Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supplementary Material

ESIPT on/off switching and crystallization-enhance emission properties of new design phenol-pyrazole modified cyclotriphosphazenes

Ceylan Mutlu Balcı[*1], *Süreyya Oğuz TÜMAY,* [1] *Serap Beşli*[1]

[1]Department of Chemistry, Gebze Technical University, Gebze, Kocaeli, Turkey

* Corresponding author

Dr. Ceylan MUTLU BALCI

Department of Chemistry, Gebze Technical University, Gebze, Kocaeli 41400, Turkey

Tel.: 90 262 6053111 Fax: 90 262 6053005 E-mail: ceylanmutlu@gtu.edu.tr

CONTENTS

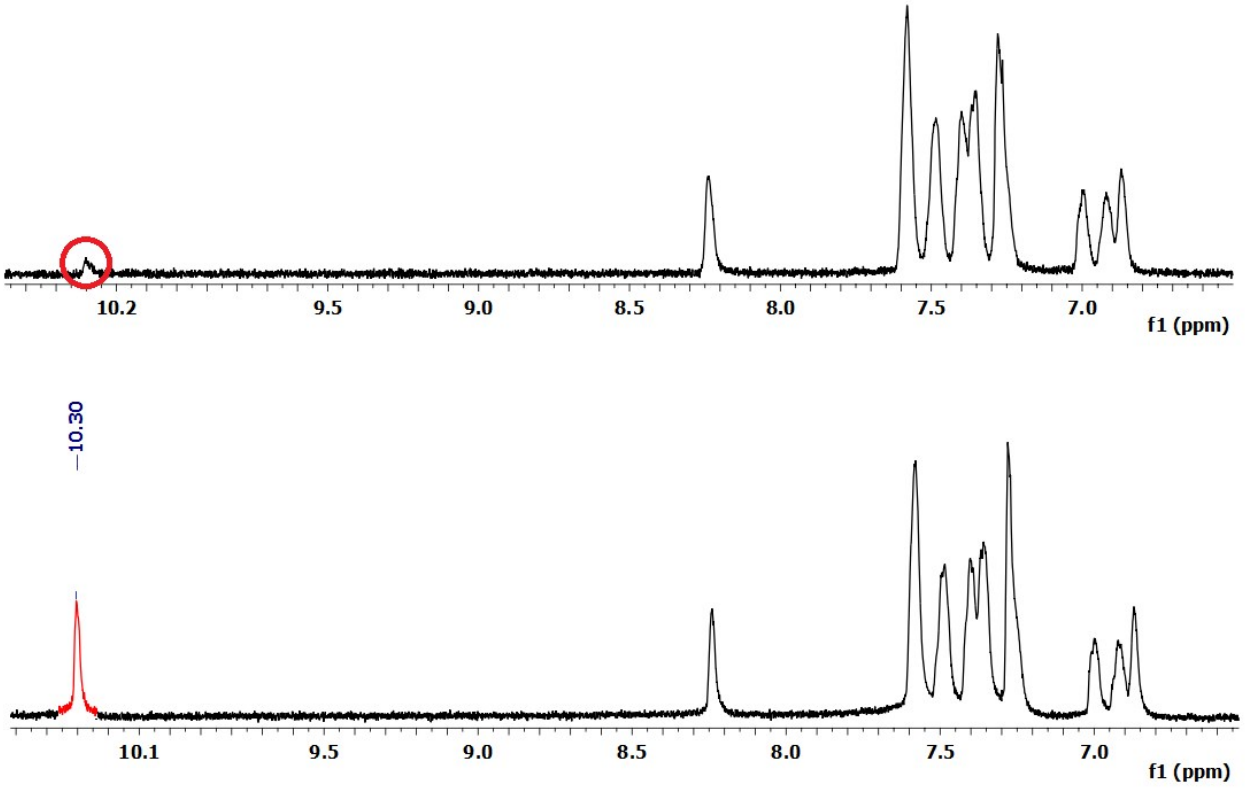
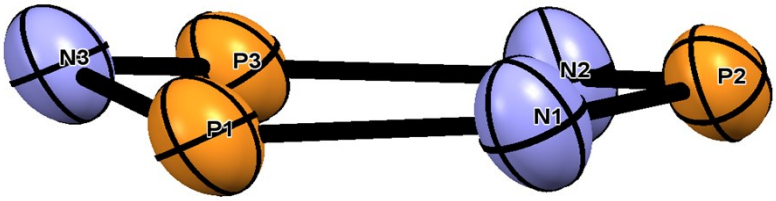


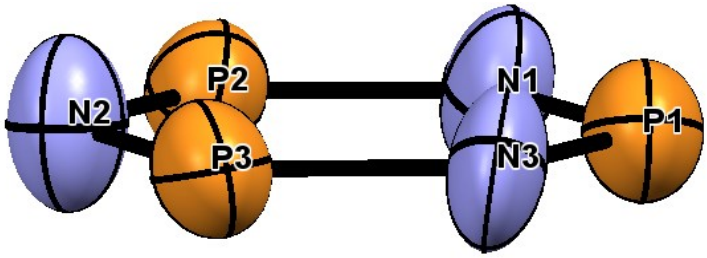
Fig. S1. a) ^{1}H NMR spectrum of compound **3 b)** D_2O exchange ^{1}H NMR spectrum of compound **3**.

Table S1. Some bond and conformational parameters of compounds **3** and **4**.

	3	**4**
Bond Lenghts		
P1-N1	1.561(2)	1.574(10)
P2-N2	1.573(2)	1.572(10)
P3-N3	1.582(2)	1.571(9)
N1-P2	1.582(2)	1.597(8)
N2-P3	1.565(2	1.572(10)
N3-P1	1.561(2)	1.597(11)
P1-N4	1.675(2)	1.669(11)
P1-N6	1.703(2)	
P1-O1		1.605(8)
P2-O2		1.614(9)
P2-O3	1.5778(18)	1.592(8)
P2-O4	1.5708(19)	
P3-O4		1.591(8)
P3-O5	1.5758(19)	1.597(8)
P3-O6	1.5828(18)	
Bond Angles		
N1-P2-N2	117.54(12)	119.5(6)
N2-P3-N3	117.14(11)	119.4(6)
N3-P1-N1	119.74(12)	119.6(5)
P1-N1-P2	120.00(13)	119.9(6)
P2-N2-P3	122.65(14)	121.1(6)
P3-N3-P1	119.70(14)	120.5(7)
Torsion Angles		
P1-N1-P2-N2	-4.4(2)	1.7(11)
N1-P2-N2-P3	9.7(2)	-3.0(11)
P2-N2-P3-N3	0.1(2)	3.4(11)
N2-P3-N3-P1	-15.5(2)	-2.6(11)
P3-N3-P1-N1	21.0(2)	1.5(11)
N3-P1-N1-P2	-10.7(2)	-1.0(10)
Puckering amplitude, Q for P_3N_3	0.1918(16)	Planar
Max. Deviation for P_3N_3 ring	-0.123(2) (N3)	-0.017(11) (N2)



a)



b)

Fig. S2. The conformation of P_3N_3 ring for **a)** compound **3** and **b)** compound **4**.

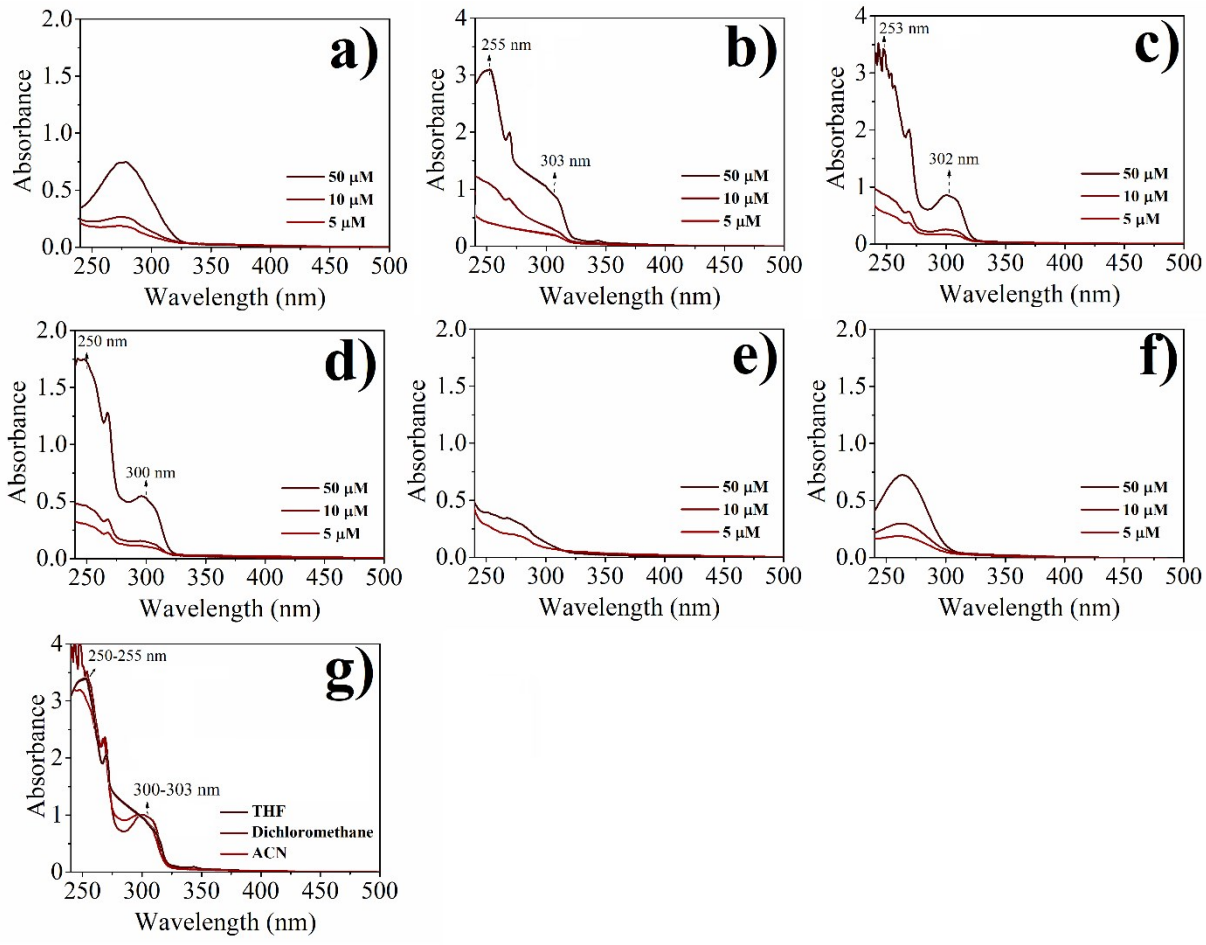


Fig. S3. UV-Vis absorption spectra of **3** in **a)** hexane, **b)** THF, **c)** dichloromethane, **d)** acetonitrile, **e)** ethanol, **f)** water and **g)** normalized UV-Vis absorption spectra of **3** in different solvents and concentrations.

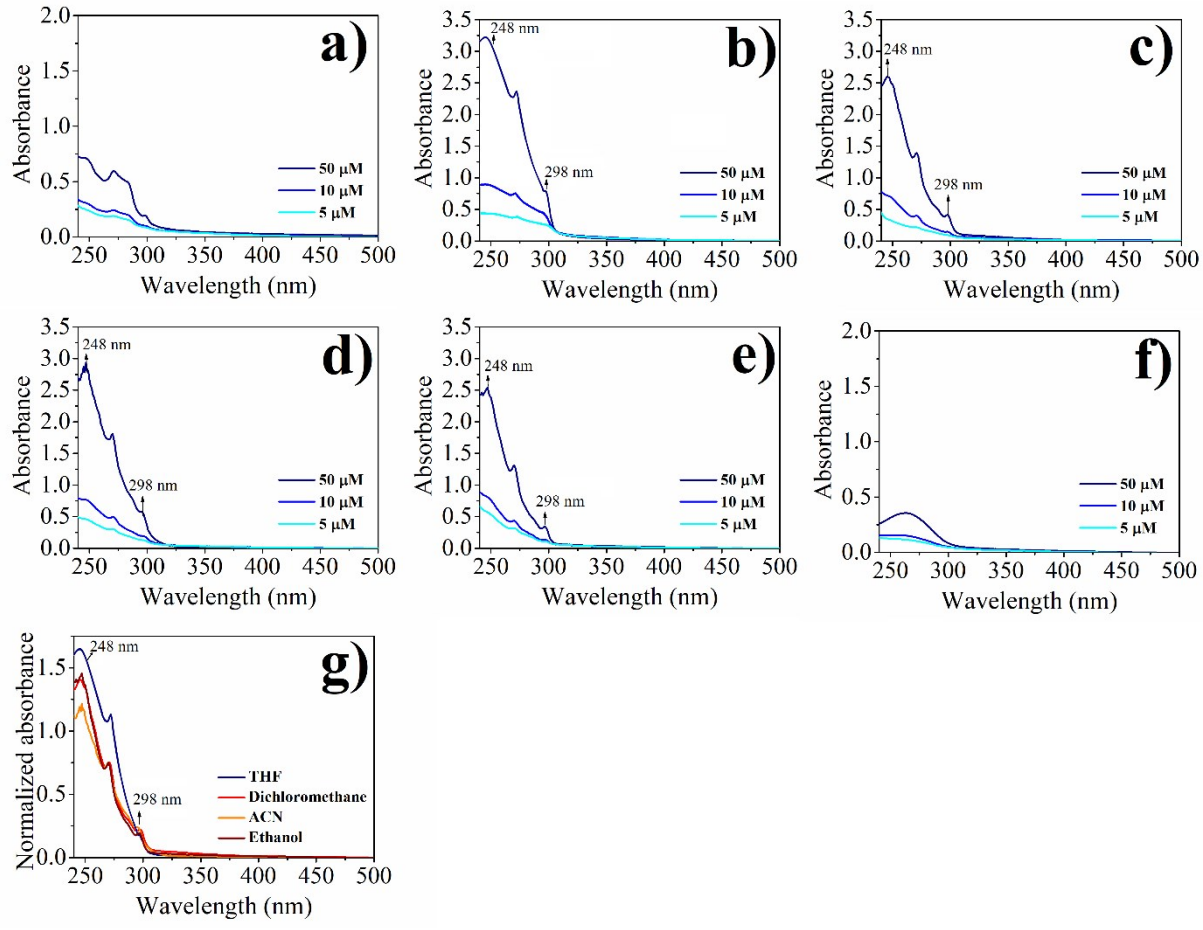


Fig. S4. UV-Vis absorption spectra of **4** in **a)** hexane, **b)** THF, **c)** dichloromethane, **d)** acetonitrile, **e)** ethanol, **f)** water and **g)** normalized UV-Vis absorption spectra of **4** in different solvents and concentrations.

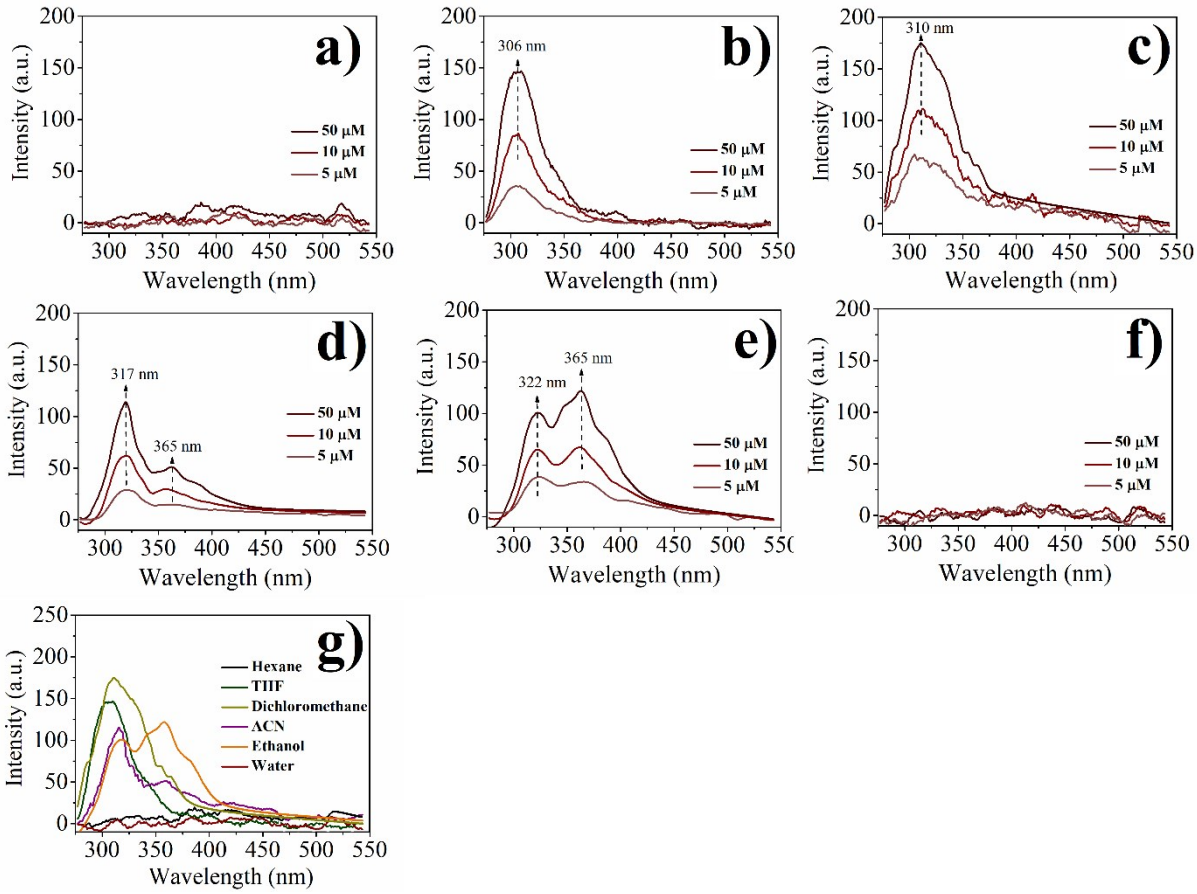


Fig. S5. Fluorescence spectra of **3** in **a)** hexane, **b)** THF, **c)** dichloromethane, **d)** acetonitrile, **e)** ethanol, and **f)** water **g)** normalized UV-Vis absorption spectra of **3** in different solvents and concentrations (λ_{ex}=265 nm).

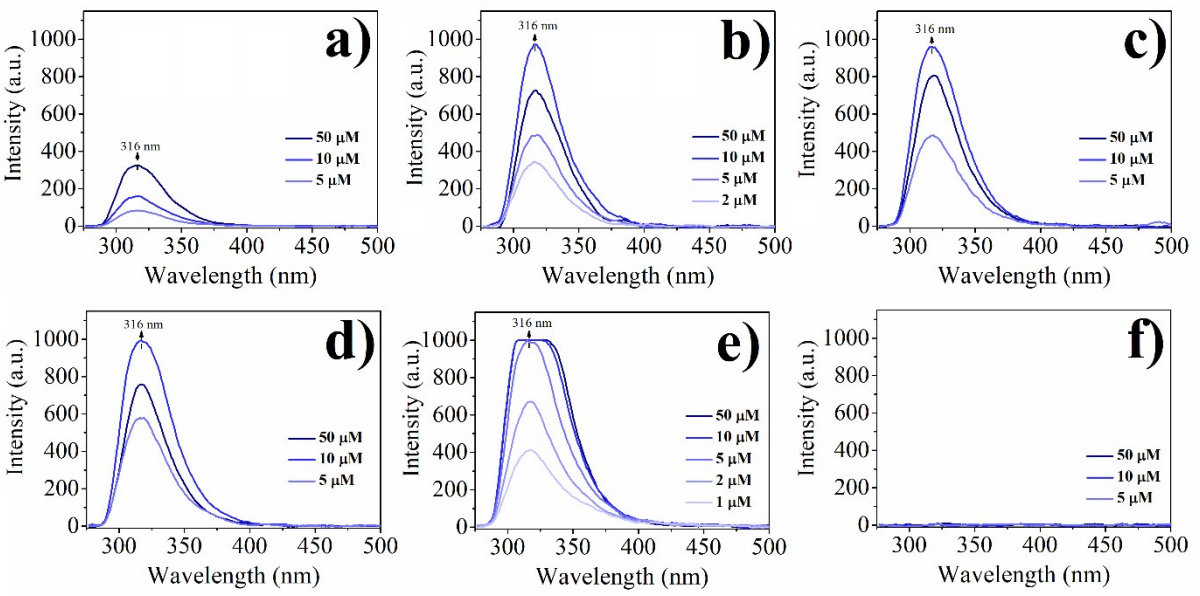


Fig. S6. Fluorescence spectra of **4** in **a)** hexane, **b)** THF, **c)** dichloromethane, **d)** acetonitrile, **e)** ethanol, and **f)** water (λ_{ex}=265 nm).

Fig. S7. Fluorescence spectra of **2** in **a)** dichloromethane, **b)** ethanol, and **c)** normalized fluorescence spectra of **2** in dichloromethane and ethanol.