Electronic Supporting Information

Applying thieno[3,2-b]thiophene as a building block in the design of rigid extended thienoacenes.

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Contents (22 pages)

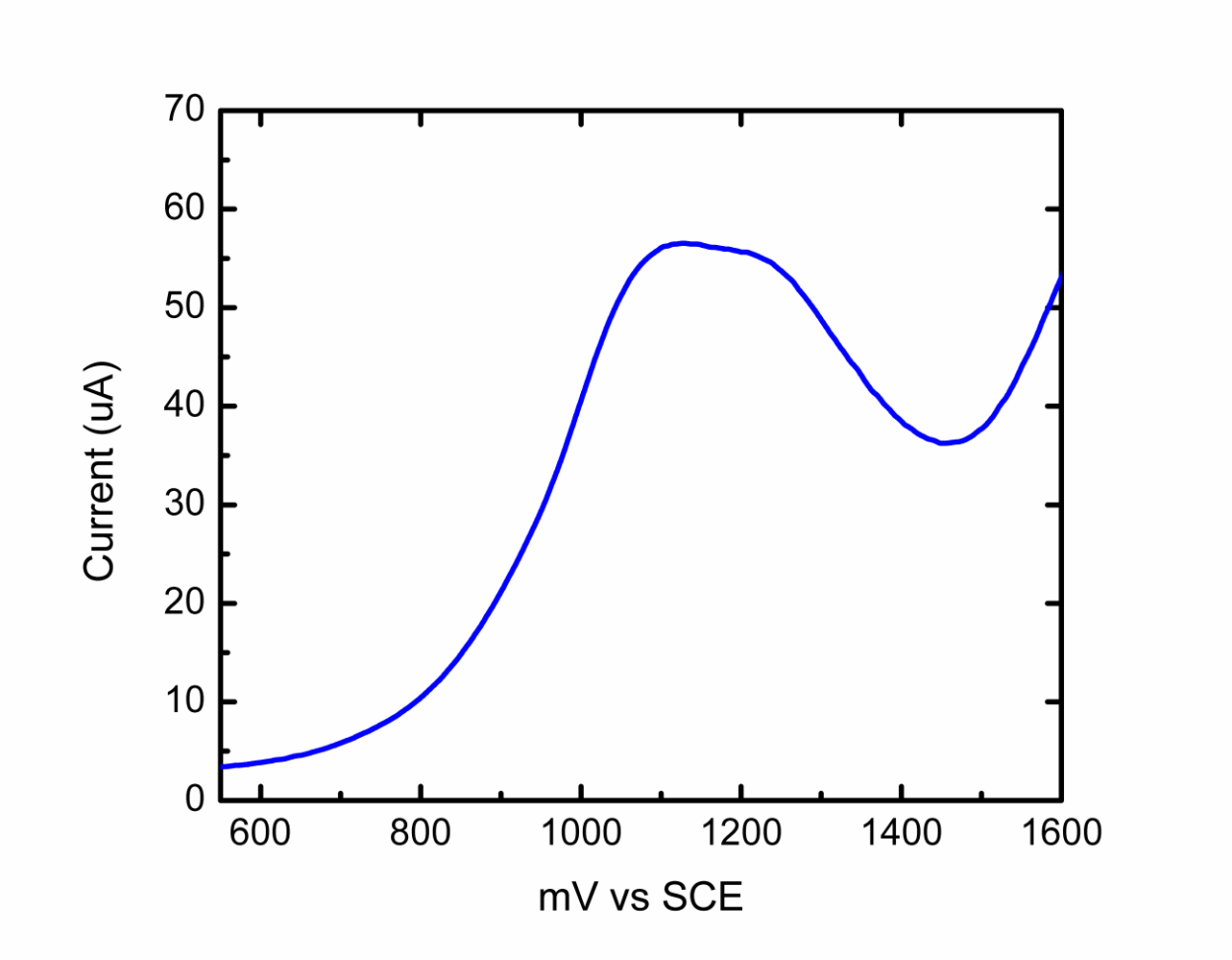

Figure S1. Differential pulse voltammetry (DPV) scan of 7.

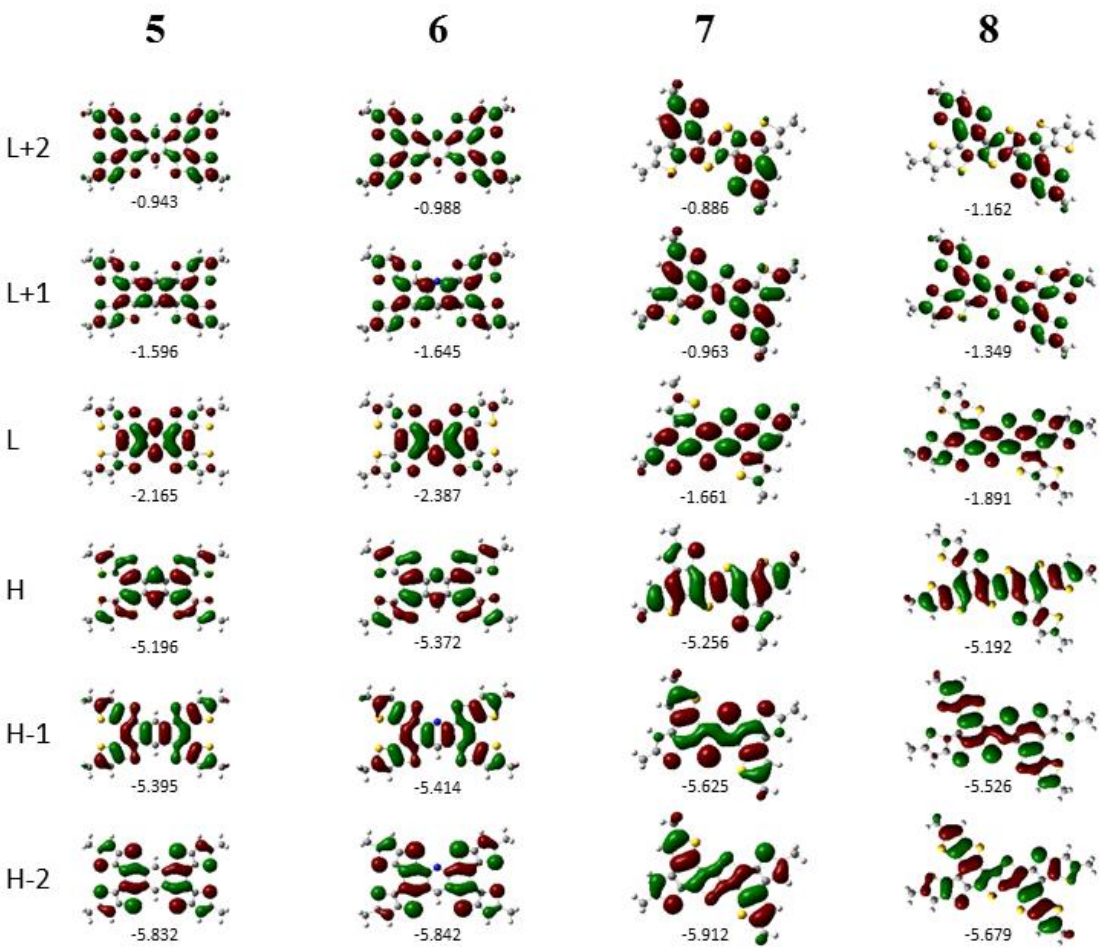

Figure S2. Frontier molecular orbitals and their corresponding energies (eV) for 5, 6, 7 and 8.

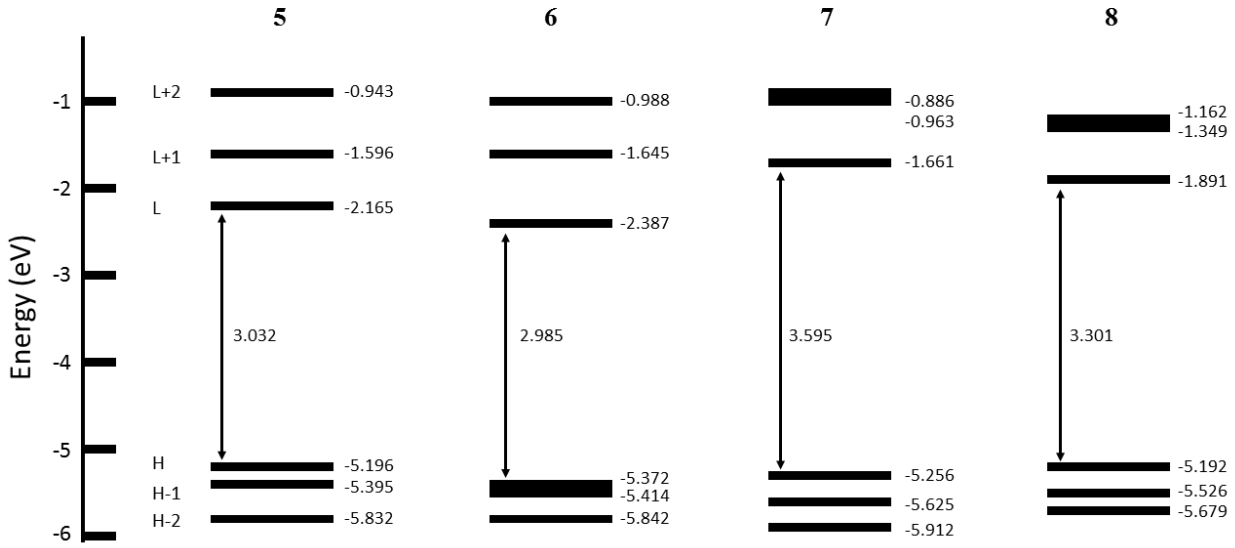

Figure S3. Energy level diagrams for the frontier molecular orbitals of 5, 6, 7 and 8.

Table S1 – DFT-calculated internal reorganization energy for oxidation (hole transfer, λ_{hole}) and reduction (electron transfer, $\lambda_{electron}$) processes.

	λ_{hole} (eV)	$\lambda_{electron}$ (eV)
1	0.122	0.109
2	0.132	0.125
3	0.148	0.108
4	0.100	0.078
5	0.113	0.125
6	0.114	0.138
7	0.202	0.203
8	0.179	0.172

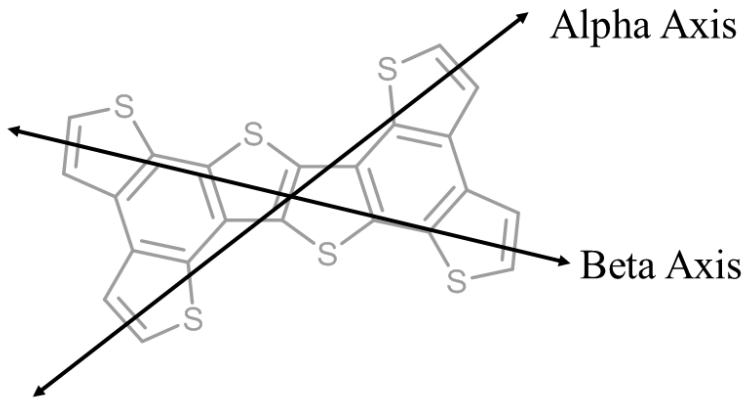

Figure S4. Schematic representation of the alpha and beta axes in 7 and 8.

Table S2. Molar extinction coefficients of 5, 6, 7 and 8.

5		**6**		**7**		**8**	
λ (nm)	ε ($M^{-1}cm^{-1}$)	λ (nm)	ε ($M^{-1}cm^{-1}$)	λ (nm)	ε ($M^{-1}cm^{-1}$)	λ (nm)	ε ($M^{-1}cm^{-1}$)
341	57712	354	94162	296	39349	325	71705
358	114394	372	178201	308	34555	340	50598
377	253227	464	19918	352	25100	375	37404
405	19292	496	34997	369	43649	396	76133
430	17909	--	--	390	47195	421	85755
440	18466	--	--	--	--	--	--
471	18899	--	--	--	--	--	--

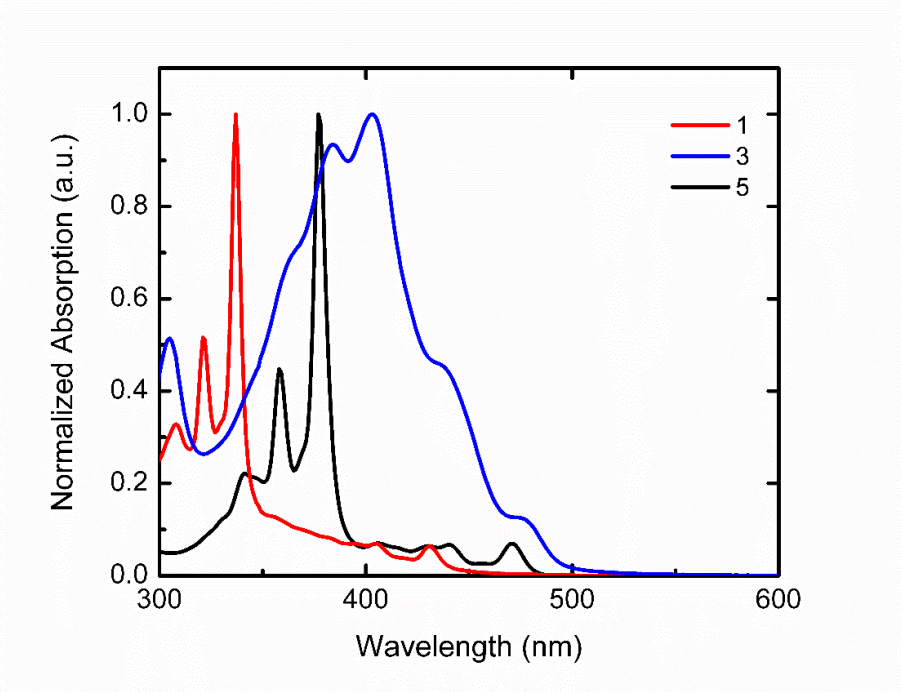

Figure S5. Normalized absorption spectra for 1, 3 and 5. Data for 1 and 3 was taken from Robertson et al.[1]; these spectra were recorded in DCM and are provided here for comparison purposes.

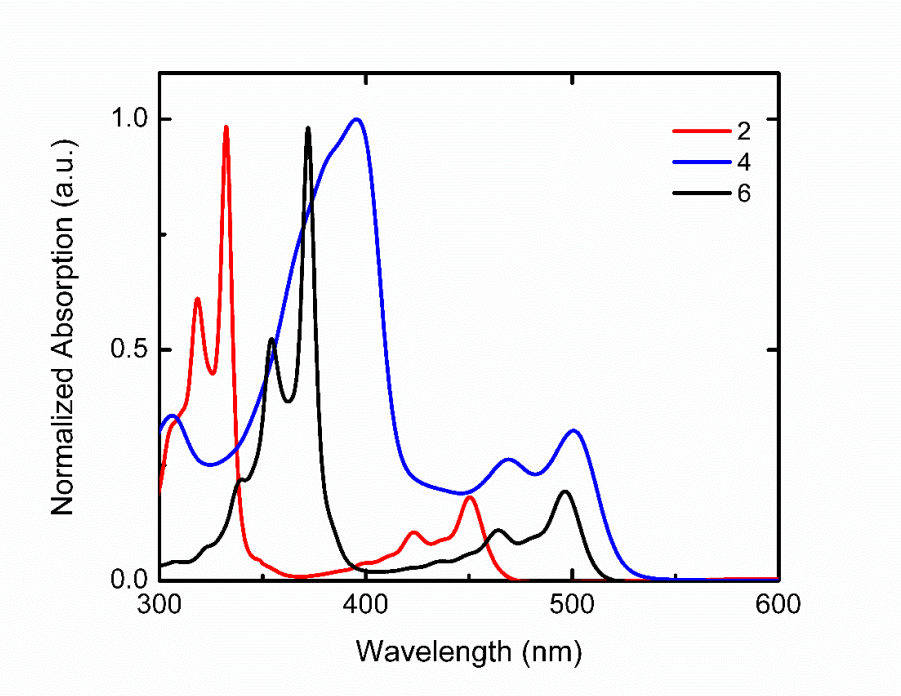

Figure S6. Normalized absorption spectra for 2,4 and 6. Data for 2 and 4 was taken from Robertson et al.[1]; these spectra were recorded in DCM and are provided here for comparison purposes.

Table S3. TD DFT optical transitions[a] for 5, 6, 7 and 8.

k	**5**		**6**		**7**		**8**	
	E(eV)	*f*	E(eV)	*f*	E(eV)	*f*	E(eV)	*f*
1	2.5844	0.0012	2.4994	0.0017	3.1585	1.0053	2.8814	1.3623
2	2.6659	0.3982	2.5040	0.6708	3.4377	0.0743	3.1553	0.1426
3	3.1367	0.0000	2.9087	0.0009	3.6433	0.0000	3.2788	0.0001
4	3.1743	2.1559	3.2268	0.0060	3.8099	0.0000	3.4304	0.0008
5	3.3815	0.0000	3.2753	1.7656	3.8990	0.0000	3.5655	0.0010
6	3.4001	0.1994	3.2810	0.0476	3.9419	0.3250	3.5955	0.5281
7	3.4545	0.4282	3.3836	0.5855	4.0167	0.0000	3.6169	0.0000
8	3.7375	0.0000	3.5249	0.0001	4.1382	0.0000	3.7884	0.0003
9	3.7980	0.0000	3.7396	0.0004	4.1892	0.0000	3.8317	0.0345
10	3.8838	0.0000	3.7695	0.1446	4.2390	0.5398	3.8567	0.9390
11	3.9209	0.0000	3.8069	0.0034	4.2592	0.0001	3.9167	0.0000
12	3.9908	0.1466	3.9171	0.0007	4.3202	0.0330	3.9582	0.1569
13	4.0053	0.0000	4.0087	0.0000	4.3842	0.0000	3.9836	0.0001
14	4.0136	0.0000	4.0321	0.0004	4.4579	0.0000	4.0215	0.0000
15	4.0512	0.0007	4.0353	0.0096	4.4880	0.3821	4.0804	0.0008
16	4.0577	0.0000	4.0593	0.0544	4.5483	0.0000	4.1464	0.2407
17	4.2035	0.0000	4.1781	0.0005	4.6176	0.0000	4.1523	0.0000
18	4.2250	0.0908	4.2027	0.0002	4.6455	0.0003	4.1794	0.0035
19	4.2906	0.0000	4.3358	0.0933	4.6704	0.0000	4.2188	0.0000
20	4.3049	0.0000	4.3566	0.0602	4.6999	0.0000	4.2545	0.0228

[a] TDDFT/B3LYP/6-311+G(2d,p) level of theory on geometry optimized structures (where R = Me for all structures) where k = order of excitation energy and f = oscillator strength.

Table S4. Selected TD DFT transitions for 5, 6, 7 and 8 (PhCl solvent cavity, where R = Me for all structures).

Compound	Calculated λ (nm)	Transition	Oscillator Strength (*f*)
5	390	HOMO-1→LUMO HOMO →LUMO+1	2.1559
	359	HOMO-4→LUMO HOMO-1→LUMO+1	0.4282
	465	HOMO-1→LUMO HOMO →LUMO+1	0.3982
	365	HOMO-4→LUMO HOMO-1→LUMO+1	0.1994
6	379	HOMO-1→LUMO HOMO →LUMO+1	1.7656
	495	HOMO-1→LUMO HOMO →LUMO+1	0.6708
	366	HOMO-4→LUMO HOMO-1→LUMO+1	0.5855
	329	HOMO-6→LUMO	0.1446
7	393	HOMO →LUMO	1.0053
	292	HOMO-1→LUMO+2	0.5398
	276	HOMO-2→LUMO+1	0.3821
	315	HOMO-1→LUMO HOMO →LUMO+2	0.3250
8	430	HOMO →LUMO	1.3623
	321	HOMO-2→LUMO+1 HOMO-1→LUMO+2	0.9390
	345	HOMO-1→LUMO HOMO →LUMO+2	0.5281
	299	HOMO-4→LUMO HOMO-3→LUMO+1	0.2407

Table S5- Crystallographic data for 6.

	6
Formula	$C_{53}H_{57}N8_4$
fw	964.48
Crystem System	Triclinic
Space Group	P-1
a (Å)	4.6484(2)
b (Å)	13.9788(7)
c (Å)	19.2908(9)
α (°)	105.132(2)
β (°)	90.170(3)
γ (°)	98.420(3)
V (Å^3)	1195.88(10)
Z	1
D_{calc} (Mg·m^{-3})	1.339
T(K)	200
u (mm^{-1})	0.411
$2\Theta_{max}$ (°)	56.924
No. of total reflections	6037
No. of unique reflections	4764
R_{int}	0.0519
R_1, wR_2 (on F^2)	0.0725, 0.1330
δ^a (Å)	3.4811
τ^b (°)	49.777

[a]δ is the mean interplanar separation between molecular planes along the π stack. [b]τ is the tilt angle between the mean molecular plane and the stacking axis.

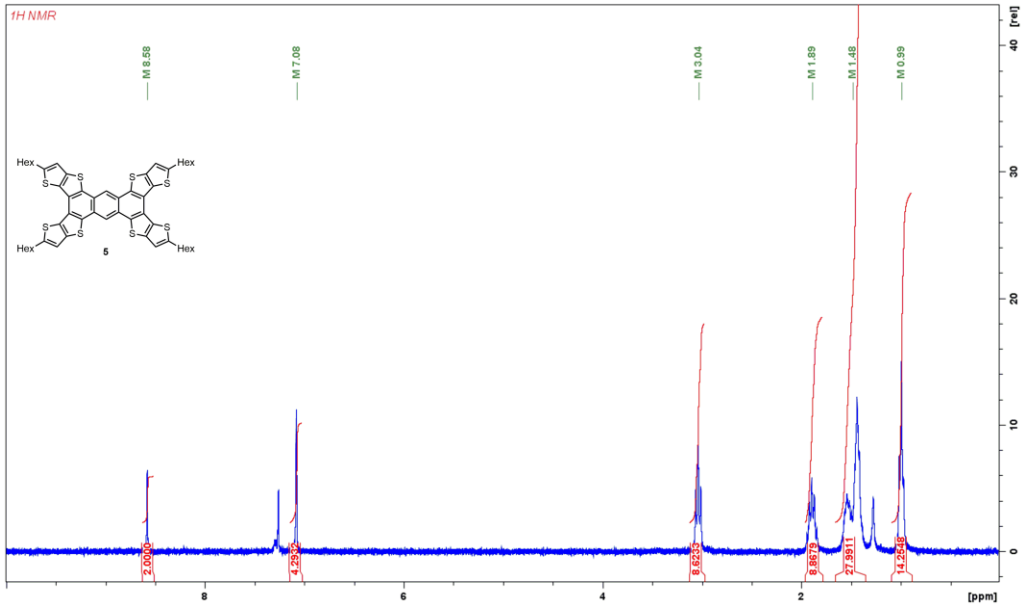

Figure 7 – ^{1}HNMR spectrum of 5

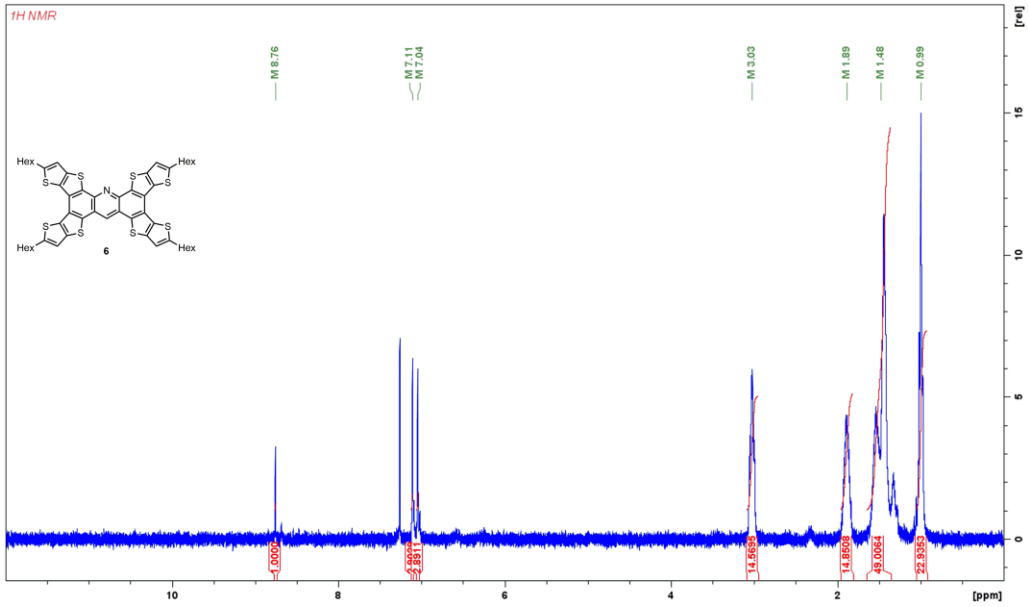

Figure 8 - ^{1}HNMR spectrum of 6

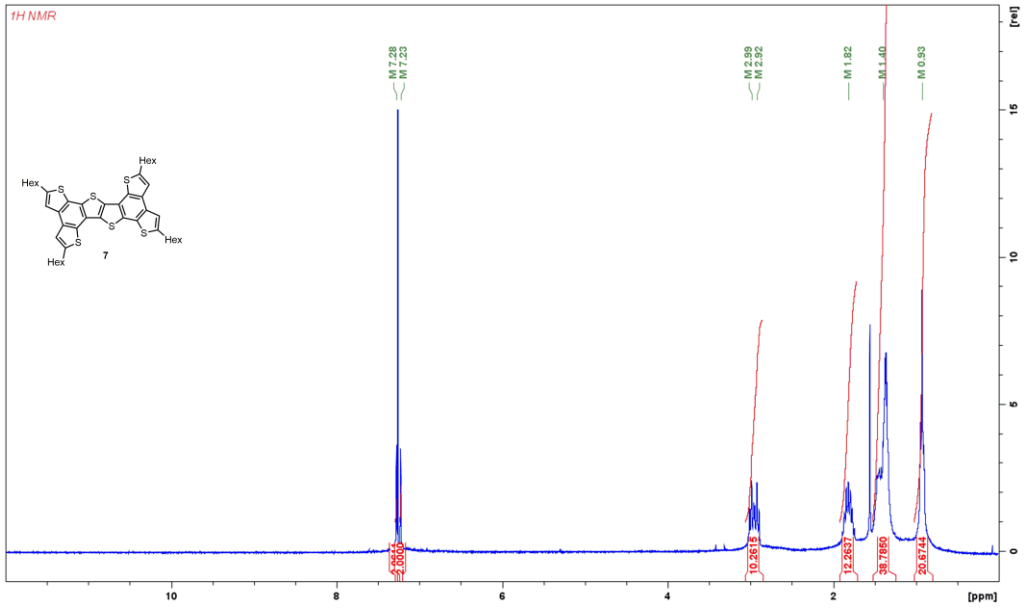

Figure 9 - ^{1}HNMR spectrum of 7

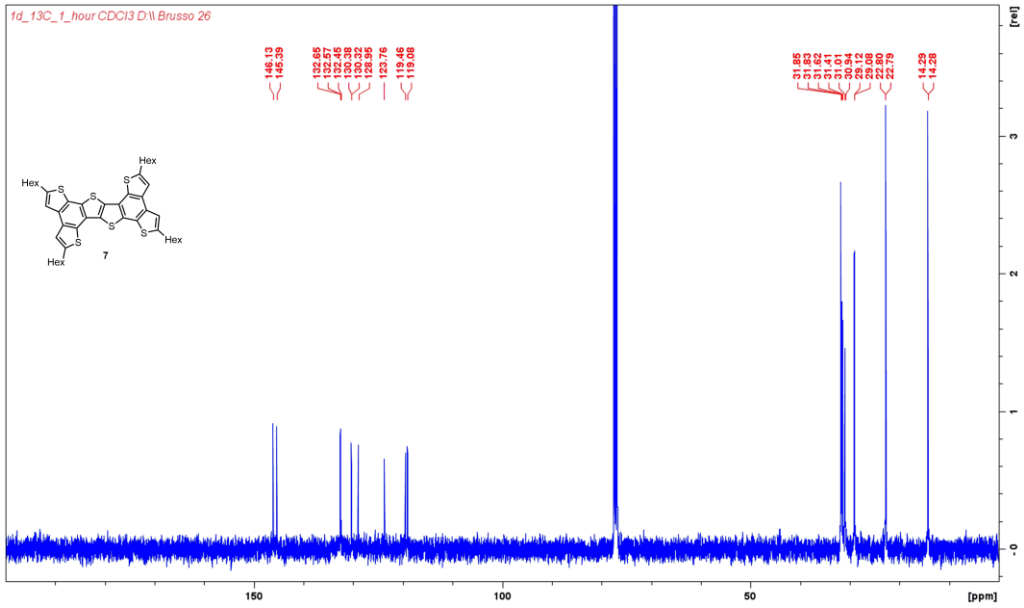

Figure 10 – ^{13}CNMR spectrum of 7

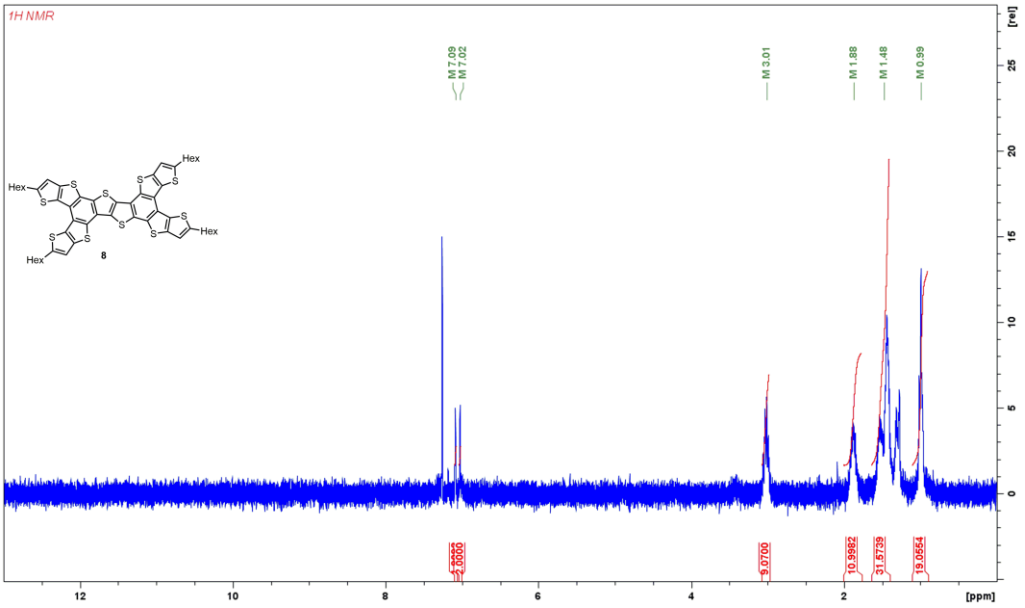

Figure 11 - ^{1}HNMR spectrum of 8

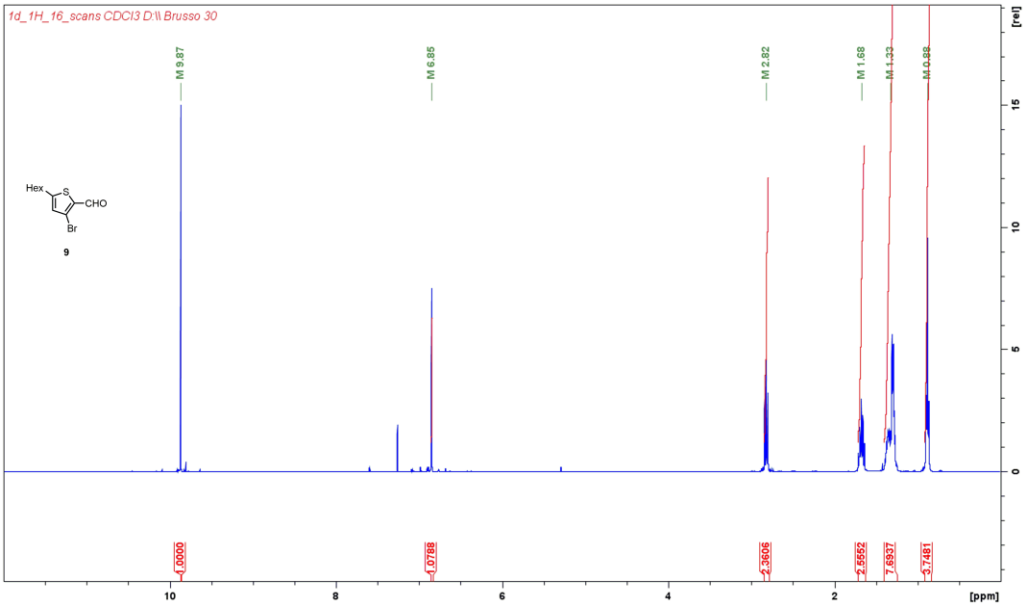

Figure 12 - ^{1}HNMR spectrum of 9

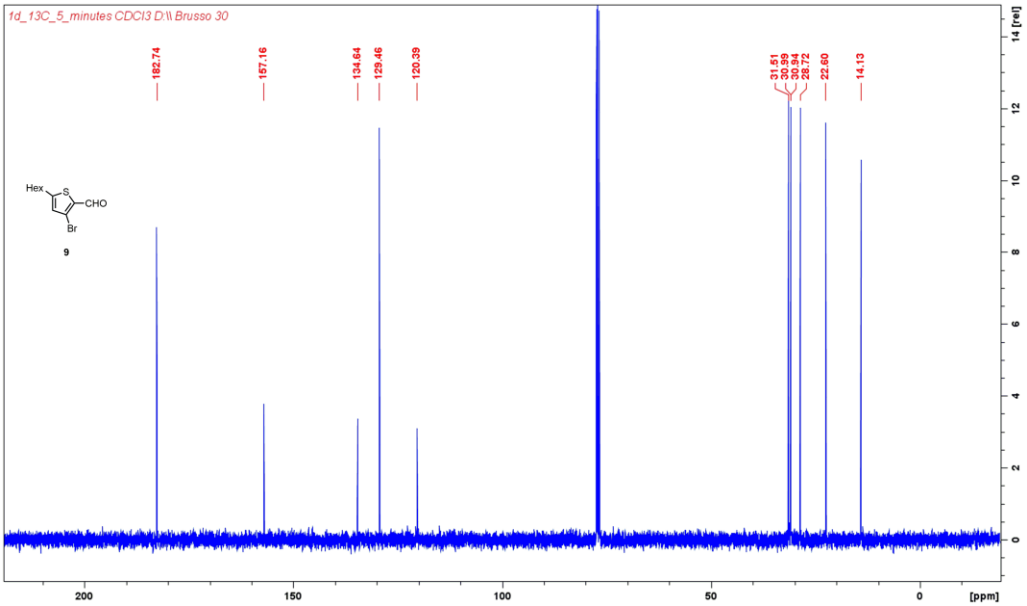

Figure 13 - ^{13}CNMR spectrum of 9

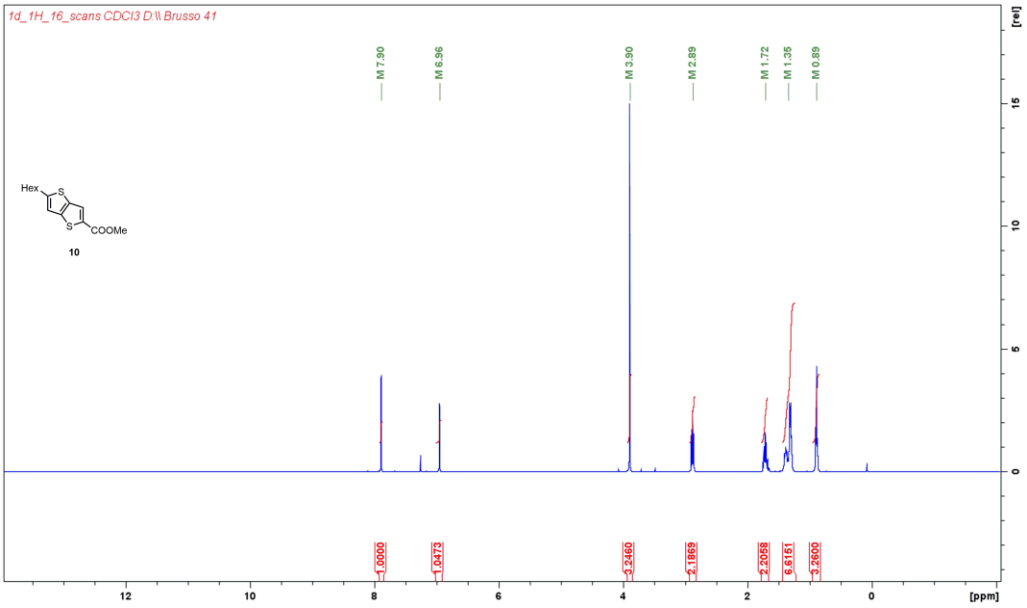

Figure 14 - ^{1}HNMR spectrum of 10

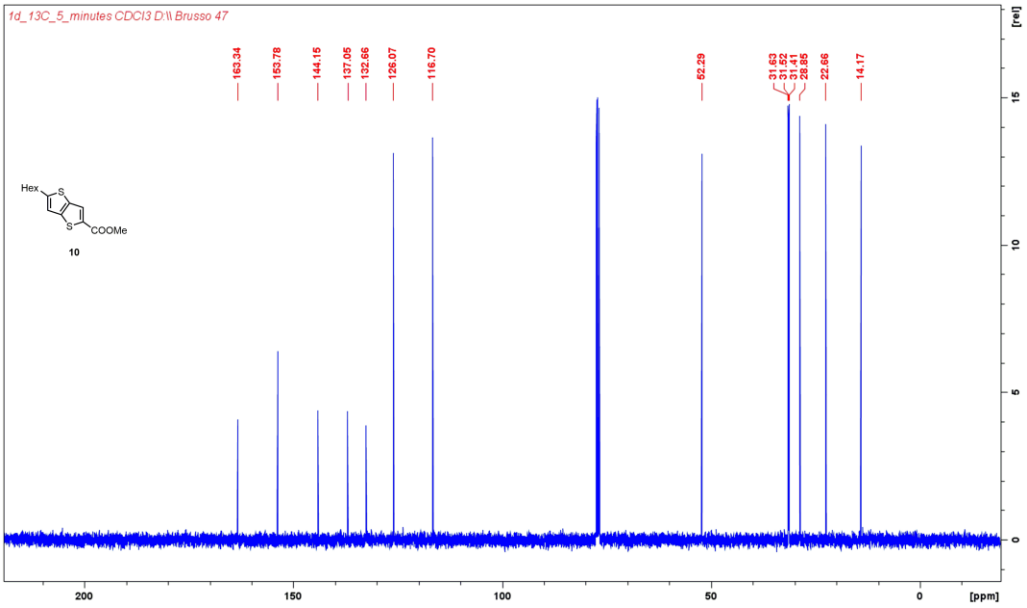

Figure 15 - ^{13}CNMR spectrum of 10

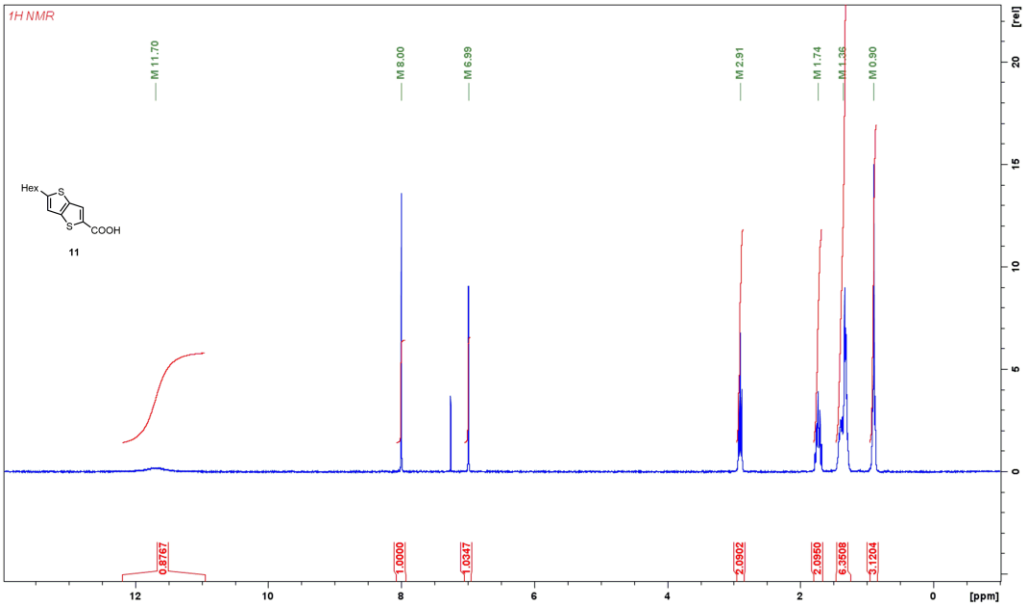

Figure 16 - ^{1}HNMR spectrum of 11

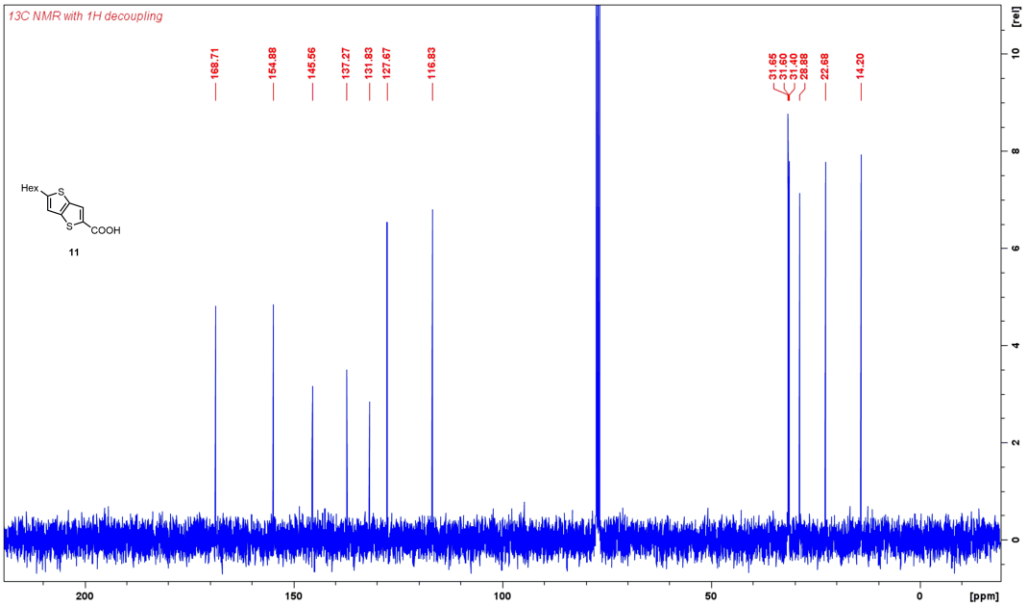

Figure 17 - ^{13}CNMR spectrum of 11

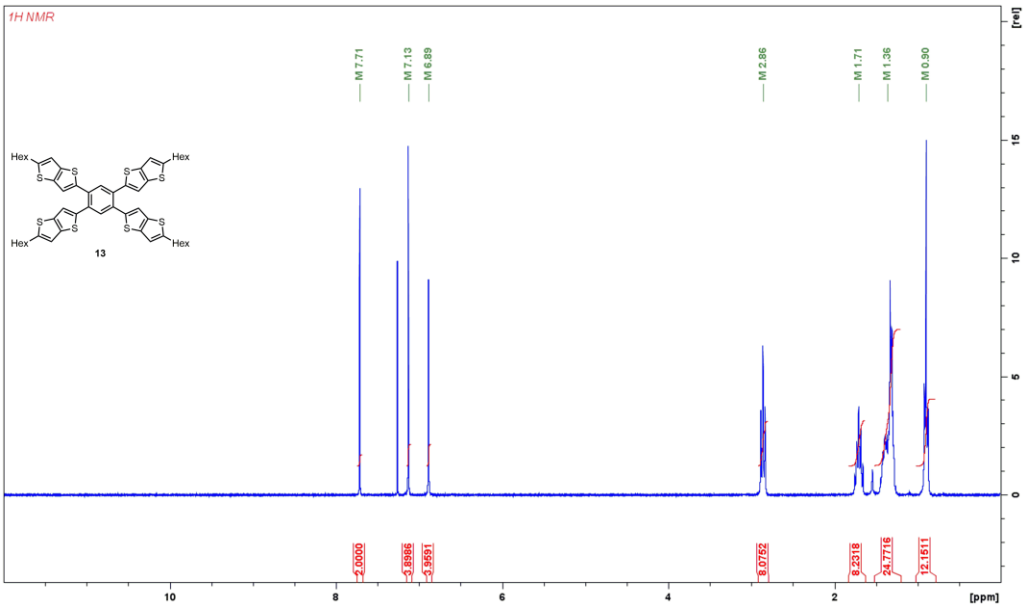

Figure 18 - - ^{1}HNMR spectrum of 13

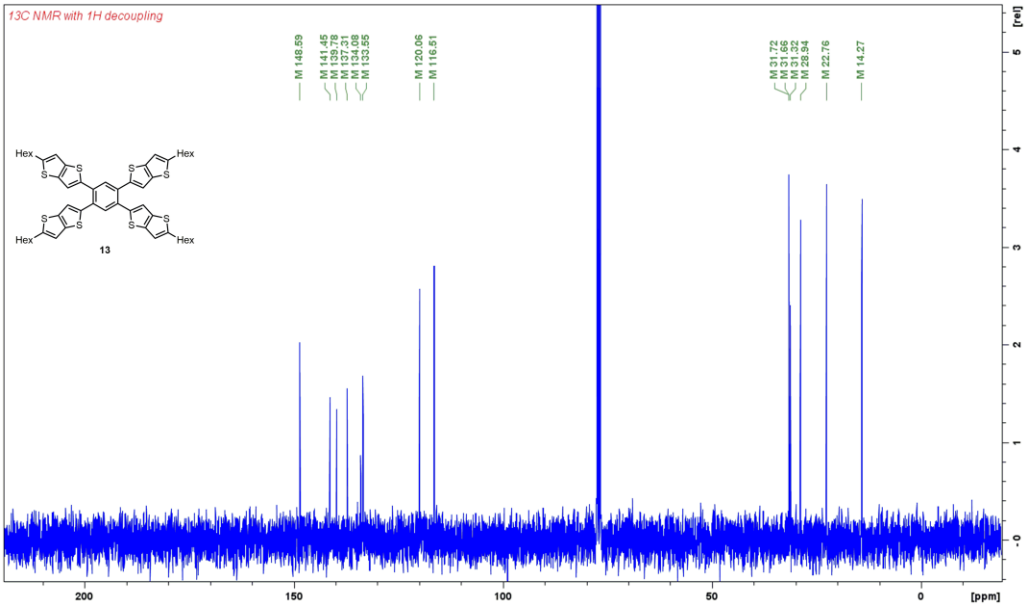

Figure 19 - ^{13}CNMR spectrum of 13

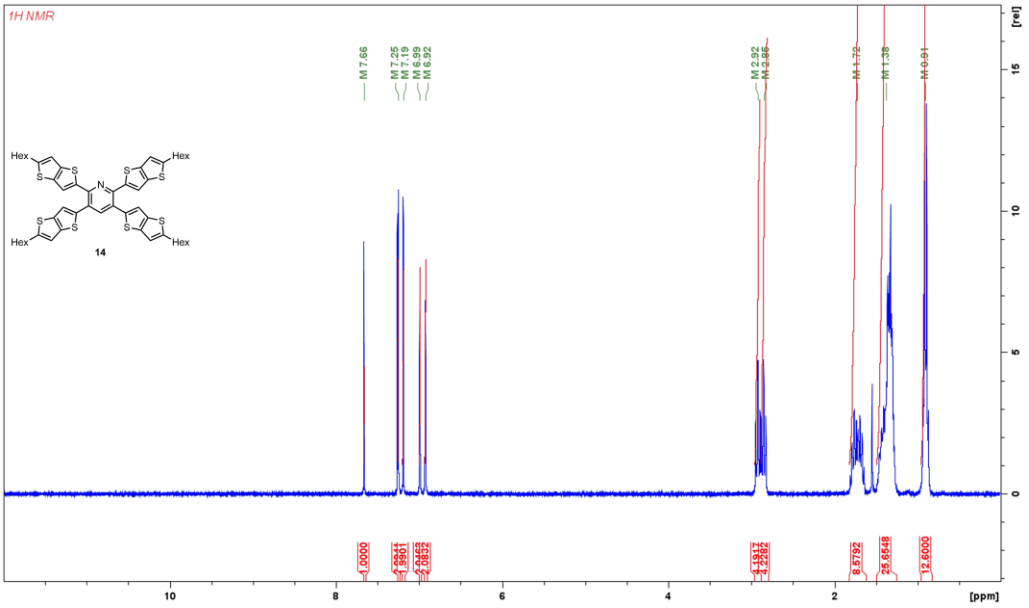

Figure 20 - - ^{1}HNMR spectrum of 14

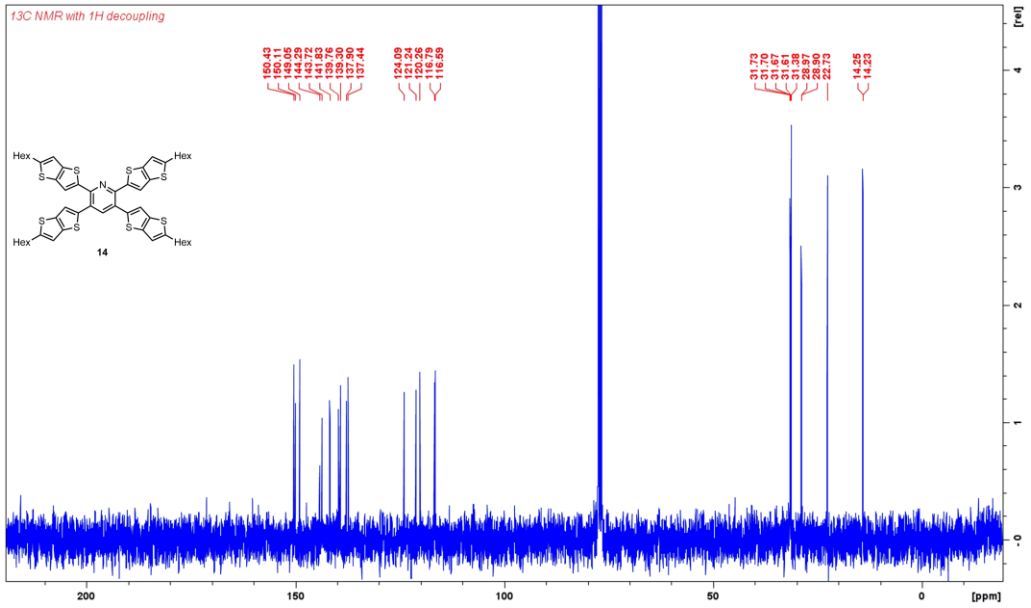

Figure 21 - ^{13}CNMR spectrum of 14

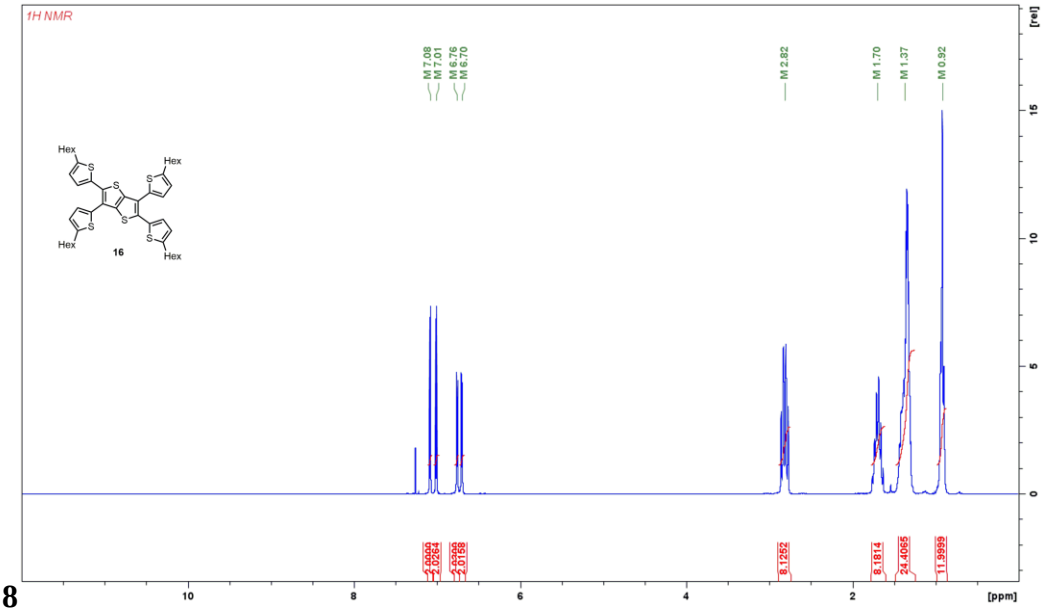

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Figure 22 - - ^{1}HNMR spectrum of 16

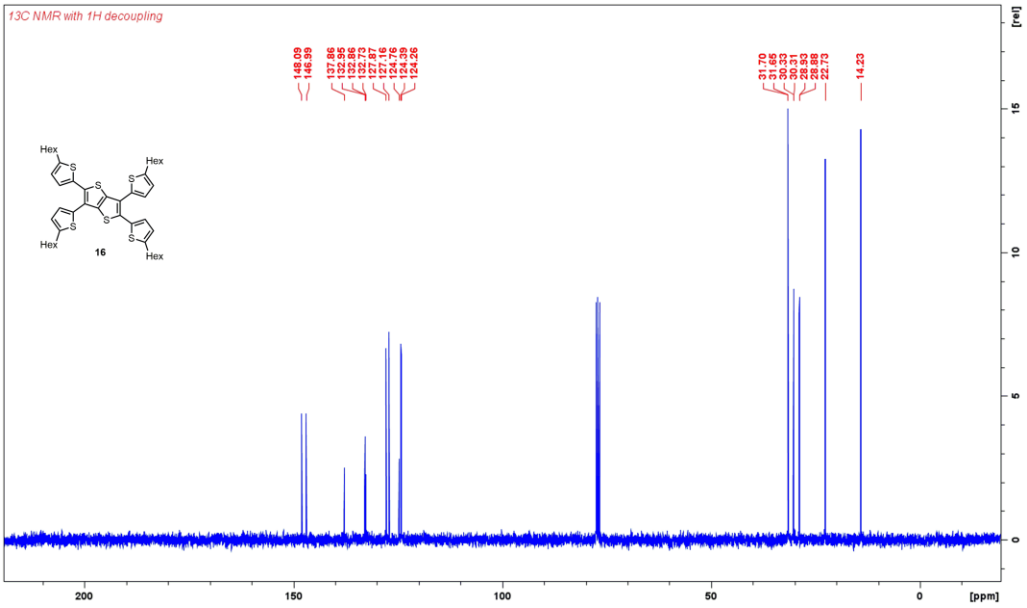

Figure 23 - ^{13}CNMR spectrum of 16

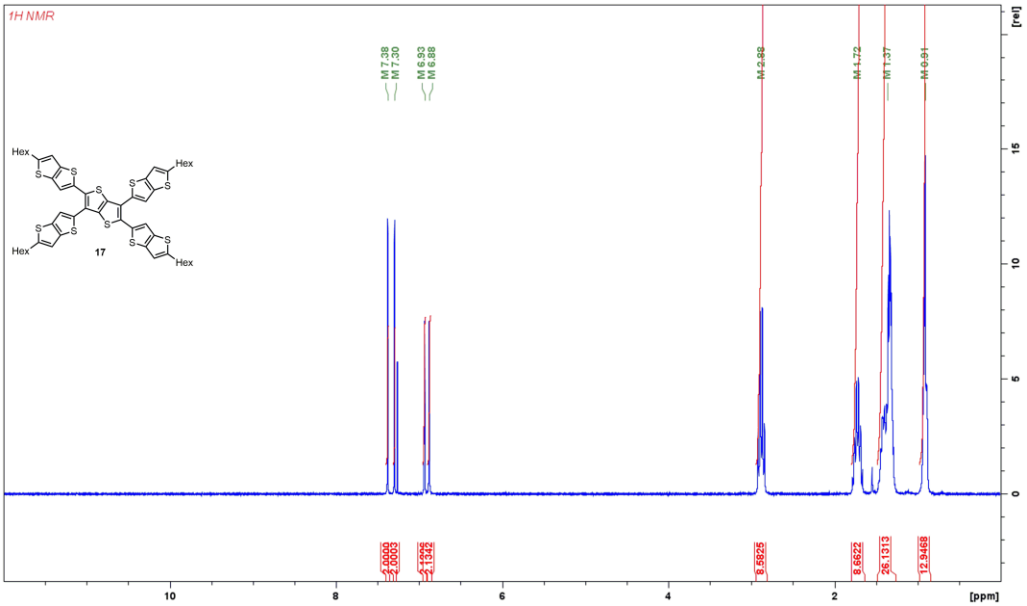

Figure 24 - - ^{1}HNMR spectrum of 17

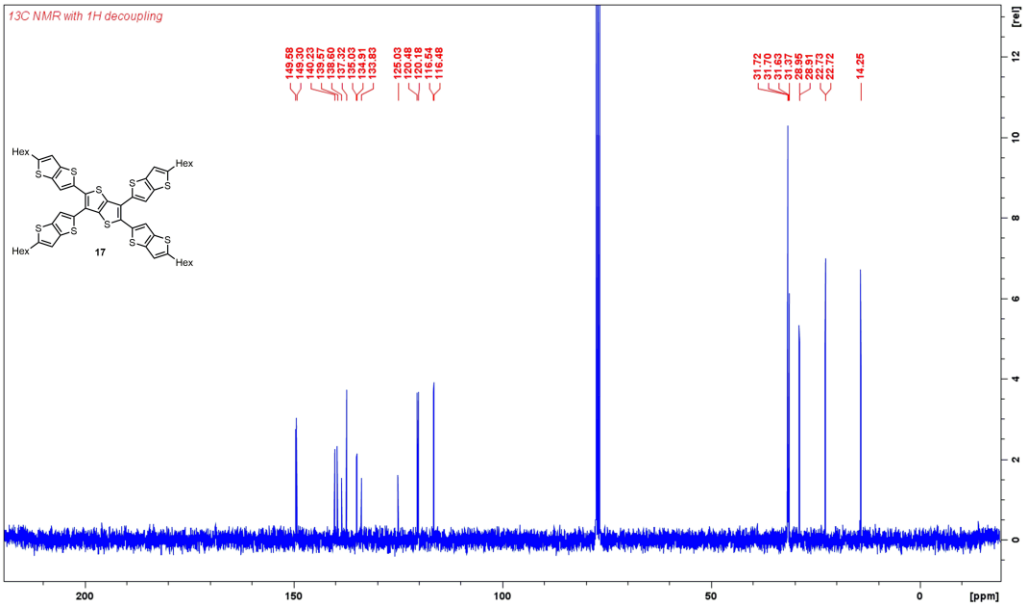

Figure 25 - ^{13}CNMR spectrum of 17

Density Functional Theory Calculations and Archival Files

Molecular geometry optimizations were performed on **5**, **6**, **7** and **8** (where R = Me in all cases) at the DFT (B3LYP) level of theory with the 6-311+G(2d,p) basis set, using the Gaussian 09W program package.[2] All geometries were optimized without symmetry constraints.

Archive file (geometry optimization) for **5** (where R = Me)

```
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Archive file (geometry optimization) for **6** (where R = Me)

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6551605161,-0.0002658364,6.4519191402\S,-3.9808584825,-0.0004633977,8.
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,0.8822056175,3.0789190801\H,-6.8710813203,-0.0004554984,6.5909987715\
C,-1.0531074699,0.0001998494,5.3228450368\C,-0.687905665,0.0004072682,
3.9364838328\S,-1.5214686062,0.0004925038,2.3998180642\H,-2.1141865395
,-0.0006681928,10.1321966487\C,0.1351764797,-0.0007374255,11.721435612
3\C,1.3556149105,-0.0007286198,12.4081893658\C,1.1236349551,-0.0011672
373,13.8246108961\C,-0.213570006,-0.0014349142,14.1804851319\S,-1.2575
80393,-0.0012223568,12.7917509061\C,-0.4653677382,-0.0020056057,15.576
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017703679,15.2709286379\C,0.8391757997,-0.002603028,17.7923814508\H,-0
.1446556087,-0.0030868324,18.2639360617\H,1.3809721235,-0.8843266074,1
8.1448533748\H,1.3803875676,0.8792459412,18.1454447079\H,-1.4493385815
,-0.0022234974,16.0250774324\C,2.5754181052,-0.000291584,11.6366432071
\C,3.9571305766,-0.0000008056,12.0190569709\C,4.835683304,0.0003718984
,10.9466266894\S,4.0146433506,0.0004048389,9.4145269721\C,2.4745926526
,-0.00007946,10.2409427473\C,6.2090937655,0.0007322254,11.301754889\C,
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.7802426082,-0.8806364863,14.0473055008\H,7.027233805,0.0010313679,10.
5941760305\H,2.088861015,0.0009026331,2.0011837854\H,1.0140637223,0.00
08940496,-0.3539099945\H,-0.5156569899,-0.8807347549,-0.3878090018\H,-

0.515474458,0.8828485801,-0.3875732574\\Version=EM64L-G09RevA.02\State
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-0.0000271,0.200485\Quadrupole=10.7171785,-33.658734,22.9415556,0.0056
077,10.489833,-0.0096091\PG=C01 [X(C33H17N1S8)]\\@

Archive file (geometry optimization) for **7** (where R = Me)

1\1\GINC-TITAN\FOpt\RB3LYP\6-311+G(2d,p)\C26H16S6\APACHE\28-Dec-2015\0
\\#N B3LYP/6-311+G(2d,p) OPT Geom=Connectivity\\T(HT)BTBT 2\\0,1\C,0.0
035184123,-0.0001596933,0.0190770651\C,0.0031858802,-0.0003507692,1.51
35331387\S,1.5227371643,-0.0002444721,2.3982267774\C,0.6831456826,-0.0
007176405,3.9322242047\C,1.2412085573,-0.000926294,5.2162454269\S,2.95
18930474,-0.0008508862,5.621847823\C,2.5646504304,-0.0013664291,7.3286
526523\C,1.2055800414,-0.0014954197,7.5458483021\C,0.4130555803,-0.001
2386109,6.3586791384\C,-0.9848814946,-0.0013386833,6.1655847734\C,-1.5
58040613,-0.001120844,4.8857657298\C,-2.9908514139,-0.0012824764,4.939
6089237\C,-3.4992657685,-0.0016280139,6.1976077074\S,-2.2211841527,-0.
001735909,7.4020553869\C,-4.9331721388,-0.0019007698,6.6201191337\H,-5
.1789334148,0.87928898,7.2188442172\H,-5.5786660124,-0.0018197085,5.74
05619517\H,-5.1786976301,-0.8833827302,7.2185109064\H,-3.6239042063,-0
.0011635211,4.0617985831\C,-0.7088175543,-0.0008004996,3.7462439774\C,
-1.0600416446,-0.0005687621,2.3563809347\H,-2.0807855136,-0.0005977849
,1.9968035388\S,0.8183354825,-0.0017263736,9.2526499632\C,2.5290187348
,-0.0016910643,9.6582557937\C,3.3571740561,-0.0014647748,8.5158201805\
C,4.7551088125,-0.0014581421,8.7089245191\S,5.991411603,-0.0012162965,
7.4724493664\C,7.2694899278,-0.0013459784,8.6768892782\C,6.7610796211,
-0.0016191521,9.9348930735\C,5.3282707397,-0.00165852,9.9887418118\C,4
.4790434071,-0.0018863496,11.1282605574\C,3.0870818103,-0.0019027028,1
0.9422767917\S,2.2474789041,-0.0021234888,12.4762671314\C,3.7670373465
,-0.0023942155,13.3609744893\C,4.830261201,-0.0021432975,12.5181242886
\H,5.8510044286,-0.002205565,12.8777061579\C,3.7666974137,-0.002790983
1,14.85542215\H,4.7925749415,-0.0027816679,15.2265888898\H,3.261469792
5,0.8783279009,15.2603285447\H,3.2616528244,-0.8842294078,15.259865030
9\H,7.3941393252,-0.0017594849,10.8126981729\C,8.7034101054,-0.0011819
004,8.2544208166\H,9.3488668358,-0.001424416,9.1340042978\H,8.94909933
05,-0.8823333699,7.6556103407\H,8.9490538228,0.8803360711,7.656129168\
H,-1.0223625883,-0.0001901593,-0.3520765857\H,0.5085925369,0.881204098
6,-0.3854826352\H,0.5087134475,-0.8813577317,-0.3856990845\\Version=EM
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4\Dipole=-0.0000118,-0.0000932,-0.0000036\Quadrupole=12.9444297,-24.70
2446,11.7580162,-0.0001509,15.3968136,-0.006134\PG=C01 [X(C26H16S6)]\\
@

Archive file (geometry optimization) for **8** (where R = Me)

1\1\GINC-TITAN\FOpt\RB3LYP\6-311+G(2d,p)\C34H16S10\APACHE\21-Dec-2015\
0\\#N B3LYP/6-311+G(2d,p) OPT Geom=Connectivity\\T(HTT)BTBT 2\\0,1\C,0
.0018968013,0.,0.0257152285\C,0.001308994,0.,1.5244772912\S,1.51446423
18,0.,2.4001172334\C,0.7016505196,0.,3.9430494297\C,1.0896104879,0.,5.
327867371\C,-0.069508379,0.,6.1387869652\C,0.0094696049,0.,7.532032629
7\C,1.2591562167,0.,8.1797006936\C,1.0849275989,0.,9.597272457\S,2.196
3747785,0.,10.9500427133\C,0.8470793796,0.,12.0766341958\C,-0.40248224
69,0.,11.4287818571\C,-0.2280358436,0.,10.0112786798\S,-1.3396069074,0
.,8.658659555\C,-1.5611657104,0.,12.2274865908\C,-1.5124024771,0.,13.6
396145827\C,-2.8510009317,0.,14.166754399\C,-3.8448034838,0.,13.203942
9044\S,-3.1967145854,0.,11.5878338024\C,-5.1705719604,0.,13.7028733937
\C,-5.2029347666,0.,15.0669074916\S,-3.5912159082,0.,15.7458306448\C,-
6.3976672584,0.,15.9721290978\H,-6.1045542185,0.,17.0226969669\H,-7.01

89304917,0.8831849643,15.8029500984\H,-7.0189304917,-0.8831849643,15.8
029500984\H,-6.0594667694,0.,13.0863839786\C,-0.2353237165,0.,14.27987
56042\C,0.1517433492,0.,15.6644907935\C,1.5178041053,0.,15.8779247423\
S,2.4221158018,0.,14.3877564476\C,0.9250194216,0.,13.4699496803\C,1.91
57671106,0.,17.2382287147\C,0.8474618448,0.,18.0857099028\S,-0.6687811
867,0.,17.2064089075\C,0.8532672858,0.,19.5811728576\H,1.8815107853,0.
,19.9459802031\H,0.352323187,0.8818456495,19.9894790155\H,0.352323187,
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6487,0.,7.380118791\S,4.0532970617,0.,8.0171961503\C,4.6985418089,0.,6
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49\S,4.4396575533,0.,3.8553446813\C,6.0560841537,0.,4.534604429\C,6.02
45632931,0.,5.8972348913\H,6.9160982377,0.,6.5095579273\C,7.2521009096
,0.,3.6366812807\H,8.1634888241,0.,4.2364556774\H,7.275417987,-0.88187
0007,2.990883819\H,7.275417987,0.881870007,2.990883819\S,-1.5683676943
,0.,5.2231000826\C,-0.666372879,0.,3.73100148\C,-1.0676242131,0.,2.373
5083404\H,-2.0954277978,0.,2.0361147867\H,1.0163628823,0.,-0.374802802
3\H,-0.5081344769,-0.8831645474,-0.367408419\H,-0.5081344769,0.8831645
474,-0.367408419\\Version=EM64L-G09RevA.02\State=1-A'\HF=-5287.8248087
\RMSD=3.813e-09\RMSF=6.134e-06\Dipole=-0.0158151,0.,-0.0115344\Quadrup
ole=5.6747217,-37.2430576,31.5683359,0.,-10.3389562,0.\PG=CS [SG(C34H8
S10),X(H8)]\\@

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2. 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, 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, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski and D. J. G. Fox, Gaussian, Inc., Wallingford CT, 2009.