

**Table III.** Geometries of methanol and protonated methanol by different methods.

Variable <sup>a</sup>	CH <sub>3</sub> OH							CH <sub>3</sub> OH <sub>2</sub> <sup>+</sup>						
	RHF/6d <sup>b</sup>	MP2/6d	DMol	DG/L	DN/L	DN/N	Exp. <sup>c</sup>	RHF/6d	MP2/6d	DMol	DG/L	DN/L	DN/N	
C1-O2	1.402	1.423	1.414	1.411	1.410	1.434	1.428	1.510	1.514	1.496	1.488	1.484	1.527	
C1-H3	1.082	1.088	1.104	1.105	1.103	1.100	1.096	1.077	1.085	1.101	1.100	1.100	1.096	
C1-H4	1.089	1.095	1.109	1.112	1.111	1.108	1.102	1.076	1.084	1.099	1.098	1.098	1.094	
C1-H5	1.089	1.095	1.109	1.112	1.111	1.108	1.102	1.076	1.084	1.099	1.098	1.099	1.095	
O2-H6	0.943	0.963	0.985	0.975	0.974	0.974	0.960	0.957	0.977	1.001	0.990	0.990	0.987	
O2-H7								0.957	0.977	1.001	0.990	0.990	0.987	
H5-C1-H4	108.700	108.840	108.790	108.293	108.312	108.736	108.5 <sup>d</sup>	112.130	111.986	110.694	110.643	110.478	111.709	
H5-C1-H3	108.332	108.505	107.913	107.580	107.541	108.115	108.5 <sup>d</sup>	113.538	113.485	112.897	112.564	112.649	113.406	
H5-C1-O2	112.043	112.252	112.487	113.026	113.063	112.590	112.6	104.532	104.274	105.068	105.459	105.463	104.353	
H4-C1-H3	108.327	108.502	107.911	107.591	107.549	108.193	108.5 <sup>d</sup>	113.537	113.491	112.891	112.574	112.709	113.545	
H4-C1-O2	112.048	112.252	112.455	113.058	113.027	112.363	112.6	104.538	104.269	105.038	105.503	105.485	104.388	
H3-C1-O2	107.255	106.340	107.078	107.013	107.066	106.657	106.8	107.611	108.400	109.652	109.603	109.548	108.545	
H7-O2-H6								111.725	109.398	107.551	110.728	110.782	109.587	
H7-O2-C1								116.763	113.891	111.295	114.373	114.706	113.813	
H6-O2-C1	109.976	107.823	107.974	108.565	108.493	107.530	108.0 <sup>d</sup>	116.764	113.898	111.204	114.373	114.778	113.880	
H5-C1-O2-H7								53.066	57.959	61.651	56.853	56.140	56.058	
H5-C1-O2-H6	-61.327	-61.533	-61.651	-61.866	-62.061	-61.627		-170.990	-175.629	-178.457	-173.962	-173.879	-177.350	
H4-C1-O2-H7								171.052	175.560	178.476	174.001	173.095	173.434	
H4-C1-O2-H6	61.164	61.450	61.598	61.610	61.444	61.559		-53.004	-58.028	-61.632	-56.813	-56.924	-59.974	
H3-C1-O2-H7								-67.940	-63.238	-59.949	-64.554	-65.340	-65.164	
H3-C1-O2-H6	179.917	179.956	179.964	179.888	179.686	179.950	<i>planar</i>	68.004	63.173	59.943	64.631	64.641	61.429	

<sup>a</sup>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.

<sup>b</sup>Methods as in Table I

<sup>c</sup>Gas phase structural parameters taken from ref. 38 except as noted.

<sup>d</sup>from ref. 37.