Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supplementary Information

Hybrid density functional theory / molecular mechanics calculations of two-photon absorption of dimethylamino nitro stilbene in solution

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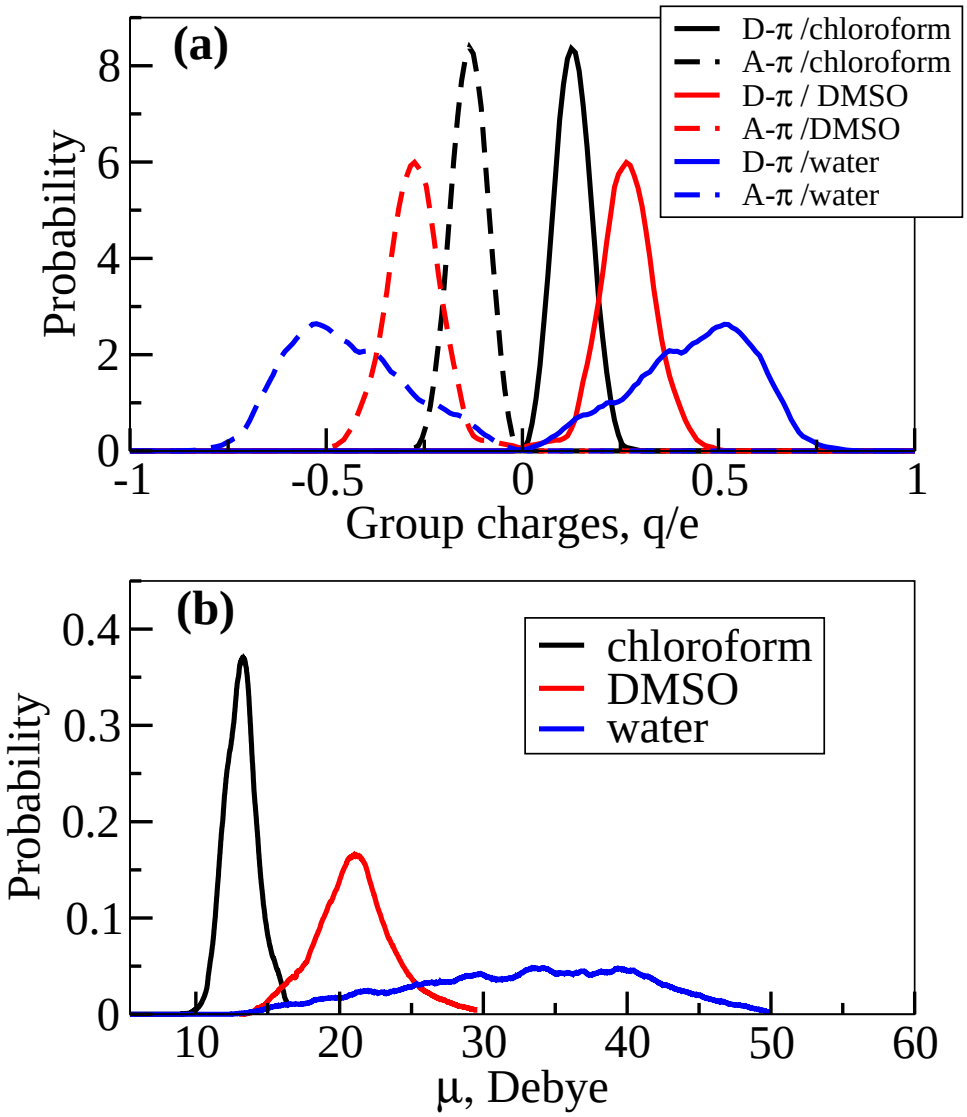

Figure 1s *(a)* Group charge distribution for DANS in chloroform, DMSO and in water *(b)* Molecular dipole moment for DANS in chloroform, DMSO and in water solvents.

Table 1s. Standard deviation in the excitation energy corresponding to different models.

Method	DANS in $CHCl_3$	DANS in DMSO	DANS in water
QM/MM-0	0.08	0.10	0.13
QM/PCM	0.11	0.14	0.16
QM/MM-1	0.13	0.24	0.21
QM/MM-2	0.14	0.24	0.26
QM/MM-3	–	–	0.21