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# Electronic Supporting Information (ESI) for

## Phase transition-induced changes in the Raman properties of DMSO/benzene binary system

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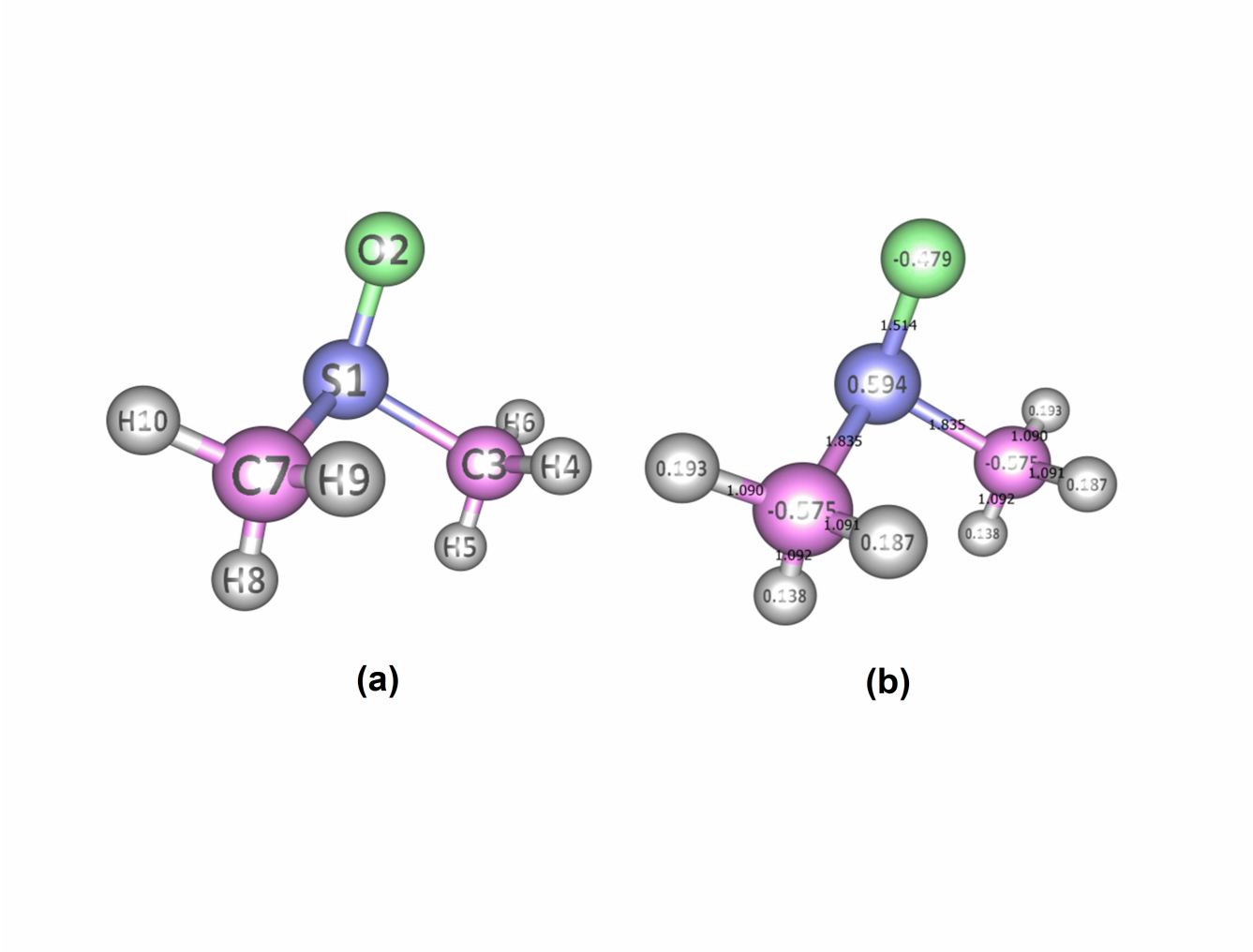


**Fig. S1.** The geometry of DMSO optimized by the DFT B3LYP/6–311++G(d,p) level of theory: (a) atoms with labels (b) atoms with charges and bond lengths.

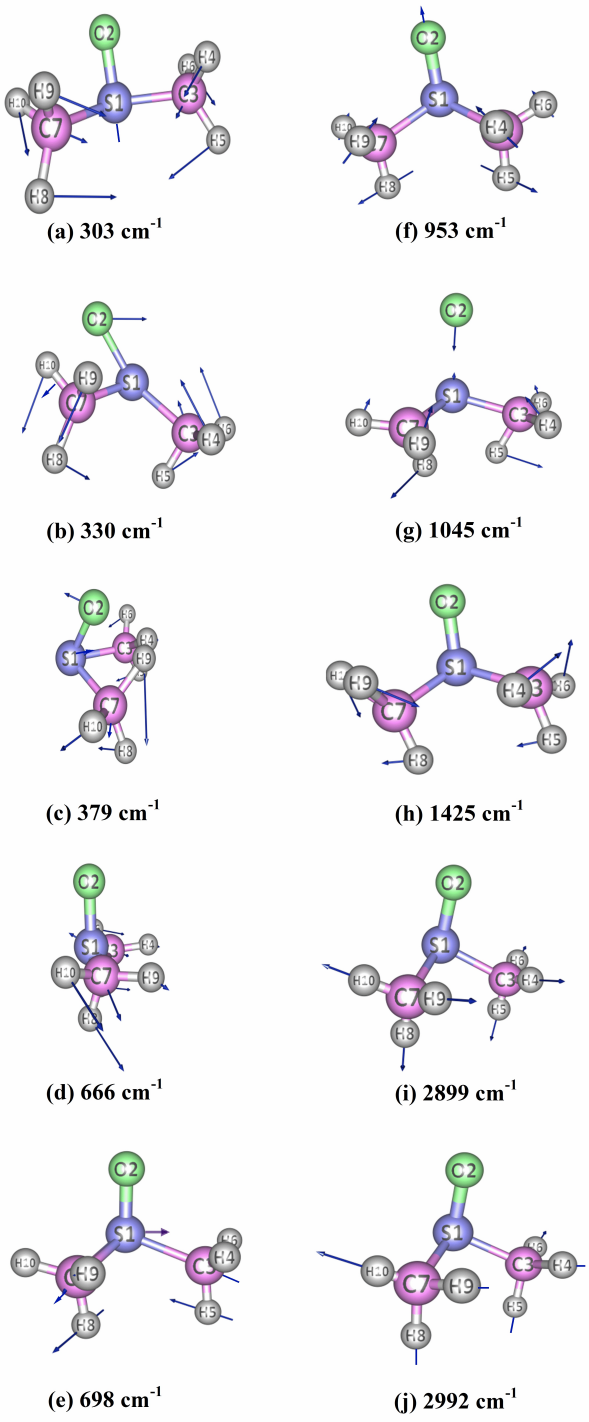


**Fig. S2.** The Raman vibration modes of DMSO arising from the calculated mode and displacement vectors are indicated by arrows. Nuclear vibration: (a) 303 $cm^{-1}$, (b) 330 $cm^{-1}$, (c) 379 $cm^{-1}$, (d) 666 $cm^{-1}$, (e) 698 $cm^{-1}$, (f) 953 $cm^{-1}$, (g) 1045 $cm^{-1}$, (h) 1425 $cm^{-1}$.

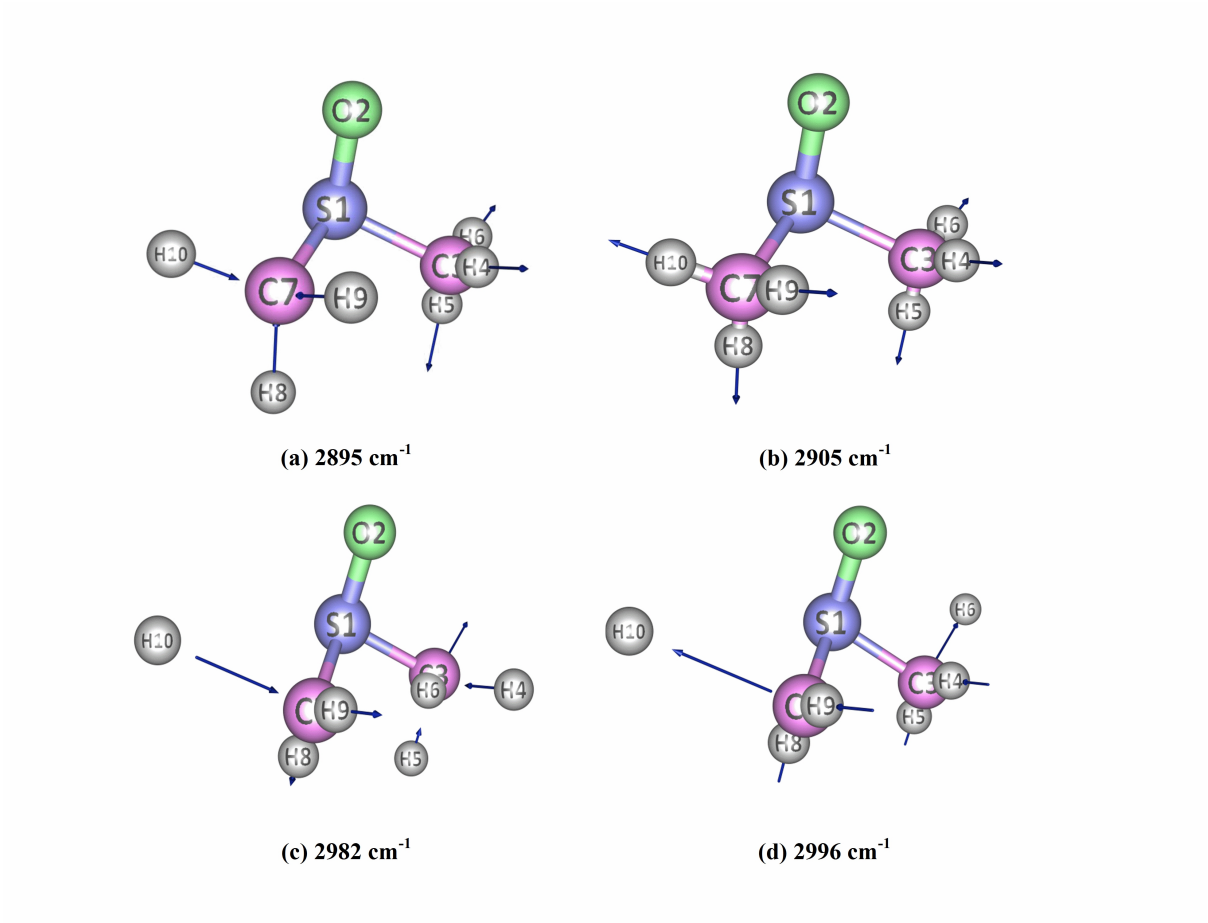


**Fig. S3.** The Raman vibrational forms of DMSO arising from the calculated mode and displacement vectors are indicated by arrows. Nuclear vibration: (a) 2895 $cm^{-1}$, (b) 2905 $cm^{-1}$, (c) 2982 $cm^{-1}$, (d) 2996 $cm^{-1}$.