

Impact of changing the core in tetrapyrrolic dendrimers designed for oxygen sensitization: New fluorescent phthalocyanines-based dendrimers with high two-photon absorption cross-sections

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1. NMR spectra of compounds **11**, **12** and dendron precursor **8c** in CDCl₃

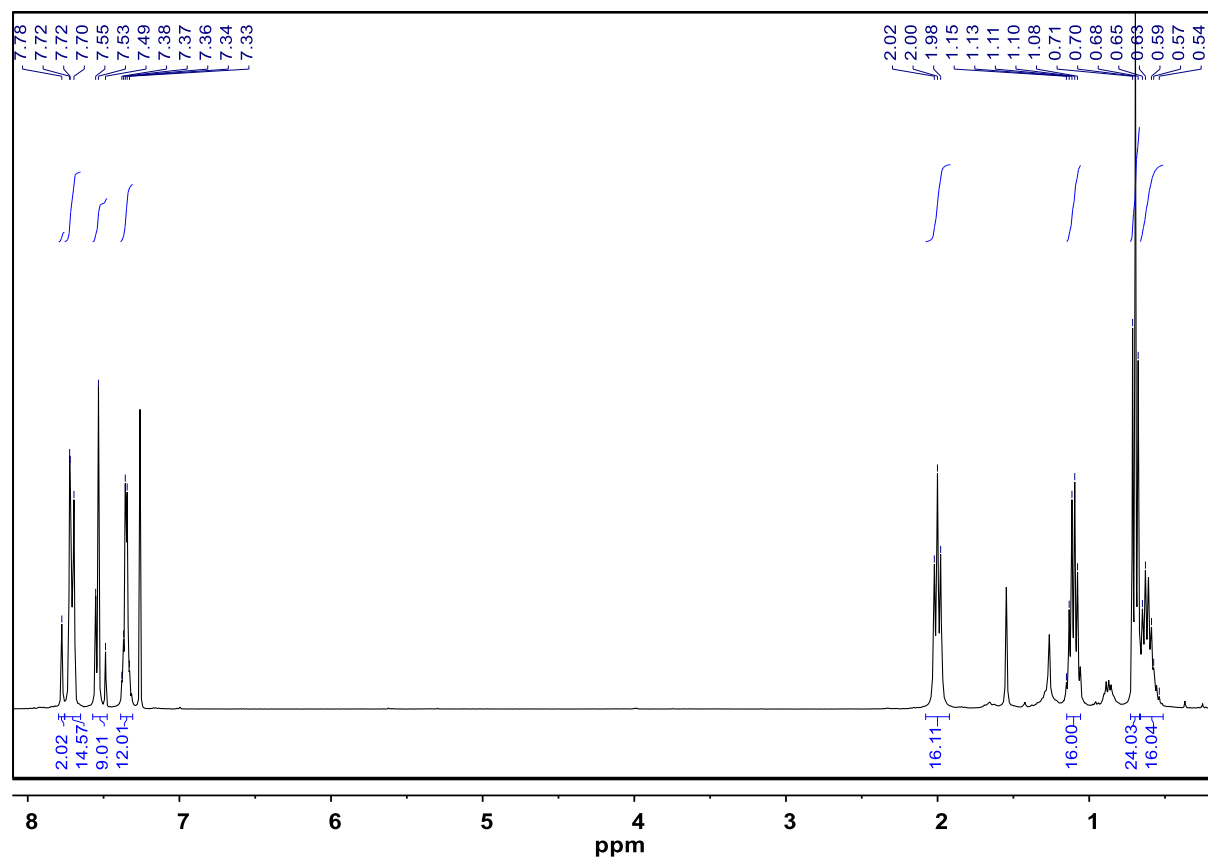
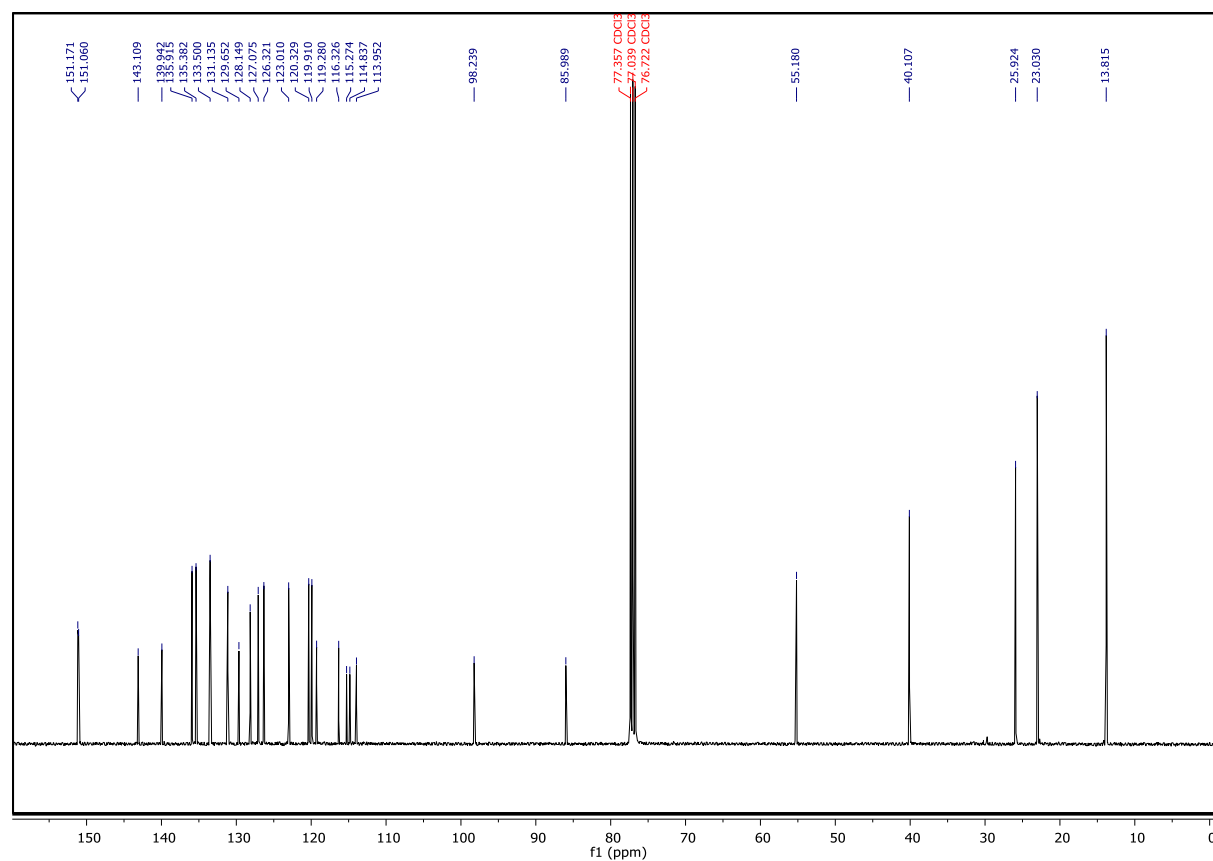
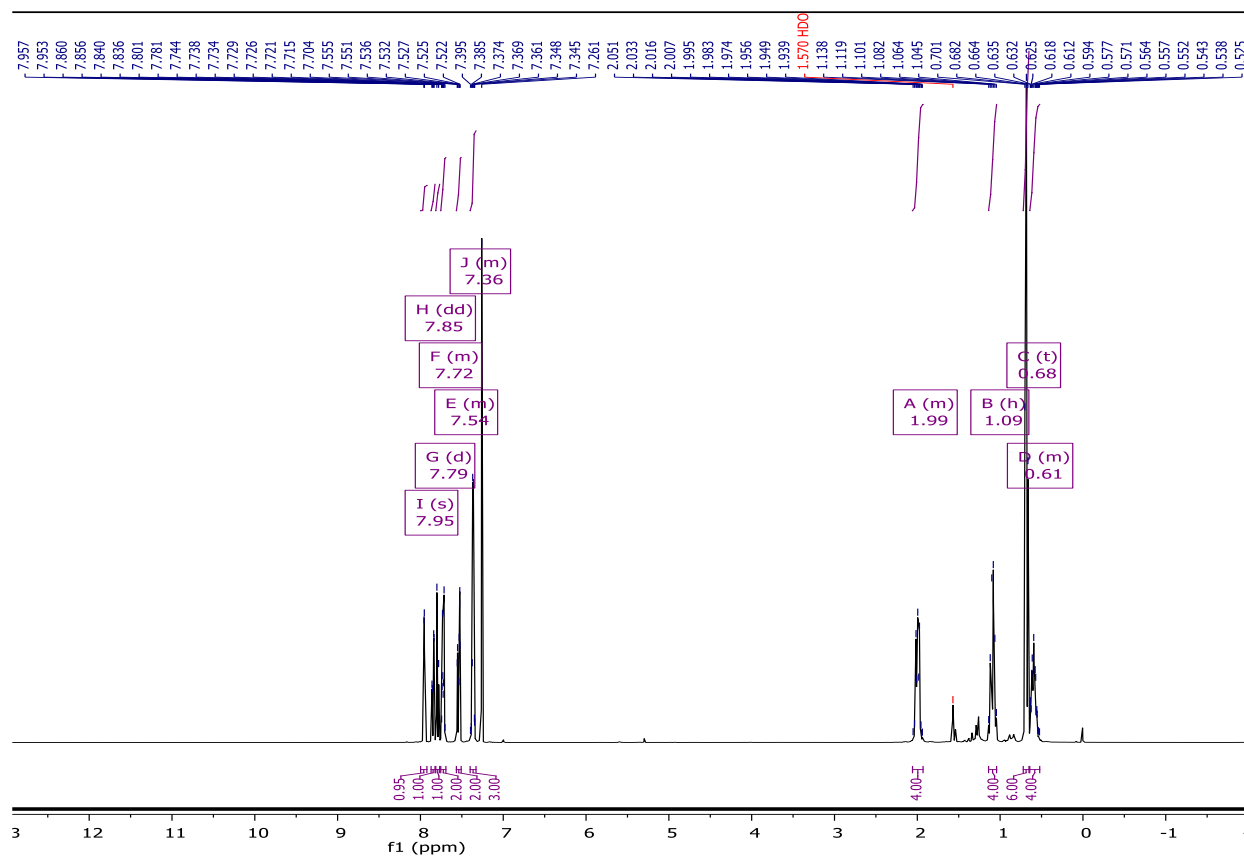


Figure S1: ¹H NMR Spectrum (400 Mz) of compound **11** in CDCl₃.

Supporting information



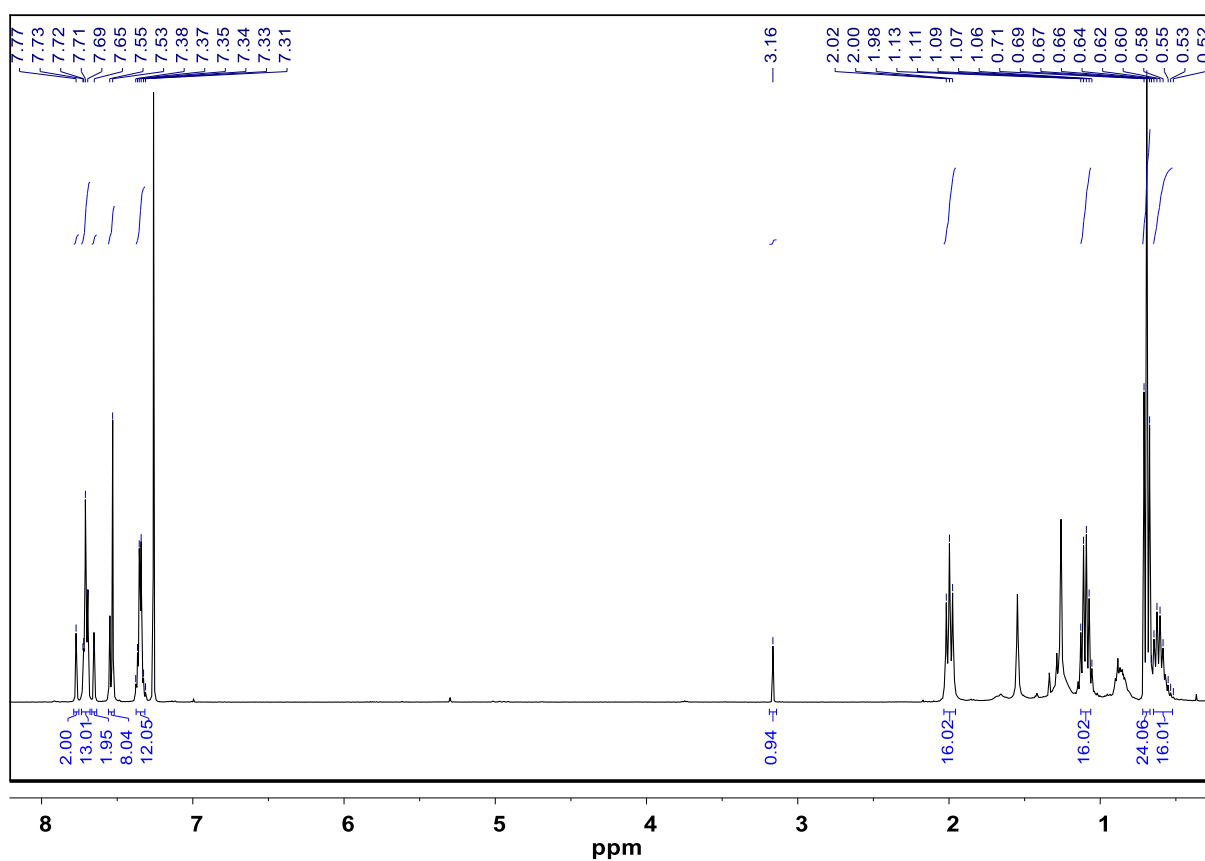


Figure S4: ¹H NMR Spectrum (400 Mz) of compound **8c** in CDCl₃.

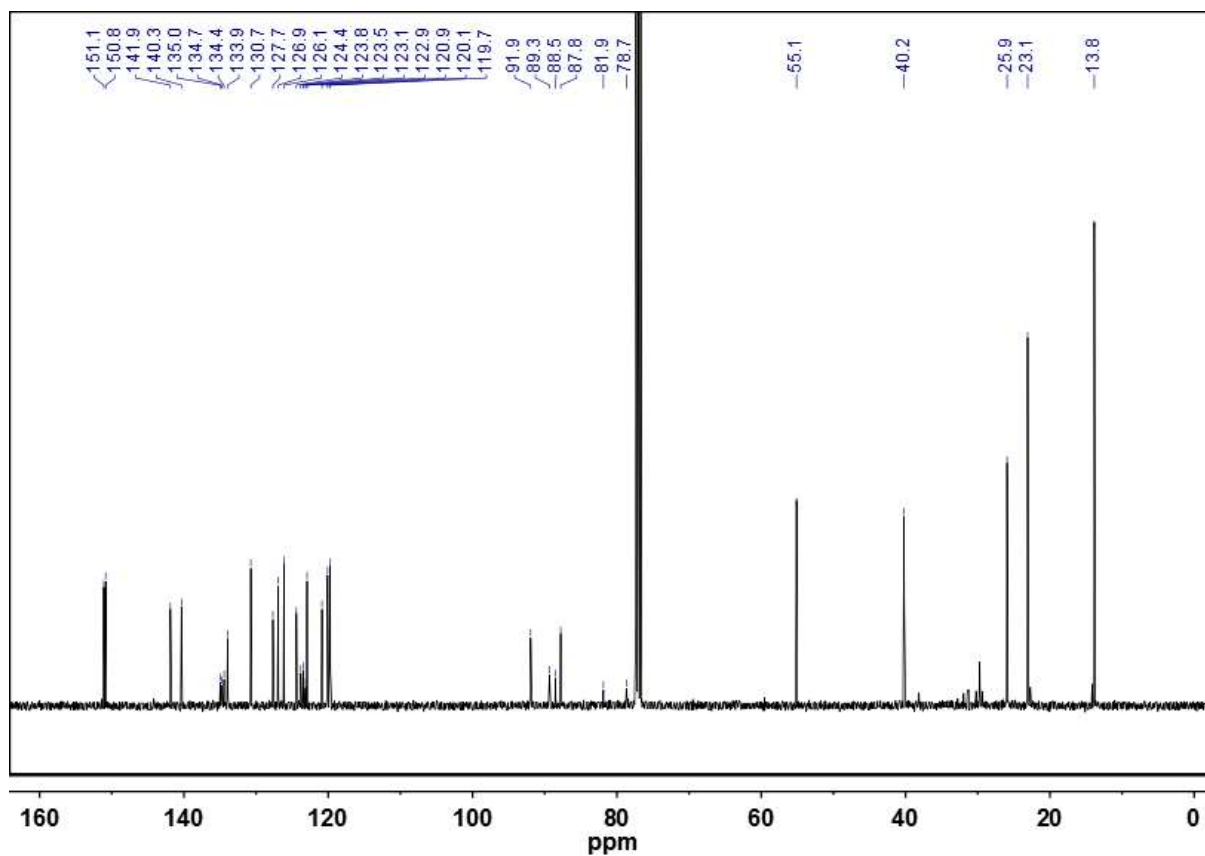


Figure S5: ¹³C{¹H} NMR Spectrum (101 MHz) of compound **8c** in CDCl₃.

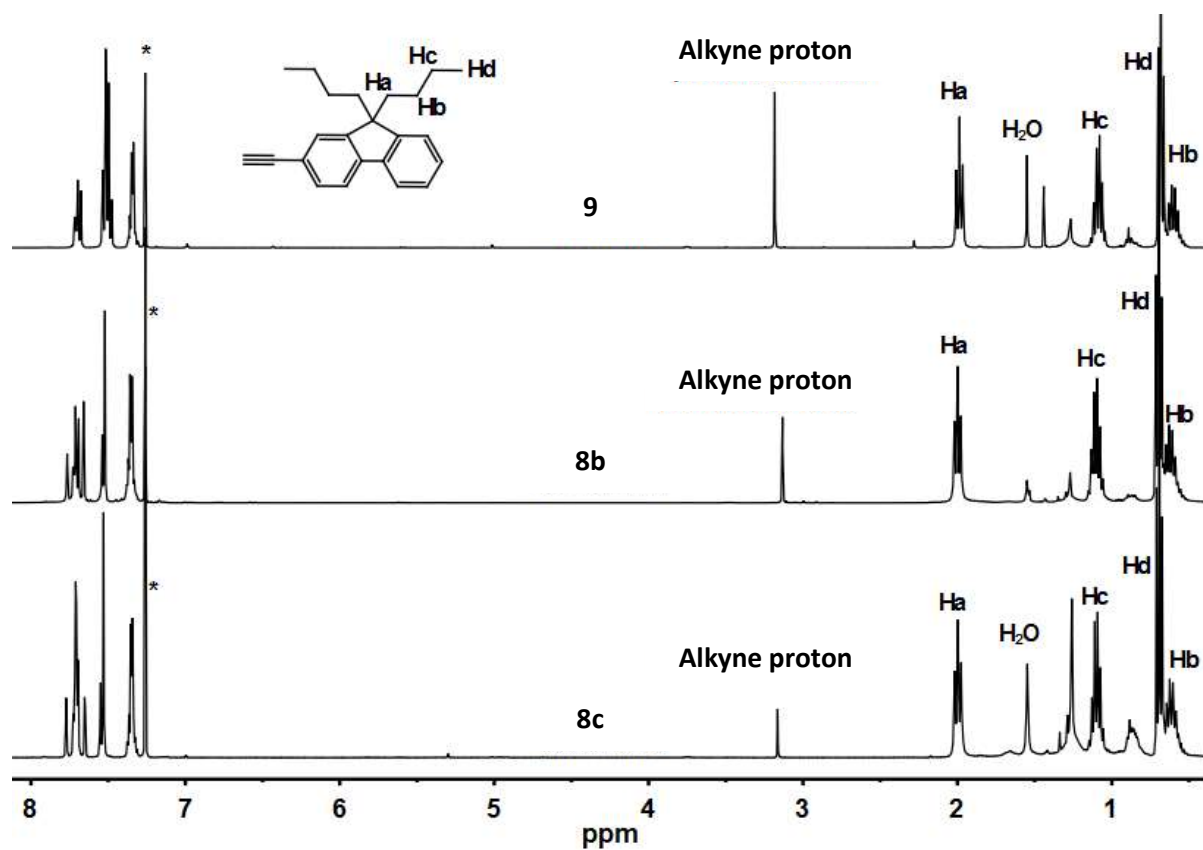
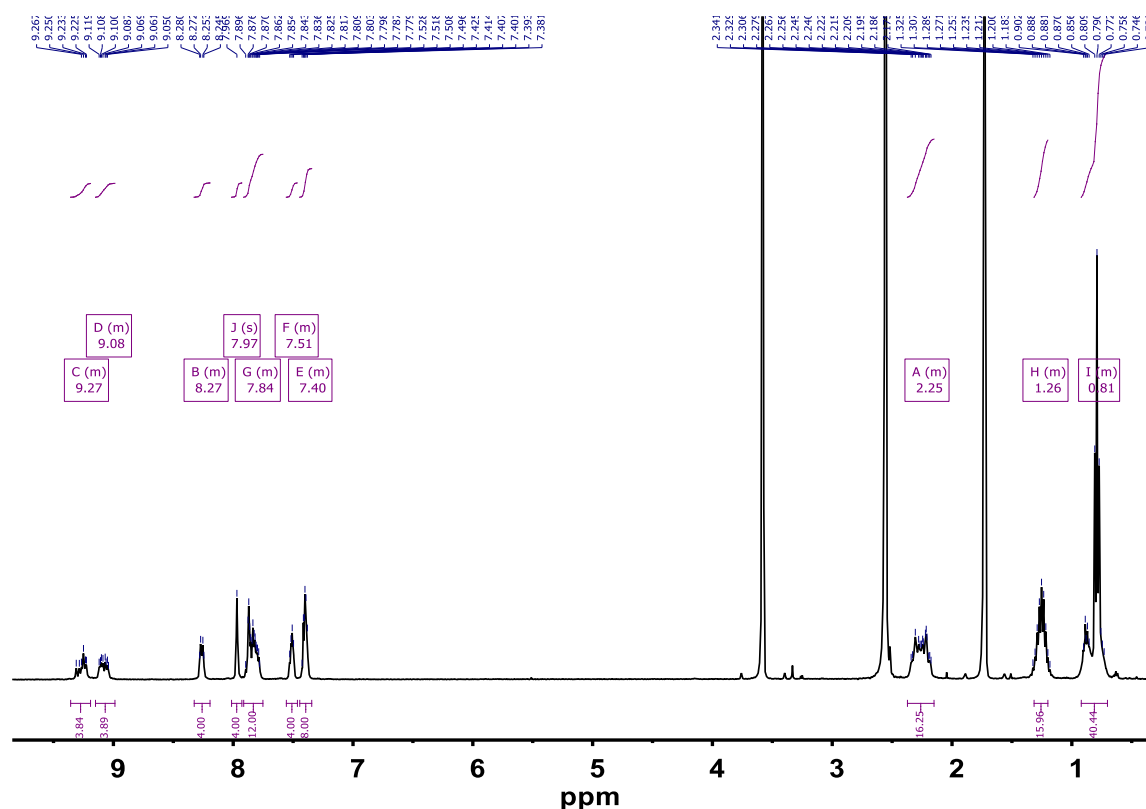
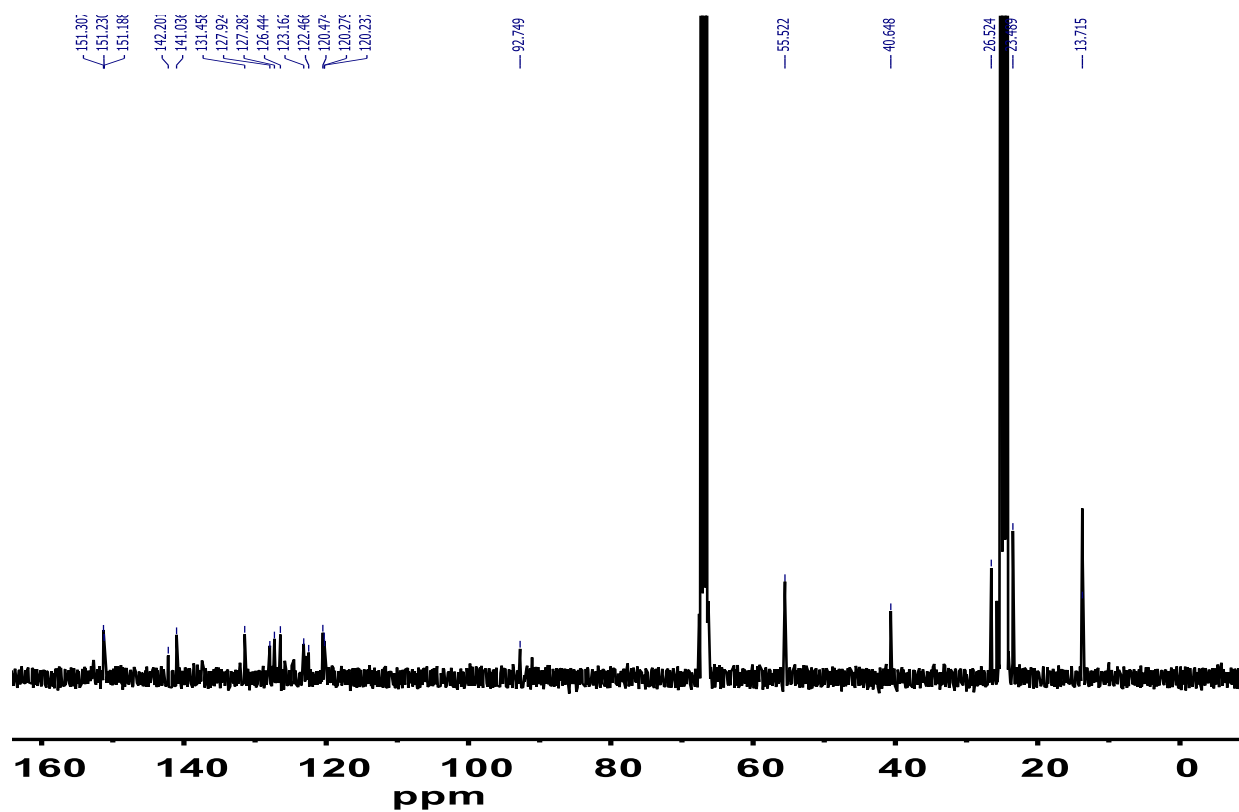


Figure S6: Comparative ^1H NMR Spectra of **8b-c** and **9** in CDCl_3 .

2. NMR spectra of phthalocyanines 6a-c and 7 in THF- d_8 Figure S7: ¹H NMR Spectrum (400 Mz) of compound 6a in THF- d_8 .Figure S8: ¹³C{¹H} NMR Spectrum (101 Mz) of compound 6a in THF- d_8 .

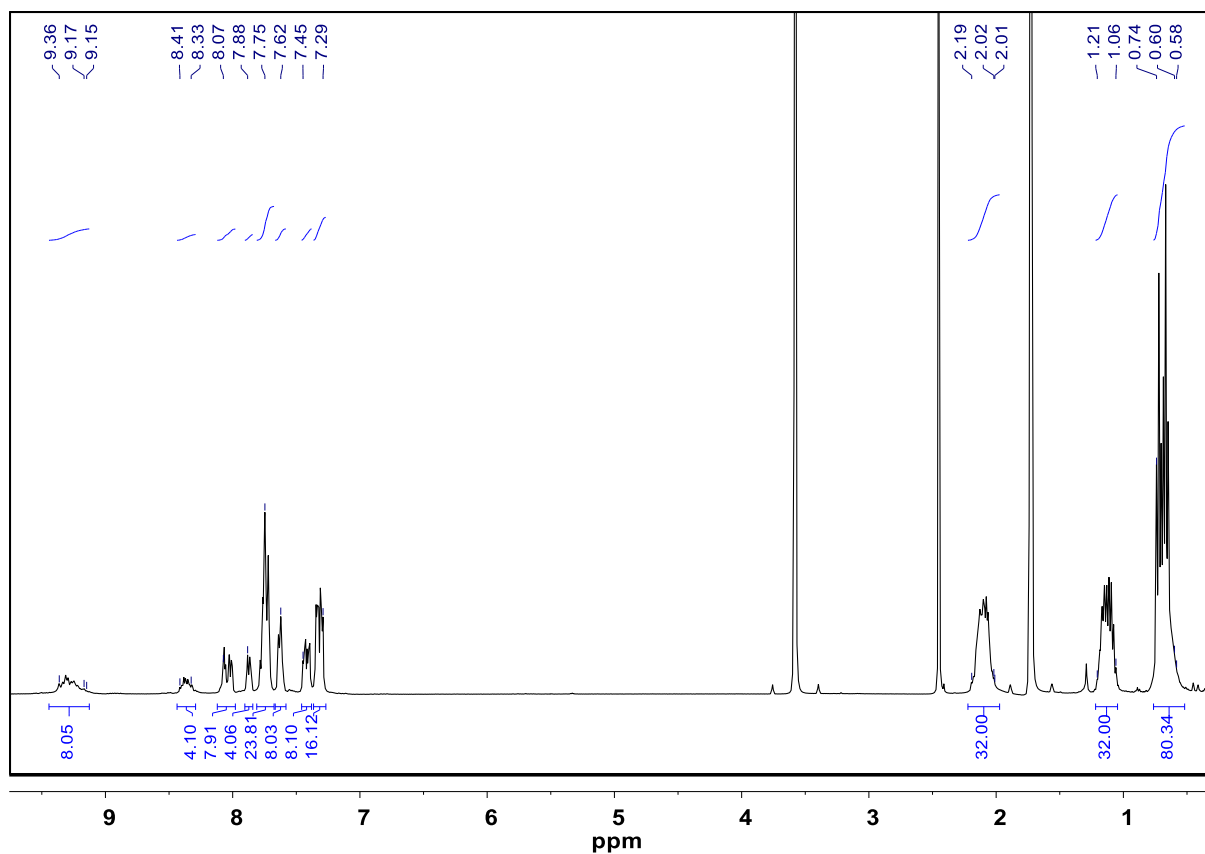


Figure S9: ¹H NMR Spectrum (400 Mz) of compound **6b** in THF-*d*₈.

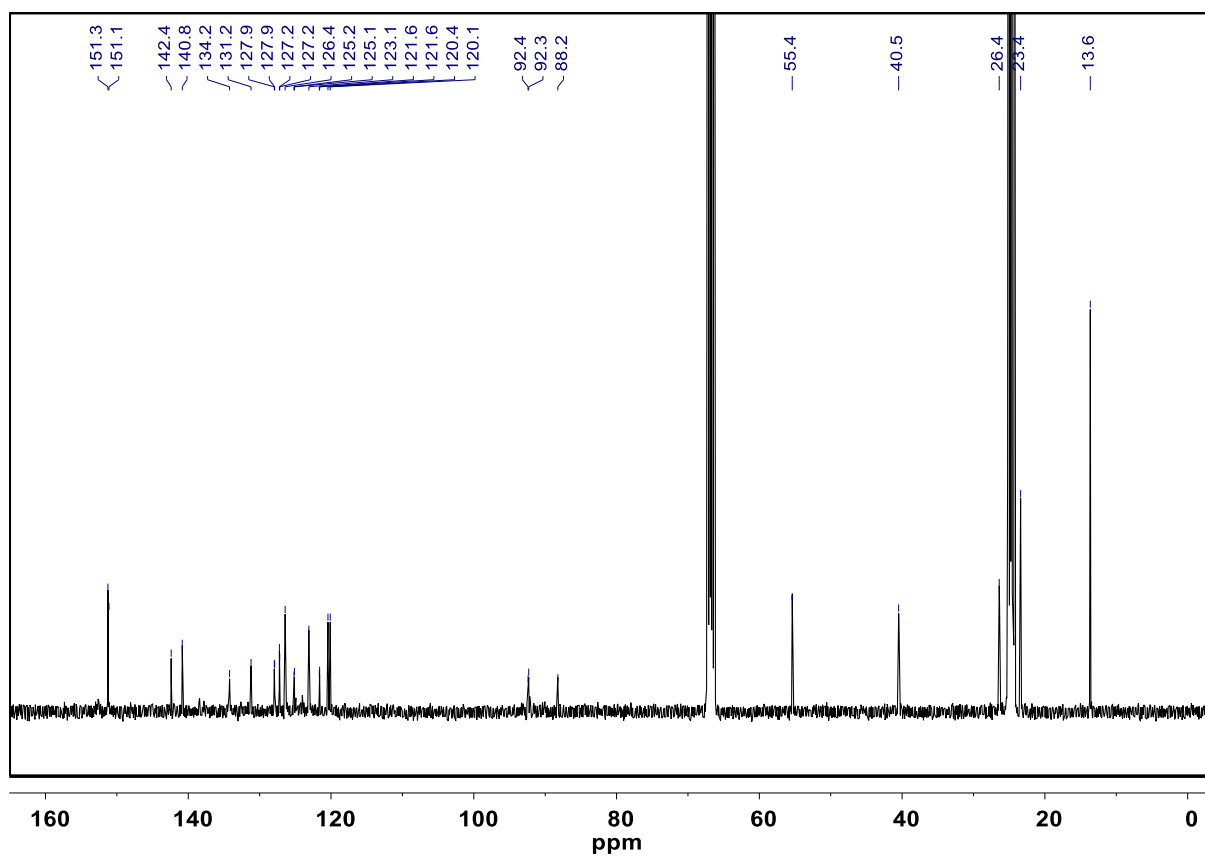


Figure S10: ¹³C{¹H} NMR Spectrum (101 MHz) of compound **6b** in THF-*d*₈.

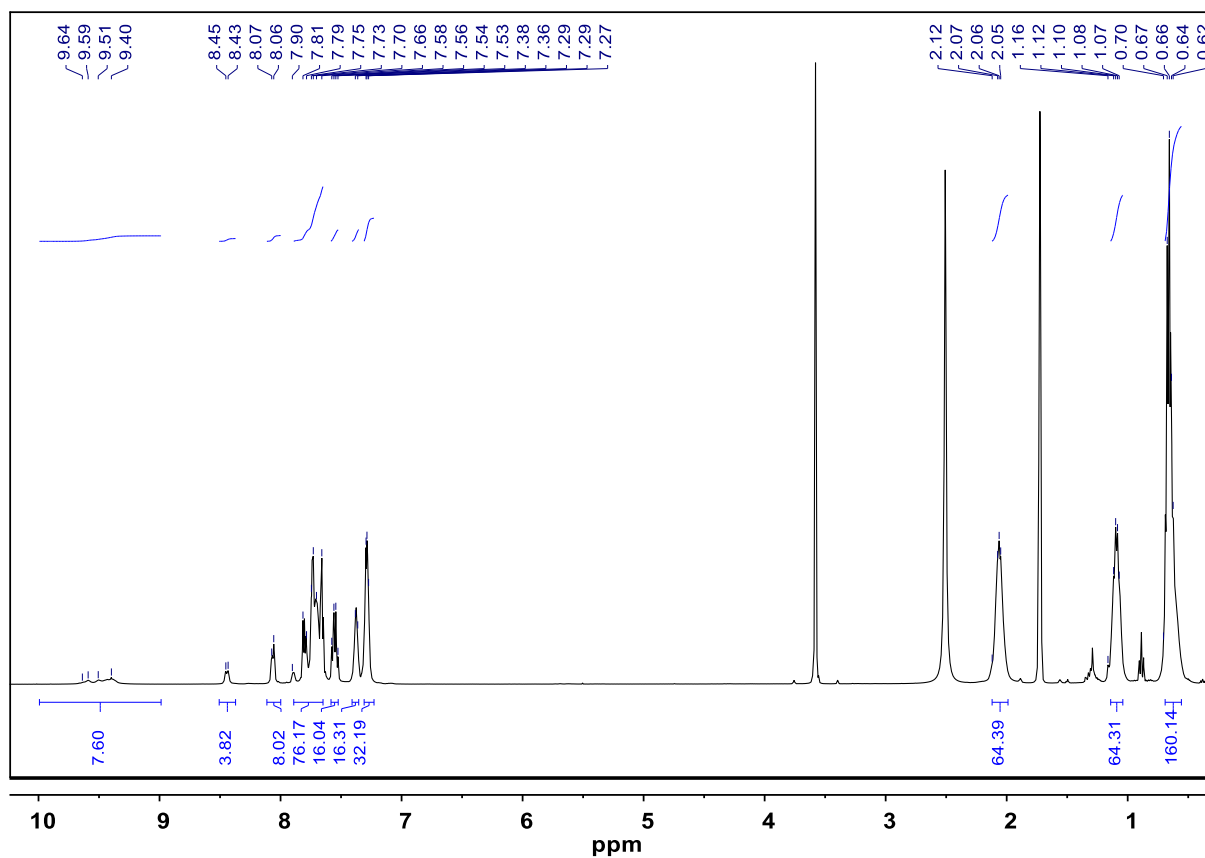


Figure S11: ¹H NMR Spectrum (400 Mz) of compound **6c** in THF-*d*₈.

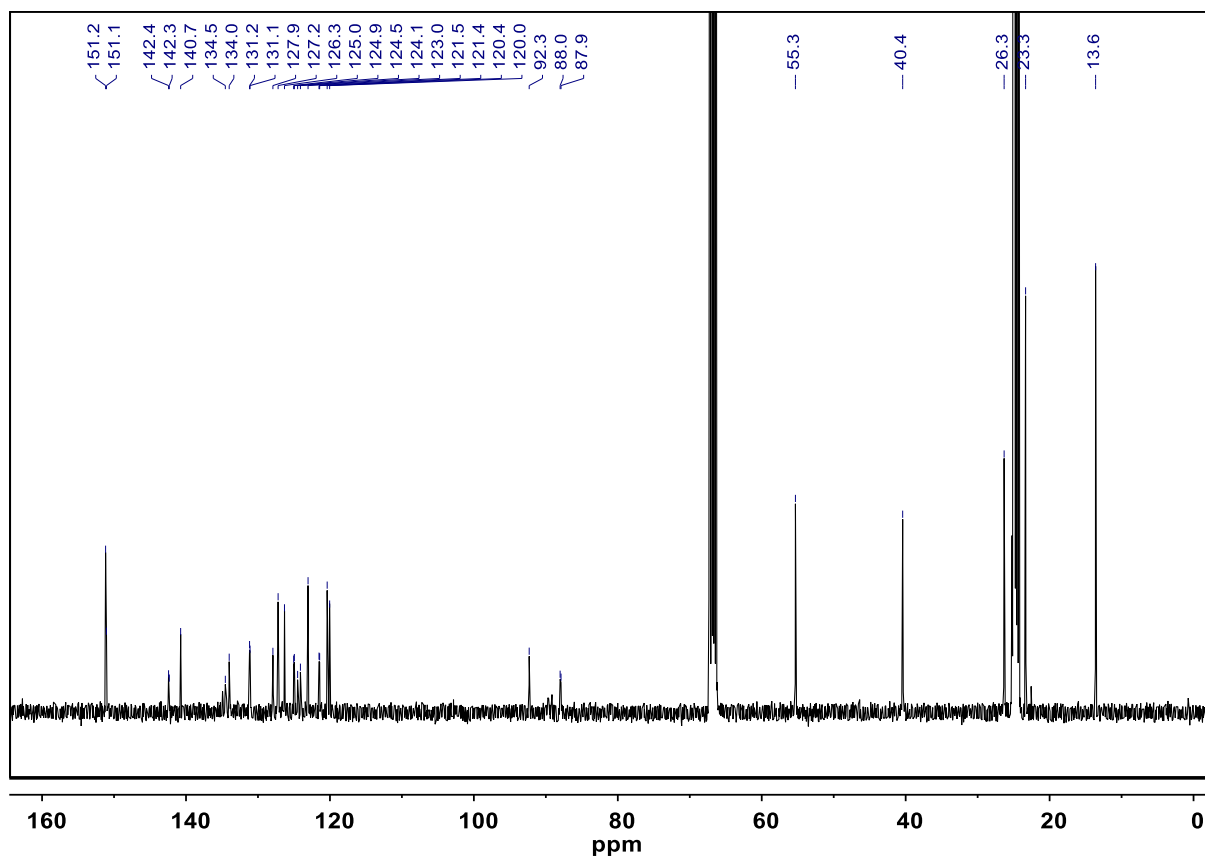


Figure S12: ¹³C{¹H} NMR Spectrum (101 MHz) of compound **6c** in THF-*d*₈.

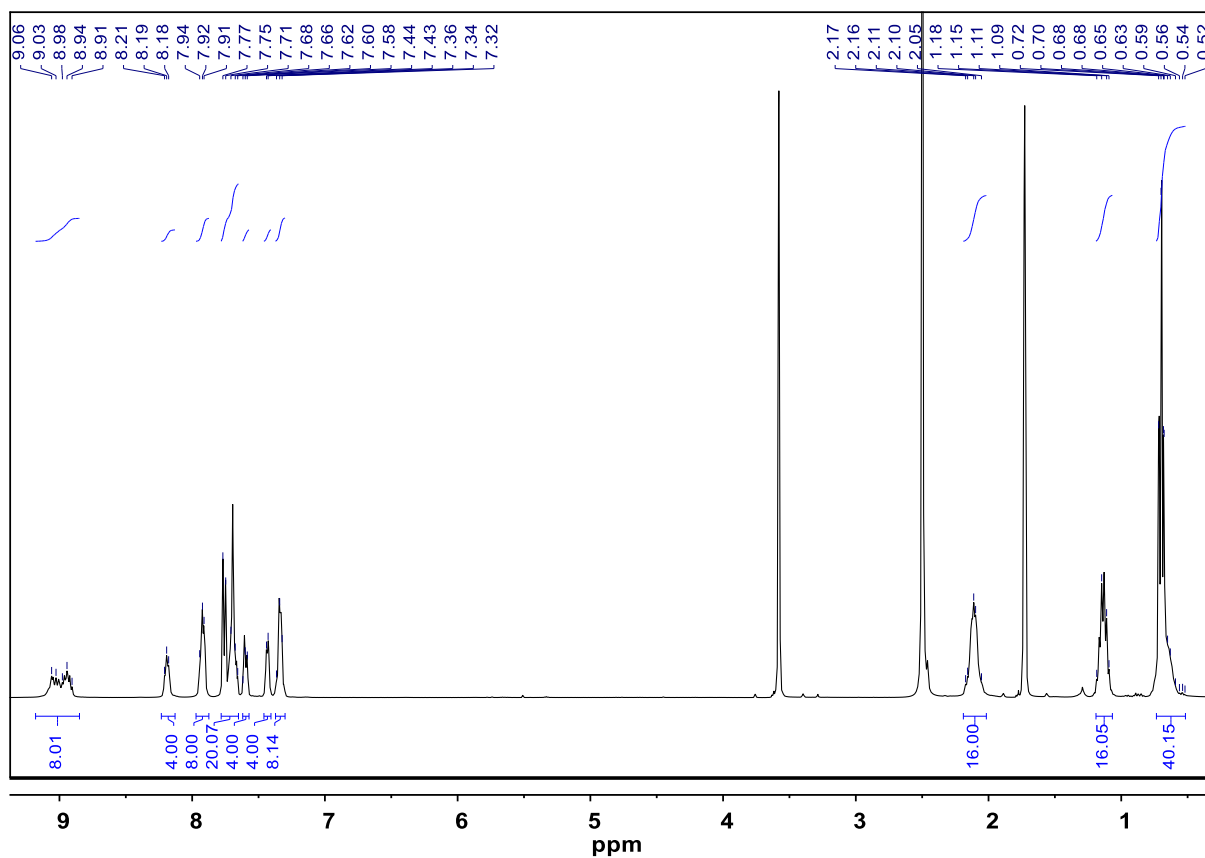


Figure S13: ¹H NMR Spectrum (400 Mz) of compound **7** in THF-*d*₈.

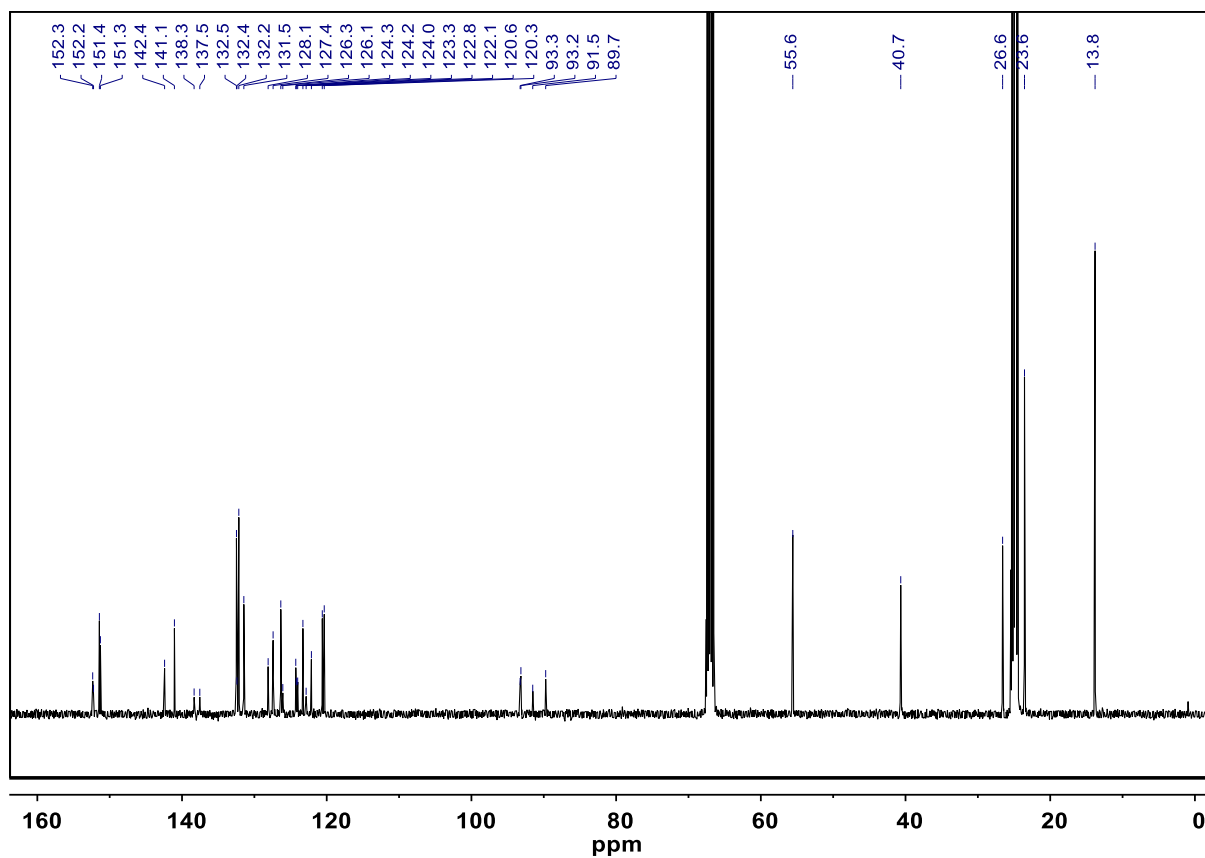


Figure S14: ¹³C{¹H} NMR Spectrum (101 MHz) of compound **7** in THF-*d*₈.

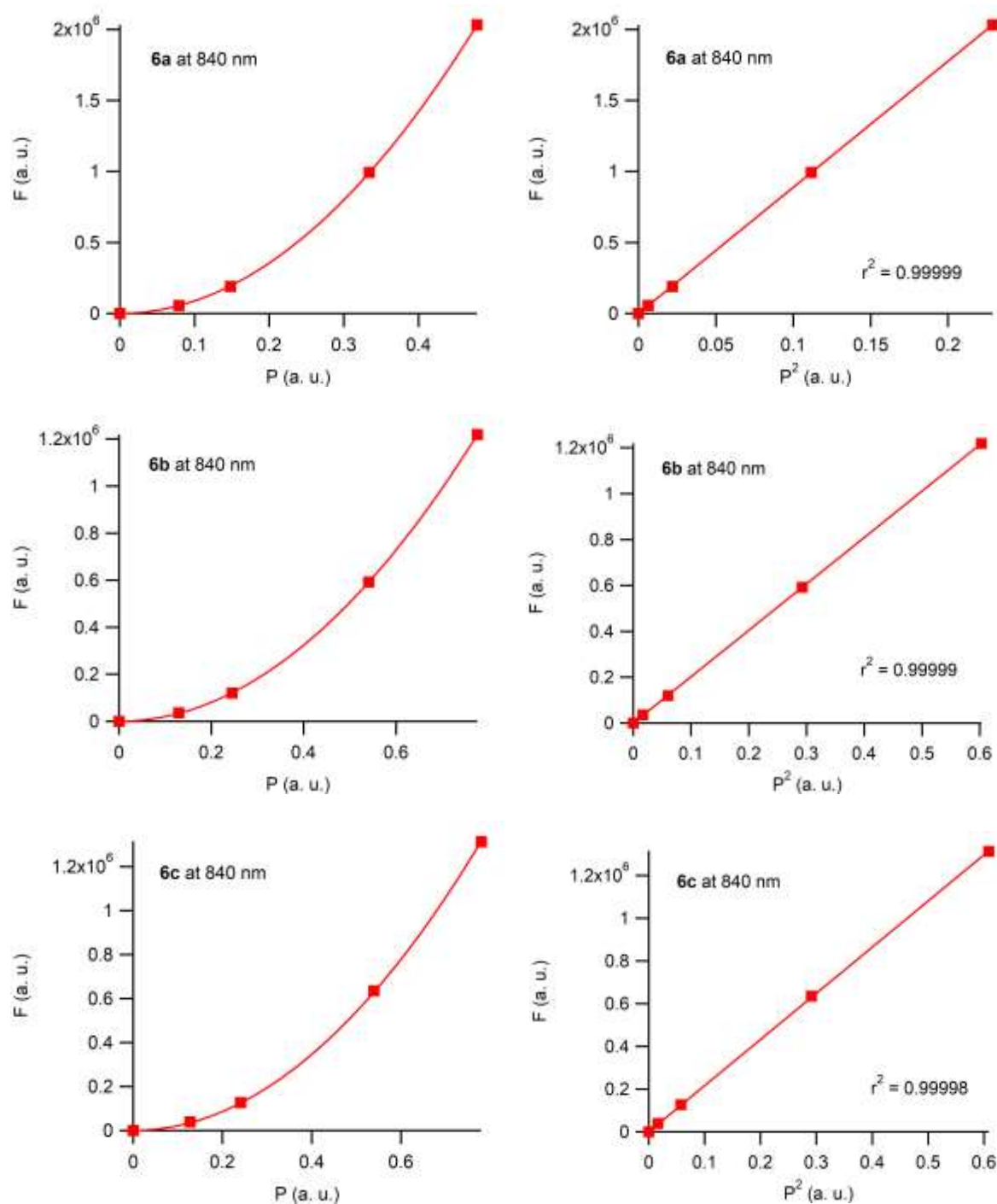
3. Complementary TPEF data on ZnI₄Pc, 6a-c and 7

Figure S15: Left: quadratic dependence of the emission intensity (F) on laser excitation power (P) for compound **6a-c** at $(\lambda_{2PA})^{lim}$ (840 nm). Right: dependence of F on P².

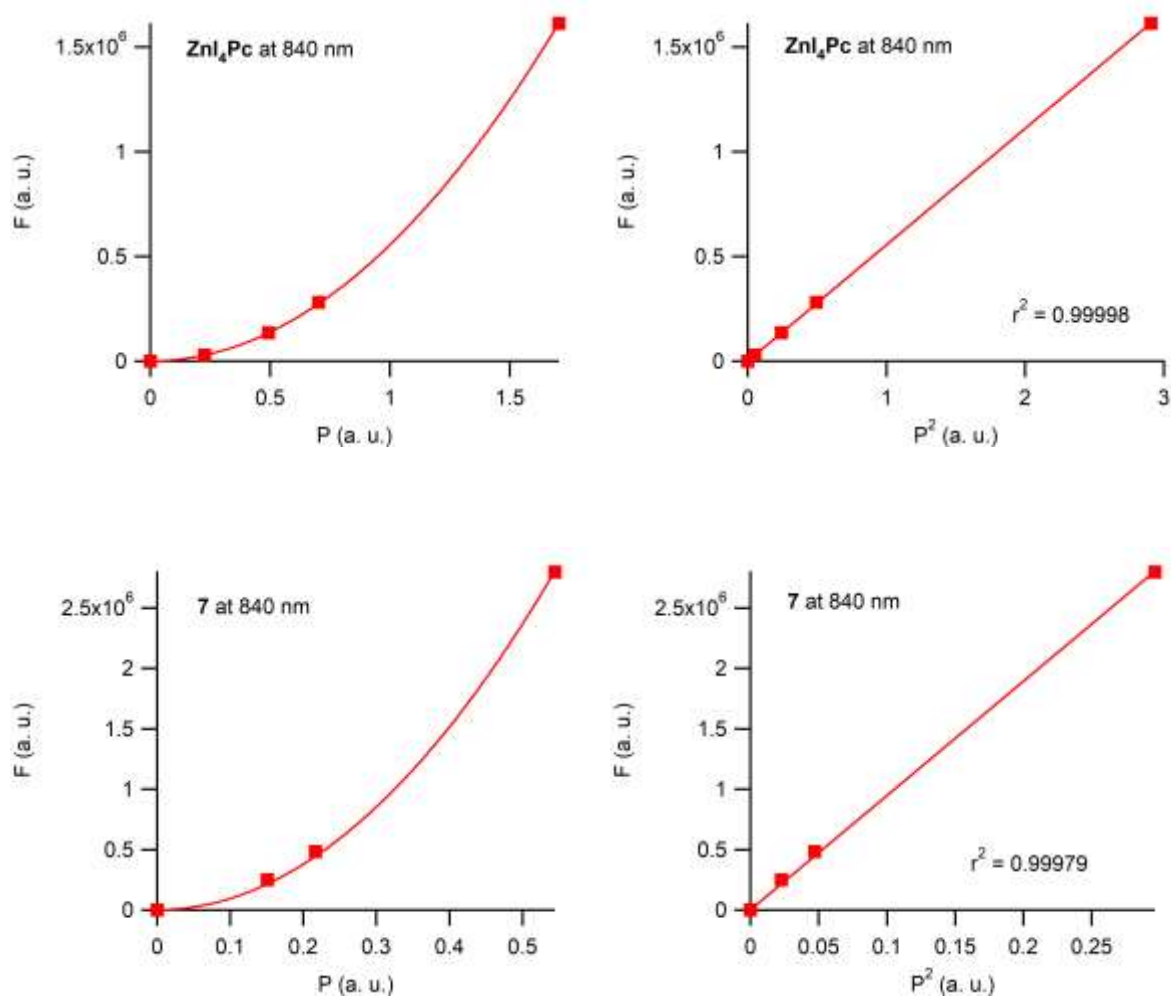


Figure S16: Left: quadratic dependence of the emission intensity (F) on laser excitation power (P) for compound **ZnI₄Pc** and **7** at $(\lambda_{2PA})^{lim}$ (840 nm). Right: dependence of F on P².

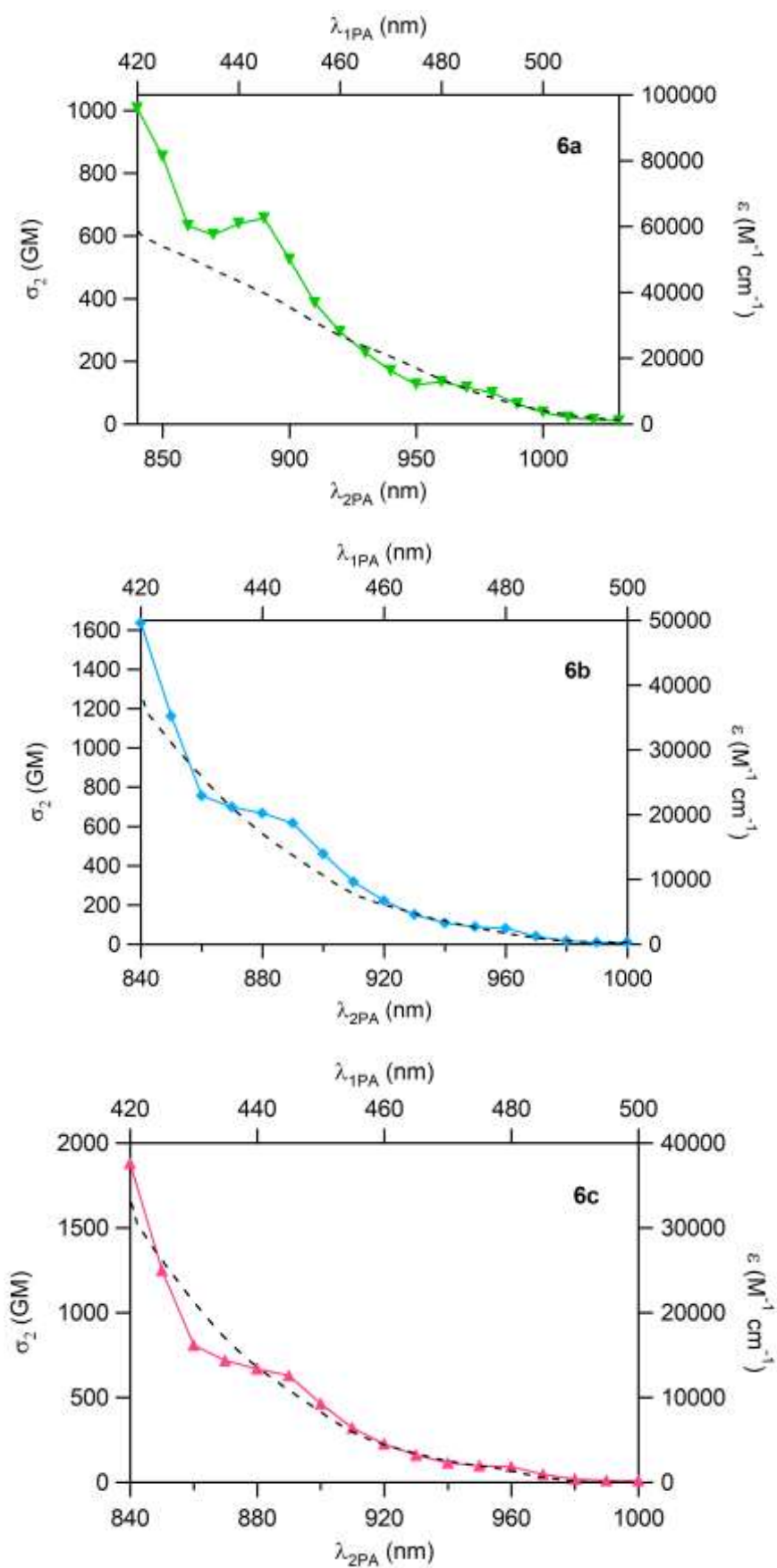


Figure S17: Overlay of one- (dotted line) and two-photon (plain line) absorption spectra for **6a-c** in THF (25 °C).

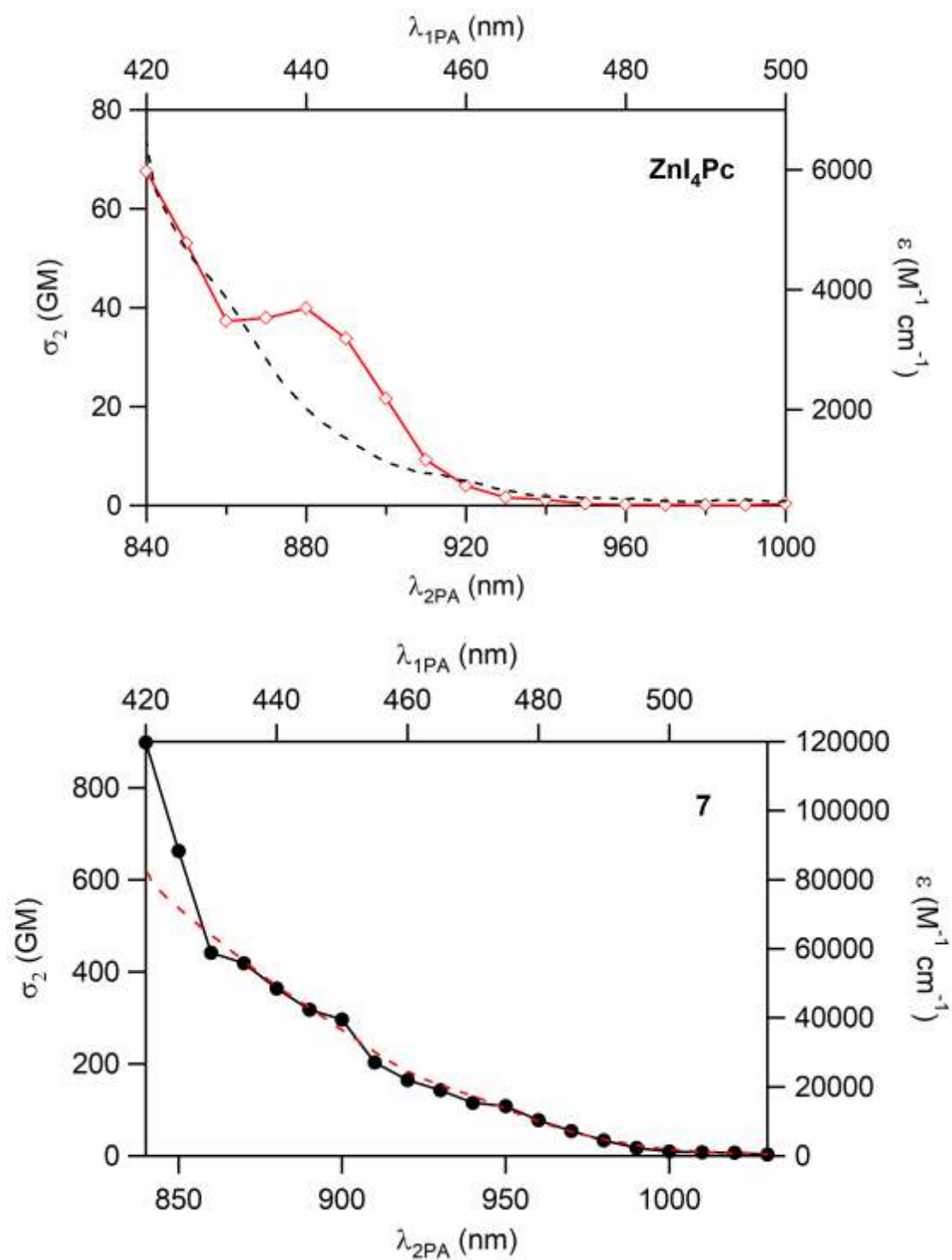


Figure S18: Overlay of one- (dotted line) and two-photon (plain line) absorption spectra for **ZnI₄Pc** and **7** in THF (25 °C).

4. Figures of merit involving effective number of electrons for 6a-c and 7

Table S1. Effective numbers (N_{eff}) of electrons for selected tetrapyrrolic derivatives mentioned in this work and associated figures of merit regarding 2PA properties.

Cpnd	σ_2^{lim} (GM)	σ_2^{max} (GM)	N_{eff}^a	n_{Flu}^b	$\sigma_2^{\text{lim}}/N_{\text{eff}}^2$ (GM)	$\sigma_2^{\text{max}}/N_{\text{eff}}^2$ (GM)	$(\sigma_2^{\text{lim}} \cdot \Phi_F)/N_{\text{eff}}^2$ (GM)	$(\sigma_2^{\text{lim}} \cdot \Phi_A)/N_{\text{eff}}^2$ (GM)
ZnPc	200	150	27.3	0	0.267	0.201	0.070	0.163
ZnI ₄ Pc	90	40	27.3	0	0.120	0.053	0.013	-
2a	380	-	45.6	4	0.183	-	0.037	0.128
2b	200	-	48.0	8	0.087	-	0.010	0.051
2c	290	-	65.0	16	0.069	-	0.009	0.038
3b	330	160	36.4	4	0.249	0.121	0.082	0.142
4	160	140	36.4	4	0.121	0.106	0.028	0.073
5	510	240	48.6	4	0.216	0.102	0.080	0.116
6a	1010	630	39.3	4	0.652	0.407	0.189	0.391
6b	1640	670	52.1	8	0.604	0.247	0.193	0.308
6c	1880	670	69.0	16	0.395	0.141	0.142	0.209
7	900	420	52.1	4	0.331	0.155	0.099	-

Unless specified, the headings of each column are similar to those in Table 2. ^a Effective number of electrons (computed considering disconnected peripheral arms). ^b Total number of fluorene units in the molecule.

5. Complementary DFT data on 6a-d and 7

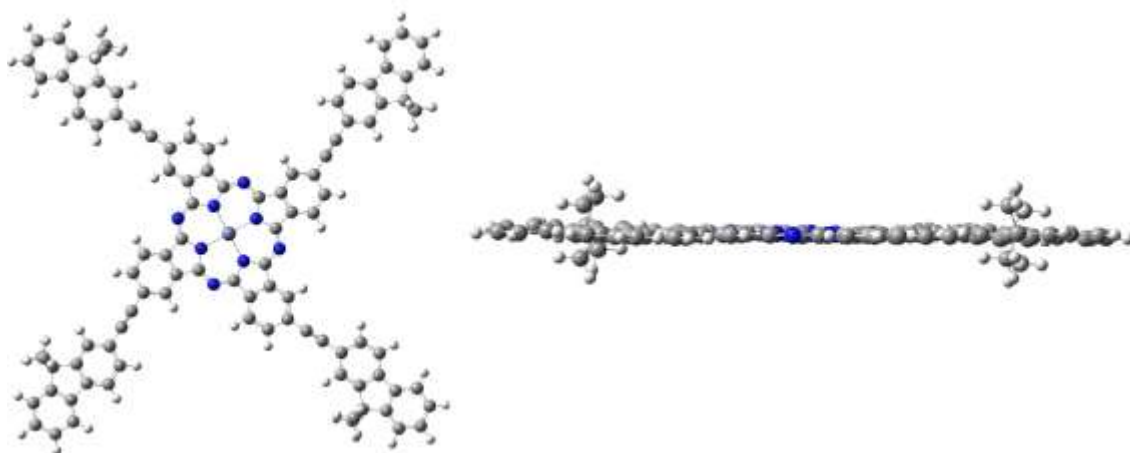


Figure S19. Optimized geometry for **6a'** (view from above and side view)

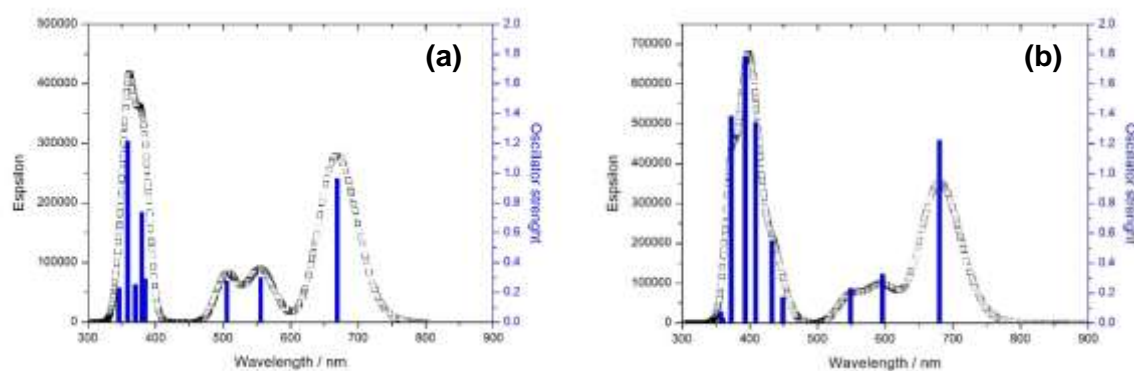


Figure S20. UV-visible absorption spectrum simulated from the vertical excitation calculated by TD-DFT (40 states) for **6a'** (a) and **7'** (b).

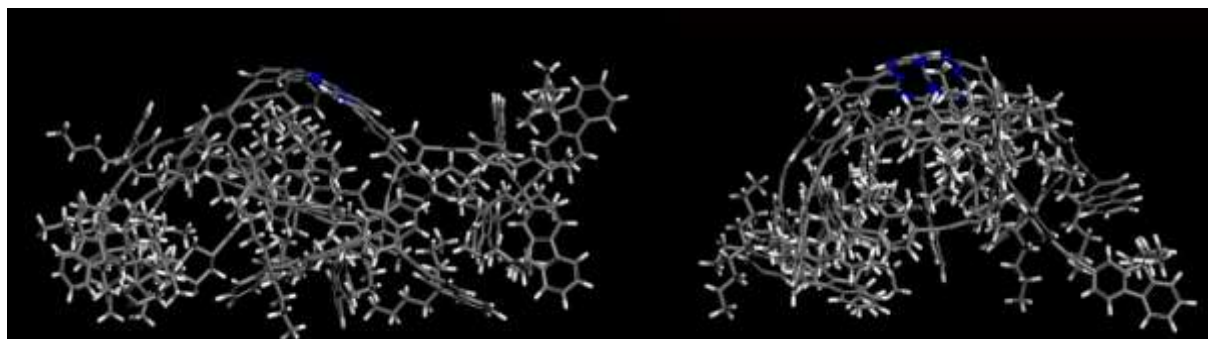
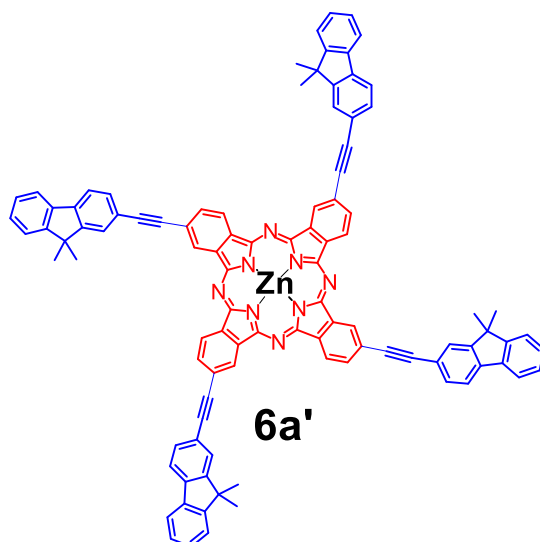


Figure S21. Two views of the molecular configuration of **6c** observed after energy relaxation and 4 ns simulation in NVT ensemble (fixed Number of molecules, Volume and Temperature) in a unit cell of $a = 75 \text{ \AA}$, $b = 75 \text{ \AA}$, $c = 75 \text{ \AA}$, $\alpha = \beta = \gamma = 90^\circ$ in vacuo.

Table S2. Cartesian coordinates of **6a'** after geometrical optimization.

Atom	x	y	z
C	6.12381481	6.75775249	-1.11987825
C	5.60557275	5.65426790	-0.96786053
C	-3.86944896	-1.82897791	0.39312340
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N	-1.65971750	-1.15346224	0.20047302
C	-2.97236486	-0.68546403	0.21377949
C	-1.87164105	3.84978356	0.36172073
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C	3.02856201	2.98756794	-0.53031714
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N	1.63827610	1.15158749	-0.24635215
C	2.95079850	0.68328994	-0.26198540
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C	1.85074251	-3.85016306	0.32866887
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N	1.15851946	-1.64834304	0.10692404
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Supporting information

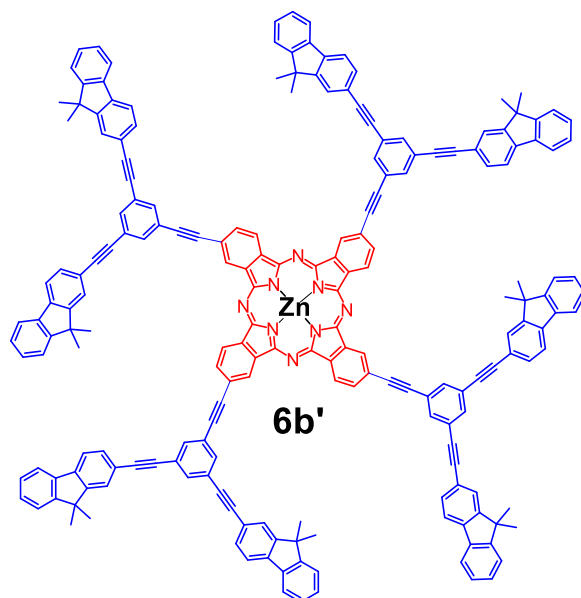
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C	-9.30675035	5.93297974	-0.27282535
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Supporting information

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Supporting information

H	12.22926268	11.91048709	-1.83292264
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H	-12.08734655	12.20737765	-0.43720070
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H	-4.87307654	-9.09624337	1.39747651
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H	-9.34713308	-15.08547021	2.23094230
H	-11.71113708	-14.32112987	2.13478577
H	-12.25186246	-11.90797091	1.80778800
H	-12.00954453	-9.41447750	2.76013475
H	-10.47334535	-9.31910780	3.65013107
H	-10.95726562	-7.99827477	2.56229667
H	-12.00962205	-9.76660453	0.20594297
H	-10.95386269	-8.35267594	0.00887144
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H	9.59636630	-12.17724746	-0.00265592
Zn	-0.01074676	-0.00102108	-0.02394208

Table S2. Cartesian coordinates of **6b'** after geometrical optimization.

Atom	x	y	z
C	4.35840196	7.76992018	3.14658871
C	3.60355794	8.85766646	2.64855078
C	5.51203797	8.02229582	3.92553347
C	3.95661361	6.42305317	2.86638691
C	5.91295509	9.34898636	4.21042908
C	3.99311748	10.19029135	2.92206946
C	5.14829832	10.42678913	3.70428853
C	3.22641811	11.28717689	2.41097088
C	7.07870674	9.59954698	5.00459734
C	2.56564185	12.22158823	1.96683835
C	1.80113097	13.31637727	1.45026612
C	0.66739413	13.07100799	0.62768813
C	2.16684160	14.65868648	1.75207076
C	1.41021082	15.70985173	1.23694110
C	0.27960794	15.45334598	0.41542905
C	-0.31541622	16.74143357	0.02179117
C	0.45088912	17.78615075	0.60262843
C	-0.09248603	14.13181316	0.11062878
C	1.61677037	17.22027013	1.42723934
C	-1.43519762	17.03013087	-0.77815437
C	0.10048880	19.12330281	0.38551941
C	-1.78476618	18.37760443	-0.99449216
C	-1.02368191	19.41701745	-0.41765435
C	8.07432156	9.82287433	5.68723120
C	9.23460714	10.07713590	6.48663699
C	9.64760431	11.41388309	6.74126856
C	9.98449908	8.99869119	7.03538364

Supporting information

C	11.10954288	9.26888909	7.81272147
C	11.51318722	10.60850447	8.06091560
C	12.72029477	10.58582859	8.90377928
C	13.05488841	9.23239957	9.17257613
C	10.78120215	11.68259432	7.52411105
C	12.05851115	8.27562160	8.50068290
C	13.49989081	11.63571170	9.42053187
C	14.17014941	8.92382573	9.95933676
C	14.62210684	11.32111043	10.21192915
C	14.95562625	9.97596546	10.48004077
C	3.61294136	5.26910357	2.62883253
C	3.21027144	3.92309818	2.35562988
C	4.09831865	2.84217358	2.65674555
C	1.93665087	3.65468629	1.79189679
C	1.58819349	2.32298306	1.54873308
C	2.47907562	1.25466023	1.85042311
C	0.36967303	1.71540808	0.99429770
C	1.79875280	0.01248853	1.47595924
C	3.74295607	1.50963477	2.40720200
C	13.45821238	0.48084724	3.11077098
C	12.59057649	0.79479571	5.48199684
C	-1.83727710	1.86765931	0.08916062
C	-3.00765827	2.63749112	-0.33978534
C	13.53449916	-15.00489757	4.58930278
C	-3.97568391	1.69989434	-0.79779053
C	-3.37901424	0.36510100	-0.64539904
C	-3.27863792	4.01542025	-0.35874354
C	-5.22285785	2.11248667	-1.27517652
C	-5.50749911	3.50188214	-1.29667727
C	-4.52642861	4.43714109	-0.83805774
C	-6.77245451	3.97355926	-1.77174861
C	12.77571730	-14.78489906	7.00797612
C	1.71602930	-2.36790628	1.27681517
C	2.31269543	-3.70269960	1.42921759
C	-14.42956316	-9.35859935	-6.83529468
C	1.34467228	-4.64029564	0.97120510
C	0.17429504	-3.87046324	0.54224946
C	3.55985992	-4.11529545	1.90662728
C	3.84449416	-5.50469241	1.92813932
C	1.61564844	-6.01822543	0.99016730
C	2.86342928	-6.43994906	1.46950216
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C	-7.85995810	4.37368205	-2.17602153
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Supporting information

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C	-12.48094059	3.43416923	-3.64880827
C	-11.03005337	9.29215188	-3.65313258
C	-11.26471575	10.69055176	-3.85151658
C	-10.22752633	11.63256961	-3.60915833
C	-12.53689394	11.15181784	-4.29362084
C	-12.74581995	12.51688575	-4.48245010
C	-11.70223219	13.44974449	-4.23773571
C	-12.20829318	14.80356600	-4.51973542
C	-13.56135559	14.69903529	-4.93705522
C	-10.44120117	13.00673449	-3.80019885
C	-14.02200481	13.23377254	-4.94894807
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C	-15.68779473	2.16551006	-4.65710641
C	-14.25721711	0.31844454	-3.89887006
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C	-16.53831216	-0.10322101	-4.67263380
C	-17.43716449	-1.25612951	-4.84905118
C	-16.74718260	-2.42917672	-4.44437708
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C	-18.76012698	-1.32659468	-5.32029282
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C	10.81785964	-5.43737365	4.28072072
C	9.36670565	-11.29527266	4.28441905
C	9.60134951	-12.69369128	4.48269288
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Supporting information

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C	12.35859873	-15.23701985	5.57997597
C	9.91375343	-18.06037071	5.06458191
C	12.62470752	-17.85052283	5.90123281
C	10.64878814	-19.21422160	5.40067944
C	11.99391787	-19.11142532	5.81603712
C	11.72469360	-4.64310793	4.51272322
C	12.77919521	-3.71166147	4.77793339
C	14.02466964	-4.16909034	5.28957898
C	12.59441609	-2.32182710	4.53121255
C	13.63514587	-1.43260641	4.79360239
C	14.87542531	-1.90045274	5.30539140
C	15.77437241	-0.74765234	5.48202907
C	15.08458944	0.42549284	5.07730025
C	15.07041035	-3.27090068	5.55376333
C	13.66242252	0.09150380	4.60228830
C	17.09725812	-0.67735780	5.95350975
C	15.71505185	1.67297978	5.14216676
C	17.72864982	0.58040495	6.01740055
C	17.04397674	1.74733784	5.61504052
C	-12.97118728	-9.41009776	-8.91936281
C	-4.65125426	-19.68503377	-0.23078337
C	-3.46172260	-2.01529172	-0.84457508
C	-4.14202927	-3.25745831	-1.21908286
C	-3.25114922	-4.32578458	-0.91738829
C	-2.03264737	-3.71821335	-0.36290754
C	-3.16468777	-19.62743552	-2.29458129
C	-5.40588628	-3.51242715	-1.77591675
C	-3.59959509	-5.65748414	-1.16058868
C	-4.87319709	-5.92589009	-1.72437106
C	-5.76123521	-4.84496297	-2.02549960
C	-5.27585155	-7.27189084	-1.99761686
C	-14.25319679	-2.79822486	-4.84947996
C	-5.61950223	-8.42582612	-2.23527315
C	-6.02126296	-9.77267329	-2.51560665
C	-5.26639838	-10.86045312	-2.01767251
C	-5.65593629	-12.19305891	-2.29131591
C	-7.17489032	-10.02499427	-3.29458091
C	-7.57578320	-11.35166306	-3.57960640
C	-6.81111149	-12.42950165	-3.07356030
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Supporting information

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C	-3.82933959	-16.66151087	-1.12197093
C	-3.07266855	-17.71269084	-0.60692469
C	-1.94226907	-17.45621794	0.21487389
C	-1.34715003	-18.74431410	0.60834095
C	-2.11319483	-19.78900329	0.02711010
C	-1.57041878	-16.13470180	0.52005050
C	-3.27897805	-19.22309193	-0.79761795
C	-0.22749369	-19.03304078	1.40845135
C	-1.76265920	-21.12615704	0.24399070
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C	-12.77236348	-11.27147212	-7.18193737
C	-13.17598792	-12.61108809	-7.43016283
C	-14.38307975	-12.58841046	-8.27304842
C	-14.71768334	-11.23498001	-8.54182913
C	-12.44398820	-13.68517910	-6.89338072
C	-13.72133931	-10.27820230	-7.86988690
C	-15.16265293	-13.63829278	-8.78983662
C	-15.83292767	-10.92640553	-9.32861362
C	-16.28485187	-13.32369071	-9.58125766
C	-16.61837970	-11.97854516	-9.84935557
C	2.98898763	17.68187441	0.85998351
C	1.50287004	17.62498209	2.92412840
C	12.76668562	7.35596800	7.46610503
C	11.30836271	7.40757104	9.55020882
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C	-14.43916793	12.78152465	-6.37689484
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H	3.03388167	14.84030921	2.38184246
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H	-2.64716878	18.62142687	-1.61052790
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H	12.45905001	0.18407767	2.76652295

Supporting information

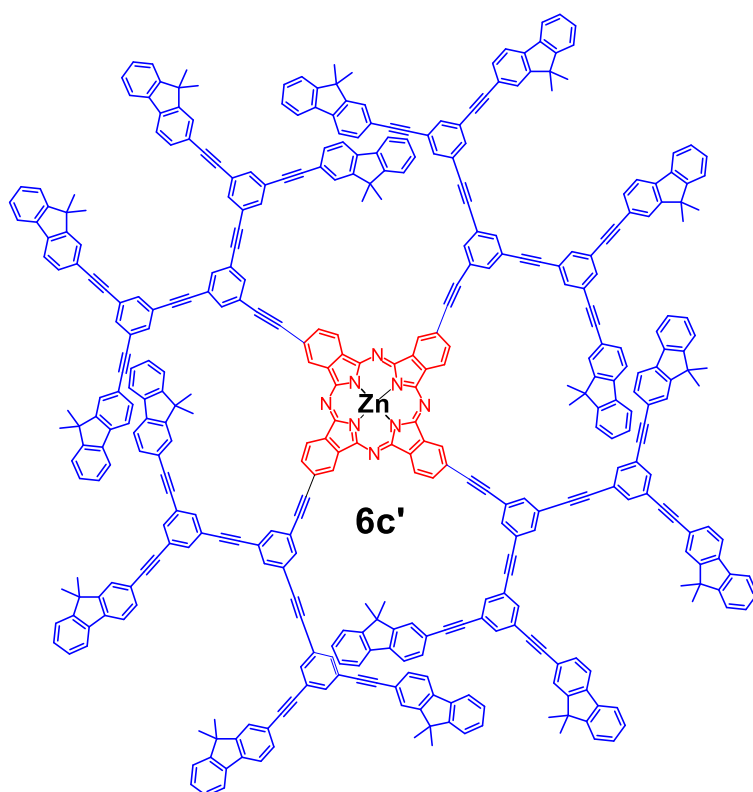
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H	-14.32819375	-3.88862903	-4.74794808
H	-13.24338277	-2.49846854	-4.54101675
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H	-15.86394169	-1.99652316	-1.83690079
H	-14.12128640	-2.18735522	-2.13404901
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H	-14.70521741	11.71666778	-6.38206490
H	-13.62478680	12.93618686	-7.09431213
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H	-14.92741608	13.31598901	-2.94333130
H	-15.47324971	11.93968995	-3.92799529
H	12.01096806	6.75049175	10.07862326
H	10.55618609	6.77550014	9.06087936
H	10.80059613	8.03533914	10.29173066
H	13.48874104	6.69910081	7.96807367
H	13.30301618	7.94711143	6.71456824
H	12.03474109	6.72226105	6.94877325
H	1.58307330	18.71401865	3.03503219
H	2.30859999	17.16471689	3.51039972
H	0.54342655	17.30593922	3.34786091
H	3.09302523	18.77127045	0.94544300
H	3.09261022	17.40816372	-0.19651997
H	3.81267160	17.21850316	1.41821136

Supporting information

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H	18.75170417	0.65522525	6.37852417
H	15.19836657	2.57948738	4.83431261
H	17.62989259	-1.57301207	6.26465862
H	16.01600554	-3.63839371	5.94473726
H	11.64089833	-1.97796128	4.13912469
H	14.15547723	-5.23185839	5.47421630
H	12.54762693	-20.01168737	6.07232618
H	10.17842979	-20.19289285	5.34050511
H	13.66179756	-17.78437906	6.22295649
H	8.87776794	-18.14550856	4.74497873
H	7.97312673	-15.71579217	4.24086254
H	11.66236996	-12.43013899	5.10795250
H	7.59687028	-13.27329187	3.90300306
H	10.94455155	-8.11140419	4.54712517
H	8.33641258	-4.85950132	3.40529019
H	6.90278627	-8.93565395	3.25628926
H	-19.20818786	-4.71467068	-5.03574465
H	-20.41450191	-2.65938448	-5.74493787
H	-16.86067922	-4.58317012	-4.20125044
H	-19.29291475	-0.43101539	-5.63139464
H	-17.67918365	1.63455899	-5.31189742
H	-13.30359388	-0.02529276	-3.50692627
H	-15.81874885	3.22825272	-4.84178614
H	-14.21105888	18.00839392	-5.44174053
H	-11.84184339	18.18967412	-4.70999867

Supporting information

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H	-13.32575191	10.42693799	-4.47669571
H	-9.26022519	11.27021162	-3.27192607
H	-12.60778957	6.10818657	-3.91544164
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H	-8.56597967	6.93274140	-2.62493993
H	3.10744589	-7.49820100	1.49715597
H	0.87456077	-6.73005276	0.64043147
H	4.29179913	-3.39252688	2.25161204
H	-4.77044816	5.49539254	-0.86570537
H	-5.95479888	1.38971634	-1.62015438
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H	4.41868272	0.69160067	2.63621113
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H	5.06750420	3.07641838	3.08806302
H	15.82479575	9.74972235	11.09330365
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H	13.24746770	12.67389825	9.21773130
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H	9.06819650	12.22975476	6.31783310
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N	-2.10310062	0.51461491	-0.11107932
N	2.32460529	-1.21771693	1.60856581
N	0.44012081	-2.51741800	0.74248862
N	-2.20394178	-2.33759735	-0.33947537
N	-3.98758162	-0.78508578	-0.97716898
N	-0.95202386	-4.40611329	0.04032102
Zn	-0.83150859	-1.00140341	0.31573905

Table S3. Cartesian coordinates of **6c'** after geometrical optimization.

Atom	x	y	z
C	7.65023	-0.81742	-3.7369
C	7.99254	0.5418	-3.7145
C	8.65613	-1.79208	-3.71961
C	6.26431	-1.20444	-3.77028
C	10.00316	-1.40777	-3.68022
C	9.33877	0.92697	-3.67417
C	10.3436	-0.04876	-3.6574
C	9.69022	2.32297	-3.64732
C	11.03808	-2.40662	-3.66264
C	9.99033	3.49075	-3.62385
C	10.35748	4.88254	-3.59481
C	9.43623	5.86233	-3.99063
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Supporting information

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Supporting information

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Supporting information

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Supporting information

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Supporting information

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Supporting information

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Supporting information

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H	-0.58707	-11.70106	-19.97226
H	0.60997	-10.7294	-20.90852
H	-0.80929	-9.9198	-20.14874
H	-13.1306	-12.80139	-13.38689
H	-14.08155	-12.63575	-11.86305
H	-12.46542	-11.85143	-12.00528
H	-15.1398	-10.34033	-11.27305
H	-14.91129	-8.94947	-12.39869
H	-13.52373	-9.55622	-11.41873
H	-12.68981	6.76854	-14.6171
H	-13.50713	7.70999	-15.92098
H	-14.16842	7.72823	-14.24258
H	-11.33548	9.83742	-12.81248
H	-11.3861	8.03677	-12.76212
H	-12.86753	8.9916	-12.38132
H	0.48916	5.10732	-23.72528

Supporting information

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H	-0.57196	8.54225	-22.44197
H	0.70421	8.91582	-23.6584
H	1.08039	9.01783	-21.89715
H	-17.79802	14.82875	3.23136
H	-18.28058	13.10166	3.03685
H	-19.47684	14.3084	3.63725
H	-19.90131	12.44603	1.12186
H	-20.51837	13.72644	0.0113
H	-21.09937	13.65325	1.7175
H	-11.7829	10.95868	-10.69612
H	-10.9278	12.4807	-11.15345
H	-11.54912	12.26018	-9.47608
H	-8.57368	12.95865	-10.09985
H	-7.81881	11.70273	-9.04771
H	-9.23042	12.65263	-8.44974
H	-11.66767	-2.67196	11.07321
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H	-11.08111	-4.06489	12.05452
H	-10.47715	-1.03391	12.69994
H	-9.89691	-2.42878	13.68239
H	-10.85427	-1.11379	14.4621
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H	-7.32864	-2.95802	19.2012
H	-7.07109	-3.49048	20.90559
H	-5.65753	-3.06768	19.8714
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H	8.23572	-13.88436	9.84976

Supporting information

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H	17.82002	-4.1026	-11.81035
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H	14.88152	-13.56258	-0.03773
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H	2.7998	10.90235	-4.23985
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H	5.76476	13.84673	-3.00542
H	5.42374	12.43774	-1.93203
H	4.19866	13.74631	-2.11609
H	18.99925	6.54173	-4.56983
H	19.86255	6.18985	-3.02567
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H	-17.31065	12.26807	0.73738
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H	-7.71351	10.38997	-14.17373
H	-8.76293	11.93831	-12.52808
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Supporting information

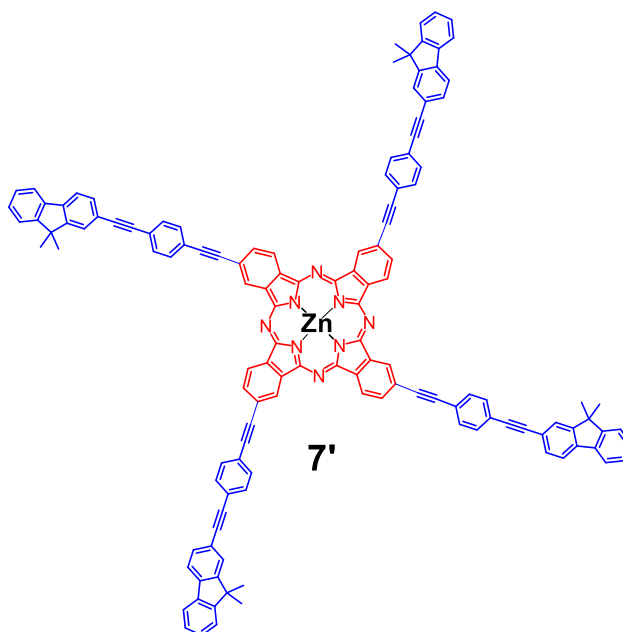
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H	-23.55699	11.39413	13.29626
H	-20.44695	13.68083	10.12968
H	-17.388	10.02443	8.67885
H	-18.78664	11.99482	9.25666
H	-19.7751	7.5505	11.30974
H	7.21414	1.29703	-3.72673
H	-11.50727	7.08045	-2.55653
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H	-11.48297	2.42018	4.52336
H	-7.58888	0.22201	4.30768
H	-5.4479	-1.04143	4.1145
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H	3.82144	-14.67296	-17.31709
H	4.36259	-13.52892	-19.45548
H	3.00972	-11.57942	-20.21304
H	1.92027	-13.876	-15.91563
H	-0.06222	-12.73057	-14.85811
H	-2.00083	-11.31995	-14.20618
H	-1.50974	-8.96963	-17.80814
H	-18.04048	-11.79131	-16.58525
H	-18.36211	-12.54075	-14.23807
H	-16.58133	-12.14993	-12.54085
H	-15.93263	-10.64226	-17.25618
H	-11.40002	-8.57626	-17.19222
H	-13.67173	-9.54585	-17.45843
H	-11.42251	-9.65814	-13.00061
H	-14.30099	13.60119	-16.3051
H	-15.62003	12.39823	-14.5767
H	-14.81409	10.2216	-13.67253
H	-12.15979	12.63827	-17.14302
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H	-10.07764	11.30536	-17.65315
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Supporting information

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H	4.85318	5.53059	-20.85176
H	0.99405	4.68269	-17.81773
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H	-6.53622	-9.28454	-15.4148
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H	-4.6939	6.76228	-17.80085
H	-2.94488	3.17938	-16.17284
H	-6.86536	4.4249	-14.91123
H	-5.44277	-0.96701	-14.52096
H	-5.44452	-2.56366	-10.52514
H	-4.92444	1.66285	-11.1503
H	-11.83098	0.50602	20.92553
H	-11.18054	-1.34185	22.4542
H	-8.87131	-2.27295	22.38574
H	-10.17589	1.43901	19.31171
H	-8.19603	2.03199	17.86195
H	-6.03667	2.2313	16.64714
H	-4.37429	-0.94611	19.07116
H	9.31817	9.77524	16.42768
H	3.32431	5.49521	14.49045
H	9.78809	-19.02479	12.38
H	10.41074	-18.70705	9.99543
H	7.87073	-17.76383	13.35315
H	3.96845	-14.72256	13.93555
H	5.88412	-16.30264	13.87697
H	4.62116	-13.76521	9.76439
H	-11.52577	-14.99178	16.60873
H	-10.49984	-16.48353	18.31056
H	-8.02237	-16.6268	18.52347
H	-10.08091	-13.6275	15.10367
H	-6.13887	-11.5527	12.86886
H	-8.24313	-12.4572	13.83212
H	-3.83315	-13.96755	15.62421
H	-0.65865	2.37306	16.73066
H	1.75023	0.56021	13.65358
H	-2.20903	-0.92606	14.44315
H	-0.32267	-13.11978	12.8668
H	-2.13229	-9.26694	12.23669
H	1.98934	-9.91164	11.16621
H	0.05474	-4.78897	12.50109
H	0.25164	-1.78579	9.42532

Supporting information

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H	22.75927	-3.06952	-13.46004
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H	22.48521	-5.85344	-10.17502
H	20.93116	-6.38261	-8.26033
H	19.13569	-6.54132	-6.54973
H	17.0689	-3.21986	-8.4032
H	15.21826	-15.38576	4.93814
H	16.55704	-14.56923	3.00279
H	12.39243	-12.17598	4.36546
H	12.09005	-8.43467	1.08997
H	12.03628	-10.21516	2.82146
H	15.74763	-10.10002	-0.519
H	2.90326	15.57989	-7.91628
H	1.71091	15.8736	-5.7561
H	2.29666	14.45235	-3.79616
H	4.69351	13.85927	-8.1357
H	7.94415	10.21037	-7.16683
H	6.40604	12.02692	-7.87791
H	6.20908	10.28444	-3.20147
H	22.28336	10.01897	0.83547
H	23.41707	9.77301	-1.36193
H	22.14262	8.97993	-3.3496
H	19.86173	9.47373	1.06425
H	15.17093	8.09842	0.09628
H	17.43954	8.81886	0.80874
H	16.62532	7.4844	-3.93456
H	-6.80392	0.43466	-3.83959
H	-6.90035	0.63176	-6.32266
H	-2.83441	-0.85197	-6.58706
H	2.46289	-3.19693	4.51162
H	-1.80619	-2.45556	4.70359
H	2.41259	-2.81403	2.04958
H	0.97852	-1.49497	-5.91146
H	3.46699	-1.3624	-5.9355
H	3.54284	-2.12191	-1.66476
H	9.12571	-17.12539	8.56291
H	6.33979	4.4016	18.31892
H	4.42852	2.90884	17.78205
H	8.14353	6.15512	18.46007
H	7.39987	9.53098	14.85745
H	9.68963	8.09559	18.22094
Zn	-2.57622	-2.12718	-0.66388

Table S4. Cartesian coordinates of **7'** after geometrical optimization.

Atom	x	y	z
C	6.34555765	8.84560592	0.38878959
C	5.97393779	9.91773083	-0.46621824
C	7.43035799	9.04032447	1.28538900
C	5.64460026	7.59967571	0.34704556
C	8.11645185	10.25810896	1.32482375
C	7.74587389	11.33055910	0.46926558
C	6.66009658	11.13541689	-0.42673208
C	8.44829181	12.57554351	0.50710488
C	5.04351816	6.52880358	0.31067145
C	4.34297156	5.28320815	0.26423256
C	4.73634046	4.21318994	1.12999509
C	3.26092321	5.10123026	-0.63564418
C	2.60879706	3.86516498	-0.64522482
C	3.00809855	2.80692686	0.21917352
C	1.47776483	3.36142393	-1.43795506
C	2.12111694	1.67407055	-0.05466350
C	4.07726272	2.97659426	1.11421050
C	12.76692851	-6.36779495	11.88171319
C	11.10514605	-5.51963817	13.61167543
C	-0.21363447	3.63215019	-3.10490451
C	-0.91364941	4.42522721	-4.11774201
C	-1.93708595	3.59705929	-4.65931555
C	-1.84725321	2.30370660	-3.96580194
C	-14.41314945	-14.09763599	-5.72163968
C	-0.73632532	5.74026217	-4.57833571

Supporting information

C	-2.79548963	4.05797037	-5.66129628
C	-2.62482149	5.38492557	-6.13435153
C	-1.59307042	6.20994222	-5.58277542
C	-3.47547295	5.90426732	-7.15956466
C	-12.80472907	-14.96978291	-7.49012057
C	-2.58552952	0.06323410	-3.58050956
C	-3.47249695	-1.06964577	-3.85437493
C	-3.07321817	-2.12785329	-2.98993551
C	-1.94220519	-1.62411023	-2.19718537
C	-11.57156410	7.25421431	-17.24611303
C	-4.54166073	-1.23934859	-4.74940547
C	-3.72537302	-3.36389788	-2.99943914
C	-4.80744598	-3.54590244	-3.89929489
C	-5.20077393	-2.47593365	-4.76512098
C	-5.50800590	-4.79149737	-3.94553113
C	-13.23259137	8.10284395	-15.51566792
C	-0.25083391	-1.89478926	-0.53021486
C	0.44922929	-2.68791063	0.48255244
C	1.47268358	-1.85975476	1.02410579
C	1.38280559	-0.56637534	0.33065721
C	12.33956227	16.70375308	3.86132472
C	0.27204183	-4.00302436	0.94296989
C	2.33122291	-2.32075007	2.02593051
C	2.16068848	-3.64777979	2.49882056
C	1.12891846	-4.47278383	1.94725933
C	3.01143281	-4.16720279	3.52391472
C	13.94848357	15.83271119	2.09277059
C	-4.20450191	6.35123413	-8.04167038
C	-5.04865178	6.87553390	-9.07023145
C	-4.87762924	8.20455748	-9.54269842
C	-6.07639746	6.08058394	-9.64490747
C	-6.89902842	6.59346851	-10.65272062
C	-6.72744693	7.92206330	-11.12683258
C	-5.70023689	8.71729319	-10.55031244
C	-7.56470085	8.44743598	-12.16017594
C	-6.10911300	-5.86236236	-3.98170926
C	-6.81008976	-7.10829124	-4.02315855
C	-6.43855102	-8.18009272	-3.16769846
C	-7.89480522	-7.30334709	-4.91977562
C	-8.58093332	-8.52113190	-4.95877466
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C	-7.12473680	-9.39777148	-3.20674989
C	-8.91294436	-10.83820724	-4.14000549
C	3.74050588	-4.61432493	4.40590578
C	4.58457033	-5.13897634	5.43435782
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Supporting information

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C	5.23627400	-6.98140528	6.91355904
C	7.10015287	-6.71190282	8.52416213
C	-8.27637805	8.90755083	-13.05003818
C	-9.10459088	9.43696346	-14.08943310
C	-8.91087269	10.76929376	-14.54871615
C	-10.12732381	8.63868989	-14.67662183
C	-10.91951173	9.17287147	-15.69125221
C	-10.71602673	10.50479833	-16.14314191
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C	-9.71071521	11.30425074	-15.57030552
C	-12.06668895	8.50307282	-16.46338606
C	-11.89688332	11.95208704	-17.97679865
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C	-13.70724500	10.79783314	-19.15468529
C	9.04797648	13.64784162	0.53197056
C	9.75168591	14.89294240	0.56519740
C	9.36859127	15.95423537	-0.30099525
C	10.84112179	15.08337996	1.46233052
C	11.51436347	16.30364206	1.47749316
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C	12.93760786	18.16541637	1.85585506
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C	12.70494466	16.72975426	2.35014447
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C	13.90098388	19.08985441	2.27462436
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C	13.93155683	20.36871215	1.67564199
C	7.81164930	-7.17226597	9.41404045
C	8.63953277	-7.70186391	10.45360133
C	8.44572890	-9.03430450	10.91252051
C	9.66200270	-6.90365533	11.04134130
C	10.45383326	-7.43800254	12.05615948
C	10.25023914	-8.77002894	12.50771225
C	11.22067142	-9.05601108	13.57726499
C	12.01764506	-7.89890910	13.78141771
C	9.24520936	-9.56942774	11.93430785
C	11.60067758	-6.76829693	12.82886850
C	11.43043009	-10.21759494	14.34158342
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C	12.44760438	-10.21351006	15.31626626

Supporting information

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C	-9.83232596	-14.21640114	-3.32954079
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H	7.72368179	8.22784308	1.94442573
H	8.94481613	10.39514015	2.01433878
H	6.36706299	11.94789564	-1.08574426
H	5.56778700	4.37956032	1.80918308
H	2.94911112	5.90124424	-1.29891587
H	4.37815121	2.16716829	1.77189620
H	0.04508559	6.36844938	-4.16235739
H	13.60440506	-5.95378196	12.45803457
H	12.43814444	-5.60338714	11.16585914
H	13.13262412	-7.23351363	11.31726580
H	11.92029629	-5.09216438	14.20967879
H	10.28191151	-5.77830313	14.28787526
H	10.75165533	-4.74505261	12.91901469
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H	-14.21140841	-13.06199616	-6.02405971
H	-14.68822193	-14.09863946	-4.66039420
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H	-12.58099288	-13.94602575	-7.81665542
H	-12.38696644	6.82670963	-17.84374915
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H	13.17728493	17.07522159	4.46540573
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H	14.80839766	16.19236767	2.67235010
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H	13.74643957	14.79686641	2.39428450
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H	-10.20540757	-16.24390032	-2.67666096
H	-11.59375588	-12.53306466	-5.75288252
H	-8.99933943	-14.06012965	-2.64952837
H	14.02144002	-9.07646574	16.27690813
H	12.62525421	-11.10207476	15.91754698
H	13.64451812	-7.01864767	14.91688439
H	10.82264070	-11.10642481	14.18913549
H	5.14562853	9.78060201	-1.15583776
H	9.80577502	-5.88661651	10.68610567
H	7.66336352	-9.63541313	10.45723958
H	14.67527814	21.09650200	1.99174634
H	13.04200045	21.70082956	0.21765194
H	14.62157660	18.83760096	3.04959051
H	11.32148969	20.05336585	-0.53328426
H	9.74242277	17.98211873	-0.95225236
H	11.12869026	14.26870730	2.12178653
H	8.53582577	15.79866652	-0.98144034
H	-14.48870861	10.81072797	-19.91089297
H	-13.09229870	12.83633958	-19.55244344
H	-14.11133226	8.75313172	-18.55066613
H	-11.28899006	12.84091416	-17.82475005
H	-9.54805126	12.32439324	-15.90927139
H	-10.27102163	7.62173399	-14.32111791
H	-8.12829182	11.37044563	-14.09386327
H	5.09563307	-7.99922560	7.26650487
H	7.21605290	-4.23930199	7.45055706
H	5.75242753	-3.32608106	5.65698999
H	3.63197387	-7.08635240	5.47326198
H	-6.83177682	-10.20999971	-2.54739665
H	-9.40924288	-8.65842037	-5.64830497
H	-8.18805065	-6.49112457	-5.57916664
H	-5.61029131	-8.04270465	-2.47807155
H	-5.55940923	9.73487067	-10.90388402
H	-7.68096649	5.97545558	-11.08516733
H	-6.21708019	5.06283966	-9.29150639
H	-4.09549394	8.82260550	-9.11053460
H	1.02041709	-5.48476809	2.32725445
H	3.10775081	-1.68133249	2.43256737
H	-0.50937214	-4.63120051	0.52698243
H	-6.03222280	-2.64231235	-5.44430519
H	-3.41357542	-4.16387883	-2.33612268

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H	-4.84254495	-0.42995422	-5.40713281
H	-1.48446387	7.22187009	-5.96289138
H	-3.57199735	3.41853319	-6.06794137
N	0.82253870	4.07245605	-2.36987203
N	-0.80450331	2.37142155	-3.04713223
N	-2.65047504	1.25378076	-4.20214460
N	-1.68694035	-0.31212858	-2.58374672
N	-1.28700474	-2.33512936	-1.26525091
N	0.33997878	-0.63405387	-0.58795683
N	2.18605004	0.48351999	0.56696875
N	1.22250976	2.04943835	-1.05140623
Zn	-0.23232976	0.86873667	-1.81747476

6. Motions videos

Video S1 and S2: MD simulations run for **6a** and **7**, with or without THF over 4 ns, reveal that these molecules remain almost flat during all the simulation time, undergoing only flapping or twisting of the peripheral fluorene arms around their initial position (Figure 7, Video S1 and S2).

Video S3: Now, when such molecules are considered in the same volume, they show some interactions through the extended arms but no tendency to stack in THF (Video S3).

Video S4: On contrary, in CH₂Cl₂ (starting from the same positions), these molecules stack readily and form well-eclipsed dimers with a good overlap of their phthalocyanine cores (Video S4), which is in line with their insolubility in dichloromethane.

Video S5: Considering the conformational evolution of **6b** in solution, a related statement can be made; the central phthalocyanine core also remains almost coplanar during the simulation, while extensive flapping and twisting of the fluorenyl groups within their peripheral arms are observed. This motion is also accompanied by large rotations of each dendron around the triple bond linking its first phenyl group to the central core (Figure 7, Video S5).

Video S6: In this compound **6b**, the extended arms are well isolated and can freely rotate and no interactions between the neighbouring arms through the butyl chains or the fluorene fragments is observed. Also, notably, a conformation with the four peripheral dendrons oriented perpendicular to the phthalocyanine core is never observed among the most stable ones for this molecule. Then, in contrast to **6b**, the dendrimer **6c** appears much more flexible in solution and strong interactions between the neighbouring arms can be observed. During the simulation the large dendrons rotate and curve to eventually interact in an intramolecular way through π -stacking interactions. This evolution contributes to flattening the molecule from a ball-shaped conformation into transitory a donut-like shaped conformation (Figure 7, bottom, Video S6).

Video S7: The bending and the clustering of the fluorene arms is driven here by strong intramolecular π - π^* interactions between fluorene fragments but also between fluorene fragments and phenyl rings of neighbouring

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arms (see white circles, on Figure 7).¹ In spite of this flattening process, the dendron shell remains too bulky to allow any intermolecular π - π stacking process to occur between phthalocyanine cores (Video S7).²

¹ In the absence of solvent, this dendrimer **6c** adopts a pocket-like conformation, with the arms all aggregated on one side of the phthalocyanine core, showing the high flexibility of this molecule (Figure S21).

² Stacking distances of 24.6 ± 3.5 Å are usually observed between phthalocyanine cores in MD simulations with the large dendrimer G₃. Note that concentrations used during these simulations ($7.874 \cdot 10^{-3}$ M) are much higher than the experimental ones.