Electronic Supplementary Information

Deprotonation Induced Formation of Möbius Aromatic [32]Heptaphyrins

Won-Young Cha,[a] Tomoki Yoneda,[b] Sangsu Lee,[a] Jong Min Lim,[a] Atsuhiro Osuka*[b] and Dongho Kim* [a]

[a]Department of Chemistry, Yonsei University, Seoul 120-749, Korea, [b]Department of Chemistry, Graduate School of Science, Kyoto University, Sakyo-ku, Kyoto, 606-8502, Japan.

E-mail: dongho@yonsei.ac.kr, osuka@kuchem.kyoto-u.ac.jp

Electronic Supplementary Material (ESI) for Chemical Communications

Contents

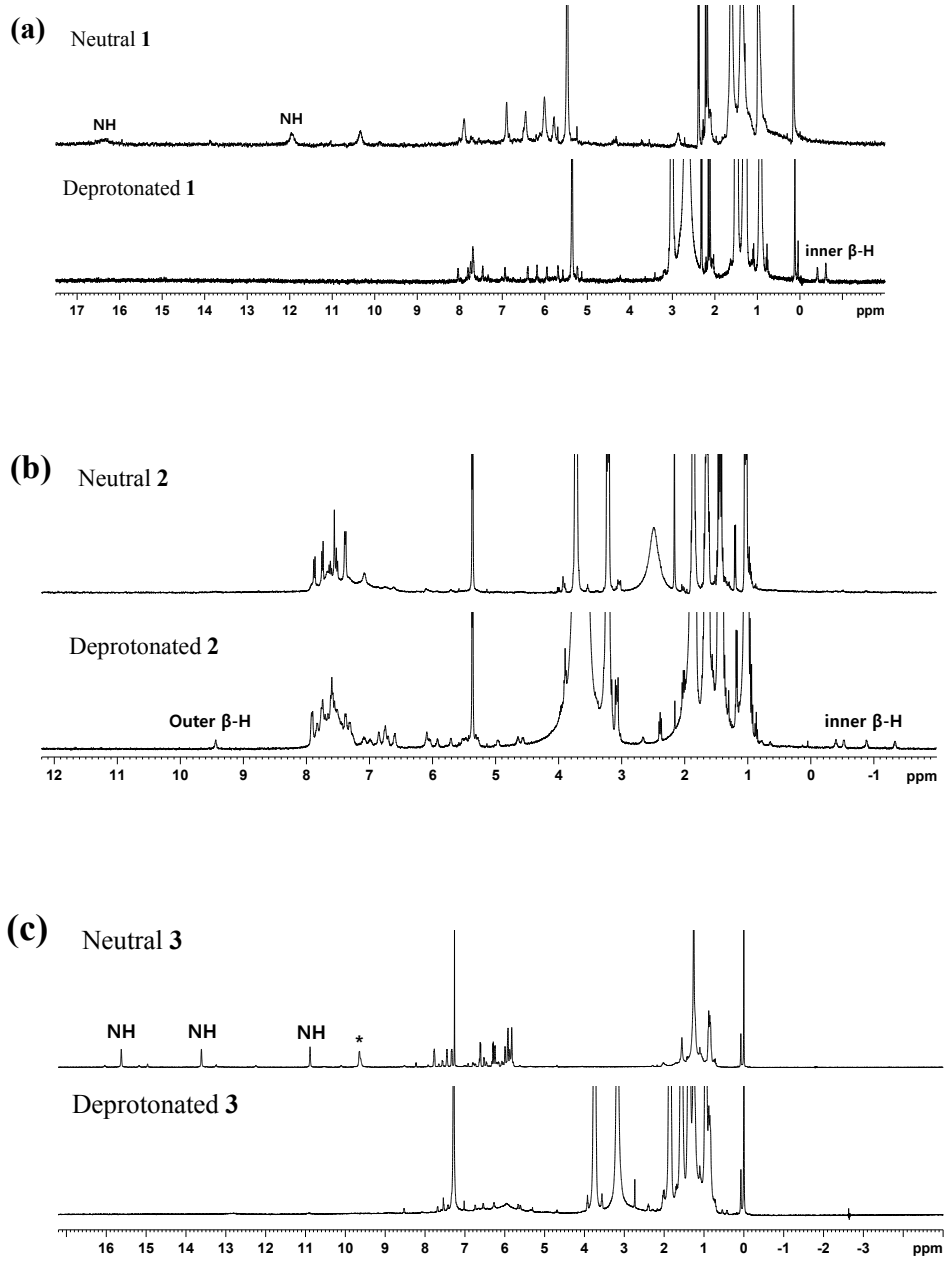


Fig. S1 ^{1}H NMR spectra of neutral and deprotonated species of (a) **1**, (b) **2** and (c) **3** in $CDCl_3$.

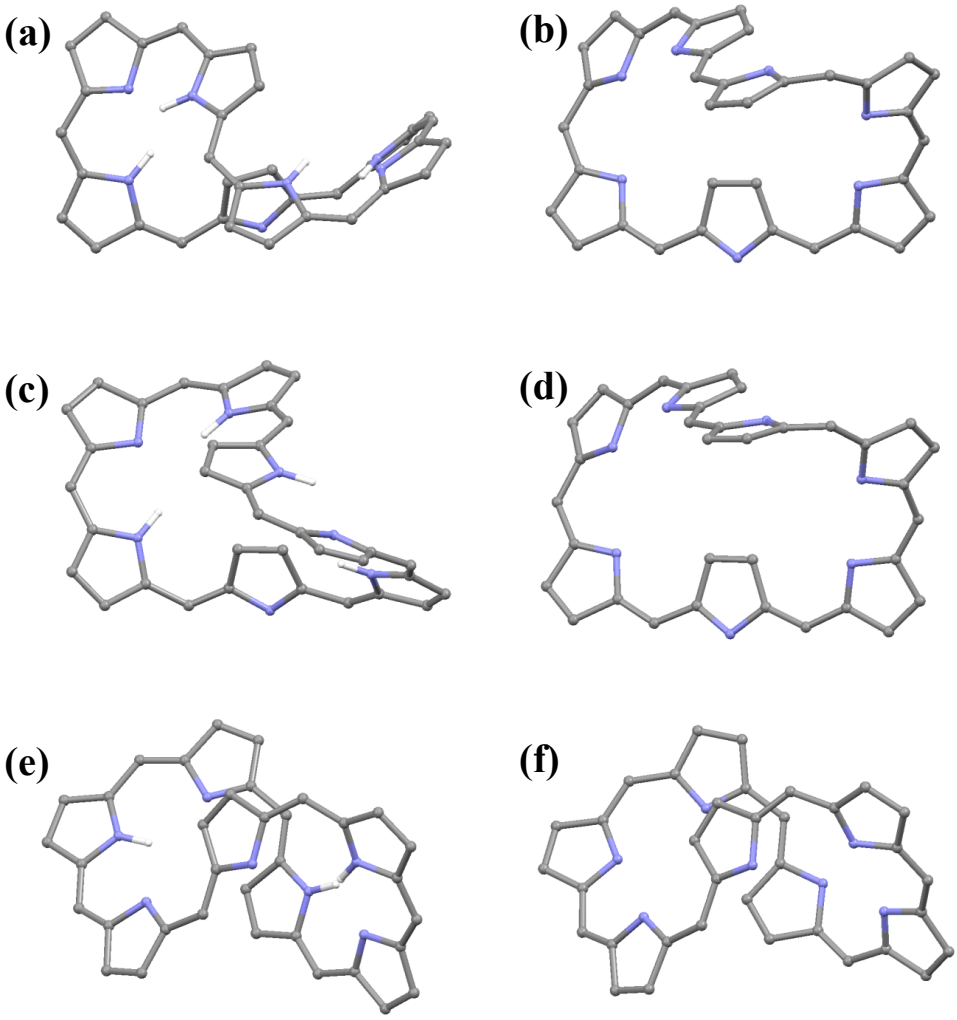


Fig. S2 Optimized molecular structures of neutral and deprotonated **1** (a, b), **2** (c, d) and **3** (e, f). All the *meso*-substituents and pyrrolic β-protons are omitted for clarity.

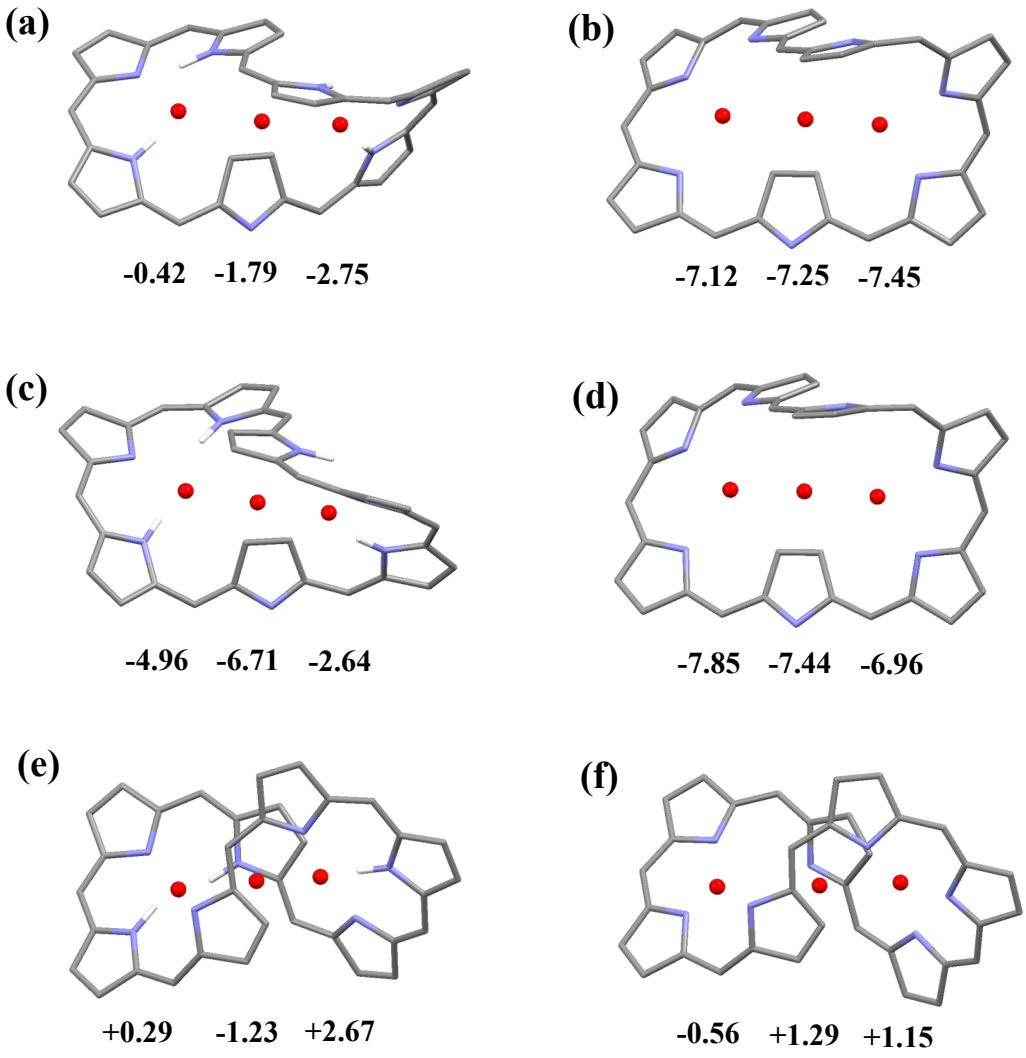
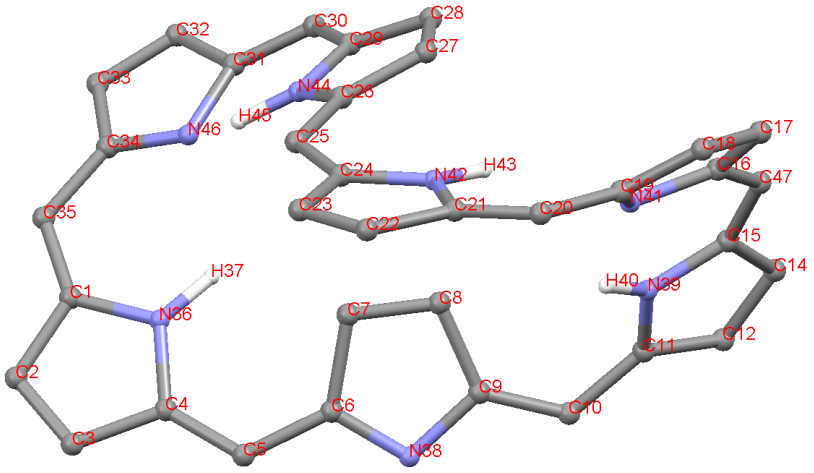


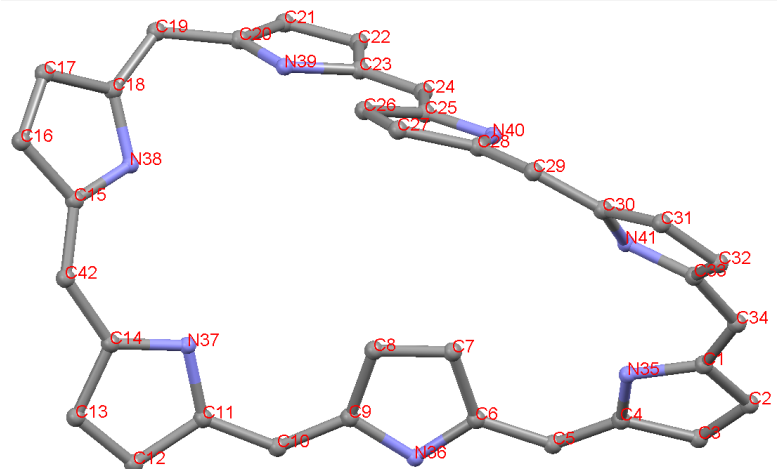
Fig S3. NICS values for neutral and deprotonated **1** (a, b), **2** (c, d) and **3** (e, f). The values were selected at z-axis of red positions. All the *meso*-substituents and pyrrolic β-protons are omitted for clarity.



Atom	Atom	Length
C1	C2	1.4586
C2	C3	1.3731
C3	C4	1.4594
C4	C5	1.3688
C5	C6	1.4464
C6	N38	1.3239
N38	C9	1.4080
C9	C10	1.3631
C10	C11	1.4444
C11	C12	1.4023
C12	C14	1.3949
C14	C15	1.4054
C15	C47	1.4280
C47	C16	1.3728
C16	N41	1.4104
N41	C19	1.3401

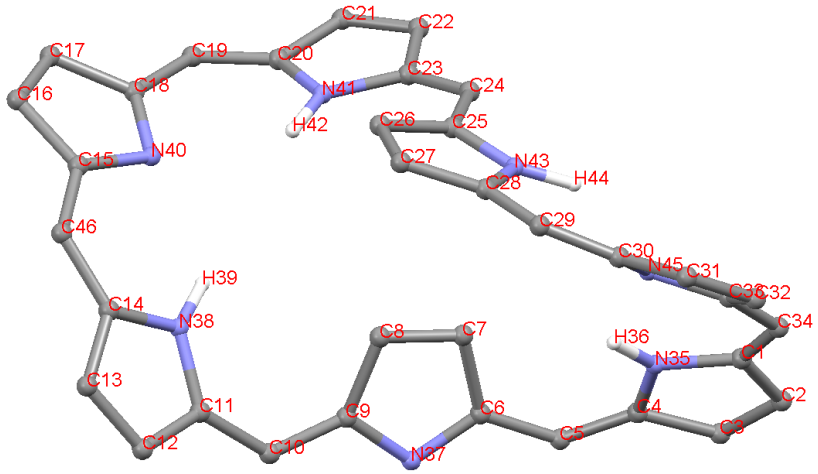
Atom	Atom	Length
C19	C20	1.4419
C20	C21	1.3712
C21	C22	1.4574
C22	C23	1.3510
C23	C24	1.4568
C24	C25	1.3659
C25	C26	1.4447
C26	C27	1.4215
C27	C28	1.4004
C28	C29	1.4070
C29	C30	1.4268
C30	C31	1.3816
C31	N46	1.4076
N46	C34	1.3397
C34	C35	1.4419
C35	C1	1.3731

Fig. S4 Calculated bond lengths of neutral **1**. *Meso*-substituents and pyrrolic β-protons are omitted for clarity.



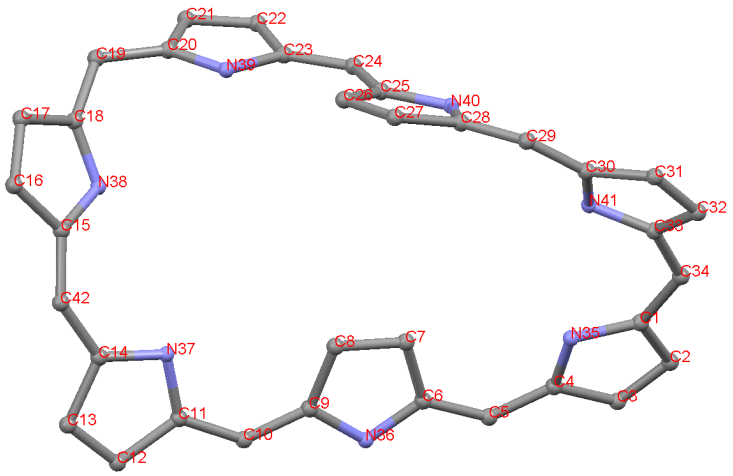
Atom	Atom	Length	Atom	Atom	Length
C1	N35	1.3561	C18	C19	1.4416
N35	C4	1.3754	C19	C20	1.4522
C4	C5	1.3848	C20	N39	1.3283
C5	C6	1.4425	N39	C23	1.4020
C6	N36	1.3374	C23	C24	1.3733
N36	C9	1.4089	C24	C25	1.4304
C9	C10	1.3740	C25	N40	1.3592
C10	C11	1.4319	N40	C28	1.3696
C11	N37	1.3719	C28	C29	1.4135
N37	C14	1.3606	C29	C30	1.3904
C14	C42	1.4478	C30	N41	1.3932
C42	C15	1.3759	N41	C33	1.3353
C15	N38	1.3968	C33	C34	1.4513
N38	C18	1.3351	C34	C1	1.4067

Fig. S5 Calculated bond lengths of deprotonated **1**. *Meso*-substituents and pyrrolic β-protons are omitted for clarity.



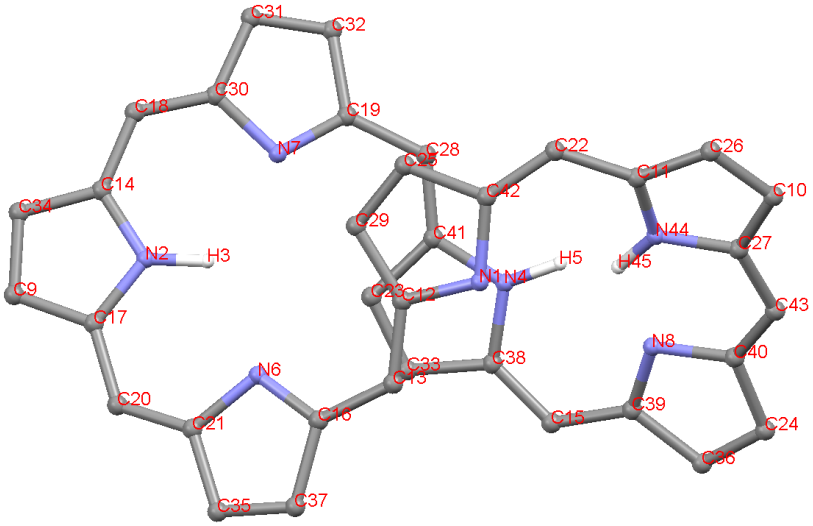
Atom	Atom	Length	Atom	Atom	Length
C1	C2	1.4588	C18	C19	1.4378
C2	C3	1.3517	C19	C20	1.3675
C3	C4	1.4612	C20	C21	1.4575
C4	C5	1.3663	C21	C22	1.3503
C5	C6	1.4434	C22	C23	1.4586
C6	N37	1.3249	C23	C24	1.3643
N37	C9	1.4083	C24	C25	1.4449
C9	C10	1.3595	C25	C26	1.4098
C10	C11	1.4438	C26	C27	1.3996
C11	C12	1.4022	C27	C28	1.4036
C12	C13	1.3949	C28	C29	1.4245
C13	C14	1.4048	C29	C30	1.3748
C14	C46	1.4264	C30	N45	1.4071
C46	C15	1.3713	N45	C33	1.3412
C12	N40	1.4105	C33	C34	1.4384
N40	C18	1.3425	C34	C1	1.3715

Fig. S6 Calculated bond lengths of neutral **2**. *Meso*-substituents and pyrrolic β-protons are omitted for clarity.



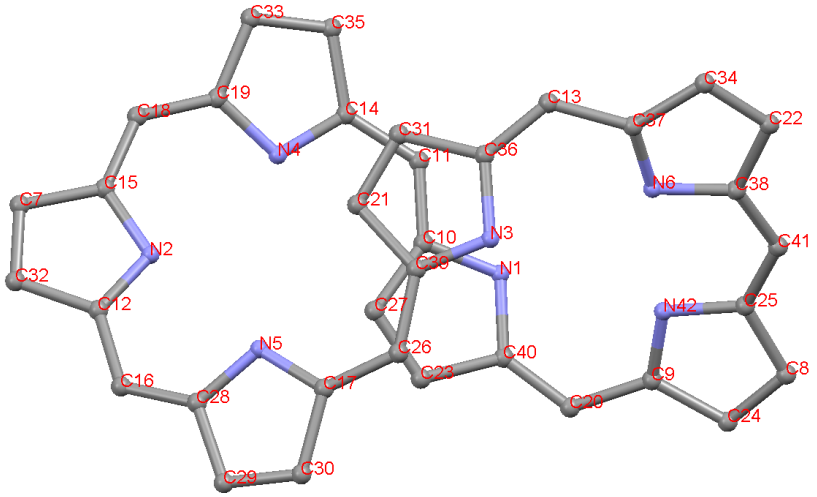
Atom	Atom	Length	Atom	Atom	Length
C1	N35	1.3572	C18	C19	1.4393
N35	C4	1.3793	C19	C20	1.4524
C4	C5	1.3816	C20	N39	1.3306
C5	C6	1.4379	N39	C23	1.4045
C6	N36	1.3410	C23	C24	1.3755
N36	C9	1.4081	C24	C25	1.4294
C9	C10	1.3749	C25	N40	1.3622
C10	C11	1.4305	N40	C28	1.3710
C11	N37	1.3765	C28	C29	1.4165
N37	C14	1.3605	C29	C30	1.3891
C14	C42	1.4527	C30	N41	1.3978
C42	C15	1.3756	N41	C33	1.3370
C15	N38	1.4014	C33	C34	1.4518
N38	C18	1.3379	C34	C1	1.4049

Fig. S7 Calculated bond lengths of deprotonated **2**. *Meso*-substituents and pyrrolic β-protons are omitted for clarity.



Atom	Atom	Length	Atom	Atom	Length
N1	C12	1.4005	C28	C41	1.3731
C12	C13	1.3807	C41	C23	1.4619
C13	C16	1.4431	C23	C33	1.3496
C16	C37	1.4705	C33	C38	1.4582
C37	C35	1.3497	C38	C15	1.3712
C35	C21	1.4627	C15	C39	1.4405
C21	C20	1.3635	C39	N8	1.3444
C20	C17	1.4379	N8	C40	1.4074
C17	C9	1.4053	C40	C43	1.3745
C9	C34	1.3915	C43	C27	1.4240
C34	C14	1.4057	C27	C10	1.4044
C14	C18	1.4320	C10	C26	1.3943
C18	C30	1.3674	C26	C11	1.4024
C30	N7	1.4063	C11	C22	1.4453
N7	C19	1.3333	C22	C42	1.3685
C19	C28	1.4496	C42	N1	1.4193

Fig. S8 Calculated bond lengths of neutral **3**. *Meso*-substituents and pyrrolic β-protons are omitted for clarity.



Atom	Atom	Length	Atom	Atom	Length
N1	C10	1.4062	C26	C39	1.4359
C10	C11	1.3785	C39	N3	1.3310
C11	C14	1.4498	N3	C36	1.4074
C14	N4	1.3434	C36	C13	1.3634
N4	C19	1.3814	C13	C37	1.4572
C19	C18	1.4033	C37	N6	1.3334
C18	C15	1.3981	N6	C38	1.3850
C15	N2	1.3901	C38	C41	1.3996
N2	C12	1.3389	C41	C25	1.4026
C12	C16	1.4542	C25	N42	1.3821
C16	C28	1.3908	N42	C9	1.3330
C28	N5	1.3642	C9	C20	1.4559
N5	C17	1.3630	C20	C40	1.3724
C17	C26	1.3939	C40	N1	1.4110

Fig. S9 Calculated bond lengths of deprotonated **3**. *Meso*-substituents and pyrrolic β-protons are omitted for clarity.

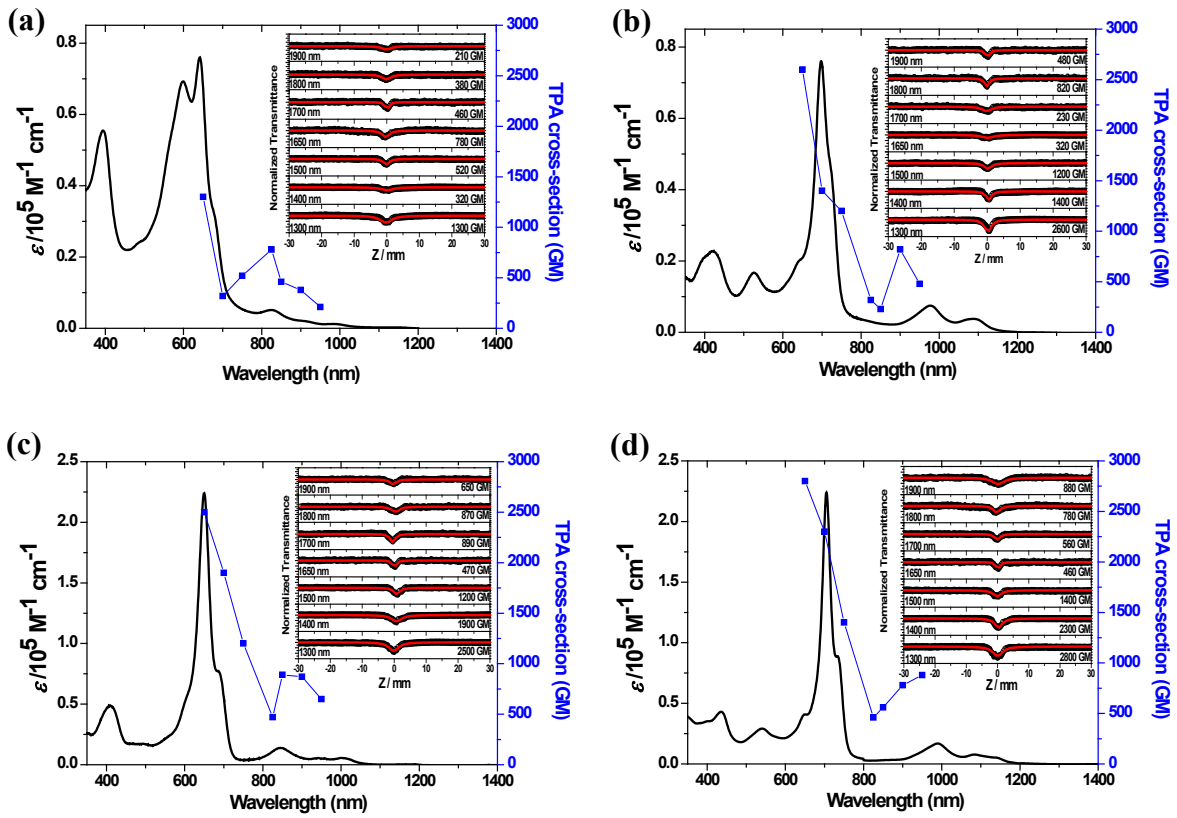


Fig S10. Two-photon absorption spectra (blue) and Z-scan traces (insets) of neutral (a, c) and deprotonated (b, d) of **1** (a, b) and **2** (c, d), respectively. The solid line indicates the steady-state absorption spectrum for comparison, and the solid line in inset is the best curve fit line of experimental data.