New Journal of Chemistry

Supporting Informations for:

Topologically diverse Polycyclic Aromatic Hydrocarbons from Pericyclic Reactions with Polyaromatic Phospholes

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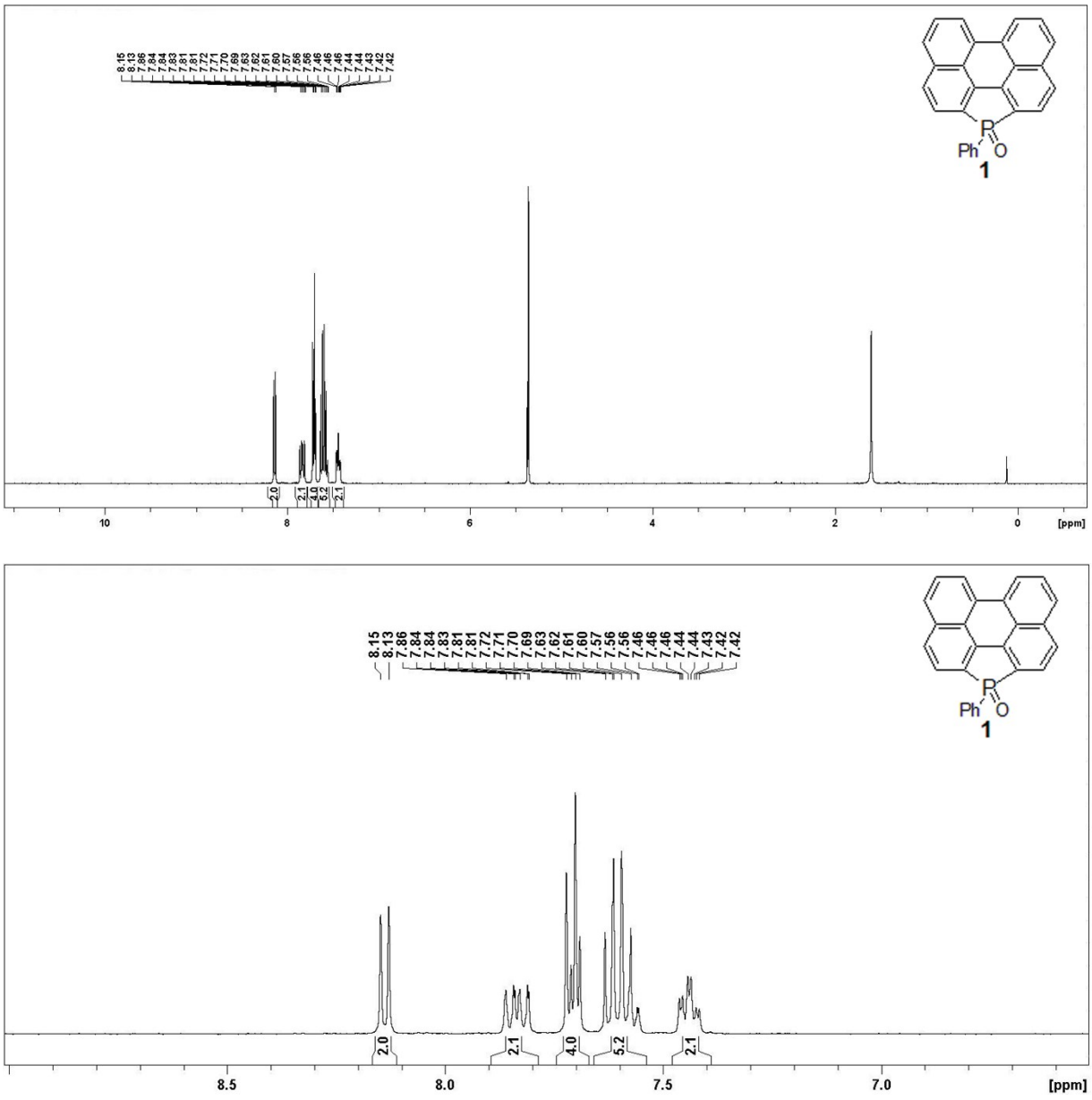
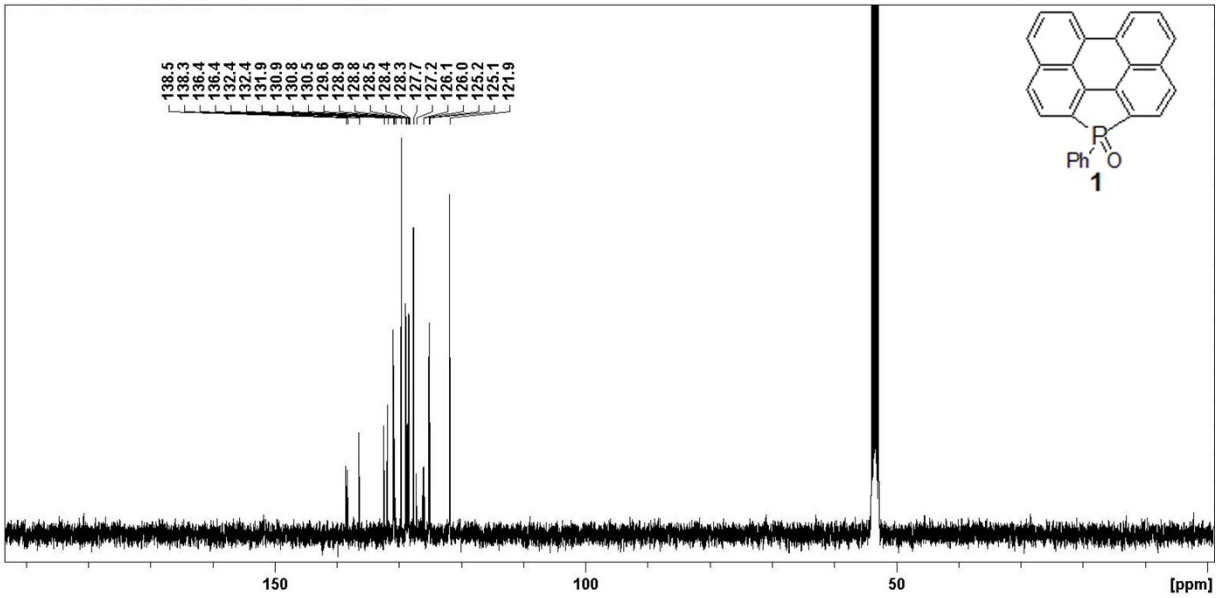
Figure S1. ^{1}H NMR (400 MHz, CD_2Cl_2), $^{13}C\{^{1}H\}$ NMR (100 MHz, CD_2Cl_2) and $^{31}P\{^{1}H\}\{^{13}C\}$ NMR of **1**.

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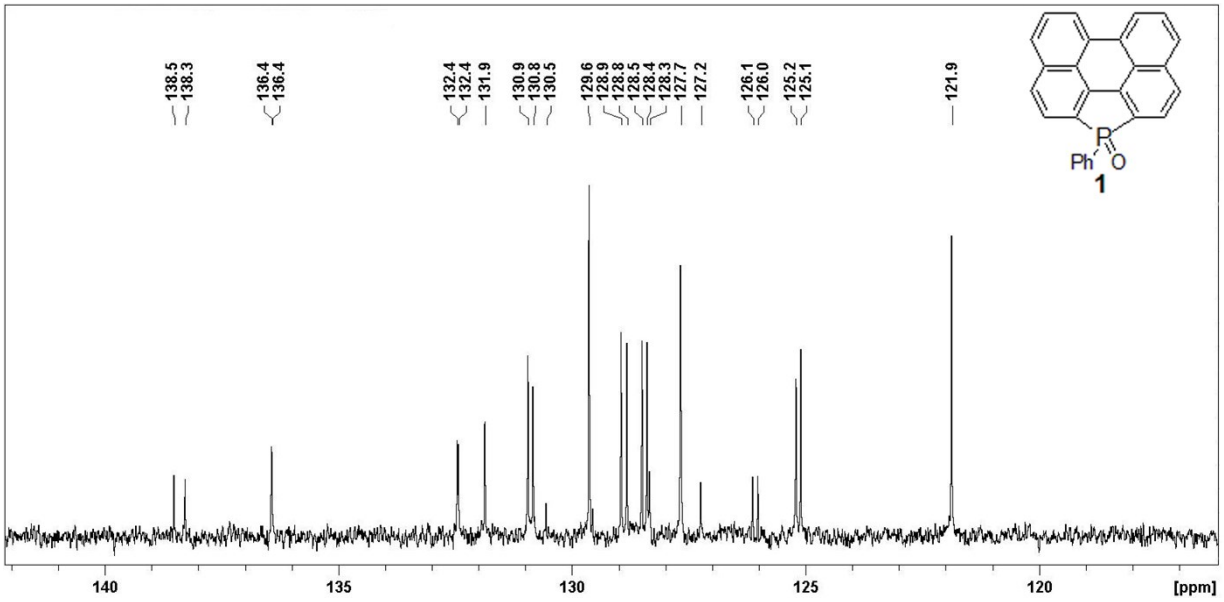
138.3
136.4
136.4
132.4
132.4
131.9
130.9
130.8
130.5
129.6
128.9
128.8
128.5
128.4
128.3
127.7
127.2
126.1
126.0
125.2
125.1
121.9
Ph
P
O
1
150
100
50
[ppm]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138.3
136.4
136.4
132.4
132.4
131.9
130.9
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130.5
129.6
128.9
128.8
128.5
128.4
128.3
127.7
127.2
126.1
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125.2
125.1
121.9
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P
O
1
140
135
130
125
120
[ppm]

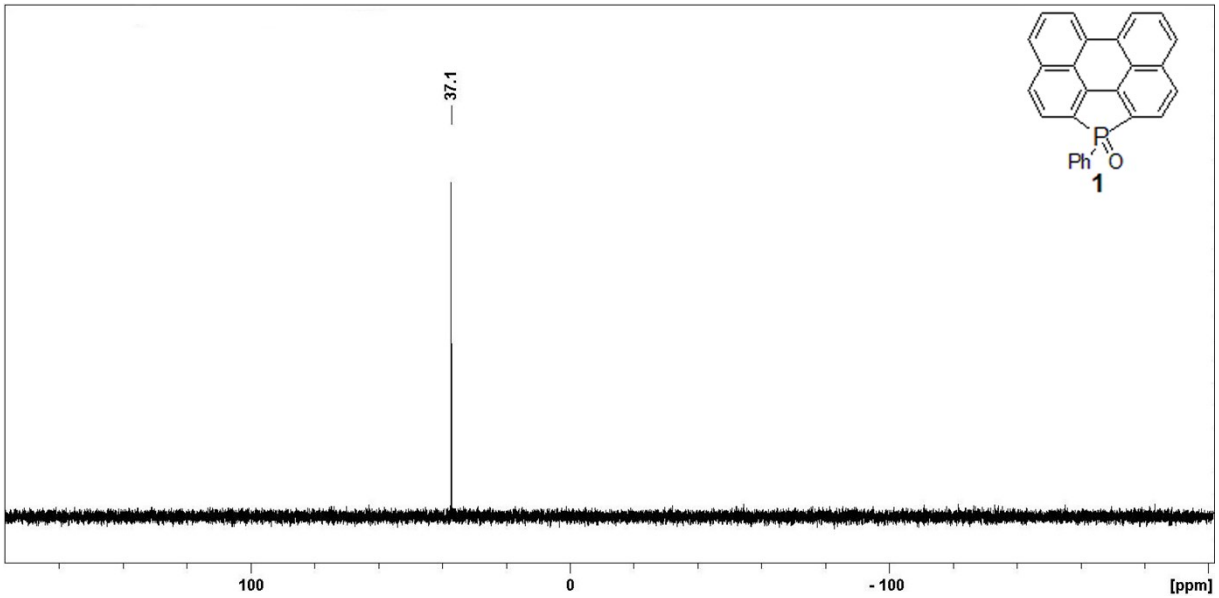
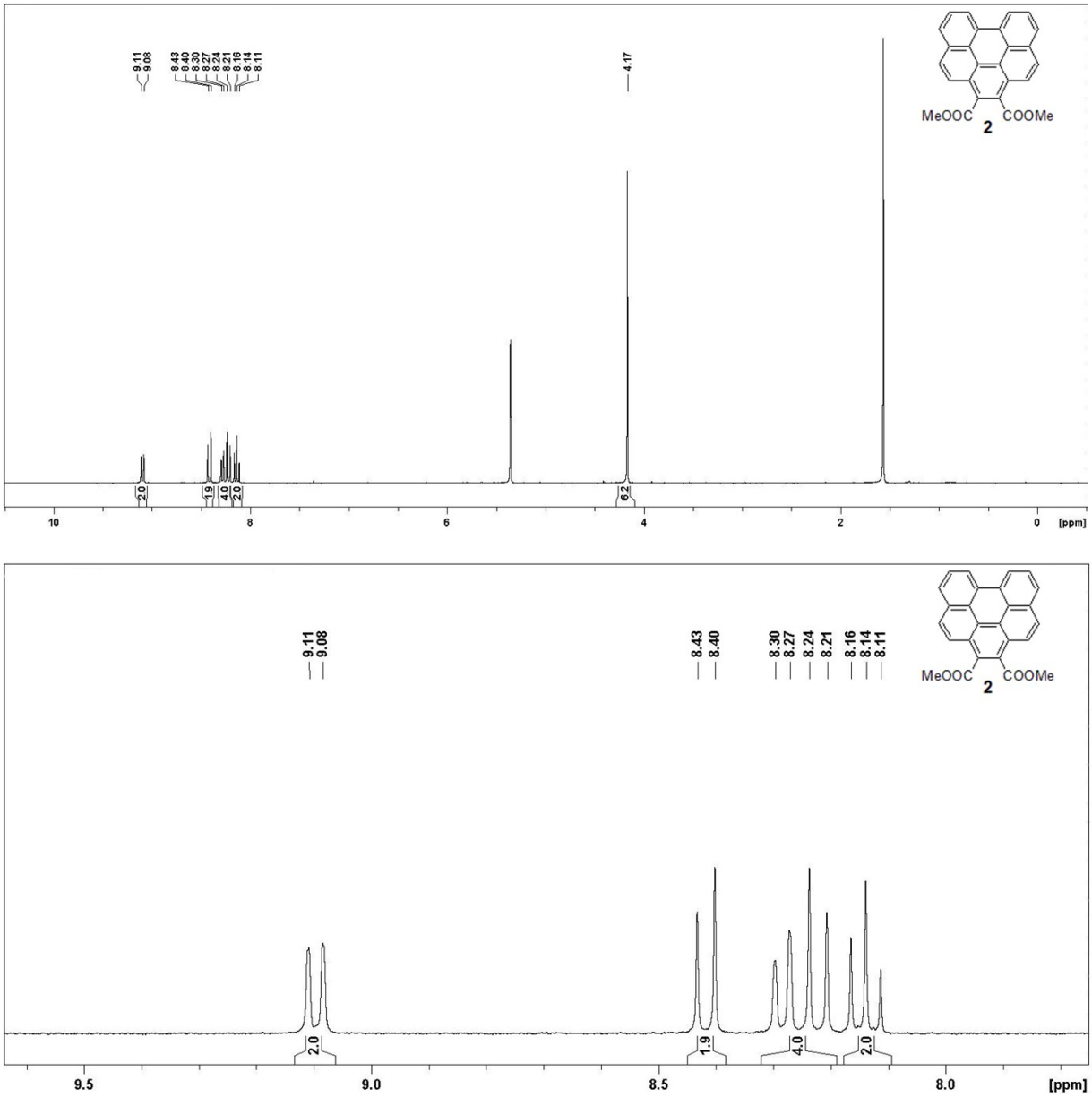
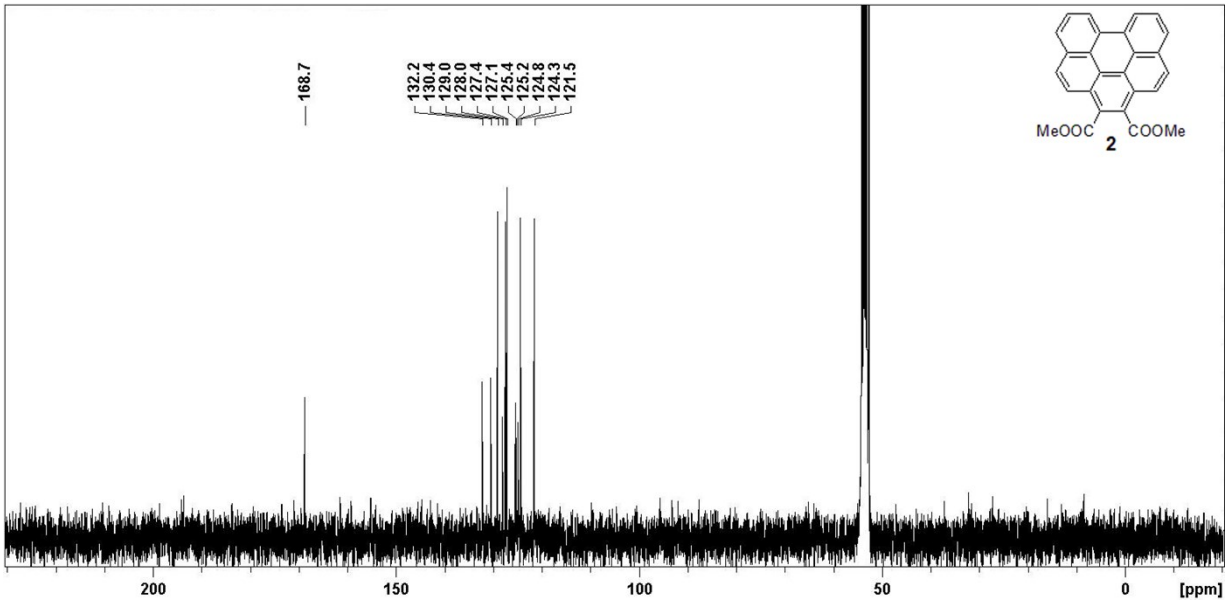

37.1
Ph
P
O
1
100
0
- 100
[ppm]

Figure S2. ^{1}H NMR (300 MHz, CD_2Cl_2) and $^{13}C\{^{1}H\}$ NMR (75 MHz, CD_2Cl_2) of **2**.




168.7
132.2
130.4
129.0
128.0
127.4
127.1
125.4
125.2
124.8
124.3
121.5
MeOOC
COOMe
2
200
150
100
50
0
[ppm]

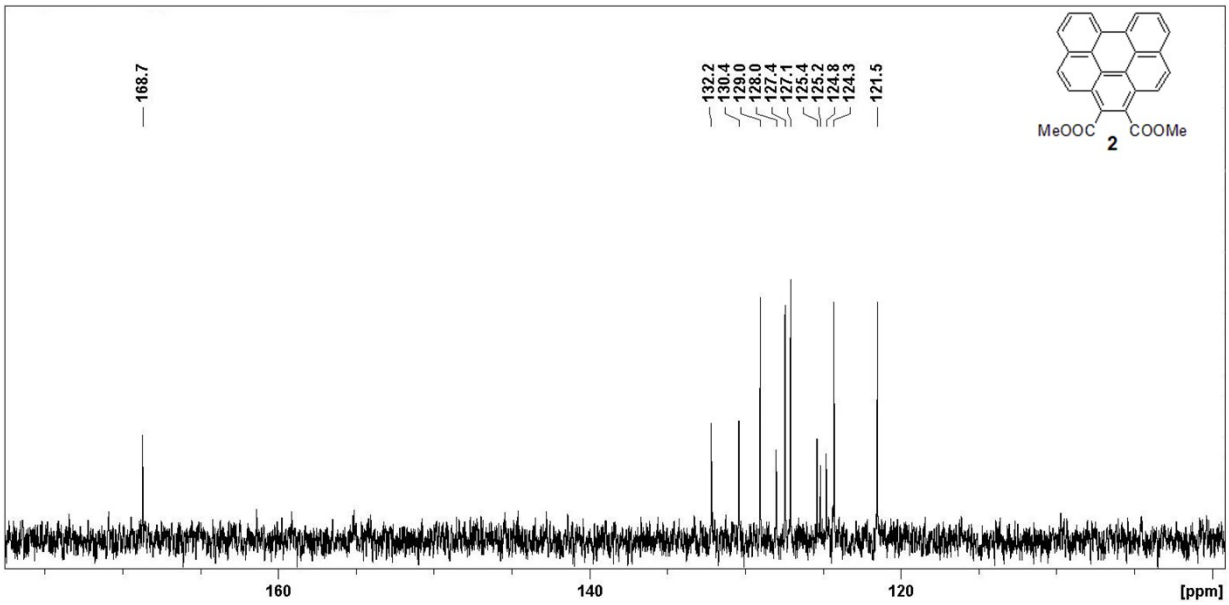
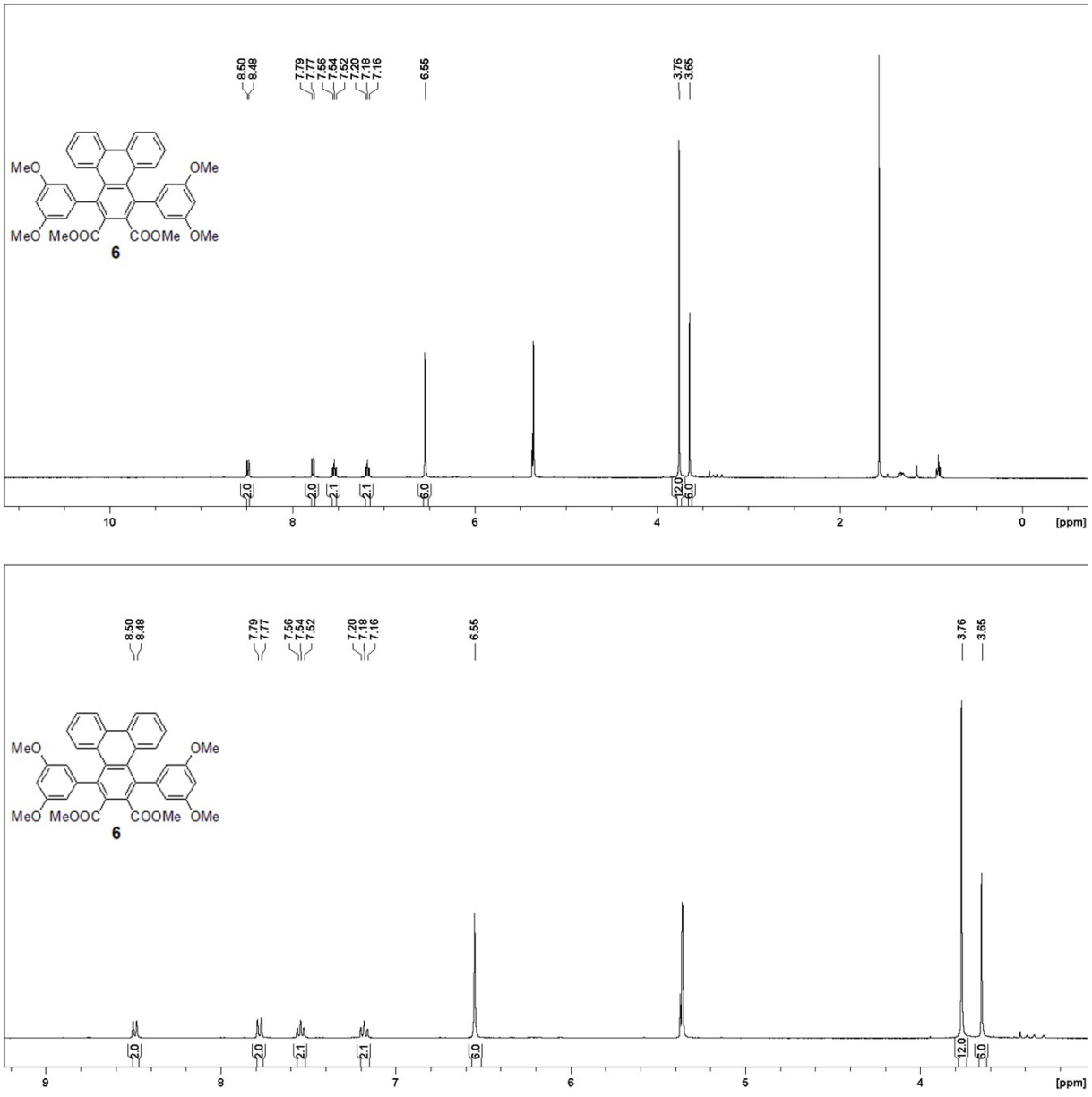

168.7
132.2
130.4
129.0
128.0
127.4
127.1
125.4
125.2
124.8
124.3
121.5
MeOOC
COOMe
2
160
140
120
[ppm]

Figure S3. ^{1}H NMR (400 MHz, CD_2Cl_2) and $^{13}C\{^{1}H\}$ NMR (100 MHz, CD_2Cl_2) of **6**.



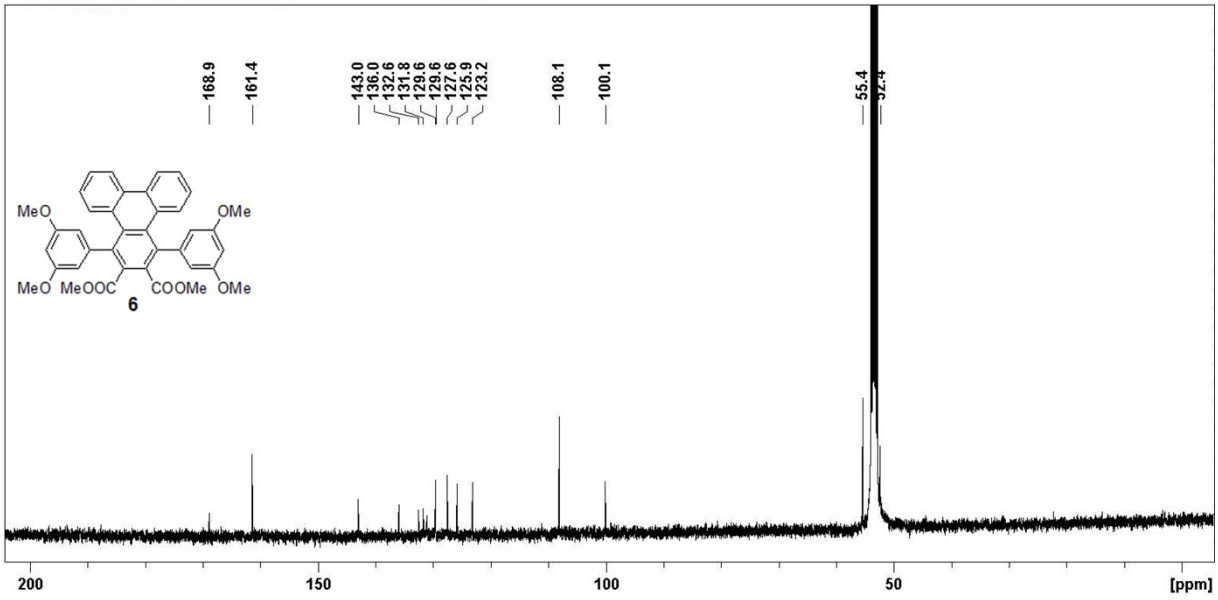
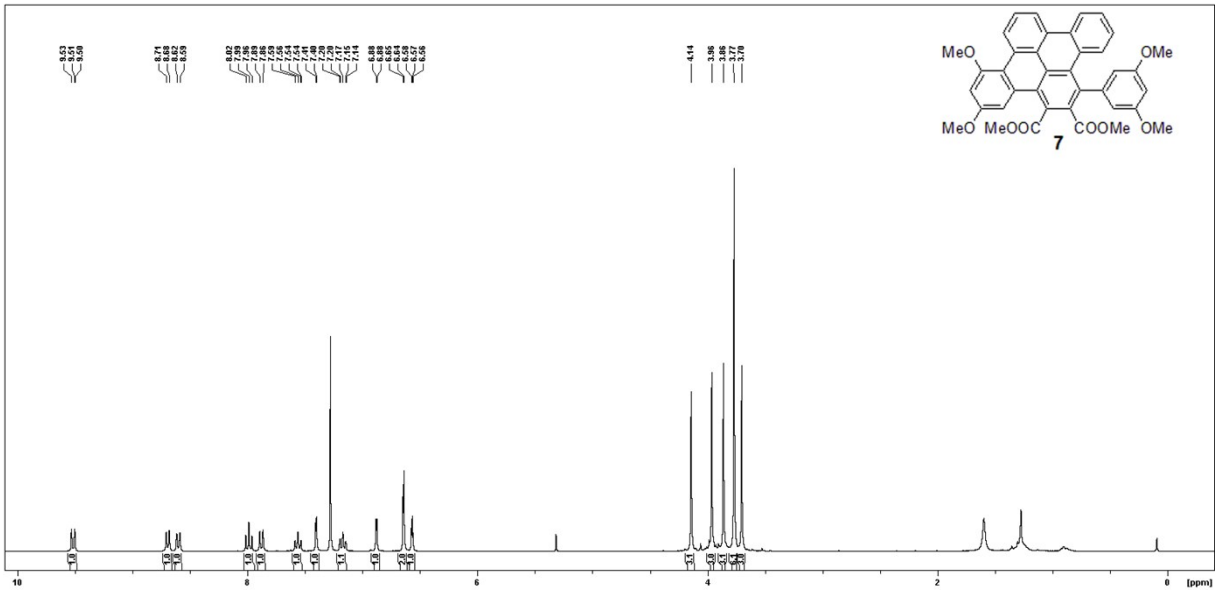
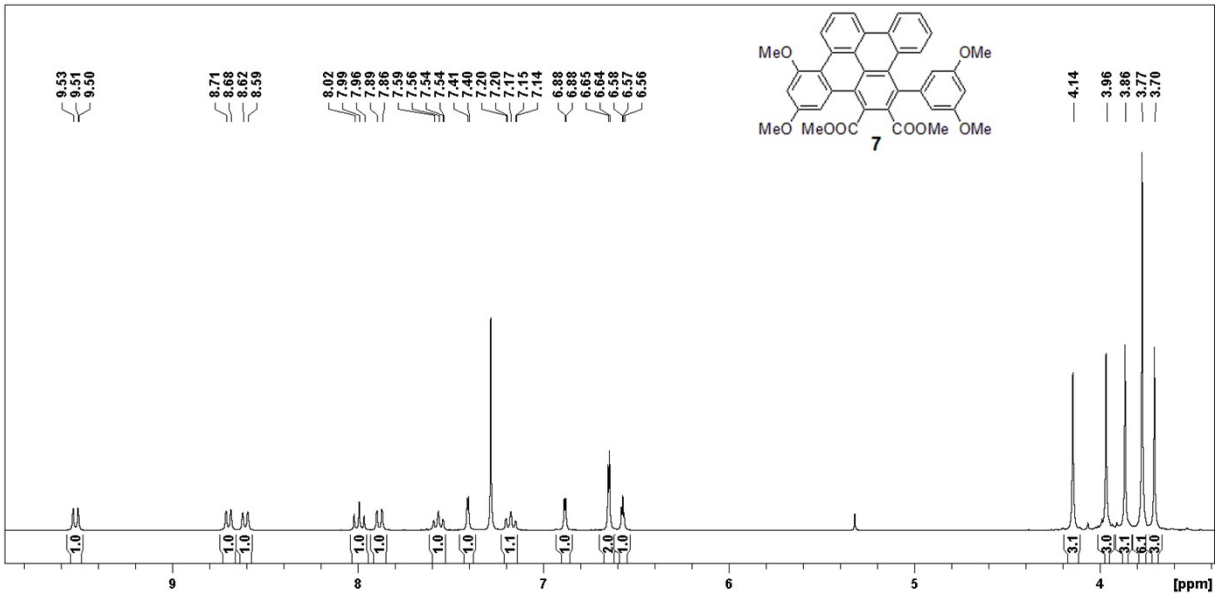


Figure S4. ^{1}H NMR (300 MHz, $CDCl_3$) and $^{13}C\{^{1}H\}$ NMR (75 MHz, $CDCl_3$) of **7**.

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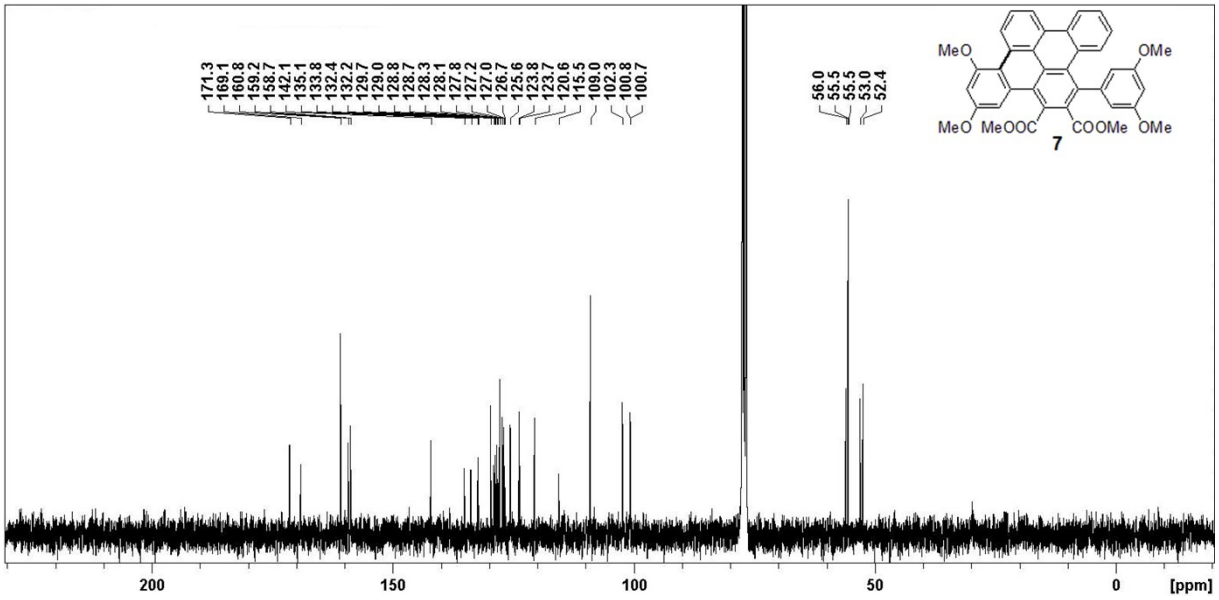
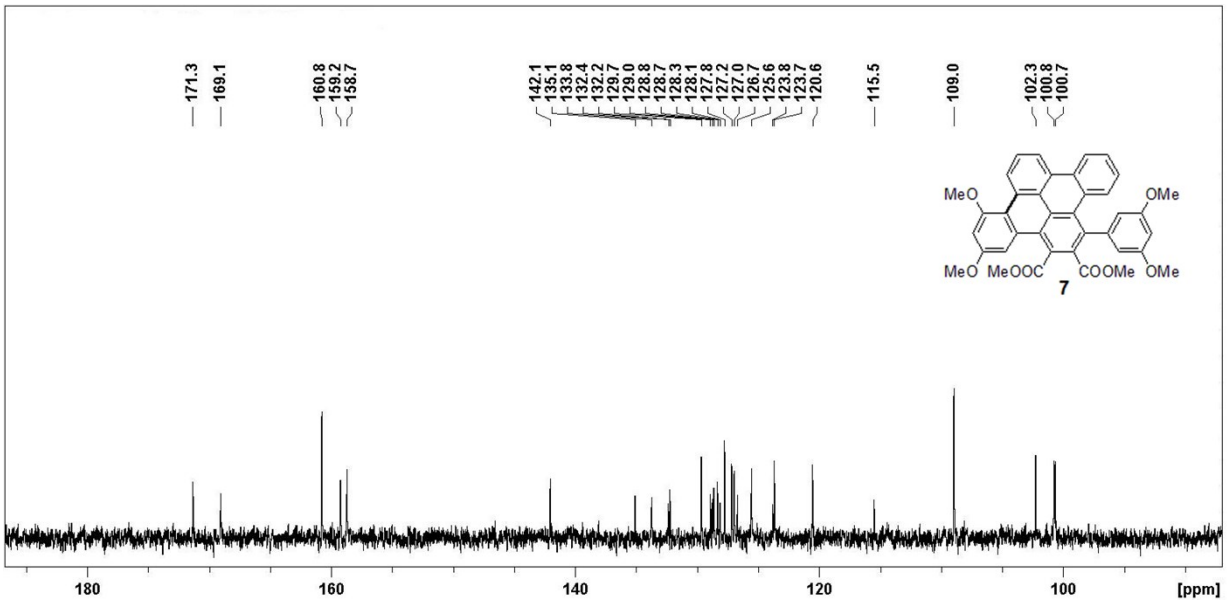
9.50
8.71
8.68
8.62
8.59
8.02
7.99
7.96
7.89
7.86
7.59
7.56
7.54
7.54
7.41
7.40
7.20
7.20
7.17
7.15
7.14
6.88
6.88
6.65
6.64
6.58
6.57
6.56
4.14
3.96
3.86
3.77
3.70
MeO
OMe
MeO MeOOC
COOMe OMe
7
[ppm]


171.3
169.1
160.8
159.2
158.7
142.1
135.1
133.8
132.4
132.2
129.7
129.0
128.8
128.7
128.3
128.1
127.8
127.2
127.0
126.7
125.6
123.8
123.7
120.6
115.5
109.0
102.3
100.8
100.7
56.0
55.5
55.5
53.0
52.4
MeO
OMe
MeO MeOOC
COOMe OMe
7
[ppm]


171.3
169.1
160.8
159.2
158.7
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132.4
132.2
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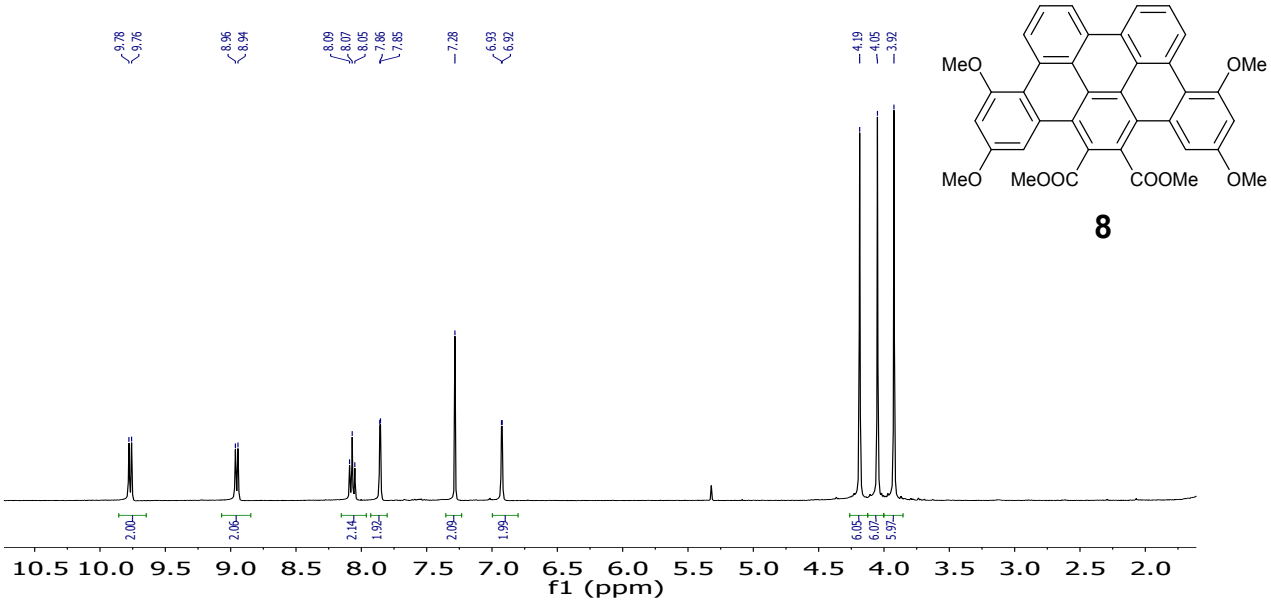
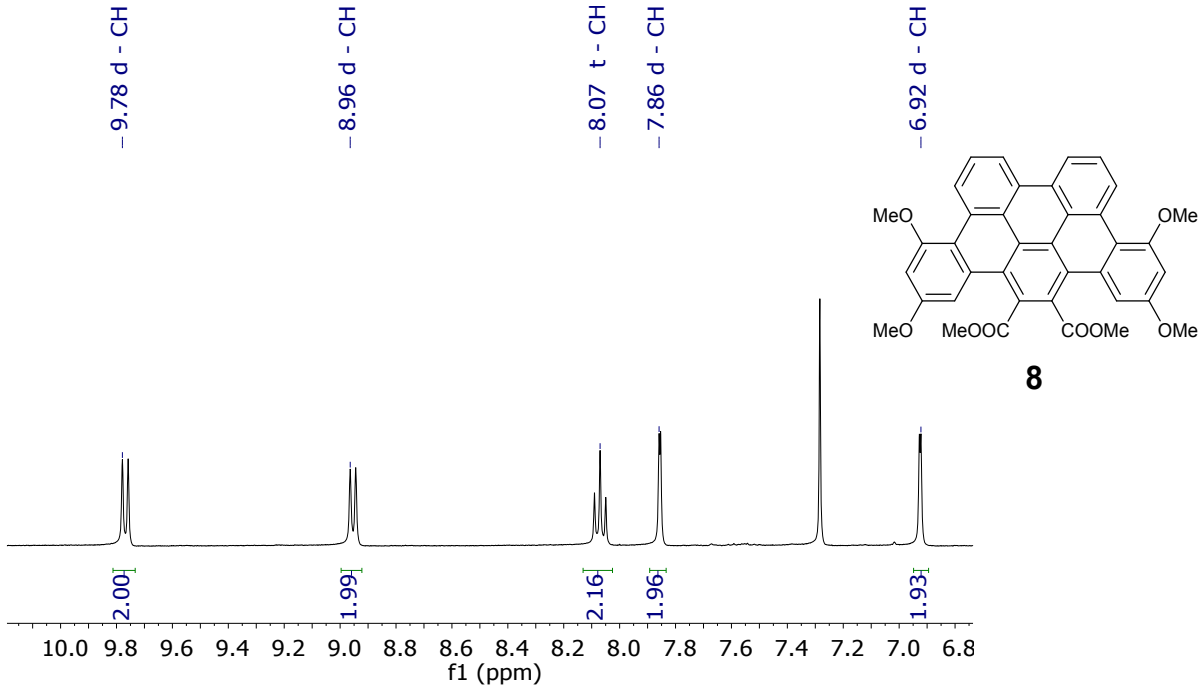
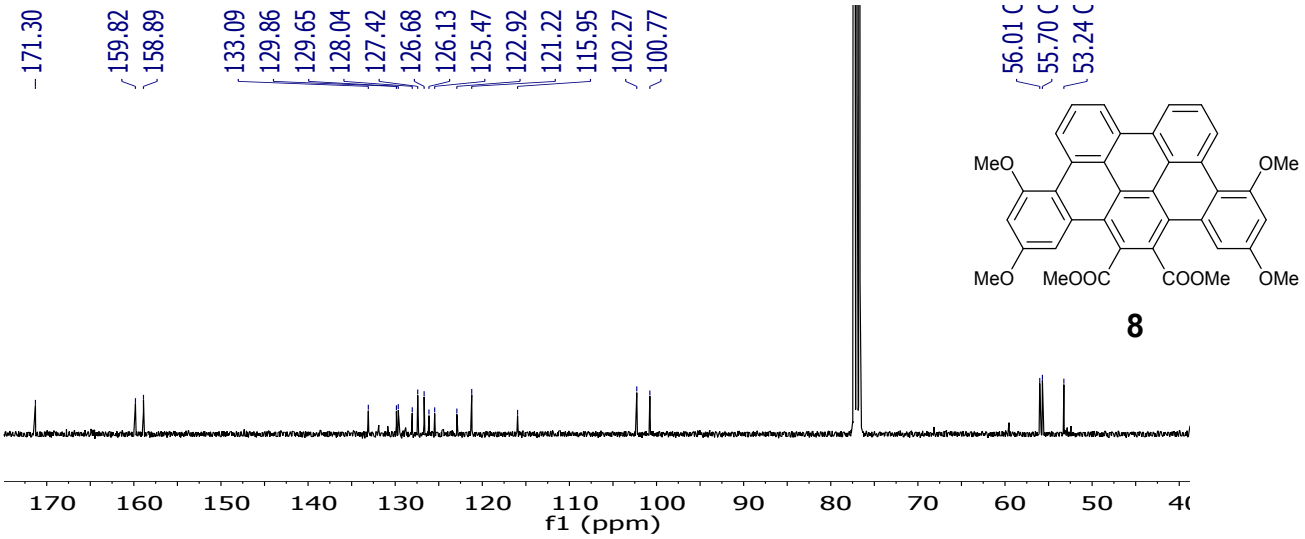
128.8
128.7
128.3
128.1
127.8
127.2
127.0
126.7
125.6
123.8
123.7
120.6
115.5
109.0
102.3
100.8
100.7
MeO
OMe
MeO MeOOC
COOMe OMe
7
[ppm]

Figure S5. ^{1}H NMR (400 MHz, CD_2Cl_2) and $^{13}C\{^{1}H\}$ NMR (100 MHz, CD_2Cl_2) of **8**.



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129.86
129.65
128.04
127.42
126.68
126.13
125.47
122.92
121.22
115.95
102.27
100.77
56.01 C
55.70 C
53.24 C
MeO
OMe
MeO
MeOOC
COOMe
OMe
8
170 160 150 140 130 120 110 100 90 80 70 60 50
f1 (ppm)

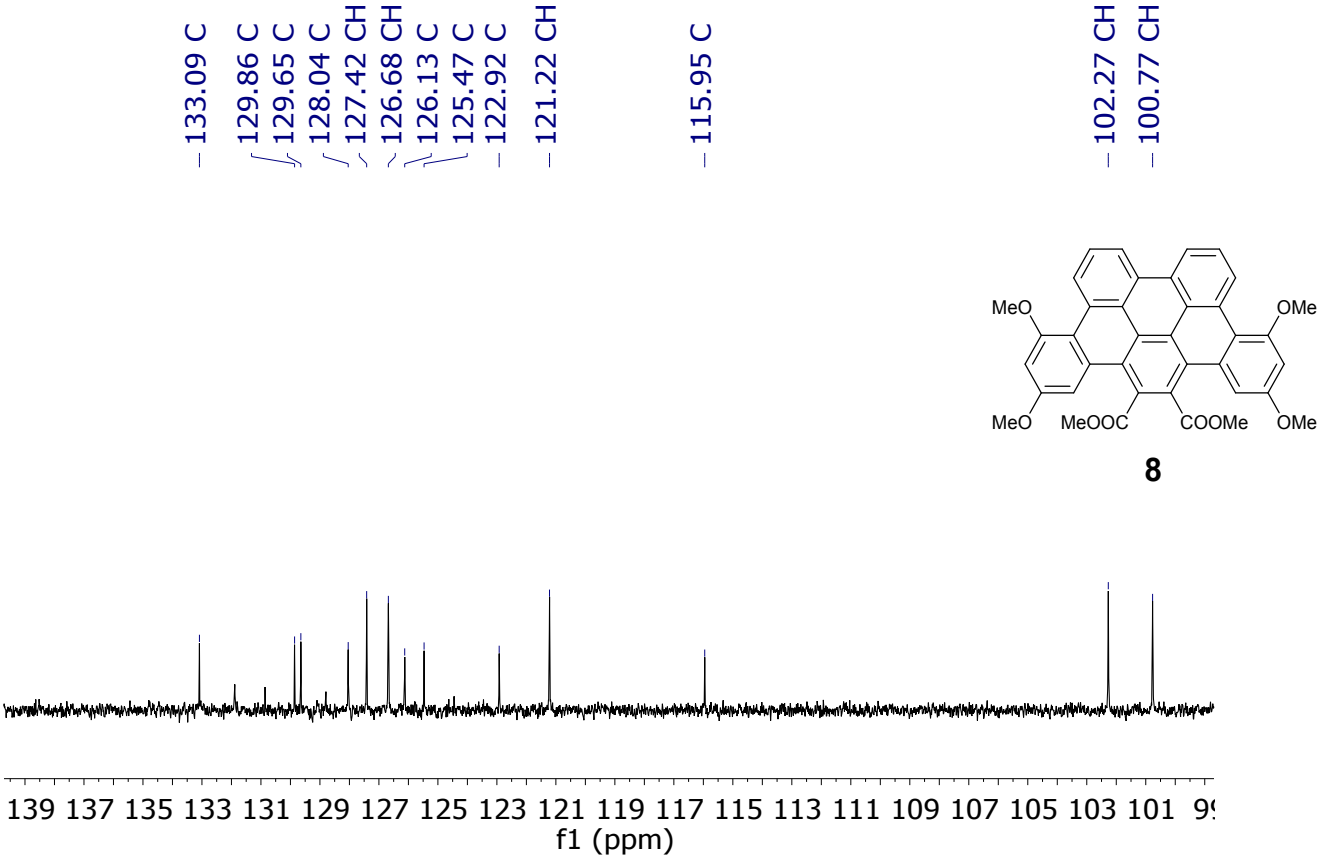
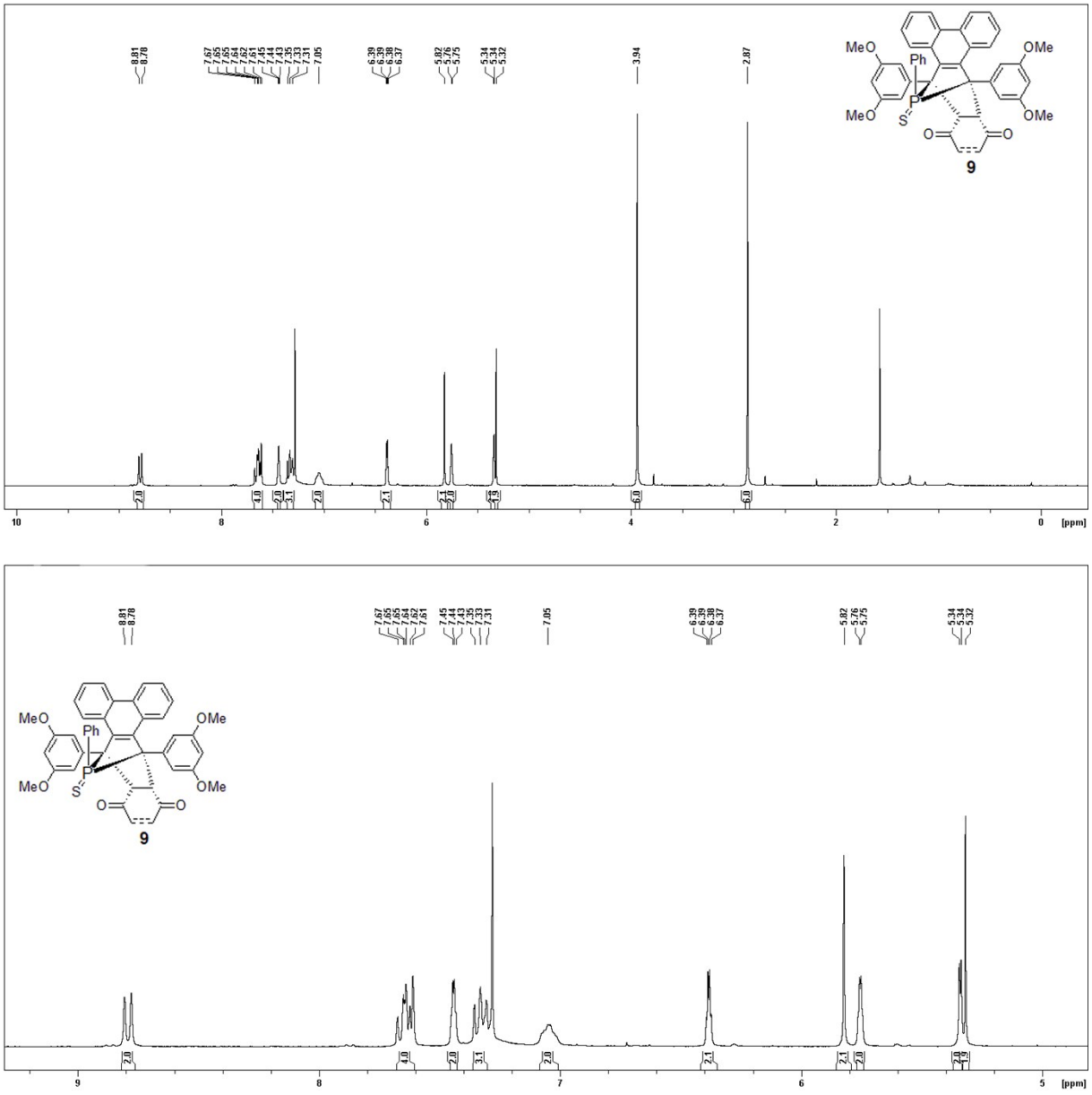
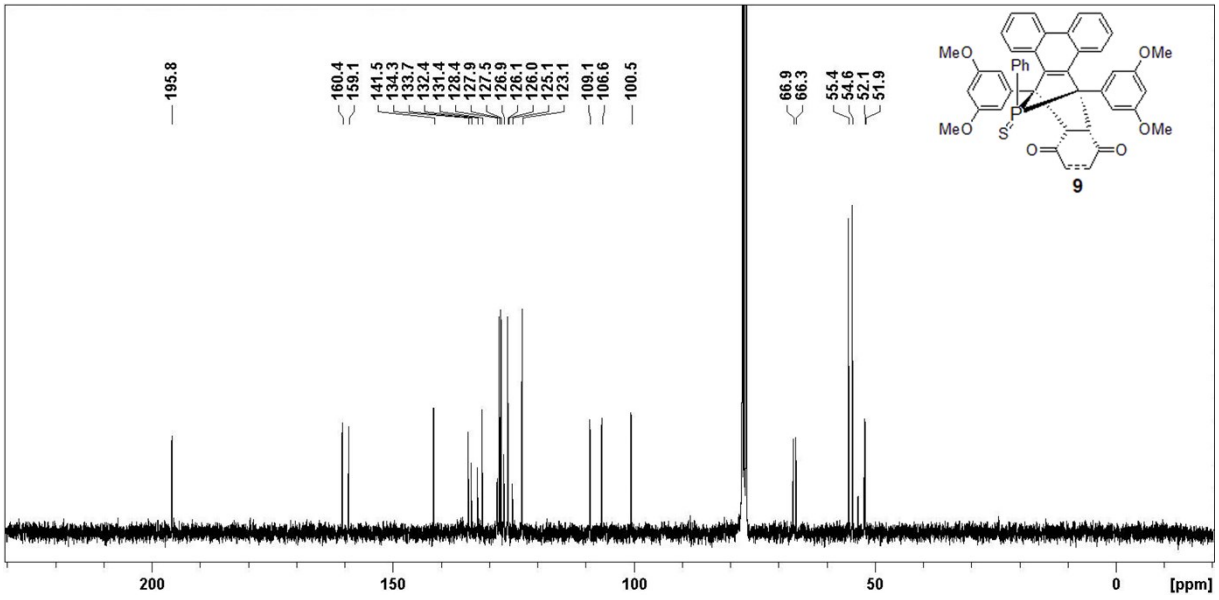
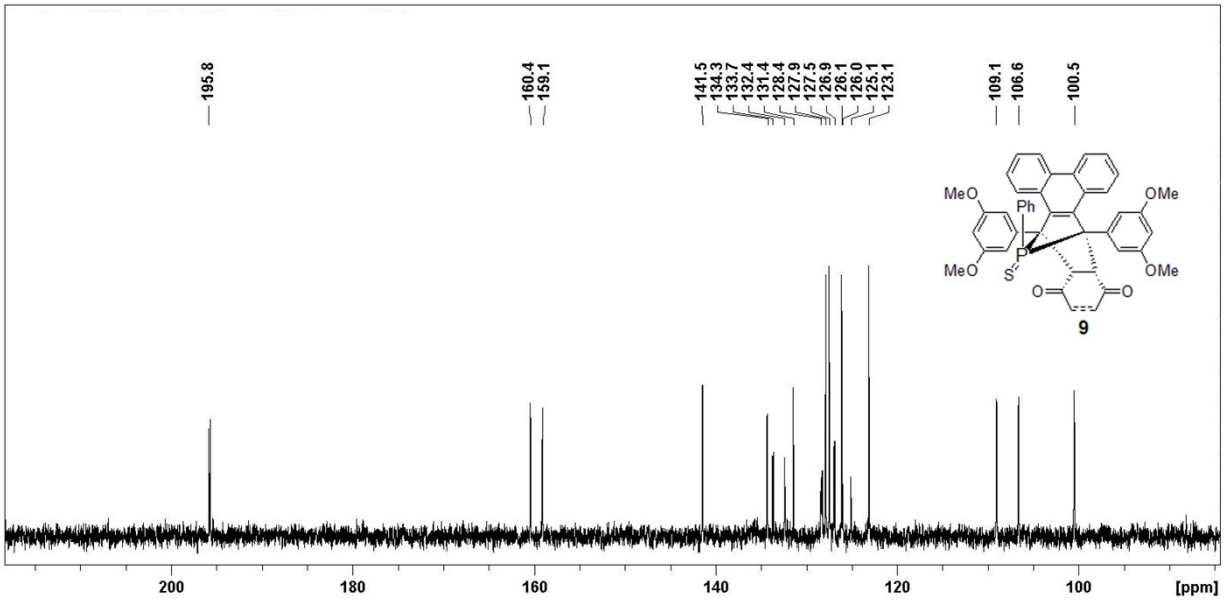

133.09 C
129.86 C
129.65 C
128.04 C
127.42 CH
126.68 CH
126.13 C
125.47 C
122.92 C
121.22 CH
115.95 C
102.27 CH
100.77 CH
MeO
OMe
MeO
MeOOC
COOMe
OMe
8
139 137 135 133 131 129 127 125 123 121 119 117 115 113 111 109 107 105 103 101
f1 (ppm)

Figure S6. ^{1}H NMR (300 MHz, $CDCl_3$), $^{13}C\{^{1}H\}$ NMR (75 MHz, $CDCl_3$) and $^{31}P\{^{1}H\}\{^{13}C\}$ NMR of **9**.




195.8
160.4
159.1
141.5
134.3
133.7
132.4
131.4
128.4
127.9
127.5
126.9
126.1
126.0
125.1
123.1
109.1
106.6
100.5
66.9
66.3
55.4
54.6
52.1
51.9
MeO
OMe
Ph
P
S
O
9
200
150
100
50
0
[ppm]


195.8
160.4
159.1
141.5
134.3
133.7
132.4
131.4
128.4
127.9
127.5
126.9
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126.0
125.1
123.1
109.1
106.6
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OMe
Ph
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S
O
9
200
180
160
140
120
100
[ppm]

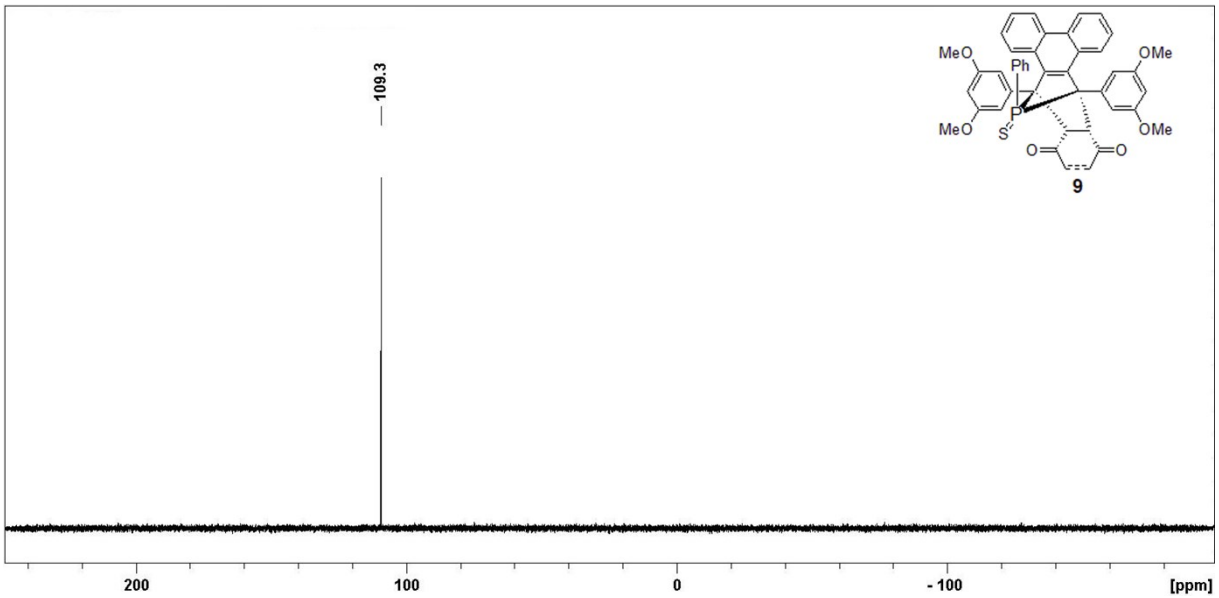
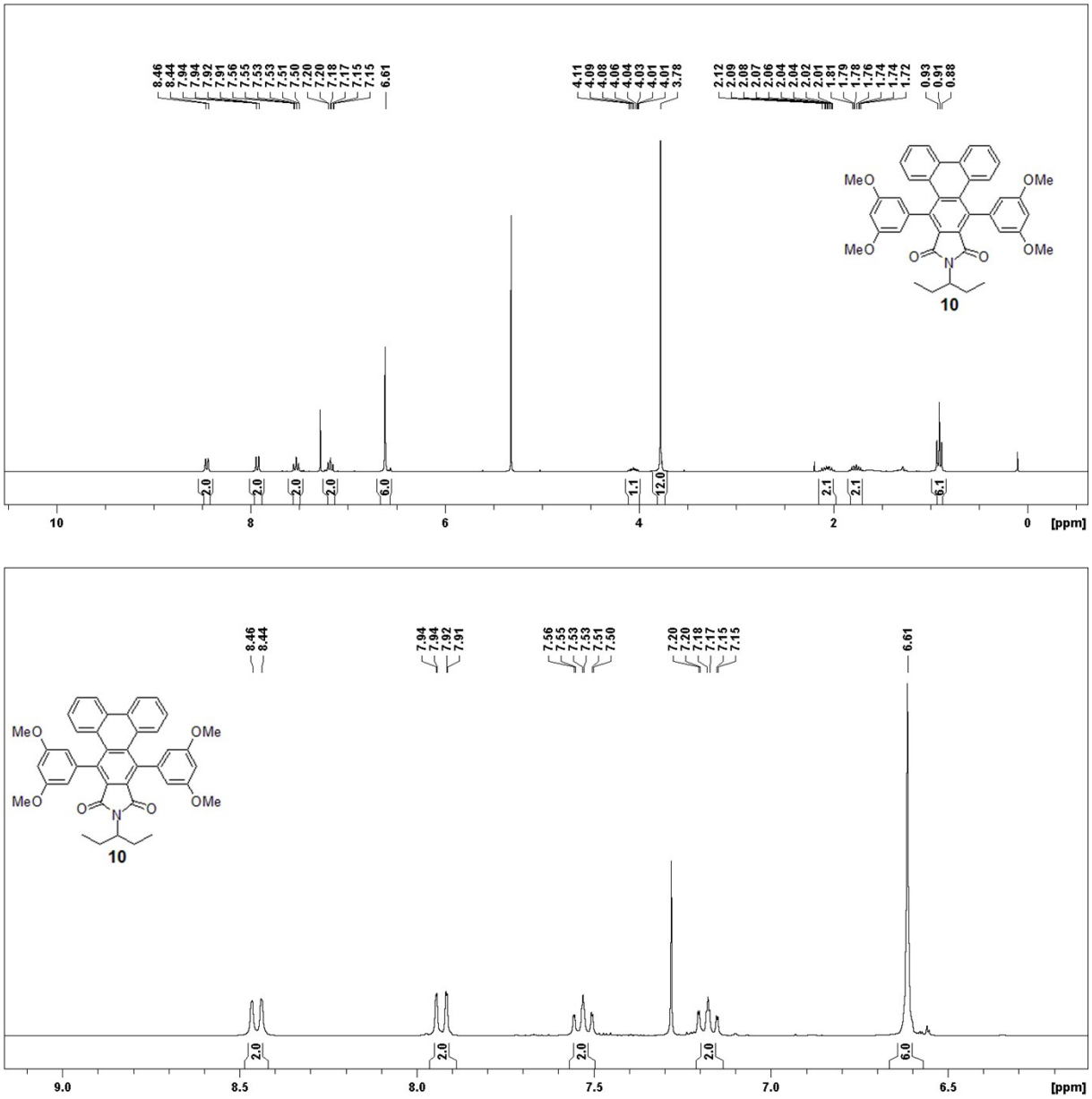
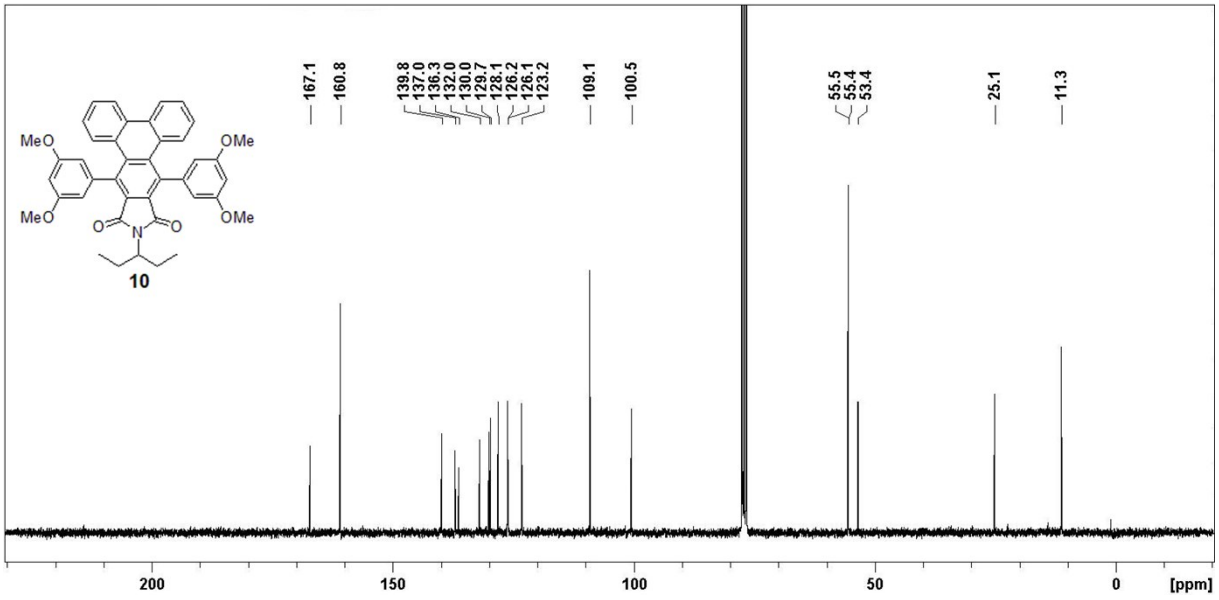

109.3
MeO
OMe
Ph
P
S
O
9
200
100
0
- 100
[ppm]

Figure S7. ^{1}H NMR (300 MHz, $CDCl_3$) and $^{13}C\{^{1}H\}$ NMR (75 MHz, $CDCl_3$) of **10**.




167.1
160.8
139.8
137.0
136.3
132.0
130.0
129.7
128.1
126.2
126.1
123.2
109.1
100.5
55.5
55.4
53.4
25.1
11.3
MeO
OMe
MeO
OMe
O
N
O
10
200
150
100
50
0
[ppm]

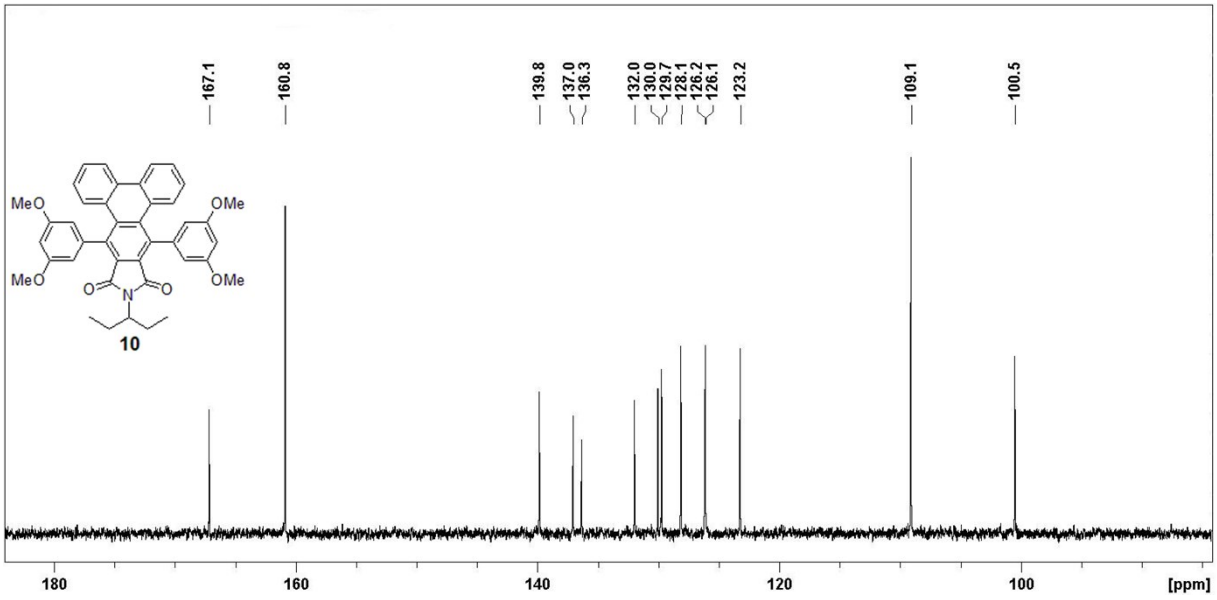

167.1
160.8
139.8
137.0
136.3
132.0
130.0
129.7
128.1
126.2
126.1
123.2
109.1
100.5
MeO
OMe
MeO
OMe
O
N
O
10
180
160
140
120
100
[ppm]

Figure S8a: $^{31}P\{1H\}$ NMR of the crude reaction mixture of **3** after 48h of heating in chlorobenzene (160°C) in absence of DMAD.

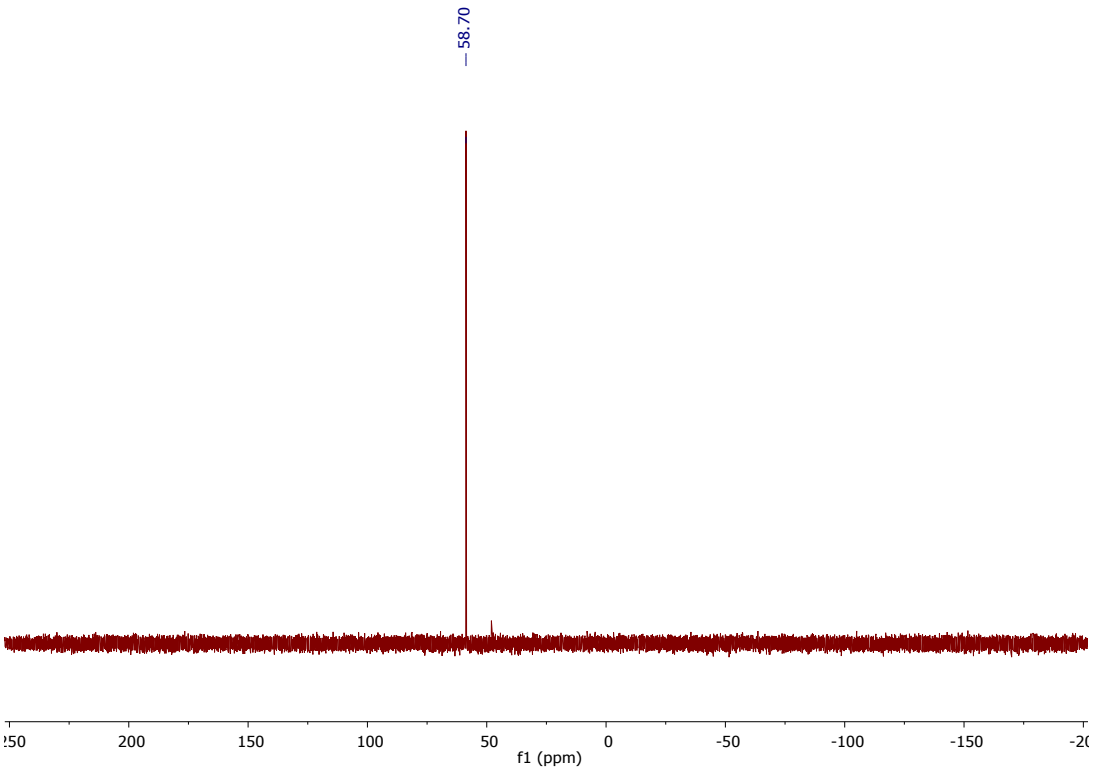
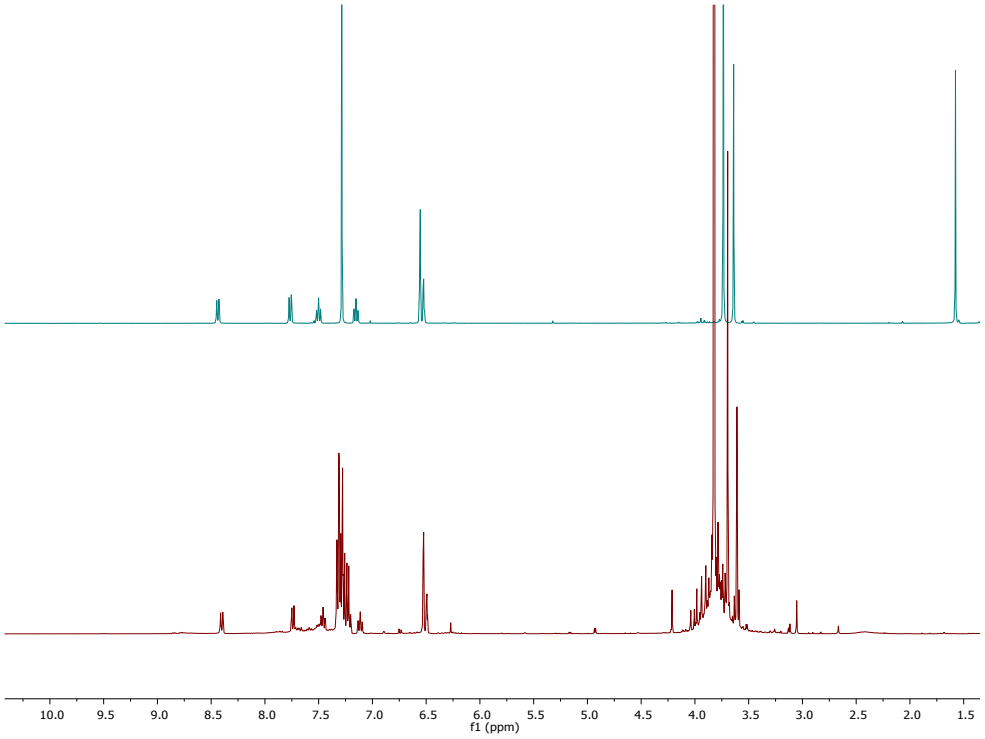


Figure S8b. ^{1}H NMR (400 MHz, $CDCl_3$) of purified **6** (top) and the crude reaction mixture (bottom).



X-ray Crystallographic Study:

Crystal structure determination: Single crystals suitable for X-Ray crystal analysis were obtained by slow diffusion of pentane vapors into a dichloromethane solution of the derivatives at room temperature. For compound **6** single crystal data collection were performed at 150 K with an APEX II Bruker-AXS diffractometer (Centre de Diffractométrie X, Institut des Sciences Chimiques de Rennes, UMR6226 CNRS-Université de Rennes 1, France) with Mo-*K*α radiation (λ = 0.71073 Å), all the others diffraction data were collected on a D8 Venture Bruker-AXS diffractometer (Mo-*K*α radiation). The crystal structures were solved by dual-space algorithm using the SHELXT[2a] program for all compounds except compound **2** that has been solved using direct methods and the *SIR97* program[1b]. Crystal structures were refined with full-matrix least-square methods based on F^2 (*SHELXL-97*)[2] with the aid of the *WINGX*[3] program. All non-hydrogen atoms were refined with anisotropic atomic displacement parameters. H atoms were finally included in their calculated positions. Data of **7** were collected at low temperature (T=150K) on a high flux X-ray microsource diffractometer, of a very thin yellow stick, showing very poor diffraction power; even using long exposition time (320 sec/deg.) during rotation scans, the quality of the final data set was quite poor (Rint~19%), leading to a low quality of the structural refinement (R1~20%). However, this crystal structure shows unambiguously the negative curvature. Note that the asymetric unit cell contains two crystallographically independent molecules of **7**, showing each of them the same curvature character.

Checkcif revealed the presence of a B alert (ADDSYM Detects New (Pseudo) Symm. Elem) for **10** which can be explained by the presence of two slightly different molecules of **10** in the asymetric unit.

[1a] G. M. Sheldrick, Acta Cryst. A71 (2015) 3-8
[1b] Altomare, A., Burla, M. C.; Camalli, M., Cascarano, G., Giacovazzo, C., Guagliardi, A., Moliterni, A. G. G., Polidori, G. R. Spagna, *J. Appl. Cryst.*, **1999**, 32, 115-119
[2] Sheldrick G.M., *Acta Cryst.* A, **2008**, 64, 112-122
[3] Farrugia, L. J. *J. Appl. Cryst.*, **2012**, 45, 849-854

TABLE S1: CRYSTAL DATA AND STRUCTURE REFINEMENT

Compound	**1**	**6**	**7**	**8**	**9**	**10**
CCDC	1973069	1895041	1956170	1895043	1895042	1973065
Formula	$C_{26}H_{15}OP$, CH_2Cl_2	C38H32O8	C38H30O8	C38H28O8	C45H37O6P1S1Cl2	$C_{41}H_{37}NO_6$
MW	459.27	616.64	614.62	612.6	807.67	639.71
a (Å)	7.7006(4)	9.1526(4)	13.107(2)	9.7076(4)	12.2704(11)	9.4795(9)
b (Å)	19.7017(12)	13.7940(6)	13.566(2)	11.8242(4)	12.9162(10)	13.3263(11)
c (Å)	27.3827(16)	15.1145(6)	32.525(6)	12.4785(4)	14.0637(11)	26.101(3)
α (°)	90	107.493(2)	90	87.7010(10)	105.461(3)	94.943(3)
β (°)	90	92.096(2)	90.549(8)	78.0410(10)	91.247(3)	98.261(4)
γ (°)	90	102.376(2)	90	89.1850(10)	115.181(3)	98.981(3)
V (Å^3)	4154.4(4)	1767.20(13)	5783.2(18)	1400.10(9)	1920.6(3)	3203.1(5)
Z	8	2	8	2	2	4
*D*c (g.cm^{-3})	1.469	1.159	1.412	1.453	1.397	1.327
Crystal system	orthorhombic	triclinic	monoclinic	triclinic	triclinic	triclinic
Space group	*P b c a*	P -1	P 2_1/c	P -1	P -1	P -1
T (K)	150	150	150	150	150	150
Wavelength Mo-Kα (Å)	0.71073	0.71073	0.71073	0.71073	0.71073	0.71073
μ (mm^{-1})	0.408	0.081	0.099	0.102	0.316	0.089
F (000)	1888	648	2576	640	840	1352
θ limit (°)	2.936-27.459	2.29-27.48	2.161-28.017	2.35-27.45	2.58- 27.48	2.914-27.484
Index ranges *hkl*	-9<h<8 -25<k<25 -35<l<35	-11<h<11 -17<k<17 -15<l<19	-16<h<16 -17<k<17 -42<l<42	-12<h<12 -15<k<15 -16<l<15	-15<h<15 -16<k<16 -18<l<17	-12<h<12 -16<k<17 -33<l<33
Reflections collected	24415	25202	49197	23410	43243	90824
Reflections [*I*>2σ(*I*)]	3800	6319	7391	5072	6557	10819
Data / restraints / parameters	4612 / 0 / 280	8015/0/ 421	13385/0/ 559	6376/0/421	8789/0/ 501	14695/0/877
Goodness-of-fit on F^2	1.018	1.113	1.112	1.040	1.088	1.014
Final *R* indices [I>2σ(I)]	R1 = 0.0634 wR2=0.1575	R1 = 0.0473 wR2=0.1405	R1 = 0.2032 wR2=0.4287	R1 = 0.0397 wR2= 0.104	R1 = 0.0542 wR2= 0.1235	R1 = 0.0456 wR2= 0.1031
R indices (all data)	*R1* = 0.0772 *wR*2 = 0.1686	R1 = 0.0587 wR2 = 0.1492	R1 = 0.2878 wR2 = 0.4658	R1 = 0.0539 wR2 = .1129	R1 = 0.0818 wR2 = 0.1359	R1 = 0.0721 wR2 = 0.1159
Largest diff peak and hole (e Å^{-3})	1.667 -1.321	0.304 -0.212	1.154 –0.817	0.325 -0.23	1.092 -1.202	0.350-0.272

Figure S9. Molecular structure of **1.**CH_2Cl_2 (thermal ellipsoids 50% probability).

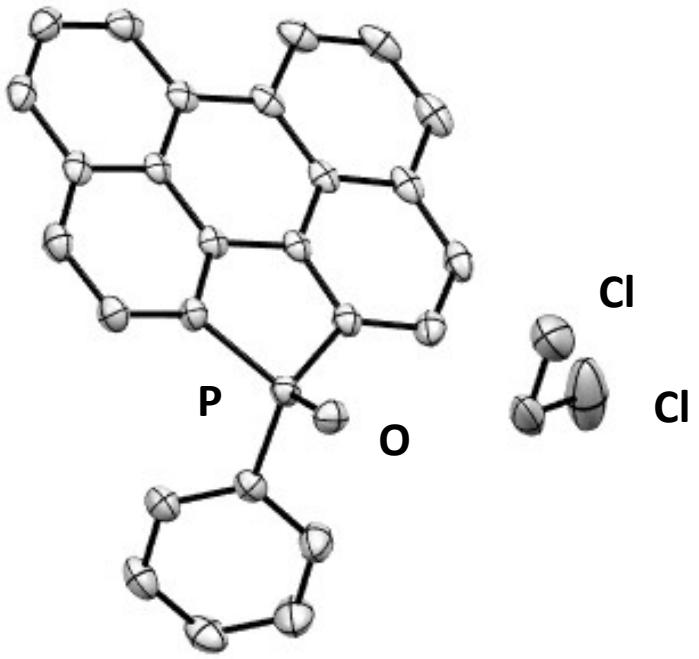


Figure S10. Molecular structure of **6** (thermal ellipsoids 50% probability).

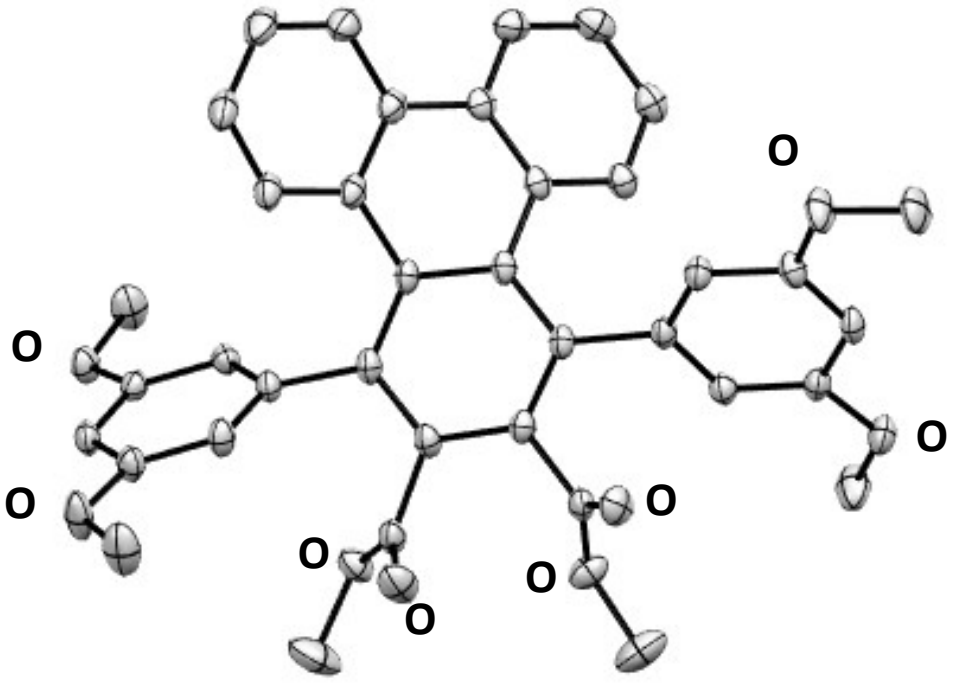


Figure S11. Molecular structure of **7** (thermal ellipsoids 50% probability).

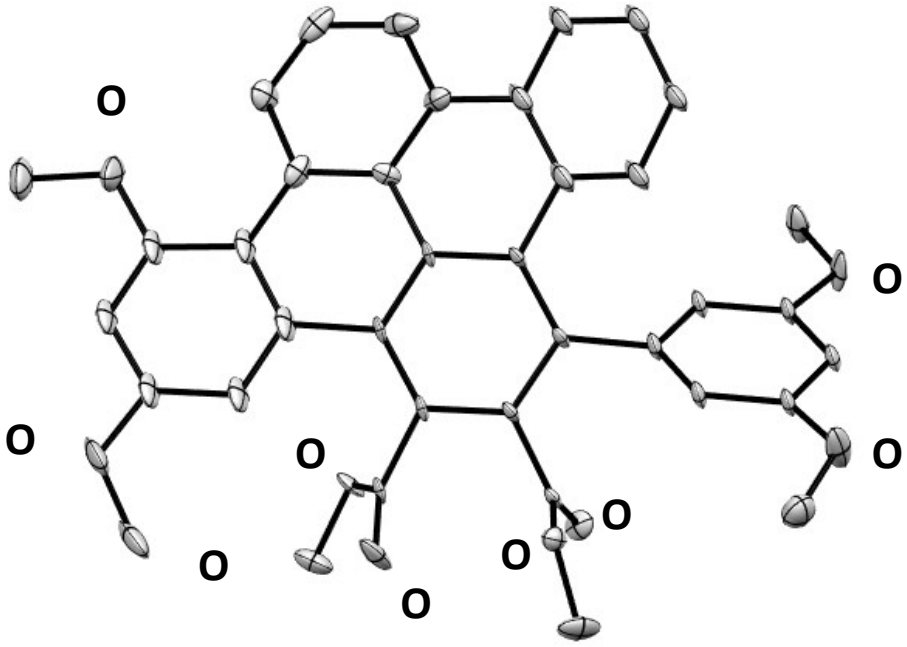


Figure S12. Molecular structure of **8** (thermal ellipsoids 50% probability).

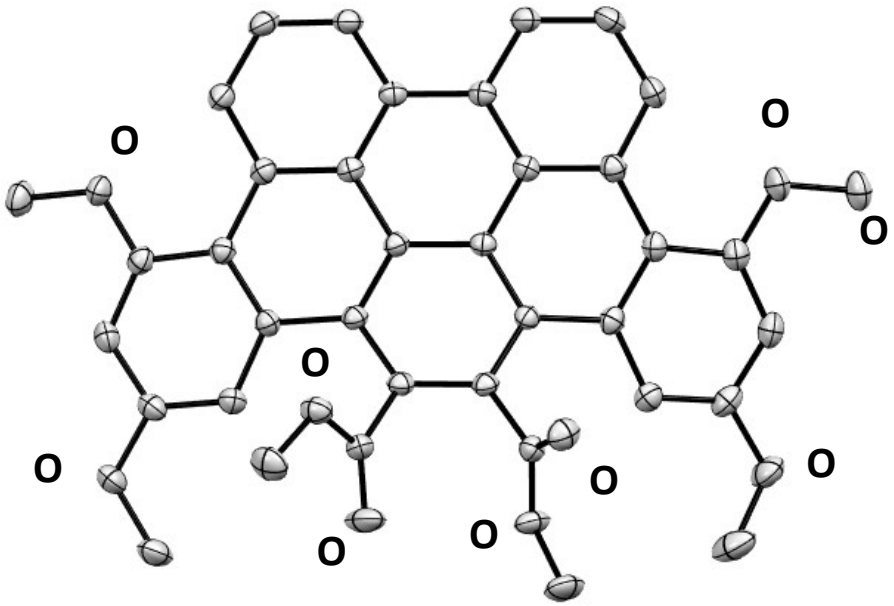


Figure S13. Molecular structure of **10** (thermal ellipsoids 50% probability).

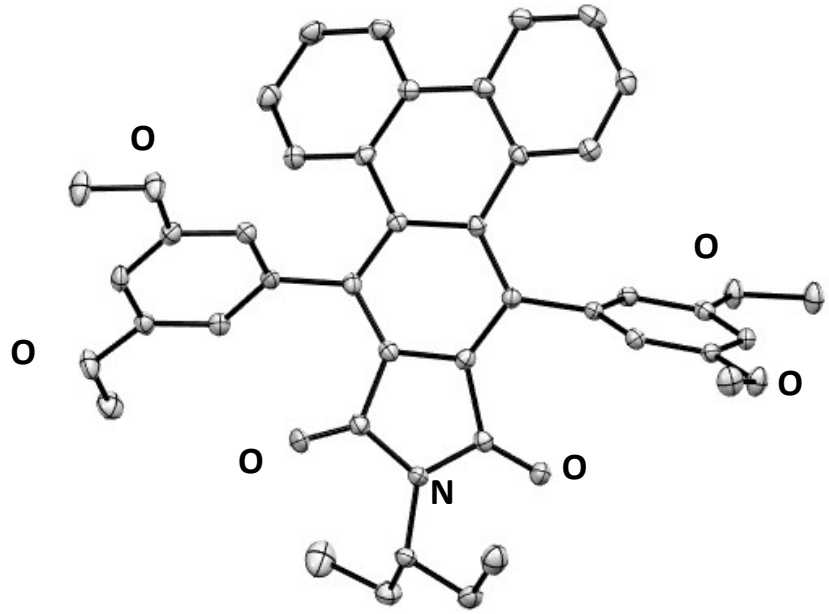


Figure S14. Molecular structure of **9.CH_2Cl_2** (thermal ellipsoids 50% probability).

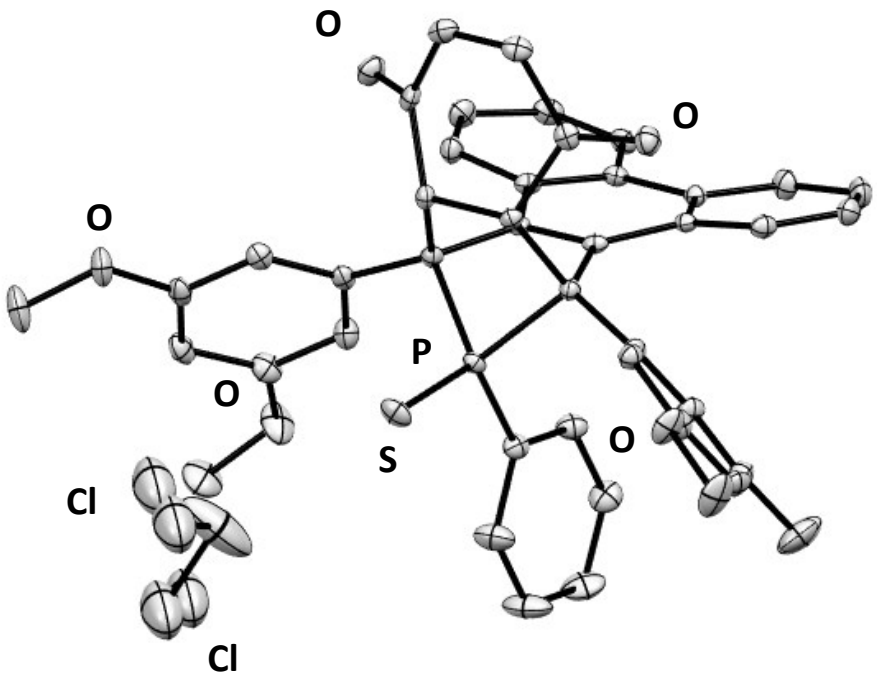
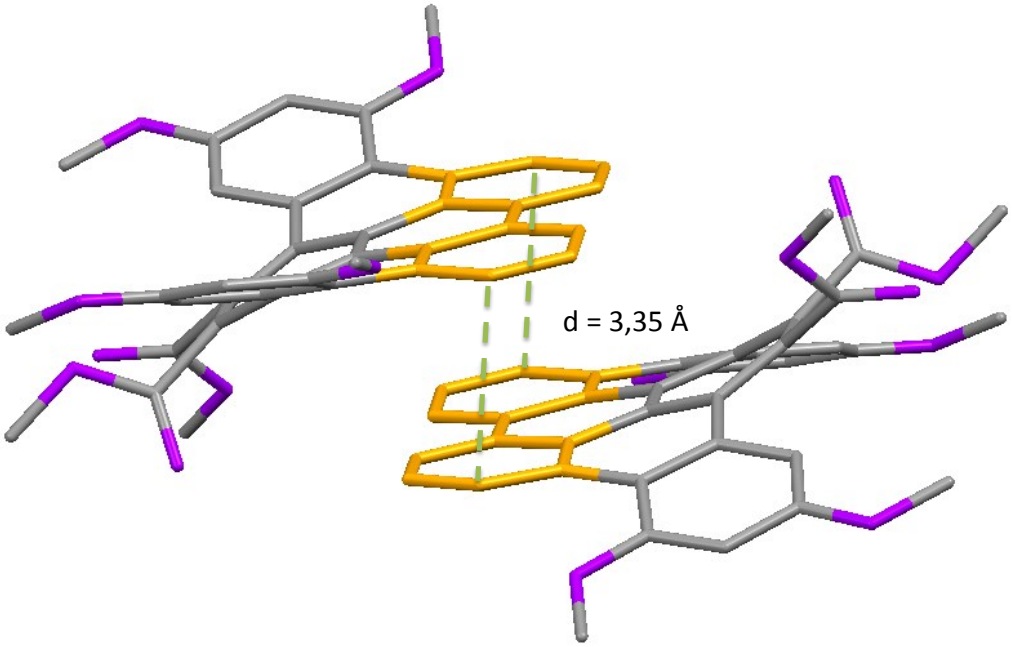


Figure S15. π-dimers observed in the packing of **8**


d = 3,35 Å

Optical and redox properties

Figure S16. Experimental absorption, excitation and emission spectra of **1**

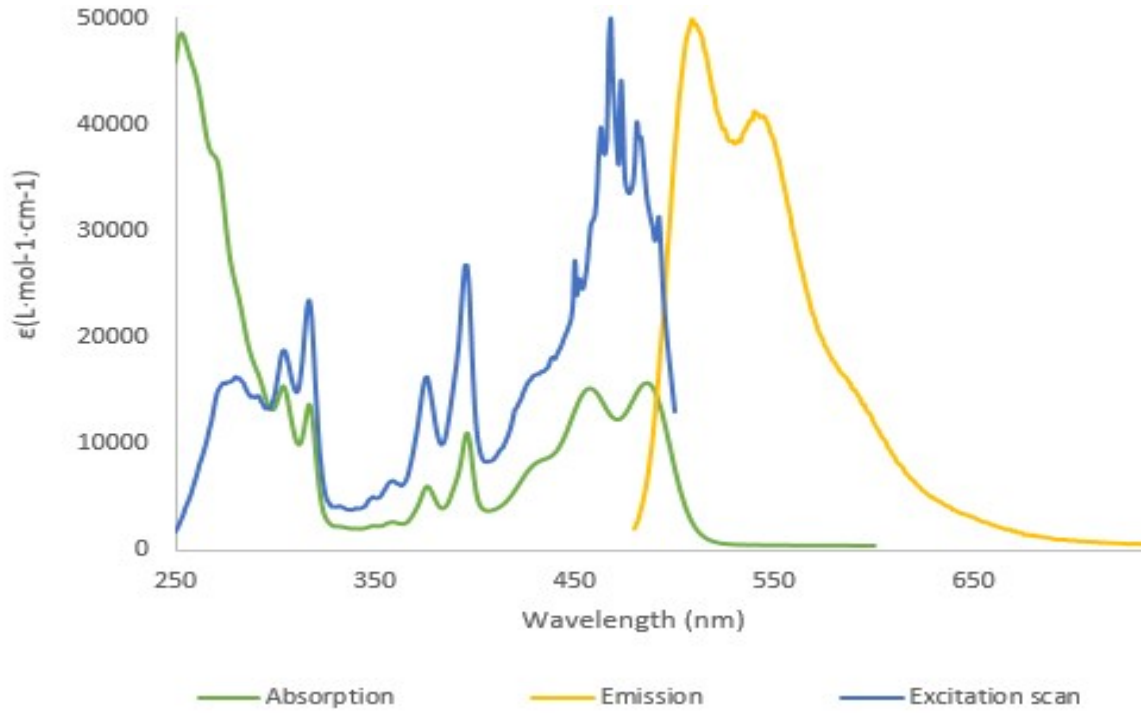


Figure S17. Experimental absorption, excitation and emission spectra of **2**

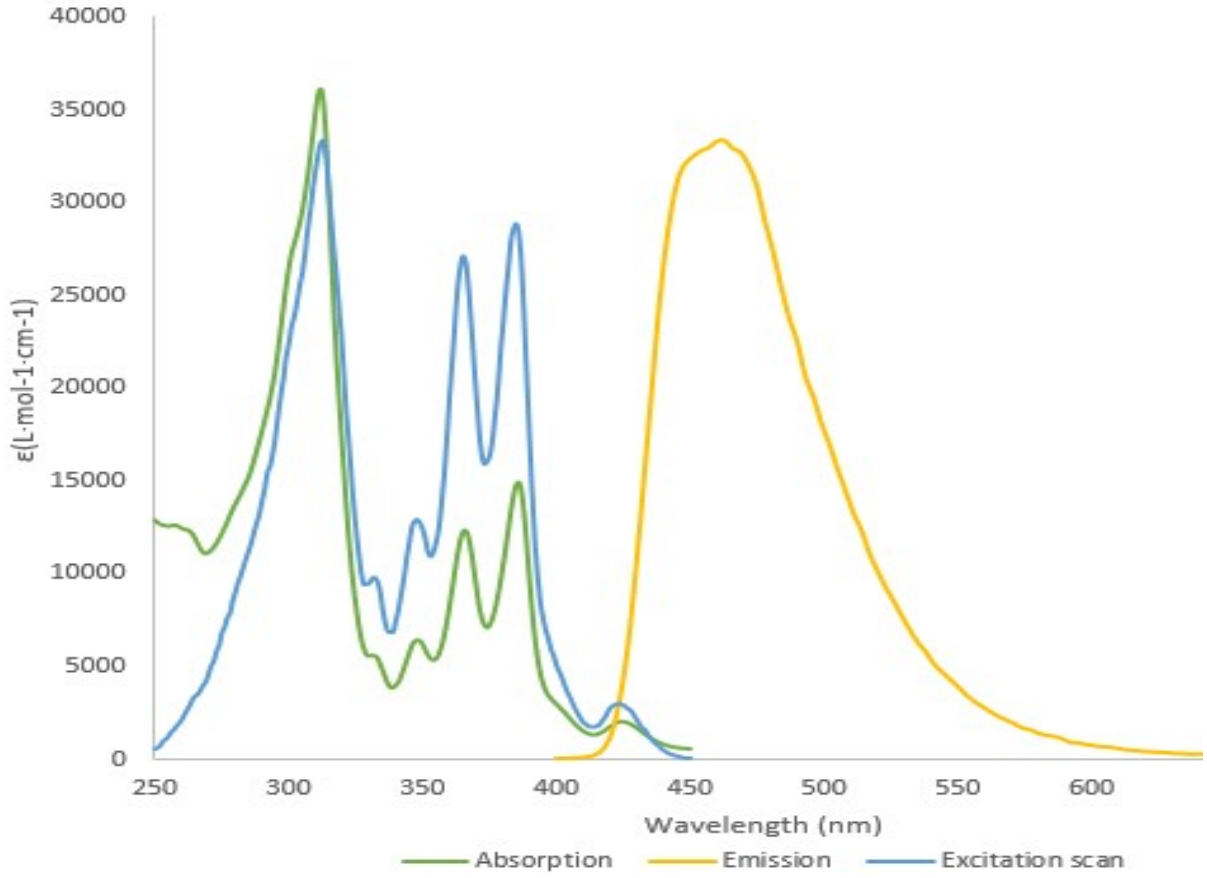


Figure S18: Experimental absorption, excitation and emission spectra of **6**

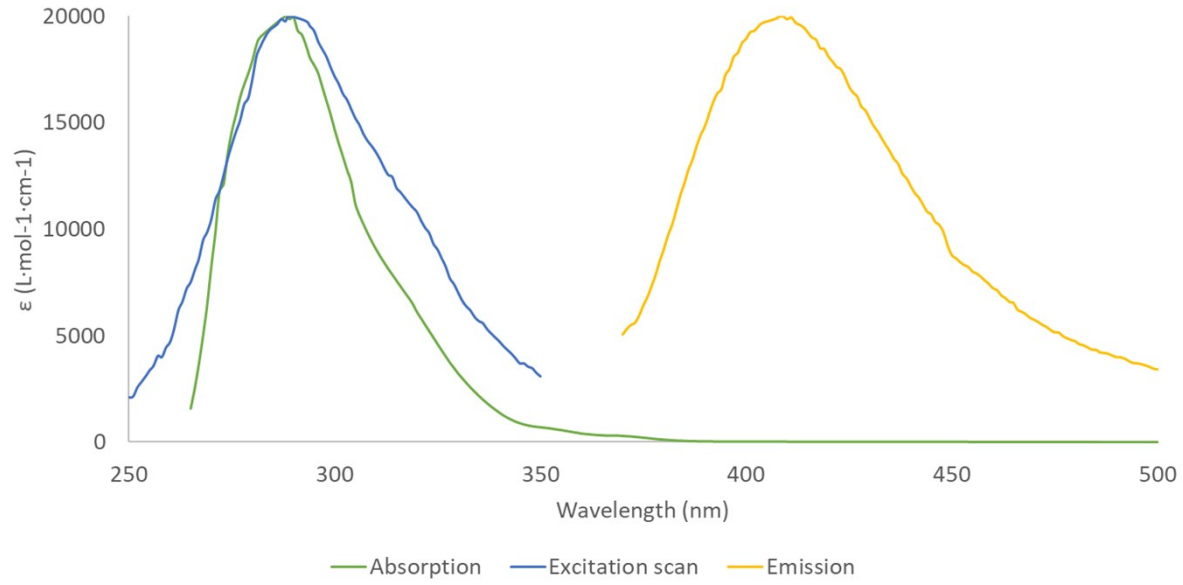


Figure S19. Experimental absorption, excitation and emission spectra of **7**

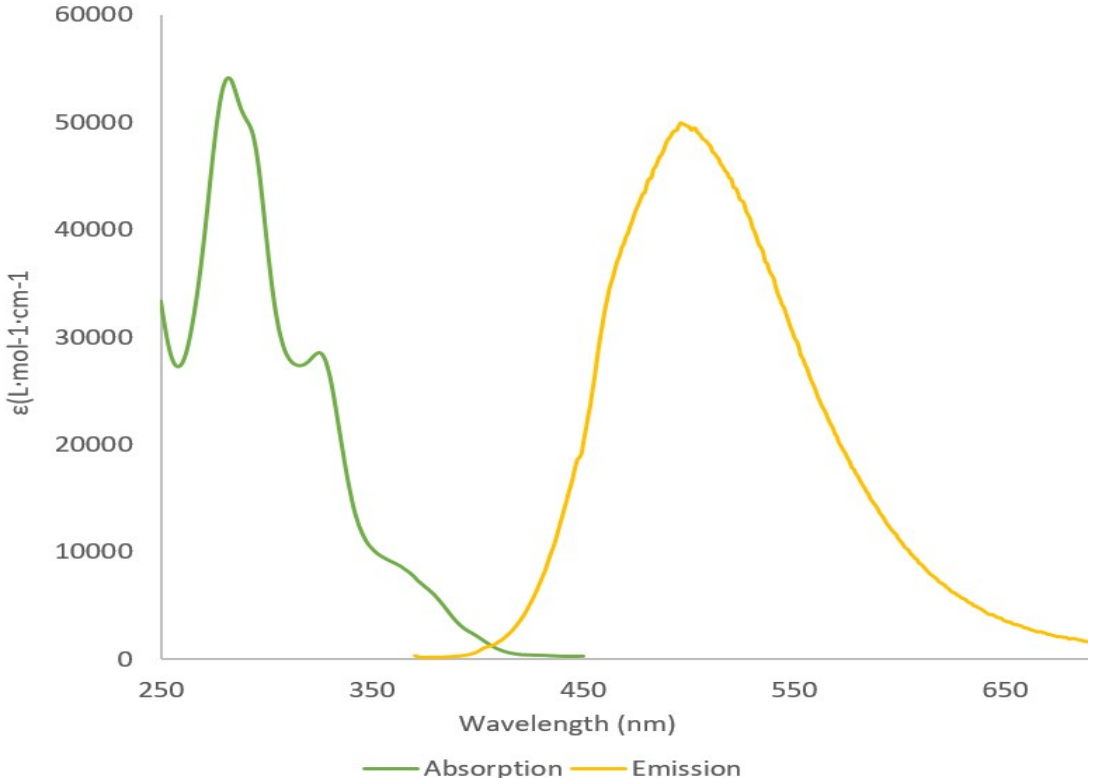
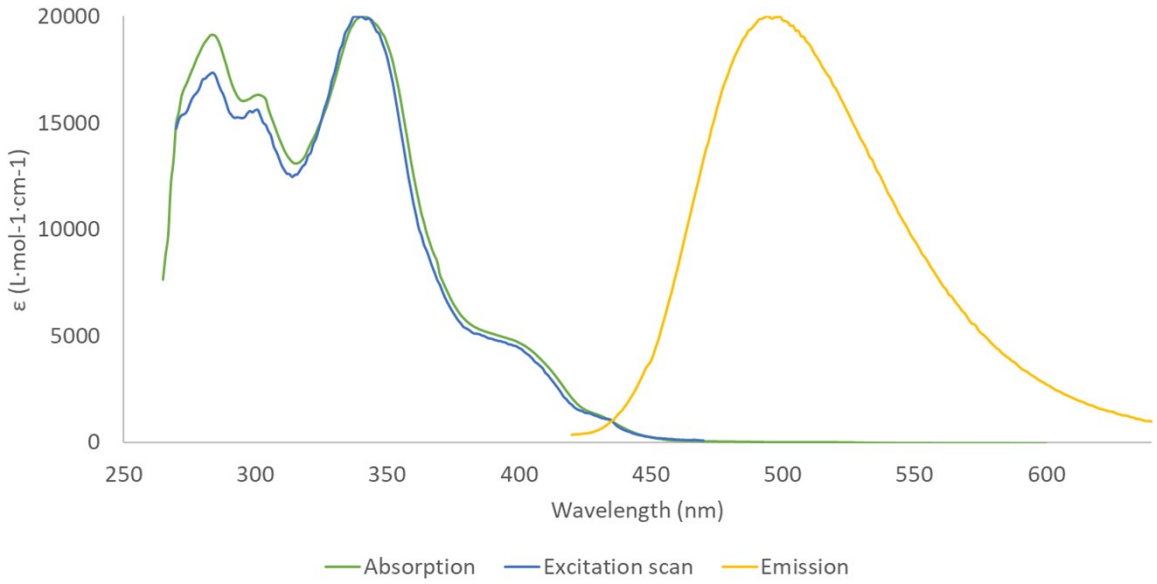


Figure S20. Experimental absorption, excitation and emission spectra of **8**



Electrochemical data

Figure S21: Cyclic voltammogram of **1** (c = 10-3 M) in DCM (Bu_4NPF_6 (0.2 M), 200 mVs−1, potentials vs Fc^+/Fc(*)).

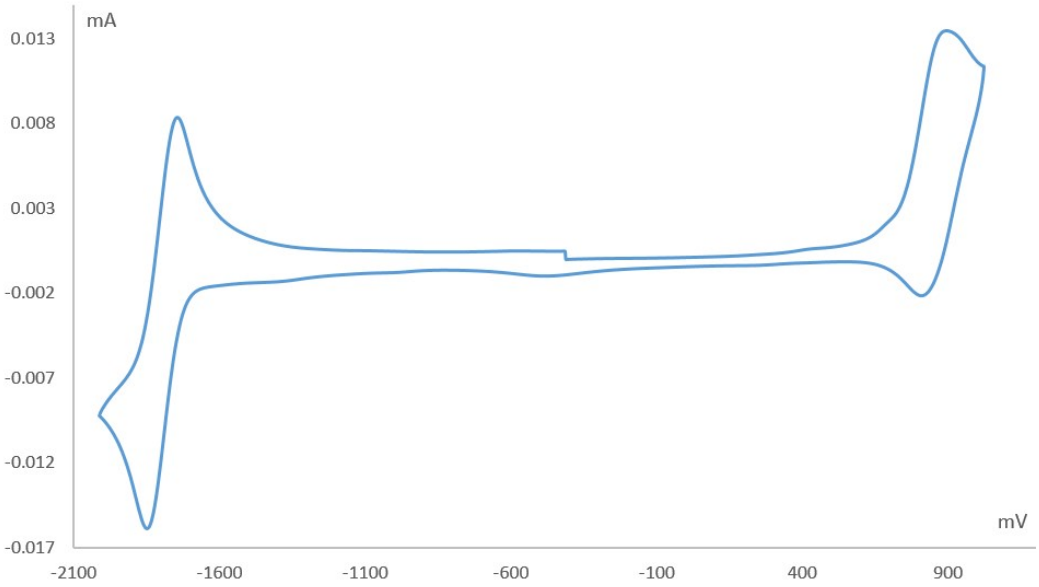


Figure S22: Cyclic voltammogram of **6** (c = 10-3 M) in DCM (Bu_4NPF_6 (0.2 M), 200 mVs−1, potentials vs Fc^+/Fc(*)).

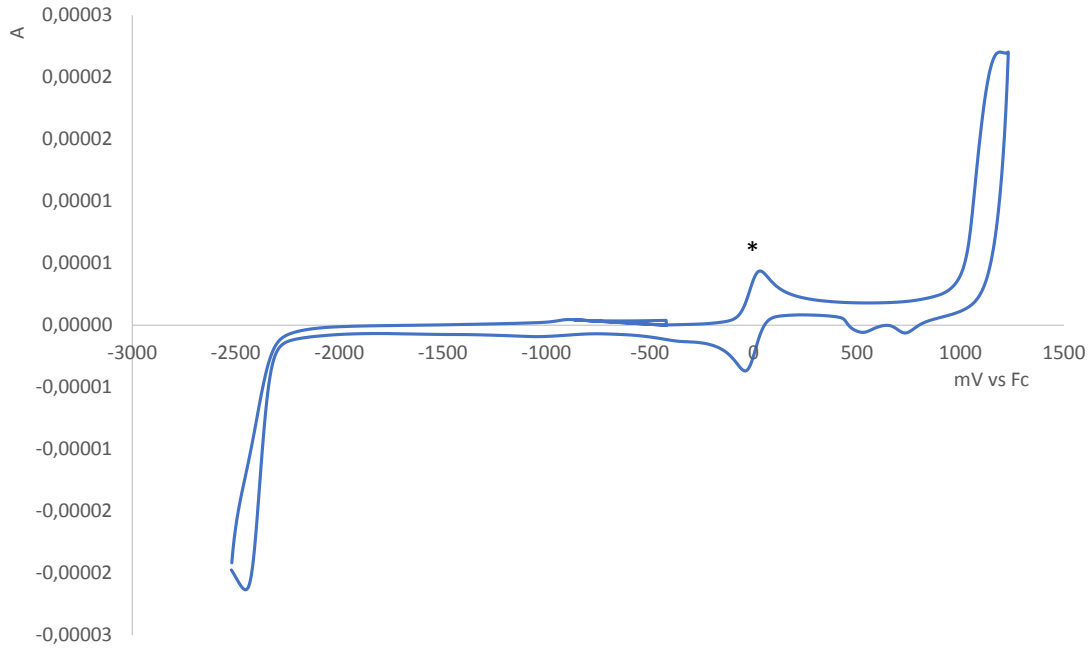


Figure S23: Cyclic voltammogram of **7** (c = 10-3 M) in DCM (Bu_4NPF_6 (0.2 M), 200 mVs−1, potentials vs Fc^+/Fc(*)).

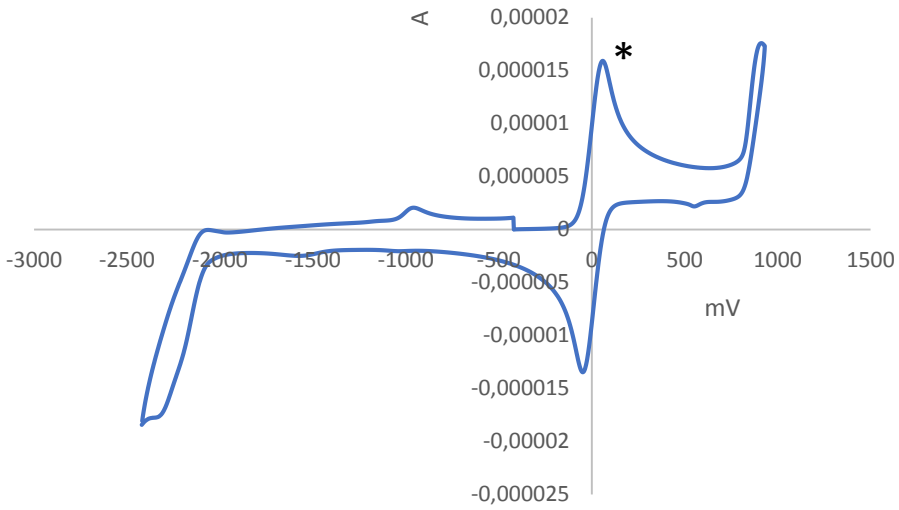
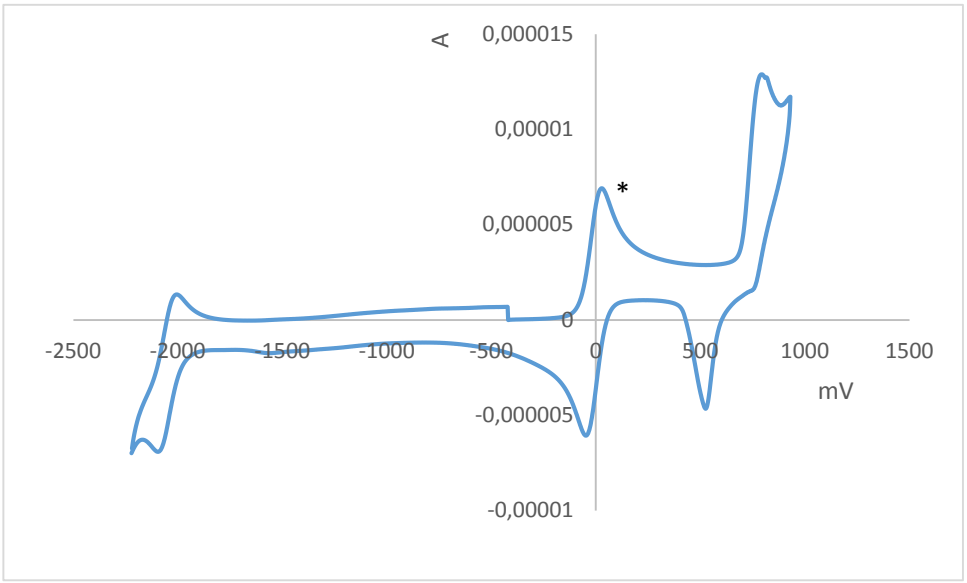


Figure S24: Cyclic voltammogram of **8** (c = 10-3 M) in DCM (Bu_4NPF_6 (0.2 M), 200 mVs−1, potentials vs Fc^+/Fc(*))



Theoretical investigations

To perform the computations the Gaussian 09[4] and MRCC[5] suites of programs were used. All structures were optimized using the B3LYP and B3LYPD3 functionals combined with the 6-31+G* and 6-311+G* basis sets. For the ADC2 method the cc-pVDZ basis set was applied. At each of the optimized structures vibrational analysis was performed to check whether the stationary point located is a minimum on the potential energy hypersurface (no imaginary frequencies were obtained) or in the case of the planar structures the stationary points are not minima, but higher order saddle points on the potential energy surface (see NImag). The molecular orbitals were visualized with Avogadro program[6]. The geometries were plotted with Molden[7,8].

Figure S25. view of the Frontiers Molecular Orbitals of **1** at the B3LYP/6-31+G* level

[4] Gaussian 09 RE 0., M. J. Frisch, G. W. Trucks, H. B. Schlegel GES, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone BM, et al Gaussian 09, Revision E.01 M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2013.

[5] Mrcc, a quantum chemical program suite written by M. Kállay, P. R. Nagy, Z. Rolik, D. Mester, G. Samu, J. Csontos, J. Csóka, B. P. Szab´o, L. Gyevi-Nagy, I. Ladjánszki, L. Szegedy, B. Ladóczki, K. Petrov, M. Farkas, P. D. Mezei, and B. Hégely. See also Z. Rolik, L. Szegedy, I. Ladjánszki, B. Ladóczki, and M. Kállay, J. Chem. Phys. 139, 094105 (2013), as well as: www.mrcc.hu

[6] https://avogadro.cc/

[7] G. Schaftenaar, J.H. Noordik *J. Comput.-Aided. Mol. Des.* **2000**, 14, 123-134.

[8] G. Schaftenaar, E. Vlieg, G. Vriend *J. Comput.-Aided. Mol. Des.* **2017**, 31, 789-800.

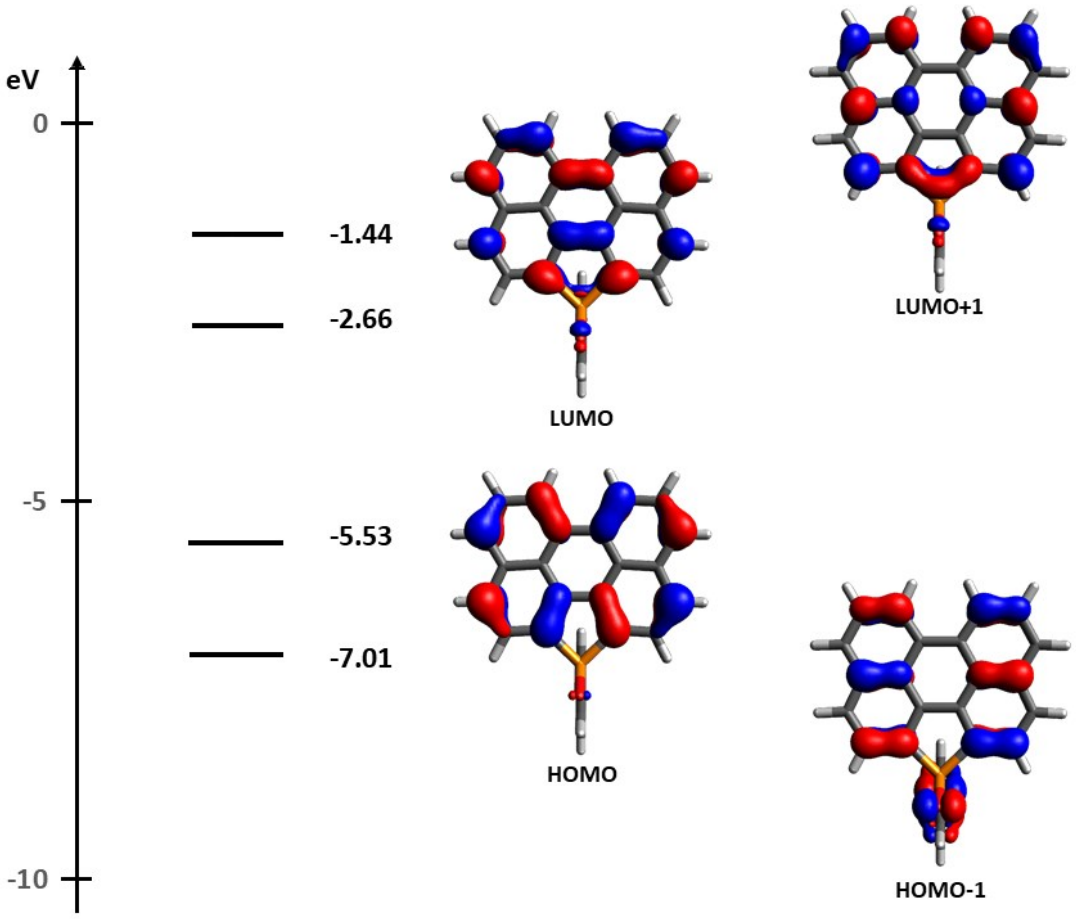


Figure S26. view of the Frontiers Molecular Orbitals of **2** at the B3LYP/6-31+G* level

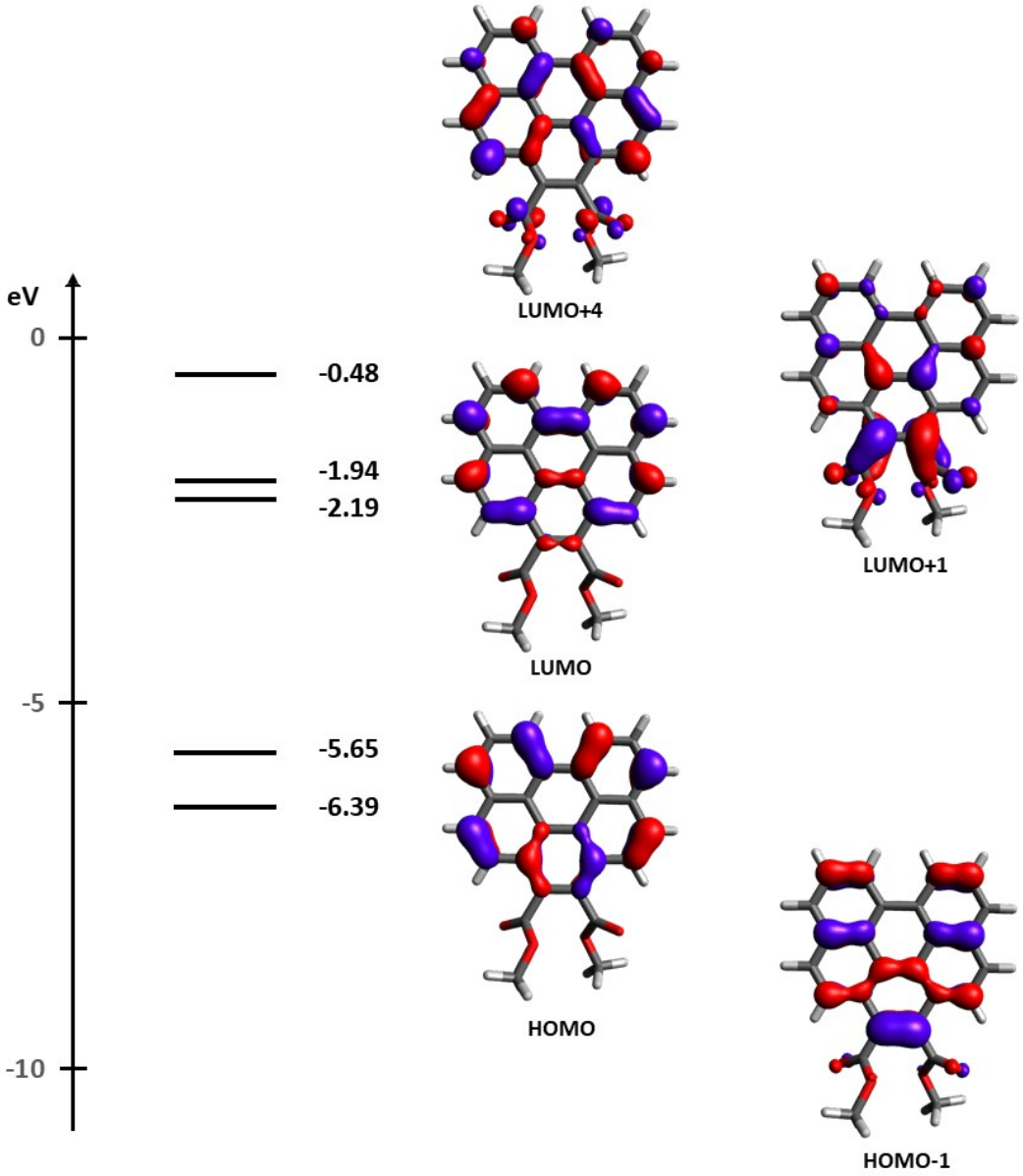


Figure S27. view of the Frontiers Molecular Orbitals of **6** at the B3LYP/6-31+G* level

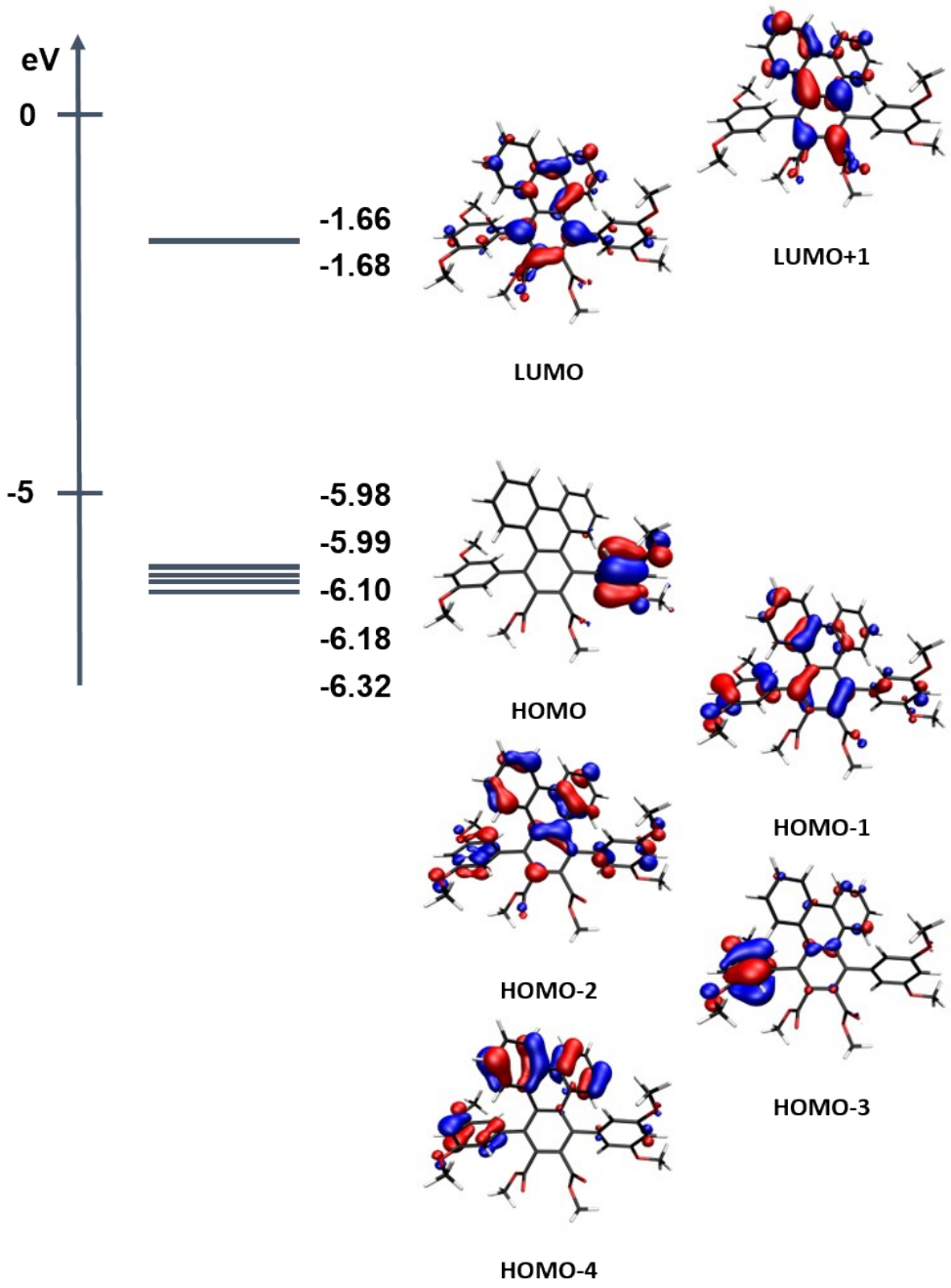


Figure S28. view of the Frontiers Molecular Orbitals of **7** at the B3LYP/6-31+G* level

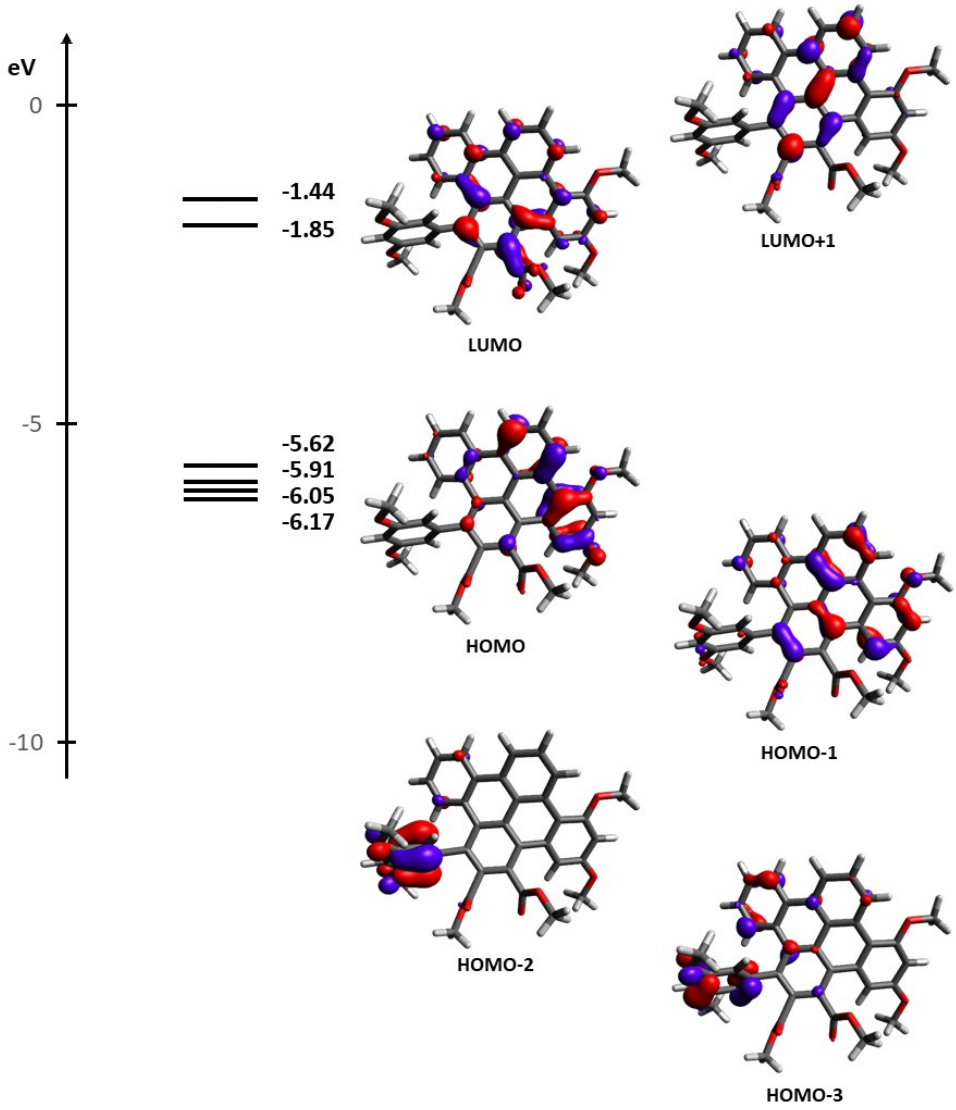


Figure S29. view of the Frontiers Molecular Orbitals of **8** at the B3LYP/6-31+G* level

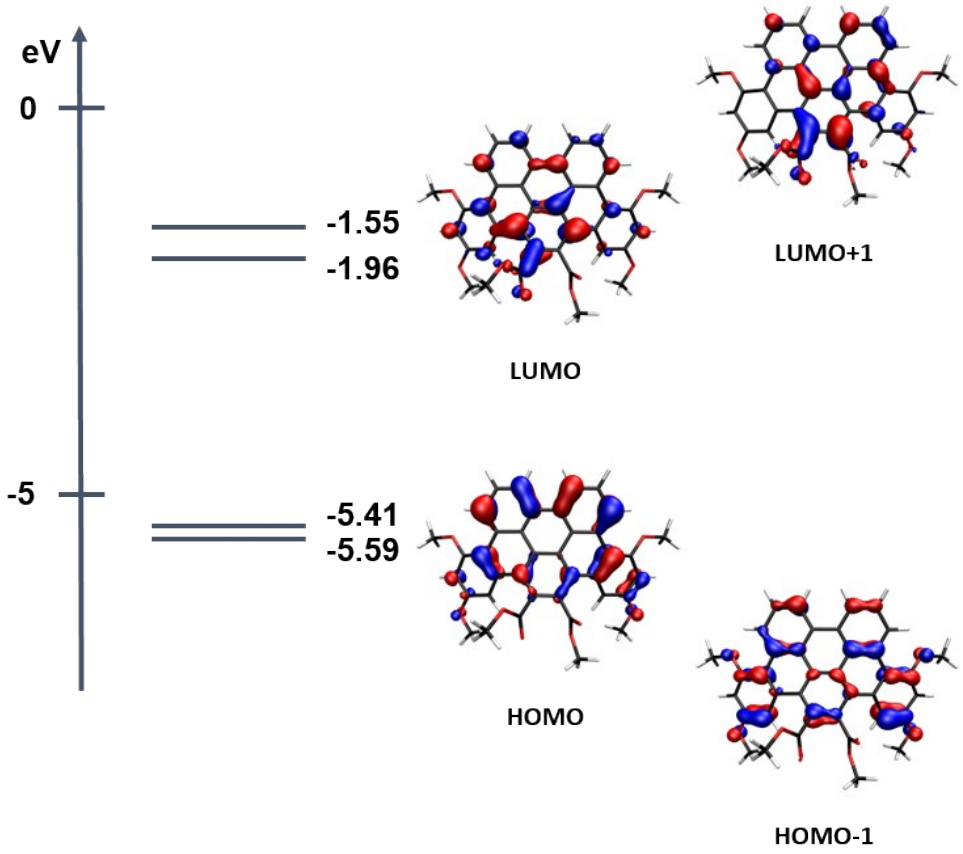


Figure S30. view of the optimized geometry of **6planar** at the B3LYP/6-31+G* level

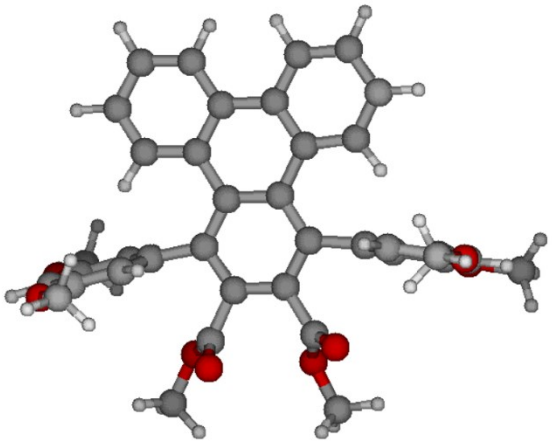


Figure S31. view of the optimized geometry of **7planar** at the B3LYP/6-31+G* level

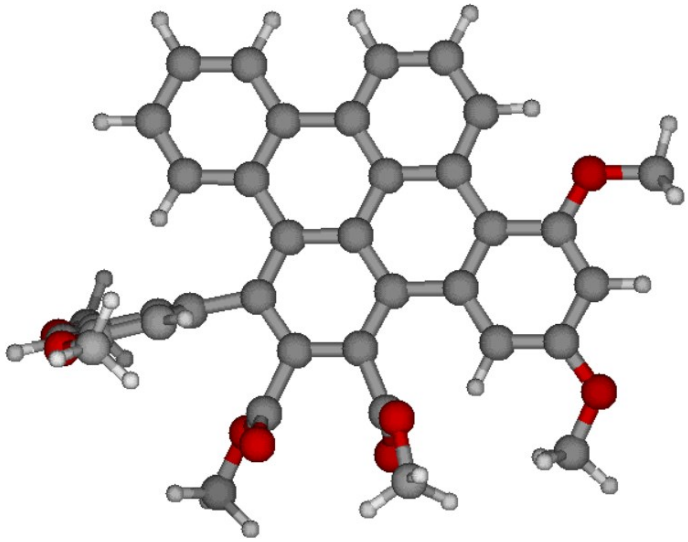


Figure S32. view of the optimized geometry of **8planar** at the B3LYP/6-31+G* level

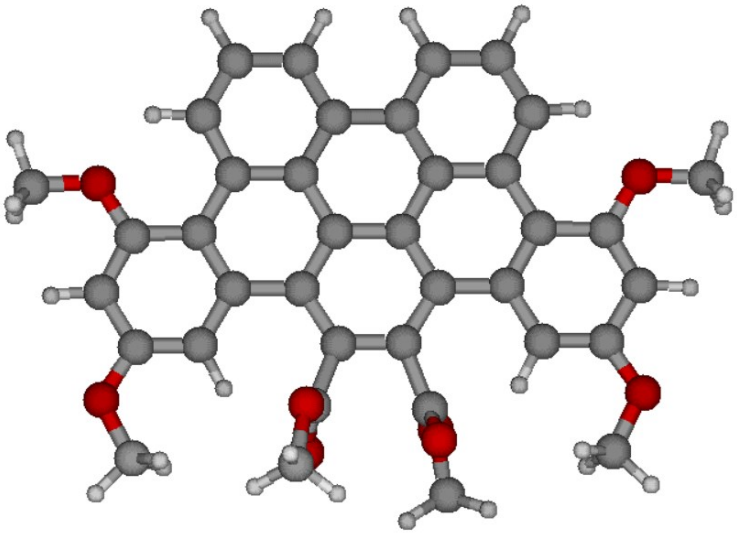


Figure S33. view of the optimized geometry of **8twisted** at the B3LYP/6-31+G* level

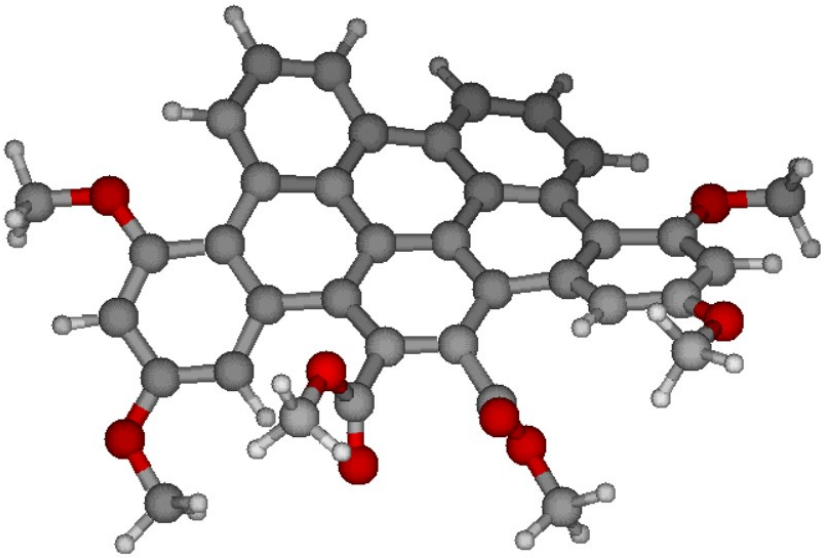


Figure S34. DFT optimized structure of **7** (top and side view)

7 possesses a negative curvature with angles between peripheral benzene ring (red and orange in **Fig. S11**) of 142.9° (140.6° from the X-ray data) and angles between the two central rings (blue and green) of 28.4° (22.2° from the X-ray data) in the opposite direction.

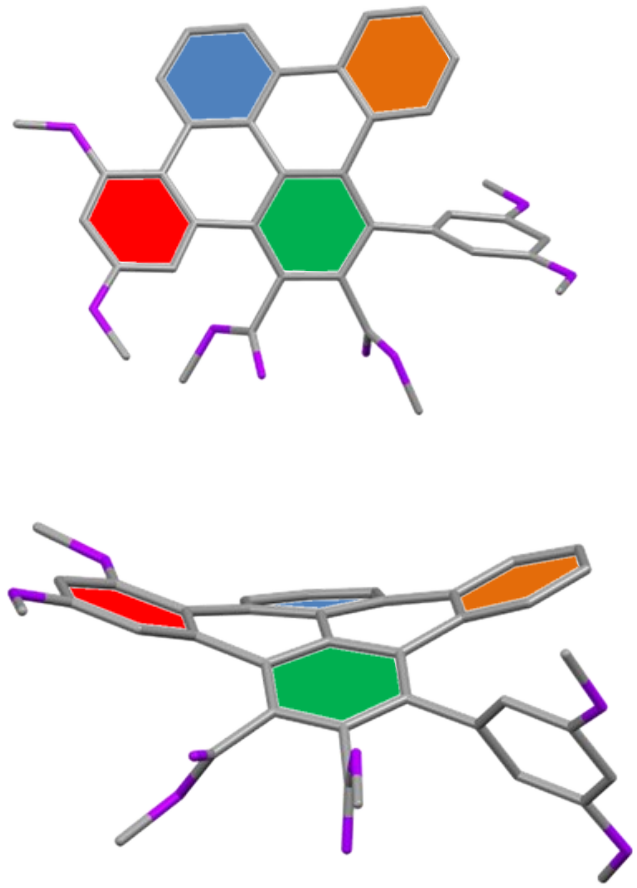


Table S2. Energy in eV of the orbitals of **6**, **6planar**, **7**, **7 planar**, **8** and **8planar** at the B3LYP/6-31+G* level

Orbitals	**6**	**6planar**	**7**	**7planar**	**8**	**8planar**
LUMO+2	-1.13	-1.11	-1.10	-1.08	-1.07	-1.02
LUMO+1	-1.66	-1.47	-1.44	-1.37	-1.55	-1.46
LUMO	-1.68	-1.54	-1.85	-1.77	-1.96	-1.84
HOMO	-5.98	-5.96	-5.62	-5.58	-5.41	-5.38
HOMO-1	-5.99	-6.09	-5.91	-5.92	-5.59	-5.57
HOMO-2	-6.10	-6.11	-6.05	-6.09	-5.83	-5.84
HOMO-3	-6.18	-6.23	-6.17	-6.29	-6.48	-6.48
HOMO-4	-6.32	-6.34	-6.42	-6.31	-6.59	-6.62

TableS3. Calculated energy differences in kcal/mol of the planar structures or twisted structures compared to the contorted structures (minima) at different levels of theory

B3LYP/6-31+G*	ΔE [kcal/mol]
6 vs. **6planar** (NImag=3)	9.6
7 vs. **7planar** (NImag=4)	10.4
8 vs. **8planar** (NImag=5)	11.6
8 vs. **8twisted** (NImag=0)	0.5
B3LYPD3/6-31+G*	ΔE [kcal/mol]
6 vs. **6planar** (NImag=3)	9.7
7 vs. **7planar** (NImag=4)	9.9
8 vs. **8planar** (NImag=5)	10.3
8 vs. **8twisted** (NImag=0)	0.7

Figure S35. Experimental absorption and calculated vertical excitations of **1** at the B3LYP/6-31+G* level

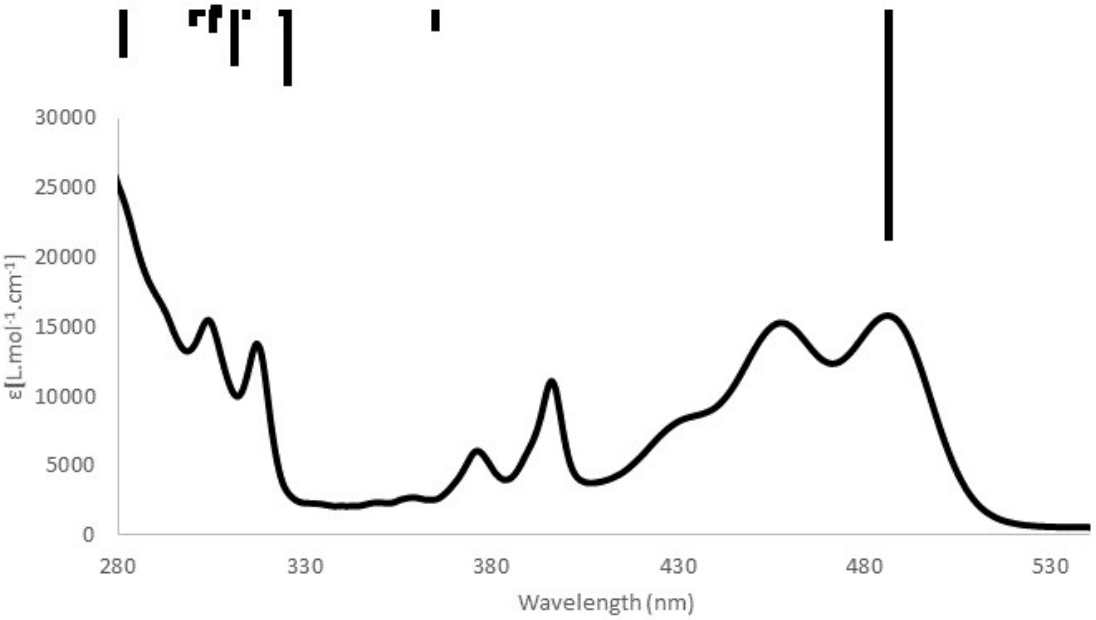


Figure S36. Experimental absorption and calculated vertical excitations of **2** at the B3LYP/6-31+G* level

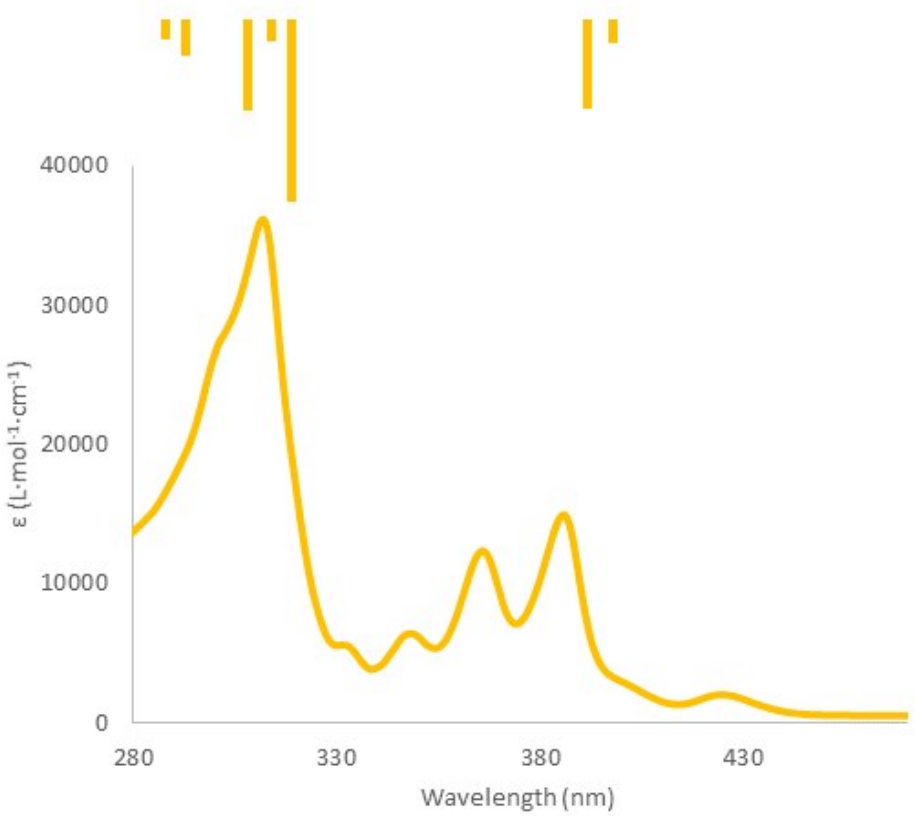


Figure S37. Experimental absorption and calculated vertical excitations of **6** at the B3LYP/6-31+G* level

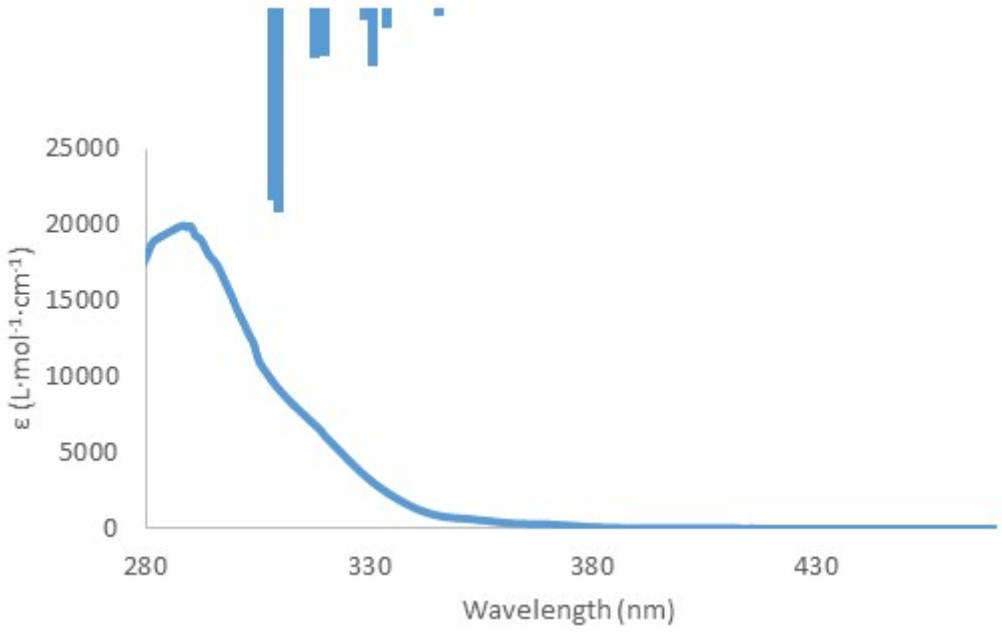


Figure S38. Experimental absorption and calculated vertical excitations of **7** at the B3LYP/6-31+G* level

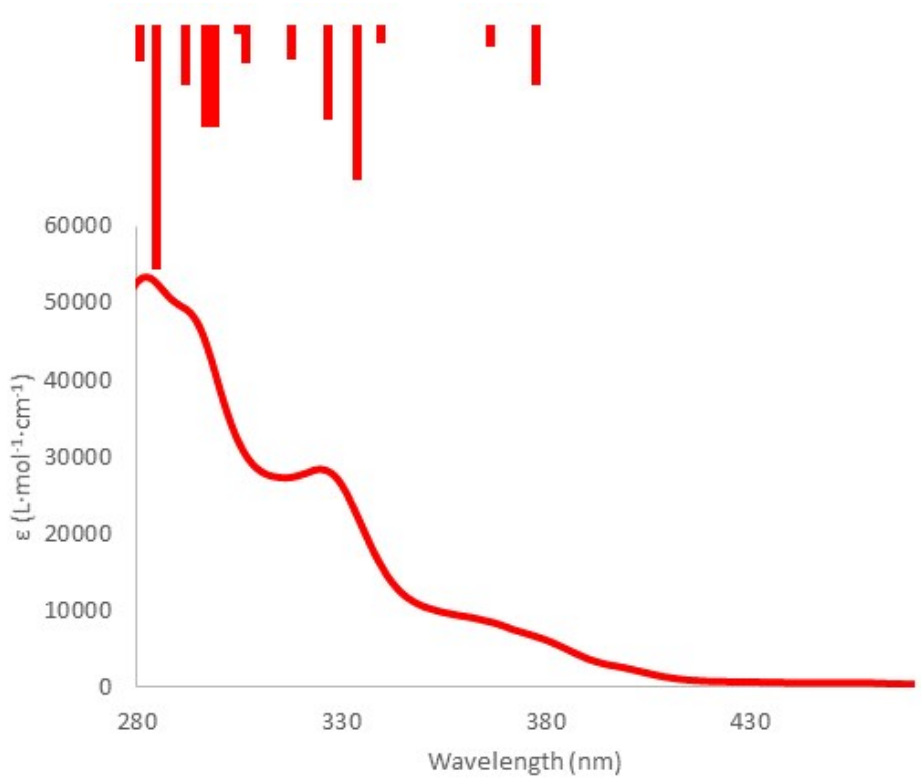
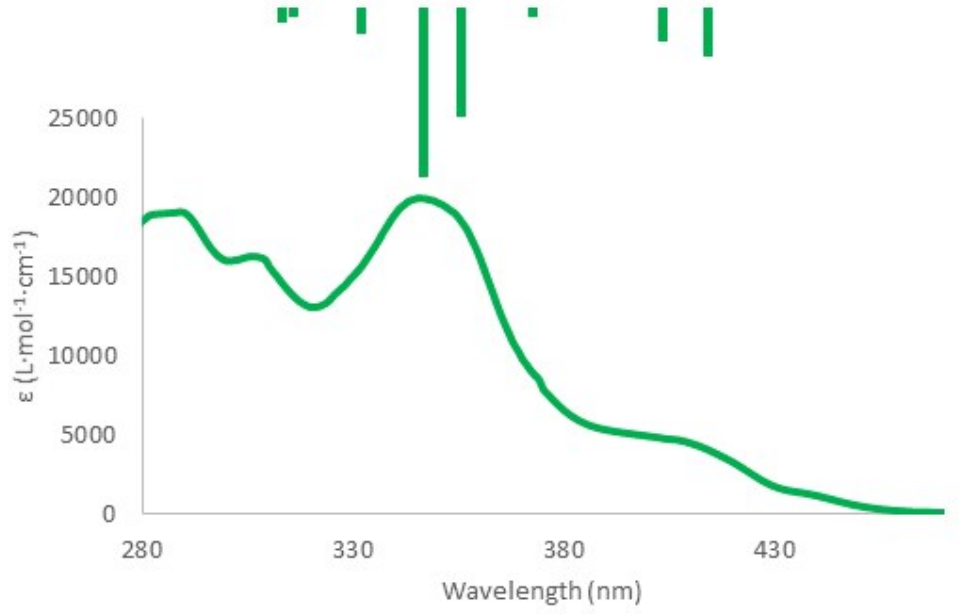


Figure S39. Experimental absorption and calculated vertical excitations of **8** at the B3LYP/6-31+G* level



TD-DFT studies

Table S4. Vertical excitation of **1** (B3LYP/6-31+G*)

λ_a (nm)	Intensity	Transition			Coefficient
486	0.1955	HOMO	→	LUMO	0.698
365	0.0151	HOMO-1	→	LUMO	0.322
		HOMO	→	LUMO+1	0.611
325	0.0630	HOMO-8	→	LUMO	0.138
		HOMO-4	→	LUMO	-0.259
		HOMO-2	→	LUMO	0.184
		HOMO-1	→	LUMO	0.521
		HOMO	→	LUMO+1	-0.276
		HOMO	→	LUMO+3	0.102
324	0.0018	HOMO-7	→	LUMO	0.112
		HOMO-3	→	LUMO	0.381
		HOMO	→	LUMO+2	0.542
		HOMO	→	LUMO+4	-0.131
		HOMO	→	LUMO+6	-0.120
317	0.0000	HOMO-8	→	LUMO	-0.102
		HOMO-5	→	LUMO	0.486
		HOMO-2	→	LUMO	-0.473
		HOMO-1	→	LUMO	0.110
314	0.0042	HOMO-5	→	LUMO	-0.212
		HOMO-4	→	LUMO	0.321
		HOMO-2	→	LUMO	-0.180
		HOMO-1	→	LUMO	0.183
		HOMO	→	LUMO+3	0.527
311	0.0445	HOMO-6	→	LUMO	0.232
		HOMO-3	→	LUMO	-0.397
		HOMO	→	LUMO+2	0.403
		HOMO	→	LUMO+4	0.178
		HOMO	→	LUMO+5	-0.253
		HOMO	→	LUMO+6	0.138
306	0.0019	HOMO-7	→	LUMO	0.528
		HOMO-6	→	LUMO	-0.354
		HOMO-3	→	LUMO	-0.243
		HOMO	→	LUMO+5	0.160
305	0.0159	HOMO-8	→	LUMO	0.139
		HOMO-5	→	LUMO	-0.191
		HOMO-4	→	LUMO	0.425
		HOMO-1	→	LUMO	0.243
		HOMO	→	LUMO+1	-0.114
		HOMO	→	LUMO+3	-0.421
302	0.0016	HOMO-8	→	LUMO	-0.102

		HOMO-5	→	LUMO	0.385
		HOMO-4	→	LUMO	0.365
		HOMO-2	→	LUMO	0.445
300	0.0104	HOMO-7	→	LUMO	0.353
		HOMO-6	→	LUMO	0.422
		HOMO	→	LUMO+2	-0.168
		HOMO	→	LUMO+4	-0.330
		HOMO	→	LUMO+5	-0.194
		HOMO	→	LUMO+6	-0.118
281	0.0380	HOMO-7	→	LUMO	0.153
		HOMO-6	→	LUMO	0.251
		HOMO-3	→	LUMO	0.113
		HOMO	→	LUMO+4	0.518
		HOMO	→	LUMO+5	0.210
		HOMO	→	LUMO+6	-0.246
278	0.0081	HOMO-8	→	LUMO	0.646
		HOMO-5	→	LUMO	0.133
		HOMO	→	LUMO+1	0.130
		HOMO	→	LUMO+3	0.121
277	0.0404	HOMO-6	→	LUMO	0.233
		HOMO-3	→	LUMO+1	0.101
		HOMO	→	LUMO+4	-0.148
		HOMO	→	HOMO+5	0.500
		HOMO	→	HOMO+6	0.374
262	0.3525	HOMO-7	→	LUMO	0.188
		HOMO-6	→	LUMO+1	-0.202
		HOMO-3	→	LUMO	0.285
		HOMO-1	→	LUMO+5	0.106
		HOMO	→	LUMO+4	0.185
		HOMO	→	LUMO+5	-0.208
		HOMO	→	LUMO+6	0.475

Table S5. Vertical emission of **1** (B3LYP/6-31+G*)

λ_e (nm)	Intensity	Transition			Coefficient
575	0.1735	HOMO	←	LUMO	0.701

Table S6. Vertical excitation of 2 (B3LYP/6-31+G*)

λ_a (nm)	Intensity	Transition			Coefficient
398	0.0384	HOMO-1	→	LUMO	-0.319
		HOMO	→	LUMO+1	0.627
392	0.1767	HOMO-1	→	LUMO+1	0.170
		HOMO	→	LUMO	0.681
319	0.3704	HOMO-1	→	LUMO	0.593
		HOMO	→	LUMO+1	0.301
		HOMO	→	LUMO+4	0.152
314	0.0335	HOMO-2	→	LUMO	-0.161
		HOMO-1	→	LUMO+1	-0.308
		HOMO	→	LUMO+2	0.596
		HOMO	→	LUMO+3	-0.115
308	0.1807	HOMO-2	→	LUMO	-0.366
		HOMO-1	→	LUMO+1	0.541
		HOMO	→	LUMO	-0.125
		HOMO	→	LUMO+2	0.175
293	0.0655	HOMO-2	→	LUMO	-0.446
		HOMO-1	→	LUMO+1	-0.178
		HOMO	→	LUMO+2	-0.134
		HOMO	→	LUMO+3	0.479
288	0.0304	HOMO-4	→	LUMO	-0.328
		HOMO-2	→	LUMO	0.345
		HOMO-1	→	LUMO+1	0.141
		HOMO	→	LUMO+2	0.226
		HOMO	→	LUMO+3	0.436
277	0.0212	HOMO-3	→	LUMO	0.592
		HOMO-2	→	LUMO+1	0.283
		HOMO	→	LUMO+4	0.215
276	0.0043	HOMO-3	→	LUMO	-0.131
		HOMO-2	→	LUMO+1	0.565
		HOMO-1	→	LUMO+2	-0.123
		HOMO	→	LUMO+4	-0.345
267	0.0175	HOMO-5	→	LUMO	0.112
		HOMO-4	→	LUMO+1	-0.350
		HOMO-3	→	LUMO	-0.172
		HOMO-1	→	LUMO+2	-0.294
		HOMO-1	→	LUMO+3	0.215
		HOMO	→	LUMO+4	0.409
266	0.0709	HOMO-5	→	LUMO+1	0.127
		HOMO-4	→	LUMO	-0.261
		HOMO-3	→	LUMO+1	0.575
		HOMO-1	→	LUMO+1	-0.119
		HOMO	→	LUMO+2	-0.148
		HOMO	→	LUMO+7	-0.124
263	0.0174	HOMO-4	→	LUMO+1	-0.355

		HOMO-3	→	LUMO	0.142
		HOMO-1	→	LUMO+2	0.399
		HOMO-1	→	LUMO+3	0.187
		HOMO	→	LUMO+4	-0.145
		HOMO	→	LUMO+5	0,328
260	0.0001	HOMO-6	→	LUMO	0.120
		HOMO-5	→	LUMO+1	0.413
		HOMO-4	→	LUMO	0.425
		HOMO-3	→	LUMO+1	0.176
		HOMO	→	LUMO+2	0.104
		HOMO	→	LUMO+3	0.149
		HOMO	→	LUMO+7	0.150
257	0.0629	HOMO-6	→	LUMO+1	0.139
		HOMO-5	→	LUMO	0.233
		HOMO-4	→	LUMO+1	0.315
		HOMO-1	→	LUMO	-0.117
		HOMO-1	→	LUMO+3	-0.146
		HOMO	→	LUMO+4	0.127
		HOMO	→	LUMO+5	0.511
252	0.0057	HOMO-5	→	LUMO+1	0.480
		HOMO-4	→	LUMO	-0.302
		HOMO-3	→	LUMO+2	-0.280
		HOMO-1	→	LUMO+3	-0.210
		HOMO	→	LUMO+5	-0.100
251	0.0001	HOMO-6	→	LUMO+1	0.283
		HOMO-5	→	LUMO	0.524
		HOMO-1	→	LUMO+2	0.121
		HOMO-1	→	LUMO+3	0.109
		HOMO	→	LUMO+5	-0.254
245	0.1021	HOMO-6	→	LUMO+1	-0.300
		HOMO-5	→	LUMO	0.240
		HOMO-3	→	LUMO	0.106
		HOMO-1	→	LUMO+2	-0.229
		HOMO	→	LUMO+4	-0.149
		HOMO	→	LUMO+6	0.400
		HOMO	→	LUMO+8	-0.247
244	0.0756	HOMO-6	→	LUMO+1	0.284
		HOMO-5	→	LUMO	-0.259
		HOMO-1	→	LUMO+2	0.145
		HOMO-1	→	LUMO+3	0.158
		HOMO	→	LUMO+4	0.107
		HOMO	→	LUMO+6	.0415
		HOMO	→	LUMO+8	-0.297
244	0.0194	HOMO-6	→	LUMO	-0.126
		HOMO-4	→	LUMO	-0.102
		HOMO-3	→	LUMO+1	0.100

		HOMO-1	→	LUMO+4	-0.181
		HOMO	→	LUMO+7	0.637
243	0.0235	HOMO-4	→	LUMO+1	0.206
		HOMO-3	→	LUMO	0.160
		HOMO-2	→	LUMO+1	-0.190
		HOMO-1	→	LUMO+2	-0.244
		HOMO-1	→	LUMO+3	0.508
		HOMO	→	LUMO+4	-0.147

Table S7. Vertical emission of **2** (B3LYP/6-31+G*)

λ_e (nm)	Intensity	Transition			Coefficient
435	0.2195	HOMO-1	←	LUMO+1	0.112
		HOMO	←	LUMO	0.693

Table S8. Vertical excitation of **6** (B3LYP/6-31+G*)

λ_a (nm)	Intensity	Transition			Coefficient
346	0.0024	HOMO-5	→	LUMO	0.100
		HOMO-3	→	LUMO	0.182
		HOMO-2	→	LUMO	0.301
		HOMO-2	→	LUMO+1	0.210
		HOMO-1	→	LUMO	-0.223
		HOMO-1	→	LUMO+1	0.475
		HOMO	→	LUMO	-0.162
334	0.0103	HOMO-2	→	LUMO+1	0.103
		HOMO-1	→	LUMO	-0.287
		HOMO	→	LUMO	0.515
		HOMO	→	LUMO+1	-0.358
331	0.0398	HOMO-2	→	LUMO	0.188
		HOMO-2	→	LUMO+1	-0.242
		HOMO-1	→	LUMO	0.394
		HOMO-1	→	LUMO+1	0.278
		HOMO	→	LUMO	0.369
		HOMO	→	LUMO+1	0.112
329	0.0046	HOMO-2	→	LUMO+1	0.163
		HOMO-1	→	LUMO	-0.223
		HOMO	→	LUMO	0.237
		HOMO	→	LUMO+1	0.592
320	0.0318	HOMO-4	→	LUMO+1	0.122
		HOMO-3	→	LUMO	-0.315
		HOMO-3	→	LUMO+1	-0.360
		HOMO-2	→	LUMO	0.435

		HOMO-1	→	LUMO+1	-0.205
318	0.0336	HOMO-4	→	LUMO	-0.121
		HOMO-3	→	LUMO	0.340
		HOMO-3	→	LUMO+1	-0.270
		HOMO-2	→	LUMO	-0.130
		HOMO-2	→	LUMO+1	0.419
		HOMO-1	→	LUMO	0.270
		HOMO-1	→	LUMO+1	-0.121
310	0.149	HOMO-5	→	LUMO	-0.131
		HOMO-4	→	LUMO	0.107
		HOMO-4	→	LUMO+1	0.383
		HOMO-3	→	LUMO	0.382
		HOMO-3	→	LUMO+1	0.122
		HOMO-2	→	LUMO	0.176
		HOMO-2	→	LUMO+1	-0.218
		HOMO-1	→	LUMO+1	-0.248
309	0.1375	HOMO-4	→	LUMO	-0.352
		HOMO-4	→	LUMO+1	0.212
		HOMO-3	→	LUMO	-0.198
		HOMO-3	→	LUMO+1	0.423
		HOMO-2	→	LUMO	0.116
		HOMO-2	→	LUMO+1	0.154
		HOMO-1	→	LUMO	0.228

Table S9. Vertical emission of **6** (B3LYP/6-31+G*)

λ_e (nm)	Intensity	Transition			Coefficient
472	0.0288	HOMO	←	LUMO	-0.703

Table S10. Vertical excitation of **7** (B3LYP/6-31+G*)

λ_a (nm)	Intensity	Transition			Coefficient
378	0.0751	HOMO-1	→	LUMO	0.212
		HOMO-1	→	LUMO+1	0.164
		HOMO	→	LUMO	0.637
367	0.0233	HOMO-1	→	LUMO	0.477
		HOMO	→	LUMO	-0.216
		HOMO	→	LUMO+1	-0.444
341	0.0181	HOMO-2	→	LUMO	0.674
		HOMO-1	→	LUMO+1	-0.147
334	0.2038	HOMO-3	→	LUMO	0.387
		HOMO-2	→	LUMO	-0.174
		HOMO-1	→	LUMO	-0.371

		HOMO-1	→	LUMO+1	0.100
		HOMO	→	LUMO+1	-0.372
327	0.1227	HOMO-3	→	LUMO	0.482
		HOMO-1	→	LUMO	0.182
		HOMO-1	→	LUMO+1	0.207
		HOMO	→	LUMO+2	-0.119
		HOMO	→	LUMO+1	0.331
		HOMO	→	LUMO+2	0.168
318	0.0406	HOMO-4	→	LUMO	-0.36375
		HOMO-3	→	LUMO	-0.28942
		HOMO-1	→	LUMO+1	0.44083
		HOMO	→	LUMO+2	0.26312
307	0.0449	HOMO-5	→	LUMO	-0.308
		HOMO-3	→	LUMO+1	0.150
		HOMO-2	→	LUMO+1	0.265
		HOMO-1	→	LUMO+1	-0.171
		HOMO-1	→	LUMO+2	0.181
		HOMO	→	LUMO+2	0.450
305	0.0064	HOMO-5	→	LUMO	0.167
		HOMO-4	→	LUMO	-0.168
		HOMO-2	→	LUMO+1	0.630
		HOMO	→	LUMO+2	-0.158
299	0.1323	HOMO-4	→	LUMO	0.504
		HOMO-3	→	LUMO+1	-0.252
		HOMO-2	→	LUMO+1	0.129
		HOMO-1	→	LUMO+1	0.311
		HOMO	→	LUMO+3	0.109
296	0.1333	HOMO-5	→	LUMO	0.335
		HOMO-4	→	LUMO	0.157
		HOMO-3	→	LUMO+1	0.559
		HOMO-1	→	LUMO+1	0.108
292	0.0753	HOMO-5	→	LUMO	-0.210
		HOMO-4	→	LUMO+1	0.124
		HOMO-3	→	LUMO+1	0.152
		HOMO-1	→	LUMO+1	0.130
		HOMO-1	→	LUMO+2	0.499
		HOMO	→	LUMO+2	-0.274
		HOMO	→	LUMO+3	0.106
285	0.3242	HOMO-5	→	LUMO	0.424
		HOMO-4	→	LUMO	-0.101
		HOMO-3	→	LUMO+1	-0.192
		HOMO-1	→	LUMO	-0.187
		HOMO-1	→	LUMO+2	0.371
		HOMO	→	LUMO+2	0.210
281	0.0435	HOMO-5	→	LUMO+1	0.183
		HOMO-4	→	LUMO+1	0.303

		HOMO-1	→	LUMO+2	-0.104
		HOMO	→	LUMO+3	0.551
279	0.0313	HOMO-6	→	LUMO	-0.257
		HOMO-5	→	LUMO+2	-0.123
		HOMO-4	→	LUMO+1	0.457
		HOMO-3	→	LUMO+2	-0.122
		HOMO-2	→	LUMO+2	-0.296
		HOMO	→	LUMO+3	-0.240
277	0.0333	HOMO-5	→	LUMO+1	-0.235
		HOMO-4	→	LUMO+1	0.298
		HOMO-3	→	LUMO+2	0.128
		HOMO-2	→	LUMO+2	0.496
		HOMO-1	→	LUMO+3	-0.174
274	0.0067	HOMO-6	→	LUMO	0.174
		HOMO-5	→	LUMO+1	-0.302
		HOMO-4	→	LUMO+2	-0.113
		HOMO-3	→	LUMO+2	0.387
		HOMO-2	→	LUMO+2	-0.359
		HOMO-1	→	LUMO+3	-0.193
271	0.0647	HOMO-6	→	LUMO	0.224
		HOMO-3	→	LUMO+2	-0.207
		HOMO	→	LUMO+3	-0.136
		HOMO	→	LUMO+4	0.567
269	0.0103	HOMO-6	→	LUMO	0.265
		HOMO-5	→	LUMO+1	0.334
		HOMO-4	→	LUMO+1	0.183
		HOMO-3	→	LUMO+2	0.296
		HOMO-1	→	LUMO+3	0.301
		HOMO	→	LUMO+3	-0.200
269	0.0185	HOMO-6	→	LUMO	0.406
		HOMO-3	→	LUMO+2	-0.368
		HOMO-2	→	LUMO+4	-0.322
		HOMO	→	LUMO+5	0.122
261	0.0088	HOMO-5	→	LUMO+1	-0.172
		HOMO-4	→	LUMO+2	0.308
		HOMO-3	→	LUMO+4	-0.119
		HOMO-3	→	LUMO+13	-0.112
		HOMO-2	→	LUMO+4	0.461
		HOMO-1	→	LUMO+3	0.100
		HOMO	→	LUMO+6	0.188

Table S11. Vertical emission of **7** (B3LYP/6-31+G*)

λ_e (nm)	Intensity	Transition			Coefficient
602	0.0335	HOMO-1	←	LUMO	0.129
		HOMO	←	LUMO	0.691

Table S12. Vertical excitation of **8** (B3LYP/6-31+G*)

λ_a (nm)	Intensity	Transition			Coefficient
415	0.1044	HOMO-1	→	LUMO	0.309
		HOMO-1	→	LUMO+1	-0.142
		HOMO	→	LUMO	0.572
		HOMO	→	LUMO+1	0.211
404	0.066	HOMO-1	→	LUMO	0.509
		HOMO	→	LUMO	-0.360
		HOMO	→	LUMO+1	0.282
373	0.0101	HOMO-2	→	LUMO	0.643
		HOMO-1	→	LUMO+1	0.230
		HOMO	→	LUMO+2	-0.137
356	0.2468	HOMO-3	→	LUMO	-0.180
		HOMO-2	→	LUMO+1	0.169
		HOMO-1	→	LUMO	-0.298
		HOMO-1	→	LUMO+1	-0.179
		HOMO	→	LUMO+1	0.540
347	0.3885	HOMO-2	→	LUMO	-0.196
		HOMO-2	→	LUMO+1	0.134
		HOMO-1	→	LUMO+1	0.603
		HOMO	→	LUMO	0.155
		HOMO	→	LUMO+1	0.141
332	0.0498	HOMO-5	→	LUMO	0.122
		HOMO-3	→	LUMO	0.170
		HOMO-2	→	LUMO+1	0.603
		HOMO-1	→	LUMO	0.142
		HOMO-1	→	LUMO+1	-0.102
		HOMO	→	LUMO+2	0.188
316	0.0081	HOMO-4	→	LUMO	0.240
		HOMO-3	→	LUMO	-0.125
		HOMO-2	→	LUMO	0.131
		HOMO-2	→	LUMO+1	-0.144
		HOMO	→	LUMO+2	0.599
313	0.0215	HOMO-5	→	LUMO	-0.148
		HOMO-3	→	LUMO	0.384

		HOMO-2	→	LUMO+1	-0.114
		HOMO-1	→	LUMO+2	0.506
		HOMO	→	LUMO+2	0.124

Table S13. Vertical emission of **8** (B3LYP/6-31+G*)

λ_e (nm)	Intensity	Transition			Coefficient
521	0.1078	HOMO-1	←	LUMO	-0.123
		HOMO	←	LUMO	-0.683

Table S14. Vertical excitation of **8twisted** (B3LYP/6-31+G*)

λ_a (nm)	Intensity	Transition			Coefficient
399	0.0066	HOMO-2	→	LUMO+1	-0.106
		HOMO-1	→	LUMO	0.538
		HOMO	→	LUMO+1	0.433
389	0.0626	HOMO-1	→	LUMO+1	-0.298
		HOMO	→	LUMO+1	0.631
362	0.1162	HOMO-2	→	LUMO	0.393
		HOMO-1	→	LUMO+1	0.522
		HOMO	→	LUMO	0.222
		HOMO	→	LUMO+2	-0.120
354	0.1869	HOMO-3	→	LUMO	0.109
		HOMO-2	→	LUMO+1	0.292
		HOMO-1	→	LUMO	-0.357
		HOMO	→	LUMO+1	0.506
345	0.4302	HOMO-2	→	LUMO	0.525
		HOMO-1	→	LUMO+1	-0.359
		HOMO	→	LUMO	-0.188
		HOMO	→	LUMO+2	-0.191
328	0.1224	HOMO-5	→	LUMO	-0.108
		HOMO-3	→	LUMO	-0.174
		HOMO-2	→	LUMO+2	0.604
		HOMO-1	→	LUMO+1	0.240
		HOMO	→	LUMO+1	-0.125
311	0.0096	HOMO-5	→	LUMO	0.111
		HOMO-4	→	LUMO+2	-0.117
		HOMO-3	→	LUMO+1	-0.206
		HOMO-1	→	LUMO+2	0.640
311	0.1038	HOMO-4	→	LUMO	0.159
		HOMO-2	→	LUMO	0.216
		HOMO	→	LUMO+2	0.630
297	0.1256	HOMO-4	→	LUMO+1	-0.180

		HOMO-3	→	LUMO	0.564
		HOMO-2	→	LUMO+1	0.116
		HOMO-2	→	LUMO+4	-0.119
		HOMO-1	→	LUMO+2	0.142
		HOMO-1	→	LUMO+3	-0.195
		HOMO	→	LUMO+1	-0.156
		HOMO	→	LUMO+6	-0.103
297	0.0279	HOMO-4	→	LUMO	0.595
		HOMO-2	→	LUMO	-0.104
		HOMO-2	→	LUMO+2	0.213
		HOMO-1	→	LUMO+4	0.119
		HOMO	→	LUMO+3	-0.240
295	0.0018	HOMO-4	→	LUMO	0.177
		HOMO-3	→	LUMO+1	0.304
		HOMO-2	→	LUMO+2	0.126
		HOMO	→	LUMO+3	0.580
288	0.0412	HOMO-5	→	LUMO	0.315
		HOMO-4	→	LUMO+1	0.356
		HOMO-3	→	LUMO	0.168
		HOMO-2	→	LUMO+3	0.455
286	0.2225	HOMO-5	→	LUMO+1	0.160
		HOMO-4	→	LUMO	-0.228
		HOMO-2	→	LUMO+2	0.605
		HOMO	→	LUMO+2	0.116
285	0.0064	HOMO-5	→	LUMO	0.549
		HOMO-4	→	LUMO+1	-0.236
		HOMO-3	→	LUMO	-0.179
		HOMO-1	→	LUMO+2	-0.162
		HOMO-1	→	LUMO+3	-0.116
		HOMO	→	LUMO+5	0.195
281	0.0742	HOMO-5	→	LUMO+1	-0.226
		HOMO-4	→	LUMO+2	0.114
		HOMO-3	→	LUMO+1	0.489
		HOMO-2	→	LUMO+2	0.157
		HOMO-1	→	LUMO+4	-0.308
		HOMO	→	LUMO+3	-0.211
277	0.1256	HOMO-5	→	LUMO+1	0.577
		HOMO-3	→	LUMO+1	0.249
		HOMO-2	→	LUMO+2	-0.138
		HOMO-2	→	LUMO+3	0.138
		HOMO	→	LUMO+3	-0.134
276	0.0112	HOMO-4	→	LUMO+1	-0.353
		HOMO-1	→	LUMO+3	0.289
		HOMO	→	LUMO+4	0.494
271	0.0258	HOMO-4	→	LUMO+1	0.306
		HOMO-3	→	LUMO	-0.104

		HOMO-2	→	LUMO+4	-0.185
		HOMO-1	→	LUMO+3	-0.248
		HOMO-1	→	LUMO+7	0.145
		HOMO	→	LUMO+4	0.400
		HOMO	→	LUMO+5	0.261
268	0.0081	HOMO-5	→	LUMO+1	-0.158
		HOMO-1	→	LUMO+4	0.205
		HOMO-1	→	LUMO+5	0.127
		HOMO-1	→	LUMO+6	0.558
		HOMO	→	LUMO+7	-0.249
267	0.0008	HOMO-4	→	LUMO+1	-0.105
		HOMO-3	→	LUMO+2	-0.147
		HOMO-2	→	LUMO+4	-0.182
		HOMO-1	→	LUMO+3	0.117
		HOMO-1	→	LUMO+7	-0.195
		HOMO	→	LUMO+4	-0.136
		HOMO	→	LUMO+5	0.441
		HOMO	→	LUMO+6	0.374

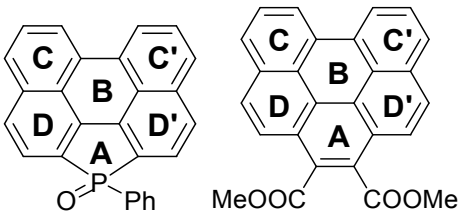
Table S15. Vertical emission of **8twisted** (B3LYP/6-31+G*)

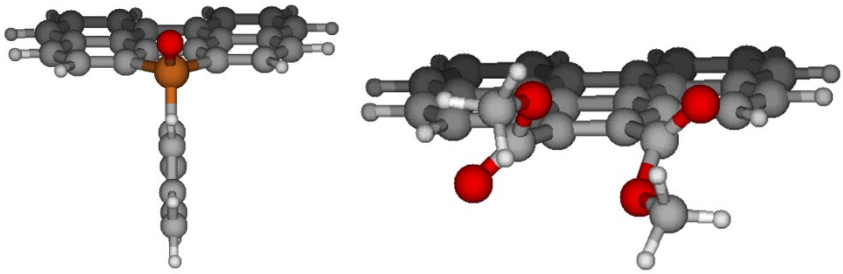
λ_e (nm)	Intensity	Transition			Coefficient
426	0.0035	HOMO-1	←	LUMO	0.523
		HOMO	←	LUMO+1	0.455

Table S16. Excitation energies and oscillator strengths of **2** at the ADC2/cc-pVDZ//B3LYP/6-31+G* level

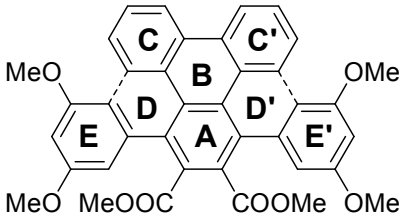
Excited state	Excitation energy [eV]	Absorption wavelength [nm]	Oscillator strength
1	3.3029	375.38	0.0229488
2	3.5854	345.80	0.2232030
3	4.1893	295.96	0.0037308
4	4.2973	288.52	0.4774374
5	4.4829	276.57	0.1966586
6	4.4829	276.57	0.1939643
7	4.7346	261.87	0.0323450
8	4.7856	259.08	0.0010719
9	5.1472	240.88	0.0407644

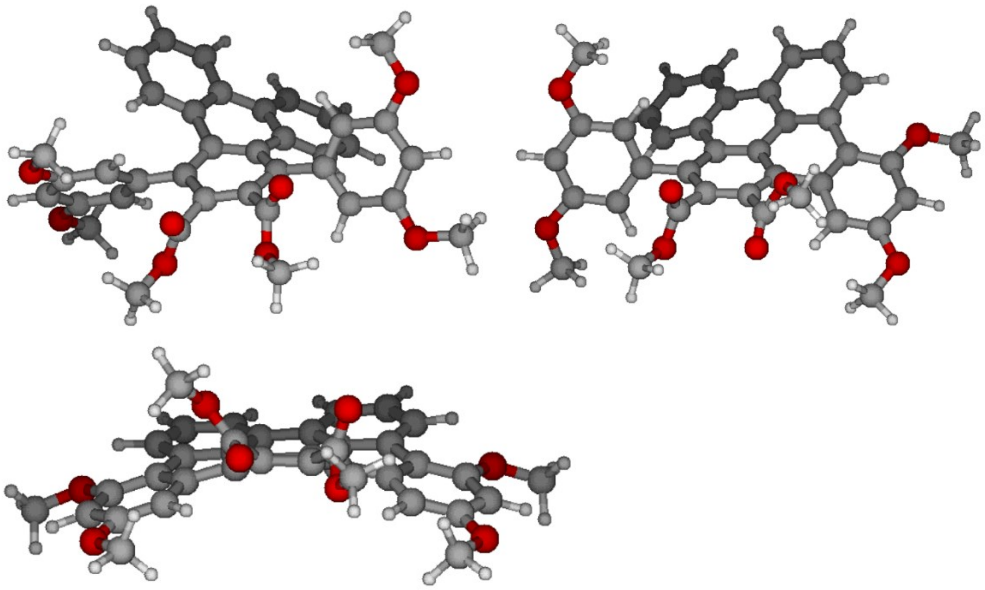
Table S17. NICS indices for calculated geometries of **1**, **2**, **6**, **7** and **8** at the B3LYP/6-311+G*//B3LYP/6-31+G* level. The NICS(-1) and NICS(1) values correspond to the direction depicted on stick representation, the NICS(1) value is calculated above the PAH.





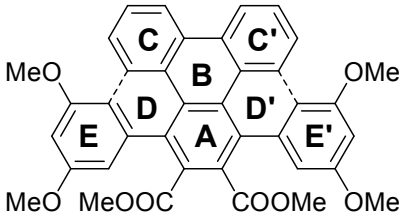
	1			**2**		
	NICS(-1)	NICS(0)	NICS(1)	NICS(-1)	NICS(0)	NICS(1)
A	3.9	7.4	3.7	-11.9	-11.1	-11.9
B	3.1	8.4	3.1	-2.0	2.5	-2.0
C	-7.5	-4.8	-7.6	-11.6	-9.4	-11.6
C'	-7.6	-4.6	-7.6	-11.6	-9.4	-11.6
D	-7.8	-5.4	-7.8	-7.0	-3.9	-7.0
D'	-7.9	-5.3	-7.7	-7.0	-4.0	-7.0

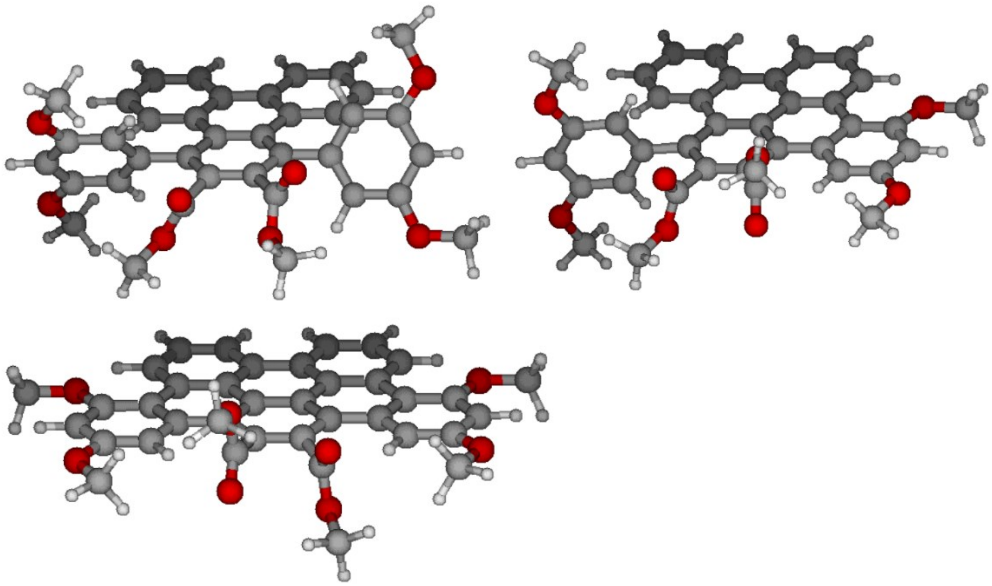




	6			7			8		
	NICS(-1)	NICS(0)	NICS(1)	NICS(-1)	NICS(0)	NICS(1)	NICS(-1)	NICS(0)	NICS(1)
A	-8.9	-7.9	-9.1	-9.0	-9.6	-11.1	-9.9	-10.0	-12.2
B	-4.1	-0.6	-4.0	-3.9	-0.2	-4.0	-2.6	0.8	-3.6
C	-10.4	-7.7	-9.0	-10.4	-7.4	-8.8	-10.3	-8.4	-10.8
C'	-9.0	-7.7	-10.3	-9.8	-8.4	-10.9	-10.1	-8.4	-11.0
D	-	-	-	-	-	-	-4.7	-0.6	-3.3
D'	-	-	-	-4.5	-0.4	-3.9	-4.6	-0.7	-3.7
E	-9.2	-9.2	-8.5	-8.9	-9.4	-8.7	-9.7	-9.3	-8.3
E'	-8.9	-9.2	-8.6	-10.1	-9.4	-8.4	-9.8	-9.2	-8.4

Table S18. NICS indices for calculated planar geometries of **6plamar**, **7planar** and **8planar** at the B3LYP/6-311+G*//B3LYP/6-31+G* level. The NICS(-1) and NICS(1) values correspond to the direction depicted on stick representation, the NICS(1) value is calculated above the PAH.





	6planar			**7planar**			**8planar**		
	NICS(-1)	NICS(0)	NICS(1)	NICS(-1)	NICS(0)	NICS(1)	NICS(-1)	NICS(0)	NICS(1)
A	-9.1	-8.8	-9.0	-10.5	-10.3	-10.7	-11.3	-10.8	-11.3
B	-4.4	-1.3	-4.4	-4.0	-0.6	-4.0	-3.2	0.6	-3.2
C	-10.0	-7.9	-10.1	-9.6	-7.5	-9.7	-11.1	-9.1	-11.1
C'	-10.1	-8.0	-10.1	-11.1	-9.1	-11.1	-11.1	-9.1	-11.1
D	-	-	-	-	-	-	-3.8	-0.7	-3.7
D'	-	-	-	-4.0	-1.1	-4.0	-3.7	-0.7	-3.8
E	-9.0	-9.1	-8.2	-8.8	-9.1	-8.3	-9.1	-9.3	-9.1
E'	-9.1	-9.1	-8.2	-9.3	-9.5	-9.2	-9.1	-9.3	-9.1

Total energies, number of imaginary frequencies (NImag) and Cartesian coordinates at the B3LYP/6-31+G* level

1

E(hartree)= -1416.488603

NImag= 0

C	0.057290	0.006945	-0.061505
C	-0.029067	-0.064050	1.381683
C	1.136638	-0.076459	2.172406
C	2.429462	-0.012148	1.552147
C	2.518292	0.060882	0.067601
C	1.308832	0.065097	-0.705341
C	0.969364	-0.159093	3.588786
C	-0.354395	-0.227187	4.119645
C	-1.476484	-0.211162	3.303946
C	-1.310735	-0.124805	1.906022
C	3.534038	-0.028449	2.396572
C	3.384601	-0.106874	3.801168
C	2.138905	-0.172162	4.394803
C	1.311720	0.122353	-2.132805
C	2.568895	0.181331	-2.791359
C	3.734724	0.180974	-2.050234
C	3.715551	0.120790	-0.636947
C	-1.152526	0.005269	-0.737995
C	-1.150299	0.056998	-2.147408
C	0.060931	0.114244	-2.821463
P	-2.513913	-0.089072	0.505838

O	-3.504823	-1.214977	0.391137
C	-3.335224	1.547542	0.537233
C	-4.733963	1.570216	0.454767
C	-5.416286	2.790725	0.474006
C	-4.705672	3.989069	0.575387
C	-3.308464	3.969529	0.657912
C	-2.624435	2.753505	0.638993
H	-5.273030	0.630116	0.376330
H	-6.501408	2.802911	0.409767
H	-5.236670	4.937614	0.590296
H	-2.753420	4.900862	0.736868
H	-1.538826	2.746158	0.703498
H	-2.468998	-0.270834	3.742587
H	-0.474979	-0.297670	5.198225
H	2.045123	-0.234886	5.476283
H	4.277400	-0.117862	4.421167
H	4.539972	0.016119	1.990705
H	-2.083221	0.046316	-2.704715
H	0.069926	0.150279	-3.908415
H	2.604798	0.225216	-3.877229
H	4.694985	0.225455	-2.557708
H	4.665784	0.119585	-0.111900

2

E(hartree)= -1301.432315

NImag= 0

C	-0.028266	-0.106413	-0.002030
C	-0.030060	-0.041459	1.433438
C	1.215392	-0.022503	2.122552
C	2.447340	-0.085105	1.384982
C	2.409404	-0.149596	-0.042438
C	1.138950	-0.156437	-0.702078
C	1.244015	0.056242	3.549570
C	0.027696	0.138111	4.284589
C	-1.211333	0.125054	3.575652
C	-1.239531	0.034171	2.188033
C	2.504175	0.055156	4.240667
C	2.522791	0.120141	5.668448
C	1.279804	0.191215	6.374957
C	0.086286	0.201521	5.718931
C	3.707842	-0.078302	2.056801
C	3.736779	-0.015361	3.522359
C	3.752064	0.114319	6.353587
C	4.944192	0.044611	5.647747
C	4.934298	-0.019115	4.251132
C	3.610989	-0.205898	-0.772907
C	4.830591	-0.197824	-0.112039
C	4.876005	-0.135005	1.283913

C	-2.493538	0.166785	4.358337
O	-3.312359	0.851115	4.011427
C	-4.581422	-0.897761	4.690832
C	-2.550464	0.058710	1.453703
O	-3.302741	1.116770	1.829899
C	-4.592189	1.228813	1.198188
O	-2.766065	0.974983	5.223035
O	-2.895921	-0.733686	0.600517
H	-4.430766	-1.027230	5.765891
H	-5.101453	-1.757619	4.268015
H	-5.141909	0.024334	4.514666
H	5.886388	-0.073344	3.735470
H	5.893415	0.039103	6.177109
H	3.753739	0.164618	7.439793
H	1.304223	0.243273	7.460953
H	-0.835230	0.280465	6.281345
H	-4.475264	1.351439	0.118140
H	-5.051518	2.113705	1.639259
H	-5.192086	0.336379	1.395988
H	5.848172	-0.129952	1.763692
H	5.758474	-0.240287	-0.676405
H	3.569623	-0.255182	-1.858372
H	1.120201	-0.208641	-1.788179
H	-0.972924	-0.137665	-0.529644

6

E(hartree)= -2069.1643725

NImag= 0

C	-0.733298	-1.424990	0.016127
C	-1.453600	-2.743843	-0.087131
O	-1.472842	-3.590079	0.786299
O	-2.052427	-2.883276	-1.282040
C	-2.818040	-4.088204	-1.469668
C	-1.444530	-0.220027	0.063658
C	-0.717526	1.006801	0.124376
C	-1.318872	2.292662	0.533539
C	-2.502229	2.350939	1.307372
C	-3.007626	3.551326	1.783505
C	-2.334718	4.750453	1.513540
C	-1.156060	4.718386	0.785139
C	-0.625827	3.508072	0.287391
C	-2.939307	-0.278479	-0.010782
C	-3.598708	0.355868	-1.071525
C	-4.994886	0.270528	-1.161850
C	-5.727667	-0.439486	-0.206038
C	-5.062060	-1.073474	0.845443
C	-3.664357	-0.997179	0.951619
O	-5.733499	0.847878	-2.156091
C	-5.061680	1.615143	-3.148205
O	-5.858182	-1.746184	1.728880

C	-5.247140	-2.417103	2.826986
C	0.671771	-1.430891	0.116527
C	1.380972	-2.725565	0.419660
O	1.963284	-2.953996	1.456844
O	1.263332	-3.610571	-0.593302
C	1.810706	-4.920416	-0.341605
C	1.395047	-0.240379	-0.012055
C	0.682857	0.988336	-0.153568
C	1.302241	2.237938	-0.639508
C	2.483425	2.230714	-1.418135
C	3.007138	3.393120	-1.963895
C	2.355687	4.617110	-1.761373
C	1.178955	4.647295	-1.029636
C	0.629588	3.476635	-0.462806
C	2.888326	-0.309194	0.080584
C	3.622149	-1.079356	-0.820025
C	5.019840	-1.160756	-0.692641
C	5.678134	-0.478482	0.328103
C	4.926357	0.288998	1.235560
C	3.539799	0.382504	1.118655
O	5.650164	-1.936703	-1.625677
C	7.064436	-2.066755	-1.557643
O	5.660634	0.908056	2.207442
C	4.978433	1.692915	3.178969
H	-2.182012	-4.967816	-1.341581

H	-3.199504	-4.029912	-2.489208
H	-3.642491	-4.123590	-0.752287
H	-3.020244	1.439063	1.567235
H	-3.914152	3.551242	2.383088
H	-2.715110	5.695377	1.892958
H	-0.616050	5.645471	0.626390
H	-3.017033	0.895009	-1.808932
H	-6.808103	-0.499418	-0.282738
H	-3.138001	-1.470159	1.771474
H	-4.528545	2.464364	-2.702143
H	-5.843981	1.984780	-3.813459
H	-4.357067	0.998378	-3.720969
H	-4.540427	-3.183674	2.486195
H	-6.065316	-2.890393	3.372544
H	-4.729700	-1.709706	3.487853
H	2.880453	-4.848965	-0.129370
H	1.635352	-5.486450	-1.256971
H	1.296868	-5.380901	0.506303
H	2.984013	1.296113	-1.626624
H	3.911114	3.343058	-2.565254
H	2.750839	5.532190	-2.195037
H	0.655370	5.591157	-0.923333
H	3.139442	-1.610776	-1.634035
H	6.752161	-0.519473	0.462058
H	2.950824	0.962580	1.817976

H 7.560304 -1.094184 -1.674479

H 7.341887 -2.718554 -2.387960

H 7.377289 -2.526139 -0.610941

H 4.447394 2.531857 2.711362

H 5.753850 2.077592 3.843755

H 4.270480 1.083894 3.755306

7

E(hartree)= -2067.982675

NImag= 0

C 3.413901 -1.573591 -0.648362

C 2.824052 -0.374725 -0.188559

C 3.597915 0.790510 0.032781

C 5.014752 0.663432 -0.145017

C 5.591049 -0.533678 -0.547036

C 4.786510 -1.650668 -0.820519

C 2.904998 2.052977 0.315178

C 1.504388 2.140204 0.025258

C 0.716372 0.937561 -0.162558

C 1.368072 -0.315310 -0.021806

C 0.842606 3.397010 0.083575

C 1.529986 4.510603 0.589895

C 2.855125 4.395776 0.990542

C 3.543788 3.195424 0.830525

C -0.703643 1.006590 -0.320081

C -1.281341 2.317505 -0.672225

C	-0.526230	3.495864	-0.425623
C	-2.535071	2.455504	-1.312200
C	-3.057358	3.697609	-1.639879
C	-2.334178	4.860353	-1.342459
C	-1.082980	4.751234	-0.756983
C	0.586014	-1.458339	0.236254
C	-0.811471	-1.380189	0.171340
C	-1.470764	-0.174326	-0.127437
C	-2.970870	-0.179402	-0.039633
C	-3.580657	0.413018	1.073257
C	-4.978733	0.398327	1.181893
C	-5.760374	-0.197773	0.188828
C	-5.142827	-0.794093	-0.912650
C	-3.744997	-0.794312	-1.033529
C	-1.604579	-2.600321	0.578756
O	-2.021107	-3.315341	-0.478967
C	-2.713729	-4.540731	-0.168955
O	-5.670477	0.945340	2.225202
C	-4.940477	1.573180	3.273229
O	-5.989900	-1.356076	-1.829091
C	-5.437587	-1.945843	-2.999037
C	1.173003	-2.738967	0.765588
O	1.855560	-2.521631	1.903604
C	2.420432	-3.683966	2.537036
O	5.778034	1.776833	0.062058

C	7.173928	1.730602	-0.208257
O	5.455745	-2.751969	-1.269897
C	4.701155	-3.906780	-1.627556
O	-1.810098	-2.911144	1.734598
O	1.004943	-3.843325	0.280321
H	-0.503604	5.653373	-0.594395
H	-2.731619	5.839176	-1.598572
H	-4.020916	3.760307	-2.138799
H	-3.101439	1.575391	-1.578568
H	-2.950808	-4.988829	-1.134408
H	-2.062455	-5.198944	0.411453
H	-3.625032	-4.330164	0.396948
H	-2.960627	0.872494	1.833214
H	-6.841593	-0.203310	0.276724
H	-3.252260	-1.253885	-1.880654
H	-5.690947	1.928875	3.981388
H	-4.272123	0.862010	3.774998
H	-4.358401	2.424835	2.898359
H	-6.289707	-2.314680	-3.572922
H	-4.886654	-1.208241	-3.597332
H	-4.773608	-2.784051	-2.752137
H	1.022333	5.462170	0.703400
H	3.367820	5.253667	1.418411
H	4.581779	3.142260	1.118920
H	2.892328	-3.312620	3.446888

H	1.634545	-4.405745	2.773194
H	3.162449	-4.150387	1.882533
H	6.658008	-0.630773	-0.700143
H	2.785099	-2.408494	-0.922492
H	7.542709	2.738267	-0.007965
H	7.685056	1.017105	0.450287
H	7.367131	1.470792	-1.256479
H	5.434011	-4.647429	-1.951831
H	4.135883	-4.297701	-0.772828
H	4.009953	-3.688572	-2.451260

8

E(hartree)= -2066.7997436

NImag= 0

C	0.751573	0.981999	0.137553
C	-0.677139	1.003319	0.105127
C	-1.402523	2.249637	0.104088
C	-0.681647	3.461771	0.301289
C	-1.400172	4.662461	0.414399
C	-2.787168	4.664905	0.366069
C	-3.497246	3.485258	0.164694
C	-2.833863	2.255332	-0.003803
C	-3.529320	0.996653	-0.302885
C	-4.894070	0.898989	-0.740746
C	-5.464698	-0.318114	-1.084517
C	-4.702816	-1.496226	-1.047453

C	-3.382688	-1.449365	-0.637212
C	-2.804422	-0.222295	-0.232876
C	-1.396007	-0.206820	0.151905
C	-0.692420	-1.380625	0.540466
C	0.702115	-1.423525	0.469559
C	1.441671	-0.255323	0.127952
C	2.871890	-0.258887	-0.192962
C	3.462307	-1.439674	-0.701471
C	4.803335	-1.455840	-1.046548
C	5.583718	-0.301992	-0.891804
C	5.008603	0.873664	-0.434521
C	3.618900	0.946040	-0.081088
C	2.926679	2.187792	0.281846
C	3.592465	3.374169	0.641890
C	2.888085	4.552107	0.870478
C	1.507647	4.595439	0.731697
C	0.782119	3.435700	0.416997
C	1.493550	2.213403	0.236773
C	-6.937771	2.019047	-1.359961
C	-4.632688	-3.851123	-1.487951
C	4.741083	-3.733379	-1.791252
C	7.104212	2.016695	-0.773926
C	-1.414971	-2.501851	1.238128
C	-2.929451	-2.983318	2.990722
C	1.371481	-2.665820	1.019006

C	1.842699	-4.949036	0.653876
O	-5.615687	2.055113	-0.836504
O	-5.354105	-2.622599	-1.460133
O	5.464779	-2.528618	-1.573083
O	5.749587	2.017520	-0.340940
O	-1.293954	-3.693536	1.016511
O	-2.192150	-2.013951	2.225474
O	1.751080	-2.757746	2.167503
O	1.437472	-3.671820	0.125303
H	-0.884321	5.604615	0.554003
H	-3.329035	5.600193	0.483366
H	-4.573530	3.522592	0.135486
H	-6.489595	-0.391927	-1.423838
H	-2.770408	-2.338208	-0.684955
H	2.846834	-2.306457	-0.883034
H	6.626400	-0.356026	-1.175865
H	4.664703	3.378200	0.746489
H	3.429544	5.451174	1.154443
H	0.999031	5.535985	0.904428
H	-6.950078	1.618692	-2.381254
H	-7.274276	3.057455	-1.370986
H	-7.604704	1.426060	-0.721593
H	-3.791002	-3.801074	-2.190157
H	-5.346748	-4.603474	-1.827035
H	-4.259449	-4.118992	-0.491942

H	4.351775	-4.137055	-0.849014
H	5.458281	-4.434684	-2.221451
H	3.911888	-3.578457	-2.493206
H	7.716358	1.334109	-0.171249
H	7.455119	3.040584	-0.631753
H	7.182760	1.746275	-1.834322
H	-3.629615	-3.522678	2.346136
H	-3.467879	-2.404696	3.741594
H	-2.247197	-3.694124	3.464031
H	2.833477	-4.881799	1.111571
H	1.851890	-5.624927	-0.201865
H	1.115293	-5.283246	1.397692

6planar

E(hartree)= -2069.149109

NImag= 3

C	-1.492350	2.524406	-0.034419
C	-0.779941	3.755512	-0.094078
C	0.680223	3.764864	-0.100876
C	1.408240	2.542888	-0.047919
C	0.690669	1.239378	0.015089
C	-0.757352	1.230053	0.021833
C	-1.441293	-0.032872	0.082829
C	-0.715649	-1.224271	0.134392
C	0.683933	-1.215254	0.127874
C	1.392070	-0.013649	0.069589

C	1.383602	4.992784	-0.160350
C	2.763383	5.059661	-0.169440
C	3.490068	3.867472	-0.117845
C	2.823343	2.655258	-0.059253
C	-2.909052	2.620126	-0.032637
C	-3.591386	3.823994	-0.084962
C	-2.879656	5.024918	-0.143232
C	-1.499176	4.974608	-0.146942
C	2.883906	-0.223419	0.017261
C	3.632569	-0.264786	1.207898
C	4.995784	-0.547850	1.143177
C	5.627744	-0.784516	-0.092222
C	4.869012	-0.758191	-1.260066
C	3.488952	-0.486936	-1.208169
O	5.374832	-0.989067	-2.508835
C	6.761264	-1.275684	-2.638077
O	5.818030	-0.627537	2.231152
C	5.246986	-0.467682	3.526023
C	1.409230	-2.532495	0.273207
O	2.062823	-2.866888	1.236563
C	-1.406188	-2.562737	0.255917
O	-1.389883	-3.232256	1.270395
C	-2.931412	-0.259195	0.072341
C	-3.616372	-0.340543	-1.147991
C	4.987690	-0.624392	-1.145118

C	-5.667505	-0.837675	0.058945
C	-4.970763	-0.780053	1.267562
C	-3.595014	-0.493867	1.281919
O	-5.752148	-0.723292	-2.274797
C	-5.138945	-0.485183	-3.536414
O	-5.712524	-1.018376	2.389061
C	-5.062263	-0.998756	3.656018
O	-1.993560	-2.951907	-0.887369
C	-2.682010	-4.216351	-0.840857
O	1.200068	-3.324838	-0.801186
C	1.801162	-4.633028	-0.735153
H	-1.986655	-5.018000	-0.578243
H	-3.080468	-4.363634	-1.844919
H	-3.490514	-4.179612	-0.106244
H	-3.514627	1.737665	0.010541
H	-4.678256	3.818688	-0.079978
H	-3.393144	5.982028	-0.184958
H	-0.966370	5.914489	-0.192440
H	-3.072925	-0.180808	-2.070977
H	-6.729669	-1.058334	0.052396
H	-3.038191	-0.445454	2.209729
H	-4.731726	0.532323	-3.596804
H	-5.932760	-0.603782	-4.276067
H	-4.340850	-1.211416	-3.737484
H	-4.271788	-1.757514	3.710299

H -5.839195 -1.228005 4.387361

H -4.639472 -0.008961 3.871146

H 2.886670 -4.544633 -0.641712

H 1.532907 -5.120141 -1.673151

H 1.405944 -5.186911 0.120708

H 3.439227 1.779674 -0.021718

H 4.576900 3.875655 -0.122961

H 3.264803 6.022945 -0.215876

H 0.839095 5.926191 -0.200852

H 2.920485 -0.469961 -2.132513

H 6.689495 -0.999195 -0.088869

H 3.132416 -0.097336 2.153063

H 7.376283 -0.441569 -2.275750

H 6.935499 -1.418934 -3.705941

H 7.031159 -2.191897 -2.096631

H 4.818697 0.535308 3.650716

H 6.071417 -0.600276 4.228846

H 4.475765 -1.224509 3.714293

7planar

E(hartree)= -2067.966022

NImag= 4

C -1.446918 0.033458 -0.019135

C -0.634256 1.200235 0.020254

C 0.805735 1.036366 -0.013009

C 1.410077 -0.267576 -0.084017

C	0.547895	-1.389478	-0.120450
C	-0.838974	-1.223985	-0.088060
C	-1.706203	-2.467529	-0.110406
O	-1.936506	-3.160842	0.861576
C	1.675319	2.203498	0.025380
C	3.108426	2.067893	-0.006454
C	3.722848	0.738461	-0.078819
C	2.885589	-0.412304	-0.117030
C	1.107032	3.512758	0.095991
C	-0.342475	3.691753	0.130122
C	-1.206920	2.566259	0.093564
C	3.888734	3.240918	0.033801
C	3.318272	4.502205	0.102234
C	1.944457	4.638829	0.133058
C	-2.601166	2.833244	0.130773
C	-3.124242	4.112961	0.199212
C	-2.263587	5.214130	0.234714
C	-0.900661	4.992343	0.200152
C	3.471381	-1.700304	-0.186970
C	4.840001	-1.879006	-0.219645
C	5.685406	-0.768260	-0.183428
C	5.149356	0.504545	-0.115077
C	-2.951647	-0.031990	0.004691
C	-3.671058	0.023739	-1.197277
C	-5.067109	-0.094336	-1.165596

C	-5.736432	-0.280668	0.047905
C	-5.007634	-0.362857	1.236538
C	-3.608873	-0.240269	1.222895
C	0.911701	-2.842708	0.086645
O	0.875120	-3.709420	-0.766127
O	-5.865575	-0.046305	-2.274803
C	-5.259569	0.174146	-3.543061
O	-5.745303	-0.566481	2.367732
C	-5.065301	-0.693889	3.612262
O	5.996693	1.577722	-0.082855
C	7.404276	1.378602	-0.118306
O	5.474107	-3.084566	-0.305965
C	4.690499	-4.267955	-0.414816
O	1.137343	-3.085008	1.391983
C	1.203119	-4.468939	1.786232
O	-2.156780	-2.733991	-1.344918
C	-2.967439	-3.918364	-1.479306
H	-0.254472	5.858857	0.228643
H	-2.651135	6.228266	0.288469
H	-4.202594	4.246323	0.224613
H	-3.310520	2.030164	0.106339
H	-3.215522	-3.976326	-2.539284
H	-2.400184	-4.798708	-1.167056
H	-3.872627	-3.826574	-0.873433
H	-3.027264	-0.303603	2.134290

H	-6.817210	-0.373363	0.064471
H	-3.135548	0.164626	-2.127891
H	-5.845094	-0.868602	4.355593
H	-4.371107	-1.543331	3.601267
H	-4.520296	0.224939	3.864514
H	-6.079597	0.180457	-4.263350
H	-4.738233	1.139584	-3.574189
H	-4.556866	-0.629806	-3.796930
H	1.531494	5.636363	0.186499
H	3.957226	5.381315	0.131436
H	4.959045	3.170362	0.011444
H	1.455479	-4.452048	2.846702
H	0.228448	-4.937986	1.629018
H	1.966093	-5.002522	1.214185
H	6.752430	-0.941590	-0.210473
H	2.868688	-2.583977	-0.217030
H	7.837801	2.379932	-0.082172
H	7.748087	0.800333	0.748184
H	7.714122	0.879745	-1.044839
H	5.405213	-5.083009	-0.541187
H	4.104315	-4.436974	0.496678
H	4.019065	-4.227280	-1.280856

8planar

E(hartree)= -2066.781267

NImag= 5

C	0.724643	1.028148	0.011761
C	1.452024	2.282951	0.023377
C	0.730294	3.511905	0.011722
C	-0.730026	3.511946	-0.011730
C	-1.451806	2.283027	-0.023257
C	-0.724501	1.028184	-0.011511
C	1.460946	-0.193925	0.023649
C	0.699541	-1.391348	0.011484
C	-0.699494	-1.391304	-0.010983
C	-1.460852	-0.193856	-0.023273
C	2.943685	-0.181039	0.047460
C	3.648048	1.058471	0.058707
C	2.890325	2.312265	0.046473
C	3.527047	3.569469	0.056633
C	2.808700	4.755091	0.045035
C	1.427934	4.730303	0.022862
C	-2.890102	2.312388	-0.046356
C	-3.526774	3.569617	-0.056646
C	-2.808382	4.755213	-0.045171
C	-1.427616	4.730375	-0.022996
C	-3.647881	1.058624	-0.058460
C	-2.943581	-0.180923	-0.047085

C	5.091378	0.988796	0.081889
C	5.770799	-0.215195	0.092863
C	5.056966	-1.414818	0.081462
C	3.676306	-1.394418	0.059289
C	-5.091221	0.989025	-0.081635
C	-5.770717	-0.214926	-0.092485
C	-5.056953	-1.414586	-0.080960
C	-3.676293	-1.394236	-0.058788
C	1.254252	-2.783354	-0.223146
O	1.435497	-2.986662	-1.540054
C	1.694587	-4.342358	-1.953320
C	-1.254390	-2.783157	0.224106
O	-1.435765	-2.985892	1.541057
C	-1.695841	-4.341247	1.954798
O	5.826615	-2.542178	0.114973
C	5.185797	-3.811457	0.170846
O	5.808195	2.153343	0.095704
C	7.229295	2.118165	0.124471
O	-5.807971	2.153597	-0.096460
C	-7.229069	2.118384	-0.125142
O	-5.826604	-2.541924	-0.114999
C	-5.185890	-3.811091	-0.174868
O	-1.414694	-3.644327	-0.621203
O	1.414220	-3.644287	0.622459
H	-0.901018	5.674211	-0.014589

H	-3.338022	5.704681	-0.053727
H	-4.597913	3.626838	-0.073851
H	-6.850639	-0.266265	-0.116195
H	-3.183456	-2.343173	-0.050824
H	3.183398	-2.343319	0.051423
H	6.850836	-0.266610	0.110211
H	4.598190	3.626645	0.073831
H	3.338375	5.704540	0.053491
H	0.901372	5.674159	0.014356
H	-7.598389	1.619259	-1.029510
H	-7.542909	3.164036	-0.133267
H	-7.635104	1.622295	0.765093
H	-4.510289	-3.880428	-1.035770
H	-5.989938	-4.542084	-0.276894
H	-4.626701	-4.012538	0.747055
H	4.510762	-3.883671	1.031967
H	5.989834	-4.542882	0.269799
H	4.625984	-4.009639	-0.751397
H	7.598504	1.618530	1.028599
H	7.543098	3.163824	0.133138
H	7.635485	1.622619	-0.765997
H	-2.580812	-4.739355	1.452745
H	-1.855231	-4.284849	3.031741
H	-0.827734	-4.963506	1.723389
H	1.854647	-4.286389	-3.030190

H	0.825760	-4.963722	-1.722235
H	2.578892	-4.741194	-1.450670

8twisted

E(hartree)= -2066.800582

NImag= 0

C	-3.397601	3.410225	0.991014
C	-2.827619	2.204680	0.535131
C	-1.426546	2.211487	0.229951
C	-0.698241	3.431697	0.218722
C	-1.326385	4.611325	0.643338
C	-2.651930	4.584762	1.056932
C	0.698213	3.431713	-0.218623
C	1.426520	2.211504	-0.229917
C	0.714636	0.971781	-0.029634
C	-0.714657	0.971767	0.029653
C	-3.593100	0.979130	0.271728
C	-2.896893	-0.193285	-0.132820
C	-1.434153	-0.244972	-0.006024
C	-0.699295	-1.457198	0.019392
C	0.699322	-1.457181	-0.019317
C	1.434148	-0.244941	0.006069
C	2.896878	-0.193244	0.132869
C	3.593074	0.979149	-0.271745
C	2.827593	2.204708	-0.535098
C	3.397595	3.410295	-0.990852

C	2.651928	4.584837	-1.056691
C	1.326367	4.611369	-0.643142
C	-3.586154	-1.282783	-0.712919
C	-4.968703	-1.279603	-0.786086
C	-5.693563	-0.200139	-0.261715
C	-5.027772	0.905810	0.246340
C	5.027748	0.905790	-0.246468
C	5.693539	-0.200128	0.261648
C	4.968681	-1.279537	0.786151
C	3.586134	-1.282721	0.713025
O	5.722240	-2.268200	1.349701
C	5.052603	-3.355729	1.982935
O	5.727558	1.978697	-0.721140
C	7.148454	1.978420	-0.655108
O	-5.727598	1.978798	0.720810
C	-7.148480	1.978600	0.654552
O	-5.722245	-2.268323	-1.349559
C	-5.052609	-3.355847	-1.982813
C	1.355538	-2.806028	-0.184979
C	-1.355455	-2.806091	0.185011
H	0.767168	5.539265	-0.696852
H	3.121438	5.492534	-1.428011
H	4.431044	3.433089	-1.292597
H	6.773602	-0.244942	0.309361
H	3.030681	-2.092049	1.159677

H	-3.030710	-2.092132	-1.159529
H	-6.773624	-0.244928	-0.309485
H	-4.431035	3.432994	1.292812
H	-3.121422	5.492425	1.428355
H	-0.767180	5.539214	0.697107
H	7.499133	1.897519	0.381229
H	7.459118	2.938483	-1.071576
H	7.575091	1.165134	-1.255346
H	4.424689	-3.004435	2.811172
H	5.842799	-4.001203	2.370047
H	4.433344	-3.916360	1.272675
H	-4.424701	-3.004541	-2.811048
H	-5.842807	-4.001317	-2.369926
H	-4.433344	-3.916489	-1.272567
H	-7.498999	1.897565	-0.381829
H	-7.459153	2.938745	1.070826
H	-7.575270	1.165432	1.254843
O	1.363030	-3.692708	0.649264
O	1.888404	-2.926924	-1.411293
C	2.472844	-4.204720	-1.726050
H	2.808513	-4.118579	-2.759648
H	3.318794	-4.410217	-1.064054
H	1.724442	-4.994255	-1.622929
O	-1.363014	-3.692672	-0.649332
O	-1.888297	-2.927100	1.411313

C	-2.472772	-4.204890	1.726001
H	-2.808931	-4.118619	2.759429
H	-3.318384	-4.410594	1.063637
H	-1.724237	-4.994365	1.623367

Total energies, number of imaginary frequencies (NImag) and Cartesian coordinates at the B3LYPD3/6-31+G* level

6

E(hartree)= -2069.261631

NImag= 0

C	3.551931	0.382067	1.087423
C	2.883823	-0.345945	0.087280
C	3.596612	-1.154663	-0.794568
C	4.994372	-1.242013	-0.683830
C	5.672293	-0.520594	0.297053
C	4.939488	0.289136	1.183183
C	1.395663	-0.259774	0.003431
C	0.660708	-1.441233	0.127633
C	-0.741123	-1.420619	0.027451
C	-1.438290	-0.208815	0.073304
C	-0.700909	1.009441	0.138185
C	0.699267	0.977316	-0.133569
C	1.335458	2.220712	-0.608772
C	0.674460	3.465643	-0.430838
C	-0.590550	3.507180	0.303180
C	-1.295195	2.297497	0.543219

C	-1.121102	4.721310	0.792206
C	-2.309969	4.760977	1.503425
C	-2.992490	3.565813	1.769651
C	-2.486181	2.361971	1.305167
C	1.245828	4.633150	-0.983048
C	2.431699	4.593335	-1.699291
C	3.069673	3.362337	-1.905386
C	2.523961	2.202956	-1.376525
C	-1.483237	-2.724337	-0.063726
O	-2.141535	-2.830649	-1.229500
C	-2.998346	-3.979759	-1.364366
C	-2.928662	-0.252976	-0.008651
C	-3.576890	0.429925	-1.043704
C	-4.972240	0.352415	-1.145534
C	-5.711100	-0.407444	-0.233298
C	-5.053302	-1.090655	0.791744
C	-3.658383	-1.009975	0.917960
O	-5.704110	0.981824	-2.112063
C	-5.022164	1.807358	-3.050437
O	-5.852047	-1.816028	1.629404
C	-5.237255	-2.557586	2.680442
C	1.354861	-2.744535	0.410105
O	1.198080	-3.616302	-0.608764
C	1.711828	-4.942305	-0.371820
O	5.603172	-2.061865	-1.592561

C	7.017850	-2.201386	-1.540158
O	5.693166	0.948989	2.112055
C	5.028149	1.790984	3.048223
O	-1.485878	-3.578734	0.802241
O	1.958704	-2.989318	1.430712
H	-2.424889	-4.902629	-1.242121
H	-3.418409	-3.910131	-2.367871
H	-3.792168	-3.937781	-0.612305
H	-3.010465	1.453101	1.562919
H	-3.906291	3.572108	2.357919
H	-2.691041	5.708991	1.874250
H	-0.575150	5.645969	0.640247
H	-2.985346	1.004681	-1.744911
H	-6.790261	-0.467053	-0.323460
H	-3.134842	-1.515387	1.719350
H	-4.489995	2.626148	-2.548479
H	-5.797787	2.219346	-3.698523
H	-4.313450	1.224709	-3.654016
H	-4.522009	-3.292407	2.288693
H	-6.052134	-3.074538	3.190227
H	-4.725921	-1.893652	3.390074
H	2.786811	-4.901445	-0.175665
H	1.504755	-5.499841	-1.285827
H	1.198044	-5.389493	0.483836
H	3.013540	1.263559	-1.588822

H 3.979811 3.305218 -2.496604

H 2.844333 5.506787 -2.119825

H 0.733812 5.583364 -0.877785

H 3.095967 -1.714212 -1.577946

H 6.747860 -0.559713 0.416499

H 2.973282 0.999021 1.762839

H 7.520287 -1.238950 -1.707077

H 7.277593 -2.891469 -2.345021

H 7.341840 -2.621433 -0.578460

H 4.492740 2.604875 2.541626

H 5.814390 2.208831 3.679573

H 4.325459 1.218637 3.668015

7

E(hartree)= -2068.077525

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C 3.583323 0.820299 0.021363

C 5.004185 0.702347 -0.128516

C 5.599625 -0.500150 -0.485035

C 4.810160 -1.630070 -0.748685

C 2.874634 2.079812 0.276043

C 1.475012 2.147565 -0.023407

C 0.704466 0.933314 -0.199880

C 1.368383 -0.310969 -0.047308

C	0.794860	3.395989	0.018722
C	1.466177	4.523770	0.514488
C	2.791371	4.430221	0.921370
C	3.495785	3.236734	0.781047
C	-0.714734	0.984293	-0.356675
C	-1.310864	2.278574	-0.727196
C	-0.575234	3.470554	-0.492442
C	-2.564620	2.383249	-1.373349
C	-3.110627	3.611678	-1.710974
C	-2.409241	4.790736	-1.421576
C	-1.155465	4.712168	-0.836220
C	0.596768	-1.461566	0.207188
C	-0.798745	-1.396843	0.148393
C	-1.469491	-0.198507	-0.144059
C	-2.961743	-0.200188	-0.018988
C	-3.542527	0.503230	1.042725
C	-4.936925	0.509430	1.180276
C	-5.741759	-0.185671	0.273153
C	-5.150511	-0.896637	-0.772627
C	-3.756554	-0.907134	-0.929513
C	-1.582358	-2.616880	0.560337
O	-2.003752	-3.327144	-0.499008
C	-2.730282	-4.531567	-0.186161
O	-5.605072	1.168514	2.172409
C	-4.848663	1.915785	3.119501

O	-6.015941	-1.556607	-1.602018
C	-5.478253	-2.304032	-2.686454
C	1.195579	-2.737806	0.724484
O	1.907594	-2.515375	1.842711
C	2.530279	-3.670516	2.432694
O	5.750903	1.829140	0.061903
C	7.151102	1.796793	-0.187458
O	5.496213	-2.741384	-1.144142
C	4.753259	-3.915619	-1.464379
O	-1.785233	-2.928174	1.715815
O	1.022849	-3.842285	0.241020
H	-0.594448	5.627635	-0.683716
H	-2.825920	5.759334	-1.685739
H	-4.074448	3.652261	-2.211476
H	-3.111786	1.488440	-1.632994
H	-2.971988	-4.981108	-1.150018
H	-2.102779	-5.202297	0.406754
H	-3.639998	-4.289626	0.371273
H	-2.900305	1.039452	1.729899
H	-6.820284	-0.179552	0.387115
H	-3.280063	-1.448369	-1.735288
H	-5.580694	2.356076	3.798977
H	-4.167131	1.267783	3.686251
H	-4.275245	2.714650	2.630782
H	-6.336719	-2.749641	-3.192439

H	-4.935398	-1.657188	-3.388886
H	-4.808181	-3.098816	-2.332433
H	0.946594	5.470309	0.615552
H	3.291293	5.299677	1.340816
H	4.531987	3.200263	1.077911
H	3.019220	-3.303904	3.335451
H	1.778251	-4.426354	2.674199
H	3.266548	-4.094471	1.742510
H	6.670399	-0.594679	-0.608747
H	2.818471	-2.400688	-0.894844
H	7.501160	2.815612	-0.010810
H	7.664302	1.110395	0.498538
H	7.363842	1.510349	-1.225486
H	5.495439	-4.669740	-1.731458
H	4.164012	-4.265181	-0.607013
H	4.082838	-3.741818	-2.315995

8

E(hartree)= -2066.891591

NImag= 0

C	1.508666	2.220123	0.218660
C	0.762900	0.991604	0.118094
C	-0.665885	1.017221	0.083887
C	-1.388576	2.264665	0.084284
C	-0.663060	3.475669	0.271822
C	0.800189	3.445297	0.391355

C	-1.387782	-0.190889	0.127725
C	-0.687103	-1.369711	0.500842
C	0.704983	-1.414852	0.433468
C	1.449788	-0.247591	0.110022
C	2.941779	2.189839	0.273034
C	3.633518	0.944307	-0.075233
C	2.883207	-0.257585	-0.188705
C	-2.799538	-0.202917	-0.238952
C	-3.524439	1.015694	-0.296107
C	-2.821212	2.273809	-0.014700
C	-3.479056	3.507607	0.147308
C	-2.764066	4.686777	0.332062
C	-1.377083	4.680008	0.375044
C	-3.386660	-1.430160	-0.625975
C	-4.719502	-1.482459	-0.987956
C	-5.482140	-0.304809	-1.013023
C	-4.899902	0.915365	-0.699546
C	5.027940	0.862151	-0.407479
C	5.609334	-0.324809	-0.827903
C	4.827401	-1.478276	-0.974411
C	3.477891	-1.445998	-0.669590
C	1.528161	4.603498	0.706492
C	2.907532	4.555976	0.853788
C	3.609105	3.374933	0.634138
O	-5.620544	2.071878	-0.788074

C	-6.956399	2.038352	-1.275394
O	-5.381759	-2.616449	-1.359521
C	-4.661246	-3.847032	-1.359445
C	-1.416365	-2.503900	1.165105
O	-2.216525	-2.033557	2.141563
C	-3.012787	-3.013756	2.829444
C	1.355013	-2.676264	0.953400
O	1.409299	-3.653533	0.027290
C	1.765279	-4.958346	0.521609
O	5.491517	-2.571172	-1.452872
C	4.769819	-3.790671	-1.589881
O	5.766956	2.007598	-0.327022
C	7.126655	2.003153	-0.743590
O	-1.295373	-3.691199	0.919565
O	1.722559	-2.809205	2.101190
H	-0.858357	5.622195	0.502916
H	-3.302315	5.625027	0.441726
H	-4.555121	3.548731	0.124767
H	-6.517075	-0.383261	-1.318381
H	-2.776014	-2.318162	-0.691536
H	2.863292	-2.308463	-0.865472
H	6.657903	-0.390518	-1.085907
H	4.680439	3.375321	0.747021
H	3.450191	5.453950	1.138753
H	1.022704	5.546462	0.874888

H -6.999297 1.627996 -2.292480

H -7.286596 3.078886 -1.287694

H -7.610107 1.456045 -0.613102

H -3.839647 -3.827299 -2.087166

H -5.384709 -4.612098 -1.646221

H -4.256424 -4.074429 -0.364833

H 4.366827 -4.120714 -0.624427

H 5.491915 -4.522275 -1.956825

H 3.948379 -3.691238 -2.311555

H 7.735320 1.336990 -0.118485

H 7.470958 3.031771 -0.619720

H 7.219753 1.709815 -1.797267

H -3.701970 -3.495531 2.128424

H -3.564631 -2.455720 3.586157

H -2.373784 -3.771442 3.291023

H 2.731658 -4.929428 1.033005

H 1.807529 -5.599494 -0.359576

H 0.991995 -5.304159 1.212853

6planar

E(hartree)= -2069.246107

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C -1.441952 2.560222 0.038720

C -0.710640 3.780274 -0.014255

C 0.749996 3.765220 -0.035066

C 1.458783 2.530790 -0.002627

C	0.719620	1.241288	0.052869
C	-0.727217	1.256980	0.073457
C	-1.429693	0.007447	0.127032
C	-0.726686	-1.196286	0.158491
C	0.669989	-1.212548	0.138656
C	1.396511	-0.023608	0.086830
C	1.474791	4.980960	-0.087796
C	2.855663	5.023194	-0.109428
C	3.562549	3.818010	-0.077975
C	2.875620	2.617217	-0.026317
C	-2.857223	2.674689	0.055423
C	-3.522085	3.888479	0.023058
C	-2.792476	5.079577	-0.028888
C	-1.412708	5.010144	-0.046634
C	2.878779	-0.258921	0.009994
C	3.639635	-0.323784	1.189671
C	4.996755	-0.626375	1.101982
C	5.606437	-0.859592	-0.144988
C	4.831476	-0.812077	-1.301851
C	3.457375	-0.520582	-1.227076
O	5.313734	-1.039670	-2.560051
C	6.692953	-1.351782	-2.712377
O	5.833559	-0.730551	2.176325
C	5.279500	-0.579091	3.480211
C	1.364782	-2.544495	0.256633

O	2.072427	-2.888683	1.177372
C	-1.449333	-2.515467	0.265327
O	-1.422909	-3.213464	1.260571
C	-2.917417	-0.201754	0.082453
C	-3.573188	-0.212929	-1.155057
C	-4.938497	-0.515624	-1.198958
C	-5.637798	-0.817802	-0.025138
C	-4.967324	-0.828954	1.198852
C	-3.597446	-0.520777	1.261019
O	-5.678579	-0.556096	-2.347633
C	-5.038037	-0.237359	-3.578358
O	-5.725350	-1.158199	2.285352
C	-5.091282	-1.234767	3.559437
O	-2.093138	-2.842962	-0.864889
C	-2.875365	-4.051031	-0.812215
O	1.049547	-3.341952	-0.787523
C	1.558023	-4.688140	-0.713164
H	-2.235765	-4.910182	-0.590667
H	-3.325611	-4.145448	-1.800654
H	-3.648294	-3.962308	-0.043571
H	-3.475032	1.800359	0.094755
H	-4.608801	3.899245	0.038557
H	-3.292510	6.044306	-0.055027
H	-0.867622	5.943385	-0.086946
H	-3.007155	0.008486	-2.050809

H	-6.694922	-1.056512	-0.068673
H	-3.053358	-0.530338	2.197116
H	-4.640704	0.786367	-3.568530
H	-5.812018	-0.320054	-4.343574
H	-4.226183	-0.942488	-3.801452
H	-4.289548	-1.984396	3.561315
H	-5.873725	-1.534223	4.258935
H	-4.685159	-0.260358	3.861740
H	2.650454	-4.678495	-0.664832
H	1.214412	-5.176744	-1.625557
H	1.158322	-5.188388	0.173856
H	3.476678	1.730955	-0.004374
H	4.649242	3.807304	-0.093476
H	3.373595	5.977939	-0.150089
H	0.947447	5.924879	-0.112814
H	2.872929	-0.486239	-2.140570
H	6.664538	-1.090107	-0.156962
H	3.150151	-0.158118	2.140148
H	7.329826	-0.531749	-2.353984
H	6.848626	-1.491376	-3.783705
H	6.953958	-2.276699	-2.180414
H	4.865741	0.428317	3.622105
H	6.109629	-0.731495	4.172378
H	4.499299	-1.327699	3.667900

7planar

E(hartree)= -2068.061736

NImag= 4

C	-0.841846	-1.198888	-0.088027
C	-1.436050	0.063040	-0.013136
C	-0.613422	1.219441	0.030391
C	0.823594	1.040786	-0.005051
C	1.412765	-0.268645	-0.082257
C	0.539834	-1.379810	-0.122567
C	0.879964	-2.843002	0.021127
O	0.817537	-3.668222	-0.870363
C	-2.936853	0.005165	0.011484
C	-3.588456	-0.239345	1.223898
C	-4.986309	-0.374576	1.233530
C	-5.714087	-0.269519	0.046647
C	-5.046127	-0.047996	-1.162076
C	-3.652540	0.084728	-1.189748
C	1.705077	2.197482	0.037411
C	1.148965	3.511855	0.114261
C	-0.299281	3.704807	0.150634
C	-1.174245	2.587781	0.110064
C	3.136891	2.045694	0.003427
C	3.735007	0.709178	-0.075317
C	2.883476	-0.429823	-0.117431
C	3.929331	3.210371	0.047928

C	3.371298	4.476989	0.122393
C	1.998786	4.628525	0.155275
C	-2.566616	2.863681	0.149616
C	-3.079350	4.146839	0.224087
C	-2.209121	5.240912	0.263580
C	-0.847600	5.009333	0.226842
C	3.449870	-1.723866	-0.193439
C	4.814577	-1.923397	-0.228612
C	5.676448	-0.825539	-0.188773
C	5.157458	0.454977	-0.114321
O	-5.844252	0.013855	-2.270340
C	-5.233166	0.253324	-3.533540
O	-5.722350	-0.615451	2.357921
C	-5.036663	-0.785814	3.595208
C	-1.727420	-2.425170	-0.097631
O	-1.913790	-3.143545	0.865986
O	5.423386	-3.141547	-0.313467
C	4.606976	-4.308811	-0.346811
O	6.015403	1.518448	-0.077038
C	7.421208	1.308817	-0.117434
O	1.109689	-3.147926	1.311490
C	1.115896	-4.551978	1.636099
O	-2.261454	-2.637787	-1.307543
C	-3.147805	-3.769837	-1.411987
H	-0.195615	5.871556	0.258587

H	-2.588834	6.257721	0.322105
H	-4.156549	4.288813	0.251062
H	-3.282123	2.066088	0.122314
H	-3.486378	-3.774295	-2.448246
H	-2.609113	-4.691390	-1.175235
H	-3.992542	-3.648821	-0.728139
H	-3.001262	-0.324815	2.129420
H	-6.793526	-0.374613	0.059520
H	-3.111995	0.247406	-2.113217
H	-5.812459	-0.991715	4.334836
H	-4.337731	-1.630985	3.549890
H	-4.494331	0.125798	3.879486
H	-6.049485	0.266676	-4.258029
H	-4.713952	1.220881	-3.549322
H	-4.525728	-0.545194	-3.794133
H	1.597736	5.630784	0.213454
H	4.019358	5.349271	0.154720
H	4.999055	3.129266	0.024176
H	1.378140	-4.601034	2.693175
H	0.117320	-4.963200	1.464425
H	1.846761	-5.090472	1.027158
H	6.740486	-1.015129	-0.217921
H	2.835680	-2.597697	-0.226467
H	7.861986	2.306940	-0.077227
H	7.763808	0.723543	0.745505

H	7.725539	0.812589	-1.047835
H	5.297009	-5.148307	-0.447347
H	4.036534	-4.413783	0.584880
H	3.916071	-4.294734	-1.199206

8planar

E(hartree)= -2066.875174

NImag= 5

C	0.724039	1.039121	0.011904
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C	0.730372	3.521324	0.011924
C	-0.730350	3.521309	-0.011882
C	-1.452343	2.292483	-0.023607
C	-0.724084	1.039076	-0.011696
C	1.458516	-0.182871	0.023916
C	0.698261	-1.379026	0.011566
C	-0.698321	-1.379087	-0.011195
C	-1.458593	-0.182911	-0.023625
C	2.938373	-0.171930	0.048033
C	3.646008	1.064659	0.059524
C	2.890983	2.319875	0.047176
C	3.528687	3.576538	0.057527
C	2.810540	4.762360	0.045783
C	1.429504	4.738960	0.023277
C	-2.891010	2.319870	-0.047054
C	-3.528672	3.576557	-0.057489

C	-2.810500	4.762363	-0.045824
C	-1.429466	4.738946	-0.023316
C	-3.646039	1.064652	-0.059317
C	-2.938429	-0.171963	-0.047743
C	5.088682	0.988664	0.083038
C	5.764450	-0.218362	0.094092
C	5.044798	-1.414408	0.082404
C	3.665312	-1.386391	0.059921
C	-5.088719	0.988661	-0.082826
C	-5.764476	-0.218360	-0.093798
C	-5.044824	-1.414409	-0.082029
C	-3.665328	-1.386423	-0.059548
C	1.251306	-2.776568	-0.169968
O	1.452677	-3.027179	-1.474808
C	1.674557	-4.406744	-1.827981
C	-1.251276	-2.776721	0.170024
O	-1.452555	-3.027623	1.474814
C	-1.674334	-4.407237	1.827827
O	5.802014	-2.549934	0.109823
C	5.138670	-3.810100	0.086597
O	5.805527	2.152196	0.095904
C	7.226507	2.120334	0.128006
O	-5.805542	2.152202	-0.096342
C	-7.226526	2.120431	-0.128343
O	-5.802064	-2.549903	-0.109550

C	-5.138704	-3.810075	-0.087372
O	-1.387106	-3.609206	-0.708216
O	1.387007	-3.609301	0.708059
H	-0.904757	5.683973	-0.014797
H	-3.340642	5.711518	-0.054496
H	-4.600009	3.633203	-0.074950
H	-6.844015	-0.275648	-0.114733
H	-3.170434	-2.332489	-0.051451
H	3.170433	-2.332466	0.051888
H	6.844051	-0.275639	0.111688
H	4.600030	3.633137	0.074985
H	3.340693	5.711509	0.054391
H	0.904806	5.683993	0.014694
H	-7.595778	1.621981	-1.033763
H	-7.537211	3.167130	-0.137737
H	-7.636717	1.626074	0.761618
H	-4.447413	-3.918424	-0.932661
H	-5.928019	-4.560433	-0.158774
H	-4.589893	-3.945460	0.853385
H	4.446370	-3.918762	0.931019
H	5.927885	-4.560479	0.158921
H	4.591045	-3.945191	-0.854911
H	7.595573	1.622269	1.033715
H	7.537279	3.167012	0.136798
H	7.636796	1.625528	-0.761660

H	-2.511874	-4.824985	1.263736
H	-1.889541	-4.399266	2.896459
H	-0.765553	-4.977993	1.617855
H	1.888982	-4.398698	-2.896770
H	0.766099	-4.977768	-1.617357
H	2.512639	-4.824236	-1.264499

8twisted

E(hartree)= -2066.892713

NImag= 0

C	-3.404658	3.414609	0.969022
C	-2.830706	2.208339	0.520244
C	-1.428098	2.217632	0.220969
C	-0.699360	3.437719	0.213352
C	-1.330995	4.616778	0.634322
C	-2.659963	4.589605	1.037452
C	0.700092	3.437460	-0.215464
C	1.428633	2.217264	-0.222082
C	0.714596	0.979333	-0.025389
C	-0.714363	0.979490	0.024502
C	-3.592107	0.979684	0.260512
C	-2.892305	-0.188250	-0.148271
C	-1.432073	-0.236891	-0.019421
C	-0.698214	-1.448306	0.008371
C	0.697907	-1.448449	-0.009683
C	1.432024	-0.237211	0.018527

C	2.892202	-0.188872	0.148126
C	3.592444	0.979035	-0.259949
C	2.831326	2.207590	-0.520909
C	3.405492	3.413332	-0.970782
C	2.660931	4.588350	-1.040434
C	1.331949	4.616073	-0.637367
C	-3.576403	-1.280692	-0.725570
C	-4.958774	-1.292875	-0.780222
C	-5.687843	-0.218819	-0.250587
C	-5.026062	0.895168	0.246512
C	5.026376	0.894729	-0.244068
C	5.687659	-0.219411	0.253361
C	4.958057	-1.293744	0.781688
C	3.575733	-1.281503	0.725738
O	5.704750	-2.295521	1.330598
C	5.022239	-3.379441	1.958409
O	5.727976	1.964855	-0.720405
C	7.148923	1.965108	-0.656336
O	-5.727195	1.964874	0.724482
C	-7.148259	1.964656	0.662964
O	-5.706017	-2.294398	-1.328844
C	-5.024134	-3.377941	-1.957993
C	1.359079	-2.794320	-0.149192
C	-1.359580	-2.794141	0.147394
H	0.774441	5.544611	-0.697289

H	3.133712	5.495917	-1.407768
H	4.440964	3.435498	-1.265350
H	6.767391	-0.276458	0.289667
H	3.016989	-2.083042	1.180472
H	-3.018088	-2.082120	-1.181018
H	-6.767612	-0.275959	-0.285599
H	-4.440102	3.437211	1.263620
H	-3.132629	5.497587	1.403911
H	-0.773344	5.545281	0.693424
H	7.501614	1.878310	0.379407
H	7.457842	2.928141	-1.067505
H	7.576291	1.155912	-1.262509
H	4.411148	-3.027799	2.799672
H	5.804217	-4.046037	2.325937
H	4.380777	-3.917857	1.249897
H	-4.413931	-3.025784	-2.799686
H	-5.806482	-4.044339	-2.325092
H	-4.381917	-3.916764	-1.250477
H	-7.502795	1.878476	-0.372200
H	-7.456783	2.927283	1.075379
H	-7.574232	1.154869	1.269327
O	1.334455	-3.680634	0.685116
O	1.948820	-2.908964	-1.349062
C	2.572934	-4.176966	-1.623774
H	2.951593	-4.096113	-2.642857

H	3.393835	-4.354628	-0.922479
H	1.838552	-4.982448	-1.540260
O	-1.335608	-3.679880	-0.687554
O	-1.948600	-2.909492	1.347528
C	-2.572586	-4.177643	1.621852
H	-2.950659	-4.097382	2.641198
H	-3.393885	-4.354889	0.920920
H	-1.838250	-4.983074	1.537439

Thermal properties

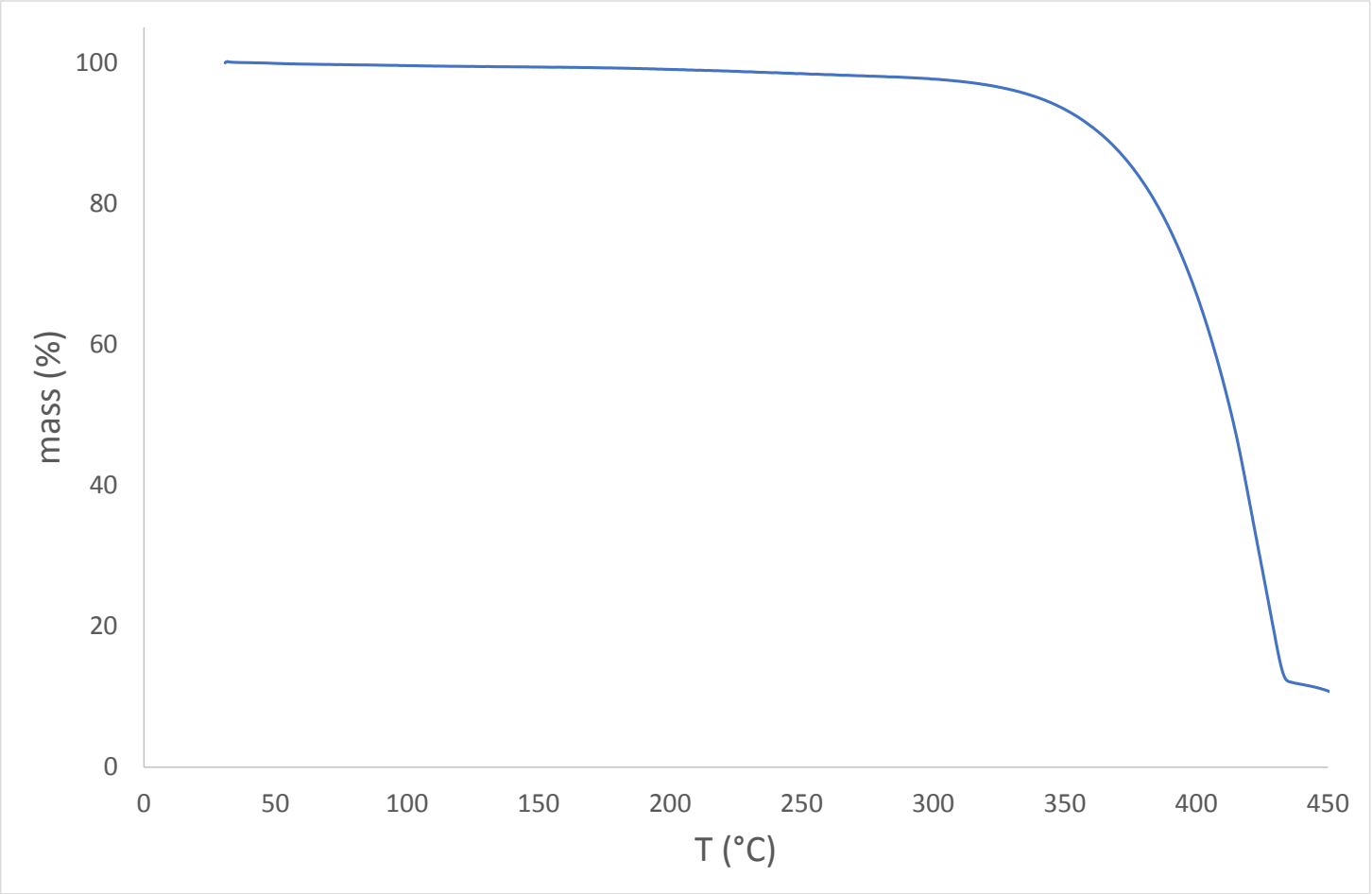

Figure S40: Thermogravimetric analyses (TGA) measurements performed on **1**. (TGA performed by using a Mettler-Toledo TGA-DSC-1 apparatus under dry nitrogen flow at a heating rate of 10 °C/min.)