

Electronic Supplementary Information (ESI) for

Expanding Donor-Acceptor toolbox with a minimal 5-(thiophen-2-yl)-1,3-thiazole core: Transition metal-free synthesis and molecular design for HOMO-LUMO energy modulations

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Table of Contents

Experimental Section	S2
Characterization Data	S3
NMR Spectra	S5
Computational Details	S13
Coordinates of the Compounds (Optimized Geometry)	S15
References	S56

EXPERIMENTAL SECTION

General Information:

Commercially available reagents were used without further purification. NMR spectra were recorded using Bruker AV III 500 MHz FTNMR spectrometer using CDCl₃ as solvent and TMS as internal standard. Mass spectra were recorded under ESI/HRMS using ThermoScientific Exactive mass spectrometer. Melting points were determined using DSC (DSC Q20, TA Instruments). TLC was performed using silica gel 60 F254 (Merck) plates and fluorescence was visualized using UV lamp of wavelength 365nm. Column chromatography was performed using 60-120 mesh silica gel.

General procedure for the syntheses of aroylthioureas

Aroylthioureas **3a-h** were prepared by the following procedure. Aroyl chloride was added slowly to a solution of KSCN (10 mmol) in acetone, refluxed for 30 min and then cooled to room temperature. A solution of secondary amine in acetone was then added slowly and stirred for 2 h. The reaction mixture was added to crushed ice, precipitated product was filtered, dried and recrystallized from appropriate solvents.

General procedure for the syntheses of thienylthiazole **5a-h**

To a solution of 2-bromomethyl-5-nitrothiophene **4** (1mmol) in DMF (2mL), thiourea (1mmol) was added followed by triethylamine (1.2 mmol) and stirred for 30-45 min. The reaction mixture was then added slowly to crushed ice with vigorous stirring. The precipitated compound was filtered and dried. (Alternatively, extraction with DCM followed by evaporation of the solvent can be performed). The residue was subjected to silica gel column chromatography (petroleum ether-ethyl acetate, 100:1) to yield the product as red solid.

N, N-dimethyl-5-(5-nitrothiophen-2-yl)-4-phenylthiazol-2-amine (**5a**)

Yield: 202 mg (61%). Red solid, m.p. 160.8 °C. ¹H NMR (500 MHz, CDCl₃, ppm): δ= 7.61(d, *J*=4.5 Hz, 1H), 7.45-7.4 (m, 2H), 7.35-7.36 (m, 3H), 6.60 (d, *J*=4.5 Hz, 1H), 3.11 (s, 6H); ¹³C NMR (125 MHz, CDCl₃, ppm): δ=168.0, 152.1, 147.1, 143.1, 133.6, 128.3, 128.2, 128.1, 128.0, 122.4, 111.6, 39.1; HRMS (ESI) calc. C₁₅H₁₄N₃O₂S₂ [M+H]⁺: 332.0524, found: 332.0528.

4-(4-bromophenyl)-N,N-dimethyl-5-(5-nitrothiophen-2-yl)thiazol-2-amine (**5b**)

Yield: 245 mg (60%). Red solid, m.p. 163.5°C. ¹H NMR (500 MHz, CDCl₃, ppm): δ=7.64 (d, *J*= 4.5 Hz, 1H), 7.47-7.48 (m, 2H), 7.35 -7.36 (m, 2H), 6.63 (d, *J*=4.5 Hz, 1H), 3.10 (s, 6H); ¹³C NMR (125 MHz, CDCl₃, ppm): δ=168.0, 150.4, 147.5, 142.5, 132.4, 131.0, 129.8, 128.3, 122.9, 122.5, 111.5, 39.1; HRMS (ESI) calc. C₁₅H₁₃BrN₃O₂S₂. [M+H]⁺: 409.9629, found: 409.9641.

N,N-dimethyl-5-(5-nitrothiophen-2-yl)-4-(p-tolyl)thiazol-2-amine (**5c**)

Yield: 217 mg (63%). Red solid, m.p. 148.3 °C. ¹H NMR (500 MHz, CDCl₃, ppm): δ=7.62 (d, *J*=4.5 Hz, 1H), 7.34-7.35 (m, 2H), 7.15-7.19 (m, 2H), 6.61 (d, *J*=4.4 Hz, 1H), 3.10 (s, 6H), 2.33 (s, 3H); ¹³C NMR (125 MHz, CDCl₃, ppm): δ=167.9, 152.4, 146.9, 143.5, 139.0, 138.4, 130.5, 128.7, 128.3, 127.9, 122.2, 39.1, 21.6; HRMS (ESI) calc. C₁₆H₁₆N₃O₂S₂. [M+H]⁺: 346.0680, found: 346.0683.

N,N-diethyl-5-(5-nitrothiophen-2-yl)-4-phenylthiazol-2-amine (**5d**)

Yield: 215 mg (60%). Red waxy solid. ¹H NMR (500 MHz, CDCl₃, ppm): δ=7.61 (d, *J*=4.5 Hz, 1H), 7.45-7.47 (m, 2H), 7.34-7.36 (m, 3H), 6.58 (d, *J*=4.5 Hz, 1H), 3.45-3.50(m, 4H), 1.20-1.23 (m, 6H); ¹³C NMR (125 MHz, CDCl₃, ppm): δ=166.6, 152, 147.5, 143.5, 133.7, 128.3, 128.3, 128.1, 127.9, 122.2, 110.6, 44.6, 11.6; HRMS (ESI) calc. C₁₇H₁₈O₂N₃S₂. [M+H]⁺: 360.0836, found: 360.0842.

N,N-diethyl-5-(5-nitrothiophen-2-yl)-4-(p-tolyl)thiazol-2-amine (**5e**)

Yield: 238 mg (64%). waxy Red solid. ¹H NMR (500 MHz, CDCl₃, ppm): δ=7.61 (d, *J*=4.5 Hz, 1H), 7.34-7.36 (m, 2H), 7.15-7.19 (m, 2H), 6.57 (d, *J*=4.5 Hz, 1H), 3.45-3.49 (m, 4H), 2.33 (s, 3H), 1.19-1.22 (m, 6H); ¹³C NMR (125 MHz, CDCl₃, ppm): δ=166.8, 152.4, 146.5, 143.7, 138.3, 128.6, 128.3, 128.0, 127.8, 122.0, 99.0, 44.6, 20.5, 11.6; HRMS (ESI) calc. C₁₈H₂₀O₂N₃S₂. [M+H]⁺: 374.0992, found: 374.0999.

5-(5-nitrothiophen-2-yl)-4-phenyl-2-(piperidin-1-yl)thiazole (**5f**)

Yield: 241 mg (65%). Red solid, m.p. 177.8 °C. ¹H NMR (500 MHz, CDCl₃, ppm): δ=7.61 (d, *J*=4.5 Hz, 1H), 7.44-7.46 (m, 2H), 7.34-7.36 (m, 3H), 6.59 (d, *J*=4.5 Hz, 1H), 3.47-3.48 (m, 4H), 1.57-1.71 (m, 6H); ¹³C NMR (125 MHz, CDCl₃, ppm): δ=168.1, 151.9, 147.1, 143.2, 133.6, 128.3, 128.3, 128.1, 127.9, 122.4, 111.2, 48.5, 24.1, 23.0; HRMS (ESI) calc. C₁₈H₁₈O₂N₃S₂. [M+H]⁺: 372.0836, found: 372.0838.

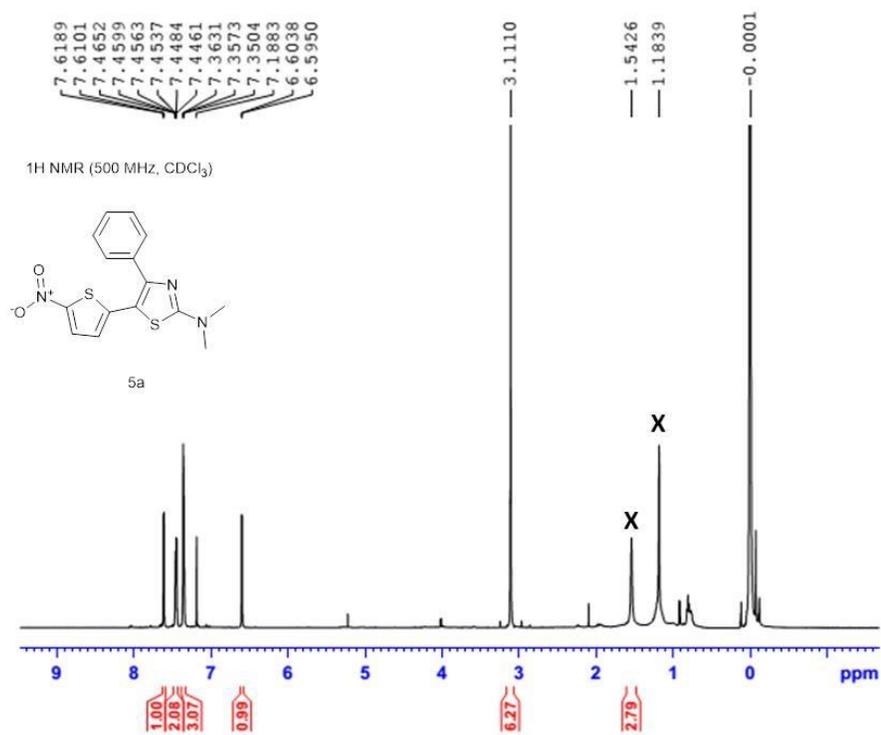
5-(5-nitrothiophen-2-yl)-2-(piperidin-1-yl)-4-(p-tolyl)thiazole (**5g**)

Yield: 223 mg (58%). Red solid, m.p. 119 °C. ¹H NMR (500 MHz, CDCl₃, ppm): δ=7.67 (d, *J*=4.5 Hz, 1H), 7.40-7.42 (m, 2H), 7.22-7.26 (m, 2H), 6.67 (d, *J*=4.5 Hz, 1H), 3.54-3.55 (m, 4H), 2.40 (s, 3H), 1.69-1.73 (m, 6H); ¹³C NMR (125 MHz, CDCl₃, ppm): δ=169.0, 153.2, 147.6, 144.6, 139.4, 131.6, 129.7, 129.3, 129.0, 123.3, 112.0, 49.5, 25.2, 24.00, 21.5; HRMS (ESI) calc. C₁₉H₂₀O₂N₃S₂. [M+H]⁺: 386.0992, found: 386.0993.

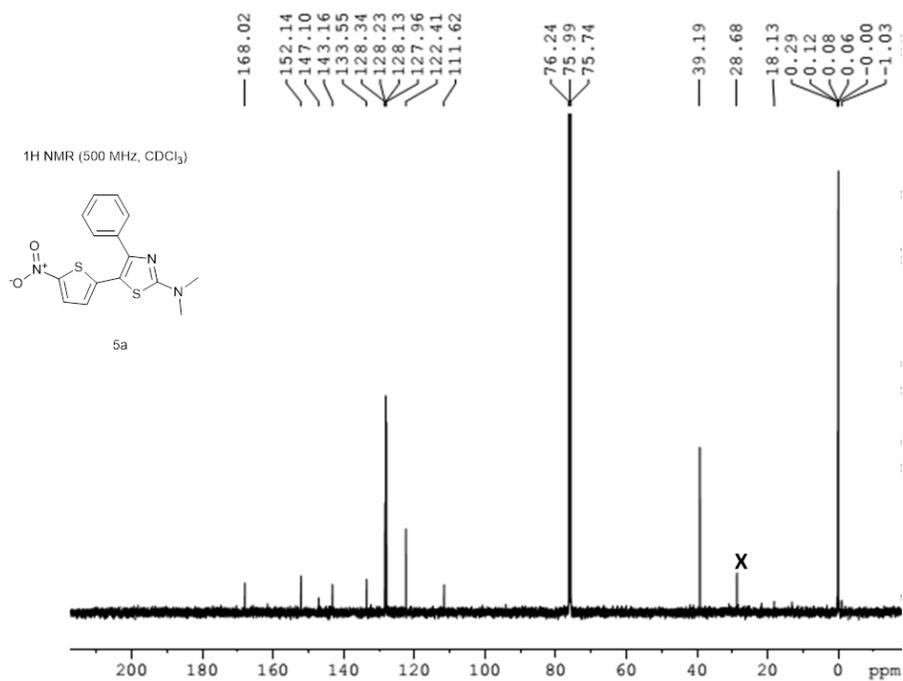
4-(furan-2-yl)-5-(5-nitrothiophen-2-yl)-N,N-diphenylthiazol-2-amine (**5h**)

Yield: 227 mg (51%). Red solid, m.p. 154.5 °C. ¹H NMR (500 MHz, CDCl₃, ppm): δ=7.71 (d, *J*=4.5 Hz, 1H), 7.33-7.40 (m, 10H), 7.21-7.24 (m, 1H), 6.97 (d, *J*=4.5 Hz, 1H), 6.74 (d, *J*=3.5 Hz, 1H), 6.42-6.43 (m, 1H); ¹³C NMR (125 MHz, CDCl₃, ppm): δ=167.4, 149.0, 144.1, 142.8, 141.7, 140.2, 129.8, 128.8, 126.8, 126.3, 126.0, 114.1, 111.9, 111.8; HRMS (ESI) calc. C₂₃H₁₆O₃N₃S₂. [M+H]⁺: 446.0629, found: 446.0630

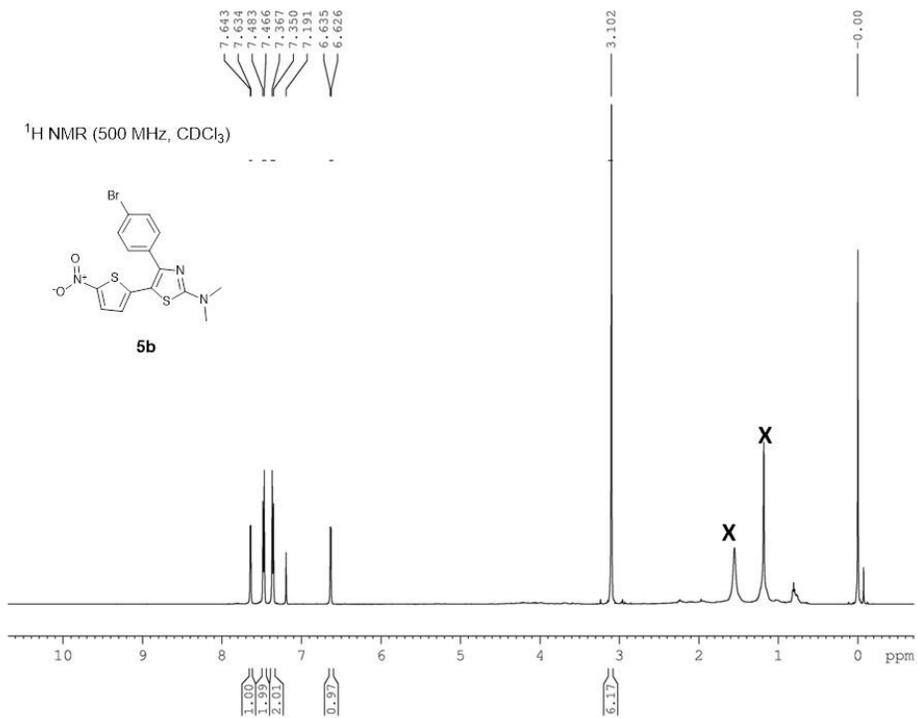
NMR Spectra of 5a-h



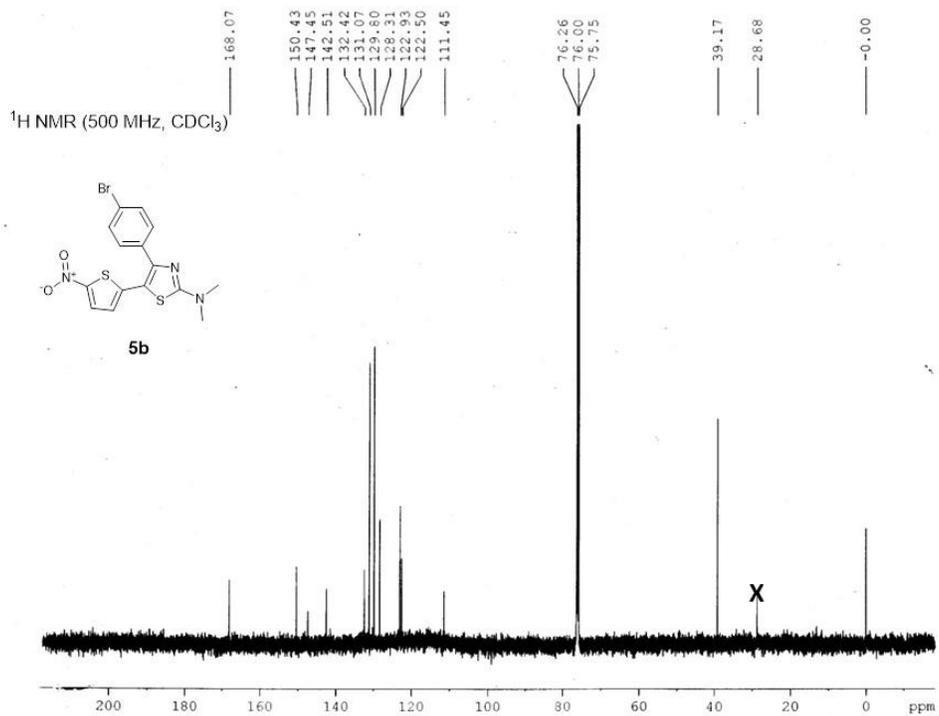
¹H NMR spectrum of 5a



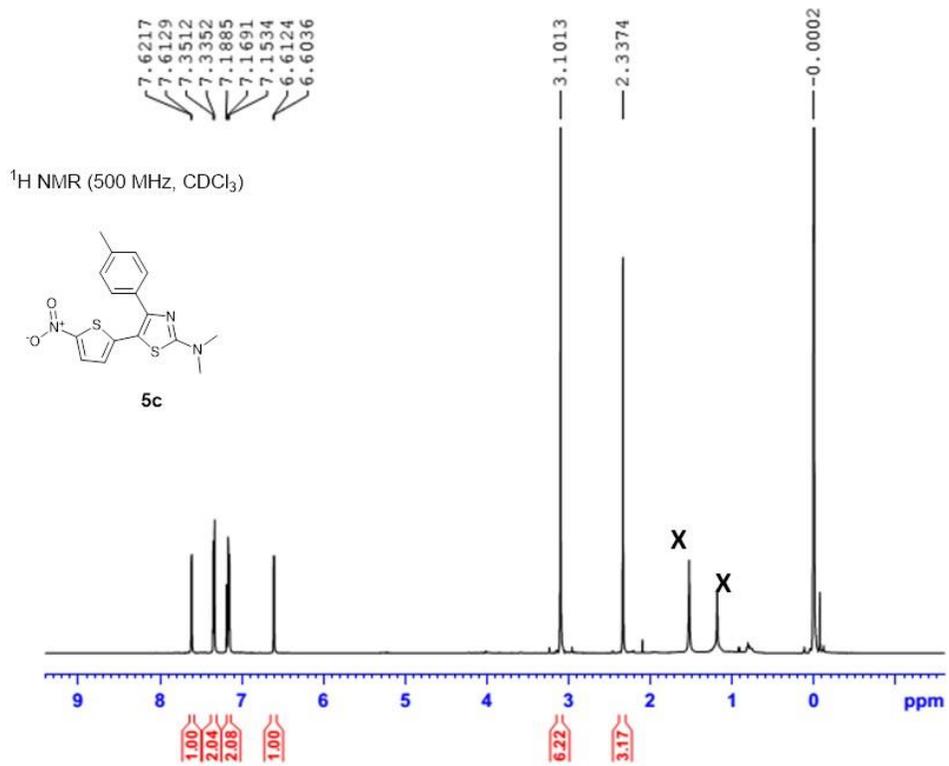
¹³C NMR spectrum of 5a



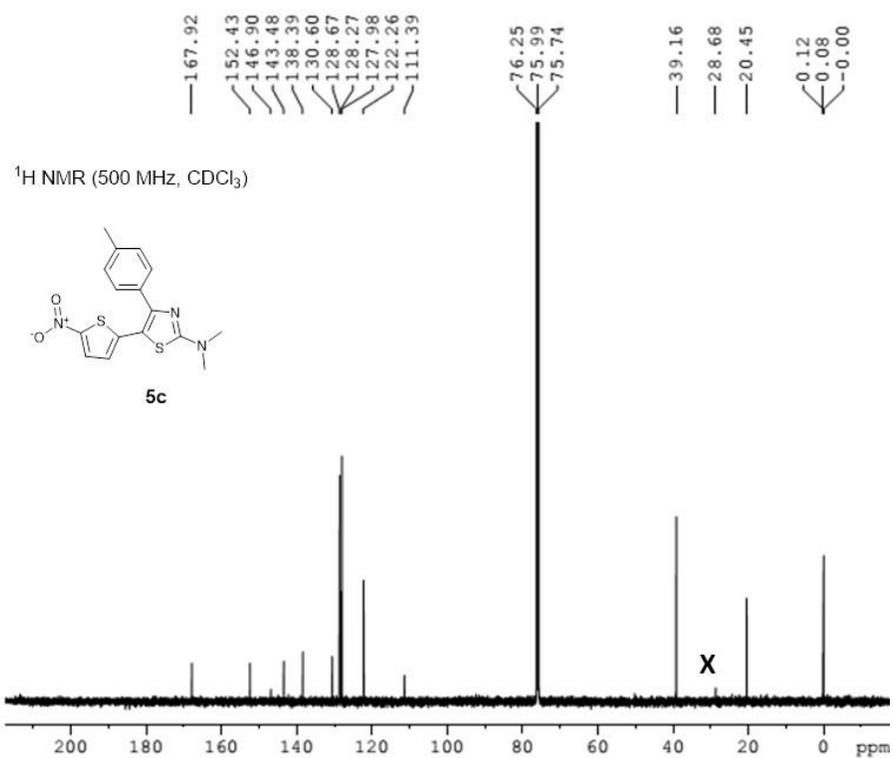
¹H NMR spectrum of **5b**



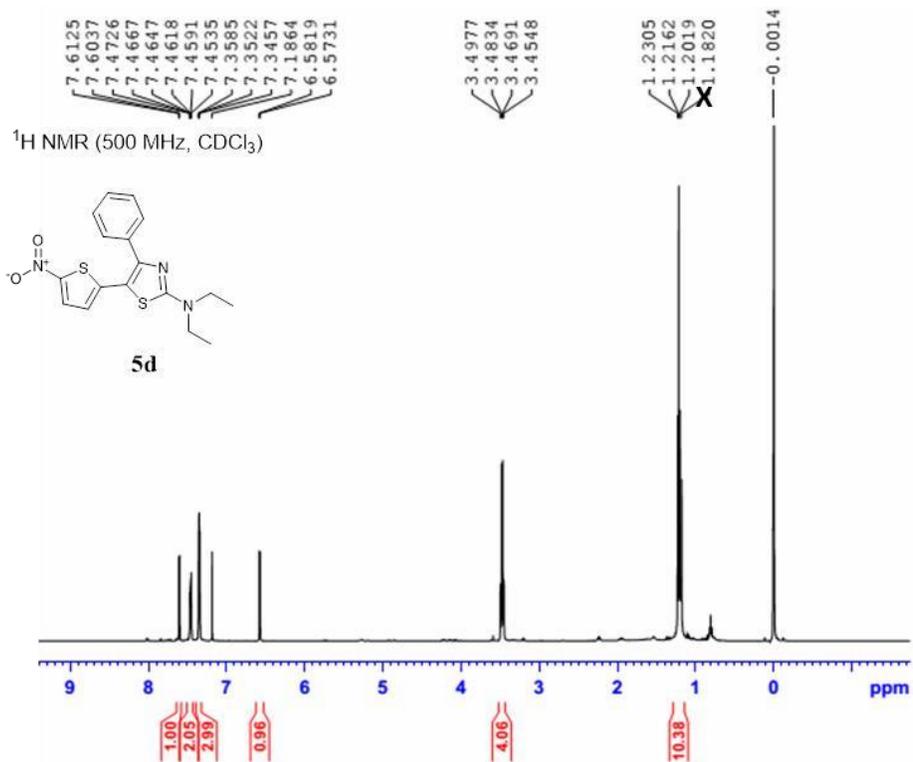
¹³C NMR spectrum of **5b**



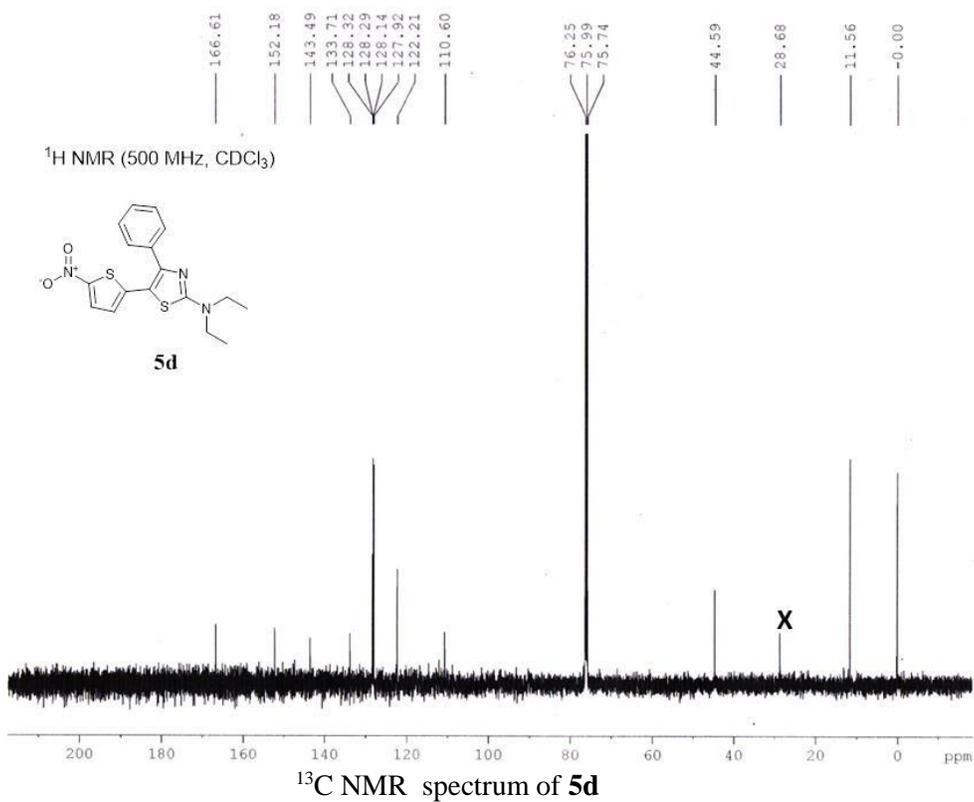
¹H NMR spectrum of **5c**



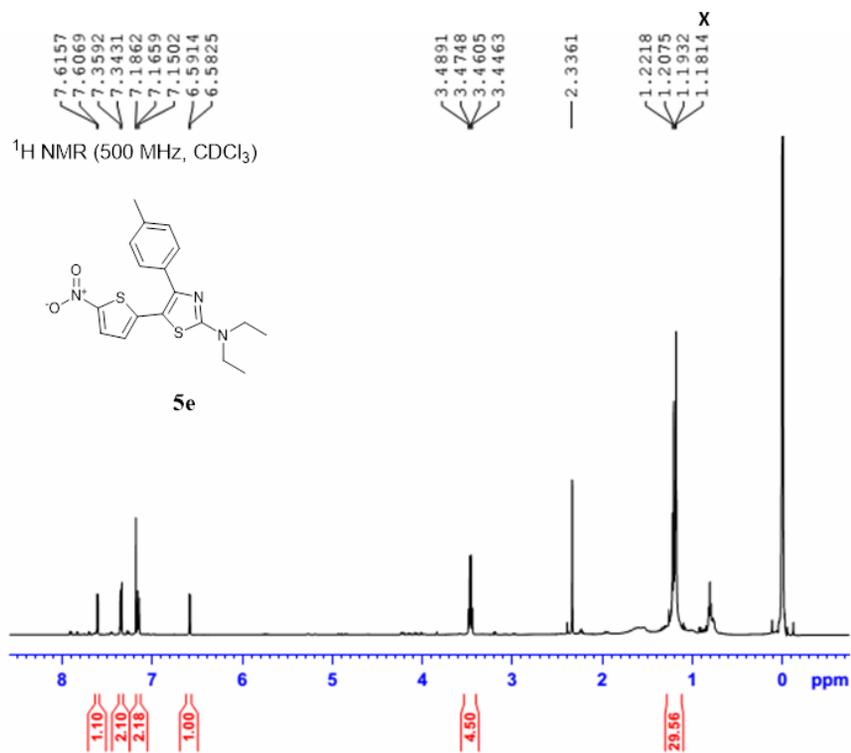
¹³C NMR spectrum of **5c**



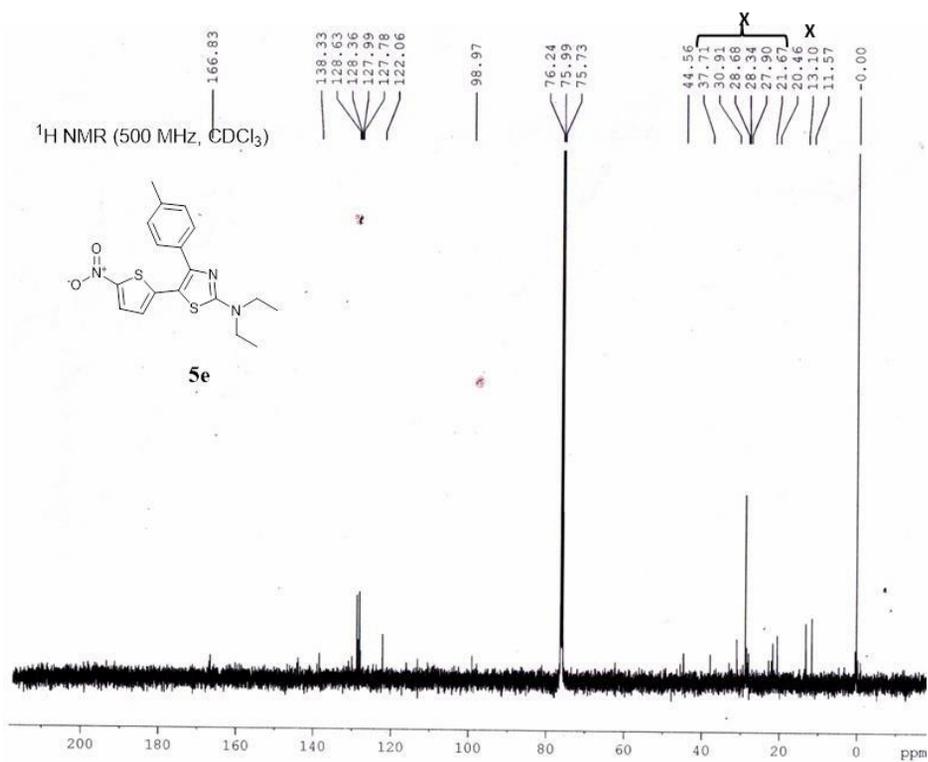
¹H NMR spectrum of **5d**



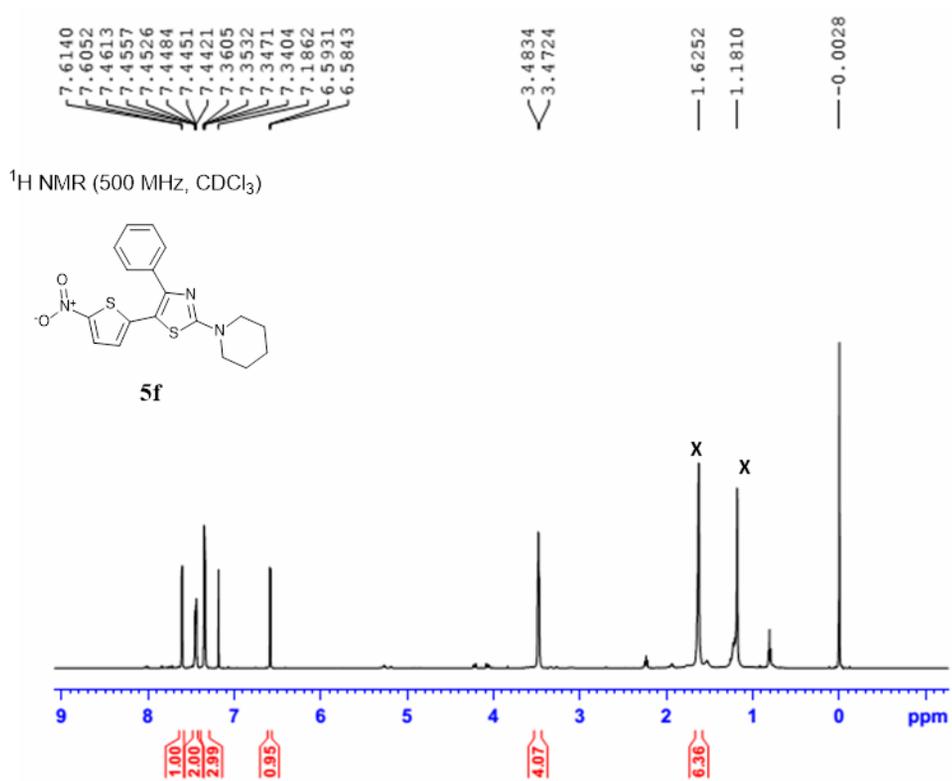
¹³C NMR spectrum of **5d**



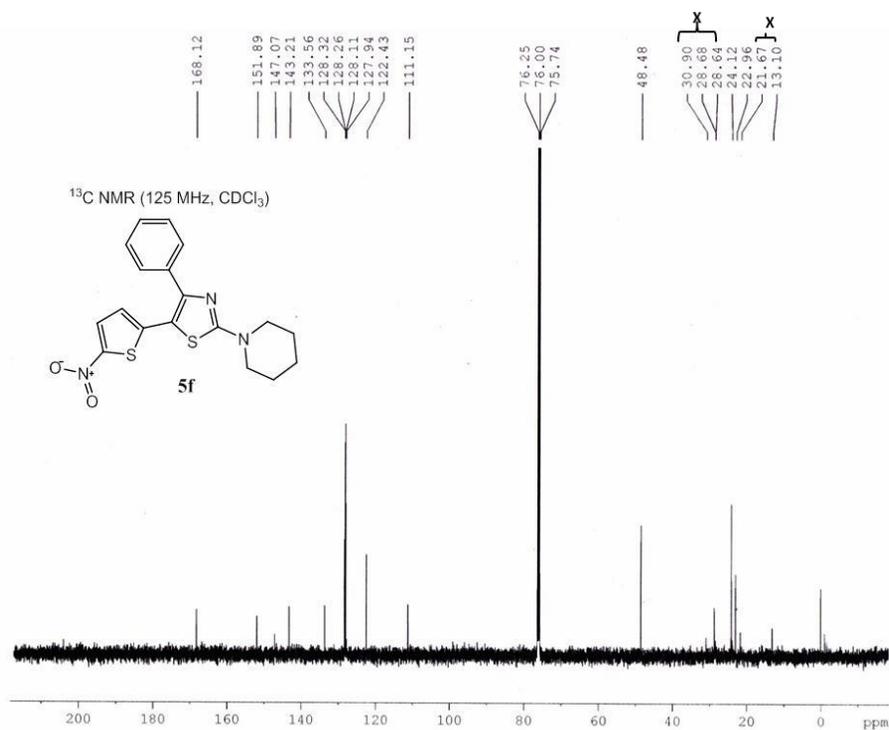
¹H NMR spectrum of **5e**



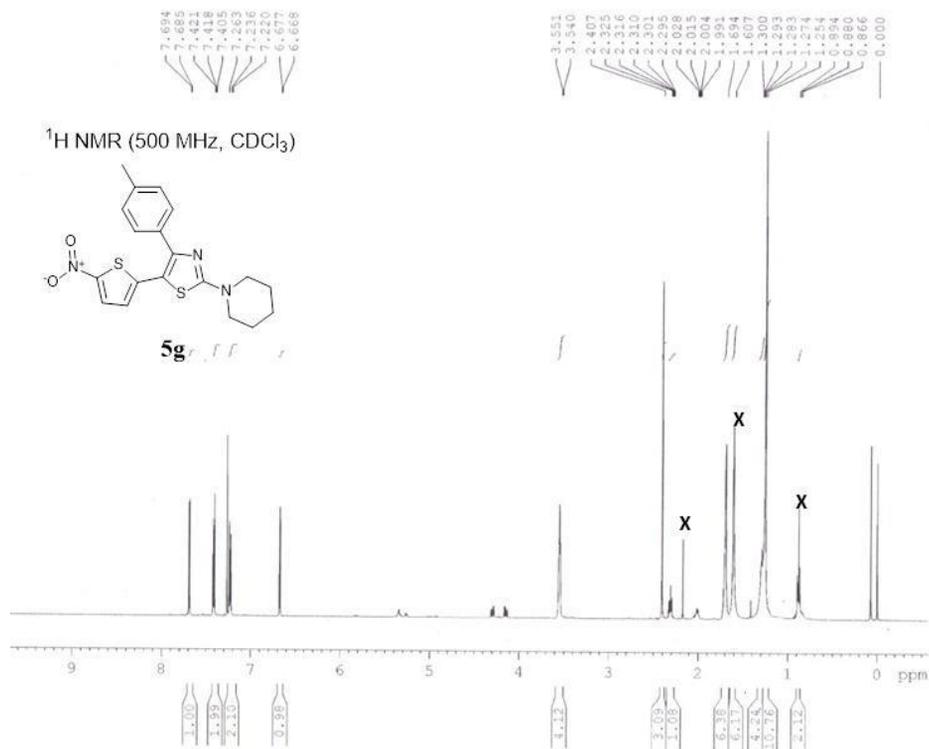
¹³C NMR spectrum of **5e**



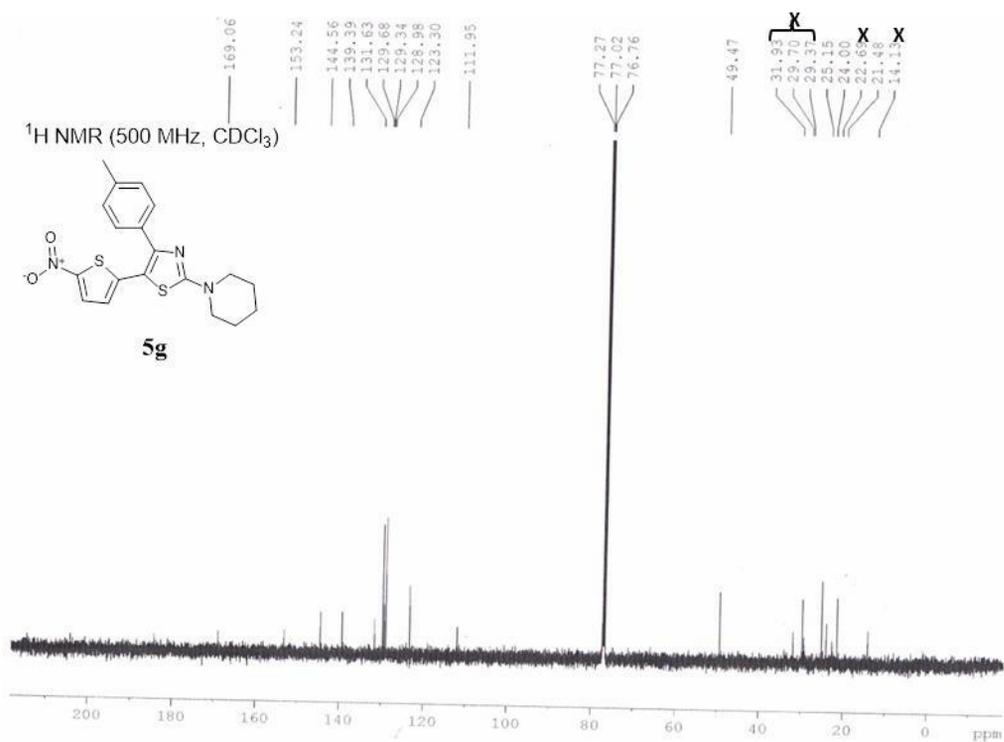
¹H NMR spectrum of **5f**



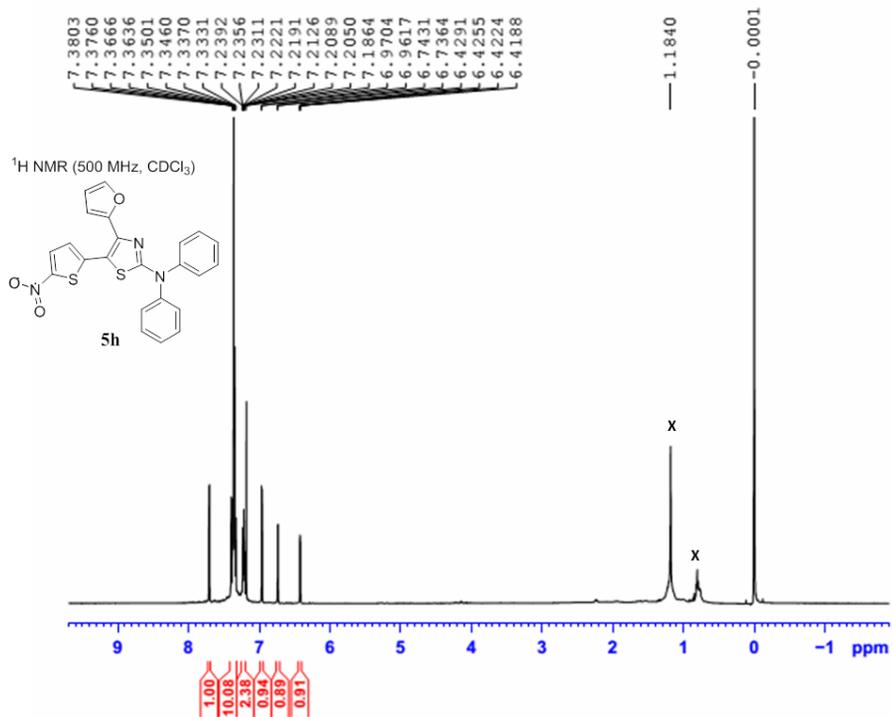
¹³C NMR spectrum of **5f**



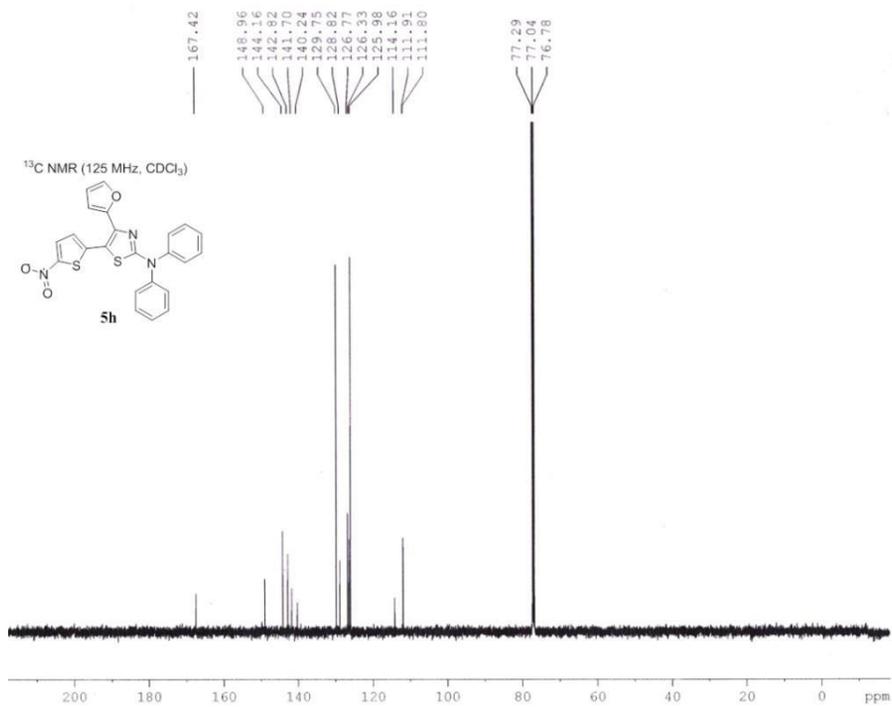
¹H NMR spectrum of **5g**



¹³C NMR spectrum of **5g**



¹H NMR spectrum of **5h**



¹³C NMR spectrum of **5h**

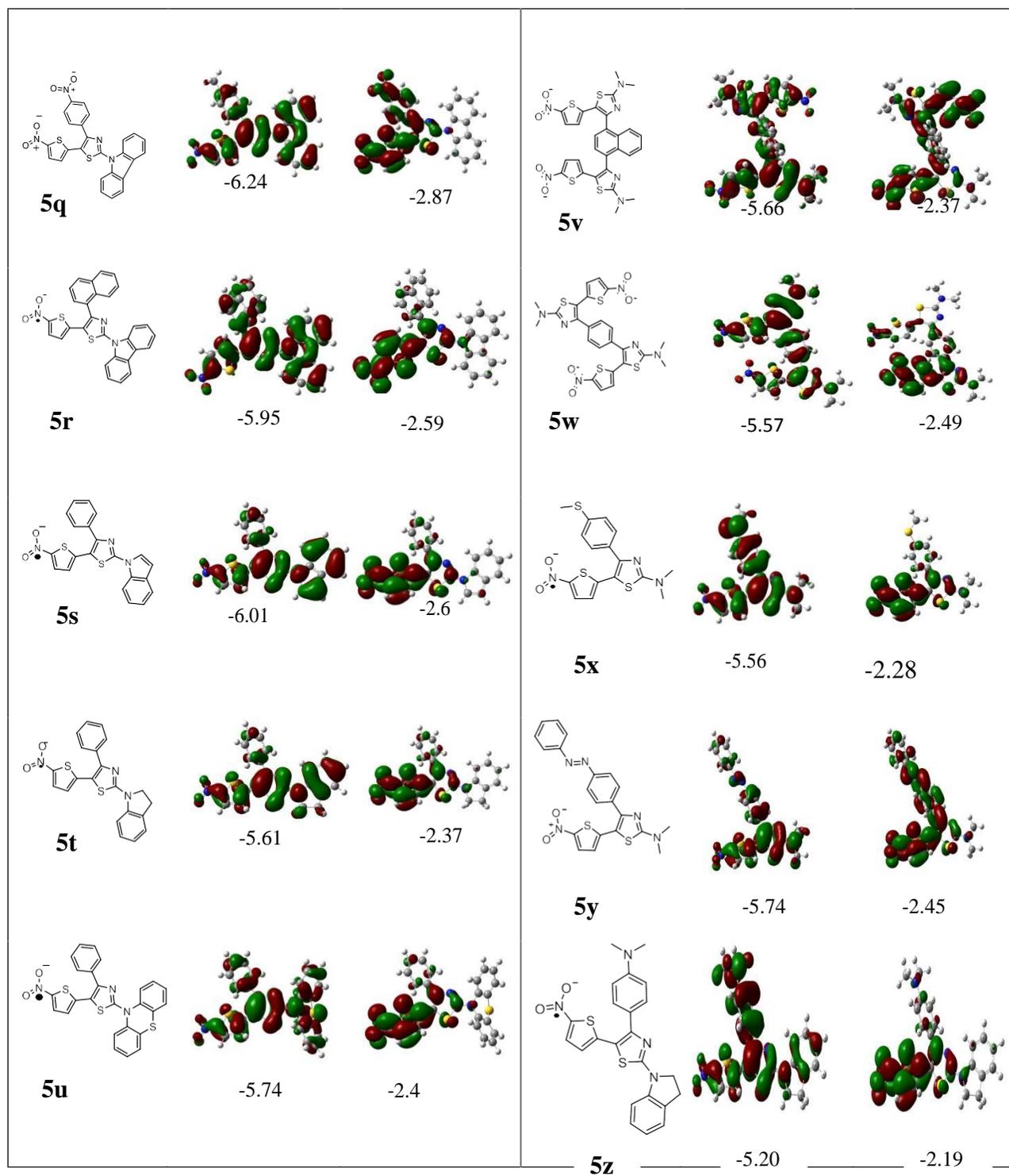
Computational Details

In order to better understand the observed properties, we performed DFT and TD-DFT calculations with Gaussian 09 package.¹ Solvent effects were taken in to consideration using polarizable continuum model. Geometry of the selected molecules were optimized using PBE0/6-31G(d,p) level and subsequent vibrational frequency calculations confirmed that the molecules were minimum in the potential energy surface. For predicting the absorption spectrum, TD-DFT calculations were performed using the same level of theory. The maximum absorption was more precisely described with TD-PBE0 compared to other functionals (results will be reported elsewhere). The frontier molecular orbital analysis confirmed the intramolecular charge transfer. The HOMO of the molecule is delocalized on whole of the molecule and LUMO is predominantly localized on the nitro acceptor suggesting an ICT from donor to acceptor.

Table 1. HOMO-LUMO energy and TD-DFT predicted absorption wavelength of compounds 5i-z

Sl. No	Compound	HOMO (eV)	LUMO (eV)	Band gap (eV)	Excitation energy (nm)	
					Gas	THF
1	5i	-5.95	-2.56	3.39	435.47	467.44
2	5j	-6.04	-2.65	3.39	436.45	462.18
3	5k	-5.89	-2.53	3.36	439.90	468.02
4	5l	-5.38	-2.39	2.99	510.61	567.07
5	5m	-5.16	-2.11	3.05	496.85	553.02
6	5n	-5.18	-2.24	2.94	514.96	554.99
7	5o	-5.63	-2.34	3.29	455.19	494.49
8	5p	-5.27	-2.26	3.01	488.29	530.34
9	5q	-6.24	-2.87	3.37	439.14	464.12
10	5r	-5.95	-2.59	3.36	435.96	463.64
11	5s	-6.01	-2.6	3.41	433.94	459.33
12	5t	-5.61	-2.37	3.24	455.98	501.80
13	5u	-5.74	-2.4	3.34	447.23	482.07
14	5v	-5.66	-2.37	3.29	445.52	479.88
15	5w	-5.57	-2.49	3.08	492.56	522.35
16	5x	-5.56	-2.28	3.28	457.61	497.88
17	5y	-5.74	-2.45	3.29	490.46	497.09
18	5z	-5.20	-2.19	3.01	501.43	557.86

Table 2. HOMO and LUMO of **5q-z**



Coordinates of **5i**

Center	Atomic	Atomic	Coordinates (Angstroms)			
Number	Number	Type	X	Y	Z	

1	16	0	-3.689706	-0.273462	-0.731792	
2	6	0	-4.745315	-1.578572	-0.346848	
3	6	0	-4.166778	-2.548298	0.427671	
4	6	0	-2.829418	-2.227291	0.727960	
5	6	0	-2.419900	-1.020099	0.186567	
6	6	0	-1.089377	-0.450630	0.249730	
7	16	0	0.282167	-1.520116	0.109849	
8	6	0	1.341374	-0.129791	0.197683	
9	7	0	0.716529	1.009024	0.297933	
10	6	0	-0.641785	0.851452	0.339331	
11	7	0	-6.093673	-1.561483	-0.810290	
12	8	0	-6.438909	-0.594948	-1.480517	
13	8	0	-6.804065	-2.510366	-0.510525	
14	7	0	2.711129	-0.226309	0.109356	
15	6	0	-1.470602	2.059129	0.510107	
16	6	0	-1.155293	3.217405	-0.209230	
17	6	0	-1.913069	4.371153	-0.050418	
18	6	0	-2.986498	4.386403	0.836865	
19	6	0	-3.295128	3.243360	1.569751	
20	6	0	-2.541648	2.086486	1.410046	

21	6	0	3.495885	-1.389846	0.222660
22	6	0	4.833256	-1.060423	-0.079455
23	6	0	4.873704	0.354030	-0.366797
24	6	0	3.563246	0.850374	-0.229779
25	6	0	5.913864	1.212354	-0.718958
26	6	0	5.632705	2.555337	-0.927356
27	6	0	4.327216	3.034999	-0.780801
28	6	0	3.273146	2.198094	-0.428839
29	6	0	3.147412	-2.685313	0.599432
30	6	0	4.152198	-3.647926	0.633228
31	6	0	5.475261	-3.337022	0.310366
32	6	0	5.823194	-2.039294	-0.039847
33	1	0	-4.703026	-3.427557	0.760456
34	1	0	-2.179422	-2.843575	1.338575
35	1	0	-0.316471	3.199592	-0.898263
36	1	0	-1.665067	5.261471	-0.620714
37	1	0	-3.577170	5.289044	0.961972
38	1	0	-4.120952	3.254229	2.274720
39	1	0	-2.770665	1.202652	1.997935
40	1	0	6.925892	0.833193	-0.826635
41	1	0	6.430382	3.239392	-1.200027
42	1	0	4.125544	4.090494	-0.937496
43	1	0	2.269014	2.573532	-0.292936
44	1	0	2.140916	-2.958970	0.889170
45	1	0	3.894537	-4.661366	0.925089

46	1	0	6.234363	-4.112098	0.344369
47	1	0	6.852743	-1.785303	-0.274195

E(RPBE1PBE) = -2070.97108191 a.u.

Coordinates of **5j**

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	16	0	-2.617845	2.106782	0.859173
2	6	0	-3.241533	3.618885	0.322101
3	6	0	-2.448984	4.248984	-0.599323
4	6	0	-1.303185	3.483913	-0.891205
5	6	0	-1.251255	2.287893	-0.196106
6	6	0	-0.175088	1.317158	-0.218893
7	16	0	1.469964	1.895994	-0.197705
8	6	0	2.026966	0.236723	-0.162343
9	7	0	1.066729	-0.644337	-0.146732
10	6	0	-0.170254	-0.061735	-0.189048
11	7	0	-4.489990	4.091406	0.826395
12	8	0	-5.066675	3.377231	1.638131
13	8	0	-4.888979	5.171603	0.416727
14	7	0	3.357645	-0.105682	-0.105700
15	6	0	-1.345128	-0.949796	-0.237759

16	6	0	-1.364813	-2.110322	0.543766
17	6	0	-2.449051	-2.976520	0.504635
18	6	0	-3.520005	-2.686098	-0.334285
19	6	0	-3.515972	-1.548724	-1.134723
20	6	0	-2.427954	-0.687266	-1.083804
21	6	0	4.468657	0.738671	-0.300965
22	6	0	5.641007	0.011003	-0.011150
23	6	0	5.239005	-1.326890	0.353386
24	6	0	3.834607	-1.382944	0.274226
25	6	0	5.965610	-2.455550	0.727817
26	6	0	5.280983	-3.627824	1.015829
27	6	0	3.886264	-3.671189	0.925343
28	6	0	3.139826	-2.557573	0.553148
29	6	0	4.540350	2.060054	-0.737816
30	6	0	5.798696	2.645463	-0.845500
31	6	0	6.963742	1.939680	-0.537022
32	6	0	6.890144	0.615660	-0.125535
33	1	0	-2.708195	5.204301	-1.037025
34	1	0	-0.540341	3.778800	-1.602722
35	1	0	-0.522281	-2.326926	1.192865
36	1	0	-2.466801	-3.870254	1.118453
37	1	0	-4.351082	-1.346278	-1.795908
38	1	0	-2.412193	0.189141	-1.724255
39	1	0	7.049059	-2.414837	0.790773
40	1	0	5.829884	-4.517943	1.307214

41	1	0	3.365624	-4.598790	1.143865
42	1	0	2.064040	-2.598661	0.462937
43	1	0	3.666447	2.633258	-1.019276
44	1	0	5.867820	3.674375	-1.184814
45	1	0	7.929314	2.426664	-0.629793
46	1	0	7.791883	0.053864	0.099348
47	35	0	-4.996239	-3.859469	-0.395725

E(RPBE1PBE)= -4641.7494261 a.u.

Coordinates of **5k**

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	16	0	-3.511214	-0.757691	-0.758158
2	6	0	-4.460676	-2.135357	-0.349562
3	6	0	-3.810170	-3.039001	0.447591
4	6	0	-2.504629	-2.605618	0.745462
5	6	0	-2.189615	-1.380997	0.179679
6	6	0	-0.908402	-0.708101	0.234046
7	16	0	0.542553	-1.673505	0.142957
8	6	0	1.491002	-0.203674	0.185850
9	7	0	0.780074	0.886496	0.240874
10	6	0	-0.563093	0.627457	0.279482

11	7	0	-5.803839	-2.235734	-0.816029
12	8	0	-6.223497	-1.313435	-1.506205
13	8	0	-6.437246	-3.232579	-0.499122
14	7	0	2.865188	-0.197487	0.110492
15	6	0	-1.482633	1.772264	0.399357
16	6	0	-1.248277	2.930592	-0.348830
17	6	0	-2.093640	4.025976	-0.235900
18	6	0	-3.190073	4.007522	0.630768
19	6	0	-3.404295	2.855701	1.393604
20	6	0	-2.566626	1.754356	1.283445
21	6	0	3.735550	-1.293766	0.262332
22	6	0	5.046708	-0.871208	-0.039017
23	6	0	4.981513	0.533558	-0.366238
24	6	0	3.635649	0.931492	-0.252961
25	6	0	5.956499	1.458544	-0.735550
26	6	0	5.576112	2.769819	-0.984348
27	6	0	4.236564	3.152060	-0.860500
28	6	0	3.246010	2.247234	-0.492391
29	6	0	3.483830	-2.601910	0.671509
30	6	0	4.558964	-3.483231	0.739166
31	6	0	5.857452	-3.080454	0.418134
32	6	0	6.108270	-1.769671	0.035074
33	1	0	-4.276171	-3.951037	0.797427
34	1	0	-1.810659	-3.154712	1.371601
35	1	0	-0.399224	2.961705	-1.024894

36	1	0	-1.899141	4.914846	-0.830946
37	1	0	-4.236107	2.825183	2.092827
38	1	0	-2.739797	0.879746	1.903513
39	1	0	6.995356	1.154706	-0.825032
40	1	0	6.321844	3.504833	-1.271061
41	1	0	3.956291	4.184213	-1.048766
42	1	0	2.214960	2.548767	-0.375177
43	1	0	2.498675	-2.944782	0.960745
44	1	0	4.376726	-4.505333	1.056559
45	1	0	6.673315	-3.793749	0.479216
46	1	0	7.117516	-1.443731	-0.198502
47	6	0	-4.121883	5.181337	0.727463
48	1	0	-3.620433	6.114561	0.457124
49	1	0	-4.974823	5.059068	0.049333
50	1	0	-4.524423	5.290487	1.738525

E(RPBE1PBE) = -2110.2435252 a.u.

Coordinates of **51**

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	16	0	-2.997347	-1.620988	-0.804940
2	6	0	-3.672561	-3.169264	-0.460827

3	6	0	-2.862810	-3.967958	0.302492
4	6	0	-1.660818	-3.312509	0.625010
5	6	0	-1.577464	-2.027244	0.111187
6	6	0	-0.437229	-1.141427	0.191378
7	16	0	1.161910	-1.842921	0.154233
8	6	0	1.837099	-0.229718	0.175175
9	7	0	0.950538	0.722887	0.189684
10	6	0	-0.331187	0.237484	0.214805
11	7	0	-4.975380	-3.495387	-0.932058
12	8	0	-5.563761	-2.638037	-1.583048
13	8	0	-5.413959	-4.604712	-0.659214
14	7	0	3.193034	0.007721	0.115989
15	6	0	-1.434311	1.200031	0.310237
16	6	0	-1.398869	2.394254	-0.419646
17	6	0	-2.420922	3.322998	-0.339830
18	6	0	-3.538076	3.102519	0.495520
19	6	0	-3.553052	1.914994	1.259538
20	6	0	-2.525502	0.994210	1.162396
21	6	0	4.230685	-0.898883	0.398684
22	6	0	5.460435	-0.291350	0.070565
23	6	0	5.167175	1.038122	-0.410678
24	6	0	3.769910	1.206328	-0.357786
25	6	0	5.978759	2.074503	-0.869539
26	6	0	5.385471	3.264090	-1.267949
27	6	0	3.996384	3.417654	-1.204210

28	6	0	3.166272	2.399154	-0.748081
29	6	0	4.188847	-2.176978	0.952271
30	6	0	5.394393	-2.847216	1.136260
31	6	0	6.616466	-2.264914	0.789408
32	6	0	6.655538	-0.981102	0.262327
33	1	0	-3.150063	-4.964204	0.612973
34	1	0	-0.875799	-3.750272	1.231099
35	1	0	-0.552941	2.588659	-1.072278
36	1	0	-2.351251	4.227190	-0.932730
37	1	0	-4.367521	1.714591	1.945203
38	1	0	-2.560731	0.102214	1.781107
39	1	0	7.056762	1.949405	-0.912968
40	1	0	6.001776	4.082978	-1.626030
41	1	0	3.548885	4.358517	-1.510692
42	1	0	2.095384	2.525893	-0.673653
43	1	0	3.263605	-2.645679	1.263188
44	1	0	5.377707	-3.843753	1.566830
45	1	0	7.538599	-2.816318	0.943864
46	1	0	7.602898	-0.514585	0.008679
47	7	0	-4.564415	4.009605	0.568840
48	6	0	-5.669696	3.776007	1.466401
49	1	0	-6.398431	4.579518	1.355470
50	1	0	-6.179198	2.830867	1.239601
51	1	0	-5.354257	3.748468	2.519277
52	6	0	-4.483961	5.250576	-0.162633

53	1	0	-5.390295	5.830514	0.013841
54	1	0	-3.625000	5.861924	0.148566
55	1	0	-4.403656	5.078674	-1.243959

E(RPBE1PBE) = -2204.7899854 a.u.

Coordinates of **5m**

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	6	0	0.834792	3.576888	-0.113740
2	6	0	-0.231219	3.988454	0.642870
3	1	0	-0.323553	4.999528	1.018035
4	6	0	-1.133703	2.935663	0.868374
5	1	0	-2.040986	3.031646	1.454033
6	6	0	-0.745073	1.734281	0.288838
7	6	0	-1.513117	0.514964	0.262685
8	6	0	-1.158059	-0.816442	0.116605
9	6	0	-3.353964	-1.093174	0.019498
10	6	0	-4.555939	-3.139129	-0.396427
11	1	0	-4.657469	-3.278722	-1.481527
12	1	0	-5.394354	-3.632808	0.102961
13	1	0	-3.618999	-3.592252	-0.074063
14	6	0	-5.771120	-0.989142	-0.169983

15	1	0	-5.786184	-0.149769	0.533183
16	1	0	-6.612054	-1.641544	0.075079
17	1	0	-5.916985	-0.596504	-1.186691
18	6	0	0.201471	-1.367557	0.141431
19	6	0	1.182303	-0.903085	1.025356
20	1	0	0.939852	-0.108706	1.724947
21	6	0	2.454271	-1.446795	1.047459
22	1	0	3.175697	-1.052907	1.753254
23	6	0	2.807820	-2.502469	0.179565
24	6	0	1.809700	-2.986230	-0.694065
25	1	0	2.027865	-3.798195	-1.377600
26	6	0	0.540768	-2.435424	-0.698357
27	1	0	-0.213931	-2.830720	-1.371258
28	7	0	1.954299	4.364919	-0.489074
29	7	0	-2.195271	-1.694770	-0.048348
30	7	0	-4.545275	-1.737062	-0.032403
31	8	0	1.964892	5.539338	-0.140331
32	8	0	2.834150	3.812346	-1.143978
33	16	0	0.758976	1.914197	-0.569703
34	16	0	-3.266713	0.643847	0.241909
35	6	0	4.428356	-4.049891	-0.777655
36	1	0	4.360324	-3.679004	-1.811063
37	1	0	5.455555	-4.370407	-0.600121
38	1	0	3.786786	-4.935705	-0.692777
39	6	0	5.102374	-2.434200	0.996391

40	1	0	5.282713	-1.386047	0.717603
41	1	0	4.851904	-2.462764	2.064281
42	1	0	6.033952	-2.985247	0.862973
43	7	0	4.069585	-3.046274	0.194802

E(RPBE1PBE) = -1822.9249107 a.u.

Coordinates of **5n**

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	6	0	-2.724025	3.611578	-0.249400
2	6	0	-3.790319	3.467236	0.598662
3	1	0	-4.337829	4.312370	0.995511
4	6	0	-4.037706	2.112306	0.881037
5	1	0	-4.824758	1.764463	1.540477
6	6	0	-3.155325	1.244407	0.253260
7	6	0	-3.212987	-0.197459	0.272705
8	6	0	-2.242320	-1.175579	0.147934
9	6	0	-4.002047	-2.519787	0.141271
10	6	0	-4.023802	-4.908012	-0.175441
11	1	0	-4.062818	-5.124234	-1.251881
12	1	0	-4.492542	-5.733304	0.367717
13	1	0	-2.979888	-4.818879	0.123489

14	6	0	-6.148625	-3.647135	0.044846
15	1	0	-6.566619	-2.897405	0.724842
16	1	0	-6.543346	-4.620804	0.343099
17	1	0	-6.494839	-3.426443	-0.975207
18	6	0	-0.786254	-0.970204	0.136470
19	6	0	-0.157087	-0.044988	0.977709
20	1	0	-0.753589	0.554357	1.658644
21	6	0	1.218660	0.117646	0.962641
22	1	0	1.684624	0.846921	1.616634
23	6	0	2.018488	-0.658904	0.111381
24	6	0	1.395261	-1.609020	-0.711903
25	1	0	2.002170	-2.230187	-1.362428
26	6	0	0.018911	-1.759867	-0.694318
27	1	0	-0.452704	-2.509679	-1.321523
28	7	0	-2.174917	4.838989	-0.710962
29	7	0	-2.699040	-2.461774	0.046415
30	7	0	-4.710080	-3.674535	0.151017
31	8	0	-2.717093	5.874421	-0.346531
32	8	0	-1.196933	4.771063	-1.449351
33	16	0	-2.011069	2.115235	-0.725930
34	16	0	-4.793549	-0.963624	0.309150
35	7	0	3.413879	-0.497661	0.090433
36	6	0	4.114641	-0.165593	1.274456
37	6	0	3.816576	-0.810053	2.480759
38	6	0	5.121879	0.805383	1.249435

39	6	0	4.506750	-0.476397	3.639957
40	1	0	3.041556	-1.569979	2.500533
41	6	0	5.818834	1.118847	2.410242
42	1	0	5.351680	1.308542	0.315536
43	6	0	5.513621	0.485469	3.612337
44	1	0	4.263899	-0.984424	4.568927
45	1	0	6.597241	1.875678	2.375509
46	1	0	6.055175	0.738557	4.518589
47	6	0	4.133575	-0.647189	-1.118944
48	6	0	3.643741	-0.101646	-2.311251
49	6	0	5.352326	-1.335061	-1.132073
50	6	0	4.357275	-0.255235	-3.493981
51	1	0	2.704524	0.442531	-2.302070
52	6	0	6.067171	-1.466946	-2.316511
53	1	0	5.732632	-1.760209	-0.208501
54	6	0	5.573427	-0.933857	-3.504535
55	1	0	3.965015	0.174949	-4.411032
56	1	0	7.012061	-2.002862	-2.311070
57	1	0	6.131710	-1.044359	-4.429054

E(RPBE1PBE) = -2205.9693634

Coordinates of **5o**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.700947	3.618509	-0.082858
2	6	0	-2.738086	3.435650	0.793229
3	1	0	-3.264878	4.261587	1.253515
4	6	0	-2.985754	2.068336	1.011411
5	1	0	-3.751182	1.688965	1.678823
6	6	0	-2.131413	1.232123	0.308304
7	6	0	-2.193040	-0.210565	0.256550
8	6	0	-1.224473	-1.186277	0.108202
9	6	0	-2.987137	-2.523203	0.021029
10	6	0	-3.011148	-4.897542	-0.386639
11	1	0	-3.030075	-5.071929	-1.471093
12	1	0	-3.493820	-5.740592	0.115326
13	1	0	-1.972987	-4.825298	-0.064031
14	6	0	-5.135542	-3.636459	-0.154804
15	1	0	-5.562369	-2.913662	0.548518
16	1	0	-5.538443	-4.619846	0.096736
17	1	0	-5.463611	-3.372716	-1.170538
18	6	0	0.233850	-0.988074	0.127510
19	6	0	0.848258	-0.071521	0.989516
20	1	0	0.241228	0.509509	1.676765
21	6	0	2.226010	0.071866	1.006322

22	1	0	2.683479	0.760560	1.709681
23	6	0	3.042292	-0.689707	0.156077
24	6	0	2.423786	-1.622385	-0.689089
25	1	0	3.030807	-2.219582	-1.364111
26	6	0	1.046881	-1.777448	-0.694513
27	1	0	0.579831	-2.508749	-1.346013
28	7	0	-1.158405	4.867264	-0.496748
29	7	0	-1.682443	-2.465819	-0.050045
30	7	0	-3.698928	-3.674130	-0.026305
31	8	0	-1.680887	5.883475	-0.058437
32	8	0	-0.206332	4.833479	-1.269633
33	16	0	-1.018765	2.146596	-0.665758
34	16	0	-3.775522	-0.970693	0.234072
35	6	0	4.492303	-0.506769	0.169445
36	6	0	5.205793	0.619101	0.506815
37	16	0	5.576605	-1.790597	-0.273837
38	6	0	6.610546	0.449722	0.403259
39	1	0	4.730125	1.551826	0.788081
40	6	0	6.959287	-0.804322	-0.011611
41	1	0	7.332556	1.228976	0.618406
42	1	0	7.949630	-1.206993	-0.174385

E(RPBE1PBE) = -2240.5977447 a.u.

Coordinates of **5p**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.021089	3.635348	0.139615
2	6	0	3.977916	3.547458	-0.837002
3	1	0	4.379999	4.418037	-1.338862
4	6	0	4.324075	2.208274	-1.092082
5	1	0	5.049613	1.899509	-1.836018
6	6	0	3.621976	1.298350	-0.316027
7	6	0	3.815449	-0.133347	-0.283829
8	6	0	2.950688	-1.191134	-0.069931
9	6	0	4.826492	-2.366499	-0.135366
10	6	0	5.090888	-4.731118	0.240390
11	1	0	5.205398	-4.906341	1.318903
12	1	0	5.607810	-5.526487	-0.303598
13	1	0	4.029231	-4.750854	-0.003972
14	6	0	7.071599	-3.286317	-0.142847
15	1	0	7.375443	-2.523086	-0.867069
16	1	0	7.538401	-4.228084	-0.439354
17	1	0	7.455389	-3.001708	0.847501
18	6	0	1.483507	-1.123753	0.019811
19	6	0	0.732648	-0.255411	-0.789662
20	1	0	1.244104	0.386745	-1.500494
21	6	0	-0.647739	-0.229453	-0.714500

22	1	0	-1.235405	0.432086	-1.341176
23	6	0	-1.316682	-1.081608	0.176187
24	6	0	-0.575180	-1.960961	0.971007
25	1	0	-1.114067	-2.617698	1.646976
26	6	0	0.808134	-1.989466	0.888523
27	1	0	1.385052	-2.681656	1.492903
28	7	0	2.417504	4.831150	0.620505
29	7	0	3.532308	-2.425457	0.039465
30	7	0	5.638467	-3.450604	-0.158998
31	8	0	2.799323	5.889777	0.138979
32	8	0	1.560670	4.713699	1.490189
33	16	0	2.534633	2.107680	0.772358
34	16	0	5.455781	-0.749226	-0.393188
35	7	0	-2.714322	-1.141123	0.336692
36	7	0	-3.352850	-0.346228	-0.402851
37	6	0	-4.740652	-0.386198	-0.259543
38	6	0	-5.473610	0.487962	-1.069260
39	6	0	-5.440330	-1.223243	0.624434
40	6	0	-6.853739	0.536865	-1.012676
41	1	0	-4.925529	1.134673	-1.748037
42	6	0	-6.816224	-1.185215	0.691312
43	1	0	-4.872526	-1.899583	1.254672
44	6	0	-7.565872	-0.303835	-0.128440
45	1	0	-7.382018	1.230883	-1.655286
46	1	0	-7.323853	-1.843658	1.386694

47	7	0	-8.934001	-0.271503	-0.063327
48	6	0	-9.637150	-1.115088	0.873802
49	1	0	-10.709843	-0.949833	0.770051
50	1	0	-9.443088	-2.179430	0.687750
51	1	0	-9.360788	-0.895678	1.914133
52	6	0	-9.672839	0.656945	-0.885220
53	1	0	-10.740015	0.529893	-0.701646
54	1	0	-9.412893	1.700891	-0.662417
55	1	0	-9.493391	0.483333	-1.954310

E(RPBE1PBE) = -2163.0567725 a.u.

Coordinates of **5q**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	16	0	3.010426	-1.597791	0.944906
2	6	0	3.836009	-3.004274	0.394970
3	6	0	3.161035	-3.700502	-0.571024
4	6	0	1.939233	-3.073837	-0.888592
5	6	0	1.717572	-1.914460	-0.167786
6	6	0	0.536338	-1.072130	-0.208991
7	16	0	-1.032625	-1.827283	-0.160536
8	6	0	-1.769789	-0.238366	-0.180655

9	7	0	-0.913924	0.744334	-0.193953
10	6	0	0.379060	0.298002	-0.221802
11	7	0	5.113822	-3.336938	0.940679
12	8	0	5.565909	-2.580664	1.791418
13	8	0	5.655399	-4.348847	0.522776
14	7	0	-3.129706	-0.050869	-0.120966
15	6	0	1.449919	1.306522	-0.312808
16	6	0	1.321418	2.510414	0.392424
17	6	0	2.301355	3.487327	0.307782
18	6	0	3.406874	3.253548	-0.500410
19	6	0	3.556297	2.078052	-1.225320
20	6	0	2.571387	1.107003	-1.128771
21	6	0	-4.133895	-1.007436	-0.368718
22	6	0	-5.382300	-0.442556	-0.037742
23	6	0	-5.138847	0.910098	0.406610
24	6	0	-3.751529	1.136448	0.330911
25	6	0	-5.988770	1.922018	0.849486
26	6	0	-5.442637	3.146338	1.208776
27	6	0	-4.063070	3.358173	1.121554
28	6	0	-3.195557	2.363884	0.680783
29	6	0	-4.046796	-2.295096	-0.892958
30	6	0	-5.226415	-3.018562	-1.043377
31	6	0	-6.465858	-2.478181	-0.692245
32	6	0	-6.550524	-1.184318	-0.195521
33	1	0	3.551474	-4.604462	-1.020382

34	1	0	1.243480	-3.439794	-1.634957
35	1	0	0.446599	2.668517	1.013845
36	1	0	2.228300	4.421889	0.850945
37	1	0	4.427915	1.949144	-1.855569
38	1	0	2.660970	0.193823	-1.707763
39	1	0	-7.059650	1.752091	0.910636
40	1	0	-6.089289	3.947059	1.553810
41	1	0	-3.652998	4.325389	1.396277
42	1	0	-2.132875	2.536761	0.589158
43	1	0	-3.109401	-2.734931	-1.209557
44	1	0	-5.174713	-4.023413	-1.450952
45	1	0	-7.366602	-3.070080	-0.820147
46	1	0	-7.512617	-0.750548	0.060261
47	7	0	4.441013	4.283916	-0.601402
48	8	0	5.395024	4.055444	-1.327438
49	8	0	4.282803	5.306314	0.046307

E(RPBE1PBE) = -2275.2688431 a.u.

Coordinates of **5r**

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	16	0	-2.930792	-2.588274	-0.551001

2	6	0	-4.551893	-2.296168	-0.049510
3	6	0	-4.732710	-1.064275	0.523082
4	6	0	-3.530249	-0.336318	0.574059
5	6	0	-2.455810	-1.023262	0.034298
6	6	0	-1.079603	-0.586549	-0.060597
7	16	0	0.231450	-1.728376	0.084709
8	6	0	1.361179	-0.390334	0.025400
9	7	0	0.800375	0.778584	-0.103967
10	6	0	-0.562717	0.689183	-0.176780
11	7	0	-5.545612	-3.297262	-0.242261
12	8	0	-5.184117	-4.346950	-0.763617
13	8	0	-6.683771	-3.038727	0.122636
14	7	0	2.723618	-0.569960	0.023802
15	6	0	3.433024	-1.697700	0.474950
16	6	0	4.794854	-1.530551	0.150135
17	6	0	4.926164	-0.250050	-0.505976
18	6	0	3.644158	0.329482	-0.560301
19	6	0	6.020072	0.427836	-1.042082
20	6	0	5.817644	1.671462	-1.624125
21	6	0	4.537218	2.233324	-1.668247
22	6	0	3.430750	1.578391	-1.137284
23	6	0	2.991655	-2.820753	1.171145
24	6	0	3.932633	-3.791219	1.502182
25	6	0	5.280651	-3.648877	1.162485
26	6	0	5.719656	-2.514320	0.492706

27	1	0	-5.693563	-0.731512	0.894241
28	1	0	-3.434876	0.653805	1.001270
29	1	0	7.011769	-0.013435	-1.004862
30	1	0	6.658170	2.214758	-2.044788
31	1	0	4.397806	3.210172	-2.121587
32	1	0	2.444722	2.022430	-1.152637
33	1	0	1.961024	-2.946571	1.479766
34	1	0	3.605493	-4.673406	2.043747
35	1	0	5.988517	-4.425586	1.434200
36	1	0	6.769211	-2.389555	0.243203
37	6	0	-1.354602	1.913011	-0.424117
38	6	0	-1.240252	3.062407	0.419785
39	6	0	-2.205593	1.941269	-1.511323
40	6	0	-0.406087	3.100943	1.566067
41	6	0	-2.024156	4.217102	0.109635
42	6	0	-2.971625	3.083823	-1.811700
43	1	0	-2.273834	1.066223	-2.150759
44	6	0	-0.344155	4.223747	2.354678
45	1	0	0.199349	2.234615	1.807333
46	6	0	-1.932955	5.359378	0.943317
47	6	0	-2.881584	4.198738	-1.017408
48	1	0	-3.625791	3.076538	-2.678138
49	6	0	-1.111829	5.366038	2.042238
50	1	0	0.302943	4.233671	3.226842
51	1	0	-2.531654	6.232056	0.695194

52	1	0	-3.467463	5.086372	-1.241907
53	1	0	-1.050943	6.247151	2.674131

E(RPBE1PBE) = -2224.4393763 a.u.

Coordinates of **5s**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	16	0	0.495180	-1.960288	0.228101
2	6	0	-0.655914	-0.644588	0.269014
3	6	0	1.769115	-0.785774	0.005306
4	6	0	0.016943	0.554213	0.140939
5	6	0	-2.068317	-0.963157	0.335063
6	7	0	1.374239	0.451425	-0.023975
7	16	0	-3.228558	-0.178920	-0.690974
8	6	0	-2.657981	-1.954123	1.100926
9	6	0	-4.044662	-2.074142	0.886464
10	6	0	-4.478718	-1.173392	-0.048915
11	7	0	-5.824869	-0.995831	-0.487501
12	8	0	-6.026383	-0.122103	-1.322823
13	8	0	-6.675245	-1.728471	-0.003417
14	1	0	-2.098193	-2.555354	1.808351
15	1	0	-4.711694	-2.763689	1.387435

16	6	0	4.208951	-0.345286	-0.071515
17	6	0	3.514540	-2.495373	-0.236878
18	6	0	5.341847	-1.181594	-0.189254
19	6	0	4.315381	1.037650	0.059883
20	6	0	4.868207	-2.534695	-0.293738
21	1	0	2.795225	-3.299527	-0.299895
22	6	0	6.618974	-0.612236	-0.180620
23	6	0	5.596904	1.573339	0.068519
24	1	0	3.432055	1.656584	0.145976
25	1	0	5.468937	-3.426049	-0.405309
26	6	0	6.735218	0.763017	-0.051710
27	1	0	7.500404	-1.240214	-0.271170
28	1	0	5.716342	2.647953	0.168944
29	1	0	7.719540	1.221421	-0.043128
30	7	0	3.082046	-1.176515	-0.100594
31	6	0	-0.567251	1.906204	0.180880
32	6	0	-0.045427	2.901288	-0.654347
33	6	0	-1.600924	2.232713	1.066162
34	6	0	-0.568699	4.188013	-0.624989
35	1	0	0.770668	2.650864	-1.324800
36	6	0	-2.119476	3.521638	1.094911
37	1	0	-1.984187	1.478210	1.746491
38	6	0	-1.609467	4.500776	0.246018
39	1	0	-0.162250	4.949652	-1.283873
40	1	0	-2.918284	3.764383	1.789220

41 1 0 -2.016865 5.507175 0.269418

E(RPBE1PBE) = -1917.4951687 a.u.

Coordinates of **5t**

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	16	0	-5.168054	-2.321288	0.063822
2	6	0	-4.023352	-0.993357	0.087616
3	6	0	-3.815476	-3.433919	-0.046101
4	6	0	-2.739591	-1.503679	0.033117
5	6	0	-4.538685	0.356952	0.059573
6	7	0	-2.638512	-2.864160	-0.057137
7	16	0	-3.804991	1.607671	-0.898698
8	6	0	-5.700659	0.807219	0.667661
9	6	0	-5.994439	2.154102	0.387784
10	6	0	-5.051505	2.705397	-0.438754
11	7	0	-5.015369	4.053760	-0.894093
12	8	0	-4.074422	4.374890	-1.612341
13	8	0	-5.925002	4.792903	-0.542607
14	1	0	-6.302491	0.176429	1.312056
15	1	0	-6.835164	2.717590	0.771331
16	6	0	-3.080749	-5.791891	-0.042763

17	6	0	-5.395644	-5.322165	-0.073427
18	6	0	-3.724675	-7.031006	-0.120003
19	6	0	-1.698116	-5.692676	0.080270
20	6	0	-5.207017	-6.833502	-0.290373
21	1	0	-5.862538	-5.102834	0.896325
22	6	0	-2.986389	-8.200831	-0.068188
23	6	0	-0.971383	-6.882314	0.132898
24	1	0	-1.220625	-4.723275	0.134399
25	1	0	-5.796761	-7.417845	0.421528
26	6	0	-1.598221	-8.123623	0.062212
27	1	0	-3.482042	-9.166083	-0.127443
28	1	0	0.108815	-6.831434	0.233678
29	1	0	-1.007693	-9.033372	0.107254
30	7	0	-4.040139	-4.766231	-0.099533
31	6	0	-1.484716	-0.730731	0.083246
32	6	0	-0.411472	-1.113807	-0.729752
33	6	0	-1.322678	0.346263	0.961845
34	6	0	0.787508	-0.412931	-0.686749
35	1	0	-0.532899	-1.964026	-1.393568
36	6	0	-0.120805	1.042790	1.005240
37	1	0	-2.136777	0.624712	1.624221
38	6	0	0.934851	0.669456	0.177341
39	1	0	1.610262	-0.712768	-1.329229
40	1	0	-0.005783	1.874598	1.693747
41	1	0	1.872733	1.216003	0.211375

42	1	0	-6.006199	-4.856803	-0.854694
43	1	0	-5.526338	-7.129737	-1.296089

E(RPBE1PBE) = - 1918.7059439 a.u.

Coordinates of **5u**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	16	0	-3.532779	-0.199780	-1.157429
2	6	0	-4.623335	-1.520149	-0.970724
3	6	0	-4.134456	-2.533095	-0.189067
4	6	0	-2.843273	-2.232697	0.283846
5	6	0	-2.377468	-0.997005	-0.134894
6	6	0	-1.065411	-0.436426	0.113715
7	16	0	0.322894	-1.500554	0.009977
8	6	0	1.354683	-0.115071	0.301058
9	7	0	0.722056	1.010304	0.462401
10	6	0	-0.636213	0.849926	0.369253
11	7	0	-5.908643	-1.474444	-1.583845
12	8	0	-6.180972	-0.470466	-2.232864
13	8	0	-6.644446	-2.438393	-1.423489
14	6	0	-1.474860	2.041395	0.590673
15	6	0	-1.024555	3.285699	0.132850

16	6	0	-1.786781	4.428681	0.340249
17	6	0	-3.000210	4.347867	1.019186
18	6	0	-3.442980	3.117928	1.499296
19	6	0	-2.685111	1.971978	1.290438
20	1	0	-4.702680	-3.428089	0.029023
21	1	0	-2.265431	-2.884153	0.929425
22	1	0	-0.070863	3.339801	-0.382477
23	1	0	-1.431684	5.386688	-0.028253
24	1	0	-3.594974	5.241908	1.181963
25	1	0	-4.378571	3.051251	2.046594
26	1	0	-3.022422	1.019855	1.688417
27	6	0	3.358841	-1.499006	0.249581
28	6	0	3.553877	0.924609	0.183545
29	6	0	4.313024	-1.741620	-0.744910
30	6	0	3.078054	-2.484722	1.196421
31	6	0	4.546841	0.924854	-0.801965
32	6	0	3.420529	2.019196	1.035823
33	6	0	4.940472	-2.984598	-0.816467
34	6	0	3.685378	-3.731593	1.102585
35	1	0	2.378506	-2.268834	1.997579
36	6	0	5.392918	2.024104	-0.939809
37	6	0	4.249890	3.123084	0.874841
38	1	0	2.646371	2.008825	1.792603
39	6	0	4.609105	-3.983947	0.091441
40	1	0	5.688495	-3.160233	-1.583455

41	1	0	3.449246	-4.499524	1.832262
42	1	0	6.170678	2.006798	-1.697097
43	6	0	5.232962	3.128480	-0.111227
44	1	0	4.130083	3.979644	1.530727
45	1	0	5.092205	-4.953615	0.022633
46	1	0	5.885881	3.987794	-0.228872
47	7	0	2.724630	-0.228903	0.298427
48	16	0	4.700970	-0.459389	-1.897115

E(RPBE1PBE) = -2468.989468 a.u.

Coordinates of **5v**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.287718	0.121037	4.072938
2	6	0	-1.810869	-0.257619	2.862075
3	6	0	-1.037881	-0.175148	1.676657
4	6	0	0.299611	0.324849	1.758651
5	6	0	0.808797	0.701682	3.027303
6	6	0	0.034698	0.602933	4.156379
7	1	0	-1.893935	0.049260	4.971230
8	1	0	-2.823352	-0.641313	2.799833
9	6	0	-1.562334	-0.561118	0.405482

10	6	0	1.088765	0.405211	0.569713
11	1	0	1.819947	1.087715	3.089980
12	1	0	0.441663	0.898496	5.118954
13	6	0	0.550510	0.006518	-0.635512
14	6	0	-0.767565	-0.471555	-0.717627
15	1	0	1.153555	0.072854	-1.535601
16	1	0	-1.170066	-0.771806	-1.680427
17	6	0	-2.940885	-1.084552	0.270797
18	6	0	-3.953549	-0.463386	-0.434114
19	7	0	-3.243417	-2.286285	0.844641
20	16	0	-5.379486	-1.489265	-0.387646
21	6	0	-4.031402	0.817533	-1.089286
22	6	0	-4.483066	-2.631578	0.598412
23	16	0	-2.856742	2.076716	-0.842060
24	6	0	-5.054225	1.245175	-1.926679
25	7	0	-5.060871	-3.763929	1.059898
26	6	0	-3.763853	3.135151	-1.860029
27	6	0	-4.902051	2.569002	-2.370107
28	1	0	-5.883957	0.608431	-2.212203
29	6	0	-4.222192	-4.781112	1.663139
30	6	0	-6.378971	-4.146223	0.614061
31	7	0	-3.286629	4.447829	-2.118316
32	1	0	-5.571368	3.099949	-3.034600
33	1	0	-3.929609	-5.546808	0.932252
34	1	0	-3.322218	-4.308582	2.054422

35	1	0	-4.768573	-5.262134	2.479408
36	1	0	-6.771039	-4.910749	1.288021
37	1	0	-7.059377	-3.289205	0.651657
38	1	0	-6.377106	-4.549475	-0.408859
39	8	0	-2.230599	4.774126	-1.584109
40	8	0	-3.960357	5.162163	-2.850001
41	6	0	2.469713	0.937174	0.594000
42	6	0	3.587350	0.255600	0.150678
43	7	0	2.670271	2.219551	1.016246
44	16	0	4.975946	1.324263	0.241703
45	6	0	3.731967	-1.113736	-0.278527
46	6	0	3.926694	2.570947	0.897177
47	16	0	4.996517	-1.566083	-1.383627
48	6	0	2.968416	-2.212246	0.089030
49	7	0	4.412837	3.781738	1.251017
50	6	0	4.484536	-3.210902	-1.320137
51	6	0	3.395843	-3.409004	-0.510299
52	1	0	2.141230	-2.142207	0.783644
53	6	0	3.478176	4.848563	1.554861
54	6	0	5.774943	4.140260	0.936135
55	7	0	5.187755	-4.201875	-2.054300
56	1	0	2.956423	-4.386672	-0.358997
57	1	0	3.290458	5.480122	0.676551
58	1	0	2.534653	4.409865	1.876476
59	1	0	3.887384	5.469139	2.357116

60	1	0	6.050456	5.022161	1.518052
61	1	0	6.458417	3.331280	1.214415
62	1	0	5.914466	4.367424	-0.130543
63	8	0	6.153774	-3.828599	-2.713832
64	8	0	4.782411	-5.354911	-1.980813

E(RPBE1PBE) = -3299.7045897 a.u.

Coordinates of **5w**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	16	0	-5.682414	-0.062962	-0.278850
2	6	0	-3.943609	0.157337	-0.173910
3	6	0	-5.423686	-1.798580	-0.319668
4	6	0	-3.334627	-1.084947	-0.214667
5	6	0	-3.417625	1.483946	0.035363
6	7	0	-6.463465	-2.661016	-0.380347
7	7	0	-4.166458	-2.164534	-0.284112
8	6	0	-1.881082	-1.325775	-0.194785
9	16	0	-1.975526	1.771404	0.963273
10	6	0	-3.999412	2.680133	-0.363888
11	6	0	-6.201053	-4.059098	-0.658445
12	6	0	-7.809205	-2.172306	-0.558541

13	6	0	-3.284650	3.818578	0.047024
14	6	0	-2.169367	3.472242	0.764872
15	7	0	-1.181160	4.354921	1.273546
16	8	0	-0.208268	3.841392	1.827566
17	8	0	-1.360746	5.555310	1.133966
18	6	0	-1.348814	-2.322646	0.630199
19	6	0	0.021944	-2.525700	0.694000
20	6	0	0.896430	-1.738301	-0.065282
21	6	0	0.357306	-0.791250	-0.944468
22	6	0	2.348801	-1.957050	0.047197
23	6	0	-1.011956	-0.588521	-1.007823
24	6	0	3.333253	-0.990090	-0.030325
25	16	0	4.901549	-1.762968	0.110242
26	6	0	3.245604	0.453413	-0.088064
27	6	0	4.086964	-3.308888	0.265663
28	7	0	2.781479	-3.240996	0.242347
29	7	0	4.786671	-4.464739	0.368536
30	6	0	2.344249	1.284367	0.555523
31	6	0	2.558057	2.651578	0.295524
32	6	0	3.632180	2.838288	-0.535374
33	16	0	4.384922	1.368636	-1.030807
34	7	0	4.155526	4.081523	-0.989118
35	8	0	3.587012	5.101537	-0.628066
36	8	0	5.143379	4.036405	-1.717404
37	6	0	4.066377	-5.678556	0.694356

38	6	0	6.210242	-4.432386	0.602732
39	1	0	-4.905105	2.718092	-0.958565
40	1	0	-6.326574	-4.287085	-1.725426
41	1	0	-5.176286	-4.288240	-0.369592
42	1	0	-6.892259	-4.679508	-0.080646
43	1	0	-8.510464	-2.971609	-0.310011
44	1	0	-8.005635	-1.335044	0.119156
45	1	0	-8.005059	-1.843981	-1.589572
46	1	0	-3.538628	4.846395	-0.178339
47	1	0	-2.023036	-2.925928	1.229982
48	1	0	0.436959	-3.291980	1.340436
49	1	0	1.016500	-0.218726	-1.588305
50	1	0	-1.418576	0.141825	-1.700773
51	1	0	1.563139	0.910216	1.205349
52	1	0	1.972586	3.465726	0.707199
53	1	0	4.583898	-6.532136	0.248112
54	1	0	3.996048	-5.834049	1.779818
55	1	0	3.058029	-5.609234	0.287335
56	1	0	6.624874	-5.420888	0.394133
57	1	0	6.692092	-3.721078	-0.076245
58	1	0	6.463915	-4.156536	1.636487

E(RPBE1PBE) = -3146.2426091 a.u.

Coordinates of **5x**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.003019	3.742000	-0.081226
2	6	0	-1.066821	3.873153	0.764279
3	1	0	-1.346407	4.820016	1.207893
4	6	0	-1.703089	2.636890	0.976878
5	1	0	-2.563384	2.500051	1.622149
6	6	0	-1.106308	1.583531	0.300206
7	6	0	-1.578541	0.219212	0.247433
8	6	0	-0.926147	-0.993964	0.126803
9	6	0	-2.995590	-1.769589	-0.013935
10	6	0	-3.686261	-4.041344	-0.418817
11	1	0	-3.710499	-4.212076	-1.503834
12	1	0	-4.411382	-4.705370	0.059610
13	1	0	-2.685234	-4.268793	-0.053608
14	6	0	-5.367206	-2.222906	-0.253666
15	1	0	-5.588599	-1.401278	0.435682
16	1	0	-6.042056	-3.047205	-0.013431
17	1	0	-5.577156	-1.885895	-1.279018
18	6	0	0.525796	-1.222807	0.194560
19	6	0	1.351299	-0.515769	1.079275
20	1	0	0.919124	0.230161	1.739029
21	6	0	2.709459	-0.773966	1.144122

22	1	0	3.330231	-0.218601	1.841560
23	6	0	3.288598	-1.754867	0.326381
24	6	0	2.468216	-2.478060	-0.544080
25	1	0	2.881420	-3.250089	-1.183391
26	6	0	1.104976	-2.216958	-0.598578
27	1	0	0.469236	-2.791277	-1.264913
28	7	0	0.891461	4.778519	-0.482493
29	7	0	-1.727984	-2.089559	-0.046912
30	7	0	-4.005958	-2.669119	-0.081490
31	8	0	0.672942	5.905791	-0.058726
32	8	0	1.811280	4.466228	-1.231663
33	16	0	0.249459	2.130302	-0.641515
34	16	0	-3.311722	-0.055176	0.178669
35	16	0	5.028392	-1.995524	0.491360
36	6	0	5.383280	-3.305397	-0.695515
37	1	0	5.142968	-2.999783	-1.716826
38	1	0	6.458723	-3.481845	-0.627880
39	1	0	4.860466	-4.231657	-0.444557

E(RPBE1PBE) = -2126.4115548 a.u.

Coordinates of **5y**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.923599	3.657437	0.094227
2	6	0	2.849094	3.576702	-0.912360
3	1	0	3.208941	4.447733	-1.444609
4	6	0	3.225317	2.242135	-1.152584
5	1	0	3.934183	1.938149	-1.914317
6	6	0	2.575679	1.330425	-0.335545
7	6	0	2.804185	-0.096626	-0.281464
8	6	0	1.962842	-1.170446	-0.058722
9	6	0	3.863289	-2.305271	-0.102516
10	6	0	4.180334	-4.659599	0.298426
11	1	0	4.296288	-4.822978	1.378534
12	1	0	4.716734	-5.447263	-0.237716
13	1	0	3.120169	-4.706186	0.051380
14	6	0	6.128824	-3.172768	-0.094508
15	1	0	6.416500	-2.413204	-0.829163
16	1	0	6.617383	-4.107662	-0.377047
17	1	0	6.503951	-2.865646	0.892296
18	6	0	0.493474	-1.134150	0.024308
19	6	0	-0.271002	-0.277529	-0.785541
20	1	0	0.230254	0.377871	-1.491148
21	6	0	-1.651719	-0.280704	-0.716006

22	1	0	-2.251052	0.370994	-1.341972
23	6	0	-2.302609	-1.151384	0.168891
24	6	0	-1.549607	-2.019126	0.963902
25	1	0	-2.077952	-2.689587	1.634578
26	6	0	-0.165367	-2.017857	0.887174
27	1	0	0.424563	-2.699829	1.490212
28	7	0	1.301462	4.846024	0.573040
29	7	0	2.569486	-2.390659	0.067227
30	7	0	4.699581	-3.370015	-0.110154
31	8	0	1.635968	5.904284	0.058277
32	8	0	0.478323	4.720493	1.473105
33	16	0	1.504633	2.130928	0.774547
34	16	0	4.457355	-0.676473	-0.374510
35	7	0	-3.701258	-1.241484	0.323285
36	7	0	-4.355433	-0.460311	-0.407972
37	6	0	-5.755536	-0.546088	-0.256817
38	6	0	-6.498330	0.319606	-1.063383
39	6	0	-6.409636	-1.418294	0.623956
40	6	0	-7.886658	0.319033	-0.995417
41	1	0	-5.960643	0.983147	-1.733620
42	6	0	-7.794076	-1.413733	0.686590
43	1	0	-5.812073	-2.080803	1.240589
44	6	0	-8.535926	-0.547469	-0.120699
45	1	0	-8.461280	0.993618	-1.622943
46	1	0	-8.305339	-2.087726	1.368095

47 1 0 -9.620646 -0.550777 -0.064249

E(RPBE1PBE) = -2029.2366038 a.u.

Coordinates of **5z**

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	16	0	1.306062	-2.346242	0.272744
2	6	0	-0.128555	-1.334029	0.276254
3	6	0	2.275237	-0.901497	0.048011
4	6	0	0.252890	-0.008051	0.143605
5	6	0	-1.417497	-1.980497	0.284360
6	7	0	1.595754	0.213534	-0.002243
7	16	0	-2.795913	-1.335015	-0.560255
8	6	0	-1.707750	-3.221674	0.836234
9	6	0	-3.024638	-3.649978	0.598808
10	6	0	-3.721386	-2.728726	-0.138412
11	7	0	-5.086567	-2.815613	-0.520563
12	8	0	-5.550940	-1.873570	-1.156627
13	8	0	-5.703900	-3.822249	-0.195224
14	1	0	-0.982404	-3.787294	1.410189
15	1	0	-3.469665	-4.571273	0.951837

16	6	0	4.550589	0.052935	-0.062689
17	6	0	4.307255	-2.293509	0.033956
18	6	0	5.843902	-0.472540	-0.151365
19	6	0	4.321704	1.424390	0.000289
20	6	0	5.785373	-1.973330	-0.248018
21	1	0	4.166402	-2.724837	1.034330
22	6	0	6.937695	0.375418	-0.172228
23	6	0	5.436542	2.262761	-0.019343
24	1	0	3.311957	1.808059	0.064210
25	1	0	6.447351	-2.470584	0.466555
26	6	0	6.730315	1.754710	-0.102645
27	1	0	7.944300	-0.028337	-0.240889
28	1	0	5.284257	3.336849	0.033945
29	1	0	7.579543	2.430849	-0.114662
30	7	0	3.621802	-1.000980	-0.041805
31	6	0	-0.633313	1.161374	0.159814
32	6	0	-0.394521	2.235727	-0.705976
33	6	0	-1.701516	1.277155	1.056574
34	6	0	-1.206902	3.355406	-0.712078
35	1	0	0.443073	2.177891	-1.394593
36	6	0	-2.519555	2.392761	1.068374
37	1	0	-1.887966	0.481974	1.772437
38	6	0	-2.299454	3.464194	0.175833
39	1	0	-0.991761	4.150680	-1.415913
40	1	0	-3.331074	2.433940	1.784883

41	1	0	3.878592	-2.988242	-0.696151
42	1	0	6.077276	-2.310702	-1.249236
43	7	0	-3.109119	4.573962	0.180661
44	6	0	-4.297974	4.588304	0.999512
45	1	0	-4.817106	5.537288	0.861067
46	1	0	-4.994316	3.777223	0.741975
47	1	0	-4.052045	4.498968	2.065003
48	6	0	-2.927593	5.596530	-0.821142
49	1	0	-3.650737	6.395391	-0.653261
50	1	0	-1.925965	6.040043	-0.762566
51	1	0	-3.071551	5.215454	-1.842908

E(RPBE1PBE) = -2052.5245857 a.u.

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