

Table I. Geometries of ethanol and protonated ethanol by different methods.

Variable ^a	CH ₃ CH ₂ OH							CH ₃ CH ₂ OH ₂ ⁺					
	RHF/6d ^b	MP2/6d ^c	DMol ^d	DG/L ^e	DN/L ^f	DN/N ^g	Exp. ^h	RHF/6d	MP2/6d	DMol	DG/L	DN/L	DN/N
C1-C2	1.523	1.523	1.506	1.511	1.509	1.529	1.5115	1.507	1.503	1.478	1.486	1.486	1.501
C1-H4	1.087	1.092	1.107	1.105	1.105	1.103	1.088	1.084	1.091	1.108	1.106	1.105	1.103
C1-H5	1.085	1.091	1.106	1.104	1.104	1.102	1.091	1.082	1.089	1.105	1.102	1.102	1.099
C1-H6	1.088	1.093	1.108	1.107	1.107	1.104	1.091	1.084	1.091	1.107	1.105	1.106	1.101
C2-O3	1.405	1.428	1.419	1.415	1.414	1.441	1.4273 ⁱ	1.544	1.545	1.536	1.525	1.520	1.580
C2-H7	1.089	1.097	1.113	1.112	1.113	1.110	1.098	1.078	1.088	1.105	1.102	1.103	1.098
C2-H8	1.083	1.091	1.106	1.106	1.105	1.101	1.098	1.077	1.086	1.103	1.101	1.101	1.097
O3-H9	0.944	0.965	0.985	0.977	0.976	0.975	0.971	0.956	0.977	1.003	0.991	0.991	0.987
O3-H10								0.956	0.977	1.000	0.991	0.990	0.987
H6-C1-H5	108.215	108.407	108.075	108.160	108.025	108.084	108.45	110.144	110.464	110.521	110.378	110.398	110.466
H6-C1-H4	107.810	107.867	107.347	107.571	107.338	107.592	108.79	107.684	107.451	106.254	106.502	106.173	106.892
H6-C1-C2	111.108	110.924	111.406	110.720	110.940	110.956	110.13	111.800	112.011	112.864	112.929	112.562	112.577
H5-C1-H4	108.594	108.709	108.405	108.309	108.391	108.242	108.79	108.516	108.341	107.307	107.538	107.245	107.572
H5-C1-C2	110.513	110.240	110.706	110.791	110.591	110.738	110.13	111.366	111.423	111.960	111.896	112.259	112.143
H4-C1-C2	110.505	110.613	110.768	111.165	111.419	111.100	110.49	107.162	106.939	107.567	107.254	107.839	106.857
H8-C2-H7	107.420	107.759	106.719	106.466	106.804	107.296	107.97	112.152	112.091	110.905	110.899	111.263	111.889
H8-C2-O3	105.830	104.900	105.160	105.734	105.522	104.916		101.863	101.652	102.005	102.699	102.625	100.977
H8-C2-C1	110.103	110.387	110.408	110.557	110.353	110.448	110.72	114.245	114.169	114.330	113.105	113.940	114.466
H7-C2-O3	110.520	110.707	110.682	111.080	111.216	110.709		104.956	105.739	106.109	106.003	106.421	105.100
H7-C2-C1	110.064	110.209	110.442	109.884	110.111	110.420	110.72	114.806	114.687	114.956	115.043	114.394	115.374
O3-C2-C1	112.697	112.653	113.119	112.861	112.588	112.785	112.35 ⁱ	107.368	107.117	107.271	108.032	107.109	107.396
H10-O3-H9								111.431	109.197	107.627	110.285	110.851	109.324
H10-O3-C2								116.991	114.114	111.514	114.407	115.173	113.813
H9-O3-C2	109.807	107.362	107.823	107.899	107.760	107.355	105.43	116.569	112.976	109.427	112.496	112.510	112.821
H6-C1-C2-H8	179.256	179.347	178.682	178.675	179.244	179.749		-176.330	-177.077	-179.255	-174.947	-178.060	-177.025
H6-C1-C2-H7	61.023	60.430	60.891	61.446	61.585	61.235		52.084	51.625	50.778	56.194	52.370	50.976
H6-C1-C2-O3	-62.843	-63.758	-63.787	-63.134	-63.145	-63.213		-64.177	-65.372	-66.944	-61.978	-65.300	-65.816
H5-C1-C2-H8	-60.600	-60.568	-61.024	-61.321	-60.909	-60.222		-52.637	-52.766	-53.788	-49.672	-52.759	-51.714
H5-C1-C2-H7	-178.833	-179.485	-178.815	-178.550	-178.567	-178.737		175.777	175.937	176.245	-178.531	177.671	176.287
H5-C1-C2-O3	57.301	56.327	56.508	56.870	56.702	56.816		59.516	58.940	58.523	63.297	60.001	59.496
H4-C1-C2-H8	59.625	59.693	59.264	59.165	59.715	60.101		65.899	65.454	63.865	68.032	65.160	65.923
H4-C1-C2-H7	-58.608	-59.224	-58.527	-58.064	-57.943	-58.414		-65.687	-65.843	-66.102	-60.828	-64.410	-66.076
H4-C1-C2-O3	177.526	176.588	176.796	177.356	177.326	177.139		178.053	177.160	176.176	-179.000	177.921	177.132
H8-C2-O3-H10								-55.772	-61.698	-64.959	-53.432	-65.115	-55.797
H8-C2-O3-H9	-178.129	179.764	-178.020	176.359	174.682	179.439		168.736	172.775	176.082	179.699	166.532	178.884
H7-C2-O3-H10								61.288	55.500	51.216	62.993	51.851	60.669
H7-C2-O3-H9	-62.129	-64.260	-63.130	-68.542	-69.872	-65.117		-74.204	-70.026	-67.743	-63.875	-76.502	-64.650
C1-C2-O3-H10								-176.127	178.241	174.562	-173.194	174.618	-175.986
C1-C2-O3-H9	61.485	59.654	61.417	55.382	54.250	59.172	54±6 ⁱ	48.381	52.715	55.603	59.938	46.265	58.695

^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.^bGeometry optimization at RHF level with DH6D basis set^cGeometry optimization at MP2 level with DH6D basis set^dGeometry optimization with DMol with DNP basis set^eGeometry optimization with DGauss at LSD level^fGeometry optimization with deMon at LSD level^gGeometry optimization with deMon with Becke-Perdew gradient corrections^hTaken for *trans* form from ref. 25 unless otherwise noted.ⁱTaken for *gauche* form from ref. 26.