

Table VI. Geometries of methanol and protonated methanol by different methods.

| Variable ^a | CH ₃ OH | | | | | | | CH ₃ OH ₂ ⁺ | | | | | | |
|-----------------------|---------------------|---------|---------|---------|---------|---------|--------------------|--|----------|----------|----------|----------|----------|--|
| | 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-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 ^d | 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 ^d | 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 ^d | 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 ^d | 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 | |

^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^cGas phase structural parameters taken from ref [Benston] except as noted.^dfrom ref [Landolt86].