Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Computing UV/vis spectra using a combined molecular dynamics and quantum chemistry approach: bis-triazin-pyridine (BTP) ligands studied in solution

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1 SUPPLEMENTARY INFORMATION

$$U^{shb} = \sum f(r)g(\psi) = d_e \left[1 - \xi \sum \exp\left(\frac{-(r-r_e)^2}{\gamma_{rt}}\right)\right] \exp\left(\frac{-(r-r_e)^2}{\gamma_r}\right) \exp\left(\frac{-(\psi-\psi_e)^2}{\gamma_\psi}\right) \tag{SI.1}$$

$$U^{pol} = \frac{1}{2}\sum_i \frac{\mu_i^2}{\alpha_i} - \sum_i \mu_i E_i^q - \frac{1}{2}\sum_i \sum_{k\neq i} \mu_i T_{ik} \mu_k. \tag{SI.2}$$

$$T_{ik} = 3\lambda_5 \frac{\mathbf{r}_i \cdot \mathbf{r}_k}{|\mathbf{r}_i - \mathbf{r}_k|^5} - \lambda_3 \frac{\mathbf{1}}{|\mathbf{r}_i - \mathbf{r}_k|^3} \tag{SI.3}$$

$$\lambda_5 = 1 - \exp(-a r_{ik}^3) \tag{SI.4}$$

$$\lambda_3 = 1 - (1 + a r_{ik}^3)\exp(-a r_{ik}) \tag{SI.5}$$

$$U^{rep} = \sum_{i<k} A_{ik} \exp\left(-B_{ik} r_{ik}\right) \tag{SI.6}$$

Table SI.1: Optimized force-field parameters according to equations (SI.1) - (SI.6).

Energy term	Unit	Parameter	Value	Parameter	Value
U^{pol}	$Å^{-3}$	a_{OC}	0.080	a_{HC} (wat/lig)	0.050
	$Å^{-3}$	a_{ON}	0.139	a_{HN} (wat/lig)	0.050
	$Å^{-3}$	a_{HH} (lig/wat)	0.500	a_{HH} (lig/lig)	0.500
	$Å^{-3}$	a_{OH} (wat/lig)	0.500		
U^{rep}	$Å^{-1}$	B_{OC}	5.694	B_{HC} (wat/lig)	6.699
	$Å^{-1}$	B_{ON}	5.113	B_{HN}	6.773
	$Å^{-1}$	B_{HH} (lig/wat)	7.000	B_{HH} (lig/lig)	6.000
	$Å^{-1}$	B_{CC}	4.140	B_{NN}	4.500
	$Å^{-1}$	B_{CN}	4.025	B_{OH} (wat/lig)	5.900
	kcal/mol	A_{OC}	2200000.0	A_{HC} (wat/lig)	2200000.0
	kcal/mol	A_{ON}	2183089.5	A_{HN}	68223.1
	kcal/mol	A_{HH} (lig/wat)	75000.0	A_{HH} (lig/lig)	75000.0
	kcal/mol	A_{CC}	500000.0	A_{NN}	100000.0
	kcal/mol	A_{CN}	1000000.0	A_{OH}	60000.0
U^{shb}_{HN}	kcal/mol	d_e	1.310		
	Å	r_e	1.604		
	$Å^2$	γ_r	2.598		
	rad^2	γ_ψ	0.115		
		ξ	0.031	γ_{rt}	0.300

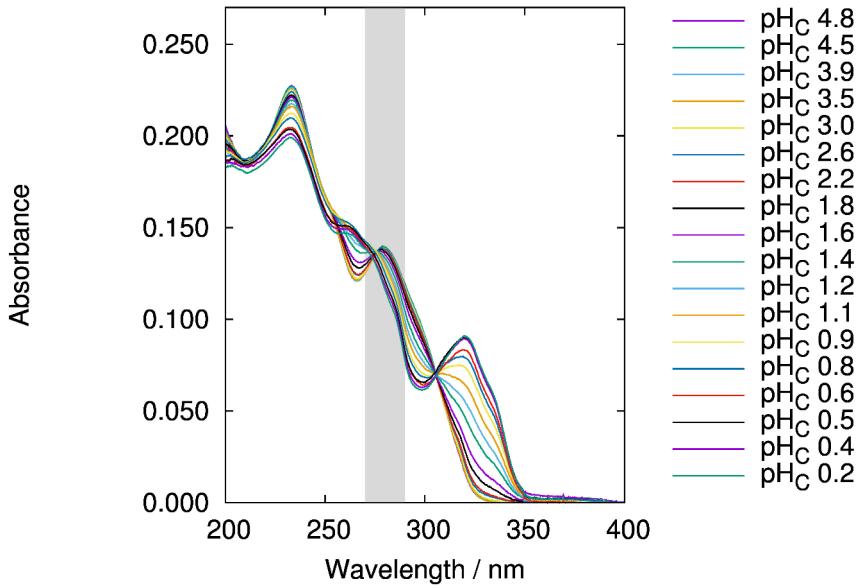


Figure SI.1: UV/vis spectra of $CyMe_4$-BTP as a function of pH.

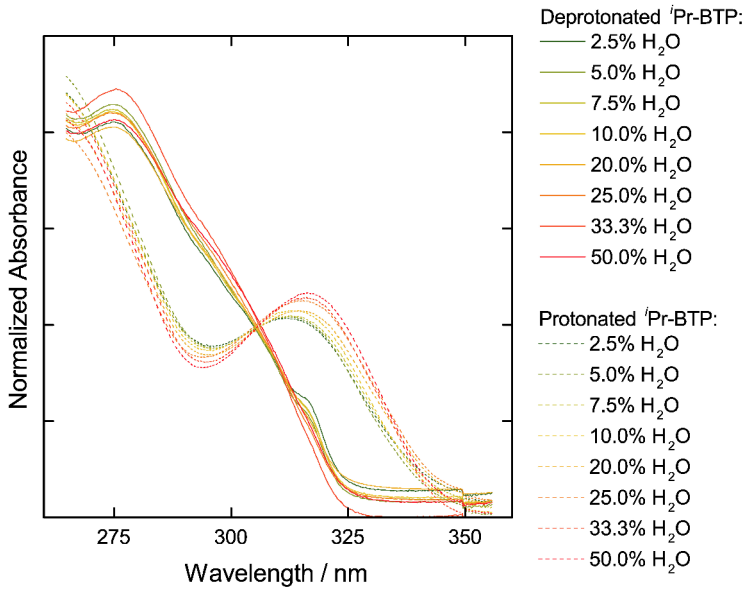
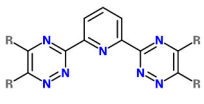
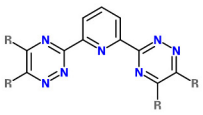
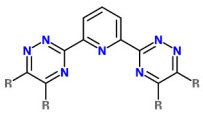


Figure SI.2: Normalized UV/vis spectra as a function of water/methanol mixtures.

Table SI.2: Molecular structures of the different ligand conformations with corresponding relative energies [kcal mol^{-1}] on the B3LYP/COSMO level using the def2-TZVP basis sets and standard COSMO radii.

	 cis/cis	 trans/cis	 trans/trans
^{i}Pr-BTP	0.0	+0.93	+2.21
$CyMe_4$	0.0	+1.89	+1.29

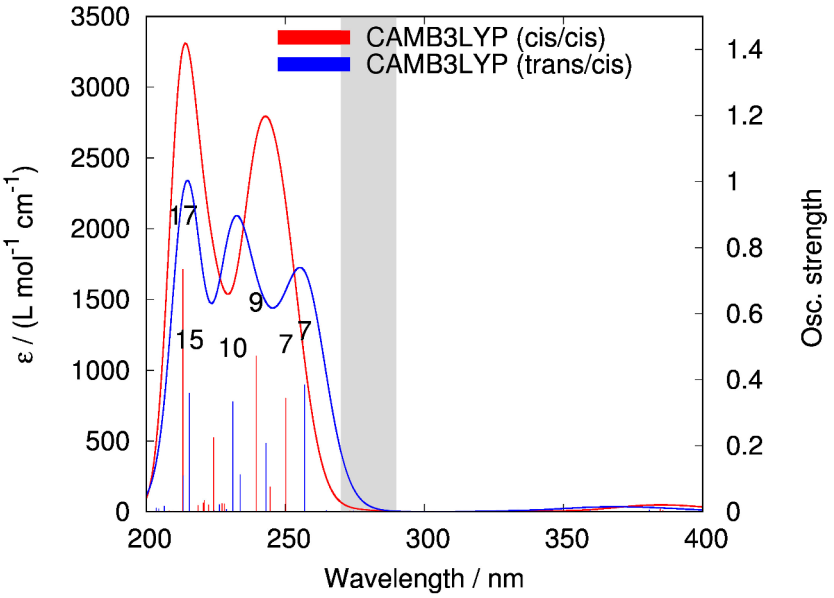


Figure SI.3: Comparison of the cis/cis and trans/cis CAM-B3LYP/def2-TZVP gas-phase spectra of ^{i}Pr-BTP.