SUPPORTING INFORMATION

Selective Bromination of 2,5-Bis(2-thienyl)pyrroles and Solid-State Polymerization Through β-Carbon of Pyrrole

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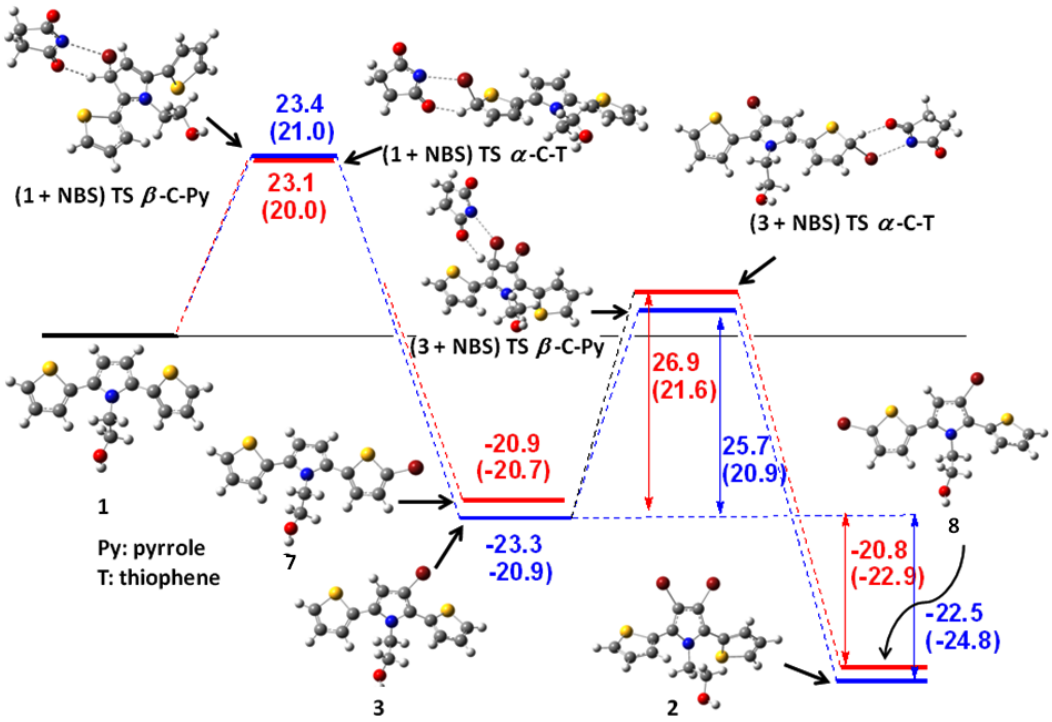


Fig. S1. DFT calculation of the reaction pathway of bromination of **1** in acetic acid and DMF (values given in parenthesis) solvents with the Polarized Continuum Model (PCM), using B3LYP/6-31G(d) level (single-point calculations). The gas phase optimized geometries are used for PCM calculation. Energy values are given in kcal/mole including ZPVE.

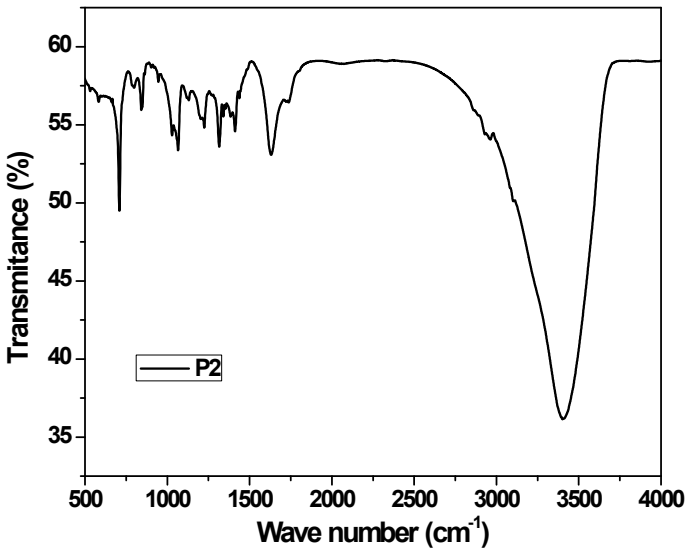


Fig. S2. FT-IR spectra of doped **P2** prepared by solid-state polymerization

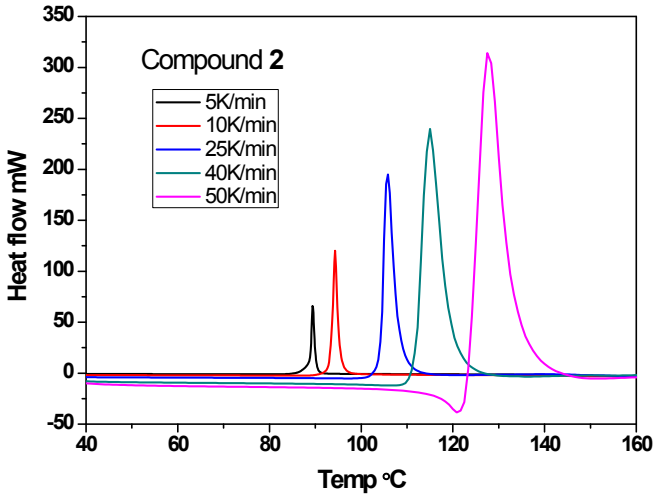


Fig. S3. DSC curves of **2** as a function of scan rates

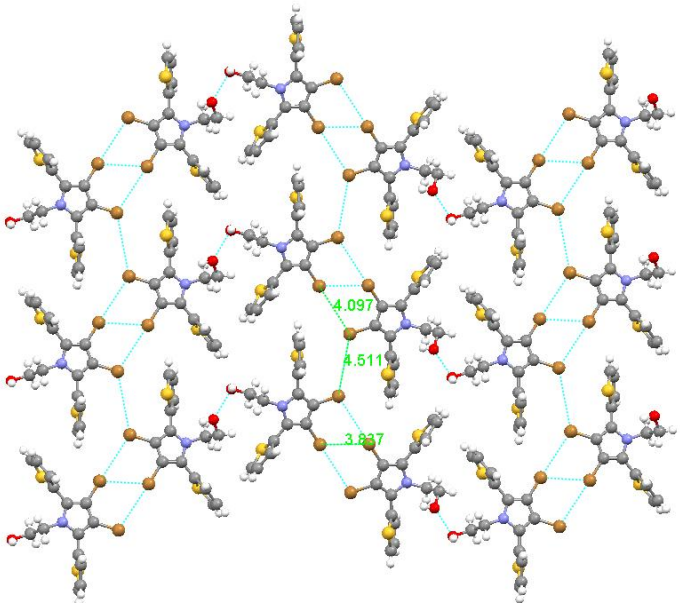


Fig. S4. Br...Br short contact in the crystal packing diagram of compound **2**.

Table S1 Crystallographic data and structure refinement parameters of compound **2**.

Formula	C_{28} H_{22} N_2 O_2 S_4 Br_4	***T* [K]**	298(2)
Crystal System	Monoclinic	***R*1**	0.0591
Space group	$P\ 2_1/c$	***θ* [°]**	2.43-22.44
***a* [Å]**	14.0099(11)	**index ranges**	$-10 \le h \le 16$ $-13 \le k \le 13$ $-25 \le l \le 25$
***b* [Å]**	10.9631(11)	***wR*2**	0.1572

***c* [Å]**	21.397(2)	R_{merge}	0.1037
***α* [°]**	90	**Parameters**	365
***β* [°]**	105.274(2)	**GOF**	1.026
***γ* [°]**	90	**reflns total**	24363
***V* [Å ^{3}]**	3170.3(5)	**unique reflns**	5623
Z	4	**obsd reflns**	3487
***λ* [Å]**	0.71073	**CCDC No.**	935851
ρ_{calcd} **[gcm^{-3}]**	1.813		
***F*[000]**	1692.7		
***μ* [mm^{-1}]**	5.371		

Table S2 Calculated absolute energies at B3LYP/6-31G(d)

Compound	E / a.u.	ZPVE / a.u.	G^0 / a.u.	E / a.u. (AcOH)[a]	E / a.u. (DMF)[a]
1	-1467.622303	0.239904	-1467.428113	-1467.630135	-1467.632336
(1 + NBS) TS *β*-C-Py	-4399.301617	0.321051	-4399.040626	-4399.333143	-4399.341402
(1 + NBS) TS *α*-C-T	-4399.299774	0.321017	-4399.039436	-4399.333497	-4399.342979
3	-4038.724115	0.229561	-4038.544025	-4038.732592	-4038.731254
9	-4038.721518	0.229843	-4038.54068	-4038.729139	-4038.731254
(3 + NBS) TS *β*-C-Py	-6970.400813	0.310789	-6970.15279	-6970.431982	-6970.440547
(3 + NBS) TS *α*-C-T	-6970.396553	0.310393	-6970.150995	-6970.429577	-6970.439050
2	-6609.824793	0.218957	-6609.658635	-6609.833611	-6609.836085
10	-6609.823204	0.219549	-6609.656509	-6609.831387	-6609.833647
NBS	-2931.731440	0.081351	-2931.683972	-2931.740425	-2931.742759
NHS	-360.6667847	0.092423	-360.604652	-360.675759	-360.677887

[a] the energy values are taken from the single point calulation in acetic acid and DMF solvents with the Polarized Continuum Model (PCM) using optimized geometries of gas phase calculations.

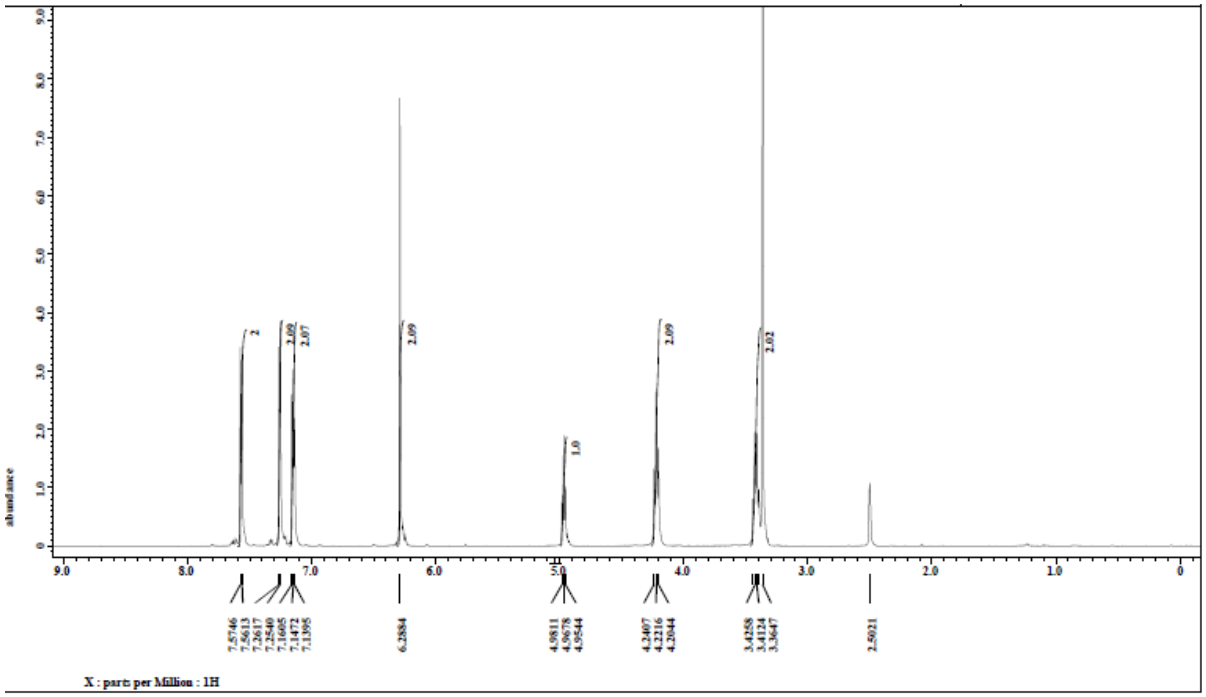
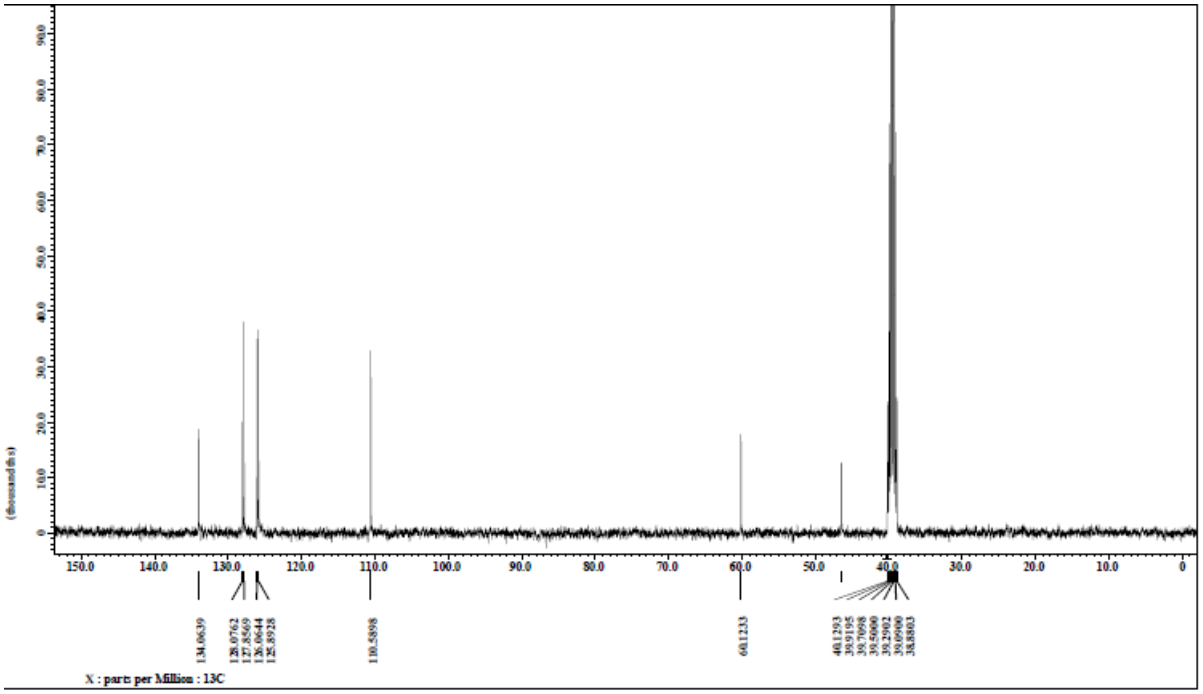


Fig. S5 ^{1}H NMR spectra of **1**



Fiig. S6. ^{13}C NMR spectra of **1**

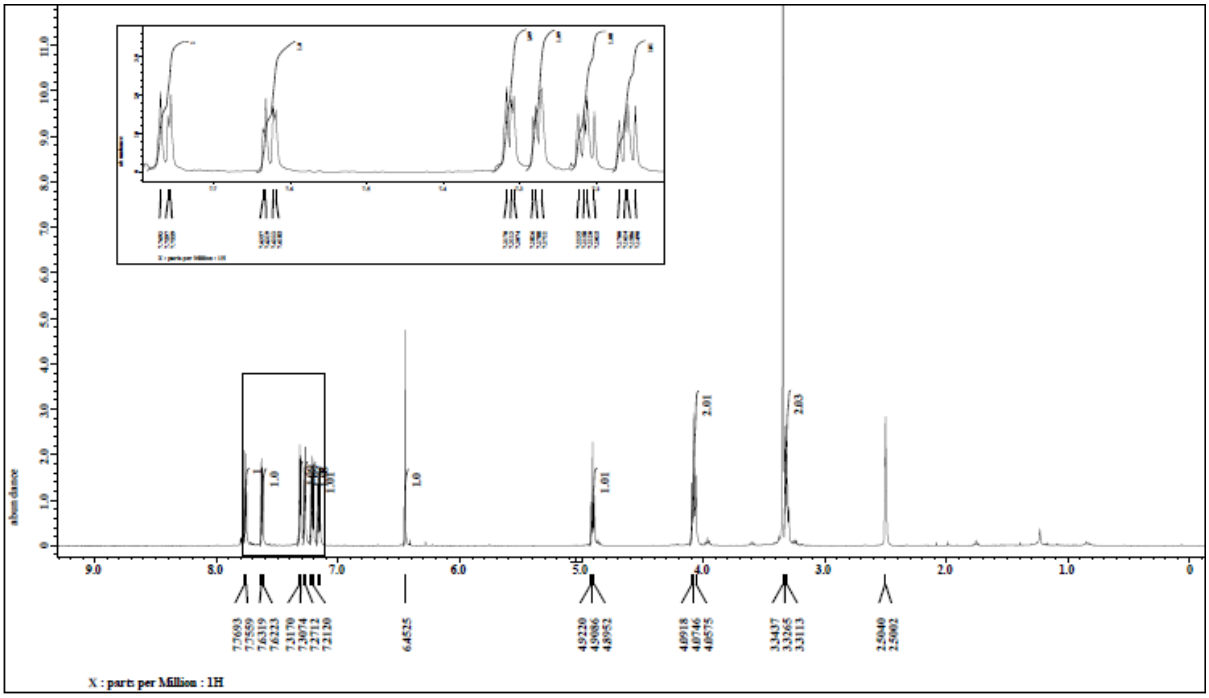


Fig. S7. ^{1}H NMR spectra of **3**

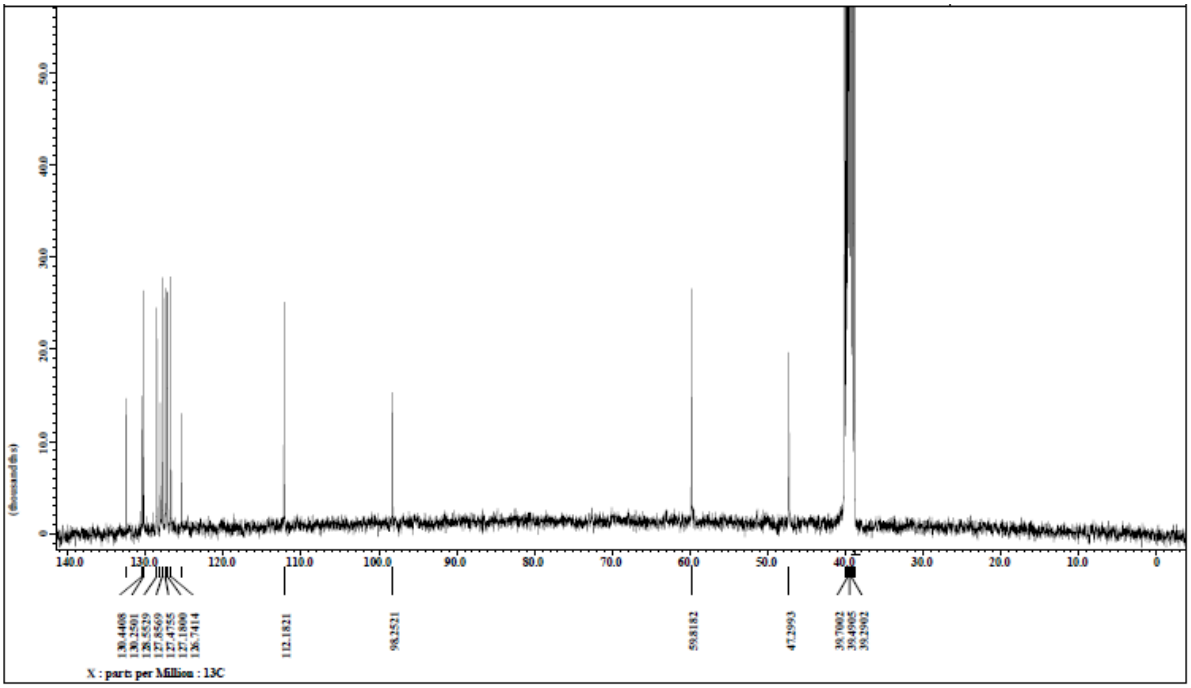


Fig. S8. ^{13}C NMR spectra of **3**

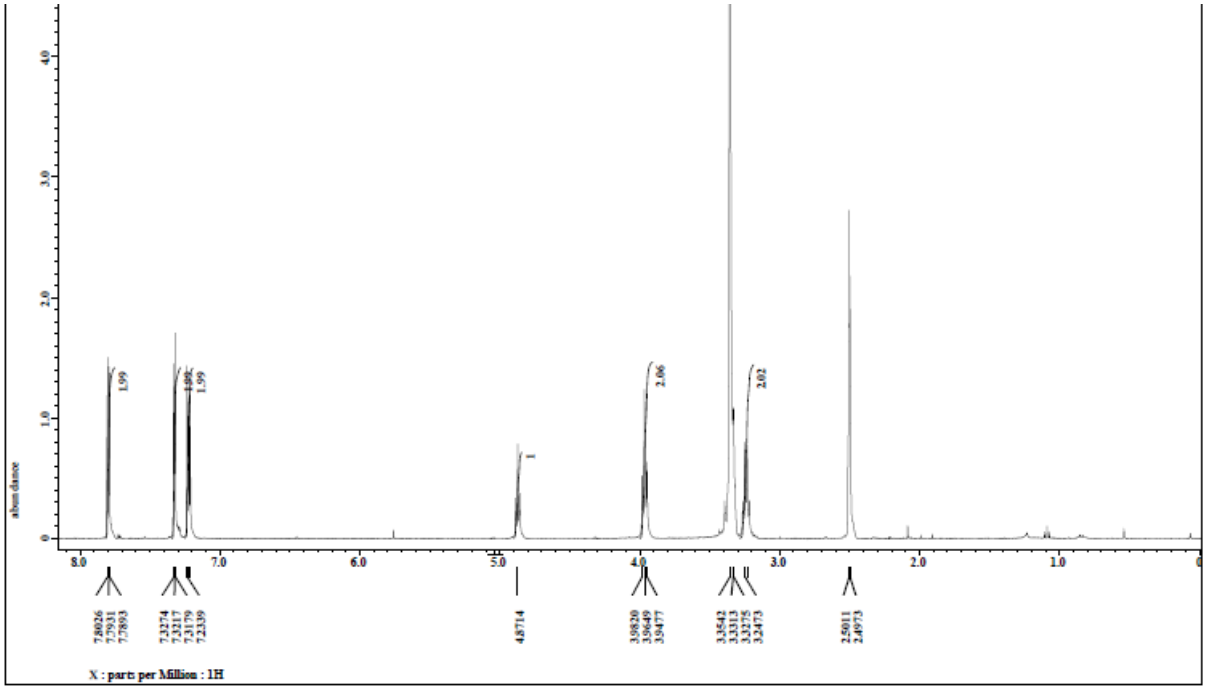


Fig. S9. ^{1}H NMR spectra of **2**

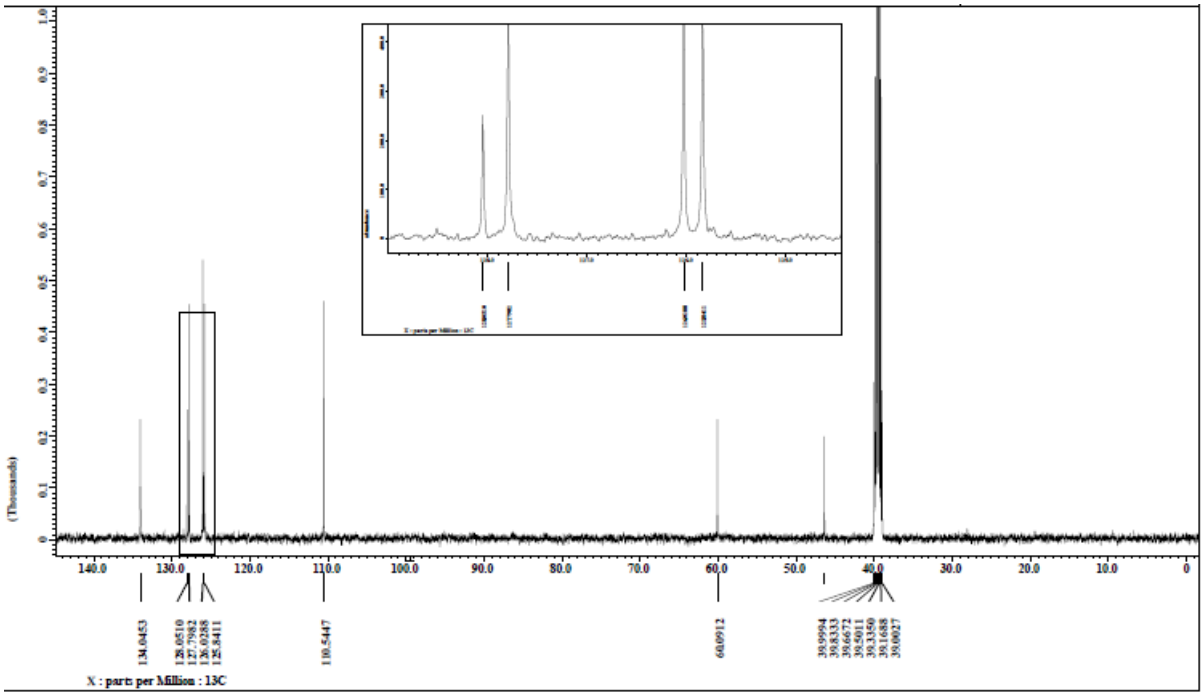


Fig. S10. ^{13}C NMR spectra of **2**

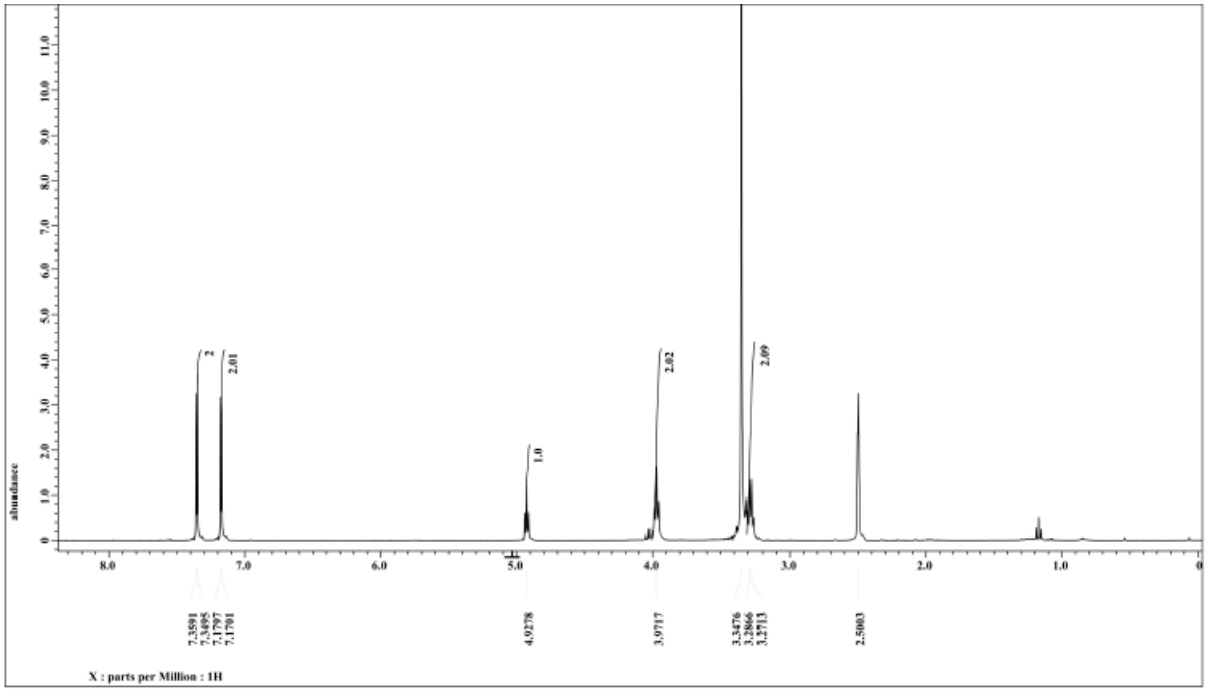


Fig. S11. ^{1}H NMR spectra of **4**

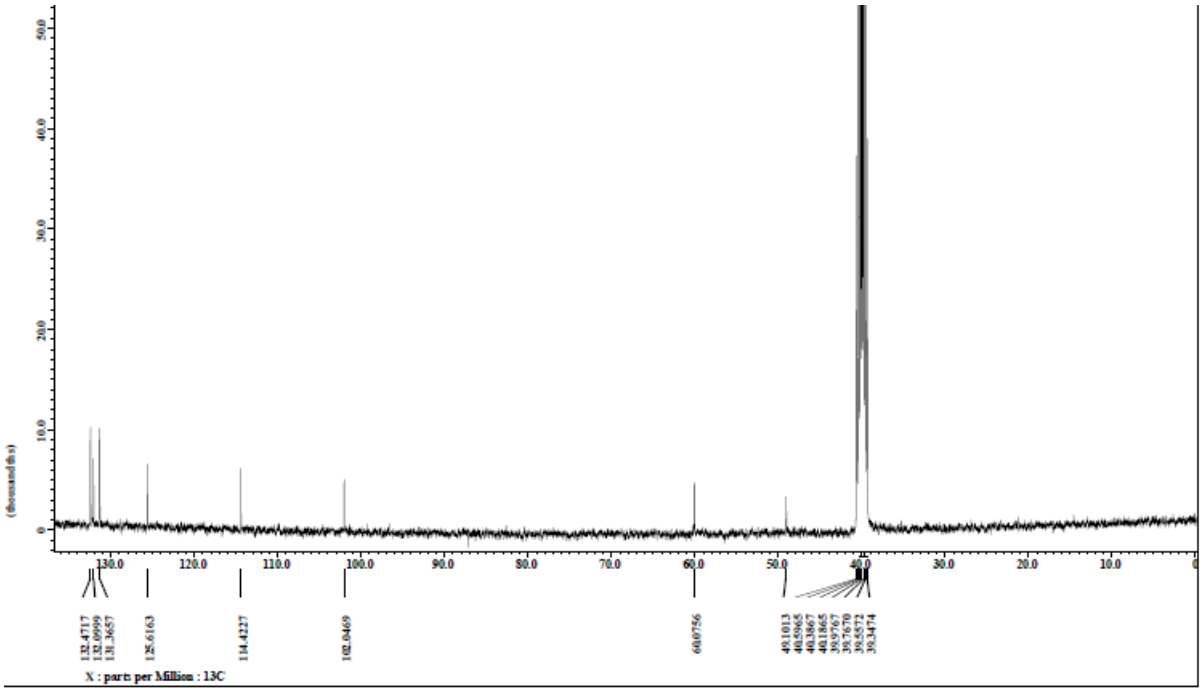


Fig. S12. ^{13}C NMR spectra of **4**

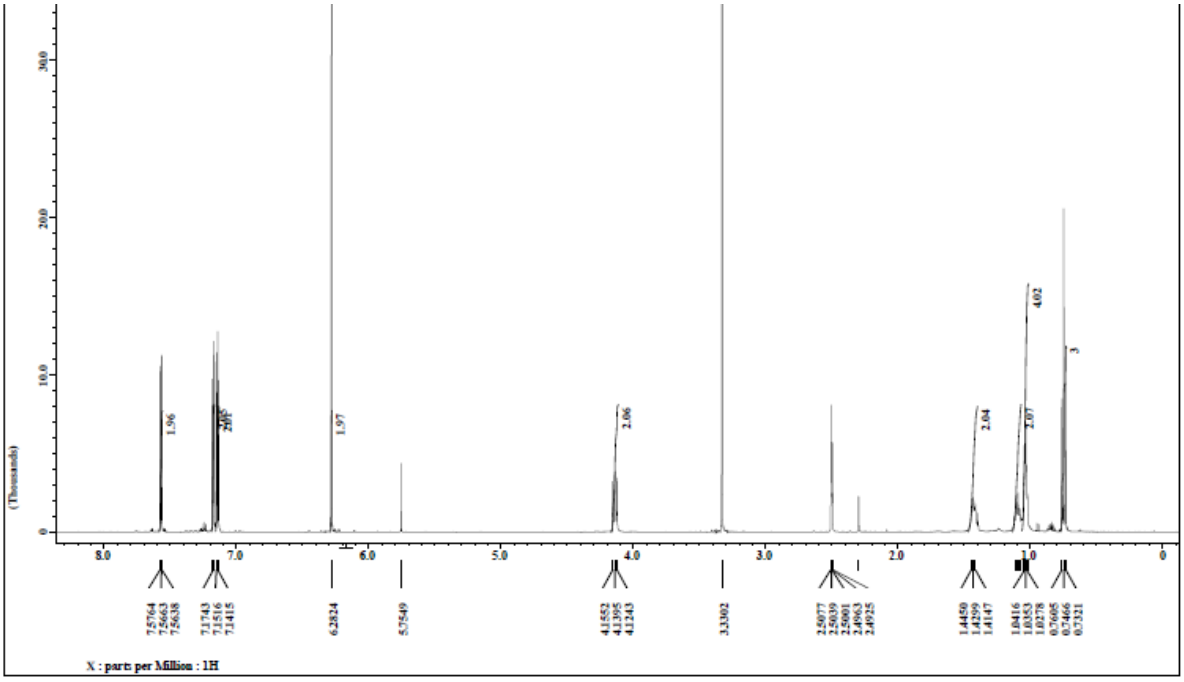


Fig. S13. ^{1}H NMR spectra of **5**

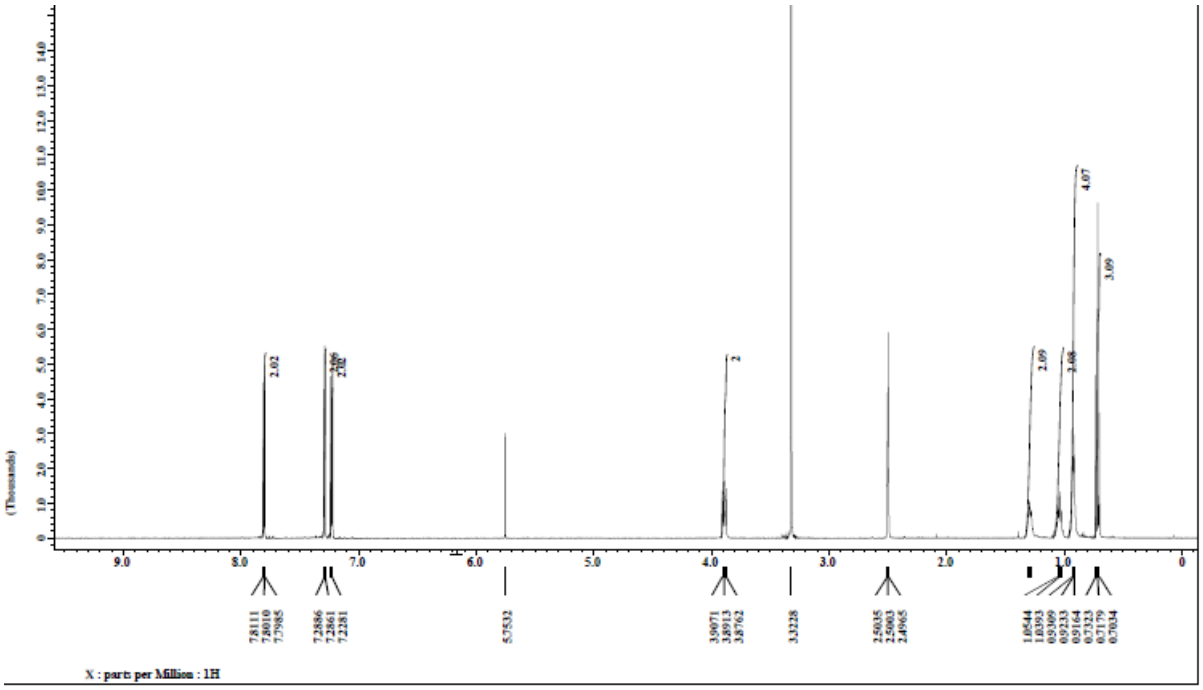


Fig. S14. ^{1}H NMR spectra of **6**

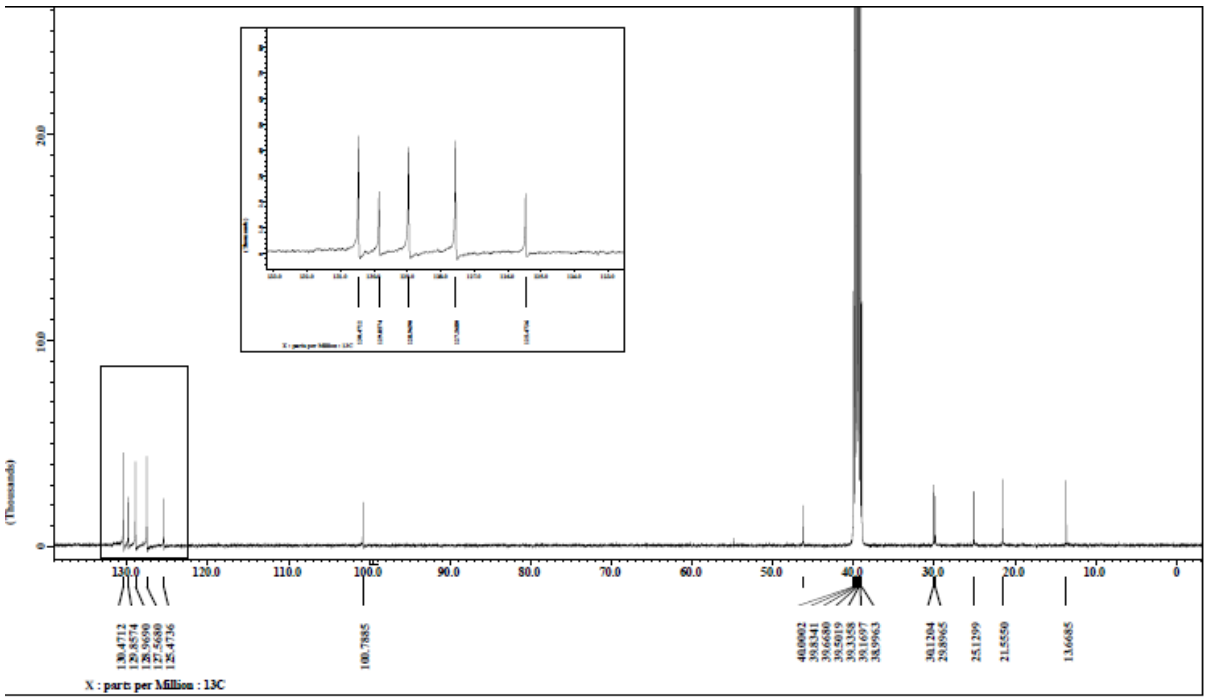


Fig. S15. ^{13}C NMR spectra of **6**

Coordinates of optimized geometries at B3LYP/6-31G(d)

1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.017239	-0.250141	-0.431565
2	6	0	4.582730	0.951666	0.054583
3	6	0	3.192978	0.953836	0.371184
4	6	0	2.563601	-0.247451	0.120846
5	16	0	3.721934	-1.397525	-0.534841
6	1	0	6.018079	-0.530514	-0.731435
7	1	0	5.232071	1.808289	0.201139
8	1	0	2.690460	1.805919	0.812549
9	6	0	1.193507	-0.693044	0.324010
10	6	0	0.768692	-1.942230	0.761892
11	7	0	0.058161	0.060298	0.036782
12	6	0	-0.635678	-1.952707	0.744846
13	1	0	1.423453	-2.738918	1.087330
14	6	0	-1.074317	-0.712639	0.286483
15	1	0	-1.279910	-2.764588	1.053679
16	6	0	-2.449800	-0.309528	0.033619
17	6	0	-3.075605	0.917245	-0.093452
18	16	0	-3.640228	-1.596951	-0.156407
19	6	0	-4.480435	0.823557	-0.319687
20	1	0	-2.573408	1.873110	-0.024874
21	6	0	-4.934498	-0.463374	-0.366874
22	1	0	-5.122569	1.690346	-0.435016
23	1	0	-5.945835	-0.816877	-0.515926
24	6	0	0.047707	1.409913	-0.506244
25	1	0	-0.769647	1.491284	-1.226674
26	1	0	0.982711	1.576304	-1.044437
27	6	0	-0.149955	2.479714	0.576797
28	1	0	0.794451	2.676363	1.105211
29	1	0	-0.871699	2.116061	1.322240
30	8	0	-0.622568	3.644969	-0.088305
31	1	0	-0.709028	4.354103	0.566516

(**1** + NBS) TS β-C-Py

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.586863	3.957442	-0.684066
2	6	0	0.374811	4.421305	-0.220495
3	6	0	-0.573748	3.392450	-0.063332
4	6	0	-0.083226	2.130715	-0.420405
5	16	0	1.604391	2.261710	-0.923273
6	1	0	2.480919	4.534201	-0.883633
7	1	0	0.176556	5.461890	0.009054
8	1	0	-1.561538	3.582678	0.334103
9	6	0	-0.680018	0.831966	-0.421066
10	6	0	0.066899	-0.438494	-0.617500
11	7	0	-1.988411	0.523462	-0.285519
12	6	0	-0.976550	-1.474182	-0.605541
13	6	0	-2.178024	-0.896749	-0.390171
14	1	0	-0.790371	-2.528435	-0.747587
15	6	0	-3.475087	-1.548707	-0.224469
16	6	0	-3.787456	-2.498461	0.720349
17	16	0	-4.815288	-1.336695	-1.342421
18	6	0	-5.096399	-3.040838	0.569645
19	1	0	-3.092446	-2.789677	1.500409
20	6	0	-5.770919	-2.505167	-0.492697
21	1	0	-5.517514	-3.793037	1.227183
22	1	0	-6.775008	-2.725506	-0.830223
23	6	0	-3.053618	1.459183	0.061789
24	1	0	-4.006120	1.022282	-0.234586
25	1	0	-2.918547	2.372104	-0.521706
26	6	0	-3.064836	1.797092	1.559133
27	1	0	-2.034350	1.894306	1.930183
28	1	0	-3.547322	0.982860	2.118603
29	8	0	-3.782274	3.017747	1.667329
30	1	0	-3.880153	3.233821	2.607189
31	1	0	0.864678	-0.483214	-1.374487
32	35	0	1.232489	-0.662288	1.025923
33	7	0	3.950477	-1.099191	0.469288
34	6	0	6.176756	-1.559083	-0.317744
35	6	0	5.269126	-1.288770	-1.518889
36	6	0	5.225679	-1.409745	0.896736
37	6	0	3.888805	-1.014148	-0.876450
38	8	0	5.587682	-1.551760	2.055002
39	8	0	2.900571	-0.751600	-1.591640
40	1	0	5.564281	-0.419546	-2.117654
41	1	0	5.177601	-2.133606	-2.210836
42	1	0	7.004189	-0.848439	-0.214952
43	1	0	6.615757	-2.562690	-0.308126

(**1** + NBS) TS α-C-T

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.964705	0.412643	0.658360
2	6	0	-1.159158	1.630635	0.659742
3	6	0	0.183552	1.453754	0.457930
4	6	0	0.577241	0.095302	0.297440
5	16	0	-0.807626	-0.965583	0.460070
6	1	0	-1.642086	2.594876	0.769798
7	1	0	0.866454	2.284235	0.352167
8	6	0	1.839592	-0.480233	0.006894
9	6	0	2.060235	-1.784948	-0.482168
10	7	0	3.102388	0.113665	0.164468
11	6	0	3.424414	-1.973782	-0.621537
12	6	0	4.073876	-0.795327	-0.205000
13	1	0	3.921905	-2.850751	-1.010942
14	6	0	5.507112	-0.598782	-0.117243
15	6	0	6.311560	0.530431	-0.101795
16	16	0	6.513252	-2.043689	-0.038717
17	6	0	7.700255	0.236748	-0.038427
18	1	0	5.946660	1.547439	-0.155583
19	6	0	7.962872	-1.106329	-0.004651

20	1	0	8.470981	0.999113	-0.026365
21	1	0	8.923978	-1.600610	0.044149
22	6	0	3.385639	1.425529	0.738839
23	1	0	4.324305	1.354755	1.292021
24	1	0	2.603296	1.662884	1.463988
25	6	0	3.534177	2.532541	-0.326656
26	1	0	2.556525	2.846265	-0.719115
27	1	0	4.101075	2.140868	-1.175532
28	8	0	4.279234	3.629378	0.172562
29	1	0	3.733957	4.117126	0.809126
30	35	0	-3.229396	0.611918	-0.906239
31	7	0	-5.839580	-0.168380	-0.339975
32	6	0	-8.002988	-0.866391	0.430614
33	6	0	-7.019446	-0.898388	1.603523
34	6	0	-7.138688	-0.380891	-0.759520
35	6	0	-5.683258	-0.436166	0.974817
36	8	0	-7.574583	-0.221014	-1.887843
37	8	0	-4.654030	-0.353661	1.667953
38	1	0	-7.277884	-0.218899	2.423204
39	1	0	-6.878622	-1.891291	2.044578
40	1	0	-8.840454	-0.174468	0.570309
41	1	0	-8.433121	-1.843222	0.184564
42	1	0	-2.715273	0.213862	1.438092
43	1	0	1.278826	-2.483641	-0.747541

3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.261915	-0.672484	0.450118
2	6	0	-5.020509	0.604854	0.029595
3	6	0	-3.638055	0.867647	-0.199577
4	6	0	-2.820848	-0.217462	0.050800
5	16	0	-3.792423	-1.578939	0.598351
6	1	0	-6.210518	-1.135918	0.685602
7	1	0	-5.800724	1.342693	-0.123771
8	1	0	-3.284216	1.829701	-0.547985
9	6	0	-1.384074	-0.417799	-0.070728
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14	6	0	0.844837	0.014255	-0.062000
15	6	0	2.083135	0.780265	0.052669
16	6	0	2.629065	1.697143	-0.816357
17	16	0	3.132676	0.574521	1.445935
18	6	0	3.871696	2.236743	-0.373766
19	1	0	2.165473	1.949349	-1.763995
20	6	0	4.271307	1.721313	0.829504
21	1	0	4.448186	2.964174	-0.934937
22	1	0	5.174833	1.941932	1.382619
23	6	0	-0.679909	1.980617	0.351965
24	1	0	0.143297	2.363478	0.958643
25	1	0	-1.594708	2.046998	0.944608
26	6	0	-0.852739	2.831713	-0.912653
27	1	0	-1.388001	2.248055	-1.676879
28	1	0	0.130873	3.098698	-1.323905
29	8	0	-1.587252	3.985825	-0.523360
30	1	0	-1.612801	4.597154	-1.274694
31	35	0	2.038302	-2.607397	-0.502564

7

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.718944	0.116121	0.002094
2	6	0	3.193732	1.307138	0.415685
3	6	0	1.788060	1.225777	0.637523
4	6	0	1.247436	-0.018012	0.390421

5	16	0	2.510051	-1.123160	-0.150696
6	1	0	3.787112	2.199775	0.573601
7	1	0	1.209522	2.060571	1.013778
8	6	0	-0.102342	-0.541913	0.516080
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17	16	0	-4.822291	-1.764400	-0.275138
18	6	0	-5.800645	0.594279	-0.543581
19	1	0	-3.989566	1.769026	-0.137345
20	6	0	-6.167329	-0.720191	-0.597184
21	1	0	-6.486897	1.415663	-0.720283
22	1	0	-7.140964	-1.140664	-0.809885
23	6	0	-1.317313	1.460090	-0.455930
24	1	0	-2.094569	1.470888	-1.223476
25	1	0	-0.363998	1.667667	-0.945746
26	6	0	-1.642389	2.546178	0.579140
27	1	0	-0.744542	2.817647	1.153898
28	1	0	-2.382343	2.158967	1.294531
29	8	0	-2.145707	3.659109	-0.148959
30	1	0	-2.310613	4.381574	0.475546
31	35	0	5.527249	-0.259463	-0.373586

(**3** + NBS) TS *β*-C-Py

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.821022	4.253727	-0.973337
2	6	0	0.643629	4.796527	-0.507219
3	6	0	-0.334005	3.818734	-0.238726
4	6	0	0.099478	2.516291	-0.512862
5	16	0	1.771431	2.544423	-1.079592
6	1	0	2.726515	4.779450	-1.248116
7	1	0	0.490008	5.858264	-0.352591
8	1	0	-1.298827	4.074696	0.178310
9	6	0	-0.545374	1.246015	-0.396233
10	6	0	0.155107	-0.061941	-0.482293
11	7	0	-1.864275	1.000709	-0.232541
12	6	0	-0.935862	-1.044801	-0.383877
13	6	0	-2.122485	-0.409964	-0.219426
14	6	0	-3.445457	-0.986960	-0.015058
15	6	0	-3.800181	-1.863153	0.984427
16	16	0	-4.769831	-0.791159	-1.155079
17	6	0	-5.130944	-2.354069	0.861433
18	1	0	-3.115988	-2.147189	1.776113
19	6	0	-5.777927	-1.858056	-0.237296
20	1	0	-5.586992	-3.043697	1.562738
21	1	0	-6.790465	-2.053887	-0.564536
22	6	0	-2.886647	2.006875	0.041976
23	1	0	-3.858315	1.594513	-0.224937
24	1	0	-2.707111	2.867083	-0.605906
25	6	0	-2.879709	2.452354	1.510977
26	1	0	-1.845131	2.521723	1.877163
27	1	0	-3.404376	1.707452	2.126239
28	8	0	-3.531522	3.713662	1.527519
29	1	0	-3.621511	4.000875	2.448970
30	1	0	0.943664	-0.214375	-1.237654
31	35	0	1.313147	-0.186860	1.166095
32	7	0	3.991935	-0.805193	0.610419
33	6	0	6.184555	-1.412320	-0.170081
34	6	0	5.273181	-1.174925	-1.375601
35	6	0	5.260281	-1.138846	1.043063
36	6	0	3.915338	-0.801124	-0.736263
37	8	0	5.633055	-1.215361	2.203661
38	8	0	2.930268	-0.539671	-1.457313
39	1	0	5.598010	-0.356856	-2.028582
40	1	0	5.134989	-2.054547	-2.014223
41	1	0	7.047698	-0.739385	-0.123123

42	1	0	6.573026	-2.434257	-0.101012
43	35	0	-0.639513	-2.880453	-0.472148

(**3** + NBS) TS α-C-T

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.569283	0.645293	0.676727
2	6	0	-1.867551	1.924283	0.690601
3	6	0	-0.510265	1.858763	0.519041
4	6	0	0.001014	0.538348	0.374244
5	16	0	-1.299389	-0.631111	0.492455
6	1	0	-2.427984	2.845479	0.801799
7	1	0	0.101396	2.745738	0.460627
8	6	0	1.319560	0.055322	0.152438
9	6	0	1.655634	-1.285089	-0.117537
10	7	0	2.522975	0.774712	0.215317
11	6	0	3.034695	-1.369482	-0.202775
12	6	0	3.583235	-0.088479	0.007314
13	6	0	4.982700	0.300158	0.069733
14	6	0	5.631364	1.386232	-0.488446
15	16	0	6.126012	-0.674745	0.983142
16	6	0	7.017901	1.438603	-0.186904
17	1	0	5.140971	2.112110	-1.124948
18	6	0	7.424635	0.395436	0.602420
19	1	0	7.683317	2.213233	-0.550485
20	1	0	8.419559	0.186397	0.973000
21	6	0	2.674049	2.197909	0.518786
22	1	0	3.678306	2.350132	0.916401
23	1	0	1.968792	2.461213	1.311747
24	6	0	2.498583	3.108131	-0.712637
25	1	0	1.485675	3.026019	-1.129713
26	1	0	3.185686	2.789271	-1.501153
27	8	0	2.842162	4.444566	-0.396043
28	1	0	2.103646	4.854910	0.079380
29	35	0	-3.818977	0.738447	-0.905938
30	7	0	-6.359222	-0.271374	-0.290929
31	6	0	-8.449994	-1.138638	0.509037
32	6	0	-7.453895	-1.079647	1.670557
33	6	0	-7.640427	-0.598504	-0.695334
34	6	0	-6.169512	-0.508728	1.023568
35	8	0	-8.097041	-0.489827	-1.821005
36	8	0	-5.146406	-0.329305	1.708984
37	1	0	-7.759557	-0.421119	2.490952
38	1	0	-7.222835	-2.054860	2.112940
39	1	0	-9.337456	-0.513030	0.652488
40	1	0	-8.804839	-2.148718	0.278040
41	1	0	-3.314236	0.383702	1.446083
42	1	0	0.956843	-2.096822	-0.258668
43	35	0	3.990579	-2.939769	-0.592326

2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.768812	1.653715	-0.634317
2	6	0	4.288174	2.340186	0.447697
3	6	0	2.962799	1.953681	0.797592
4	6	0	2.437138	0.978843	-0.021236
5	16	0	3.607602	0.529593	-1.249861
6	1	0	5.743633	1.733533	-1.097129
7	1	0	4.860567	3.086535	0.987509
8	1	0	2.421192	2.366098	1.641834
9	6	0	1.122398	0.345619	0.016129
10	6	0	0.799260	-1.002363	0.105690
11	7	0	-0.076849	1.044538	-0.073480
12	6	0	-0.604208	-1.119823	0.083525
13	6	0	-1.143372	0.155885	-0.030064
14	6	0	-2.551122	0.533894	-0.090161

15	6	0	-3.543472	0.152178	0.783312
16	16	0	-3.247825	1.429107	-1.435946
17	6	0	-4.843595	0.592073	0.401333
18	1	0	-3.337427	-0.434808	1.671002
19	6	0	-4.840808	1.302711	-0.767225
20	1	0	-5.740287	0.394914	0.978677
21	1	0	-5.676729	1.768029	-1.272473
22	6	0	-0.196267	2.501175	-0.113012
23	1	0	-0.920470	2.791712	-0.876368
24	1	0	0.773727	2.909857	-0.398569
25	6	0	-0.616945	3.092623	1.233945
26	1	0	0.078728	2.753959	2.018549
27	1	0	-1.620929	2.732691	1.499674
28	8	0	-0.584502	4.502907	1.070655
29	1	0	-0.986162	4.907108	1.853763
30	35	0	-1.564998	-2.730692	0.163915
31	35	0	2.011538	-2.428343	0.254265

8

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.171651	0.133658	0.051087
2	6	0	-3.742576	1.376519	-0.314830
3	6	0	-2.324610	1.441830	-0.448536
4	6	0	-1.680088	0.250048	-0.182292
5	16	0	-2.857794	-0.983731	0.265210
6	1	0	-4.409204	2.212015	-0.491836
7	1	0	-1.822114	2.354320	-0.743846
8	6	0	-0.280539	-0.143599	-0.220436
9	6	0	0.225676	-1.425274	-0.418490
10	7	0	0.796070	0.706810	-0.004396
11	6	0	1.623881	-1.339069	-0.315198
12	1	0	-0.351075	-2.311305	-0.640936
13	6	0	1.979851	-0.021316	-0.067468
14	6	0	3.301803	0.567833	0.132008
15	6	0	4.027046	1.385486	-0.703855
16	16	0	4.217285	0.236682	1.593314
17	6	0	5.301584	1.751600	-0.181942
18	1	0	3.666822	1.685227	-1.682106
19	6	0	5.544266	1.203538	1.048613
20	1	0	6.010643	2.382465	-0.706886
21	1	0	6.430630	1.304671	1.661041
22	6	0	0.714568	2.126918	0.311740
23	1	0	1.541163	2.380804	0.978468
24	1	0	-0.218512	2.307015	0.849805
25	6	0	0.739979	3.016716	-0.938163
26	1	0	0.196497	2.516964	-1.754515
27	1	0	1.776344	3.168928	-1.270702
28	8	0	0.122317	4.243963	-0.570638
29	1	0	0.231851	4.870769	-1.301471
30	35	0	2.836875	-2.767876	-0.513491
31	35	0	-5.948620	-0.425490	0.326321

NBS

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.912490	-1.190560	0.000002
2	6	0	-2.380765	-0.769869	-0.000523
3	1	0	-2.863626	-1.203827	-0.881396
4	1	0	-2.864871	-1.205163	0.878988
5	6	0	-2.380697	0.770062	0.000533
6	1	0	-2.863484	1.203998	0.881477
7	1	0	-2.864833	1.205494	-0.878888

8	6	0	-0.912408	1.190595	-0.000017
9	7	0	-0.166390	-0.000044	0.000119
10	8	0	-0.455664	2.306266	-0.000291
11	8	0	-0.455932	-2.306319	0.000157
12	35	0	1.698071	-0.000032	0.000002

NHS

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.178322	-0.214699	0.000099
2	6	0	-0.769650	1.259669	-0.000113
3	1	0	-1.205720	1.743632	-0.879503
4	1	0	-1.205928	1.743864	0.879038
5	6	0	0.769683	1.259684	0.000206
6	1	0	1.205775	1.743695	0.879582
7	1	0	1.205982	1.743880	-0.878929
8	6	0	1.178326	-0.214677	0.000005
9	7	0	-0.000020	-0.958927	0.000389
10	8	0	2.296897	-0.676912	-0.000357
11	8	0	-2.296924	-0.676859	-0.000259
12	1	0	0.000029	-1.972277	0.000839