

Supplementary Information

Dispersion-induced structural preference in the ultrafast dynamics of diphenyl ether

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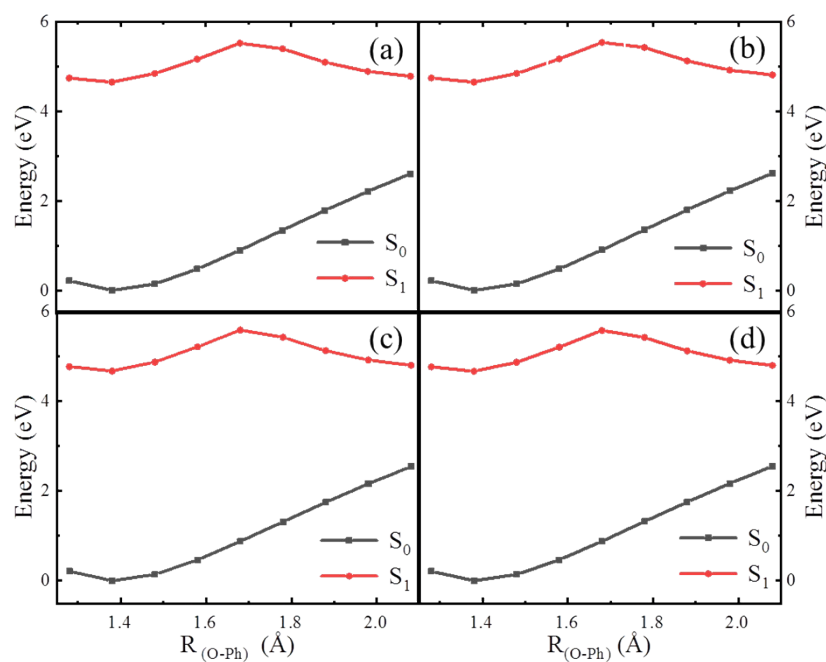


Figure S1. The potential curves of the two lowest states S_0 and S_1 of DPE in (a) cyclohexane, (b) 1,4-dioxane, (c) methanol and (d) t-butanol as a function of the O-Ph bond distance. The energies are relative to the minimum of the S_0 curve.

Table S1. Vertical excitation energies of the S_1 and T_n states using B3LYP/cc-pVDZ in cyclohexane, 1,4-dioxane, t-butanol and methanol, respectively.

solvents	Polarity	E_{S_1} (eV)	E_{T_n} (eV)	$E_{S_1 \rightarrow T_n}$ (eV)	Exp. $\cdot S_1$ (eV)		
cyclohexane	0	4.64	T ₁	3.60	1.04		
			T ₂	3.73	0.91		
			T ₃	4.08	0.56		
			T ₄	4.32	0.32		
			T ₅	4.44	0.20		
			T ₆	4.56	0.08		
1,4-dioxane	4.8	4.65	T ₁	3.60	1.05		
			T ₂	3.73	0.92		
			T ₃	4.08	0.57		
			T ₄	4.32	0.33		
			T ₅	4.44	0.21		
			T ₆	4.56	0.09		4.45 \pm 0.01 [1]
t-butanol	3.9	4.66	T ₁	3.61	1.05		
			T ₂	3.74	0.92		4.55 \pm 0.01 [2]
			T ₃	4.09	0.57		
			T ₄	4.33	0.33		
			T ₅	4.45	0.21		
			T ₆	4.56	0.10		
methanol	6.6	4.67	T ₁	3.61	1.06		
			T ₂	3.74	0.93		
			T ₃	4.10	0.57		
			T ₄	4.33	0.34		
			T ₅	4.45	0.22		
			T ₆	4.56	0.11		

1. S. E. Greenough, M. D. Horbury, J. O. F. Thompson, G. M. Roberts, T. N. V. Karsili, B. Marchetti, D. Townsend, and V. G. Stavros. *Phys. Chem. Chem. Phys.*, 2014, **16**, 16187-16195.
2. T. Hinohara, S. Cho, and T. Morita. *Bull. Chem. Soc. Jpn.*, 1971, **44**, 629-637.