Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics


# Study of structural and dynamic properties of liquid phenyltrimethoxysilane

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February 9, 2011

## Supplementary Materials

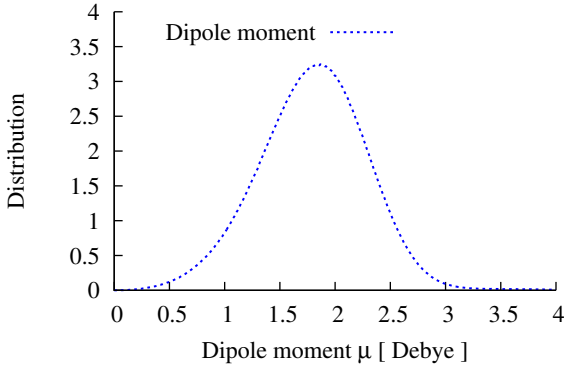


Figure 1: The distribution of the dipolemoment averaged over the trajectory of 35 ns. The average of the distribution is 1.8 Debye and the standard deviation is 0.5 Debye.

| Atom number | Atom | x | y | z |
|---|---|---|---|---|
| 1 | C | 0.356906 | -0.724015 | -0.636797 |
| 2 | C | -0.589172 | -0.022205 | 0.133592 |
| 3 | C | -0.143354 | 0.617242 | 1.304618 |
| 4 | C | 1.195055 | 0.554900 | 1.693305 |
| 5 | C | 2.116669 | -0.151489 | 0.917176 |
| 6 | C | 1.696520 | -0.791176 | -0.250241 |
| 7 | Si | -2.385729 | 0.004686 | -0.359554 |
| 8 | O | -3.259965 | -1.284147 | 0.188964 |
| 9 | C | -3.124626 | -2.615070 | -0.289472 |
| 10 | O | -3.037512 | 1.351732 | 0.327380 |
| 11 | C | -4.435023 | 1.604666 | 0.432326 |
| 12 | O | -2.528379 | -0.044066 | -2.010558 |
| 13 | C | -2.006906 | 0.946488 | -2.887164 |
| 14 | H | -0.852843 | 1.175033 | 1.909594 |
| 15 | H | 1.520456 | 1.057957 | 2.600441 |
| 16 | H | 3.159585 | -0.200975 | 1.220083 |
| 17 | H | 2.411403 | -1.338485 | -0.859580 |
| 18 | H | 0.044233 | -1.219009 | -1.553836 |
| 19 | H | -3.319475 | -2.671914 | -1.366965 |
| 20 | H | -2.119526 | -3.009589 | -0.088085 |
| 21 | H | -3.853680 | -3.238468 | 0.236991 |
| 22 | H | -4.567125 | 2.518562 | 1.019176 |
| 23 | H | -0.927261 | 1.085482 | -2.744913 |
| 24 | H | -2.185212 | 0.616709 | -3.915244 |
| 25 | H | -4.886021 | 1.754416 | -0.556993 |
| 26 | H | -2.506076 | 1.912033 | -2.736409 |
| 27 | H | -4.950035 | 0.777993 | 0.933886 |

Table 1: The coordinates of atoms of the optimized Phenyltrimethoxysilane

| Atom number | Atom | Initial charge | Optimized charge |
|---|---|---|---|
| 1 | C | 0.024 | 0.026 |
| 2 | C | -0.140 | -0.151 |
| 3 | C | -0.073 | -0.078 |
| 4 | C | -0.096 | -0.103 |
| 5 | C | -0.044 | -0.047 |
| 6 | C | -0.164 | -0.176 |
| 7 | Si | 0.845 | 0.908 |
| 8 | O | -0.472 | -0.507 |
| 9 | C | 0.184 | 0.198 |
| 10 | O | -0.479 | -0.516 |
| 11 | C | 0.207 | 0.223 |
| 12 | O | -0.432 | -0.467 |
| 13 | C | 0.136 | 0.146 |
| 14 | H | 0.081 | 0.087 |
| 15 | H | 0.089 | 0.096 |
| 16 | H | 0.082 | 0.088 |
| 17 | H | 0.099 | 0.108 |
| 18 | H | 0.065 | 0.070 |
| 19 | H | 0.003 | 0.003 |
| 20 | H | -0.026 | -0.028 |
| 21 | H | 0.038 | 0.042 |
| 22 | H | 0.016 | 0.029 |
| 23 | H | -0.025 | -0.027 |
| 24 | H | 0.039 | 0.043 |
| 25 | H | 0.007 | 0.008 |
| 26 | H | 0.007 | 0.008 |
| 27 | H | 0.007 | 0.008 |

Table 2: The charges of atoms from the ab-initio calculations and the optimized Phenyltrimethoxysilane topology.

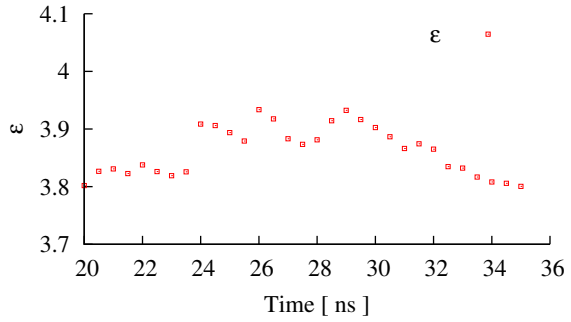


Figure 2: The dielectric constant of PhTMS from the simulation after various simulation times. The average value is 3.86 and the fluctuation over the time of 15 ns is 0.04. The standard deviation of the distribution is taken as the fluctuation.

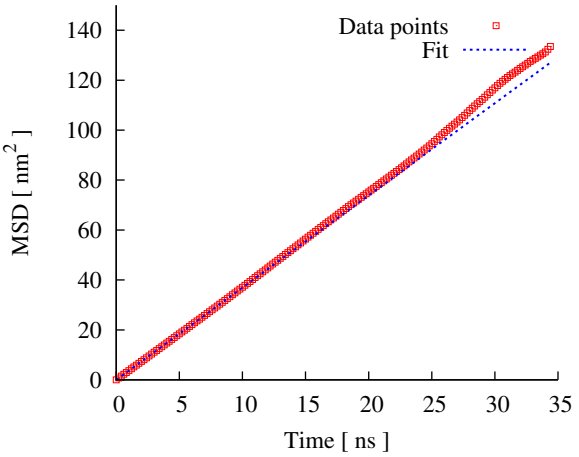


Figure 3: The mean square displacement of the molecules vs. time. The points are the data from the simulation and the straight line is the linear fit through the points. The fitting is done taking points upto 10 ns. The displacement shows a linear behavior.