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

	CH_3CH_2OH						$CH_3CH_2OH_2^+$				
Variable[a]	RHF(6d)[b]	MP2(6d)	DMol	DG(LSD)	DN(NLSD)	Exp.[c]	RHF(6d)	MP2(6d)	DMol	DG(LSD)	DN(NLSD)
C1–C2	1.523	1.523	1.506	1.511	1.529	1.5115	1.507	1.503	1.478	1.486	1.501
C1–H4	1.087	1.092	1.107	1.105	1.103	1.088	1.084	1.091	1.108	1.106	1.103
C1–H5	1.085	1.091	1.106	1.104	1.102	1.091	1.082	1.089	1.105	1.102	1.099
C1–H6	1.088	1.093	1.108	1.107	1.104	1.091	1.084	1.091	1.107	1.105	1.101
C2–O3	1.405	1.428	1.419	1.415	1.441	1.4273[d]	1.544	1.545	1.536	1.525	1.580
C2–H7	1.089	1.097	1.113	1.112	1.110	1.098	1.078	1.088	1.105	1.102	1.098
C2–H8	1.083	1.091	1.106	1.106	1.101	1.098	1.077	1.086	1.103	1.101	1.097
O3–H9	0.944	0.965	0.985	0.977	0.975	0.971	0.956	0.977	1.003	0.991	0.987
O3–H10							0.956	0.977	1.000	0.991	0.987
H6–C1–H5	108.215	108.407	108.075	108.160	108.084	108.45	110.144	110.464	110.521	110.378	110.466
H6–C1–H4	107.810	107.867	107.347	107.571	107.592	108.79	107.684	107.451	106.254	106.502	106.892
H6–C1–C2	111.108	110.924	111.406	110.720	110.956	110.13	111.800	112.011	112.864	112.929	112.577
H5–C1–H4	108.594	108.709	108.405	108.309	108.242	108.79	108.516	108.341	107.307	107.538	107.572
H5–C1–C2	110.513	110.240	110.706	110.791	110.738	110.13	111.366	111.423	111.960	111.896	112.143
H4–C1–C2	110.505	110.613	110.768	111.165	111.100	110.49	107.162	106.939	107.567	107.254	106.857
H8–C2–H7	107.420	107.759	106.719	106.466	107.296	107.97	112.152	112.091	110.905	110.899	111.889
H8–C2–O3	105.830	104.900	105.160	105.734	104.916		101.863	101.652	102.005	102.699	100.977
H8–C2–C1	110.103	110.387	110.408	110.557	110.448	110.72	114.245	114.169	114.330	113.105	114.466
H7–C2–O3	110.520	110.707	110.682	111.080	110.709		104.956	105.739	106.109	106.003	105.100
H7–C2–C1	110.064	110.209	110.442	109.884	110.420	110.72	114.806	114.687	114.956	115.043	115.374
O3–C2–C1	112.697	112.653	113.119	112.861	112.785	112.35[d]	107.368	107.117	107.271	108.032	107.396
H10–O3–H9							111.431	109.197	107.627	110.285	109.324
H10–O3–C2							116.991	114.114	111.514	114.407	113.813
H9–O3–C2	109.807	107.362	107.823	107.899	107.355	105.43	116.569	112.976	109.427	112.496	112.821
H6–C1–C2–H8	179.256	179.347	178.682	178.675	179.749		−176.330	−177.077	−179.255	−174.947	−177.025
H6–C1–C2–H7	61.023	60.430	60.891	61.446	61.235		52.084	51.625	50.778	56.194	50.976
H6–C1–C2–O3	−62.843	−63.758	−63.787	−63.134	−63.213		−64.177	−65.372	−66.944	−61.978	−65.816
H5–C1–C2–H8	−60.600	−60.568	−61.024	−61.321	−60.222		−52.637	−52.766	−53.788	−49.672	−51.714
H5–C1–C2–H7	−178.833	−179.485	−178.815	−178.550	−178.737		175.777	175.937	176.245	−178.531	176.287
H5–C1–C2–O3	57.301	56.327	56.508	56.870	56.816		59.516	58.940	58.523	63.297	59.496
H4–C1–C2–H8	59.625	59.693	59.264	59.165	60.101		65.899	65.454	63.865	68.032	65.923
H4–C1–C2–H7	−58.608	−59.224	−58.527	−58.064	−58.414		−65.687	−65.843	−66.102	−60.828	−66.076
H4–C1–C2–O3	177.526	176.588	176.796	177.356	177.139		178.053	177.160	176.176	−179.000	177.132
H8–C2–O3–H10							−55.772	−61.698	−64.959	−53.432	−55.797
H8–C2–O3–H9	−178.129	179.764	−178.020	176.359	179.439		168.736	172.775	176.082	179.699	178.884
H7–C2–O3–H10							61.288	55.500	51.216	62.993	60.669
H7–C2–O3–H9	−62.129	−64.260	−63.130	−68.542	−65.117		−74.204	−70.026	−67.743	−63.875	−64.650
C1–C2–O3–H10							−176.127	178.241	174.562	−173.194	−175.986
C1–C2–O3–H9	61.485	59.654	61.417	55.382	59.172	54±6[d]	48.381	52.715	55.603	59.938	58.695

[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] Taken for *trans* form from ref. [Landolt76] unless otherwise noted.
[d] Taken for *gauche* form from ref [Sasada71].