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

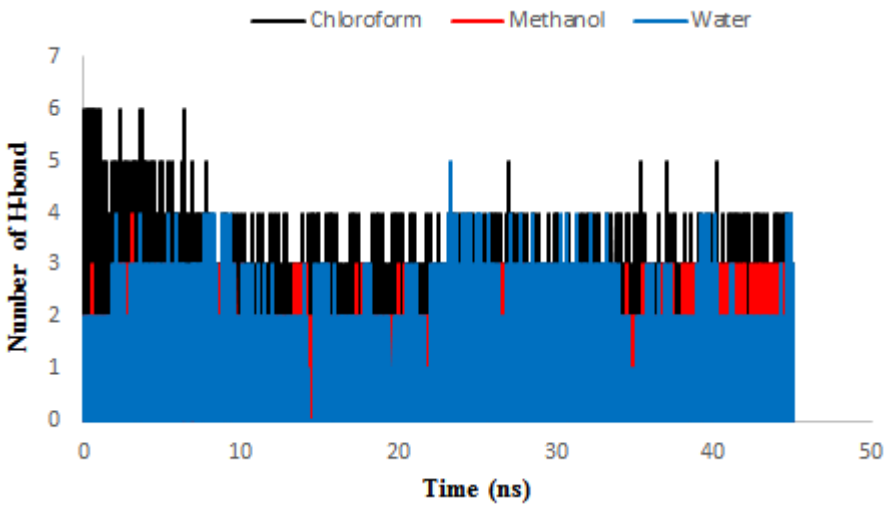

Figure S1. Calculated number of H-bond as a function of time during the 45 ns of the MD simulations in different solvents.

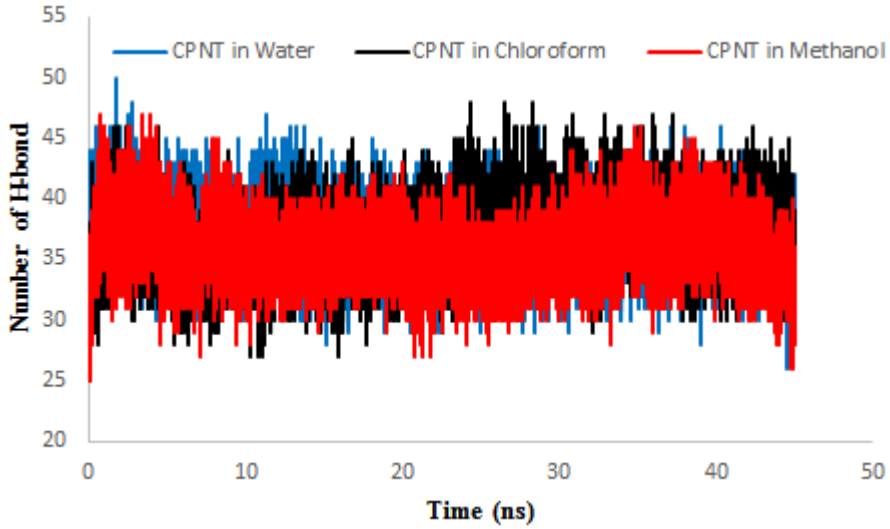

Figure S2. The number of H-bond of the CPNT during the 45 ns of the MD simulations.

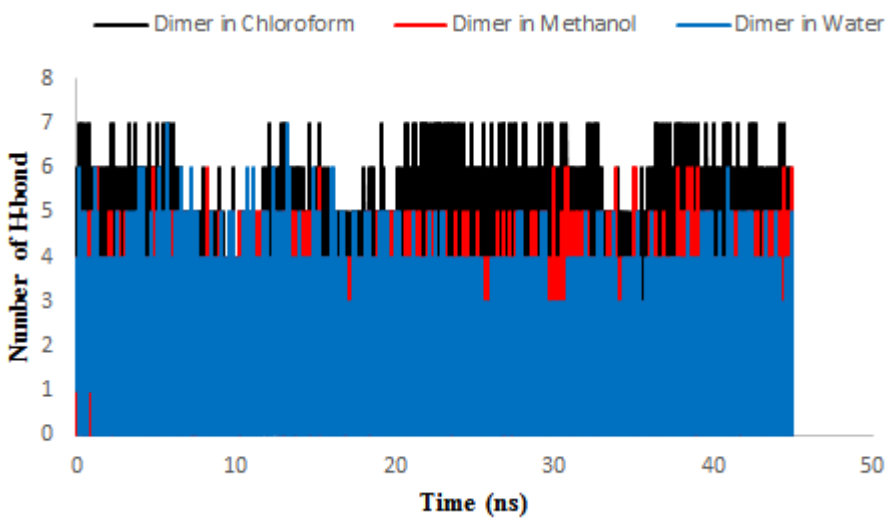

Figure S3. Calculated number of H-bonds of the dimer with guest molecule in methanol, water and chloroform.

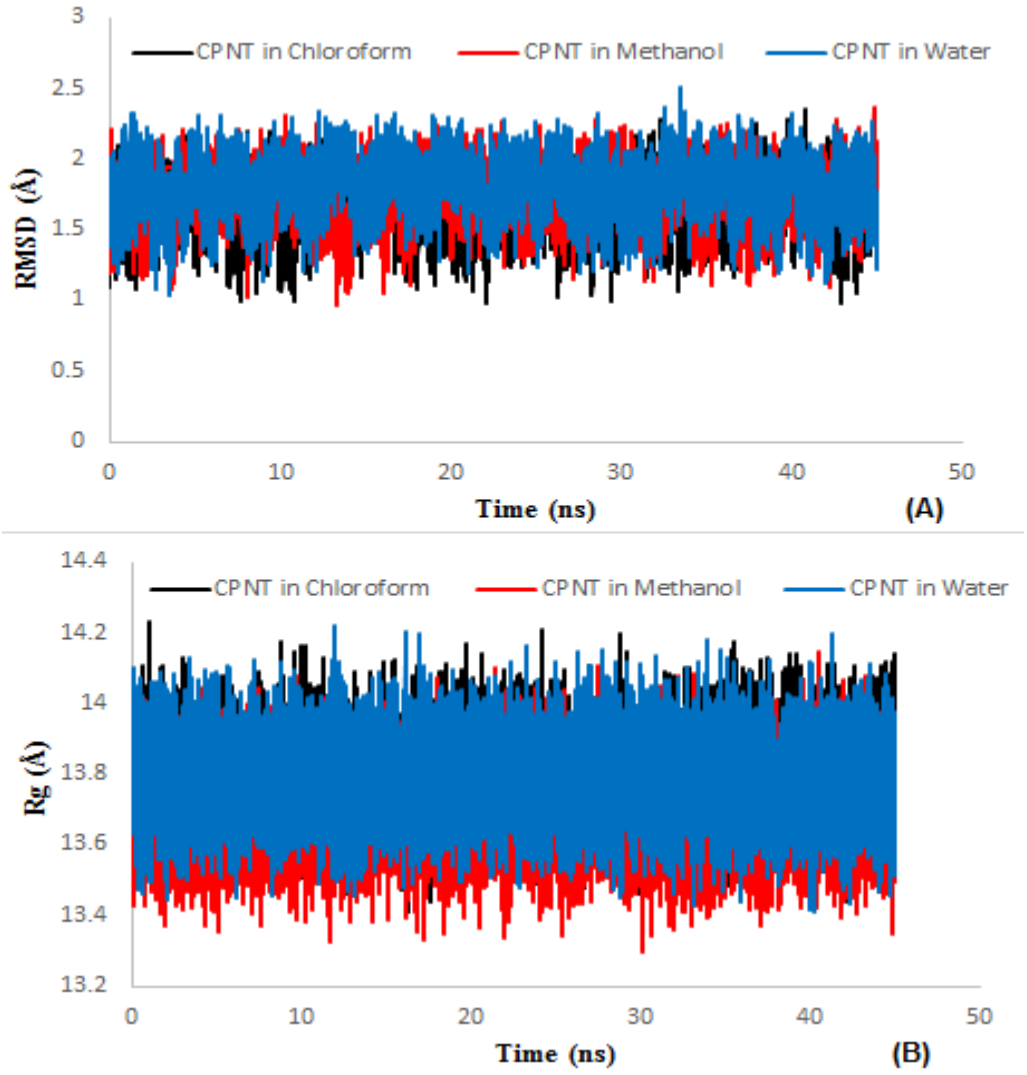

Figure S4. RMSD (A) and Rg (B) of CPNT with guest molecules in methanol, water and chloroform during the 45 ns of MD simulations.

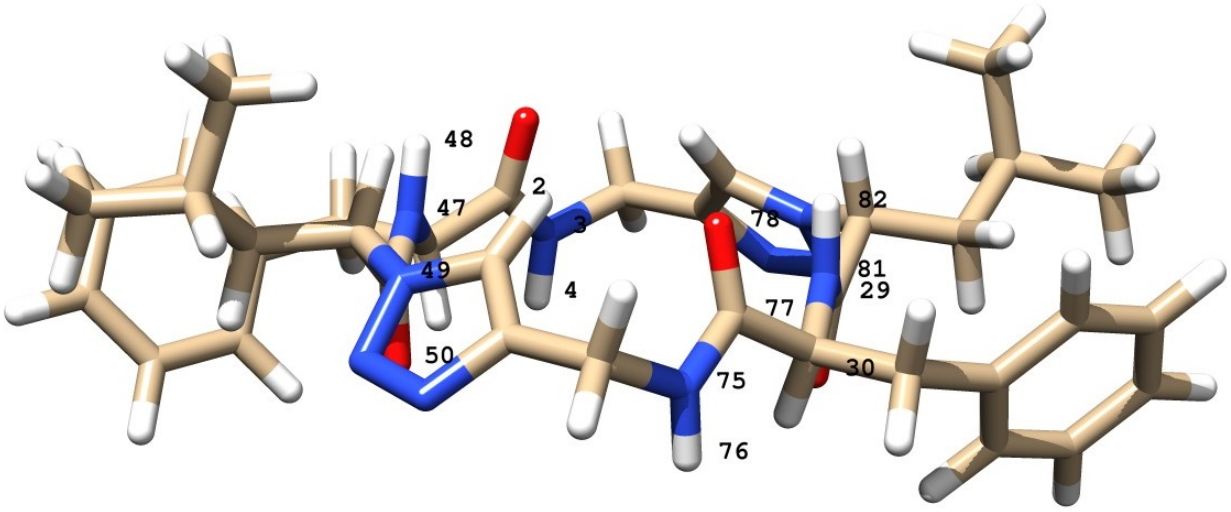

Figure S5. Optimized structure of CP monomer at M06-2X/6-31G(d) level in the gas phase.

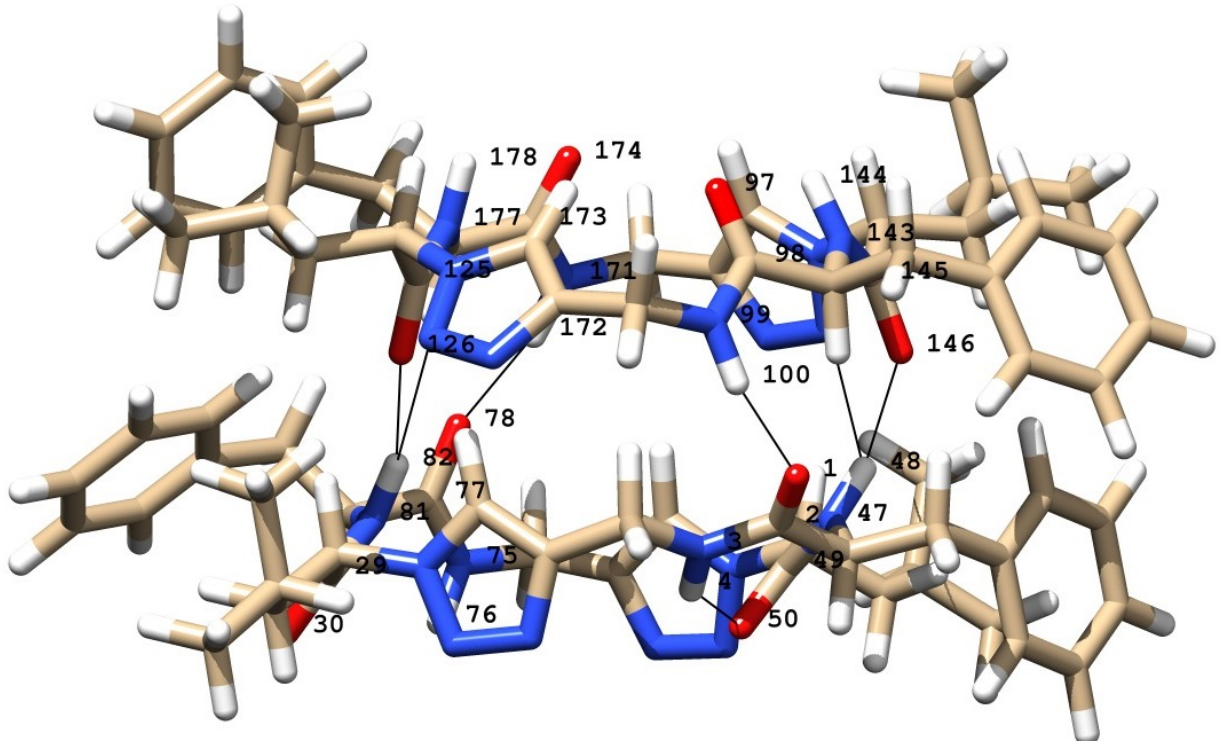

Figure S6. Optimized structure of CP dimer at M06-2X/6-31G(d) level in the gas phase.

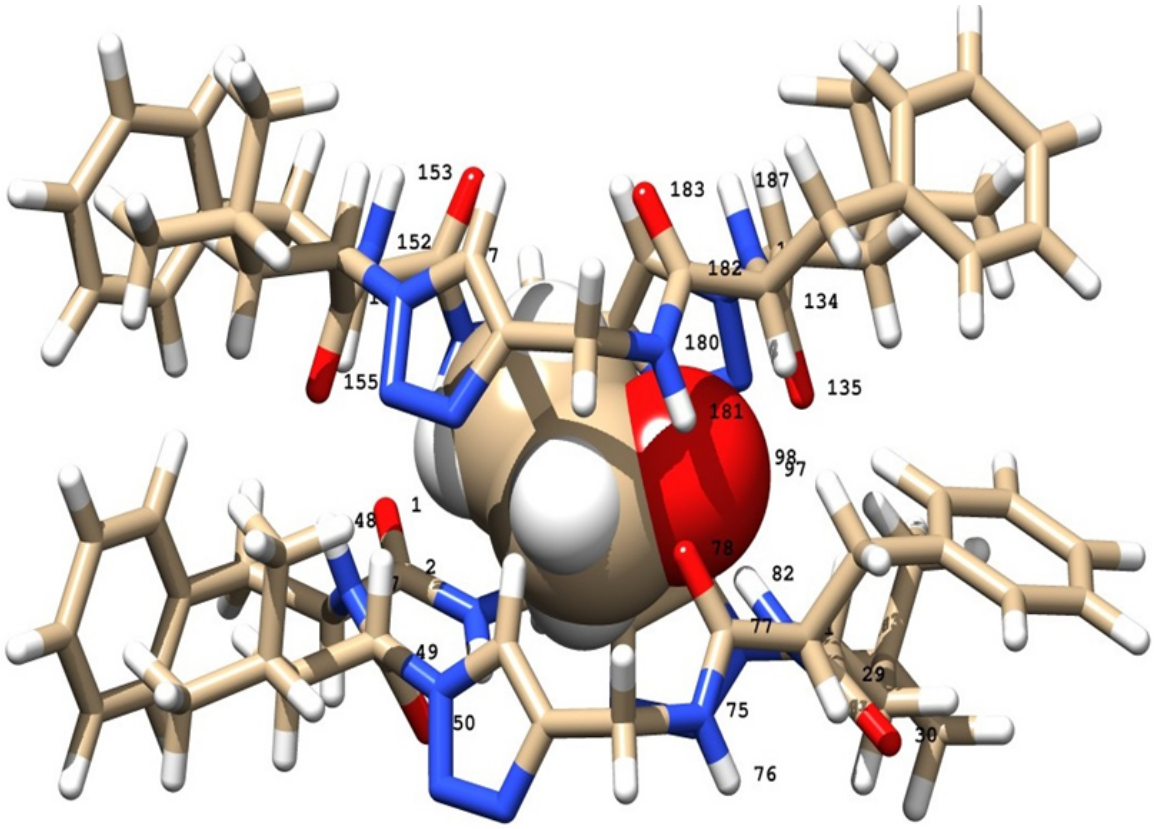

Figure S7. Optimized structure of CP dimer with a guest molecule (dimer-complex) at M06-2X/6-31G(d) level in the gas phase.

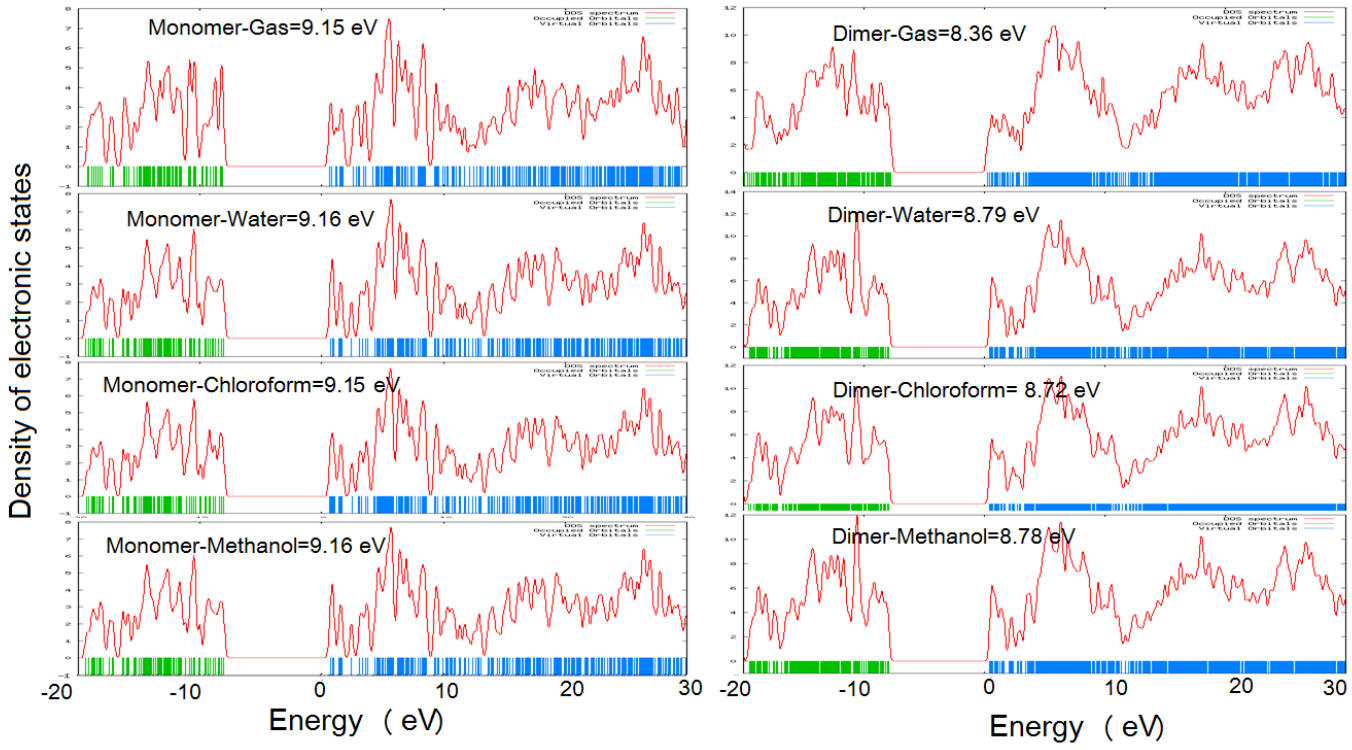

Figure S8. Calculated electronic density of sates (DOS) for the CP monomer and dimer in different solvents and gas phase (red, green and blue lines shows DOS spectrum, occupied orbitals and unoccupied orbitals, respectively.)

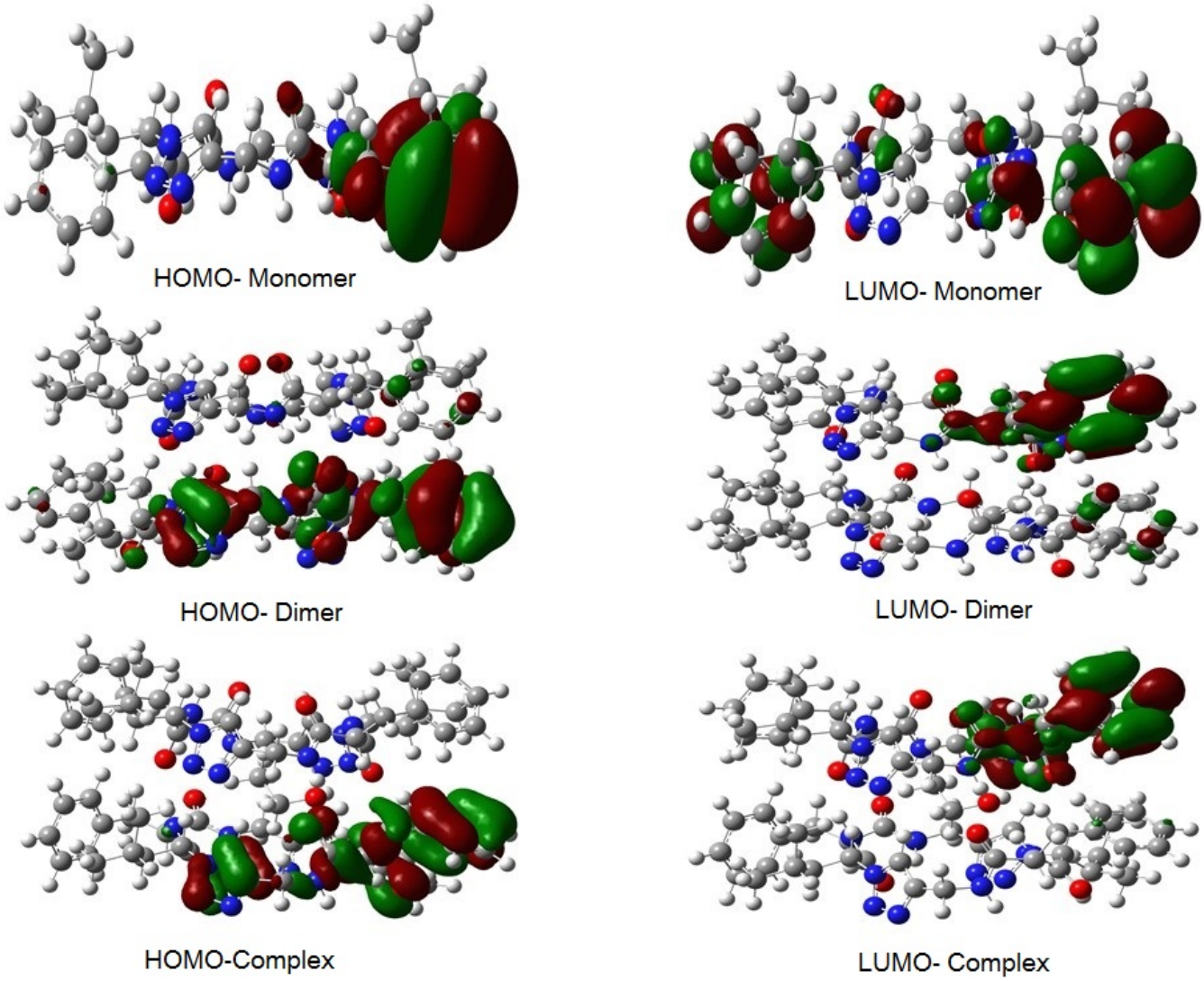

Figure S9. HOMO and LUMO orbitals of the CP monomer, dimer and dimer with guest molecule (Complex).

Table S1. Theoretical (gas phase) and experimental structural parameters of the CP monomer and

CP dimer (bond length and angles are in Å and degree, respectively)			
Parameters	**Monomer**	**Dimer**	**X-ray**
C77O78	1.22	1.23	1.23
C49O50	1.21	1.22	1.23
C2O1	1.22	1.23	1.29
C29O30	1.21	1.21	1.21
N3H4	1.01	1.02	0.99
N3C2O1	123.14	123.07	131.23
N81C29O3	124.11	123.39	122.59
N75C77O78	123.13	123.12	125.03
N47C49O50	124.16	123.07	122.73
O1C281H82	164.37	-177.98	173.08
O30C29N81H82	-168.46	166.65	174.26
O78C77N75H76	164.32	169.82	-179.27
O50C49N48H47	-168.78	-174.34	178.19

Table S2. Calculated IR vibrational frequencies (cm^{-1}) for CPs monomer and dimer in the gas phase and different solvents.

Bond	structures	Gas	Water	Chloroform	Methanol
N47H48	Monomer	3641.36	3642.94	3642.82	3642.94
	Dimer	3564.51	3543.60	3545.35	3543.78
N3H4	Monomer	3641.36	3642.94	3642.82	3642.94
	Dimer	3497.08	3504.71	3504.83	3504.79
N75H76	Monomer	3632.76	3641.20	3641.07	3641.19
	Dimer	3650.19	3641.56	3641.67	3641.57
N81H82	Monomer	3632.76	3641.20	3641.07	3641.10
	Dimer	3529.02	3531.40	3533.37	3531.59
C49O50	Monomer	1844.62	1837.82	1839.51	1837.98
	Dimer	1817.66	1805.65	1807.66	1805.84
C29O30	Monomer	1844.62	1837.82	1839.51	1837.98
	Dimer	1849.68	1841.10	1842.68	1841.35
O1C2	Monomer	1814.80	1797.63	1798.47	1797.98
	Dimer	1754.32	1740.64	1744.43	1741.03
C77O78	Monomer	1814.80	1798.63	1798.47	1797.98
	Dimer	1772.78	1755.27	1759.47	1755.64