**Supplementary Material**

**Anomalous viscoelastic response of water-dimethyl sulfoxide (DMSO) solution and molecular explanation of non-monotonic composition dependence of viscosity**

**Shubham Kumar, Sarmistha Sarkar and Biman Bagchi\***

***Solid State and Structural Chemistry Unit, Indian Institute of Science, Bangalore 560012, India*.**

**\*Email:** **bbagchi@iisc.ac.in**; **profbiman@gmail.com**

**I. Complete parameter set for Dimethyl Sulfoxide (DMSO) adapted from GROMOS96 53a6 force field**

**Table S1. Atomic mass and charge**

|  |  |  |  |
| --- | --- | --- | --- |
| **Atom type** | **O** | **S** | **CH3** |
| **Mass (amu)** | 15.9994 | 32.0600 | 15.0350 |
| **q(e)** | -0.44753 | 0.12753 | 0.16000 |
| **C61/2([kJ mol-1 nm6]1/2)** | 0.047652 | 0.10277 | 0.098050 |
| **C121/2([10-3 kJ mol-1 nm12]1/2)** | 0.86686 | 4.6366 | 5.1620 |

**Table S2. Equilibrium bond length and associated force constant**

|  |  |  |
| --- | --- | --- |
| **Bond** | **Equilibrium bond length(nm)** | **Force constant (Kb[kJ mol-1nm-2])** |
| **S=O** | 0.153 | 502080 |
| **S-CH3** | 0.1937991 | 376560 |

**Table S3. Equilibrium bond angle and associated force constant**

|  |  |  |
| --- | --- | --- |
| **Angle** | **Equilibrium bond angle****value (o)** | **Force constant (K[kJ mol-1rad-2])** |
| **O- S-CH3** | 106.75 | 460.240 |
| **CH3 -S-CH3** | 97.40 | 460.240 |

**II. Expression for **

To calculate, one need the expression for. In the liquid state, the time dependent viscosity is dominated by its potential part and hence, the equation (6) for can be approximated as,

  (S1)

where *N1* and *N2* are the numbers of particles of type A and B respectively. Also *N1* + *N2* = *N.* The potential part of the time dependent viscosity, as given in equation (19), can be separated into contributions from two, three and four particle correlation terms as,

 (S2)

And hence, can also be separated in terms of two, three and four particle correlation terms as,

 (S3)

After a few steps of algebra, one can get the final expressions for  and as follows,

 (S4)

 (S5)

where *a, b*, c = 1 indicates particles of type A and *a, b*, c= 2 indicates particles of type B. and are the number densities of A and B respectively.  and  are the partial radial distribution function and two-body interaction potential respectively. is the partial static structure factor and can be obtained by the Fourier transform of the partial pair correlation function. The integrals and  appearing in the above equation are defined as,

 (S6)

 (S7)

whereand  are the spherical Bessel functions.  and.

 contains the scalar product of velocities of four different particles and hence is equal to zero i.e. 