

Expanded Benzofuran-Decorated Twistacene Derivatives: Synthesis, Characterization and Single-Component White Electroluminescence

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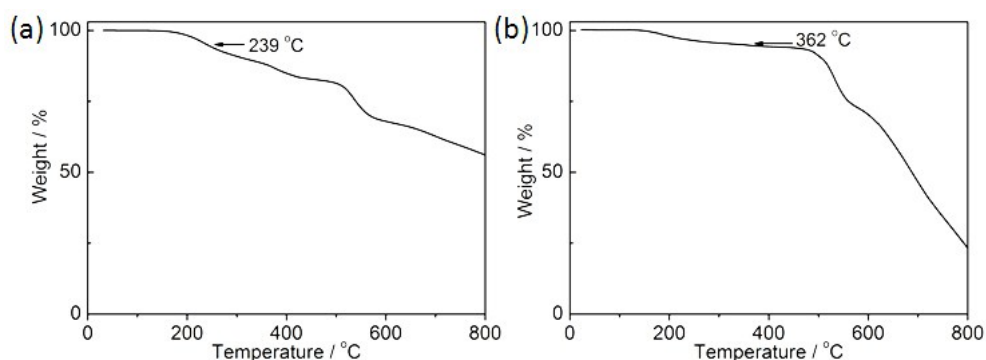


Figure S1 TGA data of **9** (a) and **10** (b) under nitrogen at a heating rate of 10 °C min⁻¹.

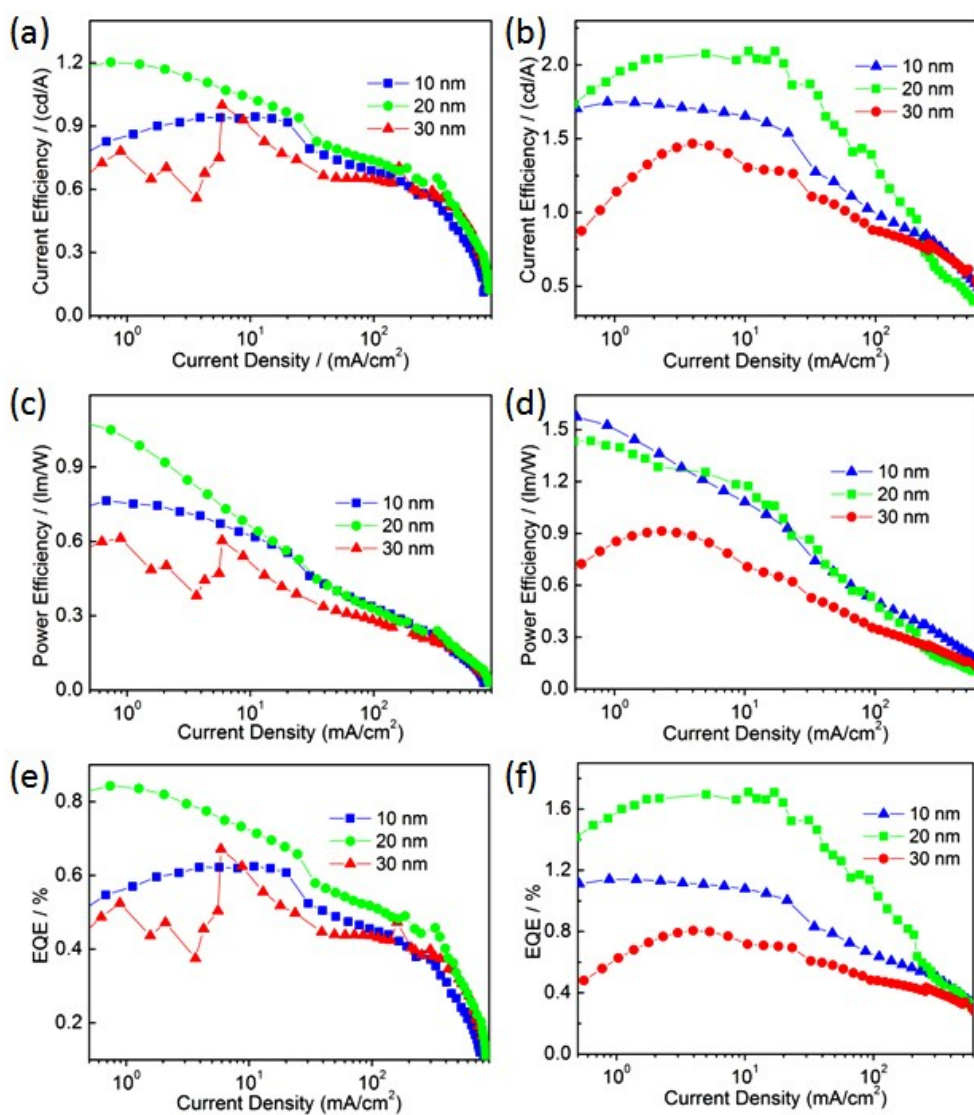


Figure S2 (a)/(c)/(e) *CE-J*, *PE-J*, and *EQE-J* curves of devices-9. (b)/(d)/(f) *CE-J*, *PE-J*, and *EQE-J* curves of devices-10.

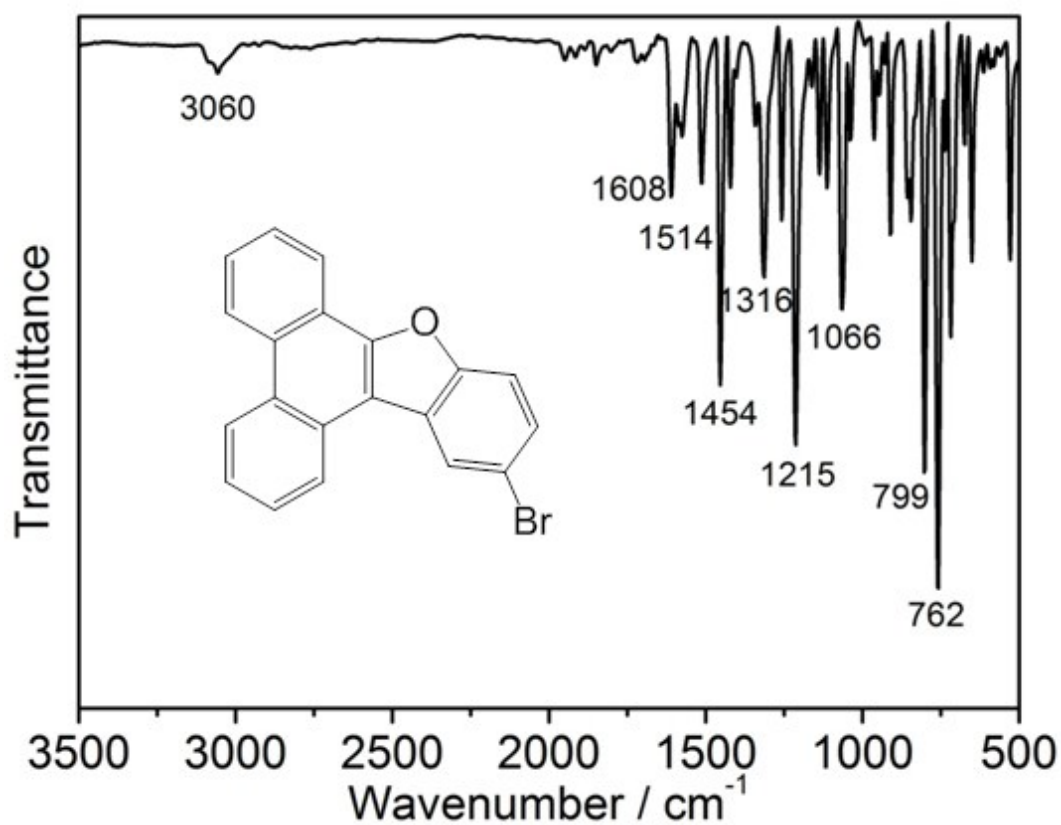


Figure S3 FT-IR spectrum of **2**.

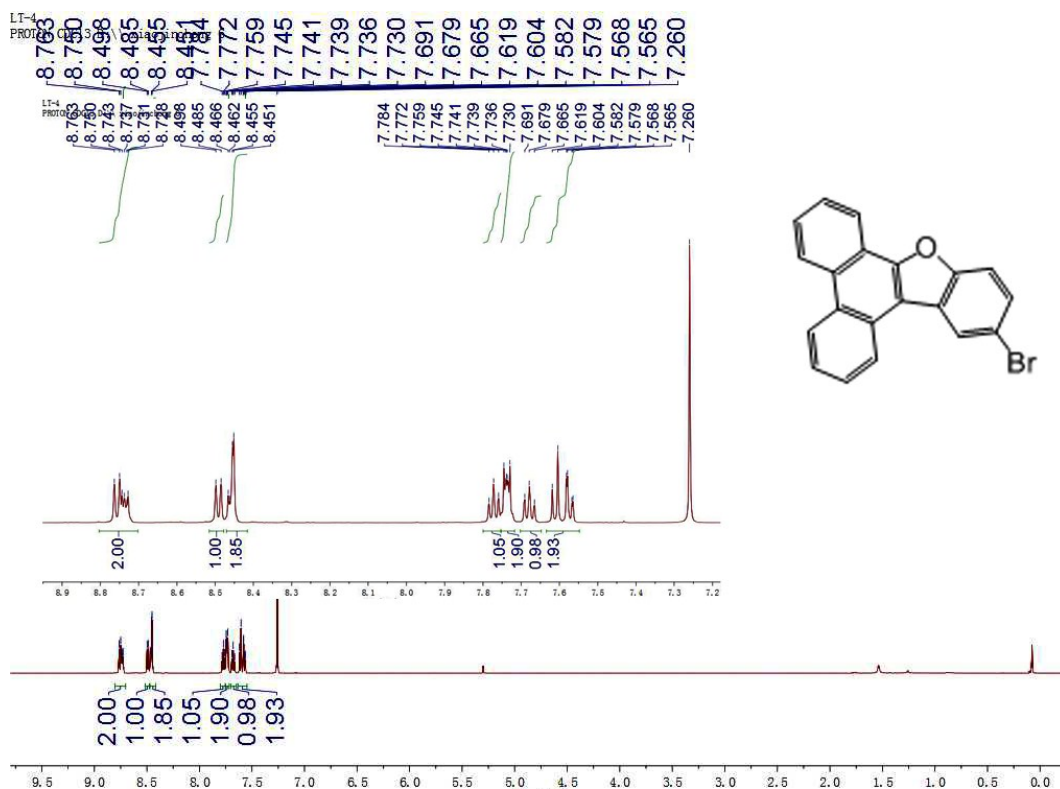


Figure S4 ^1H NMR (600 MHz) spectrum of **2**.

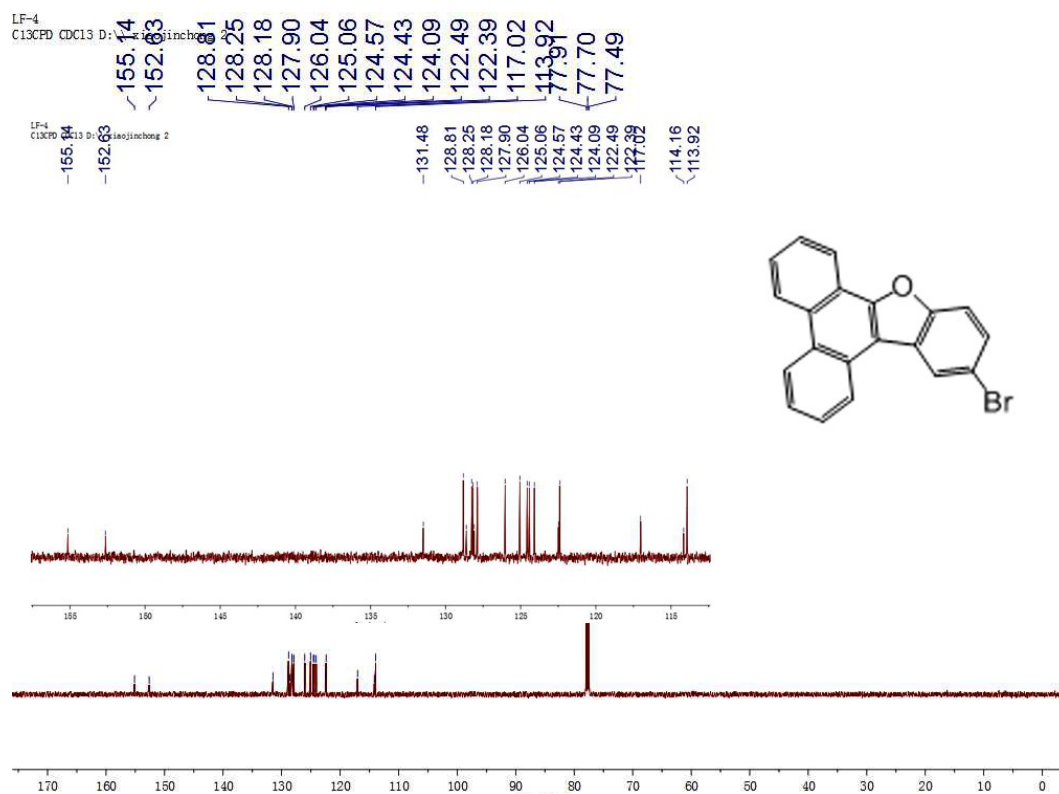


Figure S5 ^{13}C NMR spectrum of **2**.

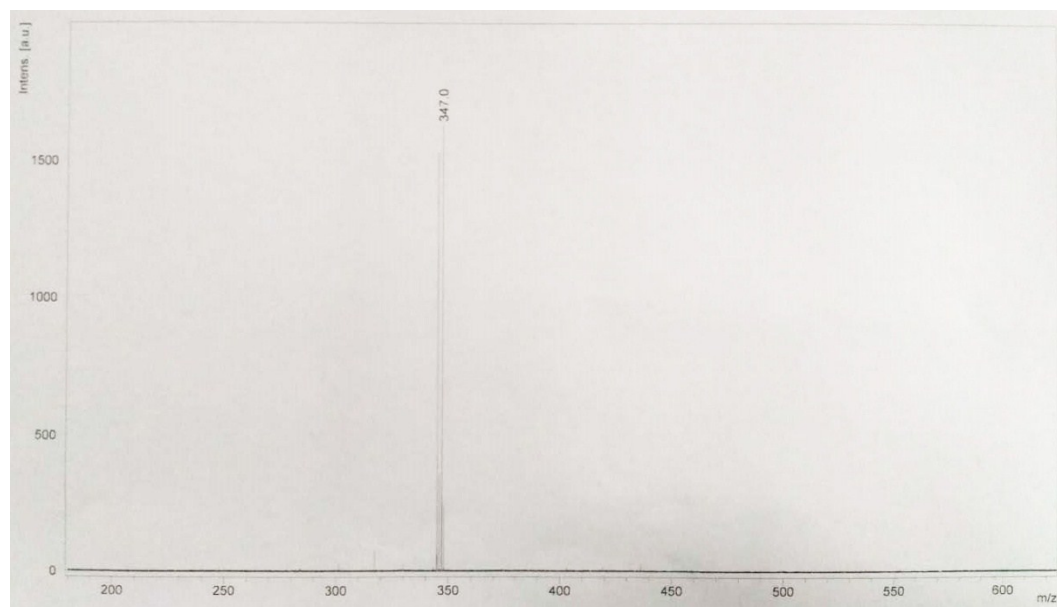


Figure S6 MALDI-TOF spectrum of **2**.

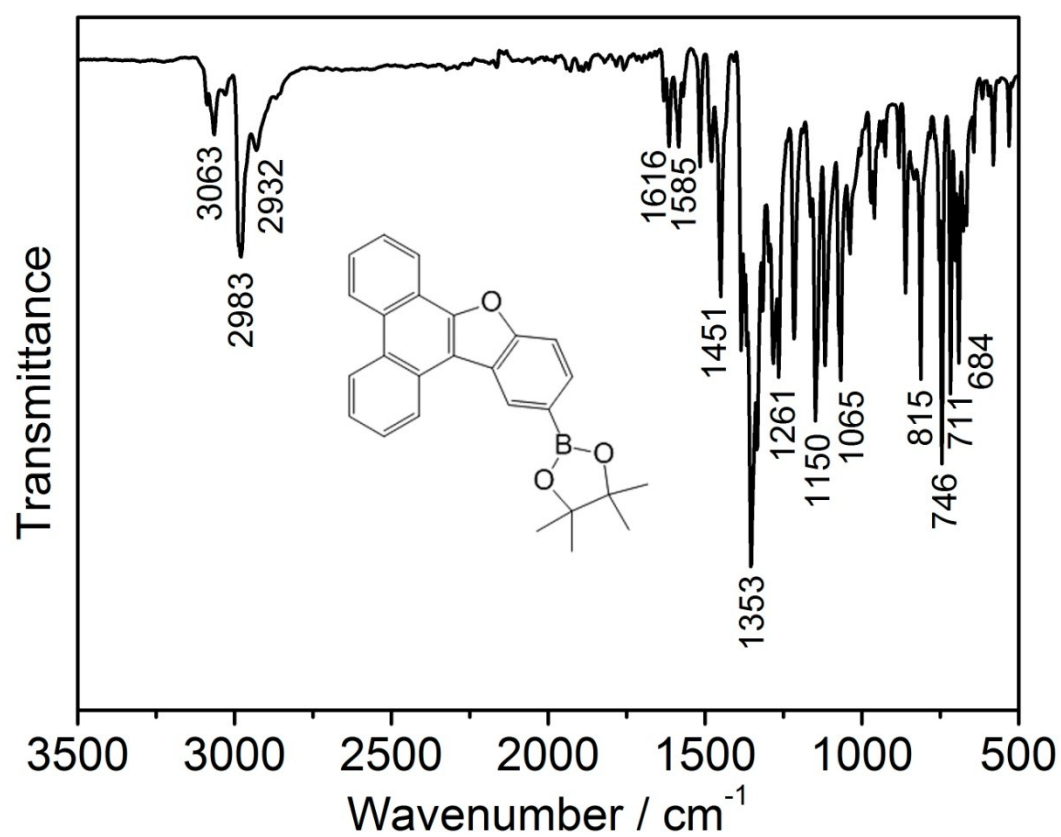


Figure S7 FT-IR spectrum of **3**.

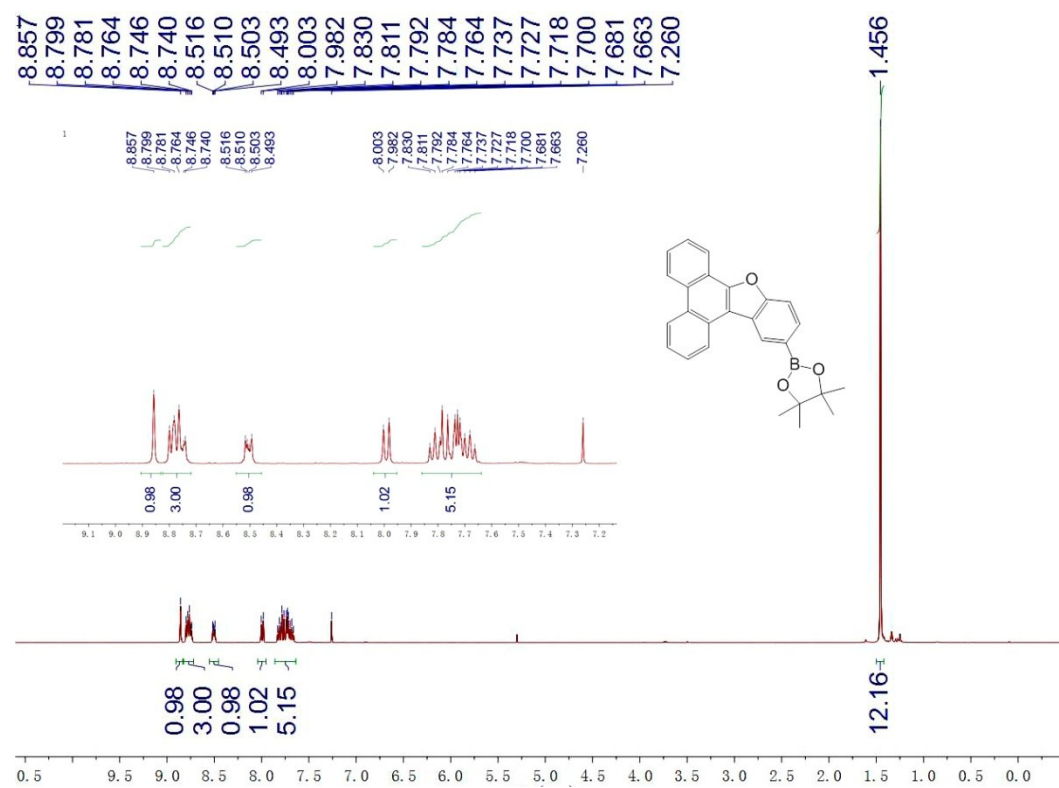


Figure S8 ^1H NMR spectrum of **3**.

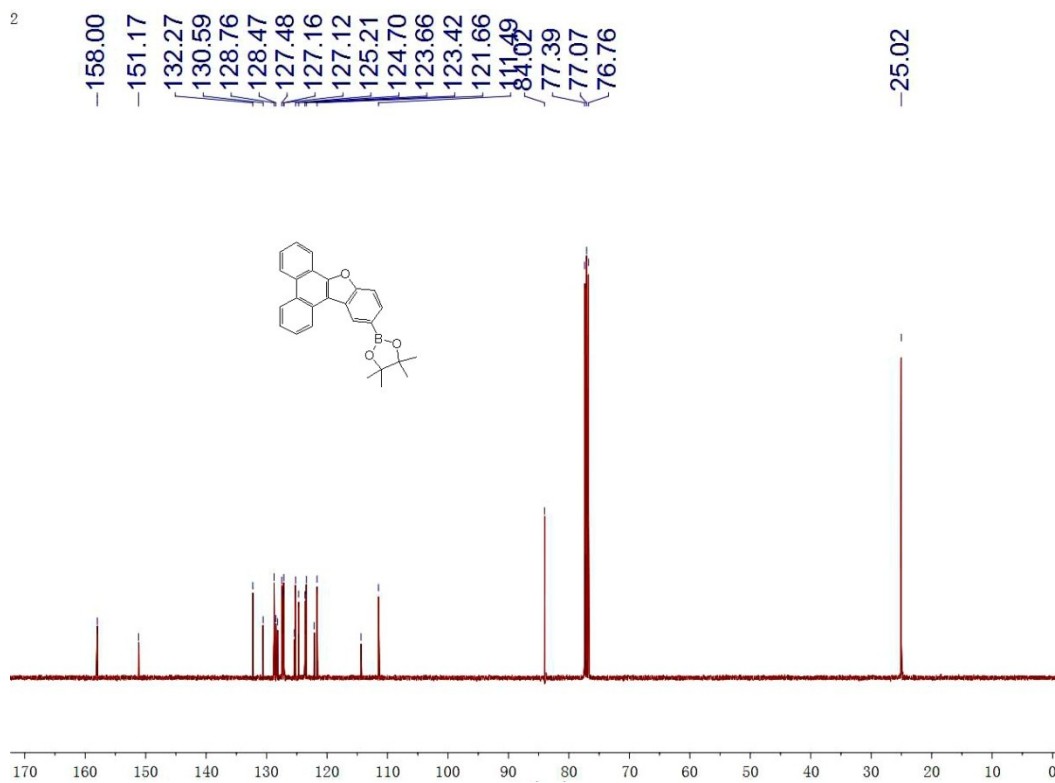


Figure S9 ^{13}C NMR spectrum of **3**.

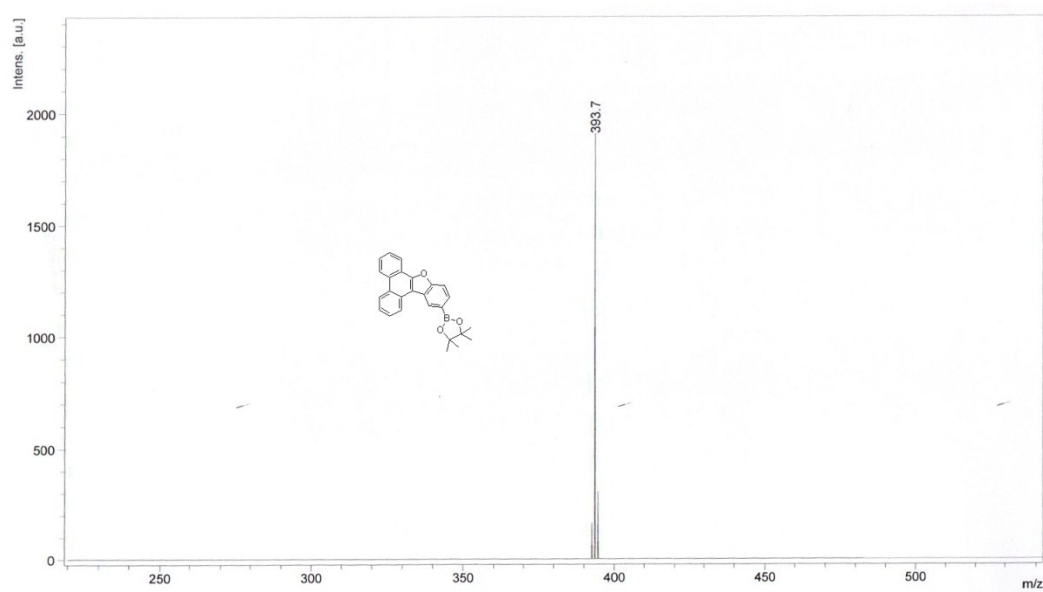


Figure S10 MALDI-TOF spectrum of **3**.

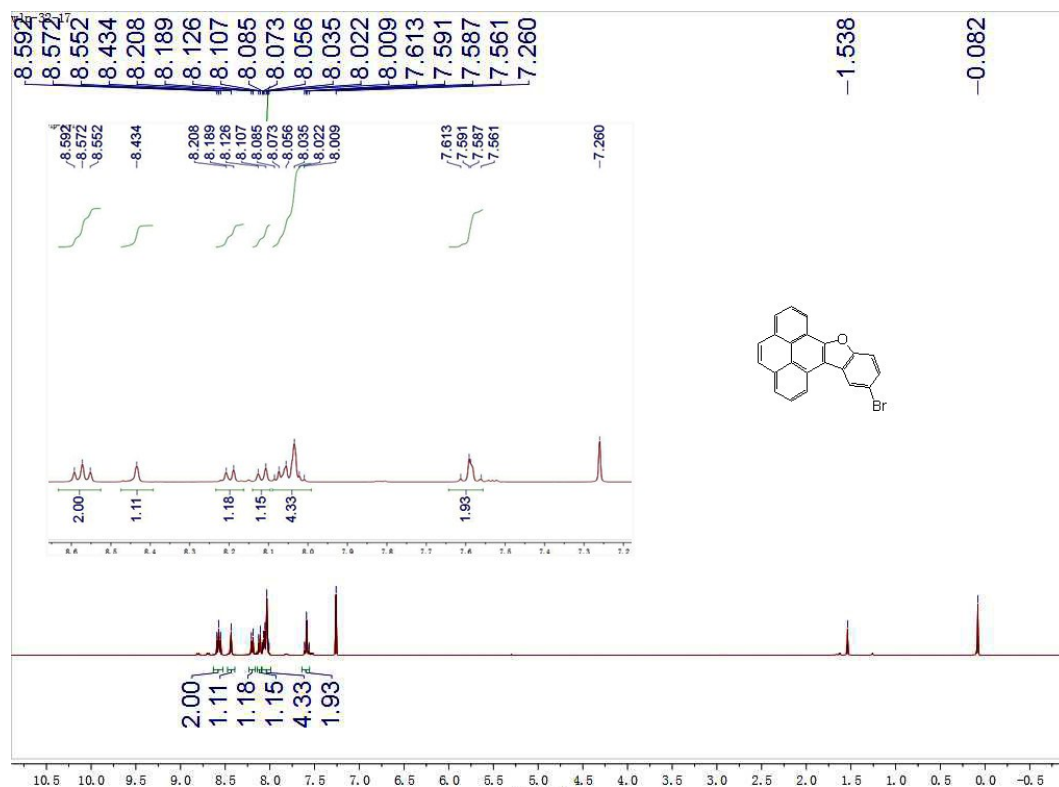


Figure S11 ¹H NMR spectrum of **5**.

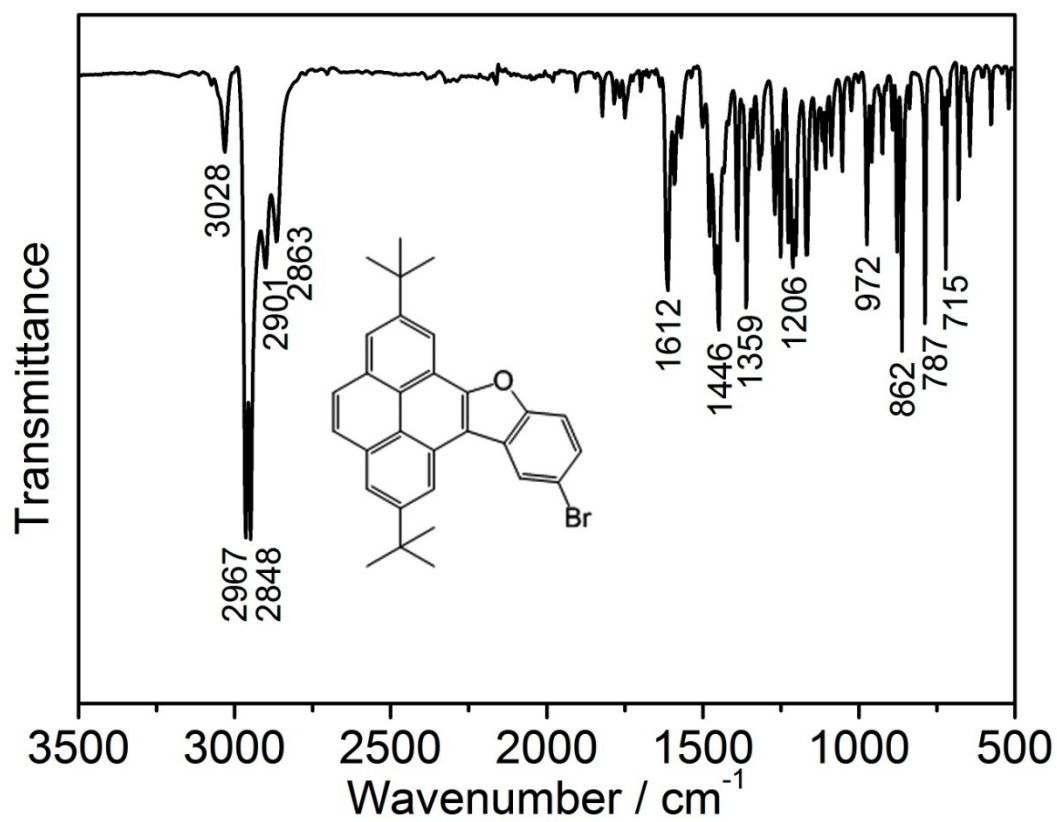


Figure S12 FT-IR spectrum of **6**.

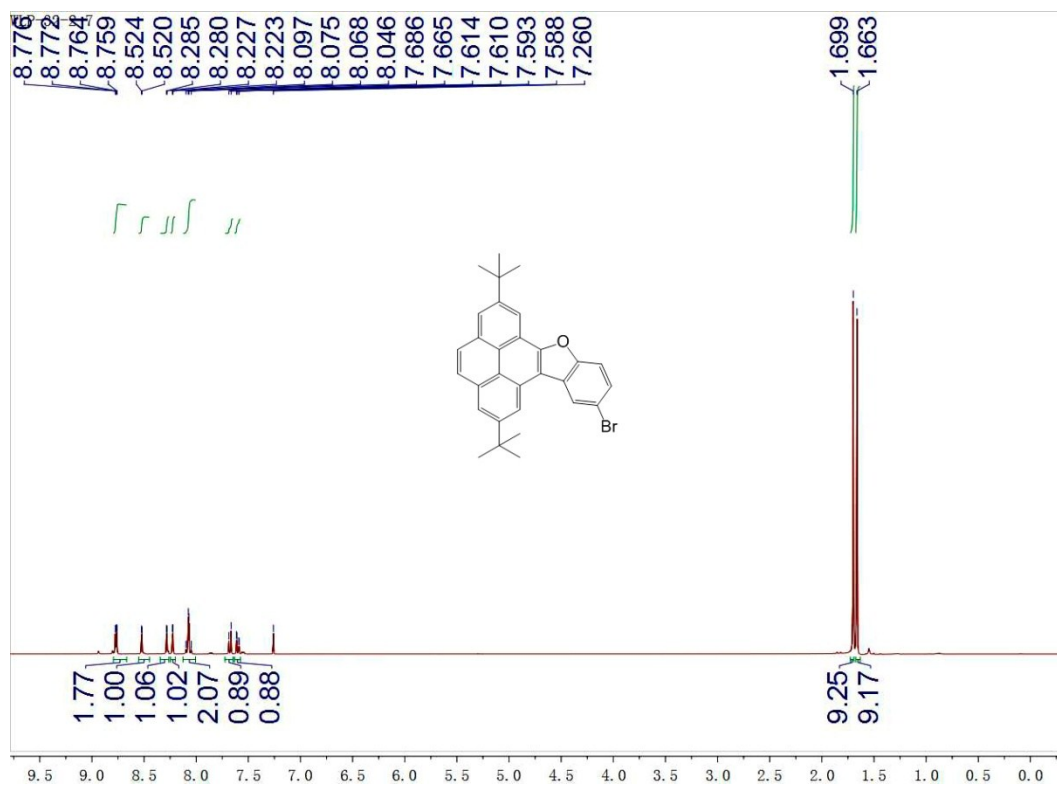


Figure S13 ¹H NMR spectrum of **6**.

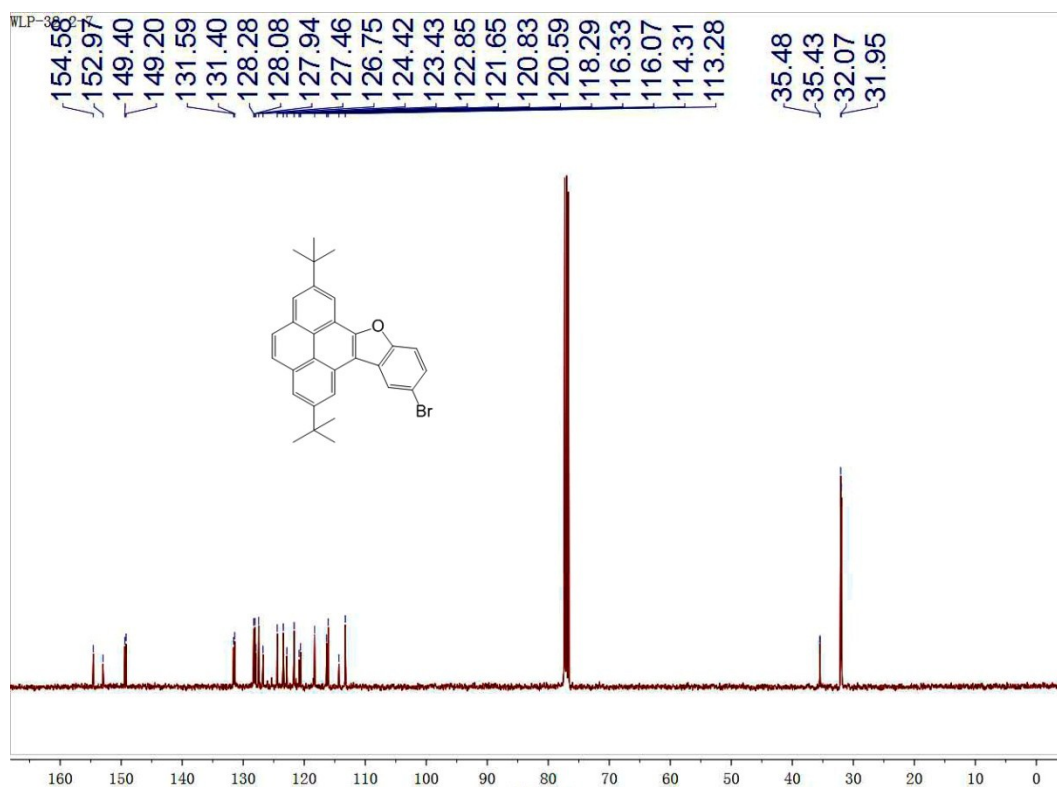


Figure S14 ¹³C NMR spectrum of **6**.

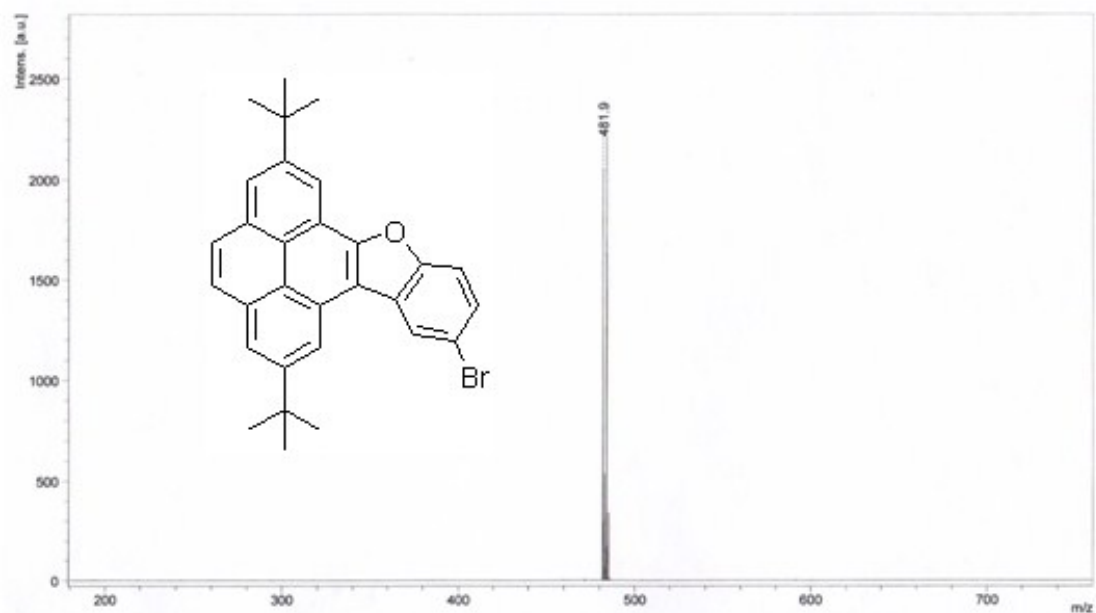


Figure S15 MALDI-TOF spectrum of 6.

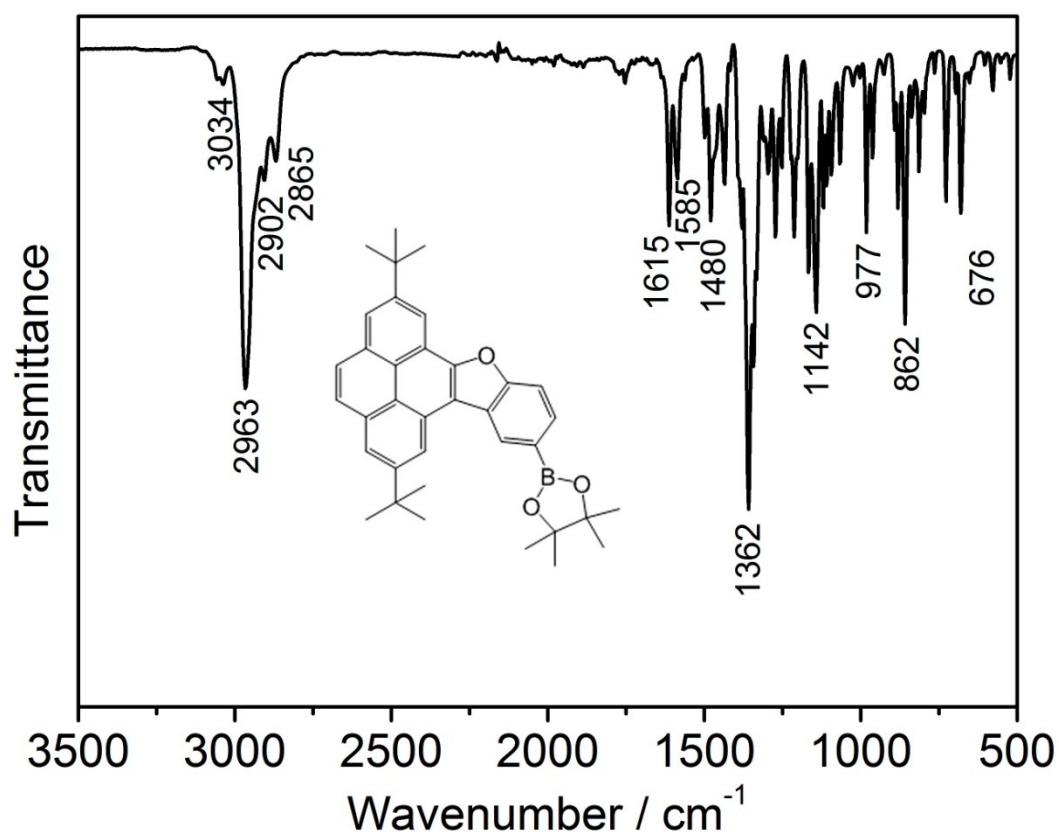


Figure S16 FT-IR spectrum of 7.

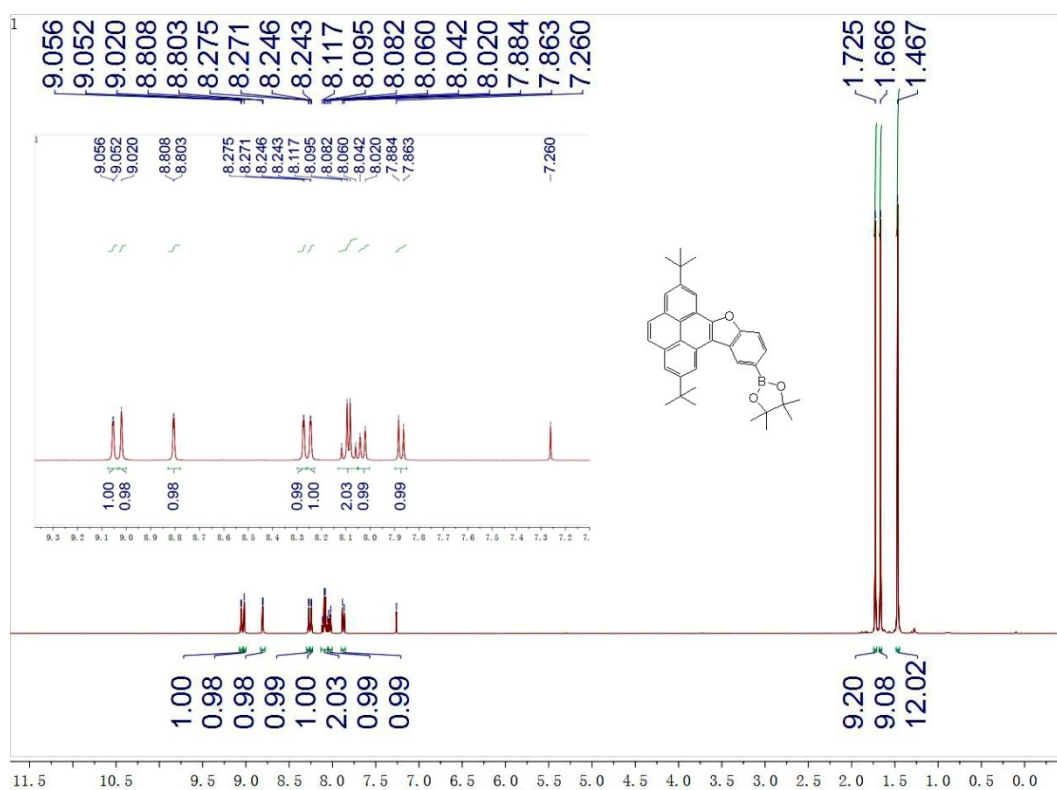


Figure S17 ¹H NMR spectrum of 7.

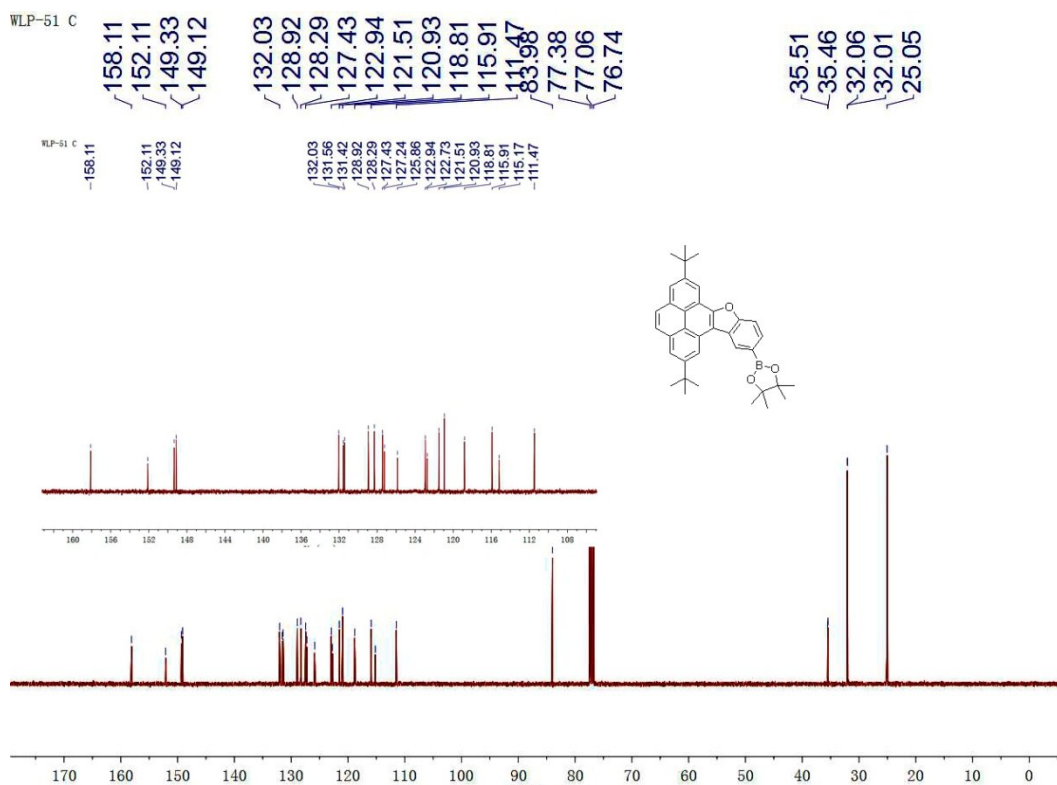


Figure S18 ¹³C NMR spectrum of 7.

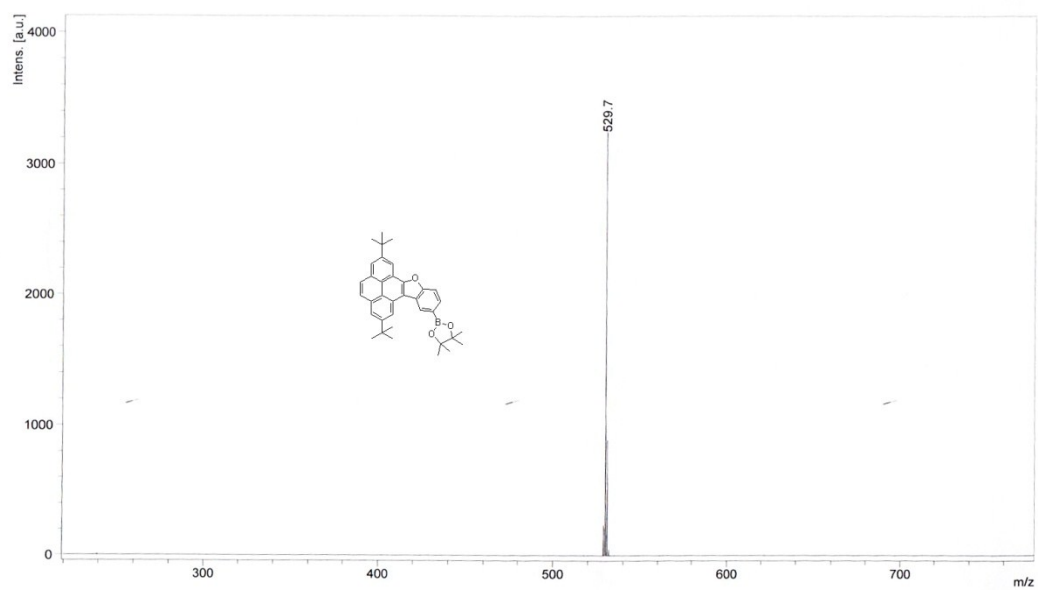


Figure S19 MALDI-TOF spectrum of 7.

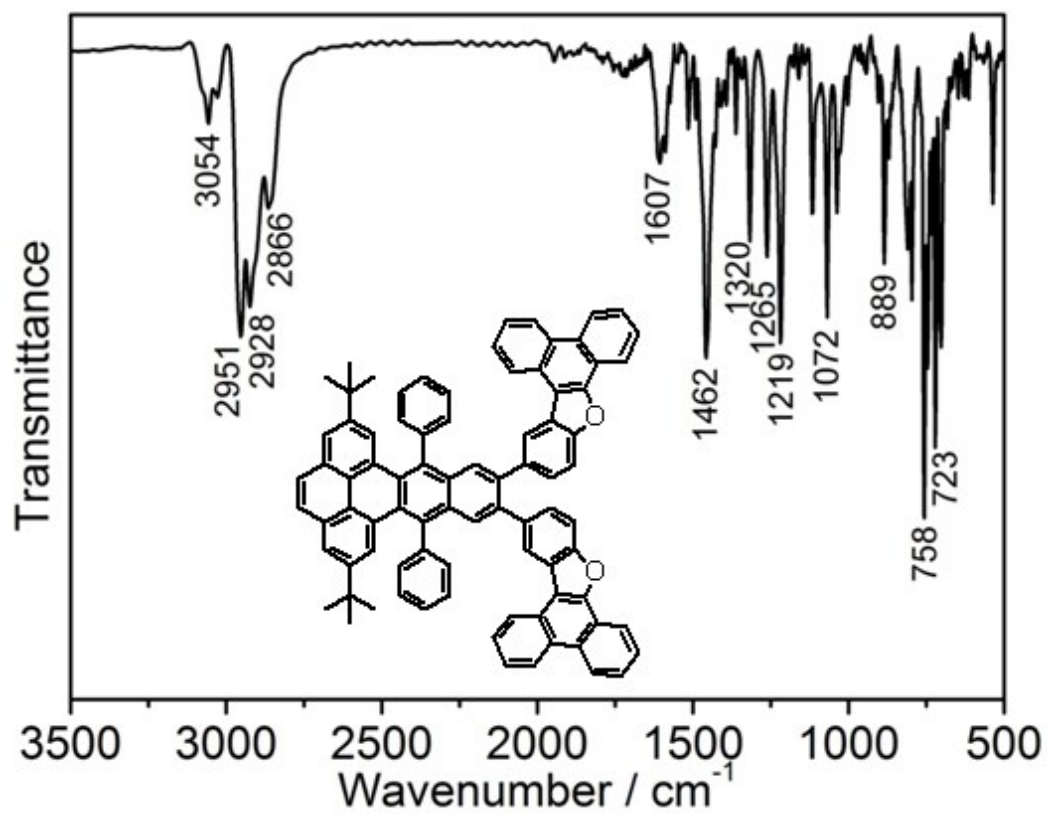


Figure S20 FT-IR spectrum of 9.

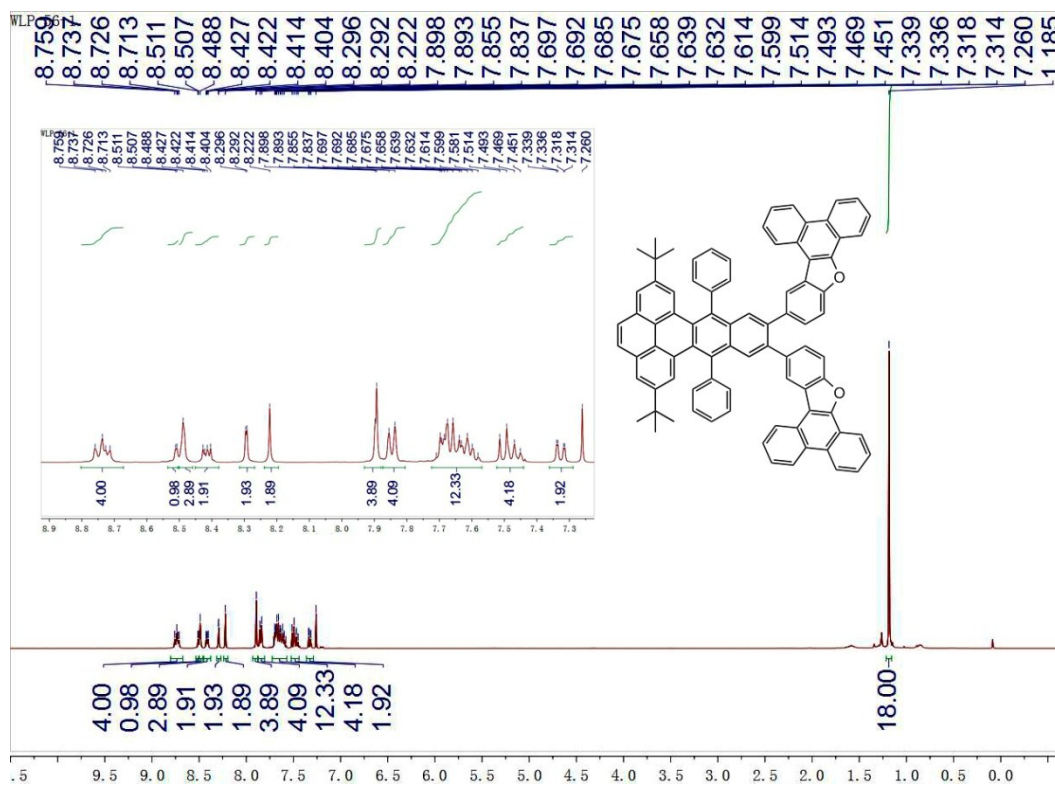


Figure S21 ¹H NMR spectrum of **9**.

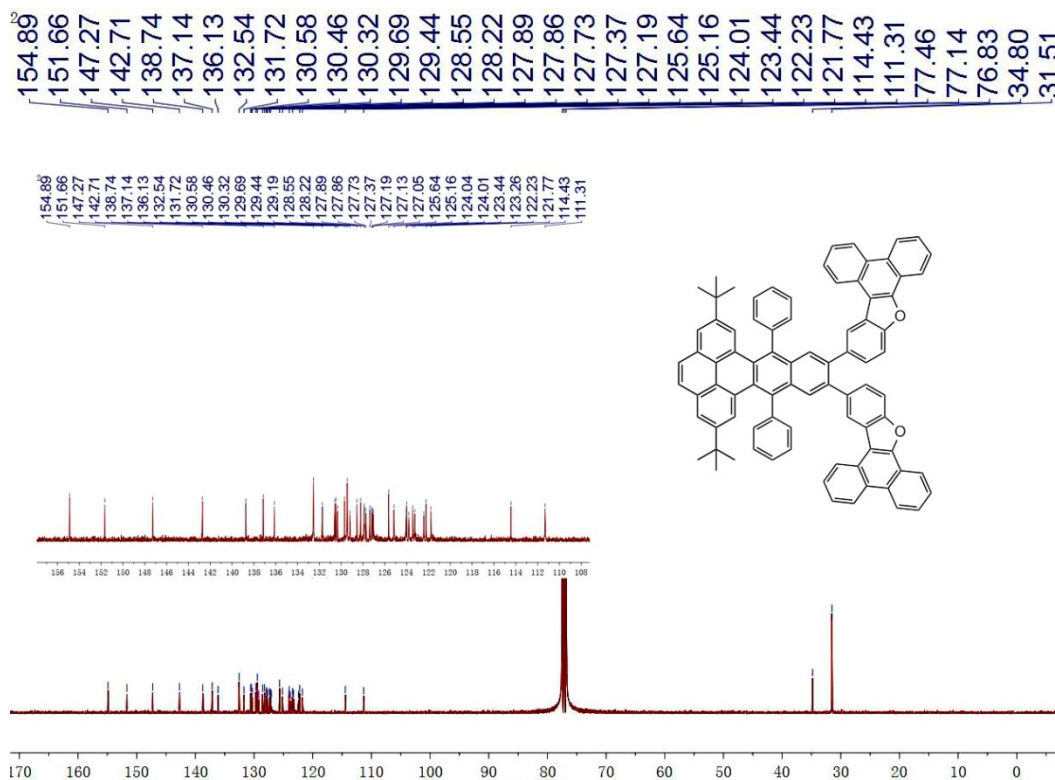


Figure S22 ¹³C NMR spectrum of **9**.

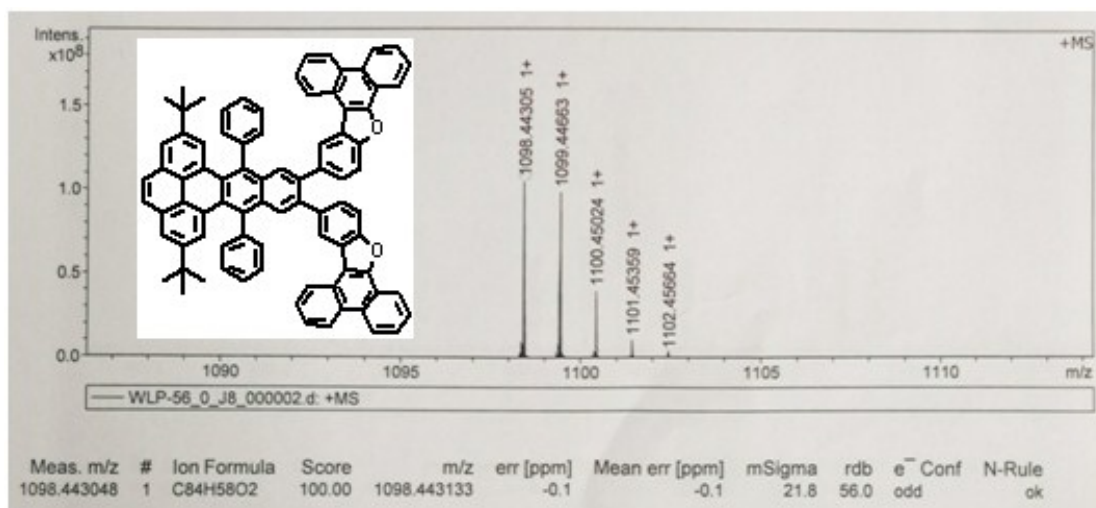


Figure S23 HR-MS spectrum of **9**.

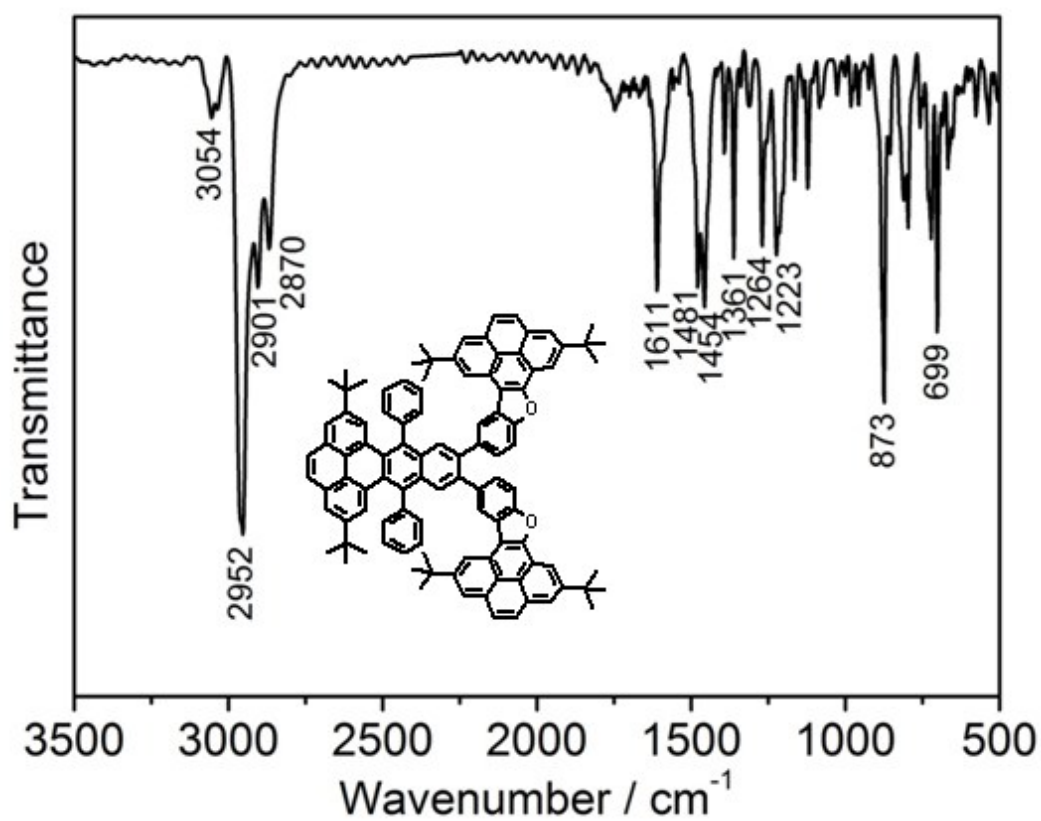


Figure S24 FT-IR spectrum of **10**.

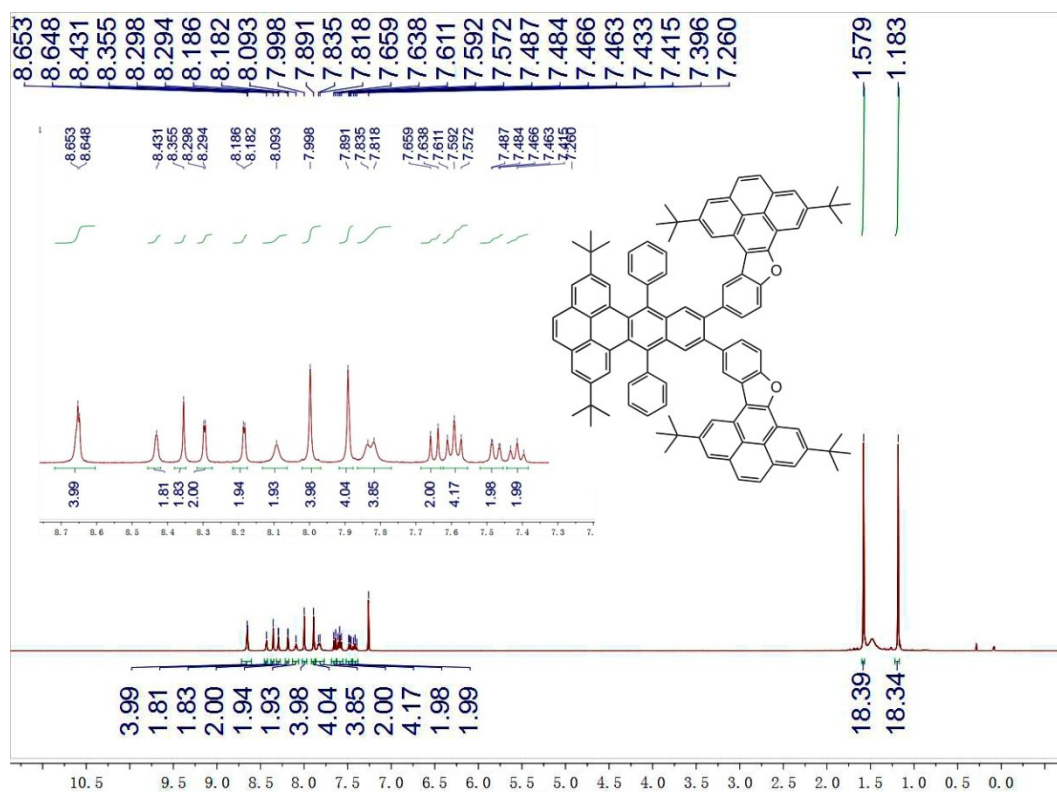


Figure S25 ¹H NMR spectrum of **10**.

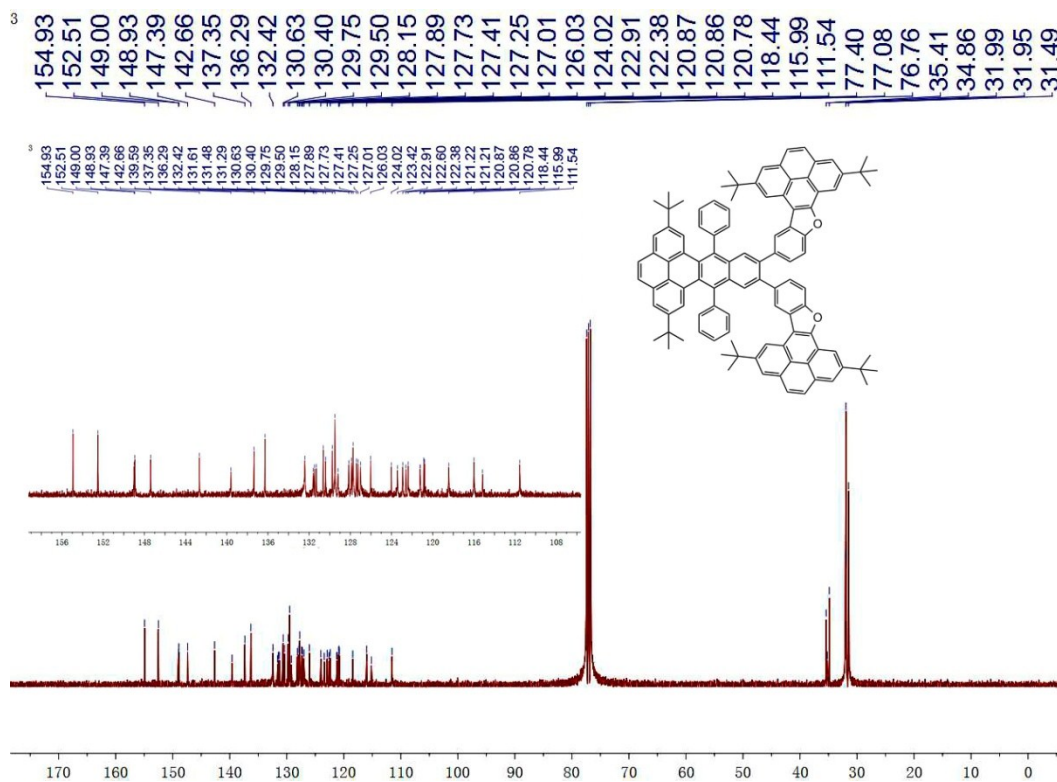


Figure S26 ¹³C NMR spectrum of **10**.

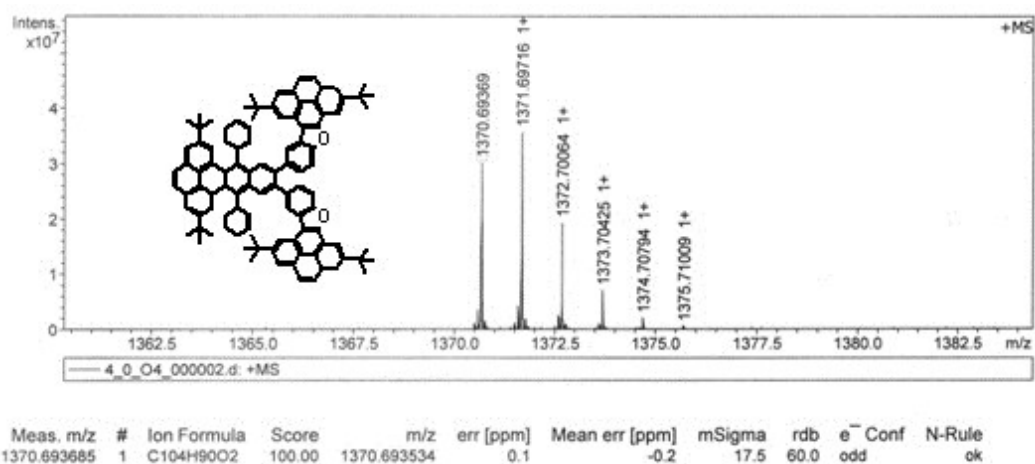
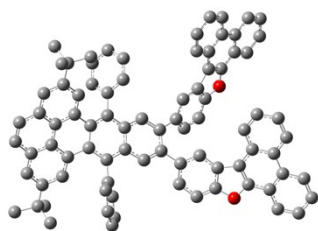


Figure S27 HR-MS spectrum of **10**.

Table S1 Cartesian coordinates of optimized species

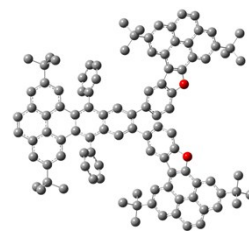
9



Optimized structure

C	-7.57792	3.33169	0.25921
C	-7.77657	1.97704	-0.04485
C	-6.67189	1.07869	-0.0024
C	-5.36713	1.58273	0.23624
C	-5.25328	2.91517	0.65945
C	-6.34084	3.80621	0.68939
C	-9.0888	1.45952	-0.31917
C	-9.31094	0.12065	-0.36864
C	-8.24301	-0.81405	-0.13931
C	-6.90568	-0.33431	-0.04114
C	-8.51038	-2.17372	0.07616
C	-7.51043	-3.05249	0.48205
C	-6.19024	-2.56708	0.52425
C	-5.84052	-1.25066	0.1859
C	-4.44115	-0.76434	0.04819
C	-4.21095	0.67674	0.03207
C	-3.35895	-1.63449	-0.17649
C	-2.03697	-1.11933	-0.35936
C	-1.82845	0.28909	-0.43777
C	-2.9344	1.17856	-0.2764
C	-0.90552	-1.96807	-0.5329
C	0.3704	-1.50236	-0.7847
C	0.56739	-0.08655	-0.92344
C	-0.51756	0.75026	-0.75125
C	-2.6614	2.61965	-0.60145
C	-3.48856	-3.11504	-0.39965
C	-1.85848	3.42592	0.22052
C	-1.53154	4.73032	-0.15373
C	-2.00312	5.25273	-1.35949
C	-2.80236	4.46037	-2.18598
C	-3.12393	3.15546	-1.81249
C	-3.93956	-3.58929	-1.64026
C	-3.96898	-4.95694	-1.91492

10



Optimized structure

C	8.7299	-3.2251	-0.1792
C	8.6844	-1.8153	-0.1713
C	7.4456	-1.1407	-0.1565
C	6.2296	-1.877	-0.1543
C	6.3168	-3.2737	-0.1542
C	7.5493	-3.9456	-0.1673
C	9.9245	-1.0768	-0.1797
C	9.9137	0.2821	-0.1654
C	8.6617	1	-0.1443
C	7.4345	0.3044	-0.1433
C	8.6842	2.4103	-0.1282
C	7.4921	3.1113	-0.1131
C	6.2714	2.4189	-0.1145
C	6.2072	1.0209	-0.1299
C	4.9367	0.279	-0.1398
C	4.9469	-1.1555	-0.1535
C	3.7124	0.9376	-0.1431
C	2.4727	0.2481	-0.1658
C	2.4815	-1.1557	-0.1769
C	3.7307	-1.8298	-0.1717
C	1.2235	0.9457	-0.181
C	0.042	0.2466	-0.1989
C	0.0498	-1.1767	-0.202
C	1.2384	-1.8645	-0.1935
C	3.7384	-3.1667	-0.1848
C	3.7028	2.2744	-0.1241
C	3.5305	-3.8769	0.9975
C	3.5387	-5.2717	0.9838
C	3.7546	-5.9561	-0.2122
C	3.9624	-5.2459	-1.3946
C	3.9543	-3.8511	-1.3809
C	3.7308	2.9891	-1.3216
C	3.721	4.3838	-1.3018

C	-3.53512	-5.87622	-0.95748	C	3.683	5.0637	-0.0845
C	-3.07688	-5.41671	0.27864	C	3.6549	4.3491	1.113
C	-3.05492	-4.04829	0.55471	C	3.6649	2.9543	1.0931
C	1.48203	-2.4944	-0.86413	C	-1.1065	-1.8478	-0.2133
C	2.65787	-2.31163	-0.12346	C	-1.1211	0.9058	-0.2135
C	3.6661	-3.28293	-0.16637	C	-1.6143	-2.2866	-1.3704
C	3.45288	-4.43146	-0.95597	C	-2.802	-2.9003	-1.3884
C	2.30661	-4.64664	-1.7046	C	-3.4616	-3.1139	-0.2452
C	1.32446	-3.66003	-1.64775	C	-2.9334	-2.7137	0.9161
C	-6.20073	5.27199	1.14669	C	-1.7559	-2.0806	0.932
C	-4.851	5.55075	1.8339	O	-4.5424	-3.6632	-0.0697
C	-6.32152	6.19351	-0.0904	C	-4.8383	-3.6479	1.512
C	-7.32071	5.61983	2.15501	C	-3.7352	-3.0251	1.9397
C	-7.86091	-4.51472	0.82507	C	-1.4514	1.6563	-1.2695
C	-9.12189	-4.57452	1.71831	C	-2.6333	2.2804	-1.3027
C	-8.13533	-5.27784	-0.49297	C	-3.485	2.154	-0.2798
C	-6.724	-5.22817	1.58096	C	-3.1458	1.4211	0.7857
C	1.87722	0.52891	-1.2891	C	-1.955	0.8147	0.8284
C	2.59194	0.08487	-2.4249	C	-3.1487	3.0559	-2.2622
C	3.78064	0.68847	-2.82351	C	-4.371	3.4825	-1.9285
C	4.23797	1.74614	-2.0515	O	-4.6973	3.0608	-0.8256
C	3.56957	2.22651	-0.90833	C	7.5858	-5.4422	-0.1684
C	2.37195	1.5998	-0.53326	C	6.1631	-5.9854	-0.1539
O	5.38737	2.45934	-2.2928	C	8.3023	-5.9308	-1.4203
C	5.45478	3.40183	-1.29667	C	8.3288	-5.9325	1.0673
C	4.39318	3.32123	-0.42044	C	7.5038	4.6081	-0.0953
C	4.97859	-3.47358	0.43166	C	8.9434	5.1053	-0.0974
C	5.42262	-4.69173	-0.03587	C	6.7835	5.1355	-1.3292
O	4.52029	-5.29289	-0.88088	C	6.7969	5.1063	1.1584
C	6.51773	4.34301	-1.2134	C	-2.6142	3.4099	-3.4355
C	6.46456	5.2707	-0.13048	C	-3.2961	4.2027	-4.2687
C	5.35478	5.22006	0.82588	C	-4.5124	4.6413	-3.9285
C	4.31636	4.24464	0.68319	C	-5.0539	4.2734	-2.7627
C	7.57718	4.37372	-2.14569	C	-5.7615	-4.0512	2.391
C	8.58454	5.31009	-2.02176	C	-5.5908	-3.8145	3.6958
C	8.54973	6.23327	-0.96139	C	-4.4942	-3.1793	4.1221
C	7.51566	6.21114	-0.04141	C	-3.5664	-2.7846	3.244
C	5.26723	6.12058	1.91159	C	-1.4027	2.962	-3.7805
C	4.22191	6.07467	2.81651	C	-0.8682	3.316	-4.9538
C	3.20832	5.11465	2.67	C	-1.5549	4.0994	-5.7919
C	3.25939	4.21787	1.61927	C	-2.7664	4.5474	-5.4469
C	5.81745	-2.7078	1.31882	C	-5.1921	5.4386	-4.7593

C	7.08053	-3.26139	1.70343	C	-6.4084	5.8771	-4.4192
C	7.50646	-4.56826	1.19395	C	-6.9563	5.4965	-3.2602
C	6.665	-5.29649	0.30053	C	-6.2735	4.7056	-2.426
C	8.73892	-5.16621	1.54151	C	-3.4434	5.3494	-6.2751
C	9.11578	-6.3992	1.03758	C	-4.6601	5.7879	-5.9351
C	8.27371	-7.10004	0.15582	C	-6.8499	-4.7012	1.9663
C	7.05926	-6.55283	-0.20828	C	-7.7732	-5.1045	2.8453
C	5.4401	-1.43817	1.80783	C	-7.6022	-4.8684	4.1501
C	6.26291	-0.72421	2.65849	C	-6.5111	-4.2231	4.5753
C	7.4985	-1.26404	3.04863	C	-4.32	-2.949	5.4275
C	7.89291	-2.50298	2.57647	C	-3.2233	-2.3142	5.8539
H	-8.43803	3.99369	0.21643	C	-2.3064	-1.8989	4.9734
H	-4.28897	3.27355	0.97752	C	-2.4753	-2.1393	3.6691
H	-9.90873	2.16355	-0.43242	C	-6.346	-3.9764	5.8789
H	-10.31304	-0.27054	-0.52234	C	-5.237	-3.3637	6.3077
H	-9.53899	-2.50902	-0.01445	C	-8.9984	-5.8203	2.3684
H	-5.41392	-3.24412	0.83354	C	-8.9482	-5.9598	0.8526
H	-1.03837	-3.036	-0.4298	C	-9.0567	-7.2036	3.0031
H	-0.36247	1.81001	-0.89837	C	-10.2363	-5.0263	2.7641
H	-1.48864	3.02364	1.15953	C	-8.334	5.9558	-2.8968
H	-0.90485	5.33569	0.49461	C	-8.8856	6.838	-4.009
H	-1.74527	6.26532	-1.65459	C	-9.24	4.7454	-2.7135
H	-3.16683	4.85438	-3.13021	C	-8.2781	6.7508	-1.599
H	-3.73935	2.54078	-2.46191	C	0.499	2.8354	-5.3291
H	-4.26886	-2.87748	-2.39085	C	1.0576	1.967	-4.2096
H	-4.32032	-5.30361	-2.88249	C	0.4146	2.0175	-6.6111
H	-3.55044	-6.94018	-1.17384	C	1.4151	4.0321	-5.5483
H	-2.73312	-6.12204	1.0295	C	-1.0912	-1.1649	5.4481
H	-2.6939	-3.6961	1.51682	C	-1.1421	-1.0239	6.9637
H	2.76517	-1.41966	0.47984	C	0.1573	-1.9425	5.0529
H	2.18875	-5.54043	-2.30686	C	-1.0524	0.2179	4.8109
H	0.41541	-3.78118	-2.22779	H	9.6976	-3.7479	-0.1947
H	-4.82449	6.58978	2.17846	H	5.389	-3.8645	-0.1435
H	-4.70398	4.90791	2.7083	H	10.8828	-1.6164	-0.1978
H	-4.00508	5.40847	1.15714	H	10.8632	0.8373	-0.1699
H	-6.23776	7.24587	0.20475	H	9.6433	2.9489	-0.1277
H	-7.28322	6.06252	-0.59615	H	5.3338	2.9941	-0.1031
H	-5.52918	5.97775	-0.81411	H	1.2097	2.0456	-0.1783
H	-8.31907	5.51166	1.72231	H	1.2349	-2.9645	-0.1995
H	-7.26747	4.97434	3.03768	H	3.3602	-3.3372	1.9407
H	-7.21825	6.65858	2.48803	H	3.3749	-5.8319	1.9162
H	-9.34304	-5.6143	1.98258	H	3.761	-7.0561	-0.223

H	-8.97391	-4.01337	2.64659	H	4.1326	-5.7857	-2.3378
H	-10.00808	-4.17178	1.22059	H	4.1182	-3.291	-2.3132
H	-8.3976	-6.32204	-0.28666	H	3.7607	2.4529	-2.2816
H	-7.25145	-5.26922	-1.13843	H	3.7432	4.9474	-2.2461
H	-8.96259	-4.82588	-1.04944	H	3.6753	6.1636	-0.0689
H	-6.46197	-4.69919	2.50348	H	3.6249	4.8853	2.073
H	-7.04559	-6.23802	1.85648	H	3.6427	2.3907	2.0375
H	-5.82065	-5.32877	0.97523	H	-1.0551	-2.1426	-2.3066
H	2.1985	-0.74327	-3.00332	H	-3.2365	-3.2296	-2.3438
H	4.32764	0.35559	-3.69831	H	-1.3214	-1.7514	1.8874
H	1.81693	1.92102	0.34	H	-0.7507	1.7603	-2.1111
H	7.58171	3.65101	-2.95434	H	-3.8464	1.3171	1.6273
H	9.39928	5.33372	-2.73873	H	-1.6612	0.2412	1.7199
H	9.34005	6.97095	-0.8608	H	6.1902	-7.0981	-0.1547
H	7.5242	6.93848	0.76166	H	5.6395	-5.6283	0.761
H	6.03522	6.8725	2.0503	H	5.6201	-5.6271	-1.057
H	4.1888	6.78224	3.63924	H	8.33	-7.0435	-1.4221
H	2.3868	5.07473	3.37892	H	9.3422	-5.5343	-1.4306
H	2.47419	3.47987	1.50991	H	7.7586	-5.572	-2.3227
H	9.41465	-4.65738	2.21852	H	8.6638	-5.0591	1.6704
H	10.07086	-6.82667	1.32748	H	7.6503	-6.5674	1.68
H	8.57676	-8.06628	-0.23538	H	9.2149	-6.5291	0.7548
H	6.39167	-7.0746	-0.8854	H	8.9521	6.2182	-0.0842
H	4.49442	-1.01015	1.49933	H	9.4698	4.7199	0.8043
H	5.95442	0.25248	3.01833	H	9.46	4.7413	-1.0136
H	8.14965	-0.70896	3.71686	H	6.7917	6.2484	-1.317
H	8.85567	-2.89037	2.88858	H	5.7313	4.7727	-1.3273
E(zp)= -3385.419086				H	7.3009	4.7709	-2.2447
E(SCF)=-3386.582061 a.u.				H	6.4436	4.2364	1.7561
				H	7.5052	5.7112	1.7675
				H	5.9256	5.7349	0.8677
				H	-0.8456	2.3021	-3.0991
				H	-1.123	4.3754	-6.7652
				H	-6.9584	6.551	-5.0926
				H	-6.7151	4.4105	-1.4627
				H	-2.9996	5.6485	-7.2361
				H	-5.2232	6.436	-6.6227
				H	-6.9858	-4.9042	0.8938
				H	-8.3591	-5.2051	4.8738
				H	-3.0751	-2.1335	6.9288
				H	-1.7165	-1.8062	2.9457
				H	-7.1217	-4.2771	6.5985

H	-5.0795	-3.201	7.3841
H	-9.8591	-6.492	0.4981
H	-8.9056	-4.9489	0.3888
H	-8.0435	-6.54	0.5634
H	-9.9673	-7.7367	2.6492
H	-9.094	-7.1016	4.1108
H	-8.1516	-7.7829	2.7133
H	-9.9289	-4.1072	3.3115
H	-10.8016	-4.7408	1.8489
H	-10.8828	-5.6503	3.421
H	-9.9099	7.1795	-3.7388
H	-8.2235	7.7226	-4.143
H	-8.9265	6.257	-4.9574
H	-10.2647	5.0858	-2.4433
H	-8.8373	4.1009	-1.9003
H	-9.2802	4.1651	-3.6624
H	-7.2267	6.7969	-1.2366
H	-8.653	7.7829	-1.7804
H	-8.9133	6.2538	-0.832
H	2.0741	1.6096	-4.4886
H	1.1193	2.5647	-3.2727
H	0.3881	1.0924	-4.0494
H	1.4306	1.6596	-6.891
H	0.0069	2.6523	-7.4293
H	-0.2551	1.1433	-6.4498
H	0.8454	4.9726	-5.3762
H	2.2688	3.9804	-4.8361
H	1.8005	4.0177	-6.5924
H	-0.2385	-0.4782	7.3166
H	-2.0544	-0.4557	7.2525
H	-1.1704	-2.0345	7.4293
H	1.0615	-1.3976	5.4054
H	0.1948	-2.0449	3.9453
H	0.128	-2.9528	5.519
H	-1.9368	0.3462	4.1475
H	-1.0718	0.994	5.6085
H	-0.1206	0.3239	4.2114

E(zp)= -4166.476863

E(SCF)=-4168.114557 a.u.