Table VII. Geometries of methylamine and its protonated from by different methods.

	CH_3NH_2							$CH_3NH_3^+$					
Variable[a]	RHF/6d[b]	MP2/6d	DMol	DG/L	DN/L	DN/N	Exp.[c]	RHF/6d	MP2/6d	DMol	DG/L	DN/L	DN/N
C1–N2	1.456	1.468	1.454	1.449	1.449	1.473	1.471	1.507	1.509	1.489	1.490	1.490	1.518
C1–H3	1.092	1.097	1.113	1.114	1.114	1.110	1.099	1.079	1.086	1.102	1.100	1.100	1.096
C1–H4	1.085	1.091	1.105	1.105	1.105	1.101	1.099	1.079	1.086	1.102	1.100	1.099	1.095
C1–H5	1.085	1.091	1.105	1.105	1.105	1.101	1.099	1.079	1.086	1.102	1.100	1.100	1.096
N2–H6	1.000	1.015	1.032	1.024	1.024	1.024	1.010	1.010	1.024	1.042	1.037	1.037	1.033
N2–H7	1.000	1.015	1.032	1.024	1.024	1.024	1.010	1.010	1.024	1.041	1.037	1.037	1.033
N2–H8								1.010	1.024	1.042	1.037	1.037	1.034
H5–C1–H4	107.368	107.464	106.758	106.051	106.245	106.969	108.0	110.730	110.833	110.200	109.972	109.904	110.582
H5–C1–H3	108.015	108.156	107.711	107.407	107.368	107.754	108.0	110.729	110.833	110.211	109.973	109.905	110.568
H5–C1–N2	109.322	108.872	109.163	109.630	109.549	109.071	109.4	108.180	108.070	108.730	108.955	109.060	108.325
H4–C1–H3	108.021	108.151	107.711	107.410	107.377	107.761	108.0	110.730	110.839	110.196	109.982	109.876	110.628
H4–C1–N2	109.322	108.866	109.165	109.639	109.553	109.067	109.4	108.182	108.071	108.728	108.965	109.019	108.251
H3–C1–N2	114.550	115.077	115.949	116.206	116.269	115.865	113.9	108.181	108.071	108.731	108.966	109.053	108.398
H8–N2–H7								107.553	107.445	107.131	107.254	107.218	107.340
H8–N2–H6								107.554	107.445	107.104	107.275	107.252	107.362
H8–N2–C1								111.326	111.428	111.722	111.574	111.589	111.474
H7–N2–H6	107.413	106.022	105.826	107.215	107.293	106.188	107.1	107.558	107.445	107.131	107.284	107.211	107.327
H7–N2–C1	110.913	109.635	109.839	111.035	111.186	109.956	110.3	111.324	111.428	111.743	111.591	111.666	111.629
H6–N2–C1	110.919	109.629	109.820	111.030	111.181	109.959	110.3	111.326	111.428	111.722	111.608	111.640	111.467
H5–C1–N2–H8								179.983	180.000	−179.980	−179.964	−179.957	−179.528
H5–C1–N2–H7	61.675	63.557	63.788	62.399	62.179	63.460		59.986	59.997	60.003	60.069	60.059	60.438
H5–C1–N2–H6	−179.047	179.556	179.779	−178.421	−178.343	−179.962		−60.018	−60.002	−60.013	−59.959	−59.949	−59.575
H4–C1–N2–H8								−60.016	−60.005	−59.983	−59.971	−59.952	−59.582
H4–C1–N2–H7	178.942	−179.573	−179.857	178.436	178.355	179.961		179.987	180.000	180.000	−179.937	−179.935	−179.617
H4–C1–N2–H6	−61.780	−63.573	−63.867	−62.383	−62.167	−63.461		59.983	59.995	59.983	60.035	60.056	60.370
H3–C1–N2–H8								59.985	60.000	60.008	60.041	60.015	60.460
H3–C1–N2–H7	−59.687	−58.013	−58.033	−59.577	−59.726	−58.286		−60.013	−60.000	−60.008	−59.926	−59.968	−59.575
H3–C1–N2–H6	59.590	57.986	57.957	59.604	59.752	58.292		179.983	180.000	179.975	−179.954	−179.977	−179.588

[a] I–J bond length in Å; I–J–K bond angle in deg; I–J–K–L torsional angle in deg. Atom numbering in Fig 1.
[b] Methods as in Table I
[c] Methylamine gas phase geometry taken from ref [Harmony].