Supplementary material (ESI) for Journal of Materials Chemistry
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Supporting Information

for

Toward Highly Efficient NLO Chromophores: Synthesis and Properties of Heterocycle-Based Electronically Gradient Dipolar NLO Chromophores

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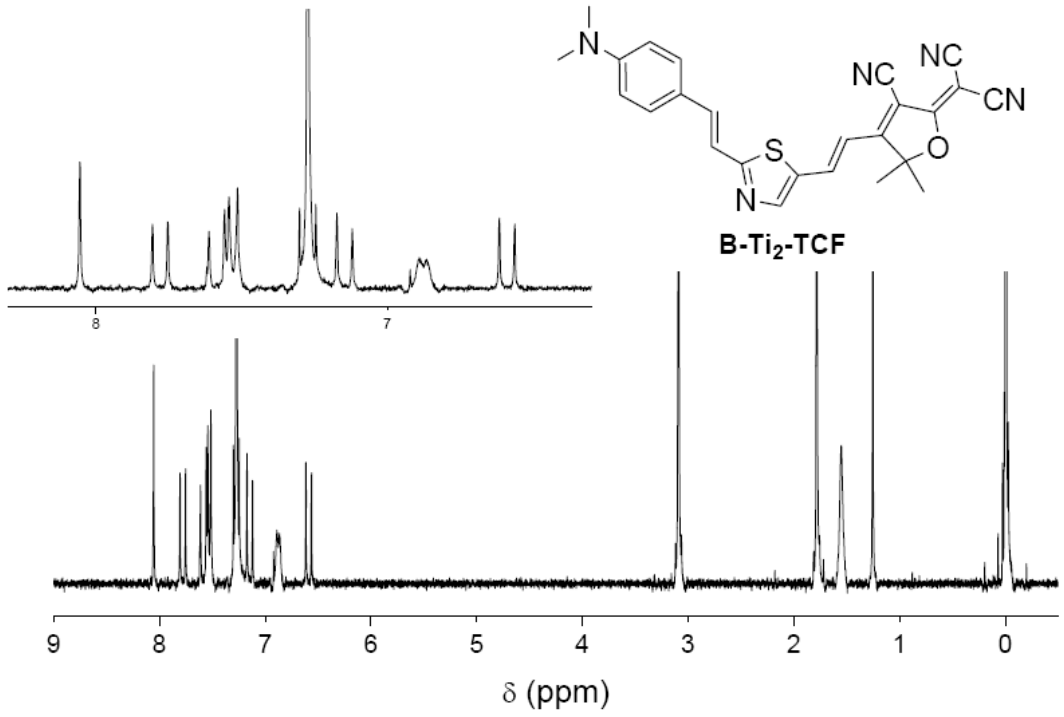

Figure 1. ^{1}H NMR spectrum of B-Ti_2-TCF in $CDCl_3$

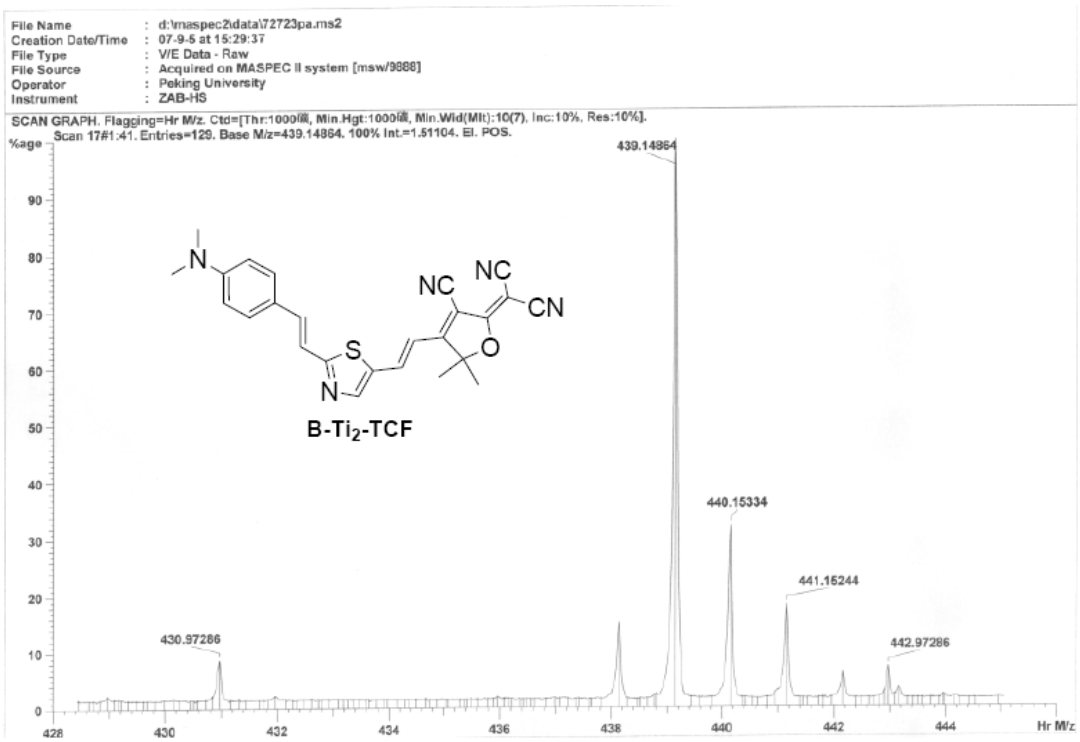

Figure 2. High resolution mass spectroscopy of B-Ti_2-TCF

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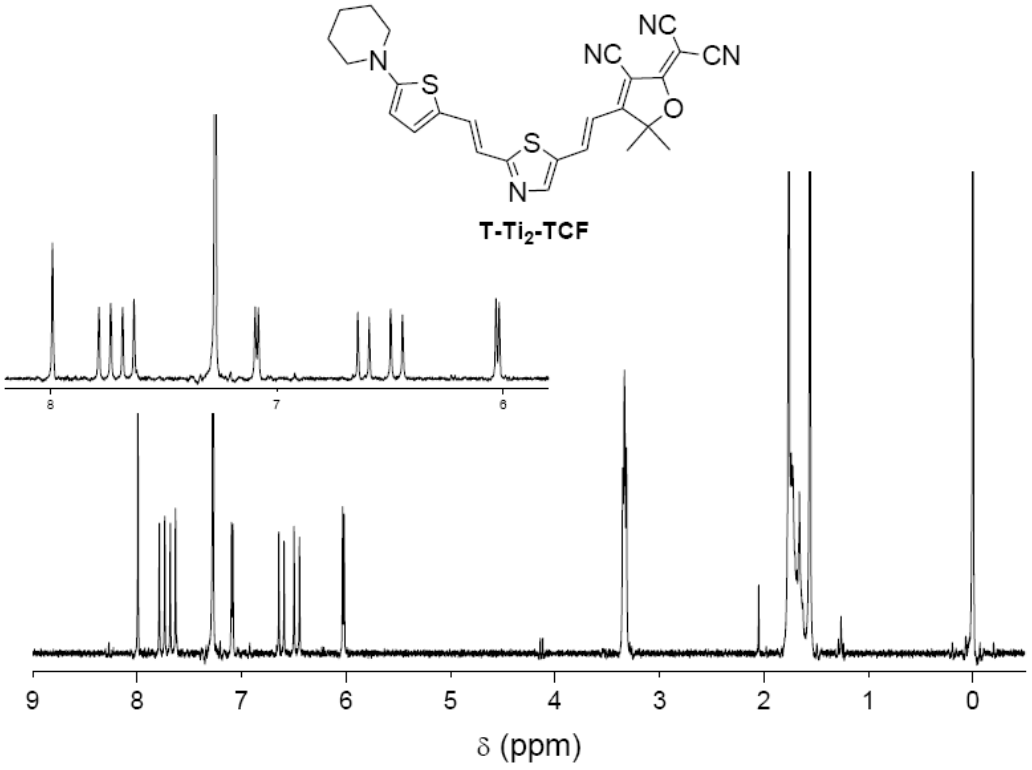

Figure 3. ^{1}H NMR spectrum of T-Ti_2-TCF in $CDCl_3$

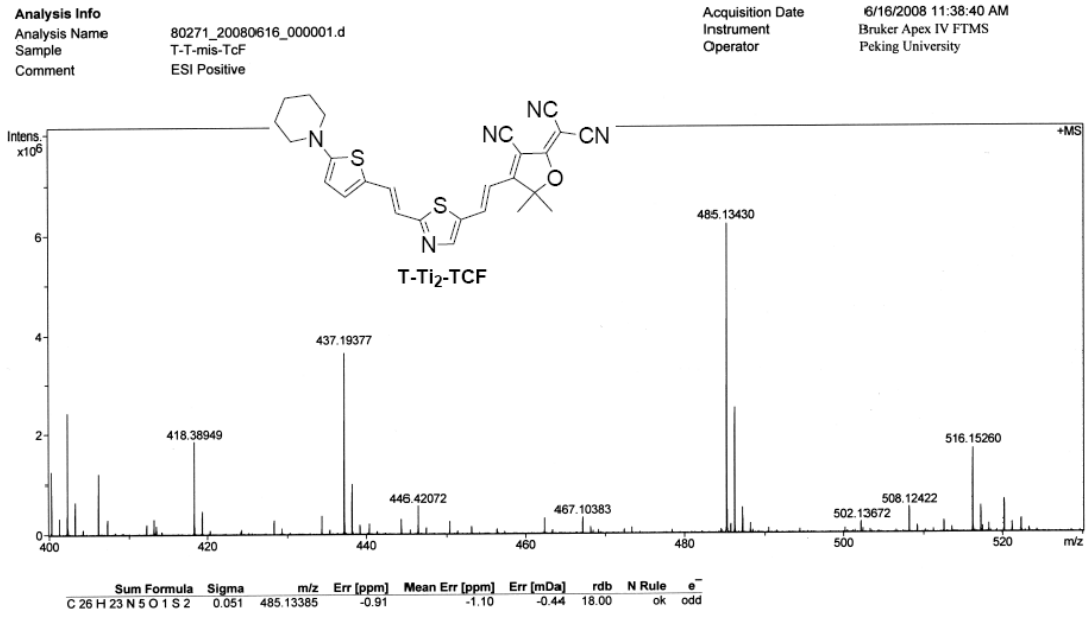

Figure 4. High resolution mass spectroscopy of T-Ti_2-TCF

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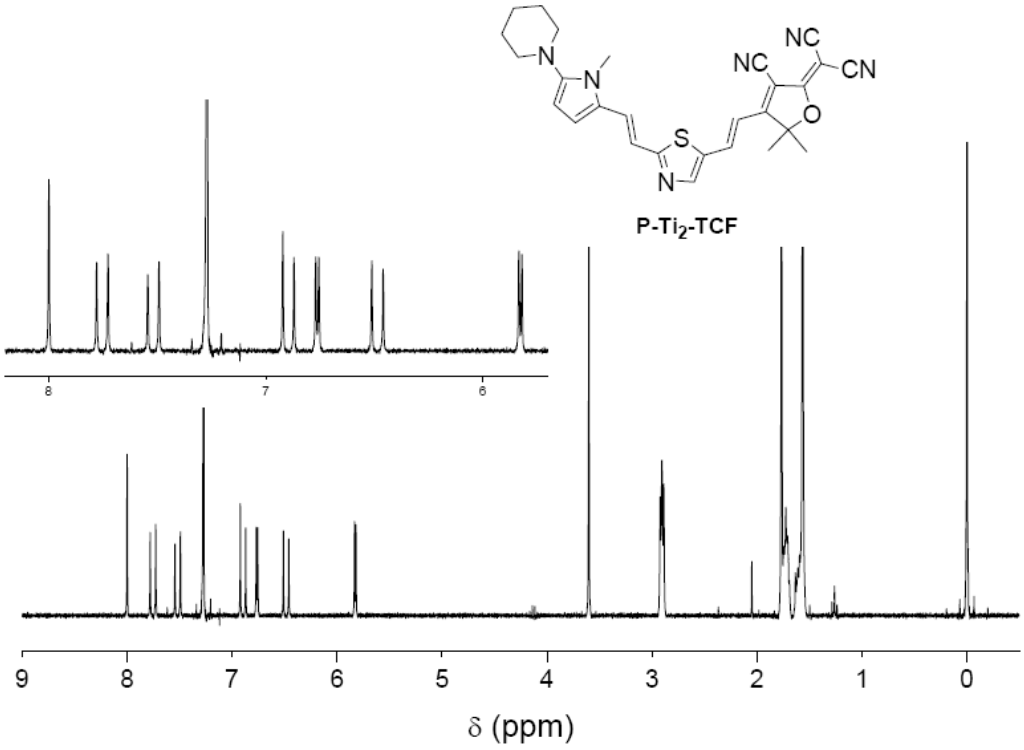

Figure 5. ^{1}H NMR spectrum of P-Ti_2-TCF in $CDCl_3$

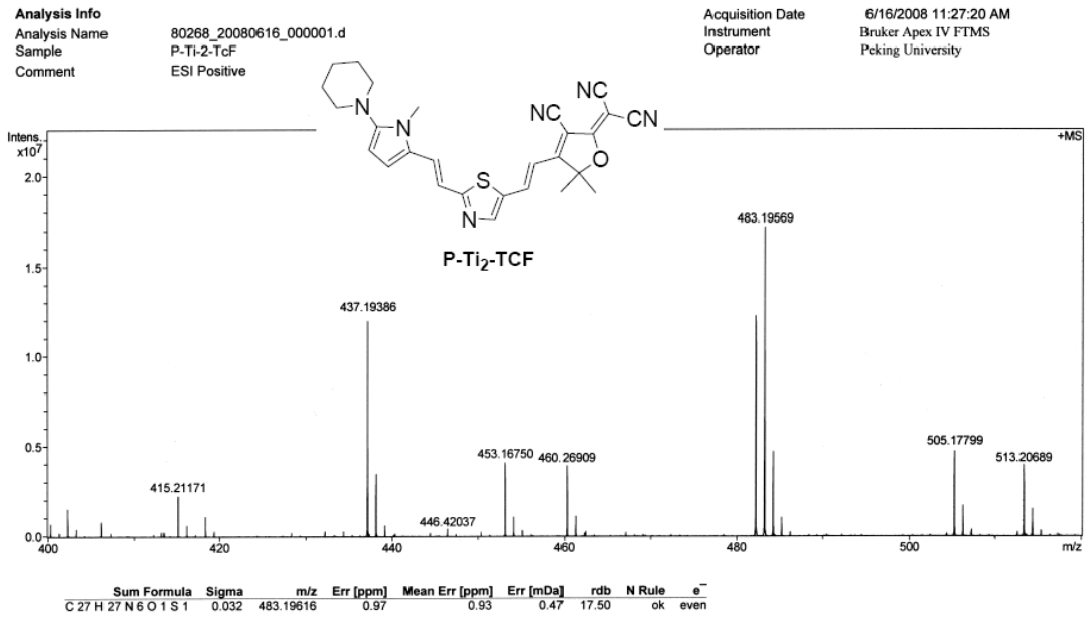

Figure 6. High resolution mass spectroscopy of P-Ti_2-TCF

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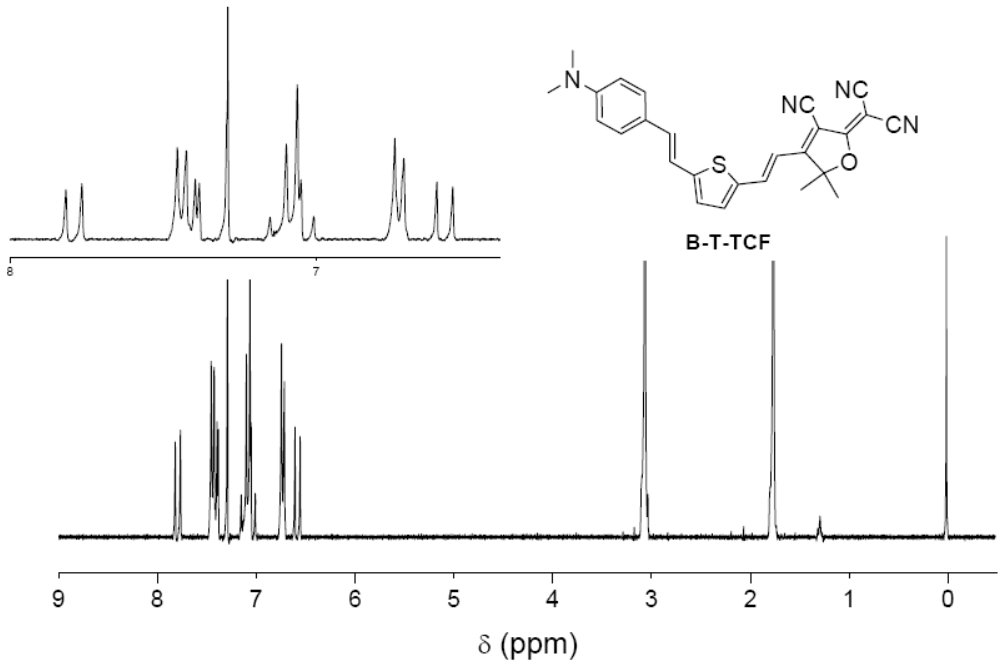

Figure 7. ^{1}H NMR spectrum of B-T-TCF in $CDCl_3$

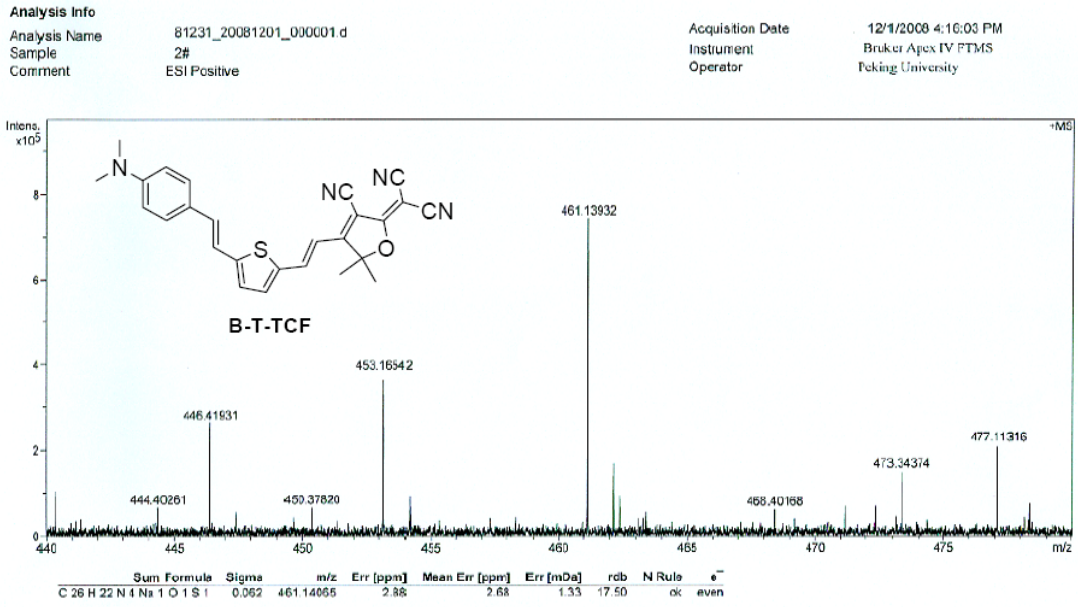

Figure 8. High resolution mass spectroscopy of B-T-TCF

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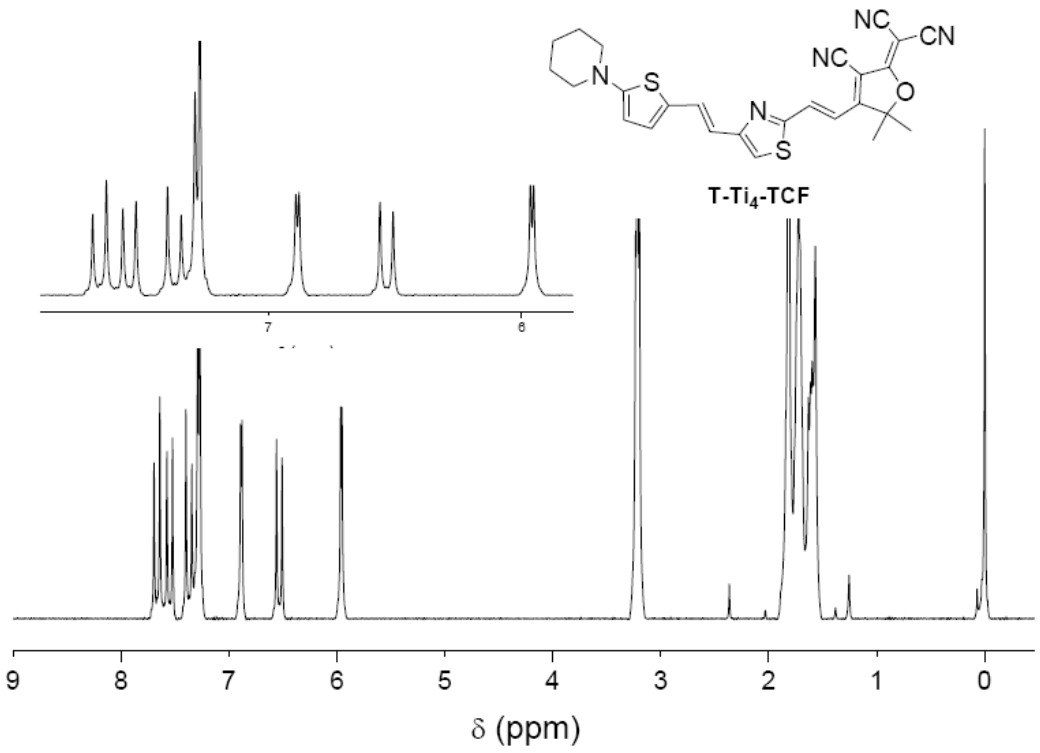

Figure 9. ^{1}H NMR spectrum of T-Ti_4-TCF in $CDCl_3$

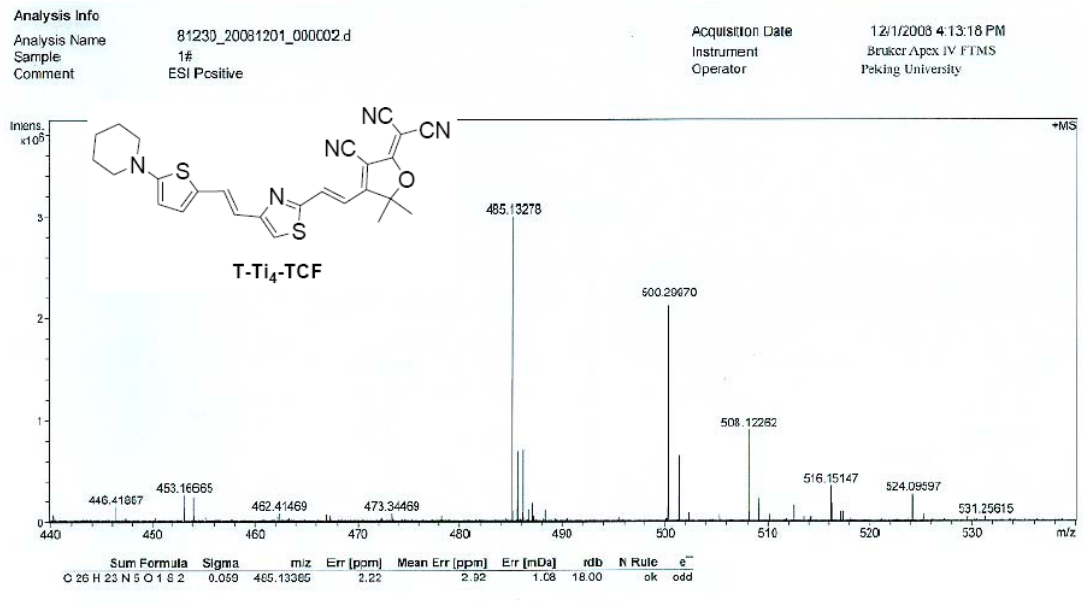

Figure 10. High resolution mass spectroscopy of T-Ti_4-TCF

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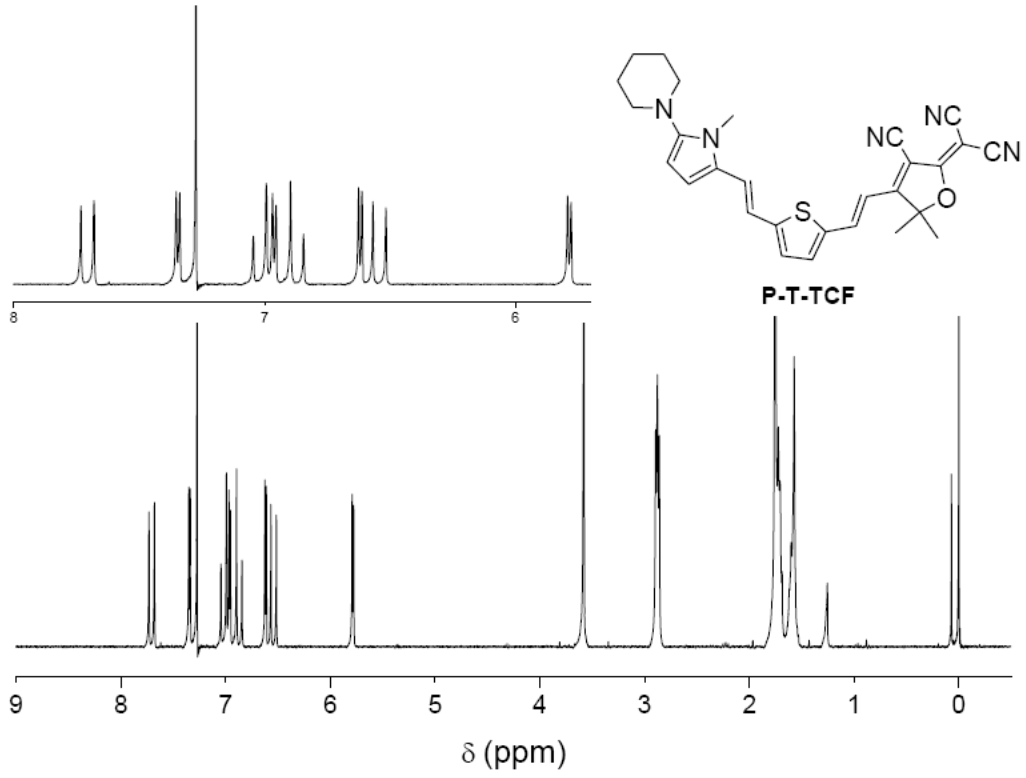

Figure 11. ^{1}H NMR spectrum of P-T-TCF in $CDCl_3$

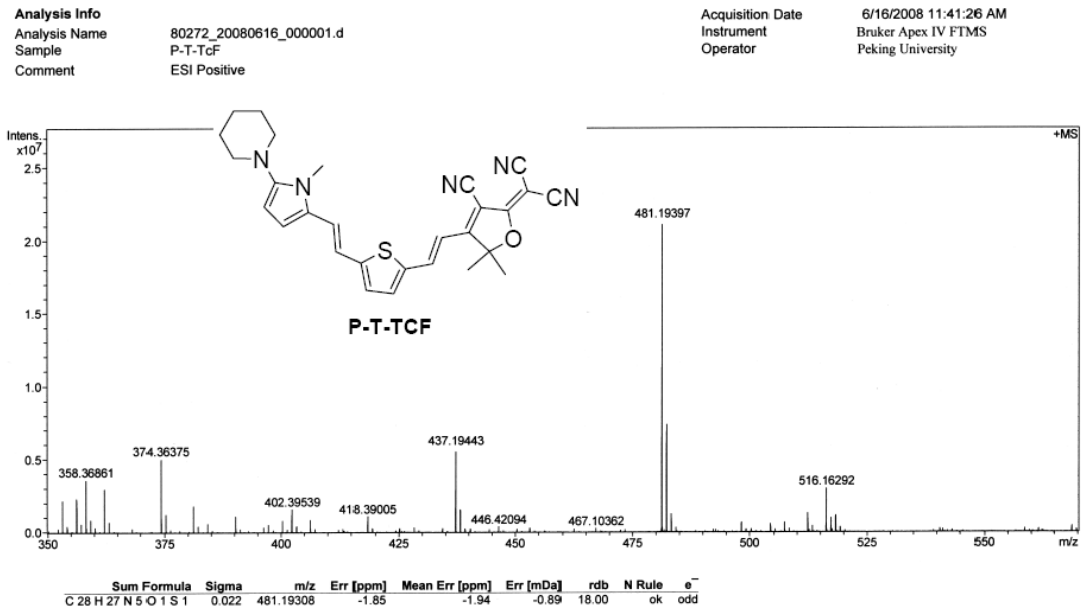

Figure 12. High resolution mass spectroscopy of P-T-TCF

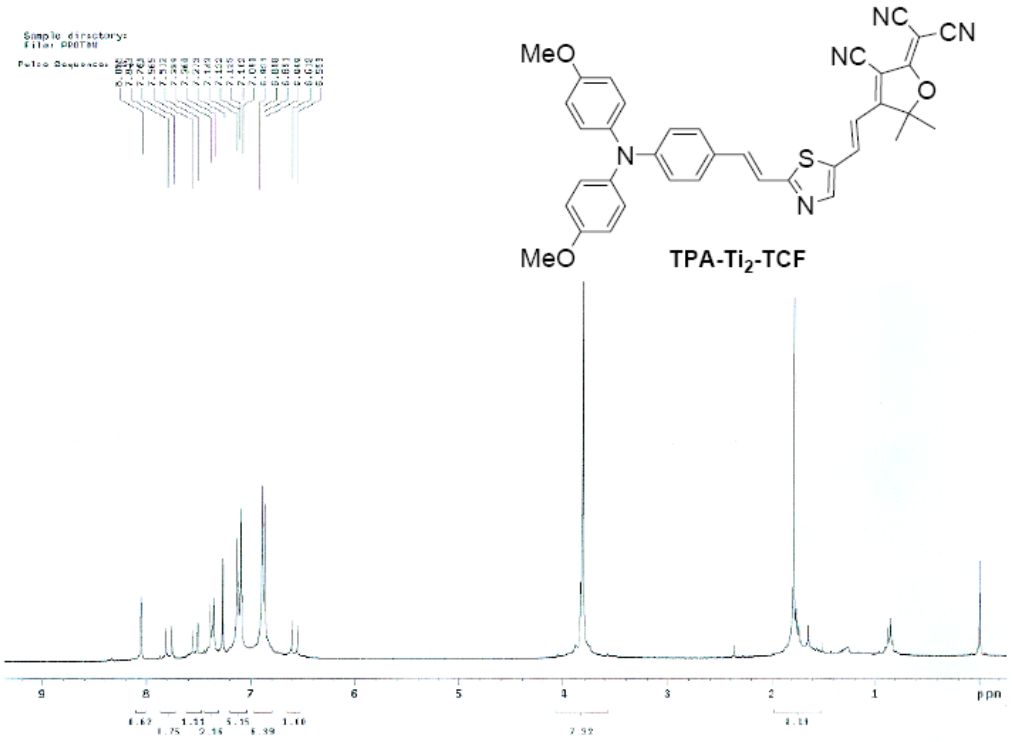

Figure 13. ^{1}H NMR spectrum of TPA-Ti_2-TCF in $CDCl_3$

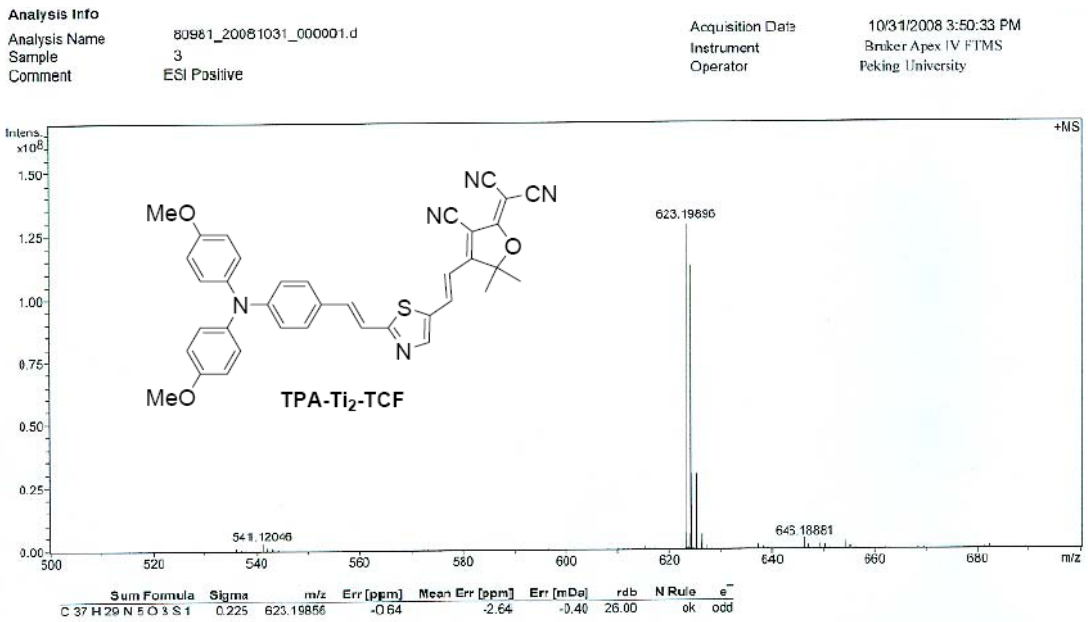

Figure 14. High resolution mass spectroscopy of TPA-Ti_2-TCF

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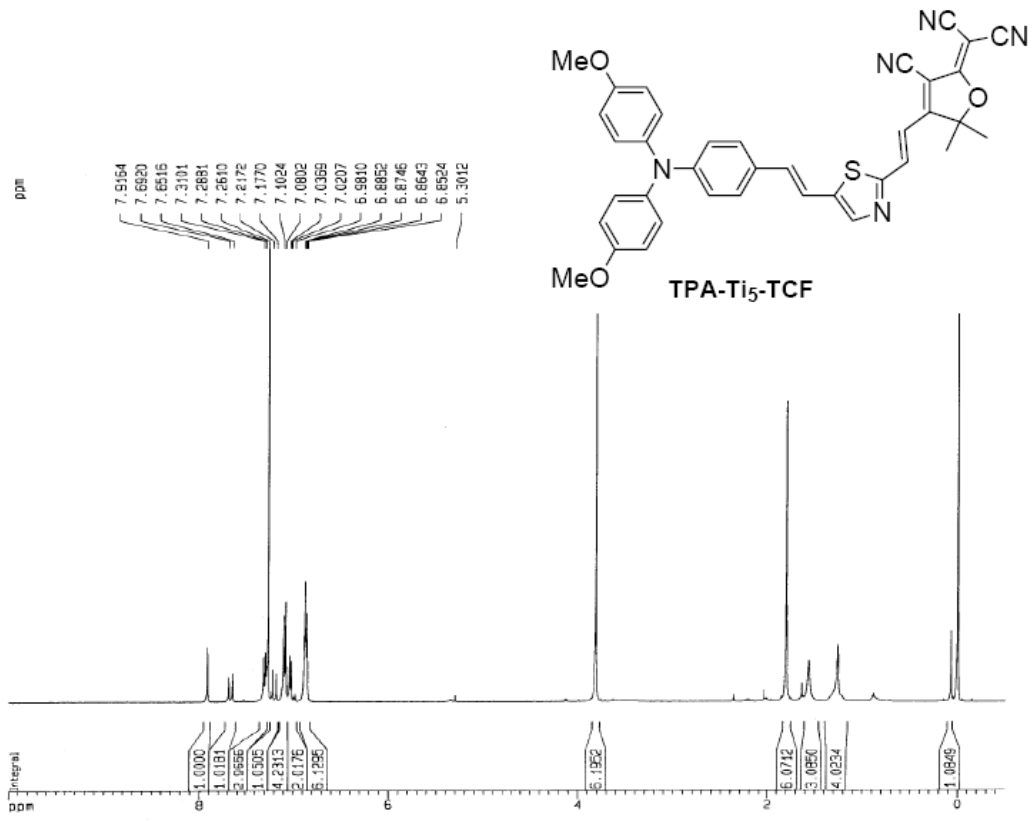

Figure 15. ^{1}H NMR spectrum of TPA-Ti_5-TCF in $CDCl_3$

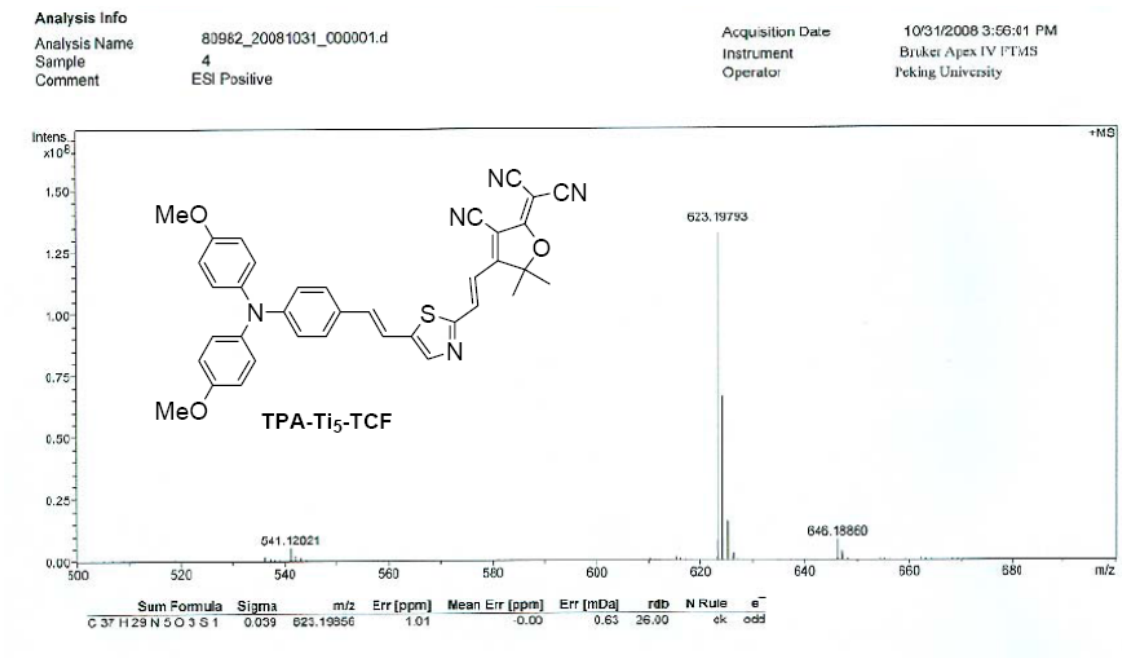

Figure 16. High resolution mass spectroscopy of TPA-Ti_5-TCF

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Molecular Modeling coordinate:

B-Ti_2-TCF

SCF FIELD WAS ACHIEVED

FINAL HEAT OF FORMATION = 196.09145 KCAL

Series No	Atom	X	Y	Z
1	C	-7.0508	2.0002	-0.0174
2	C	-5.8599	2.7687	-0.0963
3	C	-4.6182	2.1541	-0.1074
4	C	-4.4907	0.7565	-0.0363
5	C	-5.6634	-0.0067	0.0564
6	C	-6.9146	0.5914	0.0715
7	N	-8.3115	2.6054	-0.0906
8	C	-9.4608	1.8232	0.2818
9	C	-8.3944	4.0267	0.1186
10	C	-3.1703	0.1665	-0.0551
11	C	-2.9069	-1.1529	-0.1171
12	C	-1.5617	-1.6827	-0.1302
13	N	-1.2734	-2.9965	-0.2337
14	C	0.0847	-3.1763	-0.2169
15	C	0.8532	-2.0066	-0.0993
16	S	-0.1729	-0.6706	-0.0106
17	C	2.2796	-1.9915	-0.0637
18	C	3.0215	-0.8677	0.0623
19	C	4.4467	-0.8168	0.1016
20	C	5.1476	0.5273	0.2914
21	O	6.5852	0.2023	0.2829
22	C	6.7345	-1.1655	0.1091
23	C	5.4066	-1.7906	-0.0031
24	C	5.244	-3.1746	-0.1891
25	N	5.1241	-4.3231	-0.3399
26	C	7.9816	-1.7096	0.0683
27	C	8.1842	-3.1023	-0.1079
28	N	8.3716	-4.2417	-0.2504
29	C	9.147	-0.9103	0.2008
30	N	10.1004	-0.2531	0.3102
31	C	4.8984	1.4818	-0.8606
32	C	4.8395	1.1583	1.6358
33	H	-5.9033	3.8664	-0.1544
34	H	-3.7129	2.7784	-0.1741
35	H	-5.6013	-1.1043	0.1252
36	H	-7.8019	-0.0546	0.1494

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37	H	-9.5878	0.9845	-0.4549
38	H	-9.3615	1.385	1.3124
39	H	-10.3839	2.4595	0.2504
40	H	-7.9334	4.3409	1.0948
41	H	-7.859	4.5526	-0.7176
42	H	-9.4672	4.3539	0.1072
43	H	-2.3353	0.8936	-0.0195
44	H	-3.7141	-1.9055	-0.1664
45	H	0.4873	-4.1953	-0.2942
46	H	2.7596	-2.9851	-0.1459
47	H	2.5185	0.1147	0.1468
48	H	5.533	2.3924	-0.7344
49	H	3.8233	1.78	-0.873
50	H	5.1587	0.9992	-1.8328
51	H	5.0701	0.4473	2.4646
52	H	3.7598	1.4368	1.6785
53	H	5.4634	2.075	1.7697

Dipole: -11.124 7.347 1.268 Magnitude: 13.392 Debye

T-Ti_2-TCF：

SCF FIELD WAS ACHIEVED

FINAL HEAT OF FORMATION = 182.73245 KCAL

Series No	Atom	X	Y	Z
1	C	-6.2152	0.3599	-0.1662
2	N	-7.5787	0.0952	-0.2429
3	C	-2.376	-0.2459	-0.1335
4	C	-1.9706	-1.5266	-0.0097
5	C	-0.5792	-1.9087	0.0313
6	N	-0.1515	-3.1809	0.171
7	C	1.2181	-3.2118	0.1759
8	C	1.8571	-1.9687	0.0398
9	S	0.6935	-0.7543	-0.0947
10	C	3.2734	-1.7965	0.0243
11	C	3.8872	-0.601	-0.1286
12	C	5.298	-0.3907	-0.1457
13	C	5.8479	1.0092	-0.4131
14	O	7.3123	0.8512	-0.3575

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15	C	7.61	-0.4761	-0.0874
16	C	6.3583	-1.2397	0.0433
17	C	6.3472	-2.6168	0.3259
18	N	6.3537	-3.7571	0.5622
19	C	8.909	-0.8702	0.0138
20	C	9.2633	-2.2155	0.2898
21	N	9.5757	-3.3128	0.518
22	C	9.9799	0.0466	-0.1512
23	N	10.856	0.7996	-0.2865
24	C	5.5044	1.5124	-1.8021
25	C	5.4648	2.0025	0.6673
26	C	-5.5825	1.601	-0.2823
27	C	-4.1702	1.4811	-0.2935
28	C	-3.7431	0.1672	-0.1712
29	S	-5.0563	-0.8892	-0.0614
30	C	-8.0426	-1.0328	0.5558
31	C	-9.4916	-1.4165	0.2649
32	C	-10.4038	-0.2146	0.3771
33	C	-9.9194	0.8965	-0.5278
34	C	-8.4604	1.2531	-0.2483
35	H	-1.6363	0.5745	-0.213
36	H	-2.7015	-2.3526	0.0682
37	H	1.7277	-4.1788	0.2836
38	H	3.8598	-2.727	0.1452
39	H	3.2791	0.3149	-0.2575
40	H	6.0215	2.4853	-1.9851
41	H	4.4012	1.659	-1.8833
42	H	5.8375	0.7816	-2.5772
43	H	5.7456	1.6132	1.6749
44	H	6.0031	2.966	0.4956
45	H	4.3643	2.184	0.6353
46	H	-6.0965	2.561	-0.3559
47	H	-3.5024	2.342	-0.382
48	H	-7.3784	-1.9153	0.3231
49	H	-7.9451	-0.806	1.6583
50	H	-9.5694	-1.8555	-0.7638
51	H	-9.7968	-2.2059	0.9993
52	H	-11.4495	-0.5043	0.0966
53	H	-10.4267	0.1451	1.4394
54	H	-10.5368	1.8187	-0.3726
55	H	-10.0323	0.5848	-1.5991
56	H	-8.4007	1.803	0.7364
57	H	-8.1015	1.9514	-1.0571

Dipole: -12.380 5.123 -0.196 Magnitude: 13.400 Debye

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P-Ti_2-TCF

SCF FIELD WAS ACHIEVED

FINAL HEAT OF FORMATION = 202.86782 KCAL

Series No	Atom	X	Y	Z
1	C	-5.9637	-1.0251	-0.3225
2	N	-7.187	-1.633	0.0623
3	C	-2.2902	-0.9066	-0.4124
4	C	-1.6401	-2.0865	-0.3786
5	C	-0.198	-2.1797	-0.3569
6	N	0.4795	-3.346	-0.4079
7	C	1.8271	-3.1005	-0.3851
8	C	2.1998	-1.7486	-0.3098
9	S	0.8135	-0.7881	-0.273
10	C	3.5524	-1.2951	-0.2798
11	C	3.9129	0.0014	-0.1438
12	C	5.254	0.487	-0.1134
13	C	5.5166	1.9614	0.1874
14	O	6.9837	2.0955	0.1419
15	C	7.5376	0.8601	-0.1587
16	C	6.461	-0.1317	-0.3158
17	C	6.7206	-1.4749	-0.6393
18	N	6.951	-2.5829	-0.9131
19	C	8.8887	0.731	-0.2597
20	C	9.5002	-0.5124	-0.5627
21	N	10.0218	-1.5224	-0.8112
22	C	9.759	1.8361	-0.0702
23	N	10.4716	2.7422	0.086
24	C	5.0733	2.3569	1.5828
25	C	4.9516	2.8833	-0.8764
26	C	-5.7403	0.2516	-0.9053
27	C	-4.3378	0.4487	-0.9766
28	C	-3.7102	-0.7072	-0.4581
29	N	-4.7112	-1.6069	-0.048
30	C	-7.5402	-2.8395	-0.6779
31	C	-8.2872	-2.6118	-1.9914
32	C	-9.4932	-1.7224	-1.7741
33	C	-9.0969	-0.4324	-1.0877
34	C	-8.3055	-0.7078	0.191
35	C	-4.4967	-2.8439	0.631
36	H	-1.7205	0.0436	-0.4493
37	H	-2.177	-3.0514	-0.39
38	H	2.5229	-3.9494	-0.4253

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39	H	4.3154	-2.0918	-0.3671
40	H	3.1332	0.7803	-0.0416
41	H	5.397	3.4048	1.7943
42	H	3.9616	2.2919	1.6529
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44	H	5.2829	3.931	-0.6756
45	H	5.3154	2.5834	-1.8881
46	H	3.8368	2.8392	-0.8571
47	H	-6.5103	0.9424	-1.2343
48	H	-3.8261	1.3216	-1.3721
49	H	-8.2001	-3.4395	0.013
50	H	-6.6109	-3.4399	-0.8804
51	H	-8.611	-3.6043	-2.3972
52	H	-7.6004	-2.1438	-2.7436
53	H	-9.978	-1.4936	-2.7584
54	H	-10.2483	-2.2637	-1.1449
55	H	-10.0119	0.1563	-0.8209
56	H	-8.4831	0.1924	-1.7877
57	H	-8.998	-1.1782	0.9475
58	H	-7.9311	0.2647	0.6152
59	H	-5.3773	-3.0922	1.2821
60	H	-4.3501	-3.6746	-0.1134
61	H	-3.5809	-2.7663	1.2781

Dipole: -12.119 1.662 0.880 Magnitude: 12.264 Debye

P-T-TCF:

SCF FIELD WAS ACHIEVED

FINAL HEAT OF FORMATION = 189.75561 KCAL

Series No	Atom	X	Y	Z
1	C	-5.9878	-0.4572	-0.2044
2	N	-7.267	-0.9538	0.1607
3	C	-2.3178	-0.6996	-0.2601
4	C	-1.7896	-1.9384	-0.2801
5	C	-0.3806	-2.2057	-0.2442
6	C	0.1836	-3.4698	-0.3956
7	C	1.5985	-3.4329	-0.3289

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8	C	2.0787	-2.141	-0.1236
9	S	0.8078	-1.0405	-0.0225
10	C	3.4645	-1.8085	-0.0222
11	C	3.9291	-0.5635	0.2311
12	C	5.3047	-0.201	0.3314
13	C	5.6851	1.2061	0.7878
14	O	7.1591	1.216	0.7758
15	C	7.6121	-0.0247	0.3532
16	C	6.4593	-0.8976	0.08
17	C	6.6103	-2.2183	-0.3773
18	N	6.7498	-3.3089	-0.7608
19	C	8.9496	-0.2577	0.2521
20	C	9.4596	-1.5101	-0.1755
21	N	9.8984	-2.53	-0.5233
22	C	9.9063	0.7422	0.5671
23	N	10.6896	1.5622	0.8258
24	C	5.2238	2.2786	-0.1805
25	C	5.2467	1.4923	2.2113
26	C	-5.6369	0.798	-0.7661
27	C	-4.2195	0.8588	-0.8246
28	C	-3.7123	-0.3585	-0.3192
29	N	-4.7987	-1.1626	0.0695
30	C	-7.7332	-2.0933	-0.6214
31	C	-8.4545	-1.7499	-1.9241
32	C	-9.5691	-0.7563	-1.6727
33	C	-9.0497	0.4658	-0.9456
34	C	-8.2878	0.0734	0.3207
35	C	-4.7133	-2.4222	0.7339
36	H	-1.6562	0.1883	-0.2366
37	H	-2.4283	-2.8362	-0.3533
38	H	-0.3889	-4.3866	-0.5539
39	H	2.2317	-4.3186	-0.4295
40	H	4.1604	-2.6575	-0.1613
41	H	3.2154	0.2685	0.3848
42	H	5.6447	3.266	0.1289
43	H	4.1095	2.3346	-0.1745
44	H	5.5763	2.0505	-1.2147
45	H	5.6451	2.4851	2.5325
46	H	5.637	0.7109	2.9062
47	H	4.132	1.5069	2.2614
48	H	-6.3319	1.5662	-1.0901
49	H	-3.6223	1.6829	-1.2041
50	H	-8.4475	-2.6531	0.049
51	H	-6.8647	-2.7712	-0.8478

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52	H	-8.8724	-2.6922	-2.3622
53	H	-7.7262	-1.3244	-2.6623
54	H	-10.0302	-0.4495	-2.6471
55	H	-10.3721	-1.2434	-1.0588
56	H	-9.9035	1.1307	-0.6562
57	H	-8.3792	1.051	-1.6277
58	H	-9.0228	-0.3481	1.0658
59	H	-7.8183	0.9913	0.7713
60	H	-5.6021	-2.5736	1.4033
61	H	-3.7797	-2.458	1.3587
62	H	-4.6812	-3.2568	-0.0198

Dipole: -12.213 0.971 0.808 Magnitude: 12.278 Debye

T-Ti_4-TCF:

SCF FIELD WAS ACHIEVED

FINAL HEAT OF FORMATION = 187.55900 KCAL

Series No	Atom	X	Y	Z
1	C	-6.6313	0.0412	0.0568
2	N	-7.5277	1.1067	0.1327
3	C	-3.2642	-1.9054	0.1279
4	C	-2.1446	-1.157	0.1079
5	C	2.7614	-1.0758	0.0119
6	C	3.8684	-1.8469	0.0056
7	C	5.2142	-1.3693	-0.0567
8	C	6.3633	-2.3712	-0.1525
9	O	7.5787	-1.539	-0.201
10	C	7.2104	-0.2032	-0.1379
11	C	5.7429	-0.1059	-0.047
12	C	5.0807	1.1317	0.0401
13	N	4.5452	2.1623	0.1232
14	C	8.1675	0.7637	-0.1667
15	C	7.8417	2.1429	-0.106
16	N	7.5971	3.2794	-0.0584
17	C	9.5469	0.4409	-0.2598
18	N	10.676	0.1724	-0.3363
19	C	6.3236	-3.1805	-1.4347
20	C	6.4737	-3.2514	1.0778
21	C	-6.9252	-1.3227	0.0875

22	C	-5.7523	-2.1213	0.1295
23	C	-4.591	-1.3664	0.1139
24	S	-4.9413	0.285	0.0673
25	C	-7.1636	2.2766	-0.6591
26	C	-8.0605	3.4823	-0.3885
27	C	-9.5207	3.1172	-0.5432
28	C	-9.8642	1.9407	0.3437
29	C	-8.9393	0.7529	0.0831
30	C	1.4276	-1.6357	0.0746
31	N	0.3111	-0.8938	0.0449
32	C	-0.8083	-1.7197	0.1213
33	C	-0.5003	-3.0843	0.2093
34	S	1.1374	-3.3348	0.1966
35	H	-3.2125	-3.0091	0.1557
36	H	-2.2034	-0.0535	0.0788
37	H	2.8185	0.0284	-0.0353
38	H	3.7738	-2.9503	0.046
39	H	7.2413	-3.8134	-1.505
40	H	5.4214	-3.837	-1.4341
41	H	6.2884	-2.5057	-2.3231
42	H	7.4098	-3.8582	1.0187
43	H	5.5939	-3.9356	1.1288
44	H	6.5116	-2.6291	2.0036
45	H	-7.9306	-1.7472	0.08
46	H	-5.78	-3.2133	0.1621
47	H	-7.2029	2.0403	-1.7632
48	H	-6.0993	2.548	-0.4005
49	H	-7.7839	4.2922	-1.1118
50	H	-7.8755	3.8689	0.6476
51	H	-10.1624	3.9958	-0.2741
52	H	-9.7343	2.8588	-1.6137
53	H	-10.9173	1.6081	0.1544
54	H	-9.7896	2.247	1.4198
55	H	-9.2031	0.2974	-0.9163
56	H	-9.1224	-0.026	0.8769
57	H	-1.2373	-3.8824	0.2799

Dipole: -7.832 -7.020 -0.705 Magnitude: 10.542 Debye

TPA-Ti_2-TCF:

SCF FIELD WAS ACHIEVED

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FINAL HEAT OF FORMATION = 187.41563 KCAL

Series No	Atom	X	Y	Z
1	C	-7.4052	-3.5791	-0.0751
2	C	-6.9676	-2.9516	-1.2562
3	C	-6.5929	-1.6173	-1.2259
4	C	-6.634	-0.8831	-0.0187
5	C	-7.0728	-1.529	1.1549
6	C	-7.4599	-2.8659	1.1266
7	O	-7.7607	-4.9057	-0.219
8	C	-8.1851	-5.5736	0.9637
9	N	-6.2274	0.4793	0.0412
10	C	-7.1947	1.427	0.4757
11	C	-5.1182	0.9038	-0.7106
12	C	-6.8034	2.4964	1.3152
13	C	-7.7391	3.4063	1.7816
14	C	-9.0924	3.2624	1.4228
15	C	-9.4972	2.2096	0.5969
16	C	-8.5527	1.3027	0.1232
17	C	-5.0085	2.2315	-1.1909
18	C	-3.8759	2.6422	-1.8772
19	C	-2.8127	1.7588	-2.1283
20	C	-2.9196	0.4427	-1.6547
21	C	-4.0425	0.0162	-0.9616
22	O	-9.9376	4.2218	1.9453
23	C	-11.3135	4.0986	1.6038
24	C	-1.6566	2.2363	-2.8563
25	C	-0.6572	1.4629	-3.3217
26	C	0.4755	1.9985	-4.0438
27	N	1.4654	1.2387	-4.5565
28	C	2.3866	2.0372	-5.1817
29	C	2.1167	3.4154	-5.1548
30	S	0.6739	3.686	-4.3243
31	C	2.9564	4.4029	-5.7518
32	C	2.7158	5.7326	-5.7005
33	C	3.5345	6.7427	-6.2884
34	C	3.235	8.2146	-6.0113
35	O	4.2653	8.9524	-6.7644
36	C	5.0798	8.0412	-7.4201
37	C	4.6208	6.6746	-7.1224
38	C	5.2481	5.5382	-7.6623
39	N	5.7759	4.6057	-8.1184
40	C	6.1114	8.4869	-8.1884
41	C	6.9711	7.5932	-8.8767
42	N	7.69	6.8714	-9.4389

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43	C	6.3807	9.8721	-8.3421
44	N	6.6008	11.0074	-8.4662
45	C	1.8876	8.6483	-6.5563
46	C	3.4046	8.5756	-4.548
47	H	-6.932	-3.5272	-2.1926
48	H	-6.2487	-1.1328	-2.154
49	H	-7.1183	-0.9766	2.107
50	H	-7.8008	-3.3455	2.0551
51	H	-8.4002	-6.6142	0.6108
52	H	-7.3718	-5.5771	1.7294
53	H	-9.1085	-5.0981	1.3748
54	H	-5.7457	2.6132	1.6012
55	H	-7.4394	4.2393	2.434
56	H	-10.5512	2.086	0.3109
57	H	-8.8826	0.4753	-0.5254
58	H	-5.8254	2.951	-1.0221
59	H	-3.8168	3.6809	-2.239
60	H	-2.0988	-0.2721	-1.8243
61	H	-4.0914	-1.0238	-0.6014
62	H	-11.7898	4.9656	2.1282
63	H	-11.455	4.1802	0.4988
64	H	-11.7287	3.1329	1.9817
65	H	-1.6352	3.33	-3.0301
66	H	-0.6547	0.3673	-3.1785
67	H	3.2597	1.5704	-5.6571
68	H	3.8492	4.0056	-6.2714
69	H	1.8253	6.11	-5.1624
70	H	1.7908	9.7579	-6.4707
71	H	1.0727	8.161	-5.9702
72	H	1.7894	8.3648	-7.6313
73	H	4.4275	8.3036	-4.1935
74	H	3.263	9.6755	-4.4156
75	H	2.6459	8.0288	-3.9392

Dipole: -11.766 -2.690 7.453 Magnitude: 14.185 Debye

TPA-Ti_5-TCF:

SCF FIELD WAS ACHIEVED

FINAL HEAT OF FORMATION = 188.92888 KCAL

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Series No	Atom	X	Y	Z
1	C	-8.0022	-3.6861	-0.2259
2	C	-8.6553	-2.6043	-0.8454
3	C	-8.1165	-1.3306	-0.752
4	C	-6.918	-1.106	-0.0338
5	C	-6.2847	-2.2002	0.5879
6	C	-6.8179	-3.4825	0.4887
7	O	-8.6226	-4.9096	-0.3878
8	C	-7.9856	-6.0223	0.229
9	N	-6.3751	0.2056	0.0288
10	C	-7.2173	1.2454	0.5064
11	C	-4.9814	0.3873	-0.0014
12	C	-7.1572	2.5298	-0.0844
13	C	-7.9966	3.545	0.3466
14	C	-8.9238	3.2954	1.3755
15	C	-8.9998	2.0312	1.9674
16	C	-8.1479	1.0166	1.5389
17	C	-4.3607	1.4785	0.6536
18	C	-2.9894	1.666	0.5672
19	C	-2.1751	0.7777	-0.1541
20	C	-2.7877	-0.3028	-0.8053
21	C	-4.1589	-0.501	-0.737
22	O	-9.7115	4.3756	1.7232
23	C	-10.6584	4.1525	2.7616
24	C	-0.7467	1.0092	-0.205
25	C	0.1713	0.0959	-0.5759
26	C	1.5803	0.3462	-0.6196
27	C	2.5475	-0.636	-0.8922
28	N	3.8479	-0.2076	-0.886
29	C	3.8901	1.1126	-0.613
30	S	2.3418	1.8217	-0.3608
31	C	5.1186	1.8692	-0.5285
32	C	5.1392	3.2156	-0.437
33	C	6.3204	4.0159	-0.3488
34	C	6.2341	5.5239	-0.5722
35	O	7.6197	6.002	-0.4135
36	C	8.4364	4.9206	-0.1181
37	C	7.6235	3.6928	-0.0777
38	C	8.1758	2.4343	0.2204
39	N	8.6317	1.3924	0.4699
40	C	9.7692	5.1117	0.0791
41	C	10.6418	4.0358	0.3841
42	N	11.3743	3.1673	0.6349
43	C	10.3577	6.4006	-0.01

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44	N	10.8371	7.4578	-0.0833
45	C	5.3974	6.2249	0.481
46	C	5.7959	5.8763	-1.9807
47	H	-9.5865	-2.7832	-1.4024
48	H	-8.6325	-0.4883	-1.2399
49	H	-5.3504	-2.0512	1.1527
50	H	-6.3003	-4.3189	0.9791
51	H	-8.6524	-6.8822	-0.035
52	H	-7.9382	-5.8859	1.3366
53	H	-6.9618	-6.1742	-0.1912
54	H	-6.4351	2.731	-0.892
55	H	-7.952	4.5449	-0.1091
56	H	-9.7206	1.8235	2.7707
57	H	-8.2177	0.0235	2.0109
58	H	-4.9655	2.1898	1.2383
59	H	-2.5322	2.5238	1.0852
60	H	-2.178	-1.0062	-1.3939
61	H	-4.6079	-1.3567	-1.2659
62	H	-11.1658	5.1449	2.8678
63	H	-11.3921	3.3645	2.4639
64	H	-10.1433	3.8696	3.7115
65	H	-0.4255	2.0217	0.1042
66	H	-0.1271	-0.928	-0.865
67	H	2.3358	-1.6921	-1.101
68	H	6.0528	1.2756	-0.5566
69	H	4.1914	3.7886	-0.4413
70	H	5.5107	7.3308	0.3702
71	H	4.3238	5.9505	0.3509
72	H	5.7317	5.9344	1.5055
73	H	5.8418	6.9835	-2.1206
74	H	4.7492	5.5253	-2.1431
75	H	6.4669	5.3951	-2.7317

Dipole: -12.506 -0.969 0.989 Magnitude: 12.582 Debye

B-T-TCF

SCF FIELD WAS ACHIEVED

FINAL HEAT OF FORMATION = 181.41092 KCAL

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Series No	Atom	X	Y	Z
1	C	6.9302	-1.6575	0.0131
2	C	5.7859	-2.4962	0.0064
3	C	4.5097	-1.9559	0.0002
4	C	4.3004	-0.5665	0.0103
5	C	5.4279	0.266	0.031
6	C	6.713	-0.257	0.0375
7	N	8.2244	-2.1922	-0.0705
8	C	9.33	-1.3278	0.2506
9	C	8.3934	-3.5921	0.2194
10	C	2.9458	-0.0576	0.0017
11	C	2.5972	1.2433	-0.0156
12	C	1.2404	1.71	-0.0251
13	C	0.8723	3.0528	-0.0455
14	C	-0.5348	3.2193	-0.0514
15	C	-1.2057	1.9979	-0.0354
16	S	-0.1131	0.7165	-0.0139
17	C	-2.6283	1.8667	-0.0378
18	C	-3.2803	0.6814	-0.0213
19	C	-4.6964	0.516	-0.0241
20	C	-5.2909	-0.8912	-0.0035
21	O	-6.7496	-0.6802	-0.0141
22	C	-7.0048	0.6827	-0.0369
23	C	-5.7301	1.4178	-0.0428
24	C	-5.6762	2.8223	-0.0644
25	N	-5.646	3.9863	-0.0784
26	C	-8.2911	1.129	-0.0497
27	C	-8.6021	2.5124	-0.0728
28	N	-8.8781	3.6426	-0.0899
29	C	-9.3904	0.2313	-0.0406
30	N	-10.2896	-0.5065	-0.033
31	C	-4.9451	-1.687	-1.2475
32	C	-4.9573	-1.6446	1.27
33	H	5.8923	-3.5911	0.0005
34	H	3.6418	-2.6344	-0.011
35	H	5.304	1.3601	0.0457
36	H	7.5617	0.4427	0.0565
37	H	10.2896	-1.9081	0.2242
38	H	9.3927	-0.5126	-0.52
39	H	9.2235	-0.8561	1.2656
40	H	9.4825	-3.8594	0.1928
41	H	7.9792	-3.8737	1.226
42	H	7.8659	-4.1951	-0.5681
43	H	2.1573	-0.8346	0.0085

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44	H	3.3594	2.0424	-0.0252
45	H	1.5788	3.8861	-0.0561
46	H	-1.0281	4.1951	-0.0669
47	H	-3.1851	2.8227	-0.0548
48	H	-2.7014	-0.2619	-0.0043
49	H	-5.5023	-2.6551	-1.2383
50	H	-3.8485	-1.8922	-1.2666
51	H	-5.2306	-1.1213	-2.1664
52	H	-5.2572	-1.051	2.1664
53	H	-5.5096	-2.6153	1.2851
54	H	-3.8601	-1.8432	1.3095
Dipole: 12.252	-4.823	0.872	Magnitude: 13.196	Debye