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Supplementary Information: On the positional and orientational order of water and methanol around indole: a study on the microscopic origin of solubility

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1 Comparison between neutron data and molecular dynamics

The previously published neutron diffraction data¹ at a relative molar ratio 1 indole:29 methanol:30 water and for several isotopomers of indole/methanol/water has been compared against the MD data obtained at the same proportions. The MD trajectories have been converted into putative diffraction pattern similar to previous investigations.²

A comparison of the measured $F(Q)$ s and the $F(Q)$ s calculated from the MD simulation is shown in Figure 1 For the 1:29:30 solution. The total correlation function $G(r)$ is also shown in Figure 2. The overall agreement between the MD data and the neutron measurements is good. The non-deuterated sample is at the bottom of Figures 1 and 2 and the different isotopomers are shown vertically displaced.

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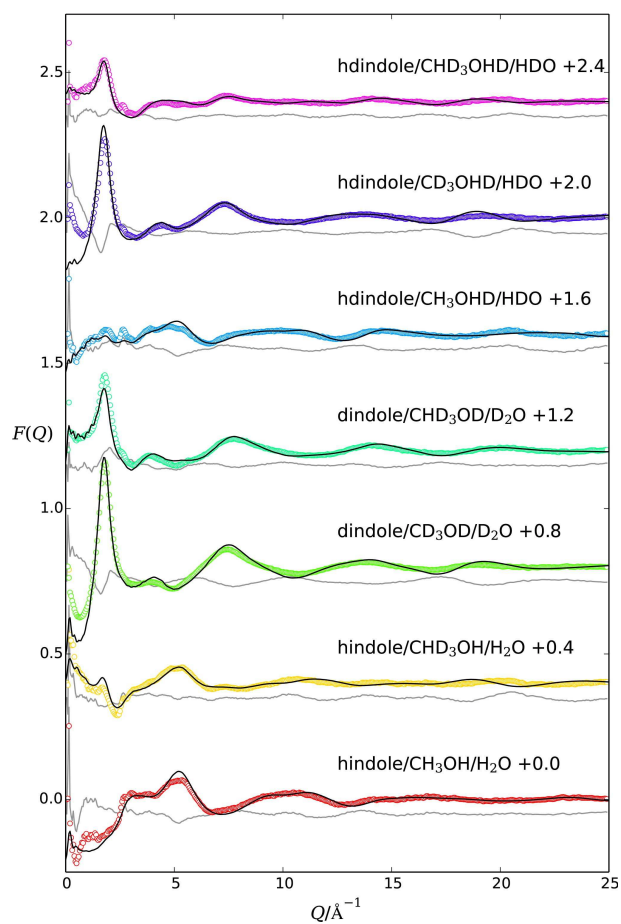


Fig. 1 (color online). Measured neutron diffraction data (colored dots), $F(Q)$ from MD (black lines) and the difference (gray lines). The data have been translated vertically in increments of 0.4 for clarity

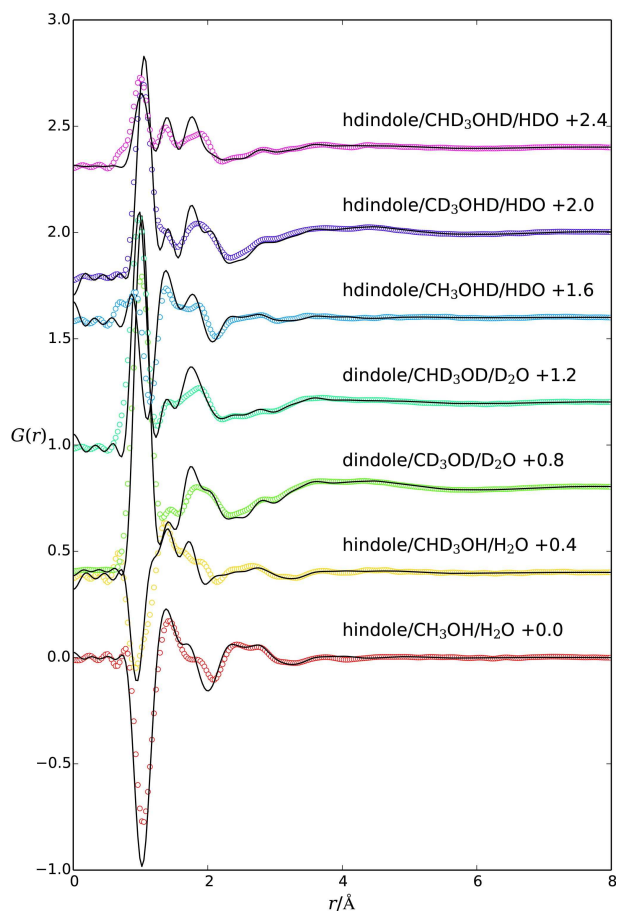


Fig. 2 (color online). $G(r)$ neutron diffraction data (colored dots) compared to the obtained $G(r)$ from MD (black lines) and the difference (gray lines). The data have been translated vertically in increments of 0.4 for clarity