

Table IV. Geometries of methylamine and its protonated form by different methods.

Variable ^a	CH ₃ NH ₂							CH ₃ NH ₃ ⁺					
	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

^aI-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.

^bMethods as in Table I

^cMethylamine gas phase geometry taken from ref. 24.