Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry

Time-dependent density functional theory (TDDFT) modelling of Pechmann dyes: from accurate absorption maximum prediction to virtual dye screening

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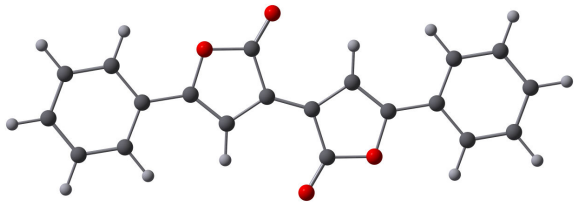
Structure plots, cartesian coordinates, SCF convergence and thermochemistry data for structures 1-12 at SMD (CH_2Cl_2)/B3LYP/DGTZVP level of theory

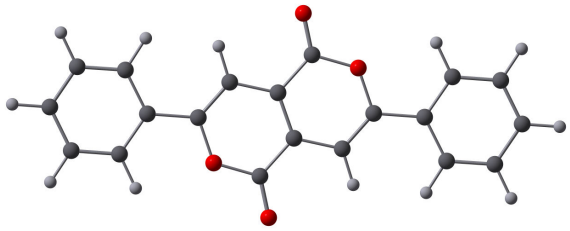
*Structure **1***



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.106403	1.598608	-0.000004
2	6	0	-0.661418	0.186390	-0.000008
3	6	0	-1.850354	-0.596711	-0.000009
4	6	0	-2.913453	0.255891	-0.000002
5	8	0	-2.495568	1.585372	0.000004
6	1	0	-1.899431	-1.671710	-0.000012
7	6	0	0.661418	-0.186389	-0.000010
8	6	0	1.106403	-1.598607	-0.000018
9	6	0	1.850354	0.596711	-0.000011
10	8	0	2.495568	-1.585372	-0.000005
11	6	0	2.913453	-0.255891	-0.000006
12	1	0	1.899431	1.671710	-0.000010
13	8	0	-0.490763	2.638005	0.000006
14	8	0	0.490763	-2.638004	-0.000003
15	6	0	4.343215	-0.029785	-0.000001
16	6	0	4.853211	1.281828	0.000000
17	6	0	5.241289	-1.111076	0.000004
18	6	0	6.221948	1.500486	0.000005
19	1	0	4.175967	2.126604	-0.000004
20	6	0	6.611809	-0.881742	0.000009
21	1	0	4.862344	-2.124167	0.000003
22	6	0	7.106897	0.420402	0.000010
23	1	0	6.603124	2.514504	0.000006
24	1	0	7.295388	-1.722305	0.000013
25	1	0	8.176095	0.595727	0.000014
26	6	0	-4.343215	0.029785	0.000002
27	6	0	-5.241289	1.111076	0.000010
28	6	0	-4.853211	-1.281828	-0.000002
29	6	0	-6.611809	0.881742	0.000013
30	1	0	-4.862344	2.124166	0.000013
31	6	0	-6.221948	-1.500487	0.000001
32	1	0	-4.175967	-2.126605	-0.000008
33	6	0	-7.106897	-0.420403	0.000009
34	1	0	-7.295388	1.722305	0.000019
35	1	0	-6.603124	-2.514504	-0.000002
36	1	0	-8.176095	-0.595728	0.000011

SCF Done: E(RB3LYP) = -1070.59391109 A.U. after 1 cycles
Convg = 0.4098D-08 -V/T = 2.0060
Zero-point correction= 0.267242 (Hartree/Particle)
Thermal correction to Energy= 0.285637
Thermal correction to Enthalpy= 0.286581
Thermal correction to Gibbs Free Energy= 0.218393
Sum of electronic and zero-point Energies= -1070.326669
Sum of electronic and thermal Energies= -1070.308275
Sum of electronic and thermal Enthalpies= -1070.307330
Sum of electronic and thermal Free Energies= -1070.375518

*Structure **2***



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.742112	1.741207	-0.000286
2	6	0	0.231441	0.651197	-0.000090
3	6	0	-0.231441	-0.651197	-0.000058
4	6	0	-1.619082	-0.948145	-0.000094
5	6	0	-2.518538	0.068693	-0.000076
6	1	0	1.938845	1.977949	-0.000049
7	6	0	1.619082	0.948145	-0.000016
8	6	0	0.742112	-1.741207	0.000103
9	1	0	-1.938845	-1.977949	-0.000055
10	6	0	2.518538	-0.068693	0.000018
11	8	0	2.072203	-1.368076	0.000036
12	8	0	-2.072203	1.368076	-0.000114
13	8	0	-0.487641	2.928304	0.000066
14	8	0	0.487641	-2.928304	-0.000081
15	6	0	-3.982030	-0.033013	-0.000010
16	6	0	-4.777449	1.124380	0.000051
17	6	0	-4.617534	-1.286837	-0.000007
18	6	0	-6.164400	1.027739	0.000113
19	1	0	-4.309597	2.098899	0.000050
20	6	0	-6.002520	-1.375296	0.000055
21	1	0	-4.035226	-2.198917	-0.000056
22	6	0	-6.783419	-0.219409	0.000116
23	1	0	-6.761523	1.931910	0.000161
24	1	0	-6.474727	-2.350445	0.000055
25	6	0	3.982030	0.033013	0.000026
26	6	0	4.777449	-1.124380	0.000012
27	6	0	4.617534	1.286837	0.000053
28	6	0	6.164400	-1.027739	0.000023
29	1	0	4.309597	-2.098899	-0.000007
30	6	0	6.002520	1.375296	0.000063
31	1	0	4.035226	2.198917	0.000069
32	6	0	6.783419	0.219409	0.000048
33	1	0	6.761523	-1.931911	0.000009
34	1	0	6.474727	2.350445	0.000085
35	1	0	7.864488	0.292545	0.000057
36	1	0	-7.864488	-0.292546	0.000163

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SCF Done:  E(RB3LYP) =  -1070.60549536     A.U. after    1 cycles
             Convg  =    0.7919D-08             -V/T =  2.0060
Zero-point correction=                           0.268441 (Hartree/Particle)
 Thermal correction to Energy=                   0.286471
 Thermal correction to Enthalpy=                 0.287415
 Thermal correction to Gibbs Free Energy=        0.220851
 Sum of electronic and zero-point Energies=          -1070.337054
 Sum of electronic and thermal Energies=             -1070.319025
 Sum of electronic and thermal Enthalpies=           -1070.318081
 Sum of electronic and thermal Free Energies=        -1070.384644
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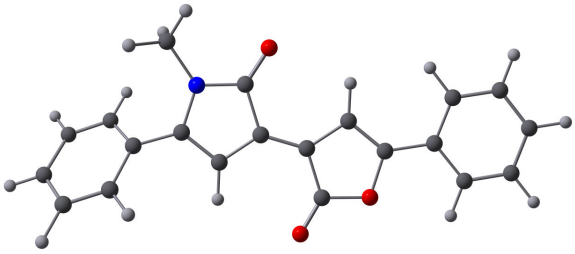
*Structure **3***

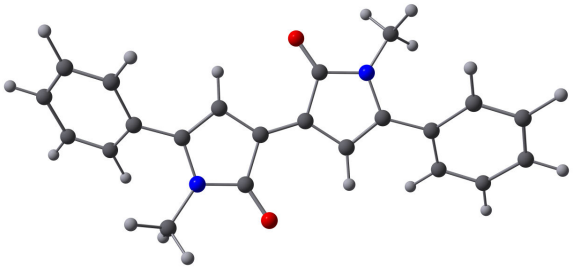


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.952942	1.574977	-0.140066
2	6	0	0.515592	0.141754	-0.079106
3	6	0	1.705504	-0.635428	-0.051889
4	6	0	2.783379	0.216079	-0.061903
5	1	0	1.761066	-1.706353	0.036710
6	6	0	-0.802343	-0.244019	-0.039648
7	6	0	-1.238006	-1.656192	0.018241
8	6	0	-2.000161	0.532185	-0.039335
9	6	0	-3.055888	-0.324075	0.015572
10	1	0	-2.051924	1.606094	-0.074705
11	8	0	0.267738	2.589476	-0.226588
12	8	0	-0.619566	-2.695519	0.036776
13	7	0	2.341196	1.550754	-0.109626
14	6	0	3.131076	2.752604	-0.353592
15	1	0	2.491040	3.475817	-0.857077
16	1	0	3.487027	3.197939	0.577540
17	1	0	3.981097	2.521764	-0.993270
18	6	0	4.193643	-0.166147	0.012669
19	6	0	5.128772	0.571079	0.757893
20	6	0	4.622309	-1.338093	-0.634212
21	6	0	6.448803	0.145318	0.852689
22	1	0	4.820283	1.460561	1.290498
23	6	0	5.944228	-1.754347	-0.541805
24	1	0	3.917605	-1.910953	-1.224030
25	6	0	6.863047	-1.014475	0.201018
26	1	0	7.154425	0.718778	1.442122
27	1	0	6.259019	-2.655063	-1.055239
28	1	0	7.894190	-1.339750	0.271752
29	6	0	-4.488279	-0.106303	0.043255
30	6	0	-5.379888	-1.189967	0.115430
31	6	0	-5.007568	1.200735	-0.000342
32	6	0	-6.751927	-0.968162	0.142091
33	1	0	-4.994654	-2.200161	0.150018
34	6	0	-6.377423	1.412363	0.026905
35	1	0	-4.335982	2.048249	-0.056615
36	6	0	-7.256113	0.329530	0.098274
37	1	0	-7.429304	-1.812030	0.197538
38	1	0	-6.764313	2.423754	-0.007664
39	1	0	-8.326038	0.499183	0.118888
40	8	0	-2.628434	-1.651408	0.052073

SCF Done: E(RB3LYP) = -1090.04400310 A.U. after 1 cycles
Convg = 0.4718D-08 -V/T = 2.0061
Zero-point correction= 0.307371 (Hartree/Particle)
Thermal correction to Energy= 0.327649
Thermal correction to Enthalpy= 0.328593
Thermal correction to Gibbs Free Energy= 0.256127
Sum of electronic and zero-point Energies= -1089.736632
Sum of electronic and thermal Energies= -1089.716354
Sum of electronic and thermal Enthalpies= -1089.715410

Sum of electronic and thermal Free Energies= -1089.787876

*Structure **4***



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.085683	-1.627732	-0.158581
2	6	0	-0.656038	-0.197517	-0.040593
3	6	0	-1.854783	0.574871	-0.015802
4	6	0	-2.926537	-0.277243	-0.081736
5	1	0	-1.912447	1.641757	0.108676
6	6	0	0.656044	0.197553	0.040409
7	6	0	1.085689	1.627771	0.158373
8	6	0	1.854788	-0.574835	0.015625
9	6	0	2.926544	0.277271	0.081646
10	1	0	1.912451	-1.641720	-0.108858
11	8	0	-0.397784	-2.641372	-0.259603
12	8	0	0.397790	2.641402	0.259483
13	7	0	-2.474483	-1.609601	-0.162557
14	7	0	2.474488	1.609626	0.162515
15	6	0	-3.251450	-2.806234	-0.460972
16	1	0	-2.596607	-3.510210	-0.972895
17	1	0	-3.625423	-3.283745	0.447194
18	1	0	-4.089464	-2.560934	-1.111250
19	6	0	3.251424	2.806253	0.461037
20	1	0	4.089388	2.560937	1.111372
21	1	0	3.625463	3.283798	-0.447085
22	1	0	2.596536	3.510206	0.972933
23	6	0	-4.341535	0.095616	-0.029064
24	6	0	-5.292524	-0.669075	0.666804
25	6	0	-4.760797	1.286592	-0.646700
26	6	0	-6.617079	-0.252288	0.741633
27	1	0	-4.994668	-1.575631	1.176459
28	6	0	-6.086324	1.695680	-0.572582
29	1	0	-4.043969	1.881418	-1.199049
30	6	0	-7.020800	0.927762	0.120577
31	1	0	-7.334647	-0.849167	1.292301
32	1	0	-6.391764	2.612703	-1.062481
33	1	0	-8.054955	1.246482	0.176121
34	6	0	4.341540	-0.095611	0.029080
35	6	0	5.292614	0.669082	-0.666670
36	6	0	4.760715	-1.286631	0.646693
37	6	0	6.617164	0.252258	-0.741403
38	1	0	4.994836	1.575669	-1.176312
39	6	0	6.086235	-1.695756	0.572671
40	1	0	4.043823	-1.881463	1.198950
41	6	0	7.020796	-0.927833	-0.120369
42	1	0	7.334796	0.849142	-1.291982
43	1	0	6.391604	-2.612812	1.062551
44	1	0	8.054946	-1.246582	-0.175840

SCF Done: E(RB3LYP) = -1109.49276409 A.U. after 1 cycles

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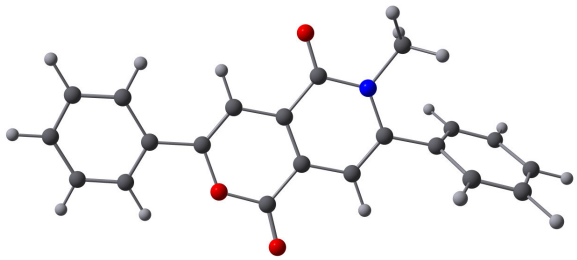
            Convg  =    0.6346D-08             -V/T =  2.0062
Zero-point correction=                          0.347613 (Hartree/Particle)
 Thermal correction to Energy=                  0.369778
 Thermal correction to Enthalpy=                0.370722
 Thermal correction to Gibbs Free Energy=       0.294439
 Sum of electronic and zero-point Energies=         -1109.145152
 Sum of electronic and thermal Energies=            -1109.122987
 Sum of electronic and thermal Enthalpies=          -1109.122042
 Sum of electronic and thermal Free Energies=       -1109.198325
```

*Structure **5***

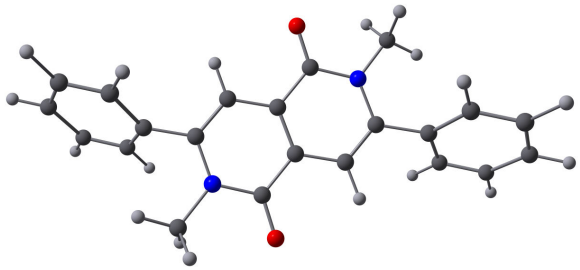


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.840927	-1.781243	-0.026872
2	6	0	-0.109210	-0.671073	-0.053936
3	6	0	0.371635	0.627055	-0.053049
4	6	0	1.770511	0.887080	-0.028047
5	6	0	2.646574	-0.145834	-0.011868
6	1	0	-1.854965	-1.949370	0.000688
7	6	0	-1.497263	-0.932828	-0.054916
8	6	0	-0.566582	1.746230	-0.076482
9	1	0	2.114695	1.908948	-0.008449
10	6	0	-2.389117	0.103600	-0.075319
11	8	0	0.561750	-2.964167	-0.019355
12	8	0	-0.212078	2.931807	-0.076479
13	7	0	-1.926450	1.411969	-0.125426
14	6	0	-2.835462	2.558601	-0.294155
15	1	0	-2.403071	3.235251	-1.028337
16	1	0	-3.802801	2.210897	-0.638181
17	1	0	-2.949423	3.102301	0.644777
18	6	0	-3.848177	-0.171611	-0.001575
19	6	0	-4.626976	0.319499	1.054857
20	6	0	-4.445894	-1.001642	-0.956810
21	6	0	-5.974141	-0.012177	1.148872
22	1	0	-4.174148	0.947304	1.813112
23	6	0	-5.796805	-1.326366	-0.863100
24	1	0	-3.853195	-1.385548	-1.778355
25	6	0	-6.563901	-0.833442	0.188833
26	1	0	-6.562499	0.365568	1.976786
27	1	0	-6.247674	-1.964283	-1.614114
28	1	0	-7.614375	-1.088915	0.263015
29	6	0	4.112262	-0.069557	0.022968
30	6	0	4.880626	-1.209630	0.306024
31	6	0	4.773893	1.145082	-0.222689
32	6	0	6.268393	-1.131895	0.350813
33	1	0	4.389786	-2.154282	0.495517
34	6	0	6.159574	1.215515	-0.176108
35	1	0	4.208483	2.036328	-0.462549
36	6	0	6.914121	0.078180	0.111636
37	1	0	6.845425	-2.021689	0.573612
38	1	0	6.653655	2.159868	-0.371649

39	1	0	7.995668	0.135849	0.144633
40	8	0	2.179037	-1.440549	-0.012539

SCF Done: E(RB3LYP) = -1090.06475538 A.U. after 1 cycles
Convg = 0.4191D-08 -V/T = 2.0061
Zero-point correction= 0.309057 (Hartree/Particle)
Thermal correction to Energy= 0.328740
Thermal correction to Enthalpy= 0.329684
Thermal correction to Gibbs Free Energy= 0.259434
Sum of electronic and zero-point Energies= -1089.755699
Sum of electronic and thermal Energies= -1089.736015
Sum of electronic and thermal Enthalpies= -1089.735071
Sum of electronic and thermal Free Energies= -1089.805321

*Structure **6***

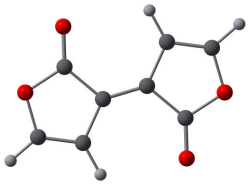


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.676352	-1.772298	-0.173870
2	6	0	0.246320	-0.646827	-0.037987
3	6	0	-0.246314	0.646857	0.037764
4	6	0	-1.642832	0.884435	0.019280
5	6	0	-2.518509	-0.155792	-0.098119
6	1	0	2.015462	-1.889780	-0.141993
7	6	0	1.642837	-0.884409	-0.019448
8	6	0	0.676361	1.772332	0.173592
9	1	0	-2.015455	1.889806	0.141837
10	6	0	2.518512	0.155812	0.098029
11	8	0	-0.305533	-2.951768	-0.254072
12	8	0	0.305531	2.951779	0.254073
13	7	0	2.036986	1.454445	0.236738
14	7	0	-2.036990	-1.454424	-0.236849
15	6	0	2.925554	2.591824	0.527085
16	1	0	2.455035	3.209607	1.289112
17	1	0	3.880689	2.226383	0.887335
18	1	0	3.076793	3.204746	-0.362823
19	6	0	-2.925597	-2.591811	-0.527042
20	1	0	-3.076702	-3.204717	0.362900
21	1	0	-3.880787	-2.226374	-0.887153
22	1	0	-2.455191	-3.209604	-1.289130
23	6	0	3.983621	-0.089259	0.033580
24	6	0	4.775074	0.500073	-0.961818
25	6	0	4.579352	-0.982303	0.931504
26	6	0	6.130790	0.203844	-1.051382
27	1	0	4.325324	1.178264	-1.677356
28	6	0	5.938515	-1.273018	0.842537
29	1	0	3.976883	-1.443073	1.705004
30	6	0	6.717695	-0.680817	-0.147478
31	1	0	6.728393	0.659499	-1.832175
32	1	0	6.386516	-1.961802	1.549120
33	1	0	7.774878	-0.908475	-0.217500
34	6	0	-3.983615	0.089261	-0.033561

35	6	0	-4.774990	-0.500105	0.961879
36	6	0	-4.579423	0.982309	-0.931431
37	6	0	-6.130704	-0.203900	1.051542
38	1	0	-4.325179	-1.178306	1.677369
39	6	0	-5.938584	1.273001	-0.842363
40	1	0	-3.977015	1.443101	-1.704965
41	6	0	-6.717686	0.680769	0.147695
42	1	0	-6.728246	-0.659580	1.832367
43	1	0	-6.386646	1.961789	-1.548904
44	1	0	-7.774867	0.908409	0.217795

SCF Done: E(RB3LYP) = -1109.52173143 A.U. after 1 cycles
Convg = 0.5341D-08 -V/T = 2.0062
Zero-point correction= 0.349743 (Hartree/Particle)
Thermal correction to Energy= 0.371089
Thermal correction to Enthalpy= 0.372033
Thermal correction to Gibbs Free Energy= 0.298084
Sum of electronic and zero-point Energies= -1109.171989
Sum of electronic and thermal Energies= -1109.150642
Sum of electronic and thermal Enthalpies= -1109.149698
Sum of electronic and thermal Free Energies= -1109.223648

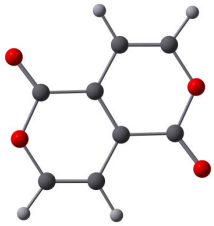
*Structure **7***



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.763306	-0.830813	0.000072
2	6	0	-0.659794	0.170253	0.000010
3	6	0	-1.301910	1.456259	-0.000151
4	6	0	-2.627616	1.230738	-0.000365
5	8	0	-2.957021	-0.113864	-0.000332
6	1	0	-0.820541	2.419021	-0.000177
7	6	0	0.659792	-0.170253	0.000140
8	6	0	1.763306	0.830813	0.000158
9	6	0	1.301908	-1.456259	0.000322
10	8	0	2.957022	0.113863	0.000136
11	6	0	2.627615	-1.230739	0.000298
12	1	0	0.820539	-2.419021	0.000403
13	8	0	-1.753628	-2.036288	-0.000034
14	8	0	1.753631	2.036289	-0.000132
15	1	0	3.468432	-1.906555	0.000354
16	1	0	-3.468434	1.906554	-0.000587

SCF Done: E(RB3LYP) = -608.317918470 A.U. after 1 cycles
Convg = 0.4304D-08 -V/T = 2.005
Zero-point correction= 0.105641 (Hartree/Particle)
Thermal correction to Energy= 0.114613
Thermal correction to Enthalpy= 0.115557
Thermal correction to Gibbs Free Energy= 0.070690
Sum of electronic and zero-point Energies= -608.212277
Sum of electronic and thermal Energies= -608.203306
Sum of electronic and thermal Enthalpies= -608.202362
Sum of electronic and thermal Free Energies= -608.247229

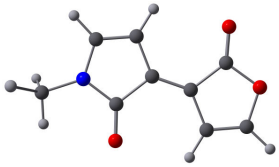
*Structure **8***



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.792936	0.638219	-0.000145
2	6	0	0.328081	0.606623	-0.000017
3	6	0	-0.328080	-0.606625	0.000044
4	6	0	0.405268	-1.832715	0.000036
5	6	0	1.746350	-1.771717	0.000031
6	1	0	0.101953	2.785655	-0.000083
7	6	0	-0.405267	1.832714	-0.000022
8	6	0	-1.792936	-0.638220	0.000184
9	1	0	-0.101950	-2.785656	0.000095
10	6	0	-1.746349	1.771717	-0.000038
11	8	0	-2.428674	0.591228	0.000017
12	8	0	2.428674	-0.591227	-0.000023
13	8	0	2.481780	1.636640	0.000040
14	8	0	-2.481783	-1.636639	-0.000087
15	1	0	2.417387	-2.618633	0.000073
16	1	0	-2.417386	2.618634	-0.000101

SCF Done: E(RB3LYP) = -608.340675802 A.U. after 1 cycles
Convg = 0.1660D-08 -V/T = 2.0058
Zero-point correction= 0.107163 (Hartree/Particle)
Thermal correction to Energy= 0.115649
Thermal correction to Enthalpy= 0.116593
Thermal correction to Gibbs Free Energy= 0.073175
Sum of electronic and zero-point Energies= -608.233513
Sum of electronic and thermal Energies= -608.225027
Sum of electronic and thermal Enthalpies= -608.224082
Sum of electronic and thermal Free Energies= -608.267501

*Structure **9***

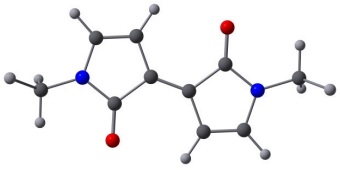


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.433261	-0.683041	-0.003767
2	6	0	-0.251405	0.260617	-0.001231
3	6	0	-0.796723	1.587462	0.000642
4	6	0	-2.149923	1.466662	-0.003481
5	1	0	-0.240875	2.508676	0.002027
6	6	0	1.044979	-0.164984	-0.000966
7	6	0	2.211164	0.754702	0.001460
8	6	0	1.598980	-1.495080	-0.001957
9	6	0	2.936187	-1.363326	-0.000051
10	1	0	1.046865	-2.418684	-0.003479
11	8	0	-1.440589	-1.908601	0.000930

12	8	0	2.290684	1.960122	0.002863
13	7	0	-2.551357	0.134203	-0.011905
14	6	0	-3.926795	-0.338685	0.010188
15	1	0	-3.919454	-1.415590	-0.147844
16	1	0	-4.398403	-0.123756	0.971934
17	1	0	-4.500985	0.134440	-0.788039
18	1	0	3.730500	-2.093180	0.000343
19	1	0	-2.898306	2.245405	-0.003779
20	8	0	3.355023	-0.041857	0.002100

SCF Done: E(RB3LYP) = -627.778697791 A.U. after 1 cycles
Convg = 0.1893D-08 -V/T = 2.0059Zero-point correction= 0.145692 (Hartree/Particle)
Thermal correction to Energy= 0.156724
Thermal correction to Enthalpy= 0.157669
Thermal correction to Gibbs Free Energy= 0.107864
Sum of electronic and zero-point Energies= -627.633006
Sum of electronic and thermal Energies= -627.621973
Sum of electronic and thermal Enthalpies= -627.621029
Sum of electronic and thermal Free Energies= -627.670834

*Structure **10***

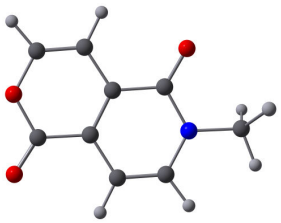


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.853426	-0.667800	-0.000024
2	6	0	-0.641800	0.231263	-0.000105
3	6	0	-1.142641	1.580431	-0.000085
4	6	0	-2.496986	1.509828	-0.000017
5	1	0	-0.548533	2.477132	-0.000168
6	6	0	0.641800	-0.231260	-0.000025
7	6	0	1.853427	0.667800	-0.000143
8	6	0	1.142639	-1.580429	-0.000066
9	6	0	2.496984	-1.509827	-0.000019
10	1	0	0.548530	-2.477128	-0.000015
11	8	0	-1.910228	-1.894859	-0.000013
12	8	0	1.910231	1.894860	0.000011
13	7	0	-2.942728	0.188149	0.000208
14	7	0	2.942727	-0.188150	-0.000187
15	6	0	-4.332913	-0.235994	0.000069
16	1	0	-4.354484	-1.324343	0.000201
17	1	0	-4.848632	0.130080	0.890574
18	1	0	-4.848418	0.129771	-0.890699
19	6	0	4.332913	0.235991	0.000232
20	1	0	4.848208	-0.129677	0.891162
21	1	0	4.848831	-0.130190	-0.890113
22	1	0	4.354492	1.324339	-0.000020
23	1	0	3.218883	-2.312924	0.000082
24	1	0	-3.218886	2.312924	-0.000034

SCF Done: E(RB3LYP) = -647.237557267 A.U. after 2 cycles
Convg = 0.8530D-08 -V/T = 2.0061
Zero-point correction= 0.186058 (Hartree/Particle)
Thermal correction to Energy= 0.198937
Thermal correction to Enthalpy= 0.199881

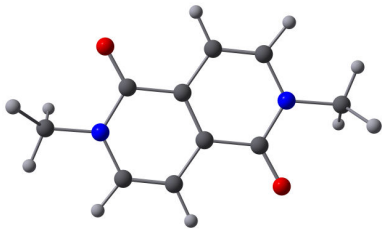
```
 Thermal correction to Gibbs Free Energy=          0.146344
 Sum of electronic and zero-point Energies=           -647.051499
 Sum of electronic and thermal Energies=              -647.038621
 Sum of electronic and thermal Enthalpies=            -647.037677
 Sum of electronic and thermal Free Energies=         -647.091214
```

*Structure **11***



```
---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0       -2.111555   -0.740692    0.000125
      2          6           0       -0.651256   -0.611601   -0.000067
      3          6           0       -0.072837    0.648016   -0.000084
      4          6           0       -0.898089    1.817017    0.000021
      5          6           0       -2.230586    1.666475    0.000048
      6          1           0       -0.296050   -2.761200   -0.000071
      7          6           0        0.152794   -1.779780   -0.000121
      8          6           0        1.381459    0.794510   -0.000309
      9          1           0       -0.456706    2.802379   -0.000016
     10          6           0        1.503320   -1.634861   -0.000055
     11          8           0       -2.733930   -1.783756   -0.000200
     12          8           0        1.967030    1.884347    0.000376
     13          7           0        2.102053   -0.400963   -0.000096
     14          6           0        3.565835   -0.286823    0.000148
     15          1           0        3.895549    0.257487    0.885091
     16          1           0        3.994748   -1.285507   -0.000085
     17          1           0        3.895773    0.257985   -0.884397
     18          1           0        2.177046   -2.480065    0.000040
     19          1           0       -2.958800    2.464709    0.000054
     20          8           0       -2.833156    0.439081    0.000052
 ---------------------------------------------------------------------SCF Done:
E(RB3LYP) =  -627.813535000     A.U. after    1 cycles
             Convg  =    0.8550D-08             -V/T =  2.0059
Zero-point correction=                           0.148328 (Hartree/Particle)
 Thermal correction to Energy=                   0.158434
 Thermal correction to Enthalpy=                 0.159378
 Thermal correction to Gibbs Free Energy=        0.112553
 Sum of electronic and zero-point Energies=           -627.665207
 Sum of electronic and thermal Energies=              -627.655101
 Sum of electronic and thermal Enthalpies=            -627.654157
 Sum of electronic and thermal Free Energies=         -627.700982
```

*Structure **12***



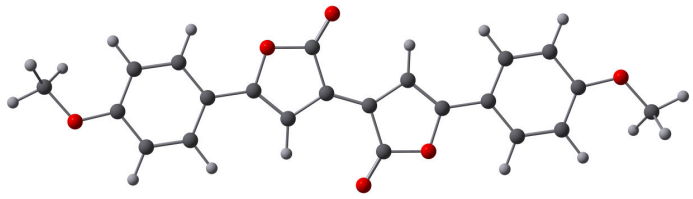
```
---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
```

Number	Number	Type	X	Y	Z
1	6	0	1.730482	0.816520	-0.000113
2	6	0	0.276740	0.638459	-0.000081
3	6	0	-0.276740	-0.638458	-0.000166
4	6	0	0.564907	-1.783798	-0.000125
5	6	0	1.909441	-1.608526	0.000026
6	1	0	-0.138584	2.775431	0.000056
7	6	0	-0.564908	1.783798	-0.000007
8	6	0	-1.730482	-0.816520	-0.000255
9	1	0	0.138582	-2.775430	-0.000162
10	6	0	-1.909441	1.608525	0.000016
11	8	0	2.292176	1.920998	0.000021
12	8	0	-2.292175	-1.920997	0.000170
13	7	0	-2.480178	0.357158	-0.000125
14	7	0	2.480178	-0.357158	0.000110
15	6	0	-3.940117	0.210869	0.000164
16	1	0	-4.260642	-0.339050	0.885236
17	1	0	-4.390890	1.200273	-0.000716
18	1	0	-4.260755	-0.340690	-0.883821
19	6	0	3.940117	-0.210870	0.000112
20	1	0	4.260568	0.340832	0.884075
21	1	0	4.390891	-1.200273	0.001246
22	1	0	4.260830	0.338908	-0.884981
23	1	0	-2.604828	2.435915	0.000117
24	1	0	2.604827	-2.435917	0.000114

SCF Done: E(RB3LYP) = -647.283571651 A.U. after 1 cycles
Convg = 0.5504D-08 -V/T = 2.0061
Zero-point correction= 0.189429 (Hartree/Particle)
Thermal correction to Energy= 0.201158
Thermal correction to Enthalpy= 0.202102
Thermal correction to Gibbs Free Energy= 0.151861
Sum of electronic and zero-point Energies= -647.094142
Sum of electronic and thermal Energies= -647.082413
Sum of electronic and thermal Enthalpies= -647.081469
Sum of electronic and thermal Free Energies= -647.131710

Structure plots, cartesian coordinates, SCF convergence and thermochemistry data for structures 13-31 at SMD(toluene)/B3LYP/DGDZVP level of theory

*Structure **13***

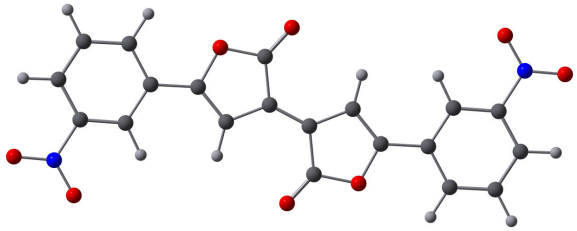


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.111038	1.602765	-0.007777
2	6	0	0.664771	0.187561	-0.005703
3	6	0	1.856360	-0.597219	-0.003633
4	6	0	2.923610	0.263104	-0.004811
5	8	0	2.503226	1.591115	-0.007752
6	1	0	1.905396	-1.676517	-0.001516
7	6	0	-0.664786	-0.187665	-0.005332
8	6	0	-1.111063	-1.602867	-0.002702
9	6	0	-1.856371	0.597123	-0.006535

10	8	0	-2.503253	-1.591203	-0.000769
11	6	0	-2.923626	-0.263189	-0.003521
12	1	0	-1.905399	1.676421	-0.008555
13	8	0	0.491447	2.644872	-0.010728
14	8	0	-0.491482	-2.644981	-0.000028
15	6	0	-4.353079	-0.041638	-0.002024
16	6	0	-4.885201	1.270753	-0.005828
17	6	0	-5.252953	-1.124917	0.003743
18	6	0	-6.252719	1.482927	-0.003974
19	1	0	-4.219446	2.129151	-0.010313
20	6	0	-6.632756	-0.920454	0.005834
21	1	0	-4.868794	-2.139756	0.006631
22	6	0	-7.143286	0.388127	0.002019
23	1	0	-6.661615	2.489371	-0.006926
24	1	0	-7.293958	-1.779529	0.010247
25	6	0	4.353067	0.041578	-0.003200
26	6	0	5.252926	1.124883	-0.004979
27	6	0	4.885208	-1.270805	0.000521
28	6	0	6.632734	0.920455	-0.002568
29	1	0	4.868752	2.139716	-0.008091
30	6	0	6.252729	-1.482946	0.003091
31	1	0	4.219464	-2.129224	0.001654
32	6	0	7.143282	-0.388118	0.001953
33	1	0	7.293925	1.779547	-0.004051
34	1	0	6.661638	-2.489384	0.006235
35	8	0	-8.465453	0.703410	0.003496
36	8	0	8.465453	-0.703367	0.005924
37	6	0	9.423562	0.362696	0.004804
38	1	0	9.321922	0.988903	0.898447
39	1	0	10.401436	-0.121147	0.013470
40	1	0	9.331984	0.977642	-0.897753
41	6	0	-9.423573	-0.362609	0.012026
42	1	0	-9.324198	-0.978399	0.913147
43	1	0	-10.401453	0.121295	0.012398
44	1	0	-9.329750	-0.987980	-0.883088

SCF Done: E(RB3LYP) = -1299.48000577 A.U. after 1 cycles
Convg = 0.4448D-08 -V/T = 2.0143
Zero-point correction= 0.332571 (Hartree/Particle)
Thermal correction to Energy= 0.355633
Thermal correction to Enthalpy= 0.356577
Thermal correction to Gibbs Free Energy= 0.278404
Sum of electronic and zero-point Energies= -1299.147435
Sum of electronic and thermal Energies= -1299.124373
Sum of electronic and thermal Enthalpies= -1299.123429
Sum of electronic and thermal Free Energies= -1299.201602

*Structure **14***

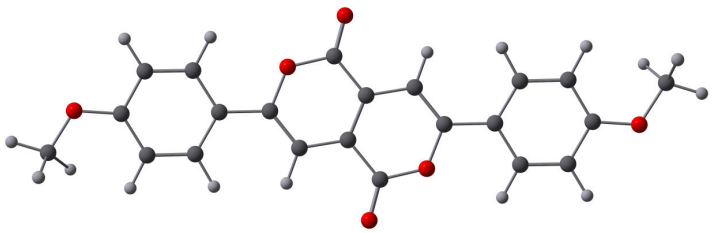


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.760957	-1.799641	-0.001996
2	6	0	0.610311	-0.319161	-0.001419

3	6	0	1.937674	0.209391	-0.001634
4	6	0	2.801074	-0.850665	-0.000591
5	8	0	2.129922	-2.065908	0.000115
6	1	0	2.204931	1.256243	-0.001933
7	6	0	-0.610311	0.319162	-0.001358
8	6	0	-0.760958	1.799642	-0.001775
9	6	0	-1.937674	-0.209390	-0.001524
10	8	0	-2.129922	2.065910	0.000176
11	6	0	-2.801074	0.850666	-0.000504
12	1	0	-2.204931	-1.256242	-0.001849
13	8	0	-0.054298	-2.691954	0.000349
14	8	0	0.054297	2.691956	0.000335
15	6	0	-4.253997	0.917895	0.000234
16	6	0	-5.014406	-0.266646	-0.000312
17	6	0	-4.918615	2.162190	0.001460
18	6	0	-6.401597	-0.175427	0.000395
19	1	0	-4.542371	-1.242066	-0.001257
20	6	0	-6.313072	2.221765	0.002132
21	1	0	-4.338352	3.079059	0.001862
22	6	0	-7.073928	1.052180	0.001623
23	1	0	-6.811513	3.186739	0.003074
24	1	0	-8.157508	1.080812	0.002152
25	6	0	4.253997	-0.917894	0.000188
26	6	0	4.918614	-2.162190	0.001467
27	6	0	5.014406	0.266646	-0.000373
28	6	0	6.313071	-2.221765	0.002178
29	1	0	4.338351	-3.079058	0.001881
30	6	0	6.401597	0.175426	0.000372
31	1	0	4.542373	1.242067	-0.001358
32	6	0	7.073928	-1.052181	0.001655
33	1	0	6.811512	-3.186739	0.003162
34	1	0	8.157508	-1.080813	0.002213
35	7	0	7.191440	1.421264	-0.000183
36	8	0	8.423581	1.321882	0.000469
37	8	0	6.580700	2.496240	-0.001373
38	7	0	-7.191439	-1.421266	-0.000141
39	8	0	-8.423580	-1.321885	0.000413
40	8	0	-6.580700	-2.496241	-0.001356

```
 ---------------------------------------------------------------------
SCF Done:  E(RB3LYP) =  -1479.46667094     A.U. after    1 cycles
             Convg  =    0.9287D-08             -V/T =  2.0139
Zero-point correction=                           0.272306 (Hartree/Particle)
 Thermal correction to Energy=                    0.294370
 Thermal correction to Enthalpy=                  0.295315
 Thermal correction to Gibbs Free Energy=         0.216495
 Sum of electronic and zero-point Energies=          -1479.194365
 Sum of electronic and thermal Energies=             -1479.172301
 Sum of electronic and thermal Enthalpies=           -1479.171356
 Sum of electronic and thermal Free Energies=        -1479.250176
```

*Structure **15***

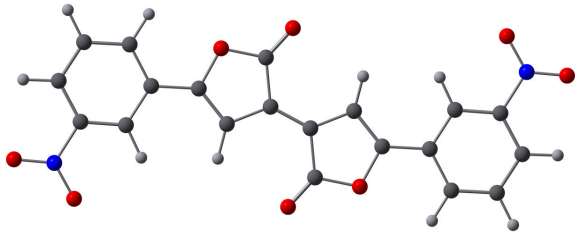


```
---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
```

1	6	0	-0.651682	1.784302	0.032618
2	6	0	0.266428	0.640691	0.012108
3	6	0	-0.266419	-0.640764	-0.009530
4	6	0	-1.671814	-0.863043	-0.014410
5	6	0	-2.519395	0.207450	0.008855
6	1	0	2.046567	1.877325	0.043385
7	6	0	1.671822	0.862976	0.016578
8	6	0	0.651693	-1.784378	-0.029670
9	1	0	-2.046552	-1.877394	-0.041291
10	6	0	2.519400	-0.207504	-0.007217
11	8	0	2.002259	-1.480969	-0.031001
12	8	0	-2.002256	1.480910	0.032861
13	8	0	-0.331846	2.958236	0.049947
14	8	0	0.331847	-2.958281	-0.048734
15	6	0	-3.985135	0.187306	0.008348
16	6	0	-4.724831	1.390719	-0.038296
17	6	0	-4.702561	-1.023205	0.052955
18	6	0	-6.112439	1.379158	-0.045769
19	1	0	-4.204753	2.341876	-0.072659
20	6	0	-6.096536	-1.046235	0.046496
21	1	0	-4.178779	-1.973158	0.101160
22	6	0	-6.815243	0.161146	-0.005111
23	1	0	-6.675301	2.307710	-0.085189
24	1	0	-6.606732	-2.002391	0.086546
25	6	0	3.985140	-0.187334	-0.007504
26	6	0	4.724887	-1.390731	0.038735
27	6	0	4.702515	1.023192	-0.052559
28	6	0	6.112499	-1.379141	0.045410
29	1	0	4.204849	-2.341898	0.073411
30	6	0	6.096494	1.046249	-0.046931
31	1	0	4.178687	1.973134	-0.100506
32	6	0	6.815254	-0.161115	0.004290
33	1	0	6.675404	-2.307680	0.084515
34	1	0	6.606649	2.002412	-0.087335
35	8	0	-8.172532	0.255705	-0.017850
36	8	0	8.172553	-0.255644	0.016174
37	6	0	8.945445	0.949497	-0.005956
38	1	0	8.737774	1.573165	0.871501
39	1	0	9.989232	0.631799	0.017924
40	1	0	8.764951	1.523611	-0.922277
41	6	0	-8.945469	-0.949418	0.003664
42	1	0	-9.989233	-0.631692	-0.020855
43	1	0	-8.737249	-1.572993	-0.873728
44	1	0	-8.765580	-1.523638	0.920037

SCF Done: E(RB3LYP) = -1299.48949249 A.U. after 1 cycles
Convg = 0.5891D-08 -V/T = 2.0143
Zero-point correction= 0.334402 (Hartree/Particle)
Thermal correction to Energy= 0.357623
Thermal correction to Enthalpy= 0.358567
Thermal correction to Gibbs Free Energy= 0.280633
Sum of electronic and zero-point Energies= -1299.155091
Sum of electronic and thermal Energies= -1299.131870
Sum of electronic and thermal Enthalpies= -1299.130925
Sum of electronic and thermal Free Energies= -1299.208859

*Structure **16***

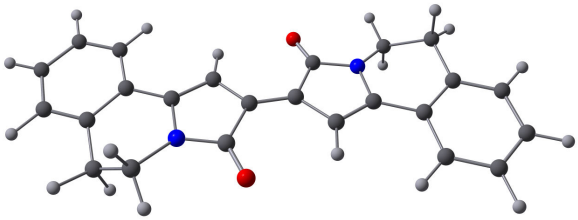


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.760957	-1.799641	-0.001996
2	6	0	0.610311	-0.319161	-0.001419
3	6	0	1.937674	0.209391	-0.001634
4	6	0	2.801074	-0.850665	-0.000591
5	8	0	2.129922	-2.065908	0.000115
6	1	0	2.204931	1.256243	-0.001933
7	6	0	-0.610311	0.319162	-0.001358
8	6	0	-0.760958	1.799642	-0.001775
9	6	0	-1.937674	-0.209390	-0.001524
10	8	0	-2.129922	2.065910	0.000176
11	6	0	-2.801074	0.850666	-0.000504
12	1	0	-2.204931	-1.256242	-0.001849
13	8	0	-0.054298	-2.691954	0.000349
14	8	0	0.054297	2.691956	0.000335
15	6	0	-4.253997	0.917895	0.000234
16	6	0	-5.014406	-0.266646	-0.000312
17	6	0	-4.918615	2.162190	0.001460
18	6	0	-6.401597	-0.175427	0.000395
19	1	0	-4.542371	-1.242066	-0.001257
20	6	0	-6.313072	2.221765	0.002132
21	1	0	-4.338352	3.079059	0.001862
22	6	0	-7.073928	1.052180	0.001623
23	1	0	-6.811513	3.186739	0.003074
24	1	0	-8.157508	1.080812	0.002152
25	6	0	4.253997	-0.917894	0.000188
26	6	0	4.918614	-2.162190	0.001467
27	6	0	5.014406	0.266646	-0.000373
28	6	0	6.313071	-2.221765	0.002178
29	1	0	4.338351	-3.079058	0.001881
30	6	0	6.401597	0.175426	0.000372
31	1	0	4.542373	1.242067	-0.001358
32	6	0	7.073928	-1.052181	0.001655
33	1	0	6.811512	-3.186739	0.003162
34	1	0	8.157508	-1.080813	0.002213
35	7	0	7.191440	1.421264	-0.000183
36	8	0	8.423581	1.321882	0.000469
37	8	0	6.580700	2.496240	-0.001373
38	7	0	-7.191439	-1.421266	-0.000141
39	8	0	-8.423580	-1.321885	0.000413
40	8	0	-6.580700	-2.496241	-0.001356

SCF Done: E(RB3LYP) = -1479.46667094 A.U. after 1 cycles
Convg = 0.9287D-08 -V/T = 2.0139
Zero-point correction= 0.272306 (Hartree/Particle)
Thermal correction to Energy= 0.294370
Thermal correction to Enthalpy= 0.295315
Thermal correction to Gibbs Free Energy= 0.216495
Sum of electronic and zero-point Energies= -1479.194365
Sum of electronic and thermal Energies= -1479.172301
Sum of electronic and thermal Enthalpies= -1479.171356

Sum of electronic and thermal Free Energies= -1479.250176

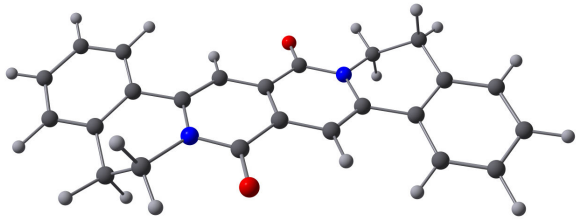
*Structure **17***



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.259132	-1.513120	0.132460
2	6	0	0.677616	-0.128056	0.023488
3	6	0	1.788000	0.775557	-0.019604
4	6	0	2.945496	0.030357	0.036355
5	1	0	1.723909	1.849452	-0.114926
6	6	0	-0.677632	0.127949	-0.025441
7	6	0	-1.259160	1.512990	-0.134620
8	6	0	-1.788013	-0.775670	0.017544
9	6	0	-2.945516	-0.030406	-0.037436
10	1	0	-1.723911	-1.849580	0.112689
11	8	0	0.684320	-2.599743	0.240953
12	8	0	-0.684348	2.599704	-0.242196
13	7	0	2.632212	-1.337213	0.100067
14	7	0	-2.632216	1.337176	-0.100828
15	6	0	3.634424	-2.369033	0.344046
16	1	0	3.828774	-2.446993	1.421545
17	1	0	3.229971	-3.324090	0.002684
18	6	0	-3.634604	2.369160	-0.343386
19	1	0	-3.829941	2.447603	-1.420670
20	1	0	-3.229793	3.324047	-0.001976
21	6	0	4.347240	0.424132	0.023061
22	6	0	5.337201	-0.573117	-0.162087
23	6	0	4.732504	1.769990	0.194932
24	6	0	6.685544	-0.197007	-0.163774
25	6	0	6.078546	2.126499	0.182417
26	1	0	3.972548	2.531305	0.348930
27	6	0	7.060342	1.139794	0.005245
28	1	0	7.450289	-0.958757	-0.301480
29	1	0	6.366076	3.166082	0.318059
30	1	0	8.113041	1.412153	0.003002
31	6	0	-4.347270	-0.424112	-0.023167
32	6	0	-5.337013	0.573095	0.163399
33	6	0	-4.732756	-1.769870	-0.195314
34	6	0	-6.685369	0.197049	0.166154
35	6	0	-6.078805	-2.126318	-0.181740
36	1	0	-3.972981	-2.531154	-0.350353
37	6	0	-7.060387	-1.139654	-0.003169
38	1	0	-7.449949	0.958765	0.304955
39	1	0	-6.366509	-3.165823	-0.317607
40	1	0	-8.113098	-1.411962	-0.000078
41	6	0	4.917695	-2.008285	-0.408301
42	1	0	4.750510	-2.152225	-1.484019
43	1	0	5.716814	-2.694950	-0.113947
44	6	0	-4.917203	2.008114	0.409964
45	1	0	-5.716556	2.694969	0.116693
46	1	0	-4.749013	2.151502	1.485599

```
SCF Done:  E(RB3LYP) =  -1185.53104509     A.U. after    1 cycles
             Convg  =    0.6432D-08             -V/T =  2.0152
Zero-point correction=                           0.365155 (Hartree/Particle)
 Thermal correction to Energy=                    0.386183
 Thermal correction to Enthalpy=                  0.387127
 Thermal correction to Gibbs Free Energy=         0.315024
 Sum of electronic and zero-point Energies=          -1185.165890
 Sum of electronic and thermal Energies=             -1185.144862
 Sum of electronic and thermal Enthalpies=           -1185.143918
 Sum of electronic and thermal Free Energies=        -1185.216022
```

*Structure **18***

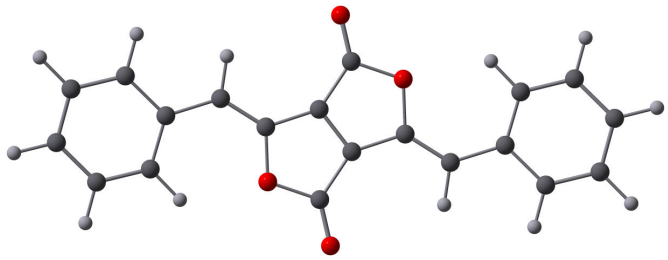


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.829288	-1.705939	0.243835
2	6	0	-0.191780	-0.665298	0.073870
3	6	0	0.191779	0.665297	-0.073882
4	6	0	1.562758	1.026837	-0.073294
5	6	0	2.533257	0.065395	0.073640
6	1	0	-1.830263	-2.064981	0.217786
7	6	0	-1.562758	-1.026839	0.073285
8	6	0	-0.829288	1.705936	-0.243850
9	1	0	1.830264	2.064980	-0.217795
10	6	0	-2.533257	-0.065396	-0.073646
11	8	0	0.550988	-2.904535	0.417659
12	8	0	-0.550989	2.904535	-0.417659
13	7	0	-2.158809	1.272641	-0.200592
14	7	0	2.158809	-1.272642	0.200584
15	6	0	-3.204891	2.306159	-0.361139
16	1	0	-2.748764	3.263909	-0.117926
17	1	0	-3.512166	2.334038	-1.413597
18	6	0	3.204891	-2.306159	0.361139
19	1	0	3.512161	-2.334036	1.413599
20	1	0	2.748767	-3.263910	0.117925
21	6	0	-3.978872	-0.383014	-0.074544
22	6	0	-4.916171	0.618427	0.257235
23	6	0	-4.439438	-1.680659	-0.374888
24	6	0	-6.279219	0.304923	0.305301
25	6	0	-5.799941	-1.982532	-0.322548
26	1	0	-3.737169	-2.455028	-0.668852
27	6	0	-6.726050	-0.989732	0.024820
28	1	0	-6.994999	1.083660	0.560809
29	1	0	-6.138069	-2.987701	-0.562067
30	1	0	-7.788018	-1.220570	0.062319
31	6	0	3.978872	0.383014	0.074545
32	6	0	4.916173	-0.618426	-0.257230
33	6	0	4.439436	1.680659	0.374890
34	6	0	6.279221	-0.304922	-0.305289
35	6	0	5.799939	1.982533	0.322555
36	1	0	3.737164	2.455028	0.668850
37	6	0	6.726049	0.989734	-0.024807
38	1	0	6.995002	-1.083659	-0.560793

39	1	0	6.138065	2.987703	0.562075
40	1	0	7.788018	1.220572	-0.062302
41	6	0	4.395207	-2.005290	-0.540600
42	1	0	4.087097	-2.091165	-1.591354
43	1	0	5.173097	-2.755405	-0.369717
44	6	0	-4.395203	2.005290	0.540605
45	1	0	-4.087088	2.091164	1.591358
46	1	0	-5.173093	2.755406	0.369726

SCF Done: E(RB3LYP) = -1185.56219704 A.U. after 1 cycles
Convg = 0.6245D-08 -V/T = 2.0152
Zero-point correction= 0.367223 (Hartree/Particle)
Thermal correction to Energy= 0.387566
Thermal correction to Enthalpy= 0.388510
Thermal correction to Gibbs Free Energy= 0.317806
Sum of electronic and zero-point Energies= -1185.194974
Sum of electronic and thermal Energies= -1185.174631
Sum of electronic and thermal Enthalpies= -1185.173687
Sum of electronic and thermal Free Energies= -1185.244391

*Structure **19***

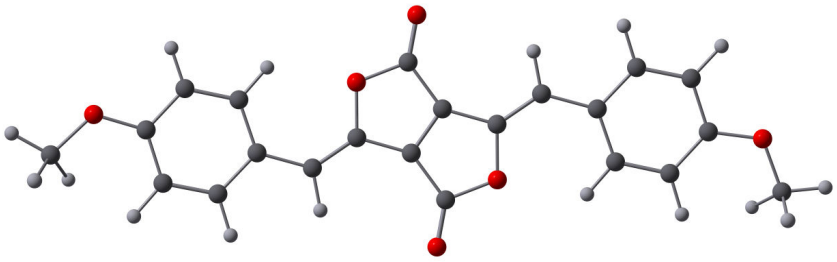


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.399287	1.757684	-0.057650
2	6	0	-0.417643	0.538336	-0.060355
3	6	0	0.417643	-0.537386	-0.060382
4	6	0	1.781570	-0.087801	-0.050590
5	6	0	-1.781670	0.088933	-0.050481
6	6	0	-0.399610	-1.756708	-0.057643
7	8	0	-1.730144	-1.308718	-0.053823
8	8	0	1.730124	1.309602	-0.053662
9	8	0	0.124633	2.934995	-0.058312
10	8	0	-0.124792	-2.934032	-0.058874
11	6	0	-2.932565	0.806315	-0.025218
12	1	0	-2.773778	1.882340	-0.018508
13	6	0	-4.319637	0.366914	0.006549
14	6	0	-5.318221	1.365223	0.092312
15	6	0	-4.727831	-0.987855	-0.037239
16	6	0	-6.670427	1.028862	0.135940
17	1	0	-5.022467	2.411591	0.125779
18	6	0	-6.081715	-1.317462	0.003625
19	1	0	-3.988149	-1.776852	-0.103448
20	6	0	-7.058232	-0.315805	0.092486
21	1	0	-7.421294	1.812177	0.203057
22	1	0	-6.379044	-2.362690	-0.032165
23	1	0	-8.111908	-0.582027	0.125440
24	6	0	2.932215	-0.805731	-0.025390
25	1	0	2.772827	-1.881653	-0.018722
26	6	0	4.319562	-0.366996	0.006434
27	6	0	4.728565	0.987493	-0.037575
28	6	0	5.317583	-1.365847	0.092521

29	6	0	6.082688	1.316320	0.003406
30	1	0	3.989590	1.777114	-0.104145
31	6	0	6.669988	-1.030277	0.136236
32	1	0	5.021317	-2.412055	0.126245
33	6	0	7.058615	0.314148	0.092557
34	1	0	6.380580	2.361378	-0.032579
35	1	0	7.420337	-1.814065	0.203610
36	1	0	8.112430	0.579811	0.125543

SCF Done: E(RB3LYP) = -1070.37475784 A.U. after 1 cycles
Convg = 0.6476D-08 -V/T = 2.0147
Zero-point correction= 0.268065 (Hartree/Particle)
Thermal correction to Energy= 0.286517
Thermal correction to Enthalpy= 0.287461
Thermal correction to Gibbs Free Energy= 0.219589
Sum of electronic and zero-point Energies= -1070.106693
Sum of electronic and thermal Energies= -1070.088241
Sum of electronic and thermal Enthalpies= -1070.087297
Sum of electronic and thermal Free Energies= -1070.155169

*Structure **20***

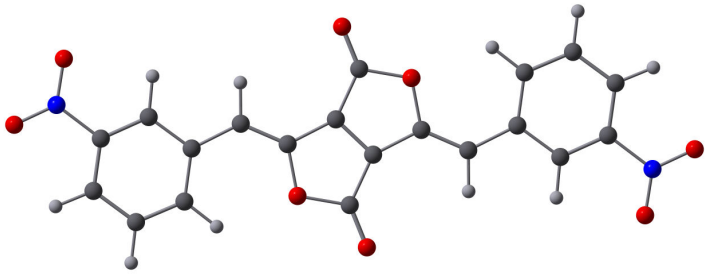


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.494976	-1.640859	-0.072003
2	6	0	-0.374182	-0.461767	-0.075744
3	6	0	0.414328	0.653142	-0.063810
4	6	0	1.794151	0.265914	-0.047693
5	6	0	-1.754340	-0.073893	-0.076259
6	6	0	-0.454644	1.832647	-0.062398
7	8	0	-1.764251	1.326202	-0.072507
8	8	0	1.804810	-1.134242	-0.056902
9	8	0	0.275006	-2.831530	-0.079268
10	8	0	-0.233785	3.022930	-0.054793
11	6	0	-2.878655	-0.837005	-0.064734
12	1	0	-2.676659	-1.906061	-0.060657
13	6	0	-4.276784	-0.454454	-0.043542
14	6	0	-5.243326	-1.480940	0.033075
15	6	0	-4.746841	0.884697	-0.086289
16	6	0	-6.610114	-1.210089	0.073086
17	1	0	-4.914661	-2.517525	0.065056
18	6	0	-6.103050	1.164888	-0.051581
19	1	0	-4.042452	1.705844	-0.146381
20	6	0	-7.050435	0.123632	0.032705
21	1	0	-7.314378	-2.032573	0.133364
22	1	0	-6.459684	2.190879	-0.084006
23	6	0	2.917661	1.029690	-0.016583
24	1	0	2.714202	2.098465	-0.006192
25	6	0	4.316377	0.649958	0.011759
26	6	0	4.788463	-0.681679	-0.030478
27	6	0	5.284197	1.683726	0.090049
28	6	0	6.151425	-0.970066	-0.000719

29	1	0	4.084998	-1.503909	-0.088995
30	6	0	6.641737	1.408223	0.123193
31	1	0	4.954068	2.719644	0.124736
32	6	0	7.091366	0.074041	0.076470
33	1	0	6.470037	-2.006215	-0.036738
34	1	0	7.375304	2.207546	0.182420
35	8	0	-8.353501	0.509412	0.067958
36	8	0	8.439318	-0.099893	0.108925
37	6	0	-9.362933	-0.497907	0.200132
38	1	0	-10.312142	0.039254	0.238124
39	1	0	-9.367504	-1.176111	-0.661105
40	1	0	-9.235009	-1.070197	1.126143
41	6	0	8.963717	-1.430792	0.030322
42	1	0	10.049232	-1.320750	0.048664
43	1	0	8.648881	-2.036429	0.888018
44	1	0	8.666418	-1.921536	-0.903505

SCF Done: E(RB3LYP) = -1299.46431300 A.U. after 1 cycles
Convg = 0.2561D-08 -V/T = 2.0143
Zero-point correction= 0.333242 (Hartree/Particle)
Thermal correction to Energy= 0.356992
Thermal correction to Enthalpy= 0.357936
Thermal correction to Gibbs Free Energy= 0.277640
Sum of electronic and zero-point Energies= -1299.131071
Sum of electronic and thermal Energies= -1299.107321
Sum of electronic and thermal Enthalpies= -1299.106377
Sum of electronic and thermal Free Energies= -1299.186673

*Structure **21***

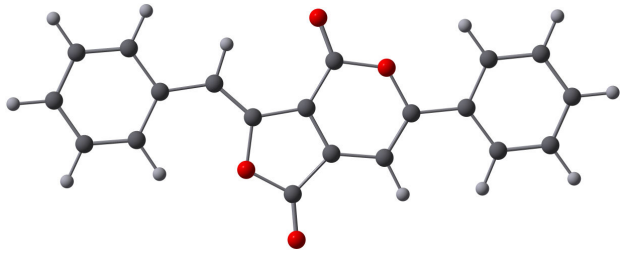


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.134843	1.798218	-0.000642
2	6	0	-0.491130	0.469222	-0.000617
3	6	0	0.491130	-0.469216	-0.000636
4	6	0	1.775024	0.178121	-0.000674
5	6	0	-1.775024	-0.178115	-0.000433
6	6	0	-0.134845	-1.798212	-0.000343
7	8	0	-1.520368	-1.550949	-0.000502
8	8	0	1.520367	1.550956	-0.000413
9	8	0	-0.312506	2.918456	-0.000116
10	8	0	0.312504	-2.918450	-0.000735
11	6	0	-3.015239	0.366732	-0.000329
12	1	0	-3.019730	1.454187	-0.000362
13	6	0	-4.321292	-0.279899	-0.000178
14	6	0	-5.455060	0.557374	0.000068
15	6	0	-4.520778	-1.681361	-0.000310
16	6	0	-6.728251	-0.005474	0.000331
17	1	0	-5.346839	1.636668	0.000095
18	6	0	-5.807891	-2.218055	-0.000097
19	1	0	-3.667891	-2.349238	-0.000573
20	6	0	-6.931348	-1.387713	0.000286

21	1	0	-5.940265	-3.296115	-0.000214
22	6	0	3.015239	-0.366726	-0.000631
23	1	0	3.019729	-1.454180	-0.000745
24	6	0	4.321294	0.279903	-0.000389
25	6	0	4.520789	1.681365	-0.000552
26	6	0	5.455059	-0.557376	-0.000008
27	6	0	5.807904	2.218053	-0.000236
28	1	0	3.667905	2.349246	-0.000932
29	6	0	6.728250	0.005470	0.000348
30	1	0	5.346835	-1.636670	0.000063
31	6	0	6.931358	1.387707	0.000272
32	1	0	5.940284	3.296113	-0.000371
33	7	0	-7.898884	0.889985	0.000739
34	8	0	-7.697041	2.110127	-0.000127
35	8	0	-9.021819	0.372521	0.002017
36	7	0	7.898879	-0.889994	0.000876
37	8	0	9.021816	-0.372530	0.001996
38	8	0	7.697023	-2.110137	0.000280
39	1	0	-7.936951	-1.792439	0.000536
40	1	0	7.936963	1.792425	0.000592

SCF Done: E(RB3LYP) = -1479.45279680 A.U. after 1 cycles
Convg = 0.5352D-08 -V/T = 2.0139
Zero-point correction= 0.272626 (Hartree/Particle)
Thermal correction to Energy= 0.296279
Thermal correction to Enthalpy= 0.297223
Thermal correction to Gibbs Free Energy= 0.215580
Sum of electronic and zero-point Energies= -1479.180170
Sum of electronic and thermal Energies= -1479.156518
Sum of electronic and thermal Enthalpies= -1479.155574
Sum of electronic and thermal Free Energies= -1479.237217

*Structure **22***

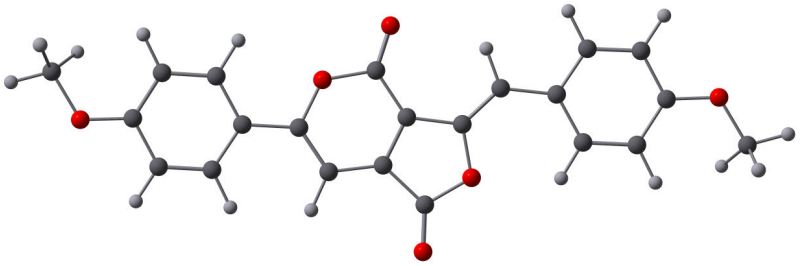


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.543700	-1.332882	-0.000014
2	6	0	-0.193719	-0.088385	-0.000021
3	6	0	0.472840	1.114928	-0.000041
4	6	0	1.881904	1.218403	-0.000069
5	6	0	2.591206	0.044074	-0.000031
6	6	0	-1.615606	0.159897	-0.000015
7	6	0	-0.551981	2.182033	-0.000091
8	1	0	2.372310	2.183201	-0.000126
9	8	0	-1.788267	1.545440	-0.000038
10	8	0	1.932584	-1.157131	0.000033
11	8	0	0.114332	-2.469230	0.000086
12	8	0	-0.446968	3.387221	-0.000177
13	6	0	4.054941	-0.105433	-0.000015
14	6	0	4.641101	-1.387504	-0.000261
15	6	0	4.898986	1.025139	0.000286
16	6	0	6.029504	-1.531332	-0.000232

17	1	0	4.008408	-2.268344	-0.000479
18	6	0	6.284408	0.874798	0.000312
19	1	0	4.482331	2.027138	0.000528
20	6	0	6.857477	-0.403783	0.000053
21	1	0	6.464749	-2.527333	-0.000425
22	1	0	6.919279	1.757119	0.000550
23	1	0	7.938537	-0.517908	0.000082
24	6	0	-2.641792	-0.726195	0.000006
25	1	0	-2.315211	-1.762933	0.000072
26	6	0	-4.081891	-0.506600	-0.000029
27	6	0	-4.912437	-1.651595	0.000070
28	6	0	-4.698955	0.767025	-0.000017
29	6	0	-6.301782	-1.534632	0.000084
30	1	0	-4.455356	-2.638680	0.000114
31	6	0	-6.088917	0.877743	0.000012
32	1	0	-4.091754	1.664466	-0.000028
33	6	0	-6.897265	-0.267404	0.000053
34	1	0	-6.919864	-2.429077	0.000136
35	1	0	-6.546881	1.863926	0.000009
36	1	0	-7.980326	-0.171756	0.000085

SCF Done: E(RB3LYP) = -1070.39361812 A.U. after 1 cycles
Convg = 0.9230D-08 -V/T = 2.0147
Zero-point correction= 0.268332 (Hartree/Particle)
Thermal correction to Energy= 0.286707
Thermal correction to Enthalpy= 0.287651
Thermal correction to Gibbs Free Energy= 0.217016
Sum of electronic and zero-point Energies= -1070.125286
Sum of electronic and thermal Energies= -1070.106911
Sum of electronic and thermal Enthalpies= -1070.105967
Sum of electronic and thermal Free Energies= -1070.176602

*Structure **23***

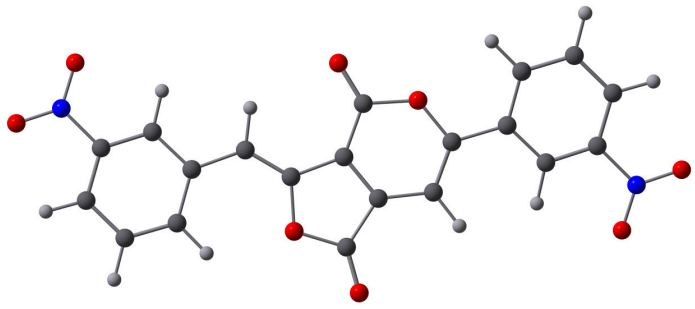


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.523838	-1.351155	-0.018045
2	6	0	-0.194778	-0.097018	0.008077
3	6	0	0.492011	1.097692	0.034903
4	6	0	1.901439	1.178585	0.038288
5	6	0	2.594746	-0.006764	0.005366
6	6	0	-1.610160	0.172496	0.011458
7	6	0	-0.515189	2.178730	0.057423
8	1	0	2.408856	2.133964	0.070700
9	8	0	-1.760992	1.561615	0.040612
10	8	0	1.915225	-1.198265	-0.022449
11	8	0	0.077525	-2.482118	-0.039104
12	8	0	-0.393857	3.383680	0.085612
13	6	0	4.049675	-0.176719	-0.002568
14	6	0	4.628579	-1.458932	0.028378
15	6	0	4.917846	0.939570	-0.040010
16	6	0	6.013178	-1.634606	0.026098

17	1	0	3.990205	-2.335526	0.057871
18	6	0	6.293379	0.776677	-0.042456
19	1	0	4.520348	1.949016	-0.075734
20	6	0	6.858510	-0.514243	-0.008586
21	1	0	6.415732	-2.641123	0.053327
22	1	0	6.955494	1.637447	-0.074663
23	6	0	-2.656396	-0.692524	-0.008781
24	1	0	-2.351367	-1.735684	-0.027707
25	6	0	-4.086687	-0.444612	-0.009083
26	6	0	-4.950844	-1.568518	-0.027226
27	6	0	-4.686256	0.834768	0.005871
28	6	0	-6.329723	-1.427817	-0.031000
29	1	0	-4.521370	-2.567797	-0.038259
30	6	0	-6.072074	0.988319	0.001562
31	1	0	-4.065936	1.723260	0.020746
32	6	0	-6.906619	-0.143510	-0.017289
33	1	0	-6.982285	-2.296497	-0.044464
34	1	0	-6.489133	1.989465	0.012885
35	8	0	8.216755	-0.565281	-0.013684
36	8	0	-8.266946	-0.103625	-0.023685
37	6	0	-8.918027	1.171576	-0.007931
38	1	0	-9.988078	0.956257	-0.014495
39	1	0	-8.669399	1.736645	0.898093
40	1	0	-8.663712	1.761785	-0.896216
41	6	0	8.856737	-1.846929	0.003533
42	1	0	8.593547	-2.435738	-0.883026
43	1	0	9.928427	-1.640810	-0.006348
44	1	0	8.605822	-2.407251	0.911677

SCF Done: E(RB3LYP) = -1299.48272101 A.U. after 1 cycles
Convg = 0.3039D-08 -V/T = 2.0143
Zero-point correction= 0.333851 (Hartree/Particle)
Thermal correction to Energy= 0.357261
Thermal correction to Enthalpy= 0.358205
Thermal correction to Gibbs Free Energy= 0.279452
Sum of electronic and zero-point Energies= -1299.148870
Sum of electronic and thermal Energies= -1299.125460
Sum of electronic and thermal Enthalpies= -1299.124516
Sum of electronic and thermal Free Energies= -1299.203269

*Structure **24***

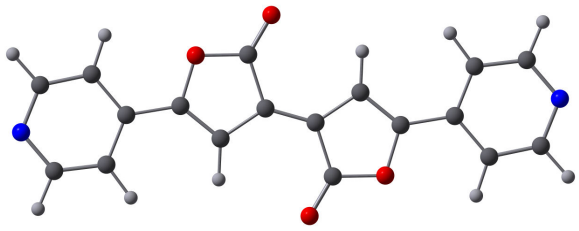


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.523838	-1.351155	-0.018045
2	6	0	-0.194778	-0.097018	0.008077
3	6	0	0.492011	1.097692	0.034903
4	6	0	1.901439	1.178585	0.038288
5	6	0	2.594746	-0.006764	0.005366
6	6	0	-1.610160	0.172496	0.011458
7	6	0	-0.515189	2.178730	0.057423

8	1	0	2.408856	2.133964	0.070700
9	8	0	-1.760992	1.561615	0.040612
10	8	0	1.915225	-1.198265	-0.022449
11	8	0	0.077525	-2.482118	-0.039104
12	8	0	-0.393857	3.383680	0.085612
13	6	0	4.049675	-0.176719	-0.002568
14	6	0	4.628579	-1.458932	0.028378
15	6	0	4.917846	0.939570	-0.040010
16	6	0	6.013178	-1.634606	0.026098
17	1	0	3.990205	-2.335526	0.057871
18	6	0	6.293379	0.776677	-0.042456
19	1	0	4.520348	1.949016	-0.075734
20	6	0	6.858510	-0.514243	-0.008586
21	1	0	6.415732	-2.641123	0.053327
22	1	0	6.955494	1.637447	-0.074663
23	6	0	-2.656396	-0.692524	-0.008781
24	1	0	-2.351367	-1.735684	-0.027707
25	6	0	-4.086687	-0.444612	-0.009083
26	6	0	-4.950844	-1.568518	-0.027226
27	6	0	-4.686256	0.834768	0.005871
28	6	0	-6.329723	-1.427817	-0.031000
29	1	0	-4.521370	-2.567797	-0.038259
30	6	0	-6.072074	0.988319	0.001562
31	1	0	-4.065936	1.723260	0.020746
32	6	0	-6.906619	-0.143510	-0.017289
33	1	0	-6.982285	-2.296497	-0.044464
34	1	0	-6.489133	1.989465	0.012885
35	8	0	8.216755	-0.565281	-0.013684
36	8	0	-8.266946	-0.103625	-0.023685
37	6	0	-8.918027	1.171576	-0.007931
38	1	0	-9.988078	0.956257	-0.014495
39	1	0	-8.669399	1.736645	0.898093
40	1	0	-8.663712	1.761785	-0.896216
41	6	0	8.856737	-1.846929	0.003533
42	1	0	8.593547	-2.435738	-0.883026
43	1	0	9.928427	-1.640810	-0.006348
44	1	0	8.605822	-2.407251	0.911677

SCF Done: E(RB3LYP) = -1479.47163641 A.U. after 1 cycles
Convg = 0.8110D-08 -V/T = 2.0139Zero-point correction= 0.273272 (Hartree/Particle)
Thermal correction to Energy= 0.296730
Thermal correction to Enthalpy= 0.297674
Thermal correction to Gibbs Free Energy= 0.216468
Sum of electronic and zero-point Energies= -1479.198364
Sum of electronic and thermal Energies= -1479.174906
Sum of electronic and thermal Enthalpies= -1479.173962
Sum of electronic and thermal Free Energies= -1479.255168

*Structure **25***

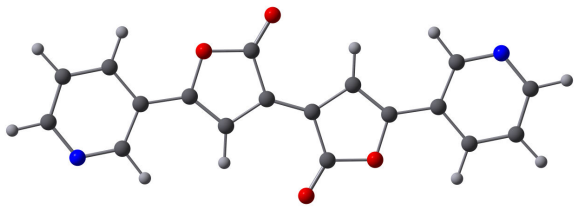


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	1.117091	-1.606481	-0.000118
2	6	0	0.662529	-0.186828	-0.000079
3	6	0	1.854098	0.602687	-0.000094
4	6	0	2.915666	-0.258672	-0.000046
5	8	0	2.507282	-1.586095	-0.000018
6	1	0	1.904638	1.681995	-0.000101
7	6	0	-0.662529	0.186828	-0.000057
8	6	0	-1.117091	1.606481	-0.000038
9	6	0	-1.854098	-0.602687	-0.000052
10	8	0	-2.507282	1.586094	0.000000
11	6	0	-2.915666	0.258671	-0.000018
12	1	0	-1.904637	-1.681995	-0.000068
13	8	0	0.499104	-2.646136	0.000005
14	8	0	-0.499104	2.646136	-0.000011
15	6	0	-4.351901	0.024694	0.000006
16	6	0	-4.880193	-1.280959	-0.000012
17	6	0	-5.261803	1.097053	0.000048
18	6	0	-6.263718	-1.445161	0.000012
19	1	0	-4.234749	-2.154158	-0.000045
20	6	0	-6.630232	0.816892	0.000069
21	1	0	-4.915188	2.124974	0.000063
22	1	0	-6.692845	-2.445557	-0.000001
23	1	0	-7.351441	1.632567	0.000102
24	6	0	4.351901	-0.024695	-0.000001
25	6	0	5.261803	-1.097053	0.000062
26	6	0	4.880193	1.280958	-0.000017
27	6	0	6.630231	-0.816893	0.000106
28	1	0	4.915187	-2.124974	0.000078
29	6	0	6.263718	1.445160	0.000031
30	1	0	4.234750	2.154158	-0.000065
31	1	0	7.351441	-1.632568	0.000155
32	1	0	6.692845	2.445557	0.000019
33	7	0	7.137701	0.424126	0.000091
34	7	0	-7.137701	-0.424127	0.000053

SCF Done: E(RB3LYP) = -1102.46623866 A.U. after 1 cycles
Convg = 0.3564D-08 -V/T = 2.0144
Zero-point correction= 0.244376 (Hartree/Particle)
Thermal correction to Energy= 0.262519
Thermal correction to Enthalpy= 0.263463
Thermal correction to Gibbs Free Energy= 0.195569
Sum of electronic and zero-point Energies= -1102.221862
Sum of electronic and thermal Energies= -1102.203720
Sum of electronic and thermal Enthalpies= -1102.202776
Sum of electronic and thermal Free Energies= -1102.270670

*Structure **26***

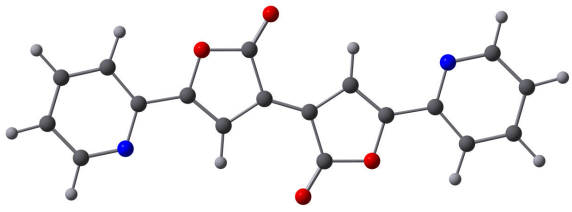


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.115311	-1.603780	-0.000084
2	6	0	0.663371	-0.186126	-0.000057
3	6	0	1.854922	0.603212	-0.000067
4	6	0	2.918734	-0.256698	-0.000033

5	8	0	2.507680	-1.584216	-0.000013
6	1	0	1.903596	1.682462	-0.000072
7	6	0	-0.663371	0.186126	-0.000041
8	6	0	-1.115311	1.603780	-0.000028
9	6	0	-1.854922	-0.603212	-0.000037
10	8	0	-2.507680	1.584216	-0.000003
11	6	0	-2.918734	0.256698	-0.000014
12	1	0	-1.903596	-1.682462	-0.000048
13	8	0	0.498487	-2.644665	0.000002
14	8	0	-0.498487	2.644665	-0.000011
15	6	0	-4.354306	0.033063	0.000003
16	6	0	-5.263748	1.108182	0.000032
17	6	0	-6.629386	0.832351	0.000047
18	1	0	-4.902885	2.131791	0.000041
19	1	0	-7.362114	1.634426	0.000069
20	6	0	4.354306	-0.033063	0.000001
21	6	0	5.263748	-1.108182	0.000045
22	6	0	6.629386	-0.832351	0.000077
23	1	0	4.902885	-2.131791	0.000055
24	1	0	7.362114	-1.634426	0.000112
25	6	0	-7.046700	-0.501740	0.000034
26	1	0	-8.106857	-0.750205	0.000046
27	6	0	7.046700	0.501740	0.000063
28	1	0	8.106857	0.750205	0.000087
29	7	0	-6.194157	-1.542085	0.000007
30	7	0	6.194157	1.542085	0.000020
31	6	0	-4.887174	-1.274556	-0.000008
32	1	0	-4.224678	-2.138619	-0.000030
33	6	0	4.887174	1.274555	-0.000010
34	1	0	4.224678	2.138618	-0.000045

SCF Done: E(RB3LYP) = -1102.46777462 A.U. after 1 cycles
Convg = 0.9524D-08 -V/T = 2.0145
Zero-point correction= 0.244382 (Hartree/Particle)
Thermal correction to Energy= 0.262562
Thermal correction to Enthalpy= 0.263506
Thermal correction to Gibbs Free Energy= 0.195657
Sum of electronic and zero-point Energies= -1102.223393
Sum of electronic and thermal Energies= -1102.205213
Sum of electronic and thermal Enthalpies= -1102.204268
Sum of electronic and thermal Free Energies= -1102.272117

*Structure **27***

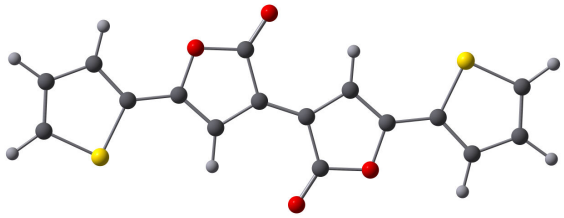


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.096938	-1.610182	-0.102559
2	6	0	0.660651	-0.185972	-0.054933
3	6	0	1.860442	0.591317	-0.041417
4	6	0	2.908596	-0.282835	-0.080847
5	8	0	2.491366	-1.606459	-0.119294
6	1	0	1.943634	1.667591	-0.009275
7	6	0	-0.662505	0.199335	-0.033775
8	6	0	-1.098748	1.623547	0.014102

9	6	0	-1.862317	-0.577914	-0.047620
10	8	0	-2.493195	1.619850	0.030807
11	6	0	-2.910451	0.296265	-0.008086
12	1	0	-1.945534	-1.654180	-0.079972
13	8	0	0.470184	-2.643844	-0.124385
14	8	0	-0.472000	2.657203	0.036206
15	6	0	-4.348730	0.057129	0.003519
16	6	0	-5.265496	1.120210	0.077858
17	6	0	-6.034743	-1.503926	-0.044971
18	6	0	-6.629234	0.821794	0.091344
19	1	0	-4.913674	2.145507	0.123097
20	1	0	-6.311449	-2.556055	-0.095868
21	1	0	-7.365252	1.619755	0.148150
22	6	0	4.346858	-0.043635	-0.093059
23	6	0	5.263698	-1.106746	-0.166186
24	6	0	6.627408	-0.808249	-0.180063
25	1	0	4.911944	-2.132122	-0.210166
26	6	0	6.032773	1.517591	-0.046499
27	1	0	7.363483	-1.606222	-0.235942
28	1	0	6.309399	2.569798	0.003166
29	7	0	-4.728519	-1.238570	-0.057582
30	7	0	4.726561	1.252154	-0.033474
31	6	0	-7.027494	-0.514382	0.030432
32	1	0	-8.077143	-0.794173	0.038374
33	6	0	7.025585	0.528028	-0.120716
34	1	0	8.075217	0.807871	-0.128986

SCF Done: E(RB3LYP) = -1102.47184759 A.U. after 1 cycles
Convg = 0.9390D-08 -V/T = 2.0145
Zero-point correction= 0.243633 (Hartree/Particle)
Thermal correction to Energy= 0.261880
Thermal correction to Enthalpy= 0.262824
Thermal correction to Gibbs Free Energy= 0.194628
Sum of electronic and zero-point Energies= -1102.228215
Sum of electronic and thermal Energies= -1102.209967
Sum of electronic and thermal Enthalpies= -1102.209023
Sum of electronic and thermal Free Energies= -1102.277219

*Structure **28***

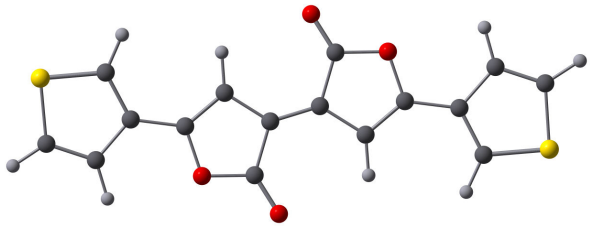


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.049035	-1.644225	-0.002288
2	6	0	-0.657240	-0.212142	-0.002032
3	6	0	-1.875476	0.528667	-0.002411
4	6	0	-2.906510	-0.375508	-0.001252
5	8	0	-2.442815	-1.686952	-0.000369
6	1	0	-1.968782	1.606047	-0.002904
7	6	0	0.657240	0.212142	-0.001935
8	6	0	1.049035	1.644225	-0.002302
9	6	0	1.875476	-0.528667	-0.001990
10	8	0	2.442815	1.686952	0.000009
11	6	0	2.906510	0.375508	-0.000656
12	1	0	1.968783	-1.606047	-0.002341

13	8	0	-0.388935	-2.659026	0.000321
14	8	0	0.388934	2.659026	0.000149
15	6	0	4.330416	0.221307	0.000488
16	6	0	5.281125	1.231310	0.001963
17	16	0	5.097258	-1.354929	0.000119
18	6	0	6.613044	0.738282	0.002797
19	1	0	5.017613	2.283400	0.002411
20	6	0	6.669829	-0.635675	0.001956
21	1	0	7.495666	1.369772	0.003968
22	1	0	7.548917	-1.269841	0.002306
23	6	0	-4.330416	-0.221307	-0.000485
24	6	0	-5.281126	-1.231310	0.000758
25	16	0	-5.097258	1.354929	-0.001102
26	6	0	-6.613045	-0.738282	0.001220
27	1	0	-5.017614	-2.283400	0.001298
28	6	0	-6.669829	0.635675	0.000326
29	1	0	-7.495667	-1.369772	0.002170
30	1	0	-7.548918	1.269841	0.000422

SCF Done: E(RB3LYP) = -1711.83428348 A.U. after 1 cycles
Convg = 0.5296D-08 -V/T = 2.0103
Zero-point correction= 0.199901 (Hartree/Particle)
Thermal correction to Energy= 0.217817
Thermal correction to Enthalpy= 0.218762
Thermal correction to Gibbs Free Energy= 0.150157
Sum of electronic and zero-point Energies= -1711.634382
Sum of electronic and thermal Energies= -1711.616466
Sum of electronic and thermal Enthalpies= -1711.615522
Sum of electronic and thermal Free Energies= -1711.684127

*Structure **29***

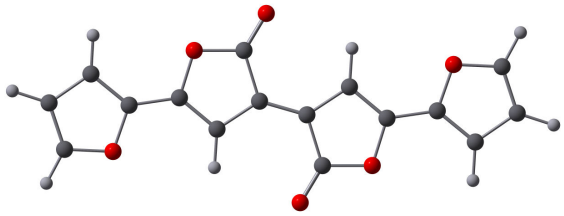


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.074698	-1.630519	-0.064396
2	6	0	-0.658937	-0.204765	-0.023303
3	6	0	-1.868038	0.554631	-0.000616
4	6	0	-2.911096	-0.331111	-0.019713
5	8	0	-2.467834	-1.648766	-0.063942
6	1	0	-1.944997	1.632146	0.025990
7	6	0	0.660948	0.198050	-0.004572
8	6	0	1.076266	1.623825	0.041068
9	6	0	1.870084	-0.561560	-0.006718
10	8	0	2.469126	1.641636	0.070263
11	6	0	2.912650	0.323701	0.044023
12	1	0	1.947418	-1.639042	-0.033592
13	8	0	-0.431465	-2.656385	-0.092243
14	8	0	0.432976	2.649924	0.053803
15	6	0	4.345743	0.138457	0.083181
16	6	0	5.297408	1.219662	0.139656
17	6	0	6.590476	0.780751	0.172845
18	1	0	5.017985	2.267228	0.153552
19	1	0	7.498867	1.369687	0.216112

20	6	0	-4.344768	-0.147302	0.001772
21	6	0	-5.296961	-1.223010	-0.115833
22	6	0	-6.590643	-0.787353	-0.071776
23	1	0	-5.017215	-2.264473	-0.228795
24	1	0	-7.499098	-1.373888	-0.138742
25	6	0	-4.968099	1.082473	0.136666
26	6	0	4.968639	-1.098921	0.078023
27	1	0	-4.507110	2.056003	0.251903
28	1	0	4.508452	-2.078702	0.041614
29	16	0	-6.681534	0.937761	0.118006
30	16	0	6.680731	-0.954496	0.138280

SCF Done: E(RB3LYP) = -1711.83136356 A.U. after 1 cycles
Convg = 0.4311D-08 -V/T = 2.0103
Zero-point correction= 0.199718 (Hartree/Particle)
Thermal correction to Energy= 0.217652
Thermal correction to Enthalpy= 0.218596
Thermal correction to Gibbs Free Energy= 0.150248
Sum of electronic and zero-point Energies= -1711.631646
Sum of electronic and thermal Energies= -1711.613712
Sum of electronic and thermal Enthalpies= -1711.612768
Sum of electronic and thermal Free Energies= -1711.681116

*Structure **30***

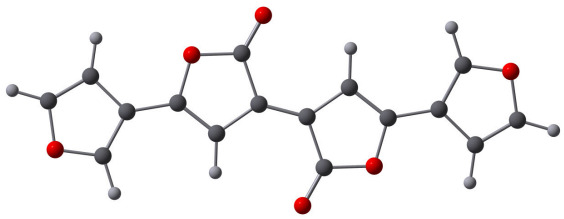


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.098560	-1.608153	0.097488
2	6	0	-0.663747	-0.188997	0.027549
3	6	0	-1.858803	0.590184	0.005955
4	6	0	-2.910596	-0.286449	0.059627
5	8	0	-2.495396	-1.608059	0.115298
6	1	0	-1.931935	1.667063	-0.041765
7	6	0	0.664240	0.192947	-0.003918
8	6	0	1.099144	1.612076	-0.073597
9	6	0	1.859256	-0.586284	0.018256
10	8	0	2.495992	1.611900	-0.091119
11	6	0	2.911125	0.290269	-0.035253
12	1	0	1.932301	-1.663154	0.066122
13	8	0	-0.472130	-2.642953	0.134777
14	8	0	0.472741	2.646858	-0.111729
15	6	0	4.323602	0.083986	-0.041904
16	6	0	5.391238	0.956227	-0.100198
17	6	0	6.567584	0.149893	-0.073155
18	1	0	5.327708	2.034934	-0.156266
19	6	0	6.139741	-1.149092	0.001890
20	1	0	7.596631	0.484005	-0.103158
21	1	0	6.654857	-2.099300	0.047282
22	6	0	-4.323077	-0.080351	0.067041
23	6	0	-5.390496	-0.952784	0.126371
24	6	0	-6.567003	-0.146680	0.099676
25	1	0	-5.326738	-2.031482	0.182176
26	6	0	-6.139430	1.152420	0.025043
27	1	0	-7.595975	-0.480978	0.130195

28	1	0	-6.654770	2.102524	-0.019838
29	8	0	-4.779159	1.213948	0.004533
30	8	0	4.779446	-1.210380	0.021104

SCF Done: E(RB3LYP) = -1065.95951194 A.U. after 1 cycles
Convg = 0.8526D-08 -V/T = 2.0139
Zero-point correction= 0.206606 (Hartree/Particle)
Thermal correction to Energy= 0.223500
Thermal correction to Enthalpy= 0.224444
Thermal correction to Gibbs Free Energy= 0.159547
Sum of electronic and zero-point Energies= -1065.752906
Sum of electronic and thermal Energies= -1065.736012
Sum of electronic and thermal Enthalpies= -1065.735068
Sum of electronic and thermal Free Energies= -1065.799965

*Structure **31***

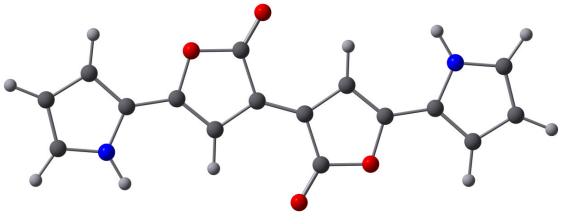


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.145206	1.580092	0.082369
2	6	0	0.667366	0.172808	0.079865
3	6	0	1.843113	-0.638806	0.084678
4	6	0	2.922221	0.201974	0.091176
5	8	0	2.538639	1.537486	0.092587
6	1	0	1.876717	-1.719006	0.089013
7	6	0	-0.668613	-0.172451	0.082919
8	6	0	-1.146165	-1.579753	0.098487
9	6	0	-1.844515	0.638977	0.083922
10	8	0	-2.539533	-1.537314	0.112128
11	6	0	-2.923428	-0.201933	0.100401
12	1	0	-1.878343	1.719173	0.079327
13	8	0	0.548914	2.634099	0.078373
14	8	0	-0.549667	-2.633657	0.101475
15	6	0	-4.344157	0.038000	0.111683
16	6	0	-5.394737	-0.950927	0.210397
17	6	0	-6.565376	-0.260825	0.189764
18	1	0	-5.273869	-2.023164	0.286009
19	1	0	-7.605582	-0.552051	0.237896
20	6	0	4.342868	-0.038417	0.100923
21	6	0	5.394216	0.950801	0.187686
22	6	0	6.564436	0.259891	0.170847
23	1	0	5.274092	2.023771	0.253277
24	1	0	7.604913	0.550996	0.213519
25	8	0	6.324426	-1.089360	0.078119
26	6	0	4.981230	-1.257791	0.036440
27	6	0	-4.983339	1.256341	0.037092
28	1	0	4.629009	-2.277516	-0.040399
29	1	0	-4.631822	2.275430	-0.050750
30	8	0	-6.326338	1.087634	0.083740

SCF Done: E(RB3LYP) = -1065.95073283 A.U. after 1 cycles
Convg = 0.6730D-08 -V/T = 2.0139
Zero-point correction= 0.206649 (Hartree/Particle)
Thermal correction to Energy= 0.223643

```
 Thermal correction to Enthalpy=                  0.224587
 Thermal correction to Gibbs Free Energy=         0.158865
 Sum of electronic and zero-point Energies=          -1065.744083
 Sum of electronic and thermal Energies=             -1065.727090
 Sum of electronic and thermal Enthalpies=           -1065.726146
 Sum of electronic and thermal Free Energies=        -1065.791868
```

*Structure **32***



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---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0       -1.013320   -1.663413    0.000033
      2          6           0       -0.653807   -0.225800    0.000011
      3          6           0       -1.888682    0.487597   -0.000157
      4          6           0       -2.899859   -0.441924   -0.000300
      5          8           0       -2.404977   -1.739933   -0.000220
      6          1           0       -2.001998    1.562661   -0.000195
      7          6           0        0.653807    0.225800    0.000149
      8          6           0        1.013320    1.663414    0.000150
      9          6           0        1.888682   -0.487597    0.000336
     10          8           0        2.404977    1.739933    0.000254
     11          6           0        2.899859    0.441924    0.000391
     12          1           0        2.001998   -1.562661    0.000405
     13          8           0       -0.329107   -2.664936    0.000060
     14          8           0        0.329106    2.664936   -0.000069
     15          6           0        4.321185    0.319790    0.000553
     16          6           0        5.310118    1.311938    0.000635
     17          6           0        6.565576    0.662198    0.000682
     18          1           0        5.121379    2.377519    0.000589
     19          6           0        6.323314   -0.708886    0.000619
     20          1           0        7.541527    1.130851    0.000687
     21          1           0        7.008683   -1.546373    0.000594
     22          6           0       -4.321185   -0.319790   -0.000522
     23          6           0       -5.310119   -1.311938   -0.000666
     24          6           0       -6.565576   -0.662198   -0.000810
     25          1           0       -5.121380   -2.377519   -0.000631
     26          6           0       -6.323315    0.708886   -0.000748
     27          1           0       -7.541527   -1.130851   -0.000915
     28          1           0       -7.008683    1.546373   -0.000802
     29          7           0        4.971480   -0.904319    0.000757
     30          7           0       -4.971480    0.904319   -0.000667
     31          1           0        4.518213   -1.810360    0.001004
     32          1           0       -4.518214    1.810360   -0.000715
 ---------------------------------------------------------------------
SCF Done:  E(RB3LYP) =  -1026.24802616     A.U. after    1 cycles
             Convg  =    0.5294D-08             -V/T =  2.0143
Zero-point correction=                           0.231690 (Hartree/Particle)
 Thermal correction to Energy=                   0.249060
 Thermal correction to Enthalpy=                 0.250004
 Thermal correction to Gibbs Free Energy=        0.183839
 Sum of electronic and zero-point Energies=          -1026.016336
 Sum of electronic and thermal Energies=             -1025.998966
 Sum of electronic and thermal Enthalpies=           -1025.998022
 Sum of electronic and thermal Free Energies=        -1026.064187
```
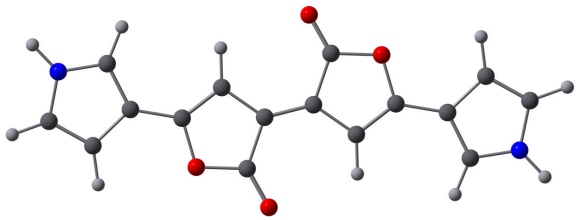
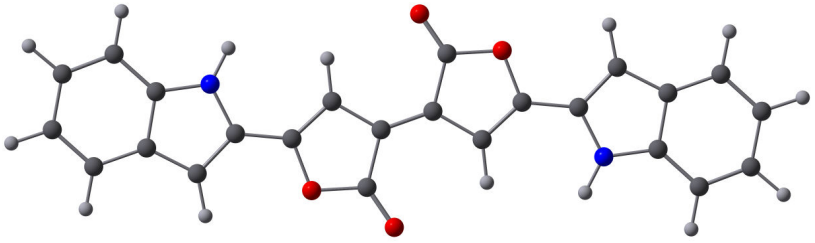

*Structure **33***



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.060822	-1.638356	-0.025763
2	6	0	-0.659118	-0.211561	0.029551
3	6	0	-1.875545	0.535482	0.046087
4	6	0	-2.913334	-0.359137	0.001751
5	8	0	-2.452495	-1.672370	-0.043104
6	1	0	-1.963585	1.611911	0.082586
7	6	0	0.659616	0.201628	0.053363
8	6	0	1.061199	1.628483	0.107575
9	6	0	1.876125	-0.545323	0.037106
10	8	0	2.452868	1.662701	0.124034
11	6	0	2.913827	0.349446	0.080474
12	1	0	1.964239	-1.621760	0.001138
13	8	0	-0.406842	-2.659955	-0.053017
14	8	0	0.407070	2.650000	0.134181
15	6	0	4.341170	0.187544	0.091444
16	6	0	5.325552	1.233103	0.168266
17	6	0	6.563970	0.630841	0.157442
18	1	0	5.129135	2.295418	0.223569
19	1	0	7.559216	1.052046	0.198467
20	6	0	-4.340646	-0.196938	-0.009736
21	6	0	-5.325290	-1.241805	-0.092501
22	6	0	-6.563525	-0.639190	-0.080352
23	1	0	-5.129190	-2.303939	-0.152326
24	1	0	-7.558859	-1.059882	-0.124415
25	6	0	-5.036928	1.014616	0.048971
26	6	0	5.037776	-1.024068	0.037776
27	1	0	-4.680472	2.033380	0.118891
28	1	0	4.681580	-2.043284	-0.026556
29	7	0	-6.368199	0.726576	0.004901
30	7	0	6.369035	-0.735303	0.077567
31	1	0	7.108565	-1.426860	0.048544
32	1	0	-7.107492	1.418359	0.034509

SCF Done: E(RB3LYP) = -1026.24584566 A.U. after 1 cycles
Convg = 0.3189D-08 -V/T = 2.0143
Zero-point correction= 0.231730 (Hartree/Particle)
Thermal correction to Energy= 0.249111
Thermal correction to Enthalpy= 0.250055
Thermal correction to Gibbs Free Energy= 0.184243
Sum of electronic and zero-point Energies= -1026.014116
Sum of electronic and thermal Energies= -1025.996735
Sum of electronic and thermal Enthalpies= -1025.995790
Sum of electronic and thermal Free Energies= -1026.061603

*Structure **34***

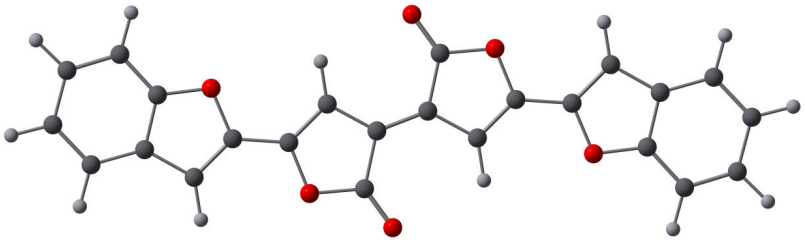


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.117811	-1.594833	-0.134477
2	6	0	0.663864	-0.181938	-0.144969
3	6	0	1.848457	0.609675	-0.179915
4	6	0	2.917397	-0.251437	-0.190663
5	8	0	2.510904	-1.578437	-0.162694
6	1	0	1.891625	1.689793	-0.194929
7	6	0	-0.668918	0.187359	-0.122654
8	6	0	-1.122758	1.600277	-0.131826
9	6	0	-1.853552	-0.604193	-0.087644
10	8	0	-2.515856	1.583996	-0.102741
11	6	0	-2.922422	0.257005	-0.075732
12	1	0	-1.896807	-1.684310	-0.072957
13	8	0	0.501788	-2.638335	-0.108705
14	8	0	-0.506636	2.643703	-0.157829
15	6	0	-4.332514	0.030998	-0.040074
16	6	0	-5.367941	0.961966	-0.046046
17	6	0	-6.592831	0.232686	-0.000288
18	1	0	-5.240320	2.036144	-0.079404
19	6	0	-6.252215	-1.155337	0.035136
20	6	0	4.327521	-0.025475	-0.225373
21	6	0	5.362925	-0.956392	-0.212841
22	6	0	6.587892	-0.227351	-0.260104
23	1	0	5.235242	-2.030396	-0.174440
24	6	0	6.247358	1.160515	-0.302559
25	7	0	-4.878380	-1.248353	0.007939
26	7	0	4.873481	1.253683	-0.277547
27	1	0	-4.350310	-2.111781	0.028253
28	1	0	4.345415	2.116911	-0.305553
29	6	0	7.223215	2.166567	-0.368256
30	6	0	8.555641	1.764218	-0.386333
31	1	0	6.952705	3.219121	-0.402444
32	1	0	9.337643	2.517888	-0.435905
33	6	0	7.951551	-0.601492	-0.278651
34	6	0	8.917546	0.393608	-0.342219
35	1	0	8.235289	-1.650654	-0.243344
36	1	0	9.970699	0.124847	-0.358236
37	6	0	-7.956473	0.606683	0.021920
38	6	0	-8.922347	-0.388771	0.081390
39	1	0	-8.240168	1.656141	-0.003507
40	1	0	-9.975499	-0.120146	0.099581
41	6	0	-7.227930	-2.161738	0.097199
42	6	0	-8.560343	-1.759541	0.118873
43	1	0	-6.957311	-3.214367	0.127841
44	1	0	-9.342174	-2.513372	0.168776

SCF Done: E(RB3LYP) = -1333.56793121 A.U. after 1 cycles
Convg = 0.2233D-08 -V/T = 2.0147
Zero-point correction= 0.324588 (Hartree/Particle)
Thermal correction to Energy= 0.347473
Thermal correction to Enthalpy= 0.348417

```
Thermal correction to Gibbs Free Energy=          0.269811
Sum of electronic and zero-point Energies=          -1333.243343
Sum of electronic and thermal Energies=             -1333.220458
Sum of electronic and thermal Enthalpies=           -1333.219514
Sum of electronic and thermal Free Energies=        -1333.298120
```

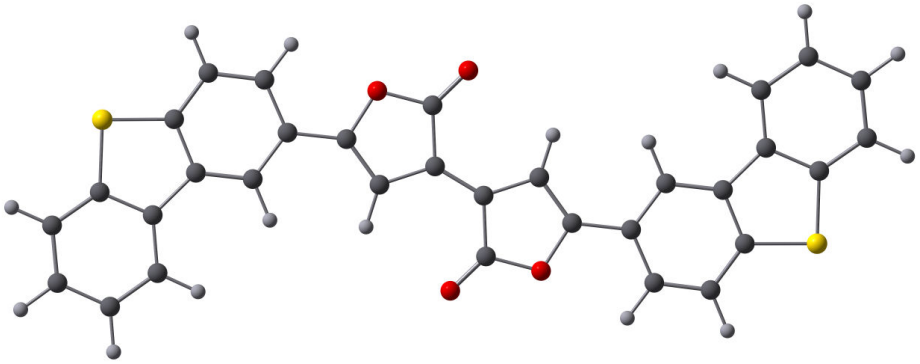
*Structure **35***



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.827829	-3.026779	3.244525
2	6	0	-4.295588	-2.078343	4.289634
3	6	0	-4.890228	-0.984950	3.594124
4	6	0	-4.783821	-1.256529	2.254981
5	8	0	-4.154385	-2.466421	2.007755
6	1	0	-5.340366	-0.104272	4.029322
7	6	0	-4.136238	-2.306444	5.643595
8	6	0	-4.603953	-1.357984	6.688703
9	6	0	-3.541612	-3.399843	6.339109
10	8	0	-4.277404	-1.918340	7.925470
11	6	0	-3.647971	-3.128234	7.678250
12	1	0	-3.091500	-4.280538	5.903916
13	8	0	-3.267845	-4.096411	3.320317
14	8	0	-5.163971	-0.288368	6.612909
15	6	0	-3.230016	-3.863410	8.827815
16	6	0	-3.338728	-3.592120	10.171746
17	6	0	-2.731096	-4.698272	10.853290
18	1	0	-3.795390	-2.710486	10.602607
19	6	0	-2.290445	-5.576719	9.838450
20	6	0	-5.201758	-0.521331	1.105422
21	6	0	-5.092999	-0.792579	-0.238515
22	6	0	-5.700416	0.313697	-0.920052
23	1	0	-4.636285	-1.674181	-0.669386
24	6	0	-6.141432	1.191937	0.094810
25	8	0	-5.837124	0.684412	1.331784
26	8	0	-2.594810	-5.069242	8.601470
27	6	0	-6.792762	2.395807	-0.154664
28	6	0	-7.002228	2.717175	-1.498417
29	1	0	-7.118911	3.046245	0.651663
30	1	0	-7.507871	3.646278	-1.748068
31	6	0	-5.922304	0.661289	-2.268648
32	6	0	-6.572962	1.862114	-2.539318
33	1	0	-5.595287	0.008780	-3.073993
34	1	0	-6.756934	2.152940	-3.570282
35	6	0	-1.639146	-6.780595	10.087939
36	6	0	-1.429359	-7.101778	11.431678
37	1	0	-1.313276	-7.431192	9.281628
38	1	0	-0.923671	-8.030856	11.681331
39	6	0	-2.508953	-5.045713	12.201881
40	6	0	-1.858256	-6.246514	12.472563
41	1	0	-2.835653	-4.393024	13.007209
42	1	0	-1.674055	-6.537210	13.503522

```
SCF Done:  E(RB3LYP) =  -1373.28874065     A.U. after    1 cycles
             Convg  =    0.5368D-08             -V/T =  2.0144
Zero-point correction=                           0.300573 (Hartree/Particle)
 Thermal correction to Energy=                    0.322482
 Thermal correction to Enthalpy=                  0.323426
 Thermal correction to Gibbs Free Energy=         0.247529
 Sum of electronic and zero-point Energies=          -1372.988168
 Sum of electronic and thermal Energies=             -1372.966259
 Sum of electronic and thermal Enthalpies=           -1372.965315
 Sum of electronic and thermal Free Energies=        -1373.041212
```

*Structure **36***

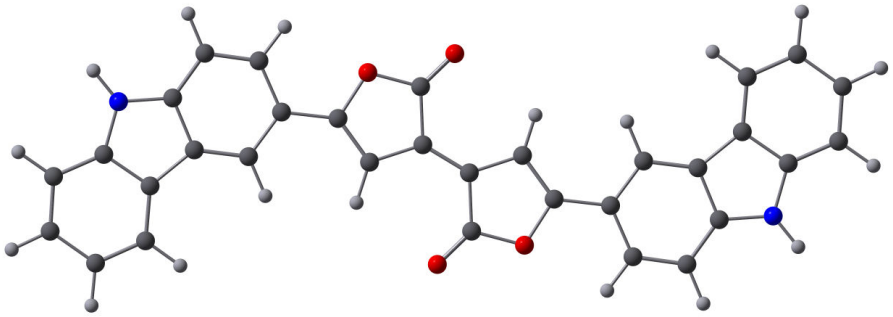


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.571450	1.858867	-0.066741
2	6	0	-0.575323	0.374128	-0.094967
3	6	0	-1.948863	-0.012444	-0.078215
4	6	0	-2.703167	1.130819	-0.041315
5	8	0	-1.901501	2.268215	-0.033407
6	1	0	-2.322895	-1.025913	-0.091611
7	6	0	0.577448	-0.385388	-0.130955
8	6	0	0.575426	-1.869775	-0.173145
9	6	0	1.950320	0.003146	-0.149957
10	8	0	1.905922	-2.276817	-0.223713
11	6	0	2.705889	-1.138390	-0.205700
12	1	0	2.322802	1.017023	-0.129703
13	8	0	0.335181	2.662298	-0.069697
14	8	0	-0.330064	-2.674438	-0.170018
15	6	0	4.139652	-1.355194	-0.251014
16	6	0	5.024947	-0.263661	-0.177409
17	6	0	4.659994	-2.669263	-0.369273
18	6	0	6.405018	-0.474899	-0.219353
19	1	0	4.639916	0.748106	-0.085067
20	6	0	6.030480	-2.894953	-0.415622
21	1	0	3.976673	-3.509692	-0.426027
22	6	0	6.898984	-1.799280	-0.339704
23	1	0	6.412658	-3.908134	-0.507602
24	6	0	-4.136574	1.352479	-0.009413
25	6	0	-4.652774	2.673031	0.022367
26	6	0	-5.025102	0.260912	-0.010963
27	6	0	-6.022412	2.906024	0.051818
28	1	0	-3.966546	3.512976	0.023633
29	6	0	-6.404524	0.479380	0.019365
30	1	0	-4.643555	-0.756181	-0.035193
31	6	0	-6.894215	1.810442	0.050146
32	1	0	-6.401204	3.924312	0.075615
33	6	0	8.756140	-0.100469	-0.220299

34	6	0	9.933459	0.653862	-0.174661
35	6	0	7.481361	0.506078	-0.148824
36	6	0	9.828203	2.040696	-0.054220
37	1	0	10.908631	0.177027	-0.230631
38	6	0	7.399592	1.904018	-0.026899
39	6	0	8.568002	2.662541	0.018886
40	1	0	10.731759	2.643972	-0.017162
41	1	0	6.429837	2.392184	0.031283
42	1	0	8.506111	3.743669	0.112288
43	6	0	-8.757127	0.114242	0.058064
44	6	0	-9.937109	-0.637243	0.067738
45	6	0	-7.484644	-0.500237	0.024540
46	6	0	-9.836788	-2.029359	0.043011
47	1	0	-10.910607	-0.154237	0.093517
48	6	0	-7.407861	-1.903366	0.000139
49	6	0	-8.578869	-2.659199	0.009757
50	1	0	-10.742435	-2.630616	0.049995
51	1	0	-6.439723	-2.397205	-0.025794
52	1	0	-8.520924	-3.744407	-0.008748
53	16	0	-8.651712	1.880629	0.085235
54	16	0	8.656812	-1.861099	-0.372680

SCF Done: E(RB3LYP) = -2326.48949315 A.U. after 1 cycles
Convg = 0.3432D-08 -V/T = 2.0118
Zero-point correction= 0.388213 (Hartree/Particle)
Thermal correction to Energy= 0.416835
Thermal correction to Enthalpy= 0.417779
Thermal correction to Gibbs Free Energy= 0.324750
Sum of electronic and zero-point Energies= -2326.101280
Sum of electronic and thermal Energies= -2326.072658
Sum of electronic and thermal Enthalpies= -2326.071714
Sum of electronic and thermal Free Energies= -2326.164743

*Structure **37***



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.641861	1.838021	0.019732
2	6	0	-0.591004	0.358887	-0.073951
3	6	0	-1.949051	-0.077309	-0.089085
4	6	0	-2.748369	1.034655	-0.010437
5	8	0	-1.985786	2.198869	0.053777
6	1	0	-2.283846	-1.102510	-0.150761
7	6	0	0.590712	-0.357678	-0.123939
8	6	0	0.641880	-1.836856	-0.216727
9	6	0	1.948659	0.078767	-0.108336
10	8	0	1.985899	-2.197534	-0.249488
11	6	0	2.748221	-1.033100	-0.185645
12	1	0	2.283182	1.104041	-0.046744
13	8	0	0.234665	2.674747	0.067871

14	8	0	-0.234528	-2.673687	-0.264987
15	6	0	4.186249	-1.200717	-0.213828
16	6	0	5.031876	-0.072091	-0.177777
17	6	0	4.753402	-2.503421	-0.277151
18	6	0	6.413198	-0.248192	-0.204945
19	1	0	4.610246	0.928088	-0.131326
20	6	0	6.128427	-2.699486	-0.302392
21	1	0	4.092694	-3.363185	-0.306055
22	6	0	6.954867	-1.567858	-0.265273
23	1	0	6.544659	-3.702452	-0.349854
24	6	0	-4.186351	1.202704	0.018974
25	6	0	-4.752836	2.505527	0.086406
26	6	0	-5.032514	0.074569	-0.019181
27	6	0	-6.127735	2.702155	0.113615
28	1	0	-4.091706	3.364883	0.117027
29	6	0	-6.413746	0.251203	0.010028
30	1	0	-4.611311	-0.925636	-0.068993
31	6	0	-6.954687	1.570987	0.074550
32	1	0	-6.543478	3.705175	0.164248
33	7	0	8.331350	-1.478895	-0.277606
34	1	0	8.965544	-2.266741	-0.323329
35	7	0	-8.331197	1.482670	0.088447
36	1	0	-8.964914	2.270762	0.136570
37	6	0	8.716206	-0.141171	-0.229016
38	6	0	9.999835	0.415102	-0.223104
39	6	0	7.546044	0.664116	-0.182883
40	6	0	10.098809	1.807479	-0.168782
41	1	0	10.889224	-0.209557	-0.258883
42	6	0	7.672590	2.060109	-0.128928
43	6	0	8.949958	2.623496	-0.122530
44	1	0	11.082771	2.269838	-0.162758
45	1	0	6.791688	2.696741	-0.092684
46	1	0	9.062974	3.703622	-0.081068
47	6	0	-8.716785	0.145306	0.036644
48	6	0	-10.000703	-0.410304	0.031081
49	6	0	-7.547106	-0.660478	-0.013156
50	6	0	-10.100498	-1.802482	-0.026799
51	1	0	-10.889709	0.214723	0.069717
52	6	0	-7.674484	-2.056266	-0.070610
53	6	0	-8.952152	-2.618980	-0.076711
54	1	0	-11.084709	-2.264304	-0.032685
55	1	0	-6.793973	-2.693276	-0.109603
56	1	0	-9.065785	-3.698935	-0.120794

```
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SCF Done:  E(RB3LYP) =  -1640.89556239     A.U. after    1 cycles
            Convg  =    0.3315D-08             -V/T =  2.0149
Zero-point correction=                           0.418929 (Hartree/Particle)
 Thermal correction to Energy=                    0.446954
 Thermal correction to Enthalpy=                  0.447898
 Thermal correction to Gibbs Free Energy=         0.358220
 Sum of electronic and zero-point Energies=          -1640.476633
 Sum of electronic and thermal Energies=             -1640.448608
 Sum of electronic and thermal Enthalpies=           -1640.447664
 Sum of electronic and thermal Free Energies=        -1640.537342
```