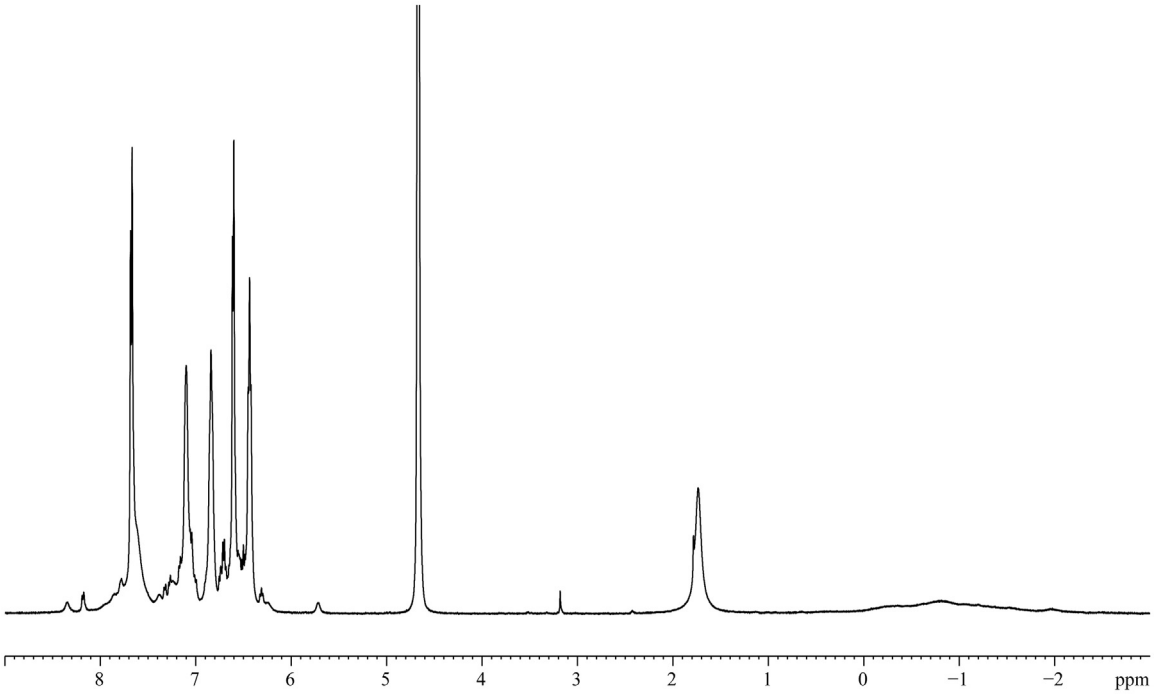

Fig. S5. ^{1}H NMR spectrum of 1 equivalent of *N*-methylazetidine in **1**.

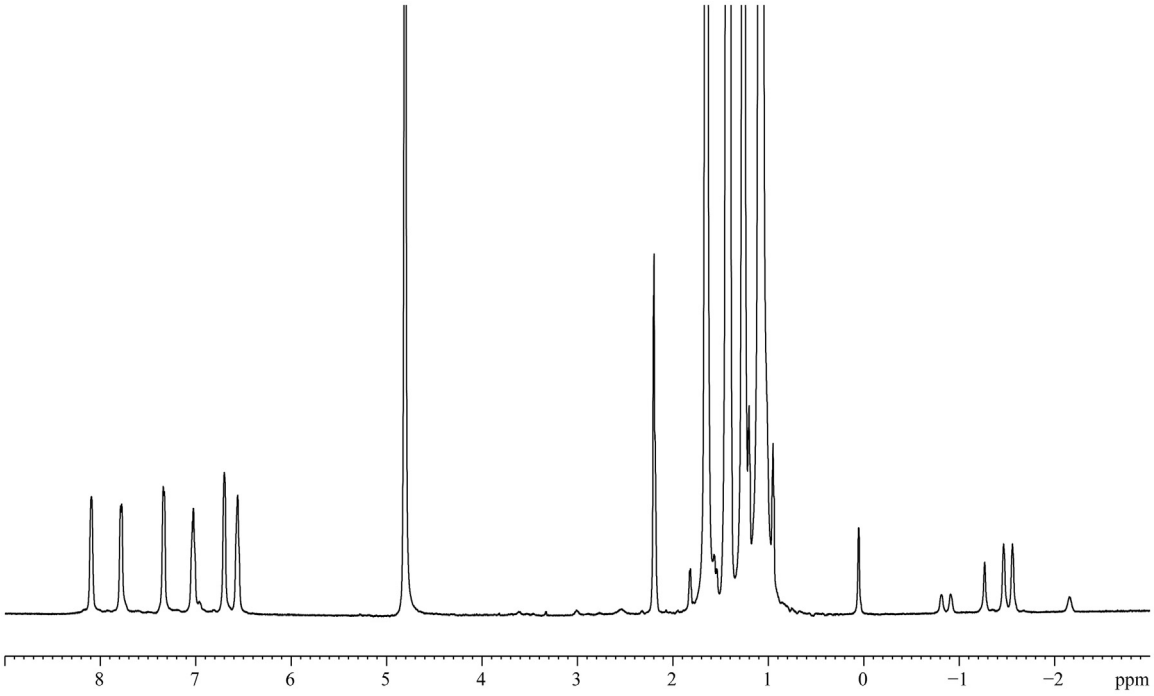

Fig. S6. ^{1}H NMR spectrum of 2 equivalents of *N*-isopropylaziridine in **1**.

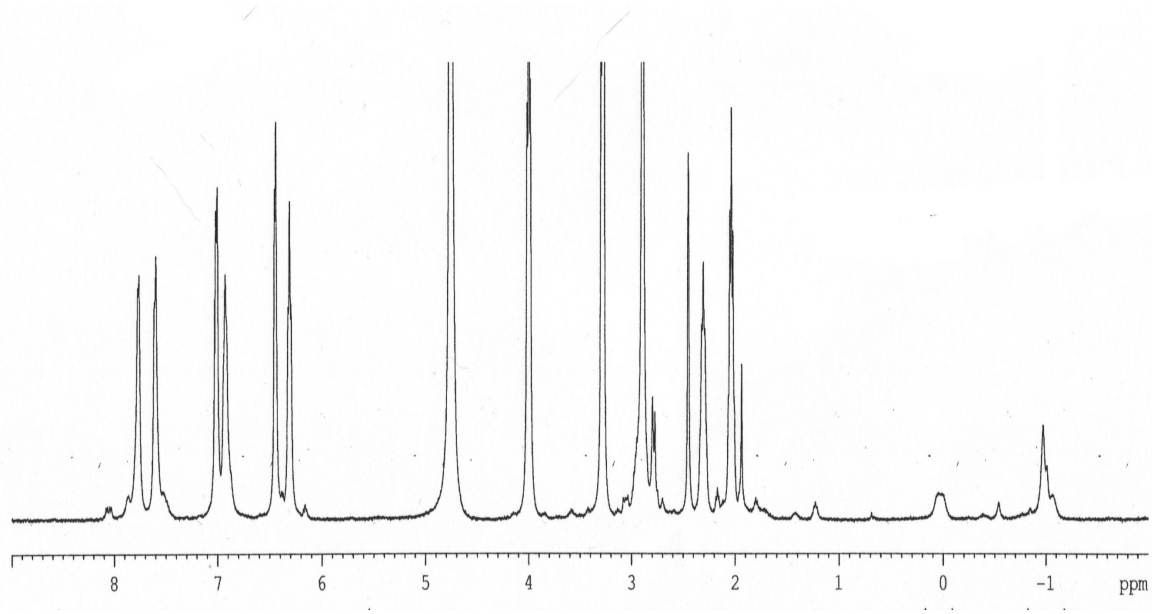

Fig. S7. ^{1}H NMR spectrum of 1 equivalent of *N*-methylazetidine in **1**.

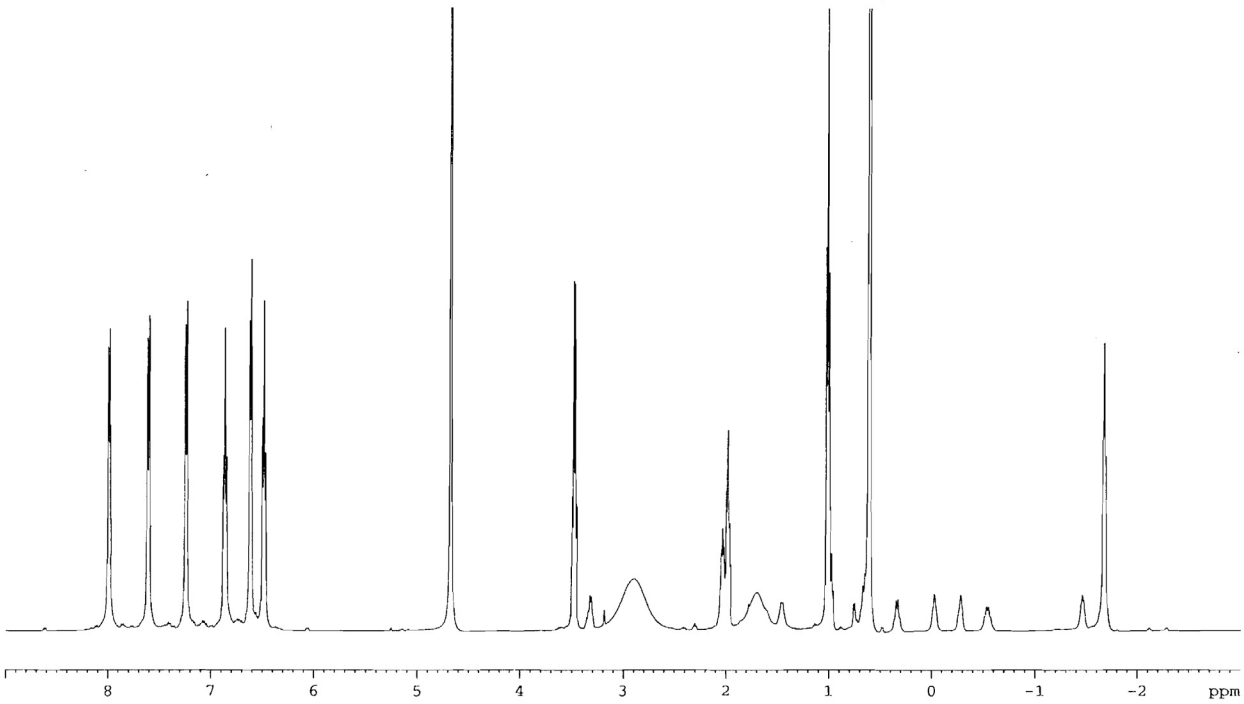

Fig. S8. ^{1}H NMR spectrum of 2 equivalents of *N*-isopropylazetidine in **1**.

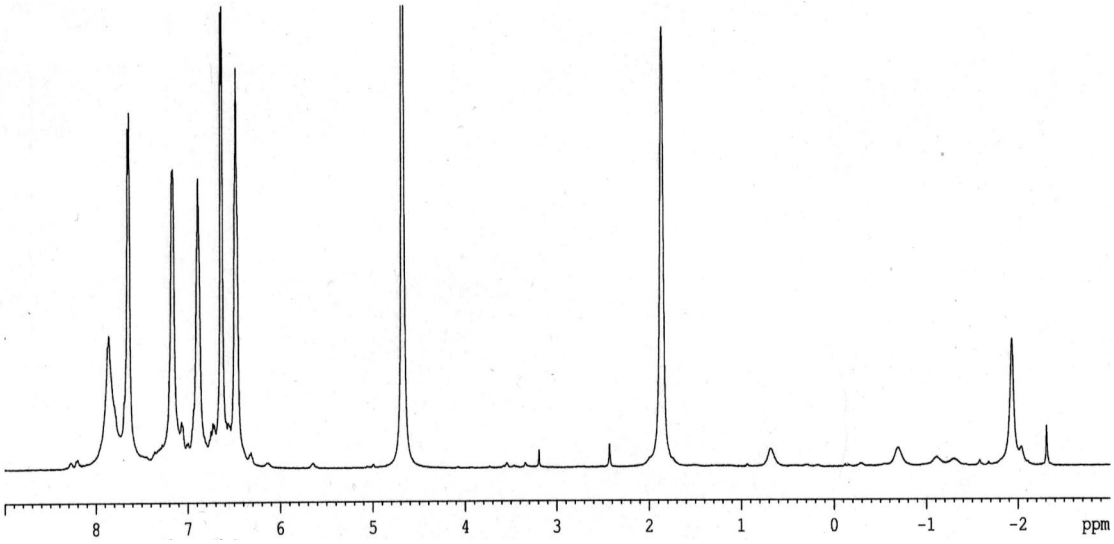

Fig. S9. ^{1}H NMR spectrum of 2 equivalents of *N*-tertbutylazetidine in **1**.

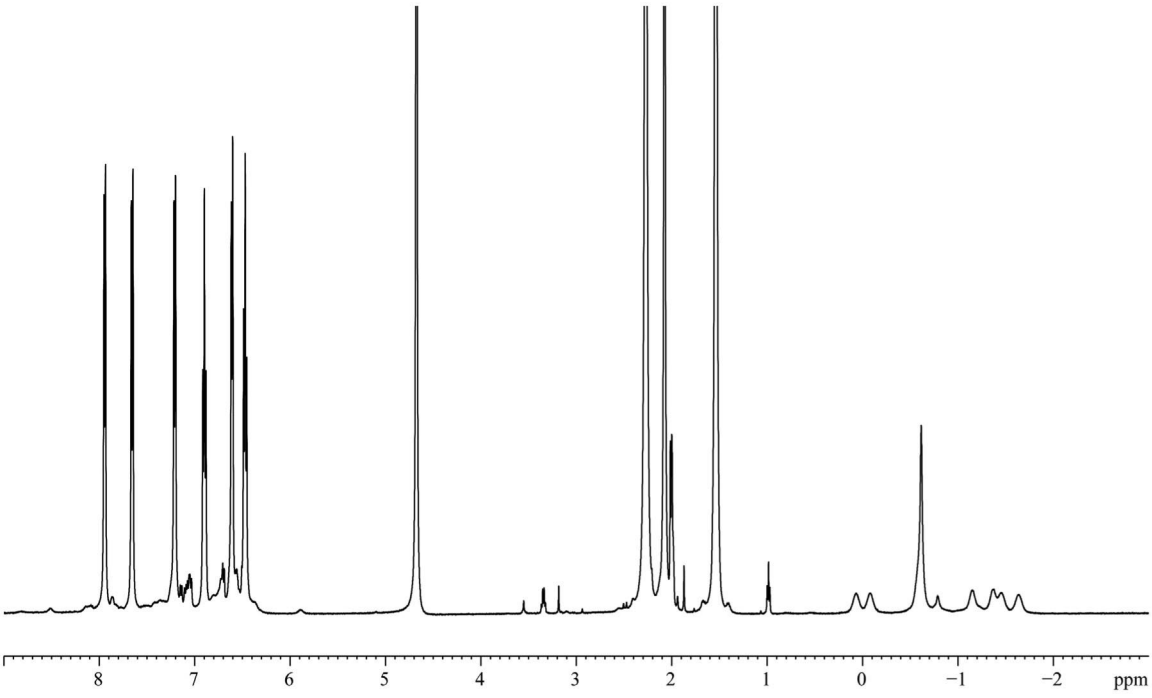

Fig. S10. ^{1}H NMR spectrum of 2 equivalents of *N*-methylpyrrolidine in **1**.

Table S1. Calculated volumes of $[B{\cdot\cdot}H{\cdot\cdot}OH_2]^+$ and $[B{\cdot\cdot}H{\cdot\cdot}B]^+$ complexes

Compound	Volume, Å^3	Compound	Volume, Å^3
$[2{\cdot\cdot}H{\cdot\cdot}OH_2]^+$	80	$[2{\cdot\cdot}H{\cdot\cdot}2]^+$	123
$[3{\cdot\cdot}H{\cdot\cdot}OH_2]^+$	95	$[3{\cdot\cdot}H{\cdot\cdot}3]^+$	153
$[4{\cdot\cdot}H{\cdot\cdot}OH_2]^+$	109	$[4{\cdot\cdot}H{\cdot\cdot}4]^+$	182
$[5{\cdot\cdot}H{\cdot\cdot}OH_2]^+$	125	$[5{\cdot\cdot}H{\cdot\cdot}5]^+$	212
$[6{\cdot\cdot}H{\cdot\cdot}OH_2]^+$	93	$[6{\cdot\cdot}H{\cdot\cdot}6]^+$	150
$[7{\cdot\cdot}H{\cdot\cdot}OH_2]^+$	108	$[7{\cdot\cdot}H{\cdot\cdot}7]^+$	179
$[8{\cdot\cdot}H{\cdot\cdot}OH_2]^+$	124	$[8{\cdot\cdot}H{\cdot\cdot}8]^+$	210
$[9{\cdot\cdot}H{\cdot\cdot}OH_2]^+$	125	$[9{\cdot\cdot}H{\cdot\cdot}9]^+$	240
$[10{\cdot\cdot}H{\cdot\cdot}OH_2]^+$	107	$[10{\cdot\cdot}H{\cdot\cdot}10]^+$	176
$[14{\cdot\cdot}H{\cdot\cdot}OH_2]^+$	121	$[14{\cdot\cdot}H{\cdot\cdot}14]^+$	204

Table S2. Comparison of the calculated and experimentally known proton affinities

	Proton affinity, kcal/mol			
Substrate	B3LYP	G3MP2	G3	Exp.
NH_3	203.1	202.9	203.1	204.0
$MeNH_2$	213.9	213.9	214.0	214.9
Me_2NH	220.7	221.1	221.2	222.2
Me_3N	224.9	225.7	225.7	226.8

Table S3. Comparison of calculated an known experimental values for hydrogen bond enthalpies in $[B\cdot\cdot H\cdot\cdot OH_2]^+$ and $[B\cdot\cdot H\cdot\cdot B]^+$

	ΔH $[B\cdot\cdot H\cdot\cdot OH_2]^+$, kcal/mol				ΔH $[B\cdot\cdot H\cdot\cdot B]^+$, kcal/mol			
Substrate	B3LYP	G3MP2	G3	Exp.	B3LYP	G3MP2	G3	Exp.
NH_3	20.4	18.3	18.7	20.2	27.9	24.0	24.7	25.2
$MeNH_2$	17.9	16.5	17.0	17.8	25.9	24.0	24.5	23.6
Me_2NH	16.2	15.4	15.9	15.0	23.0	23.9	24.3	22.5
Me_3N	15.1	14.9	15.4	14.5	19.8	23.7	24.3	22.2

Table S4. Calculated raw energies for model amines

	B3LYP, hartrees		G3MP2, hartrees		G3, hartrees	
Substrate	Neutral	Protonated	Neutral	Substrate	Neutral	Protonated
NH_3	−56.856471	−56.532727	−56.796378	−56.473101	−56.832128	−56.508481
$MeNH_2$	−96.148881	−95.807973	−96.032391	−95.691533	−96.103862	−95.762781
Me_2NH	−135.440887	−135.089099	−135.270206	−134.917819	−135.377362	−135.024850
Me_3N	−174.731448	−174.373028	−174.509246	−174.149617	−174.652008	−174.292324

Table S5. Calculated raw energies for $[B{\cdot\cdot}H{\cdot\cdot}OH_2]^+$ complexes for model amines

	Energy of $[B{\cdot\cdot}H{\cdot\cdot}OH_2]^+$, hartrees		
Substrate	B3LYP	B3LYP	B3LYP
NH_3	−133.301827	−133.171026	−133.245677
$MeNH_2$	−172.590269	−172.404252	−172.514576
Me_2NH	−211.879611	−211.640307	−211.786325
Me_3N	−251.168426	−250.878529	−251.060216

Table S6. Calculated raw energies for $[B{\cdot\cdot}H{\cdot\cdot}B]^+$ complexes for model amines

	Δ Energy of $[B{\cdot\cdot}H{\cdot\cdot}B]^+$, hartrees		
Substrate	B3LYP	G3MP2	G3
NH_3	−113.433622	−113.307799	−113.379911
$MeNH_2$	−191.998057	−191.762195	−191.905741
Me_2NH	−270.566565	−270.226092	−270.440989
Me_3N	−349.135987	−348.696711	

Table S7. Calculated raw energies for cyclic amines

	B3LYP, hartrees		G3MP2, hartrees		G3, hartrees	
Substrate	Neutral	Protonated	Neutral	Protonated	Neutral	Protonated
2	−173.505371	−173.150384	−173.279971	−172.926786	−173.424649	−173.071187
3	−212.801463	−212.442610	−212.523529	−212.166763	−212.703695	−212.346720
4	−252.097301	−251.735471	−251.768814	−251.409465	−251.984512	−251.625016
5	−291.388412	−291.021442	−291.011679	−290.647105	−291.262973	−290.898249
6	−212.808310	−212.445000	−212.531367	−212.168582	−212.711473	−212.348712
7	−252.100343	−251.736509	−251.771469	−251.408371	−251.987051	−251.624105
8	−291.398586	−291.028387	−291.019650	−290.650850	−291.270764	−290.902090
9	−330.689121	−330.315221	−330.262260	−329.889693	−330.549007	−330.176597
10	−252.126398	−251.761411	−251.800097	−251.435468	−252.015620	−251.651050
14	−291.419354	−291.056277	−291.047576	−290.680085	−290.931228	−290.564238

Table S8. Calculated raw energies for $[B{\cdot\cdot}H{\cdot\cdot}OH_2]^+$ complexes for cyclic amines

	Energy of $[B{\cdot\cdot}H{\cdot\cdot}OH_2]^+$, hartrees		
Substrate	B3LYP	G3MP2	G3
2	−249.943483	−249.650066	−249.833672
3	−289.238114	−288.892683	−289.111795
4	−328.532862	−328.137340	−328.392032
5	−367.823002	−367.379704	−367.670004
6	−289.244239	−288.899900	−289.119074
7	−328.538409	−328.142384	−328.396935
8	−367.829129	−367.383552	−367.673627
9	−407.121601	−406.628677	−406.954438
10	−328.561304	−328.168100	−328.422584
14	−367.857603	−367.414809	−367.337163

Table S9. Calculated raw energies for $[B\cdot\cdot H\cdot\cdot B]^+$ complexes for cyclic amines

	Energy of $[B\cdot\cdot H\cdot\cdot B]^+$, hartrees		
Substrate	B3LYP	G3MP2	G3
2	−346.692624	−346.246475	−346.536453
3	−425.278547	−424.730523	−425.091574
4	−503.863769	−503.218394	−503.650494
5	−582.436972	−581.697703	—
6	−425.285390	−424.738598	−425.099670
7	−503.866732	−503.219863	−503.570702
8	−582.445861	−581.702005	—
9	−661.022700	−660.185955	—
10	−503.916075	−503.274407	—
14	−582.501997	—	—

Table S10. Calculated Cartesian coordinates for *N*-methylaziridine

Atom	*x*	*y*	*z*	Atom	*X*	*y*	*z*
C	0.00000	0.00000	0.00000	N	0.74696	−0.38291	1.19616
C	1.49393	0.00000	0.00000	C	0.74695	0.58201	2.29067
H	−0.49746	0.97093	0.00000	H	−0.14067	0.42193	2.91119
H	−0.55286	−0.79747	−0.49021	H	1.63453	0.42190	2.91124
H	1.99139	0.97093	0.00000	H	0.74698	1.63229	1.94721
H	2.04679	−0.79747	−0.49021				

Table S11. Calculated Cartesian coordinates for H^+-*N*-methylaziridine

Atom	*x*	*y*	*z*	Atom	*X*	*y*	*z*
C	0.00000	0.00000	0.00000	H	0.74079	−1.24758	1.56896
C	1.48158	0.00000	0.00000	N	0.74079	−0.27174	1.27362
H	−0.53387	0.94448	0.00000	C	0.74078	0.69363	2.40665
H	−0.53762	−0.85342	−0.39963	H	−0.15686	0.52910	3.00460
H	2.01546	0.94447	0.00000	H	1.63832	0.52898	3.00471
H	2.01920	−0.85342	−0.39963	H	0.74087	1.70709	2.00427

Table S12. Calculated Cartesian coordinates for *N*-ethylaziridine.

Atom	*x*	*y*	*z*	Atom	*X*	*y*	*z*
C	1.16204	0.90058	0.18083	C	−0.82012	−0.60000	0.20543
C	1.65685	−0.49756	0.00719	H	−1.00386	−1.62420	−0.14135
H	0.85190	1.19618	1.18421	H	−0.63349	−0.65570	1.29515
H	1.55457	1.70730	−0.43304	C	−2.04335	0.27189	−0.06792
H	1.67818	−1.13085	0.89511	H	−2.25448	0.31053	−1.14097
H	2.41556	−0.72812	−0.73652	H	−2.92432	−0.12771	0.44590
N	0.35235	−0.09919	−0.51493	H	−1.88298	1.29739	0.28277

Table S13. Calculated Cartesian coordinates for H^+-*N*-ethylaziridine

Atom	*x*	*y*	*z*	Atom	*X*	*y*	*z*
C	−1.24084	0.89533	−0.22243	H	1.06553	−1.62676	0.13155
C	−1.70857	−0.49891	−0.03964	H	0.68448	−0.66662	−1.30942
H	−0.89943	1.21683	−1.20078	C	2.09011	0.30110	0.05248
H	−1.60315	1.67626	0.43761	H	2.30942	0.34968	1.12393
H	−1.70331	−1.17708	−0.88648	H	2.97673	−0.10187	−0.44441
H	−2.40963	−0.73274	0.75452	H	1.92725	1.31512	−0.32396
N	−0.34183	−0.10960	0.42619	H	−0.24504	−0.00575	1.43646
C	0.90762	−0.61084	−0.24080				

Table S14. Calculated Cartesian coordinates for *N*–isopropylaziridine

Atom	*x*	*y*	*z*	Atom	*X*	*y*	*z*
C	0.00000	0.00000	0.00000	C	2.01498	0.37115	3.14402
C	1.49312	0.00000	0.00000	H	2.91414	0.51802	2.53627
H	−0.49441	0.97252	0.00000	H	2.04771	1.08191	3.97663
H	−0.55515	−0.79453	−0.49233	H	2.04381	−0.64469	3.55243
H	1.98769	0.97244	0.00014	C	−0.52187	0.37086	3.14416
H	2.04813	−0.79460	−0.49237	H	−0.55047	−0.64500	3.55253
N	0.74656	−0.38535	1.19555	H	−0.55471	1.08159	3.97680
C	0.74650	0.57214	2.31158	H	−1.42111	0.51755	2.53647
H	0.74638	1.60933	1.92024				

Table S15. Calculated Cartesian coordinates for H^+-*N*–isopropylaziridine

Atom	*x*	*y*	*z*	Atom	*X*	*y*	*z*
C	0.00000	0.00000	0.00000	C	2.02171	0.48307	3.24176
C	1.48262	0.00000	0.00000	H	2.91841	0.62358	2.63119
H	−0.52905	0.94714	0.00000	H	2.05510	1.21261	4.05498
H	−0.53957	−0.84824	−0.40740	H	2.05270	−0.51446	3.69361
H	2.01154	0.94724	0.00019	C	−0.53999	0.48462	3.24053
H	2.02249	−0.84796	−0.40759	H	−0.57265	−0.51288	3.69235
N	0.74144	−0.27424	1.26756	H	−0.57322	1.21420	4.05372
C	0.74135	0.69128	2.43757	H	−1.43599	0.62623	2.62917
H	0.74219	1.68323	1.97279	H	0.74145	−1.25207	1.56040

Table S16. Calculated Cartesian coordinates for *N*–tertbutylaziridine

Atom	*x*	*y*	*z*	Atom	*X*	*y*	*z*
C	0.00000	0.00000	0.00000	H	−0.55393	0.42630	4.18464
C	1.49641	0.00000	0.00000	H	−1.41862	0.21728	2.65105
H	−0.49022	0.97286	0.00000	C	0.74817	1.90291	2.25878
H	−0.55523	−0.78451	−0.50981	H	−0.14027	2.25920	1.72726
H	1.98663	0.97287	0.00000	H	0.74834	2.38067	3.24386
H	2.05164	−0.78445	−0.50989	H	1.63649	2.25914	1.72700
N	0.74820	−0.42362	1.17655	C	2.00918	−0.05825	3.20324
C	0.74815	0.36894	2.43379	H	2.04998	0.42635	4.18476
C	−0.51298	−0.05826	3.20309	H	2.01605	−1.14282	3.34682
H	−0.51984	−1.14283	3.34666	H	2.91488	0.21731	2.65130

Table S17. Calculated Cartesian coordinates for H^+-*N*–tertbutylaziridine

Atom	*x*	*y*	*z*	Atom	*X*	*y*	*z*
C	0.00000	0.00000	0.00000	H	1.63458	2.35849	1.65725
C	1.48301	0.00000	0.00000	C	2.01326	0.15263	3.30273
H	−0.52305	0.94857	0.00000	H	2.91677	0.40288	2.73833
H	−0.54265	−0.84211	−0.41598	H	2.05374	0.69123	4.25288
H	2.00601	0.94858	−0.00004	H	2.02673	−0.91812	3.53440
H	2.02559	−0.84212	−0.41604	H	0.74149	−1.28970	1.50093
N	0.74147	−0.29822	1.26137	C	−0.53064	0.15263	3.30261
C	0.74135	0.55634	2.54679	H	−0.54398	−0.91806	3.53461
C	0.74130	2.04764	2.20599	H	−0.57138	0.69148	4.25260
H	−0.15178	2.35827	1.65680	H	−1.43407	0.40256	2.73794
H	0.74102	2.60330	3.14717				

Table S18. Calculated Cartesian coordinates for *N*-methylazetidine

Atom	*x*	*y*	*z*	Atom	*X*	*y*	*z*
C	0.00000	0.00000	0.00000	H	0.06149	1.95739	−1.02276
C	1.54838	0.00000	0.00000	H	−0.53377	2.12342	0.65867
C	0.12258	1.54352	0.00000	N	1.51645	1.40079	0.47504
H	−0.50126	−0.46303	−0.85223	C	2.51734	2.32534	−0.01668
H	−0.41997	−0.38794	0.93089	H	2.30395	3.33368	0.35439
H	1.95612	−0.09366	−1.02276	H	3.50562	2.03279	0.35439
H	2.07450	−0.70020	0.65867	H	2.56053	2.36525	−1.12373

Table S19. Calculated Cartesian coordinates for H^+-*N*-methylazetidine

Atom	*x*	*y*	*z*	Atom	*X*	*y*	*z*
C	0.00000	0.00000	0.00000	H	−0.54709	2.09750	0.72438
C	1.54412	0.00000	0.00000	N	1.53897	1.48959	0.37990
C	0.05034	1.54330	0.00000	C	2.50101	2.42076	−0.27781
H	−0.47769	−0.46236	−0.86327	H	2.27030	3.44281	0.02836
H	−0.42872	−0.41497	0.91408	H	3.51500	2.15685	0.02836
H	1.99454	−0.10040	−0.98868	H	2.39894	2.32197	−1.35907
H	2.07855	−0.61518	0.72438	H	1.63456	1.58211	1.39486
H	−0.03532	1.99675	−0.98868				

Table S20. Calculated Cartesian coordinates for *N*-ethylazetidine

Atom	*x*	*y*	*z*	Atom	*X*	*y*	*z*
C	1.24790	0.59350	0.25755	H	−0.46039	−1.24068	1.21818
H	1.16572	0.63140	1.36451	H	−0.47748	−1.95138	−0.42580
C	2.39966	−0.32909	−0.13977	H	−1.18909	1.44757	0.95157
H	2.52409	−0.34317	−1.22717	H	−1.46734	1.74229	−0.79320
H	3.33765	0.00606	0.31571	H	−2.78098	−0.45684	0.76062
H	2.21731	−1.35687	0.19388	H	−2.49987	−0.55572	−1.00050
C	−0.67729	−1.04306	0.15261	N	−0.00962	0.18322	−0.34480
C	−1.22215	0.97744	−0.04766	H	1.45791	1.61656	−0.07966
C	−2.04149	−0.33574	−0.03348				

Table S21. Calculated Cartesian coordinates for H^+-*N*-ethylazetidine

Atom	*x*	*y*	*z*	Atom	*X*	*y*	*z*
C	1.44728	−0.13809	−0.62662	H	−0.34266	−1.31267	1.09543
H	1.77682	0.60104	−1.36280	H	−1.21233	−1.95470	−0.33030
C	2.05239	0.14144	0.74104	H	−0.29861	1.56205	0.66518
H	1.72743	−0.57090	1.50390	H	−1.15294	1.78659	−0.89098
H	3.13738	0.03890	0.65019	H	−2.26793	0.24093	1.44143
H	1.85518	1.15782	1.09062	H	−2.80798	−0.00308	−0.23614
C	−0.91001	−1.05265	0.20245	N	−0.06673	−0.11138	−0.66973
C	−0.87665	1.07091	−0.11622	H	1.72975	−1.13054	−0.99074
C	−1.93639	0.08147	0.41578	H	−0.33662	−0.25426	−1.64637

Table S22. Calculated Cartesian coordinates for *N*-isopropylazetidine

Atom	*x*	*y*	*z*	Atom	*X*	*y*	*z*
C	0.00000	0.00000	0.00000	C	−0.00816	−2.05526	1.48193
H	1.11233	0.00000	0.00000	C	−0.00816	−0.22931	2.52342
C	−0.47508	1.45659	0.00000	C	0.00187	−1.70448	2.98832
H	−0.12320	1.99533	0.88607	H	1.01207	−2.23709	1.09871
H	−0.09523	1.98314	−0.88193	H	−0.66617	−2.86047	1.13857
H	−1.56981	1.49962	−0.01286	H	1.01207	0.19311	2.48484
C	−0.47508	−0.74149	−1.25374	H	−0.66617	0.47614	3.04170
H	−1.56981	−0.75232	−1.29732	H	0.86017	−2.03883	3.57451
H	−0.09523	−0.25042	−2.15590	H	−0.92351	−1.99221	3.49279
H	−0.12320	−1.77841	−1.26638	N	−0.48810	−0.68183	1.19540

Table S23. Calculated Cartesian coordinates for H^+-*N*-isopropylazetidine

Atom	*x*	*y*	*z*	Atom	*X*	*y*	*z*
C	0.00000	0.00000	0.00000	C	0.18394	−0.13974	2.63613
H	1.09570	0.00000	0.00000	C	0.38553	−1.59088	3.12200
C	−0.52780	1.43322	0.00000	H	1.11263	−2.19506	1.10814
H	−0.13709	2.02233	0.83466	H	−0.51361	−2.86102	1.45160
H	−0.21601	1.92815	−0.92321	H	1.11263	0.39354	2.42722
H	−1.62312	1.45705	0.03111	H	−0.51361	0.50707	3.16788
C	−0.52780	−0.84234	−1.15956	H	1.35406	−1.81760	3.56692
H	−1.62312	−0.88152	−1.16055	H	−0.40685	−1.93182	3.79107
H	−0.21601	−0.38629	−2.10258	N	−0.38061	−0.66763	1.31019
H	−0.13709	−1.86386	−1.14564	H	−1.40388	−0.69410	1.36214
C	0.18394	−2.05066	1.66238				

Table S24. Calculated Cartesian coordinates for *N*-tbutylazetidine

Atom	*x*	*y*	*z*	Atom	*X*	*y*	*z*
C	0.00000	0.00000	0.00000	H	−0.16083	−0.73732	−2.71520
C	1.53883	0.00000	0.00000	H	0.79868	0.74801	−2.97048
H	1.91914	1.02637	0.00000	H	−2.50377	0.09903	−1.28962
H	1.92518	−0.51704	0.88484	H	−2.32491	1.86305	−1.06984
H	1.93662	−0.51173	−0.88361	H	−2.08862	0.46806	−3.70725
C	−0.51524	−1.45971	0.00757	H	−1.31831	2.04297	−3.36521
H	−0.15954	−2.01969	−0.86389	N	−0.43691	0.77748	−1.17423
H	−0.15984	−1.98440	0.90109	C	−0.51790	0.73254	1.25030
H	−1.60958	−1.50329	0.01612	H	−0.17462	0.23134	2.16160
C	−0.13846	0.35446	−2.56082	H	−0.15772	1.76608	1.26194
C	−1.86535	0.97091	−1.51006	H	−1.61329	0.75212	1.27471
C	−1.46305	1.02208	−3.00417				

Table S25. Calculated Cartesian coordinates for H^+-*N*-tbutylazetidine

Atom	*x*	*y*	*z*	Atom	*X*	*y*	*z*
C	0.00000	0.00000	0.00000	H	−2.46856	1.05034	−0.78396
C	1.53475	0.00000	0.00000	H	−2.32319	0.11320	−2.30018
H	1.94575	1.01421	0.00000	H	−0.05241	2.69298	−0.74578
H	1.89427	−0.49886	0.90334	H	0.79820	2.23530	−2.25086
H	1.94295	−0.54693	−0.85762	H	−2.07947	3.10816	−2.13684
C	−0.56292	−1.42739	−0.03360	H	−1.40287	2.14395	−3.46963
H	−0.18489	−1.99518	−0.89148	N	−0.42381	0.65421	−1.33382
H	−0.25096	−1.95825	0.86918	H	−0.01436	0.06897	−2.06763
H	−1.65693	−1.43726	−0.05811	C	−0.55641	0.78972	1.18808
C	−1.89213	0.91237	−1.69748	H	−0.17736	1.81416	1.23161
C	−0.11629	2.11970	−1.66942	H	−1.64917	0.81152	1.20877
C	−1.48007	2.23226	−2.38421	H	−0.23181	0.29233	2.10583

Table S26. Calculated Cartesian coordinates for *N*-methylpyrrolidine

Atom	*x*	*y*	*z*	Atom	*X*	*y*	*z*
C	0.00000	0.00000	0.00000	H	2.09651	1.84982	−1.03930
C	1.55847	0.00000	0.00000	H	−1.28981	1.71295	0.56780
C	1.93761	1.49314	0.00000	H	−0.53792	1.84970	−1.03967
C	−0.37934	1.49319	−0.00019	N	0.77896	2.14768	0.60814
H	−0.41946	−0.52044	−0.86611	C	0.77916	3.59471	0.49785
H	−0.38414	−0.49353	0.89743	H	−0.10671	4.00628	0.99241
H	1.97793	−0.52053	−0.86606	H	1.66473	4.00604	0.99317
H	1.94255	−0.49371	0.89737	H	0.77959	3.94291	−0.55503
H	2.84778	1.71333	0.56833				

Table S27. Calculated Cartesian coordinates for H^+-*N*-methylpyrrolidine

Atom	*x*	*y*	*z*	Atom	*X*	*y*	*z*
C	0.00000	0.00000	0.00000	H	2.30763	1.82641	−0.98430
C	1.55690	0.00000	0.00000	H	−1.36186	1.76081	0.08107
C	1.98102	1.48350	0.00000	H	−0.36457	1.65842	−1.39245
C	−0.39927	1.44021	−0.32158	N	0.70861	2.25952	0.31644
H	−0.41919	−0.69269	−0.73214	C	0.74076	3.70562	−0.07595
H	−0.38972	−0.29244	0.97991	H	−0.20151	4.17347	0.21219
H	1.96042	−0.49710	−0.88432	H	1.57233	4.19413	0.43366
H	1.94931	−0.52520	0.87308	H	0.87533	3.76855	−1.15636
H	2.74263	1.74767	0.73560	H	0.56757	2.21681	1.33092

Table S28. Calculated Cartesian coordinates for *N*-methylpiperidine

Atom	*x*	*y*	*z*	Atom	*X*	*y*	*z*
C	1.90010	−0.00001	0.24028	H	−0.85190	2.07924	−0.21440
C	1.15670	−1.25922	−0.22709	H	−0.38873	1.27349	1.29679
C	−0.31710	−1.21156	0.18887	H	1.21188	1.33551	−1.32056
C	−0.31710	1.21157	0.18887	H	1.62249	2.16160	0.18757
C	1.15671	1.25922	−0.22708	H	−0.38874	−1.27347	1.29680
H	−0.85193	−2.07923	−0.21438	N	−0.97279	0.00000	−0.30766
H	1.21186	−1.33552	−1.32057	C	−2.39876	0.00000	−0.01570
H	1.62246	−2.16161	0.18756	H	−2.86749	0.88631	−0.45580
H	1.96017	−0.00001	1.33832	H	−2.86748	−0.88632	−0.45578
H	2.93155	−0.00001	−0.13213	H	−2.61788	0.00001	1.07128

Table S29. Calculated Cartesian coordinates for H^+-*N*-methylpiperidine

Atom	*x*	*y*	*z*	Atom	*X*	*y*	*z*
C	0.00000	0.00000	0.00000	H	−0.24701	2.80392	0.26063
C	1.53527	0.00000	0.00000	H	−0.31096	0.35050	2.12555
C	2.10115	1.41853	0.00000	H	−1.63064	0.92277	1.12106
C	0.03426	2.25248	1.16290	H	1.81458	1.97208	−0.89931
C	−0.54037	0.83747	1.16782	N	1.55571	2.22104	1.17236
H	3.19028	1.43279	0.08690	C	2.14884	3.59976	1.23785
H	1.91733	−0.54857	0.87184	H	1.76457	4.11065	2.12155
H	1.93001	−0.51387	−0.88219	H	3.23495	3.51737	1.29448
H	−0.37099	0.40538	−0.95015	H	1.86200	4.14406	0.33745
H	−0.37365	−1.02511	0.07102	H	1.83626	1.72585	2.02608
H	−0.27520	2.83099	2.03670				

Table S30. Calculated Cartesian coordinates for *N*-methylaziridine + H_3O^+

Atom	*x*	*y*	*z*	Atom	*X*	*y*	*z*
N	−0.31610	0.17341	−0.00044	H	−0.25254	−1.58974	1.27503
C	−0.91042	1.53181	0.00016	H	−1.85646	−0.68317	1.27344
H	−0.57743	2.05919	0.89549	H	0.72394	0.15838	−0.00138
H	−0.57816	2.05965	−0.89516	H	−0.25508	−1.58987	−1.27588
H	−1.99827	1.45131	0.00057	O	2.45867	−0.02192	−0.00022
C	−0.95216	−0.95404	−0.74102	H	3.03765	0.01838	0.77386
H	−1.85898	−0.68330	−1.27120	H	3.03840	0.01791	−0.77378
C	−0.95070	−0.95396	0.74150				

Table S31. Calculated Cartesian coordinates for *N*-ethylaziridine + H_3O^+

Atom	*x*	*y*	*z*	Atom	*x*	*y*	*z*
C	0.11399	1.40340	0.92182	H	1.09295	−0.66005	−1.63385
H	1.11080	1.59157	1.30630	H	2.09442	0.38352	−0.61113
H	−0.68177	1.35152	1.65669	C	1.61334	−1.54212	0.29222
C	−0.20468	1.78133	−0.47610	H	2.51109	−2.03687	−0.08793
H	−1.23114	1.99935	−0.74998	H	1.81314	−1.23221	1.32228
H	0.56363	2.23988	−1.08940	H	0.80382	−2.27794	0.29333
N	0.05471	0.35447	−0.13523	O	−2.35779	−1.06541	−0.01815
H	−0.79713	−0.23884	−0.10342	H	−2.70870	−1.56098	0.73493
C	1.28689	−0.35373	−0.60207	H	−2.94908	−1.25024	−0.76122

Table S32. Calculated Cartesian coordinates for *N*-isopropylazidine + H_3O^+

Atom	*x*	*y*	*z*	Atom	*X*	*y*	*z*
H	−0.87434	−0.39535	−0.00012	H	1.29584	−0.11234	−2.17598
N	−0.24169	0.42708	0.00000	H	2.62955	−0.88480	−1.31302
C	−0.77117	1.60413	−0.74159	H	1.03490	−1.64497	−1.30774
H	−0.01467	2.17541	−1.26887	C	1.55601	−0.68234	1.27907
H	−1.69705	1.42487	−1.27696	H	1.03543	−1.64518	1.30764
C	−0.77126	1.60411	0.74153	H	2.62972	−0.88426	1.31321
H	−0.01472	2.17534	1.26881	H	1.29553	−0.11249	2.17601
C	1.22814	0.08513	0.00002	O	−2.17359	−1.62255	0.00001
H	1.74484	1.05153	0.00002	H	−2.53731	−2.07617	0.77314
H	−1.69718	1.42493	1.27685	H	−2.53590	−2.07758	−0.77296
C	1.55593	−0.68238	−1.27904				

Table S33. Calculated Cartesian coordinates for *N*-tertbutylaziridine + H_3O^+

Atom	*x*	*y*	*z*	Atom	*X*	*y*	*z*
H	−1.18841	−0.17378	−0.00017	H	2.25038	1.13081	−0.89233
N	−0.34632	0.42777	−0.00006	C	0.88654	−1.25891	−1.26997
C	−0.56274	1.69982	−0.74181	H	0.88912	−0.64265	−2.17445
H	0.30655	2.07972	−1.26414	H	1.76381	−1.90986	−1.30756
H	−1.50363	1.74997	−1.27859	H	−0.00092	−1.89980	−1.28135
C	−0.56286	1.69974	0.74177	C	0.88643	−1.25888	1.27001
H	0.30637	2.07956	1.26426	H	1.76361	−1.90995	1.30760
C	0.94561	−0.39943	0.00001	H	0.88912	−0.64260	2.17448
H	−1.50383	1.74986	1.27843	H	−0.00112	−1.89963	1.28142
C	2.18273	0.50229	0.00005	O	−2.85332	−0.89818	−0.00003
H	2.25022	1.13093	0.89236	H	−3.34541	−1.21007	−0.77227
H	3.06666	−0.14045	0.00018	H	−3.34597	−1.20881	0.77235

Table S34. Calculated Cartesian coordinates for *N*-methylazetidine + H_3O^+

Atom	*x*	*y*	*z*	Atom	*X*	*y*	*z*
H	0.88858	0.01384	0.00083	H	−2.58831	−1.30942	0.00141
C	−0.91805	−0.25394	−1.07130	N	−0.06488	0.42763	−0.00030
C	−0.91900	−0.25047	1.07224	C	0.05781	1.90919	−0.00295
C	−1.50440	−1.19784	0.00175	H	0.60325	2.22078	0.88979
H	−0.31756	−0.67808	−1.87660	H	0.60552	2.21730	−0.89549
H	−1.63091	0.46880	−1.47196	H	−0.93868	2.35340	−0.00493
H	−0.31899	−0.67226	1.87910	O	2.54204	−0.67667	0.00097
H	−1.63222	0.47350	1.47005	H	3.10550	−0.83177	0.77178
H	−1.03868	−2.18474	0.00368	H	3.08216	−0.89302	−0.77178

Table S35. Calculated Cartesian coordinates for *N*-ethylazetidine + H_3O^+

Atom	*x*	*y*	*z*	Atom	*x*	*Y*	*z*
C	−2.19637	−0.15521	−0.32556	C	1.02564	−1.07729	0.63731
C	−1.38371	−0.14111	0.98776	H	1.31952	−0.72482	1.63082
C	−0.89696	−0.55683	−1.05796	H	0.59979	−2.07919	0.74307
H	−3.01552	−0.87219	−0.37558	C	2.19971	−1.05939	−0.33300
H	−2.56194	0.83214	−0.61248	H	2.98455	−1.71976	0.04503
H	−1.46515	−1.05643	1.57637	H	1.91508	−1.42221	−1.32537
H	−1.44720	0.73316	1.63603	H	2.62584	−0.05642	−0.43049
H	−0.79678	−1.62893	−1.23606	O	0.78716	2.53059	−0.04377
H	−0.59822	0.00192	−1.94496	H	0.99981	3.01884	−0.85127
N	−0.08540	−0.17924	0.18244	H	0.96989	3.13634	0.68793
H	0.28101	0.78648	0.07873				

Table S36. Calculated Cartesian coordinates for *N*-isoprpopylazetidine + H_3O^+

Atom	*x*	*y*	*z*	Atom	*x*	*y*	*z*
C	−1.23799	−1.92576	0.34382	H	1.08517	0.92514	−1.41258
C	−0.36459	−0.94902	1.16270	C	2.36135	−0.47811	−0.39214
C	−0.68055	−1.26574	−0.93665	H	2.20689	−1.31505	−1.07796
H	−1.01839	−2.98560	0.47143	H	3.26610	0.03946	−0.72198
H	−2.30791	−1.75852	0.47838	H	2.56381	−0.87120	0.60855
H	0.58020	−1.37447	1.49850	C	1.42714	1.67985	0.58306
H	−0.82718	−0.37751	1.96740	H	2.34885	2.20753	0.32522
H	−0.84218	0.64685	−0.11500	H	0.60765	2.40406	0.54746
H	0.14213	−1.81034	−1.39763	H	1.53387	1.31549	1.61044
H	−1.38265	−0.92473	−1.69788	O	−2.24825	1.83059	−0.25076
N	−0.13604	−0.11116	−0.09651	H	−2.55678	2.27736	−1.05131
C	1.21172	0.52684	−0.39871	H	−2.76390	2.20658	0.47612

Table S37. Calculated Cartesian coordinates for *N*-tertbutylazetidine + H_3O^+

Atom	*x*	*y*	*z*	Atom	*x*	*y*	*z*
H	−1.18841	−0.17378	−0.00017	H	2.25038	1.13081	−0.89233
N	−0.34632	0.42777	−0.00006	C	0.88654	−1.25891	−1.26997
C	−0.56274	1.69982	−0.74181	H	0.88912	−0.64265	−2.17445
H	0.30655	2.07972	−1.26414	H	1.76381	−1.90986	−1.30756
H	−1.50363	1.74997	−1.27859	H	−0.00092	−1.89980	−1.28135
C	−0.56286	1.69974	0.74177	C	0.88643	−1.25888	1.27001
H	0.30637	2.07956	1.26426	H	1.76361	−1.90995	1.30760
C	0.94561	−0.39943	0.00001	H	0.88912	−0.64260	2.17448
H	−1.50383	1.74986	1.27843	H	−0.00112	−1.89963	1.28142
C	2.18273	0.50229	0.00005	O	−2.85332	−0.89818	−0.00003
H	2.25022	1.13093	0.89236	H	−3.34541	−1.21007	−0.77227
H	3.06666	−0.14045	0.00018	H	−3.34597	−1.20881	0.77235

Table S38. Calculated Cartesian coordinates for *N*-methylpyrrolidine + H_3O^+

Atom	*x*	*y*	*z*	Atom	*x*	*y*	*z*
C	−1.42958	−0.95517	0.73766	H	−2.73390	−0.04408	−0.76150
C	−0.58932	0.21853	1.23088	H	−1.86671	−1.45190	−1.36281
C	−0.64234	0.36445	−1.18846	N	0.26164	0.55668	0.02579
C	−1.77882	−0.57354	−0.72049	C	0.93322	1.88996	0.08571
H	−0.84354	−1.87955	0.77583	H	1.57363	1.92659	0.96832
H	−2.31622	−1.10382	1.35727	H	1.53485	2.02511	−0.81420
H	0.06409	0.00253	2.07823	H	0.17295	2.67005	0.14651
H	−1.19877	1.09851	1.45647	O	2.39471	−1.32223	−0.13093
H	1.01151	−0.15982	−0.02833	H	3.29900	−1.17162	0.17777
H	−1.00610	1.35009	−1.48451	H	2.39077	−2.20934	−0.51634
H	−0.02967	−0.03701	−1.99750				

Table S39. Calculated Cartesian coordinates for *N*-methylpiperidine + H_3O^+

Atom	*x*	*y*	*z*	Atom	*X*	*y*	*z*
C	0.00000	0.00000	0.00000	H	−0.29943	0.34718	2.12543
C	1.53445	0.00000	0.00000	H	−1.62672	0.91870	1.12878
C	2.09933	1.41945	0.00000	H	1.82411	1.96130	−0.91057
C	0.03881	2.25010	1.16478	N	1.55447	2.23020	1.15896
C	−0.53610	0.83472	1.17062	C	2.12210	3.61598	1.17567
H	3.18802	1.42772	0.09344	H	1.75298	4.14044	2.05807
H	1.91499	−0.54540	0.87354	H	3.21071	3.55388	1.20691
H	1.92926	−0.51494	−0.88160	H	1.80692	4.14218	0.27328
H	−0.37129	0.40934	−0.94854	H	1.86645	1.77161	2.03791
H	−0.37521	−1.02510	0.06729	O	2.52669	1.16698	3.63201
H	−0.26585	2.82067	2.04553	H	3.07231	1.64711	4.27040
H	−0.26461	2.80298	0.26997	H	2.36969	0.29633	4.02287

Table S40. Calculated Cartesian coordinates for (*N*-methylazirdine)$_2$H$^+$

Atom	*x*	*y*	*z*	Atom	*X*	*y*	*z*
N	1.36097	0.14111	−0.06318	C	−2.12602	0.39109	−1.05880
C	1.87867	1.45559	−0.50191	H	−3.01365	0.99208	−0.88001
H	1.50289	1.66679	−1.50479	H	−1.56107	0.65831	−1.94738
H	1.53259	2.22116	0.19507	C	−2.11293	−1.01038	−0.56871
H	2.97039	1.44315	−0.51695	H	−2.99166	−1.38267	−0.04869
C	2.09924	−0.65031	0.95486	C	−1.85085	0.47839	1.43249
H	3.00059	−0.18075	1.33491	H	−1.49336	1.49158	1.63682
C	2.06323	−1.10824	−0.45576	H	−2.94732	0.48676	1.45085
H	1.41082	−1.92898	−0.73387	H	−1.49646	−0.19344	2.21921
H	2.93876	−0.96412	−1.08023	H	1.47072	−1.13981	1.69140
H	0.25346	0.07616	−0.00059	H	−1.54103	−1.76470	−1.10117
N	−1.32435	0.02770	0.13067				

Table S41. Calculated Cartesian coordinates for (*N*-ethylaziridine)$_2$H$^+$

Atom	*x*	*y*	*z*	Atom	*X*	*y*	*z*
N	−1.32350	−0.37483	0.13477	C	2.07226	−0.06549	−1.02463
C	−2.10422	0.14106	−1.02648	H	3.08698	0.35331	−0.97293
H	−1.61050	−0.23930	−1.92563	H	−0.68355	−2.28981	0.93700
C	−1.57714	−1.73896	0.66320	H	1.52630	0.13322	2.32804
H	−2.33925	−2.30166	0.13421	H	−3.10276	−0.30440	−0.97860
C	−1.97810	−0.55111	1.45625	C	−2.17447	1.66307	−1.02441
H	−1.38075	−0.24718	2.30900	H	−2.74829	1.99720	−1.89307
H	−3.02541	−0.26873	1.48807	H	−2.67461	2.04312	−0.12846
H	−0.26395	−0.06489	0.15958	H	−1.17973	2.11336	−1.08937
N	1.29364	0.35804	0.16424	H	1.58846	0.37498	−1.90390
C	1.62216	1.68710	0.72128	C	2.13704	−1.58486	−1.14475
H	2.37725	2.26386	0.19343	H	1.14024	−2.02585	−1.25456
H	0.78104	2.26548	1.09323	H	2.71961	−1.86560	−2.02675
C	2.04906	0.45535	1.43214	H	2.61898	−2.03430	−0.27053
H	3.09939	0.17783	1.39249				

Table S42. Calculated Cartesian coordinates for (*N*-isopropylaziridine)$_2$H$^+$

Atom	*x*	*y*	*z*	Atom	*x*	*y*	*z*
N	1.24085	0.66939	−0.16698	H	−0.21721	−2.49573	0.44506
C	2.46955	−0.10348	0.23031	C	2.68441	−1.26007	−0.74454
H	3.30050	0.60582	0.13695	H	3.61738	−1.77331	−0.49716
C	1.31249	1.67993	−1.25287	H	1.87667	−1.99600	−0.68100
H	2.28578	1.77949	−1.72183	H	2.76057	−0.91212	−1.77913
C	1.14297	2.11534	0.15446	C	2.33896	−0.54279	1.68777
H	0.16939	2.44185	0.50244	H	3.25600	−1.05113	1.99705
H	1.99707	2.52080	0.68658	H	2.18789	0.30977	2.35649
H	0.29178	0.13194	−0.12553	H	1.50743	−1.24149	1.82235
N	−1.20009	−0.64484	−0.18065	C	−2.69279	1.25604	−0.70672
C	−1.34821	−1.62349	−1.27862	H	−2.74715	0.94168	−1.75376
H	−2.33465	−1.71302	−1.72681	H	−3.63981	1.74194	−0.45563
H	−0.52121	−1.67842	−1.98138	H	−1.90444	2.01253	−0.61354
C	−1.17104	−2.09106	0.11889	C	−2.34567	0.48007	1.69487
H	−2.03613	−2.49961	0.63517	H	−1.53234	1.19711	1.85571
C	−2.44515	0.06929	0.22542	H	−3.27560	0.95634	2.01815
H	−3.28822	−0.63110	0.11833	H	−2.16981	−0.38481	2.34184
H	0.45777	1.68698	−1.92087				

Table S43. Calculated Cartesian coordinates for (*N*-tertbutylaziridine)$_2$H$^+$

Atom	*x*	*y*	*z*	Atom	*x*	*y*	*z*
N	−1.33806	0.54073	−0.22340	C	−2.03930	−0.81524	1.69027
C	−2.45527	−0.37856	0.27883	H	−2.79296	−1.49422	2.09766
C	−1.34418	2.01856	−0.06443	H	−1.08050	−1.34088	1.68780
H	−2.22774	2.43198	0.40464	H	−1.96265	0.04293	2.36522
C	−1.46821	1.41880	−1.41447	C	3.80631	−0.37472	0.31055
H	−0.60725	1.40279	−2.07421	H	4.10866	−0.76298	−0.66650
H	−2.43752	1.41146	−1.89818	H	4.56936	0.34791	0.61270
H	−0.34925	0.11614	−0.14621	H	3.83635	−1.18990	1.03856
N	1.29704	−0.51054	−0.23866	C	2.05772	0.74912	1.70788
C	1.35693	−1.97934	−0.10864	H	1.94191	−0.12908	2.35150
H	2.24526	−2.41603	0.33415	H	2.83615	1.38207	2.14360
H	0.43040	−2.47011	0.17547	H	1.11914	1.31278	1.73034
C	1.49271	−1.34069	−1.44258	C	−2.51365	−1.56277	−0.69595
H	2.47269	−1.34304	−1.90975	H	−1.55290	−2.07953	−0.76933
C	2.43894	0.33625	0.27760	H	−3.25191	−2.28757	−0.34335
H	−0.39820	2.44168	0.25259	H	−2.81355	−1.24357	−1.69902
H	0.66151	−1.35448	−2.14361	C	2.53492	1.56202	−0.64478
C	−3.80716	0.34428	0.32170	H	3.29141	2.25939	−0.27449
H	−4.56846	−0.38358	0.61370	H	2.81710	1.27368	−1.66261
H	−3.83319	1.14486	1.06566	H	1.58574	2.10569	−0.69765
H	−4.11113	0.74399	−0.65016				

Table S44. Calculated Cartesian coordinates for (*N*-methylazetidine)$_2$H$^+$

Atom	*x*	*y*	*z*	Atom	*x*	*y*	*z*
C	2.71418	1.05998	0.00050	H	−2.82656	0.59757	−1.48825
C	2.13545	0.09386	−1.05820	H	−1.52040	−0.56177	1.86894
C	2.13531	0.09314	1.05848	H	−2.82602	0.59824	1.48853
H	3.79562	1.19677	0.00062	H	−2.29142	−2.05659	0.00065
H	2.23344	2.04130	0.00080	H	−3.81586	−1.14237	0.00071
H	2.88018	−0.61812	−1.43415	N	−1.27000	0.54760	−0.00014
H	1.58713	0.51287	−1.90784	C	1.17861	−1.99695	−0.00065
H	−0.25172	0.11894	−0.00019	H	0.64006	−2.33851	0.88902
H	2.87999	−0.61909	1.43404	H	0.64049	−2.33789	−0.89081
H	1.58688	0.51160	1.90832	H	2.17365	−2.46340	−0.00057
N	1.26500	−0.53019	−0.00013	C	−1.17375	2.02631	−0.00053
C	−2.12101	−0.12336	−1.07004	H	−0.63326	2.34976	0.89155
C	−2.12063	−0.12287	1.07039	H	−0.63399	2.34931	−0.89322
C	−2.72946	−1.05710	0.00049	H	−2.17438	2.46405	−0.00023
H	−1.52109	−0.56262	−1.86863				

Table S45. Calculated Cartesian coordinates for (*N*-ethylazetidine)$_2$H$^+$

Atom	*x*	*y*	*z*	Atom	*x*	*y*	*z*
C	2.19459	−1.85803	0.41725	H	−1.64186	2.67539	−0.50595
C	2.12484	−0.44810	1.04510	H	−3.32841	2.26407	−0.13183
C	1.89855	−1.16224	−0.92961	N	−1.40542	−0.07227	0.17689
H	3.14417	−2.38747	0.49929	C	1.90964	1.34365	−0.73402
H	1.39221	−2.52025	0.75261	H	2.99424	1.27174	−0.91435
H	3.11648	0.00751	1.15961	C	−1.84899	−1.43156	0.62365
H	1.56718	−0.31731	1.97741	H	−1.29265	−1.65450	1.53943
H	−0.33279	−0.04799	0.01808	H	−2.90774	−1.34714	0.88761
H	2.81195	−0.95265	−1.50021	C	−1.64191	−2.50843	−0.43400
H	1.16062	−1.60477	−1.60590	H	−2.01036	−3.46100	−0.04350
N	1.42333	0.05843	−0.18932	H	−2.19967	−2.29414	−1.35051
C	−1.81609	1.10585	1.05505	H	−0.58800	−2.63969	−0.68844
C	−2.13858	0.56948	−0.99770	H	1.43658	1.49006	−1.71284
C	−2.31192	1.87478	−0.18957	C	1.63297	2.53415	0.17986
H	−0.97404	1.51598	1.61329	H	2.08381	2.39650	1.16802
H	−2.60506	0.79776	1.74325	H	2.06528	3.44114	−0.25221
H	−1.52907	0.59887	−1.90153	H	0.56184	2.71405	0.31369
H	−3.06862	0.03341	−1.19410				

Table S46. Calculated Cartesian coordinates for (*N*-isopropylazetidine)$_2$H$^+$

Atom	*x*	*y*	*z*	Atom	*X*	*y*	*z*
C	1.89236	2.09720	0.88752	C	1.96108	−1.19273	−0.24553
C	1.99596	1.38026	−0.47794	H	1.43994	−1.91489	0.39869
C	1.72363	0.69186	1.50859	C	−1.95528	−1.22960	0.25464
H	2.76275	2.67145	1.20635	H	−1.40250	−1.92753	−0.38465
H	1.00332	2.72610	0.98229	C	3.47155	−1.38030	−0.02565
H	3.03398	1.24535	−0.79889	H	3.77311	−1.21433	1.01201
H	1.42093	1.77886	−1.31957	H	3.74430	−2.40981	−0.27580
H	−0.34107	0.11701	−0.01414	H	4.06722	−0.72346	−0.66755
H	2.65953	0.30556	1.92271	C	1.59222	−1.48219	−1.70533
H	0.92975	0.53970	2.24751	H	1.92858	−2.48212	−1.99239
N	1.41377	0.14027	0.14497	H	0.51112	−1.43738	−1.87502
C	−1.97749	1.40018	0.49243	H	2.07376	−0.76840	−2.38306
C	−1.70283	0.72058	−1.52099	C	−1.59769	−1.48765	1.72006
C	−1.92034	2.10862	−0.87892	H	−2.12930	−0.80181	2.38824
H	−1.35060	1.77500	1.30149	H	−1.89365	−2.50410	1.99164
H	−2.98985	1.22646	0.85650	H	−0.52416	−1.39450	1.90403
H	−0.86531	0.58657	−2.20598	C	−3.45230	−1.39401	−0.00888
H	−2.60516	0.28434	−1.94615	H	−3.72240	−1.26081	−1.05937
H	−1.06092	2.77278	−0.98520	H	−3.73682	−2.41396	0.26359
H	−2.82284	2.63994	−1.18105	H	−4.05994	−0.71837	0.60087
N	−1.41789	0.13243	−0.14314				

Table S47. Calculated Cartesian coordinates for (*N*-tertbutylazetidine)$_2$H$^+$

Atom	*x*	*y*	*z*	Atom	*X*	*y*	*z*
C	1.37658	−2.06758	−1.52997	H	4.31005	−0.03798	−0.42239
C	1.54566	−1.86111	−0.00831	H	4.49986	0.74961	1.13857
C	1.80716	−0.59164	−1.67552	H	4.01572	−0.93878	1.07705
H	2.01645	−2.81580	−1.99919	C	1.90071	0.52251	2.02908
H	0.34198	−2.24897	−1.83292	H	2.53838	1.15331	2.65528
H	2.51936	−2.21583	0.34411	H	0.88135	0.91843	2.08669
H	0.77618	−2.25290	0.66461	H	1.90345	−0.48134	2.46745
H	−0.50028	0.06598	−0.10069	C	−1.90739	−0.61290	2.02523
H	2.87406	−0.49989	−1.90716	H	−1.96416	0.36899	2.50598
H	1.25245	0.05300	−2.36501	H	−2.52664	−1.29858	2.60942
N	1.49993	−0.37386	−0.22082	H	−0.87464	−0.96797	2.07743
C	−1.53155	1.89218	0.09002	C	−3.87998	−0.08478	0.54641
C	−1.75840	0.68875	−1.66973	H	−4.27686	0.00377	−0.46864
C	−1.44168	2.17909	−1.42379	H	−4.49538	−0.82601	1.06288
H	−0.70920	2.20786	0.73041	H	−4.02567	0.86453	1.06789
H	−2.48281	2.17243	0.53793	C	−2.30967	−1.94363	−0.09625
H	−1.10422	0.11646	−2.32594	H	−1.28259	−2.31590	−0.09170
H	−2.80033	0.49318	−1.91846	H	−2.92408	−2.66430	0.44933
H	−0.44053	2.46613	−1.74893	H	−2.67188	−1.92134	−1.12866
H	−2.16641	2.89172	−1.81786	C	2.36131	1.91663	−0.02444
N	−1.50303	0.38946	−0.19208	H	1.33897	2.30680	−0.03899
C	2.41853	0.50477	0.58194	H	2.97105	2.60740	0.56470
C	−2.42419	−0.57121	0.58102	H	2.74704	1.93190	−1.04888
C	3.88974	0.02974	0.58530				

Table S48. Calculated Cartesian coordinates for (*N*-methylpyrrolidine)$_2$H$^+$

Atom	*x*	*y*	*z*	Atom	*x*	*Y*	*z*
C	2.42544	0.60636	1.25520	C	1.70375	0.84458	1.04448
C	2.28407	−0.76615	0.58611	C	2.29400	−0.79446	−0.50827
C	1.69302	0.81532	−1.09194	C	2.10418	1.62820	−0.21928
C	2.12188	1.64326	0.13294	H	0.89463	1.30731	1.61850
H	1.71348	0.70843	2.07867	H	2.56551	0.73172	1.72014
H	3.42443	0.72861	1.67823	C	2.46578	0.53234	−1.26545
H	1.90765	−1.55744	1.23701	H	3.24138	−1.09702	−0.03547
H	3.22214	−1.10023	0.13223	H	1.95877	−1.62692	−1.13486
H	0.29875	−0.46012	−0.11069	H	2.94195	2.29789	−0.01314
H	2.52196	0.65112	−1.78634	H	1.28132	2.25566	−0.57578
H	0.84858	1.22683	−1.64808	H	3.48309	0.63893	−1.64825
H	2.99468	2.25219	−0.11113	H	1.79750	0.58182	−2.13165
H	1.32894	2.32858	0.44090	N	1.28845	−0.49279	0.54466
N	1.30433	−0.53189	−0.53515	C	1.26773	−1.50906	1.61046
C	1.27399	−1.62002	−1.55228	H	0.98144	−2.48115	1.19758
H	0.97532	−2.55265	−1.07104	H	0.54595	−1.22769	2.38303
H	0.55410	−1.36310	−2.33084	H	2.25353	−1.61615	2.08622
H	2.26610	−1.73613	−1.99361				

Table S49. Calculated Cartesian coordinates for (*N*-methylpiperidine)$_2$H$^+$

Atom	*x*	*y*	*z*	Atom	*x*	*Y*	*z*
C	3.91013	−1.00963	−0.34943	C	−1.72646	−0.86902	−0.91485
C	3.56136	0.32849	−1.01841	C	−2.04324	0.51397	1.07882
C	2.04829	0.53498	−1.09667	C	−3.23814	−1.10970	−1.03859
C	1.71848	−0.90405	0.91135	H	−1.28533	−1.67935	−0.31884
C	3.22676	−1.13000	1.02095	H	−1.24479	−0.88416	−1.89879
H	1.78608	1.51576	−1.50107	C	−3.56527	0.31681	1.02310
H	4.03141	1.15932	−0.47869	H	−1.60694	−0.26129	1.72369
H	3.95560	0.36740	−2.03911	H	−1.79070	1.48645	1.51573
H	3.58625	−1.83746	−0.99441	C	−3.92060	−1.00984	0.33445
H	4.99430	−1.10451	−0.23960	H	−3.39919	−2.09852	−1.48229
H	1.22695	−0.91398	1.88744	H	−3.68057	−0.38495	−1.73308
H	1.25994	−1.68079	0.29134	H	−3.95842	0.34174	2.04551
H	3.66785	−0.42094	1.73177	H	−4.03492	1.15416	0.49255
H	3.38368	−2.12597	1.44786	H	−5.00582	−1.10692	0.22954
H	1.59013	−0.22937	−1.73262	H	−3.59165	−1.84741	0.96601
N	1.37022	0.41292	0.25079	C	−1.63044	1.58735	−1.10204
C	1.62433	1.58986	1.13643	H	−1.29750	2.49487	−0.58917
H	1.29052	2.49293	0.62310	H	−1.07193	1.48846	−2.03763
H	1.05550	1.46351	2.05881	H	−2.68899	1.71376	−1.35378
H	2.68358	1.67909	1.37286	N	−1.36068	0.41327	−0.24429
H	0.28700	0.39947	0.05671	N	−1.36068	0.41327	−0.24429