Supplementary Material for Organic & Biomolecular Chemistry

Supporting Information:

Design principles for α-tocopherol analogues

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i. Table of calculated *vs* experimental IP values for reference compounds.

compound	calculated IP / eV	Experimental IP / eV		
		Median	Lowest	Highest
4-methoxyphenol	7.51	7.75	7.50	8.00
4-methoxytoluene	7.63	7.90	7.83	8.30
dimethyl telluride	7.82	7.89	7.85	7.93
thioanisole	7.77	7.94	7.90	8.90
hydroquinone	7.77	7.94	7.93	7.95
2-methoxythiophene	7.76	8.14	8.02	8.30
anisole	7.95	8.20	8.10	8.80
4-methylphenol	7.93	8.34	8.13	8.97
benzo[b]thiophene	7.98	8.17	8.13	8.73
2-methylthiophene	8.26	8.61	8.14	8.63
phenol	8.30	8.49	8.21	9.10
tellurophene	8.33	8.36	8.27	8.60
benzenethiol	8.18	8.30	8.28	9.00
Benzo[b]furan	8.16	8.36	8.29	8.85
2-methylfuran	8.31	8.38	8.31	8.57
2-methylselenophene	8.09	8.39	8.37	8.40
tetrahydrothiophene	8.31	8.38	8.38	8.62
2-acetylselenophene	8.71	9.01	8.72	9.30
selenophene	8.60	8.96	8.78	9.01
thiophene	8.77	8.86	8.80	9.12
furan	8.88	8.88	8.83	9.00
2-acetylfuran	9.02	9.15	9.02	9.27
tetrahydrofuran	8.99	9.40	9.38	9.54
ethyl 4-methylphenyl selenide	7.25	7.10		
2,2-Dimethyl-2,3-dihydrobenzo[b]selenophene	7.28	7.30		
2-(methylthio)tellurophene	7.38	8.15		
ethyl phenyl selenide	7.47	7.60		
methyl 2-methylphenyl selenide	7.49	7.50		
benzo[b]tellurophene	7.55	7.76		
2-(methylthio)selenophene	7.56	8.75		
selenoanisole	7.59	7.40		
2-(methylthio)thiophene	7.68	8.10		
benzo[b]selenophene	7.82	8.03		
2-methyltellurophene	7.91	8.25		
benzeneselenol	8.00	7.70		

resorcinol	8.10	8.20		
2-acetyltellurophene	8.36	8.60		
2-acetylthiophene	8.94	9.20		

Table of calculated *vs* experimental BDE values for reference compounds

Phenol	Calc. BDE / kcal mol^{-1}	Exp. BDE / kcal mol^{-1}
unsubstituted	86.98	87.20
4-methyl-	84.12	85.10
4-*t*-butyl-	84.96	84.20
4-methoxy-	80.94	81.71
2,6-dimethyl-	82.32	83.40
2,6-dimethoxy-	81.66	82.06
3,5-di-*t*-butyl-	85.11	85.52
3,5-dimethoxy-	84.55	85.60
2,4,6-trimethyl-	80.36	81.63
2,4,6-trimethoxy-	77.79	78.90
2,3,6-trimethyl-4-methoxy-	76.61	78.10
2,3,5,6-tetramethyl-4-methoxy-	79.07	80.78
6a	75.19	77.15

ii. Geometrical parameters and ΔBDE values for compounds **4-7 a-d**.[a]

Compound	dihedral ϕ / °	bonding angle σ / °	sum of aromatic angles λ / °	ΔBDE / kcal mol^{-1}
4a	0.0	87.8	187.2	-1.79
5a	9.4	107.7	221.5	-1.46
6a	16.6	118.5	242.5	0.00
7a	0.0	118.4	234.0	5.75
4b	0.0	72.2	200.1	-0.18
5b	16.2	89.9	226.6	0.81
6b	16.6	102.3	246.4	0.71
7b	0.0	102.5	236.7	6.14
4c	0.0	69.3	202.7	0.19
5c	16.5	86.3	227.6	1.14
6c	6.7	100.3	247.2	0.94
7c	0.0	99.9	237.6	6.28
4d	0.0	65.3	206.2	0.54
5d	16.1	81.8	229.1	1.37
6d	30.4	97.4	238.2	1.67
7d	0.0	96.8	238.8	7.04

[a] BDE values given relative to the calculated value for HPMC (**6a**).

iii. Absolute energies (a.u.), energy corrections (a.u.) and cartesian coordinates for compounds **4-6**.

4a antioxidant

E(RB+HF-LYP) = -617.239609424 (LANL2DZ)
E(RB+HF-LYP) = -617.422407455 (LANL2DZdp)
Zero-point correction= 0.253377
Thermal correction to Enthalpy= 0.269845

1	6	0	0.354517	2.858704	0.000000
2	6	0	-0.065560	1.407001	0.000000
3	6	0	-0.984045	-1.406088	0.000000
4	6	0	0.795867	0.318037	0.000000
5	6	0	-1.441444	1.030042	0.000000
6	6	0	-1.909183	-0.309851	0.000000
7	6	0	0.343211	-1.002593	0.000000
8	6	0	3.054046	0.011863	1.283334
9	8	0	-2.344305	2.119263	0.000000
10	6	0	-3.410788	-0.556929	0.000000
11	8	0	1.632333	-1.637519	-0.000001
12	6	0	-1.384486	-2.867523	0.000000
13	1	0	-3.276904	1.826885	-0.000001
14	1	0	1.446064	2.952880	0.000010
15	1	0	-0.042816	3.382832	0.878420
16	1	0	-0.042799	3.382827	-0.878430
17	1	0	-3.898330	-0.128574	0.890060
18	1	0	-3.640012	-1.624764	0.000008
19	1	0	-3.898329	-0.128586	-0.890066
20	1	0	-1.979626	-3.129813	0.885552
21	1	0	-0.491329	-3.500393	-0.000003
22	1	0	-1.979630	-3.129811	-0.885551
23	6	0	2.252801	-0.183456	0.000000
24	6	0	3.054047	0.011863	-1.283334
25	1	0	2.441145	-0.219162	-2.160243
26	1	0	3.932648	-0.644601	-1.286001
27	1	0	3.398998	1.051841	-1.361312
28	1	0	2.441144	-0.219164	2.160243
29	1	0	3.398997	1.051841	1.361314
30	1	0	3.932648	-0.644601	1.286001

4a phenoxyl radical

E(ROB+HF-LYP) = -616.794678799
Thermal correction to Enthalpy= 0.256470

1	6	0	-0.464296	2.881407	0.000000
2	6	0	0.005055	1.449920	0.000000
3	6	0	1.086197	-1.347636	0.000000
4	6	0	-0.787873	0.331258	0.000000
5	6	0	1.456499	1.158185	0.000000
6	6	0	1.958254	-0.235459	0.000000
7	6	0	-0.265282	-0.980492	0.000000
8	6	0	-3.026429	-0.106857	-1.284368
9	8	0	2.302034	2.140637	0.000000
10	6	0	3.460894	-0.393744	0.000000
11	8	0	-1.497278	-1.669569	0.000000
12	6	0	1.522005	-2.799126	0.000000
13	1	0	-1.558024	2.947927	-0.000002
14	1	0	-0.074991	3.415207	-0.876087
15	1	0	-0.074993	3.415207	0.876088
16	1	0	3.898876	0.104255	-0.874496
17	1	0	3.767993	-1.443034	0.000000
18	1	0	3.898876	0.104255	0.874496
19	1	0	2.126266	-3.038393	-0.884549
20	1	0	0.648963	-3.459620	0.000000
21	1	0	2.126266	-3.038393	0.884549
22	6	0	-2.218447	-0.245666	0.000000
23	6	0	-3.026429	-0.106857	1.284368
24	1	0	-2.401258	-0.296330	2.162411
25	1	0	-3.862640	-0.815936	1.286772
26	1	0	-3.435179	0.909486	1.360674
27	1	0	-2.401258	-0.296330	-2.162411
28	1	0	-3.435179	0.909486	-1.360673
29	1	0	-3.862640	-0.815935	-1.286772

4a radical cation

E(UB+HF-LYP) = -616.986015523
Zero-point correction= 0.253932

1	6	0	0.406234	2.882526	0.000000
2	6	0	-0.007257	1.435521	0.000000
3	6	0	-1.036871	-1.395319	0.000000
4	6	0	0.816894	0.341387	0.000000
5	6	0	-1.416175	1.053287	0.000000
6	6	0	-1.928362	-0.307214	0.000000
7	6	0	0.324109	-0.990857	0.000000
8	6	0	3.063604	-0.062237	1.289230
9	8	0	-2.266598	2.116813	0.000000
10	6	0	-3.431600	-0.500782	0.000000
11	8	0	1.514277	-1.659936	0.000000
12	6	0	-1.427897	-2.852671	0.000000
13	1	0	-3.225249	1.902323	0.000000
14	1	0	1.494997	2.982376	0.000002
15	1	0	0.005763	3.403846	0.877924
16	1	0	0.005766	3.403845	-0.877927
17	1	0	-3.901560	-0.060586	0.892213
18	1	0	-3.697313	-1.558686	0.000000
19	1	0	-3.901560	-0.060586	-0.892212
20	1	0	-2.025935	-3.107040	0.884273
21	1	0	-0.541022	-3.492091	-0.000001
22	1	0	-2.025936	-3.107040	-0.884272
23	6	0	2.271224	-0.178502	0.000000
24	6	0	3.063604	-0.062236	-1.289229
25	1	0	2.441301	-0.241414	-2.170894
26	1	0	3.893889	-0.776132	-1.288410
27	1	0	3.487596	0.948146	-1.363634
28	1	0	2.441301	-0.241414	2.170894
29	1	0	3.487596	0.948146	1.363634
30	1	0	3.893889	-0.776132	1.288410

4b antioxidant

E(RB+HF-LYP) = -552.145325717 (LANL2DZ)
E(ROB+HF-LYP) = -552.324294912 (LANL2DZdp)
Zero-point correction= 0.251542
Thermal correction to Enthalpy= 0.268303

1	6	0	0.140908	2.888354	-0.000031
2	6	0	-0.258268	1.428566	-0.000015
3	6	0	-1.142688	-1.360914	-0.000042
4	6	0	0.636806	0.357175	0.000010
5	6	0	-1.627987	1.052629	-0.000052
6	6	0	-2.086699	-0.288431	-0.000009
7	6	0	0.196377	-0.974730	-0.000031
8	6	0	2.877437	0.631317	1.281398
9	8	0	-2.535174	2.134711	0.000043
10	6	0	-3.586011	-0.549063	0.000160
11	16	0	1.858612	-1.802067	-0.000062
12	6	0	-1.546171	-2.822922	-0.000067
13	1	0	3.910812	0.263247	1.298787
14	1	0	1.229275	3.005103	0.000592
15	1	0	-0.266432	3.405385	0.877980
16	1	0	-0.265349	3.405067	-0.878748
17	1	0	-3.807544	-1.618196	0.000423
18	1	0	-4.077006	-0.124582	-0.889872
19	1	0	-4.076798	-0.124184	0.890108
20	1	0	-2.141336	-3.083983	0.885787
21	1	0	-0.658238	-3.463714	-0.000662
22	1	0	-2.142344	-3.083698	-0.885312
23	6	0	2.161059	0.188519	0.000037
24	6	0	2.877473	0.631462	-1.281253
25	1	0	2.361554	0.260747	-2.172470
26	1	0	3.910867	0.263448	-1.298634
27	1	0	2.908959	1.730119	-1.330244
28	1	0	2.361463	0.260546	2.172559
29	1	0	2.908988	1.729967	1.330497
30	1	0	-3.466683	1.838339	-0.000779

4b phenoxyl radical
E(ROB+HF-LYP) = -551.693871113
Thermal correction to Enthalpy= 0.254795

1	6	0	-0.268525	2.914457	0.000002
2	6	0	0.189112	1.476956	-0.000004
3	6	0	1.246850	-1.289460	-0.000001
4	6	0	-0.634977	0.372185	-0.000004
5	6	0	1.635897	1.195009	-0.000013
6	6	0	2.133774	-0.194782	-0.000003
7	6	0	-0.119341	-0.949605	-0.000002
8	6	0	-2.890957	0.503460	-1.281987
9	8	0	2.478980	2.178886	0.000000
10	6	0	3.635740	-0.361323	0.000002
11	16	0	-1.704521	-1.860803	0.000000
12	6	0	1.696005	-2.738271	0.000005
13	1	0	-3.898990	0.071432	-1.297741
14	1	0	-1.360244	2.996632	-0.000020
15	1	0	0.127031	3.444096	-0.875844
16	1	0	0.126992	3.444077	0.875878
17	1	0	3.939626	-1.411086	-0.000025
18	1	0	4.075933	0.135325	0.874365
19	1	0	4.075944	0.135376	-0.874326
20	1	0	2.302265	-2.972639	-0.884480
21	1	0	0.833355	-3.413418	0.000026
22	1	0	2.302295	-2.972623	0.884474
23	6	0	-2.148258	0.114721	0.000001
24	6	0	-2.890949	0.503463	1.281992
25	1	0	-2.353400	0.168613	2.174515
26	1	0	-3.898983	0.071439	1.297752
27	1	0	-2.992063	1.597538	1.330763
28	1	0	-2.353412	0.168611	-2.174513
29	1	0	-2.992075	1.597534	-1.330759

4b radical cation
E(UB+HF-LYP) = -551.892750515
Zero-point correction= 0.252107

1	6	0	-0.211216	2.911796	0.000001
2	6	0	0.194558	1.459786	-0.000003
3	6	0	1.186746	-1.338606	0.000001
4	6	0	-0.661982	0.379110	-0.000003
5	6	0	1.592650	1.088109	-0.000004
6	6	0	2.096376	-0.264862	-0.000003
7	6	0	-0.184015	-0.961621	0.000000
8	6	0	-2.918353	0.547343	-1.286668
9	8	0	2.445692	2.154261	0.000004
10	6	0	3.598690	-0.470369	-0.000004
11	16	0	-1.730347	-1.849798	0.000002
12	6	0	1.601065	-2.791593	0.000003
13	1	0	-3.929989	0.127341	-1.294926
14	1	0	-1.298442	3.024427	-0.000038
15	1	0	0.193534	3.430327	-0.877527
16	1	0	0.193468	3.430304	0.877573
17	1	0	3.860391	-1.529026	-0.000028
18	1	0	4.071568	-0.031971	0.891618
19	1	0	4.071572	-0.031931	-0.891603
20	1	0	2.203106	-3.037026	-0.883975
21	1	0	0.730830	-3.454753	0.000034
22	1	0	2.203157	-3.037010	0.883951
23	6	0	-2.183471	0.177859	-0.000001
24	6	0	-2.918349	0.547349	1.286667
25	1	0	-2.388460	0.210775	2.182863
26	1	0	-3.929988	0.127353	1.294926
27	1	0	-3.015495	1.641482	1.338866
28	1	0	-2.388462	0.210769	-2.182864
29	1	0	-3.015505	1.641475	-1.338869
30	1	0	3.402528	1.934333	0.000008

4c antioxidant
E(RB+HF-LYP) = -551.267770617 (LANL2DZ)
E(ROB+HF-LYP) = -551.438499535 (LANL2DZdp)
Zero-point correction= 0.250443
Thermal correction to Enthalpy= 0.267664

1	6	0	0.897624	3.002997	0.000014
2	6	0	0.926496	1.489525	-0.000001
3	6	0	1.117042	-1.422871	-0.000007
4	6	0	-0.206236	0.668764	-0.000002
5	6	0	2.166515	0.798839	-0.000012
6	6	0	2.292226	-0.611640	0.000004
7	6	0	-0.095855	-0.733389	-0.000010
8	6	0	-2.269636	1.582393	-1.280365
9	8	0	3.306034	1.632265	-0.000003
10	6	0	3.685421	-1.224020	0.000034
11	34	0	-2.019833	-1.161703	0.000000
12	6	0	1.164060	-2.938837	-0.000004
13	1	0	-3.365672	1.534473	-1.301766
14	1	0	-0.127522	3.384379	-0.000187
15	1	0	1.419842	3.403519	-0.878089
16	1	0	1.419479	3.403499	0.878347
17	1	0	3.644485	-2.315080	0.000310
18	1	0	4.264190	-0.929233	0.889800
19	1	0	4.264044	-0.929680	-0.889980
20	1	0	1.681292	-3.333343	-0.885509
21	1	0	0.150229	-3.352936	-0.000044
22	1	0	1.681217	-3.333343	0.885544
23	6	0	-1.717243	0.938508	0.000001
24	6	0	-2.269619	1.582402	1.280369
25	1	0	-1.883312	1.084536	2.175320
26	1	0	-3.365655	1.534510	1.301773
27	1	0	-1.978724	2.643021	1.321917
28	1	0	-1.883321	1.084539	-2.175318
29	1	0	-1.978772	2.643020	-1.321914
30	1	0	4.139487	1.121876	-0.000303

4c phenoxyl radical
E(ROB+HF-LYP) = -550.807462674
Thermal correction to Enthalpy= 0.254128

1	6	0	0.789626	3.068540	0.000003
2	6	0	0.868943	1.561256	-0.000002
3	6	0	1.208205	-1.371900	-0.000001
4	6	0	-0.211044	0.700397	-0.000003
5	6	0	2.200917	0.932836	-0.000003
6	6	0	2.340390	-0.534764	-0.000002
7	6	0	-0.037230	-0.711136	-0.000002
8	6	0	-2.323970	1.498780	-1.281125
9	8	0	3.260659	1.678712	-0.000002
10	6	0	3.754325	-1.068991	0.000003
11	34	0	-1.908038	-1.231401	0.000001
12	6	0	1.290197	-2.886831	0.000002
13	1	0	-3.415458	1.390364	-1.302205
14	1	0	-0.244502	3.425912	-0.000040
15	1	0	1.307185	3.480254	-0.875640
16	1	0	1.307107	3.480246	0.875696
17	1	0	3.788599	-2.161321	-0.000033
18	1	0	4.303801	-0.696912	0.874366
19	1	0	4.303829	-0.696850	-0.874316
20	1	0	1.820515	-3.262794	-0.884488
21	1	0	0.289023	-3.332130	-0.000005
22	1	0	1.820502	-3.262791	0.884500
23	6	0	-1.735112	0.893643	-0.000001
24	6	0	-2.323965	1.498784	1.281123
25	1	0	-1.909068	1.026272	2.176941
26	1	0	-3.415453	1.390374	1.302205
27	1	0	-2.093326	2.573689	1.321625
28	1	0	-1.909072	1.026269	-2.176943
29	1	0	-2.093337	2.573686	-1.321629

4c radical cation
E(UB+HF-LYP) = -551.018811884
Zero-point correction= 0.251090

1	6	0	0.840652	3.046920	0.000000

2	6	0	0.869959	1.538318	-0.000004
3	6	0	1.138773	-1.407604	-0.000003
4	6	0	-0.234337	0.706333	-0.000004
5	6	0	2.132216	0.839133	-0.000003
6	6	0	2.287245	-0.593013	-0.000005
7	6	0	-0.100686	-0.712493	-0.000002
8	6	0	-2.337263	1.538948	-1.285692
9	8	0	3.222429	1.664525	0.000005
10	6	0	3.692862	-1.163895	-0.000001
11	34	0	-1.932103	-1.216956	0.000003
12	6	0	1.192370	-2.918431	0.000000
13	1	0	-3.428792	1.445130	-1.299447
14	1	0	-0.182338	3.430423	-0.000046
15	1	0	1.363079	3.446775	-0.877398
16	1	0	1.362996	3.446767	0.877451
17	1	0	3.685748	-2.254379	-0.000042
18	1	0	4.259343	-0.855279	0.891444
19	1	0	4.259377	-0.855215	-0.891402
20	1	0	1.717374	-3.301806	-0.883962
21	1	0	0.188723	-3.354974	-0.000024
22	1	0	1.717332	-3.301802	0.883988
23	6	0	-1.750226	0.952906	-0.000002
24	6	0	-2.337256	1.538956	1.285688
25	1	0	-1.930367	1.067254	2.185446
26	1	0	-3.428786	1.445147	1.299446
27	1	0	-2.100725	2.612116	1.329506
28	1	0	-1.930372	1.067247	-2.185449
29	1	0	-2.100741	2.612110	-1.329514
30	1	0	4.094381	1.214311	0.000016

4d antioxidant

E(RB+HF-LYP) = -550.091183384 (LANL2DZ)
E(ROB+HF-LYP) = -550.253496841 (LANL2DZdp)
Zero-point correction= 0.250311
Thermal correction to Enthalpy= 0.267482

1	6	0	1.684066	2.910110	-0.000006
2	6	0	1.459525	1.411710	0.000005
3	6	0	1.197233	-1.484872	0.000000
4	6	0	0.203707	0.784941	0.000011
5	6	0	2.577482	0.539633	-0.000002
6	6	0	2.484765	-0.872548	0.000006
7	6	0	0.096194	-0.622216	0.000003
8	6	0	-1.606020	2.135376	-1.279377
9	8	0	3.832528	1.186312	-0.000008
10	6	0	3.766421	-1.693374	0.000019
11	52	0	-2.035025	-0.765150	-0.000007
12	6	0	1.014871	-2.991547	-0.000003
13	1	0	-2.683821	2.340520	-1.304016
14	1	0	0.741180	3.462581	0.000173
15	1	0	2.267116	3.215534	-0.878125
16	1	0	2.267437	3.215497	0.877909
17	1	0	3.558246	-2.765100	0.000194
18	1	0	4.383190	-1.490893	0.890000
19	1	0	4.383050	-1.491148	-0.890118
20	1	0	1.466107	-3.460338	-0.885429
21	1	0	-0.049779	-3.248948	-0.000114
22	1	0	1.465915	-3.460314	0.885536
23	6	0	-1.219448	1.370576	0.000008
24	6	0	-1.606038	2.135354	1.279403
25	1	0	-1.341417	1.571617	2.179636
26	1	0	-2.683844	2.340477	1.304039
27	1	0	-1.081790	3.102814	1.313601
28	1	0	-1.341405	1.571647	-2.179616
29	1	0	-1.081752	3.102827	-1.313559
30	1	0	4.576078	0.551653	-0.000097

4d phenoxyl radical

E(ROB+HF-LYP) = -549.621797402
Thermal correction to Enthalpy= 0.253847

1	6	0	1.631205	2.974821	-0.000007
2	6	0	1.431462	1.477679	0.000001
3	6	0	1.260745	-1.458066	0.000000
4	6	0	0.209332	0.825483	0.000003
5	6	0	2.635691	0.631470	0.000003
6	6	0	2.521904	-0.835572	-0.000001
7	6	0	0.137066	-0.600282	0.000002
8	6	0	-1.649839	2.109292	-1.279690
9	8	0	3.807483	1.185417	-0.000004
10	6	0	3.821969	-1.606886	-0.000002
11	52	0	-1.959958	-0.810068	0.000000
12	6	0	1.086918	-2.966136	-0.000002
13	1	0	-2.733917	2.277124	-1.304400
14	1	0	0.684397	3.521581	0.000059
15	1	0	2.217369	3.281882	-0.875430
16	1	0	2.217492	3.281873	0.875336
17	1	0	3.666899	-2.688735	-0.000079
18	1	0	4.427528	-1.336045	0.874539
19	1	0	4.427597	-1.335925	-0.874456
20	1	0	1.545731	-3.427199	-0.884339
21	1	0	0.024990	-3.237782	0.000014
22	1	0	1.545760	-3.427205	0.884316
23	6	0	-1.234077	1.363517	0.000003
24	6	0	-1.649844	2.109287	1.279698
25	1	0	-1.363121	1.558570	2.181253
26	1	0	-2.733923	2.277111	1.304407
27	1	0	-1.160460	3.094365	1.311964
28	1	0	-1.363118	1.558576	-2.181247
29	1	0	-1.160448	3.094367	-1.311953

4d radical cation

E(UB+HF-LYP) = -549.847772828
Zero-point correction= 0.250929

1	6	0	1.661579	2.945158	-0.000003
2	6	0	1.424804	1.453280	0.000001
3	6	0	1.192669	-1.480921	0.000001
4	6	0	0.186111	0.826065	0.000003
5	6	0	2.550723	0.559237	0.000000
6	6	0	2.464378	-0.873773	0.000000
7	6	0	0.079565	-0.597810	0.000002
8	6	0	-1.660288	2.134691	-1.284126
9	8	0	3.766842	1.192616	-0.000002
10	6	0	3.754161	-1.673653	0.000002
11	52	0	-1.981425	-0.797526	-0.000003
12	6	0	1.003625	-2.982229	0.000002
13	1	0	-2.740653	2.317842	-1.300167
14	1	0	0.725701	3.507914	0.000064
15	1	0	2.247550	3.245012	-0.877169
16	1	0	2.247673	3.244998	0.877083
17	1	0	3.565446	-2.747739	-0.000056
18	1	0	4.364418	-1.463555	0.891225
19	1	0	4.364474	-1.463466	-0.891161
20	1	0	1.459142	-3.446551	-0.883726
21	1	0	-0.057355	-3.253184	0.000024
22	1	0	1.459181	-3.446554	0.883708
23	6	0	-1.239032	1.407688	0.000003
24	6	0	-1.660295	2.134679	1.284137
25	1	0	-1.381772	1.585998	2.189462
26	1	0	-2.740659	2.317836	1.300170
27	1	0	-1.164226	3.115580	1.321518
28	1	0	-1.381754	1.586021	-2.189455
29	1	0	-1.164222	3.115594	-1.321491
30	1	0	4.548413	0.600199	0.000006

5a antioxidant

E(RB+HF-LYP) = -656.594996547 (LANL2DZ)
E(ROB+HF-LYP) = -656.786666463 (LANL2DZdp)
Zero-point correction= 0.283252
Thermal correction to Enthalpy= 0.300548

1	6	0	-1.010529	2.974792	-0.046127
2	6	0	-0.908486	1.459438	-0.041015
3	6	0	-0.777543	-1.422370	-0.051107
4	6	0	0.321017	0.788406	-0.091455

5	6	0	-2.074334	0.651061	0.009058
6	6	0	-2.035199	-0.761061	0.002533
7	6	0	0.364850	-0.613847	-0.095906
8	6	0	1.740521	1.323278	-0.193046
9	8	0	-3.358979	1.244561	0.067377
10	6	0	-3.322628	-1.561018	0.053579
11	8	0	1.678933	-1.115894	-0.162348
12	6	0	-0.661675	-2.932732	-0.061975
13	1	0	1.969619	2.088480	0.559014
14	1	0	1.929615	1.765411	-1.181843
15	6	0	2.625937	0.048020	0.026494
16	6	0	3.737108	-0.118980	-1.013636
17	6	0	3.152781	-0.043199	1.469034
18	1	0	-3.308420	2.220606	0.062066
19	1	0	-1.492712	3.360176	0.865913
20	1	0	-1.582937	3.346343	-0.910424
21	1	0	-0.019924	3.435201	-0.101345
22	1	0	-3.352139	-2.209800	0.940477
23	1	0	-3.417004	-2.216256	-0.823921
24	1	0	-4.189735	-0.899190	0.083604
25	1	0	-1.136783	-3.378358	0.823098
26	1	0	0.388400	-3.236043	-0.077571
27	1	0	-1.156909	-3.366822	-0.942064
28	1	0	3.317876	-0.122380	-2.026197
29	1	0	4.267739	-1.065661	-0.859273
30	1	0	4.462078	0.702290	-0.936900
31	1	0	2.328880	0.052214	2.186691
32	1	0	3.881435	0.754511	1.666823
33	1	0	3.640362	-1.010782	1.633034

5a phenoxyl radical

E(ROB+HF-LYP) = -656.158559072

Thermal correction to Enthalpy= 0.287327

1	6	0	-0.990893	3.026576	-0.000926
2	6	0	-0.895088	1.520752	-0.000586
3	6	0	-0.854572	-1.400376	-0.000109
4	6	0	0.299972	0.825336	-0.000821
5	6	0	-2.141676	0.742608	-0.000204
6	6	0	-2.085413	-0.726784	0.000182
7	6	0	0.308405	-0.595464	-0.000593
8	6	0	1.736657	1.323376	-0.001548
9	8	0	-3.282887	1.362591	-0.000101
10	6	0	-3.393134	-1.483765	0.001016
11	8	0	1.587345	-1.121222	-0.000891
12	6	0	-0.745968	-2.912012	-0.000195
13	1	0	1.954715	1.937207	0.881224
14	1	0	1.954468	1.934679	-0.886159
15	6	0	2.602281	0.016815	0.000268
16	6	0	3.436555	-0.159243	-1.274591
17	6	0	3.432329	-0.158067	1.278108
18	1	0	-1.551951	3.377210	0.874593
19	1	0	-1.552669	3.376753	-0.876163
20	1	0	-0.003212	3.499717	-0.001460
21	1	0	-3.481451	-2.128116	0.887649
22	1	0	-3.476642	-2.138917	-0.878004
23	1	0	-4.229108	-0.780999	-0.004974
24	1	0	-1.245685	-3.346190	0.876406
25	1	0	0.300496	-3.227379	0.010602
26	1	0	-1.226161	-3.344624	-0.888570
27	1	0	2.804618	-0.079007	-2.166711
28	1	0	3.921823	-1.141644	-1.283187
29	1	0	4.213897	0.614040	-1.328919
30	1	0	2.797470	-0.076687	2.168056
31	1	0	4.209690	0.615077	1.334175
32	1	0	3.917298	-1.140587	1.289371

5a radical cation

E(UB+HF-LYP) = -656.348266316

Zero-point correction= 0.284109

1	6	0	-1.005649	3.008906	0.000009
2	6	0	-0.880422	1.500494	-0.000304
3	6	0	-0.810096	-1.437992	-0.000463
4	6	0	0.326819	0.830854	-0.000293
5	6	0	-2.062846	0.666471	-0.000563
6	6	0	-2.045307	-0.778357	-0.000325
7	6	0	0.352006	-0.606816	-0.000503
8	6	0	1.751725	1.343427	-0.000378
9	8	0	-3.304748	1.231150	-0.000225
10	6	0	-3.344720	-1.548788	0.001055
11	8	0	1.602800	-1.099989	-0.000830
12	6	0	-0.681724	-2.941329	-0.000554
13	1	0	1.957609	1.959921	0.882778
14	1	0	1.957711	1.959263	-0.883962
15	6	0	2.647855	0.059846	0.000197
16	6	0	3.465509	-0.135911	-1.278953
17	6	0	3.463127	-0.135859	1.280899
18	1	0	-3.323997	2.212877	-0.000166
19	1	0	-1.535341	3.376142	0.891216
20	1	0	-1.536183	3.376519	-0.890558
21	1	0	-0.023308	3.486568	-0.000457
22	1	0	-3.418775	-2.182824	0.894700
23	1	0	-3.400111	-2.218184	-0.867366
24	1	0	-4.209498	-0.885812	-0.020297
25	1	0	-1.185023	-3.379071	0.871264
26	1	0	0.364689	-3.252580	0.015752
27	1	0	-1.155308	-3.376180	-0.890585
28	1	0	2.840520	-0.047487	-2.174789
29	1	0	3.946163	-1.119098	-1.283874
30	1	0	4.250485	0.628526	-1.330062
31	1	0	2.836309	-0.048284	2.175561
32	1	0	4.247279	0.629317	1.333842
33	1	0	3.944709	-1.118577	1.286496

5b antioxidant

E(RB+HF-LYP) = -591.481843503 (LANL2DZ)

E(ROB+HF-LYP) = -591.671296585 (LANL2DZdp)

Zero-point correction= 0.281137

Thermal correction to Enthalpy= 0.298681

1	6	0	1.000609	3.006195	-0.162820
2	6	0	0.983365	1.486382	-0.110600
3	6	0	1.069047	-1.381136	-0.043874
4	6	0	-0.201754	0.732890	-0.194357
5	6	0	2.203444	0.773608	0.010889
6	6	0	2.274438	-0.633758	0.043340
7	6	0	-0.141898	-0.676918	-0.159272
8	6	0	-1.607398	1.285700	-0.384668
9	8	0	3.431679	1.464765	0.107593
10	6	0	3.619410	-1.325505	0.166768
11	16	0	-1.803552	-1.463110	-0.308827
12	6	0	1.098464	-2.897802	-0.025085
13	1	0	-1.780801	1.480284	-1.454857
14	1	0	-1.767124	2.231476	0.149553
15	6	0	-2.641646	0.238284	0.115757
16	6	0	-2.829882	0.322681	1.644445
17	6	0	-3.986050	0.333195	-0.622408
18	1	0	3.312807	2.433363	0.054459
19	1	0	1.604372	3.379166	-1.005203
20	1	0	1.406705	3.445899	0.761705
21	1	0	-0.003439	3.415703	-0.295168
22	1	0	3.752010	-2.080504	-0.619387
23	1	0	3.714405	-1.844200	1.131873
24	1	0	4.432537	-0.601247	0.093590
25	1	0	1.381139	-3.303270	-1.007958
26	1	0	0.116555	-3.309469	0.231150
27	1	0	1.825457	-3.278476	0.701649
28	1	0	-1.869196	0.250428	2.166779
29	1	0	-3.475183	-0.486261	2.005253
30	1	0	-3.298223	1.282271	1.911836
31	1	0	-3.854892	0.220974	-1.704639
32	1	0	-4.448864	1.311902	-0.429143
33	1	0	-4.685765	-0.439279	-0.279689

5b phenoxyl radical

E(ROB+HF-LYP) = -591.040229917
Thermal correction to Enthalpy= 0.286123

1	6	0	0.886212	3.062569	-0.148926
2	6	0	0.943324	1.551939	-0.101447
3	6	0	1.161440	-1.345035	-0.041942
4	6	0	-0.191445	0.757138	-0.182597
5	6	0	2.250211	0.897158	0.019076
6	6	0	2.327944	-0.569039	0.041276
7	6	0	-0.081571	-0.665224	-0.144864
8	6	0	-1.610569	1.260810	-0.385177
9	8	0	3.331621	1.611712	0.099815
10	6	0	3.699498	-1.196731	0.156538
11	16	0	-1.692812	-1.496834	-0.262881
12	6	0	1.214544	-2.861900	-0.036186
13	1	0	-1.774655	1.454146	-1.456637
14	1	0	-1.790996	2.205155	0.143952
15	6	0	-2.618545	0.185191	0.102316
16	6	0	-2.851649	0.275696	1.624133
17	6	0	-3.941595	0.202552	-0.677904
18	1	0	1.898631	3.470387	-0.107829
19	1	0	0.314270	3.468664	0.697892
20	1	0	0.400934	3.417475	-1.068925
21	1	0	3.886208	-1.909028	-0.658373
22	1	0	3.808995	-1.750155	1.100739
23	1	0	4.463718	-0.417265	0.127979
24	1	0	1.365413	-3.256041	-1.051905
25	1	0	0.282658	-3.292499	0.347098
26	1	0	2.037884	-3.233448	0.582091
27	1	0	-1.903960	0.266675	2.174375
28	1	0	-3.462589	-0.560731	1.982038
29	1	0	-3.378884	1.211475	1.861116
30	1	0	-3.773717	0.079128	-1.753723
31	1	0	-4.450582	1.163533	-0.517070
32	1	0	-4.618096	-0.592553	-0.340999

5b radical cation
E(UB+HF-LYP) = -591.233281326
Zero-point correction= 0.281788

1	6	0	0.968247	3.038720	-0.133909
2	6	0	0.946204	1.523278	-0.080821
3	6	0	1.110310	-1.384701	-0.044475
4	6	0	-0.215145	0.764732	-0.143358
5	6	0	2.187308	0.802232	0.018725
6	6	0	2.290323	-0.629867	0.029750
7	6	0	-0.130426	-0.675168	-0.114861
8	6	0	-1.622839	1.300025	-0.323126
9	8	0	3.374901	1.473002	0.100201
10	6	0	3.648787	-1.286992	0.123198
11	16	0	-1.712981	-1.472397	-0.196422
12	6	0	1.160957	-2.896734	-0.050275
13	1	0	-1.767379	1.573394	-1.378649
14	1	0	-1.798051	2.205139	0.269164
15	6	0	-2.673465	0.228136	0.078929
16	6	0	-3.026863	0.288363	1.580412
17	6	0	-3.922238	0.230033	-0.814561
18	1	0	3.307555	2.451941	0.094106
19	1	0	1.566918	3.406906	-0.980102
20	1	0	1.375915	3.475137	0.790020
21	1	0	-0.032593	3.454225	-0.262297
22	1	0	3.770943	-2.048421	-0.656319
23	1	0	3.770997	-1.794925	1.090213
24	1	0	4.453230	-0.557897	0.025242
25	1	0	1.533228	-3.269254	-1.014753
26	1	0	0.180960	-3.349825	0.122227
27	1	0	1.842287	-3.272787	0.720716
28	1	0	-2.133821	0.306450	2.215399
29	1	0	-3.647940	-0.561370	1.882826
30	1	0	-3.602002	1.204665	1.770059
31	1	0	-3.672014	0.103224	-1.873473
32	1	0	-4.438772	1.192382	-0.700515
33	1	0	-4.627941	-0.556995	-0.526483

5c antioxidant
E(RB+HF-LYP) = -590.600953467 (LANL2DZ)
E(ROB+HF-LYP) = -590.781507241 (LANL2DZdp)
Zero-point correction= 0.280088
Thermal correction to Enthalpy= 0.298023

1	6	0	-1.567846	3.039065	-0.241987
2	6	0	-1.398820	1.530434	-0.139405
3	6	0	-1.214682	-1.325257	0.015237
4	6	0	-0.143400	0.893190	-0.192280
5	6	0	-2.547303	0.710144	-0.003346
6	6	0	-2.487038	-0.695653	0.072814
7	6	0	-0.070186	-0.516973	-0.115305
8	6	0	1.192244	1.598840	-0.390246
9	8	0	-3.835467	1.285672	0.062480
10	6	0	-3.763434	-1.505228	0.209928
11	34	0	1.772061	-1.182303	-0.233061
12	6	0	-1.105599	-2.837556	0.079681
13	1	0	1.215268	2.591068	0.080192
14	1	0	1.364613	1.745413	-1.468599
15	6	0	2.353902	0.745120	0.190546
16	6	0	3.697797	1.048456	-0.493711
17	6	0	2.457507	0.910016	1.721766
18	1	0	-3.806431	2.259771	-0.010646
19	1	0	-2.023411	3.465578	0.665645
20	1	0	-2.199655	3.320632	-1.099202
21	1	0	-0.610555	3.544870	-0.383565
22	1	0	-3.823759	-1.992143	1.194212
23	1	0	-3.815529	-2.298764	-0.547015
24	1	0	-4.638631	-0.862467	0.100248
25	1	0	-1.827839	-3.267228	0.782935
26	1	0	-0.103757	-3.149030	0.396591
27	1	0	-1.299590	-3.293905	-0.902542
28	1	0	3.641622	0.888528	-1.576641
29	1	0	4.503511	0.419407	-0.094530
30	1	0	3.977564	2.097469	-0.314273
31	1	0	1.502279	0.691297	2.211840
32	1	0	2.742956	1.945502	1.966231
33	1	0	3.216169	0.239326	2.141191

5c phenoxyl radical
E(ROB+HF-LYP) = -590.149904798
Thermal correction to Enthalpy= 0.285461

1	6	0	-1.457599	3.111862	-0.211786
2	6	0	-1.361599	1.604303	-0.125628
3	6	0	-1.297872	-1.293335	0.001593
4	6	0	-0.149763	0.926053	-0.181637
5	6	0	-2.598836	0.828574	0.006487
6	6	0	-2.536679	-0.638621	0.062269
7	6	0	-0.121945	-0.499604	-0.109198
8	6	0	1.202163	1.588298	-0.395432
9	8	0	-3.744115	1.437283	0.068235
10	6	0	-3.848051	-1.385881	0.186642
11	34	0	1.670168	-1.219098	-0.187380
12	6	0	-1.176999	-2.805990	0.047276
13	1	0	1.247194	2.578687	0.076174
14	1	0	1.354699	1.740002	-1.475648
15	6	0	2.350639	0.701606	0.158132
16	6	0	3.678867	0.922111	-0.585197
17	6	0	2.520756	0.885825	1.681247
18	1	0	-0.932138	3.596087	0.624041
19	1	0	-2.506467	3.415125	-0.180736
20	1	0	-1.009372	3.491057	-1.140805
21	1	0	-3.893458	-1.968846	1.117366
22	1	0	-3.993118	-2.087827	-0.645697
23	1	0	-4.674425	-0.672029	0.188634
24	1	0	-2.123458	-3.288277	0.300829
25	1	0	-0.429700	-3.116310	0.790455
26	1	0	-0.851011	-3.204474	-0.924775
27	1	0	3.574760	0.739997	-1.660881
28	1	0	4.471839	0.268981	-0.199741
29	1	0	4.009213	1.961659	-0.444322

30	1	0	1.572915	0.741950	2.211934
31	1	0	2.879735	1.905374	1.889233
32	1	0	3.251514	0.178708	2.090361

5c radical cation

E(UB+HF-LYP) = -590.355317859

Zero-point correction= 0.280873

1	6	0	-1.514274	3.085181	-0.186760
2	6	0	-1.349641	1.579063	-0.101043
3	6	0	-1.250213	-1.322613	-0.007128
4	6	0	-0.119598	0.929144	-0.145276
5	6	0	-2.520783	0.754843	0.010157
6	6	0	-2.495614	-0.677066	0.050233
7	6	0	-0.074368	-0.512074	-0.089688
8	6	0	1.220945	1.616907	-0.335866
9	8	0	-3.765331	1.320319	0.075813
10	6	0	-3.789688	-1.452666	0.155001
11	34	0	1.686420	-1.204145	-0.153165
12	6	0	-1.179075	-2.834559	0.017326
13	1	0	1.272761	2.566308	0.209423
14	1	0	1.344876	1.854295	-1.403011
15	6	0	2.405524	0.724409	0.127440
16	6	0	3.673766	0.920750	-0.719340
17	6	0	2.689773	0.876484	1.639027
18	1	0	-3.782583	2.300736	0.050147
19	1	0	-1.967092	3.499940	0.726120
20	1	0	-2.140942	3.375964	-1.042812
21	1	0	-0.558392	3.593311	-0.320943
22	1	0	-3.865281	-1.958407	1.127800
23	1	0	-3.845913	-2.230533	-0.616029
24	1	0	-4.655422	-0.798441	0.050682
25	1	0	-1.782120	-3.246431	0.834663
26	1	0	-0.158800	-3.209008	0.141978
27	1	0	-1.575247	-3.258687	-0.915399
28	1	0	3.494371	0.739080	-1.784837
29	1	0	4.490600	0.270050	-0.387131
30	1	0	4.017895	1.958143	-0.608145
31	1	0	1.785065	0.759781	2.246437
32	1	0	3.094972	1.881862	1.819630
33	1	0	3.435105	0.153618	1.988032

5d antioxidant

E(RB+HF-LYP) = -589.419798910 (LANL2DZ)

E(ROB+HF-LYP) = -589.592041002 (LANL2DZdp)

Zero-point correction= 0.279325

Thermal correction to Enthalpy= 0.297495

1	6	0	-2.079526	2.999691	-0.310766
2	6	0	-1.780952	1.513574	-0.169463
3	6	0	-1.378887	-1.311456	0.050568
4	6	0	-0.474444	0.978140	-0.203038
5	6	0	-2.862202	0.610184	-0.015223
6	6	0	-2.697125	-0.785964	0.091237
7	6	0	-0.293228	-0.422397	-0.089327
8	6	0	0.784476	1.811951	-0.423107
9	8	0	-4.190766	1.086322	0.033435
10	6	0	-3.914690	-1.682255	0.238868
11	52	0	1.761015	-0.991558	-0.170805
12	6	0	-1.135972	-2.807496	0.139391
13	1	0	0.677290	2.831414	-0.027061
14	1	0	0.961410	1.904428	-1.507101
15	6	0	2.046418	1.176807	0.229321
16	6	0	3.341975	1.701346	-0.419097
17	6	0	2.059706	1.420443	1.755451
18	1	0	-4.235937	2.059447	-0.043361
19	1	0	-2.556996	3.410959	0.592857
20	1	0	-2.746171	3.200355	-1.164381
21	1	0	-1.173823	3.583866	-0.483192
22	1	0	-3.909775	-2.208781	1.203840
23	1	0	-3.946514	-2.446480	-0.549060
24	1	0	-4.831009	-1.092401	0.182446
25	1	0	-1.971846	-3.339062	0.602204
26	1	0	-0.235652	-3.021047	0.731410
27	1	0	-0.982608	-3.244200	-0.859313
28	1	0	3.362841	1.508662	-1.498187
29	1	0	4.232695	1.242543	0.029194
30	1	0	3.420446	2.789133	-0.264031
31	1	0	1.135618	1.068234	2.227330
32	1	0	2.158402	2.499959	1.956781
33	1	0	2.901700	0.908020	2.235127

5d phenoxyl radical

E(ROB+HF-LYP) = -588.960104619

Thermal correction to Enthalpy= 0.284965

1	6	0	-1.959046	3.087595	-0.276427
2	6	0	-1.739737	1.594578	-0.157300
3	6	0	-1.456225	-1.281160	0.025579
4	6	0	-0.474453	1.013275	-0.200079
5	6	0	-2.914156	0.730740	-0.005778
6	6	0	-2.742138	-0.725315	0.077251
7	6	0	-0.336487	-0.407693	-0.097707
8	6	0	0.802985	1.808173	-0.434778
9	8	0	-4.102598	1.251929	0.047277
10	6	0	-3.993916	-1.566411	0.219661
11	52	0	1.675903	-1.030735	-0.140796
12	6	0	-1.224559	-2.780586	0.098741
13	1	0	0.713051	2.829893	-0.041115
14	1	0	0.961694	1.899451	-1.521355
15	6	0	2.056926	1.141322	0.197091
16	6	0	3.356594	1.591332	-0.496715
17	6	0	2.120917	1.407354	1.718162
18	1	0	-1.473774	3.632590	0.546063
19	1	0	-3.029431	3.303104	-0.247244
20	1	0	-1.547274	3.481948	-1.215881
21	1	0	-3.979799	-2.158810	1.145064
22	1	0	-4.104923	-2.269708	-0.617236
23	1	0	-4.869089	-0.913625	0.241169
24	1	0	-2.151467	-3.338174	0.247675
25	1	0	-0.546251	-3.031880	0.926873
26	1	0	-0.761704	-3.152377	-0.827550
27	1	0	3.341446	1.374238	-1.571152
28	1	0	4.239456	1.107712	-0.059432
29	1	0	3.482152	2.677842	-0.371028
30	1	0	1.192231	1.113622	2.219937
31	1	0	2.278630	2.483553	1.893251
32	1	0	2.948676	0.864190	2.188907

5d radical cation

E(UB+HF-LYP) = -589.178591604

Zero-point correction= 0.280116

1	6	0	-2.007941	3.057691	-0.258765
2	6	0	-1.723220	1.570948	-0.135326
3	6	0	-1.407291	-1.302378	0.023629
4	6	0	-0.441790	1.015232	-0.163912
5	6	0	-2.829762	0.669748	-0.002434
6	6	0	-2.699529	-0.750490	0.071480
7	6	0	-0.289069	-0.417407	-0.078195
8	6	0	0.824377	1.835016	-0.368159
9	8	0	-4.115546	1.145769	0.053305
10	6	0	-3.932626	-1.618251	0.199136
11	52	0	1.691592	-1.018785	-0.135807
12	6	0	-1.240702	-2.806905	0.080841
13	1	0	0.747342	2.817515	0.112936
14	1	0	0.950067	2.020148	-1.445734
15	6	0	2.110473	1.151865	0.177789
16	6	0	3.372719	1.584785	-0.591551
17	6	0	2.271379	1.372162	1.701811
18	1	0	-4.201255	2.121139	0.004714
19	1	0	-2.474875	3.460851	0.652311
20	1	0	-2.674027	3.271509	-1.107841
21	1	0	-1.101567	3.639176	-0.430445
22	1	0	-3.959017	-2.122229	1.175352
23	1	0	-3.945385	-2.402345	-0.567851

24	1	0	-4.843803	-1.027572	0.103360
25	1	0	-1.796417	-3.236413	0.922502
26	1	0	-0.196140	-3.116798	0.191120
27	1	0	-1.629979	-3.279970	-0.830752
28	1	0	3.299546	1.381555	-1.666106
29	1	0	4.275705	1.097672	-0.205532
30	1	0	3.511237	2.668061	-0.465594
31	1	0	1.369451	1.100327	2.261785
32	1	0	2.472899	2.438416	1.880527
33	1	0	3.115713	0.807549	2.112706

6a antioxidant

E(RB+HF-LYP) = -695.903412762 (LANL2DZ)
E(ROB+HF-LYP) = -696.104937888 (LANL2DZdp)
Zero-point correction= 0.313189
Thermal correction to Enthalpy= 0.331238

1	6	0	-0.464426	2.901490	-0.110809
2	6	0	-0.788306	1.416836	-0.080135
3	6	0	-1.311692	-1.393420	-0.027791
4	6	0	0.262772	0.469166	-0.130415
5	6	0	-2.119207	0.945702	-0.004299
6	6	0	-2.352687	-0.449942	0.029016
7	6	0	0.019784	-0.922352	-0.120428
8	8	0	1.567288	1.003237	-0.222222
9	6	0	-3.308462	1.893116	0.047931
10	8	0	-3.667952	-0.965644	0.113975
11	6	0	1.178401	-1.906471	-0.207267
12	6	0	-1.621551	-2.878461	0.004826
13	1	0	-0.852480	3.418160	0.777978
14	1	0	-0.901415	3.391386	-0.992280
15	1	0	0.615813	3.048642	-0.145499
16	1	0	-3.883299	1.778224	0.980890
17	1	0	-3.998507	1.727422	-0.794376
18	1	0	-2.995985	2.937578	-0.001707
19	1	0	-2.684509	-3.042290	0.189814
20	1	0	-1.048567	-3.390392	0.790063
21	1	0	-1.365039	-3.362865	-0.948891
22	1	0	-4.333826	-0.253311	0.178021
23	1	0	1.328377	-2.392276	0.769594
24	6	0	2.485211	-1.229295	-0.665573
25	1	0	0.927108	-2.716032	-0.904793
26	6	0	2.723775	0.109590	0.064139
27	1	0	2.435069	-1.020804	-1.743042
28	1	0	3.339212	-1.898938	-0.497667
29	6	0	2.850768	-0.054893	1.593113
30	6	0	3.926617	0.863268	-0.515940
31	1	0	1.934793	-0.464163	2.032380
32	1	0	3.041872	0.918925	2.058378
33	1	0	3.682875	-0.727579	1.839774
34	1	0	4.011034	1.855182	-0.057241
35	1	0	3.811107	0.995775	-1.597764
36	1	0	4.855694	0.310601	-0.325862

6a phenoxyl radical

E(ROB+HF-LYP) = -695.475204466
Thermal correction to Enthalpy= 0.318720

1	6	0	0.558385	-2.890414	-0.102472
2	6	0	0.858805	-1.403262	-0.069605
3	6	0	1.315670	1.439312	-0.020948
4	6	0	-0.212771	-0.454595	-0.100051
5	6	0	2.171114	-0.933828	-0.001513
6	6	0	2.439787	0.504956	0.036925
7	6	0	0.006781	0.956488	-0.097567
8	8	0	-1.487580	-1.002417	-0.151811
9	6	0	3.349378	-1.879847	0.043765
10	8	0	3.659858	0.948659	0.115710
11	6	0	-1.178826	1.908033	-0.186472
12	6	0	1.621518	2.920475	-0.002150
13	1	0	0.906274	-3.382709	0.816642
14	1	0	1.078213	-3.376049	-0.939318
15	1	0	-0.511793	-3.074018	-0.206067
16	1	0	3.277746	-2.569652	0.896654
17	1	0	4.277962	-1.311421	0.128356
18	1	0	3.398772	-2.499616	-0.863228
19	1	0	2.691870	3.069852	0.154582
20	1	0	1.068922	3.438468	0.793902
21	1	0	1.343764	3.400478	-0.952462
22	1	0	-4.789843	-0.410252	-0.450319
23	1	0	-1.360330	2.371843	0.794950
24	6	0	-2.454912	1.200172	-0.682273
25	1	0	-0.936631	2.734915	-0.865420
26	6	0	-2.694562	-0.133573	0.052238
27	1	0	-2.367027	0.988272	-1.756619
28	1	0	-3.328024	1.851218	-0.545926
29	6	0	-2.894076	0.035702	1.571334
30	6	0	-3.836522	-0.938359	-0.578066
31	1	0	-2.024086	0.500634	2.046892
32	1	0	-3.052598	-0.942262	2.039153
33	1	0	-3.772638	0.662602	1.771000
34	1	0	-3.918101	-1.922719	-0.103687
35	1	0	-3.659285	-1.087070	-1.649150

6a radical cation

E(UB+HF-LYP) = -695.658611294
Zero-point correction= 0.314069

1	6	0	0.483808	-2.909168	-0.063863
2	6	0	0.825134	-1.435886	-0.042184
3	6	0	1.300372	1.430005	-0.012669
4	6	0	-0.249056	-0.453035	-0.053211
5	6	0	2.137562	-0.970100	-0.002678
6	6	0	2.357067	0.450648	0.020762
7	6	0	-0.012112	0.969025	-0.063508
8	8	0	-1.491452	-0.968901	-0.049926
9	6	0	3.342214	-1.891216	0.023506
10	8	0	3.620231	0.963525	0.069035
11	6	0	-1.194553	1.917935	-0.129540
12	6	0	1.637031	2.903764	-0.001647
13	1	0	0.871646	-3.417171	0.828528
14	1	0	0.928280	-3.402144	-0.938006
15	1	0	-0.593942	-3.064891	-0.099770
16	1	0	3.938246	-1.756337	0.938447
17	1	0	3.998656	-1.727596	-0.844113
18	1	0	3.048921	-2.940755	-0.003276
19	1	0	2.687074	3.070090	0.240050
20	1	0	1.021262	3.444195	0.726524
21	1	0	1.446121	3.354765	-0.985919
22	1	0	4.343071	0.299252	0.085433
23	1	0	-1.387462	2.335539	0.869450
24	6	0	-2.460599	1.229002	-0.678895
25	1	0	-0.945488	2.773396	-0.766803
26	6	0	-2.768709	-0.100694	0.029437
27	1	0	-2.344328	1.039135	-1.753928
28	1	0	-3.324609	1.892951	-0.561036
29	6	0	-3.079461	0.032488	1.529228
30	6	0	-3.811423	-0.941539	-0.709125
31	1	0	-2.298105	0.571802	2.074931
32	1	0	-3.198307	-0.956001	1.984032
33	1	0	-4.021995	0.578811	1.654069
34	1	0	-3.944682	-1.914049	-0.224587
35	1	0	-3.522591	-1.106032	-1.752570
36	1	0	-4.775647	-0.419336	-0.698018

6b antioxidant

E(RB+HF-LYP) = -630.781669237 (LANL2DZ)
E(ROB+HF-LYP) = -630.982751938 (LANL2DZdp)
Zero-point correction= 0.310777
Thermal correction to Enthalpy= 0.329292

1	6	0	0.960693	-2.910444	-0.004921
2	6	0	1.115794	-1.395506	-0.033784
3	6	0	1.423772	1.440638	-0.046263
4	6	0	-0.015867	-0.537932	-0.126139
5	6	0	2.410406	-0.824968	0.026657

6	6	0	2.533291	0.581939	0.034364
7	6	0	0.126652	0.871833	-0.150538
8	16	0	-1.672535	-1.371801	-0.266525
9	6	0	3.677804	-1.667449	0.075503
10	8	0	3.801386	1.197885	0.118474
11	6	0	-1.044718	1.850431	-0.238741
12	6	0	1.639097	2.943910	-0.028936
13	1	0	1.607240	-3.364034	0.755247
14	1	0	1.221348	-3.360432	-0.974000
15	1	0	-0.064969	-3.207680	0.226188
16	1	0	4.186524	-1.591575	1.049951
17	1	0	4.393610	-1.360941	-0.703110
18	1	0	3.474151	-2.725351	-0.094969
19	1	0	2.686558	3.173315	0.172714
20	1	0	1.022813	3.431530	0.738138
21	1	0	1.373891	3.400364	-0.993786
22	1	0	4.519253	0.543846	0.226673
23	1	0	-1.164402	2.339708	0.740950
24	6	0	-2.404512	1.290529	-0.690207
25	1	0	-0.772343	2.657824	-0.930954
26	6	0	-2.887042	0.066370	0.112912
27	1	0	-2.362258	1.013986	-1.752219
28	1	0	-3.156297	2.090246	-0.593309
29	6	0	-2.932827	0.329210	1.632056
30	6	0	-4.258148	-0.416819	-0.399661
31	1	0	-1.939571	0.537718	2.042728
32	1	0	-3.335546	-0.542095	2.161357
33	1	0	-3.582454	1.192315	1.844430
34	1	0	-4.560593	-1.352870	0.086574
35	1	0	-4.242343	-0.582571	-1.483290
36	1	0	-5.021503	0.341979	-0.176520

6b phenoxyl radical

E(ROB+HF-LYP) = -630.351867628

Thermal correction to Enthalpy= 0.316752

1	6	0	0.984638	-2.882960	-0.045075
2	6	0	1.184565	-1.376109	-0.038983
3	6	0	1.440955	1.484273	-0.033801
4	6	0	0.037035	-0.507870	-0.084486
5	6	0	2.465265	-0.821662	0.017977
6	6	0	2.625832	0.632634	0.034029
7	6	0	0.161216	0.916094	-0.106284
8	16	0	-1.574623	-1.372537	-0.129607
9	6	0	3.726345	-1.659779	0.075163
10	8	0	3.810545	1.163270	0.103674
11	6	0	-1.037721	1.859978	-0.181487
12	6	0	1.660628	2.982069	-0.025713
13	1	0	0.392575	-3.208529	0.821079
14	1	0	1.936656	-3.415350	-0.020081
15	1	0	0.441436	-3.210215	-0.942233
16	1	0	4.595560	-1.000534	0.121930
17	1	0	3.825333	-2.302460	-0.810307
18	1	0	3.739123	-2.313492	0.957996
19	1	0	2.718587	3.191696	0.144567
20	1	0	1.068639	3.477230	0.755779
21	1	0	1.373953	3.437361	-0.985475
22	1	0	-1.213522	2.295967	0.813985
23	6	0	-2.350697	1.264404	-0.717087
24	1	0	-0.770074	2.707330	-0.824286
25	6	0	-2.866992	0.045388	0.071190
26	1	0	-2.228493	0.977963	-1.770597
27	1	0	-3.126596	2.045003	-0.683317
28	6	0	-3.062400	0.339378	1.573256
29	6	0	-4.165605	-0.504095	-0.551742
30	1	0	-2.124485	0.611627	2.067559
31	1	0	-3.467770	-0.538216	2.089727
32	1	0	-3.772431	1.170348	1.699541
33	1	0	-4.481363	-1.436721	-0.067740
34	1	0	-4.044791	-0.697086	-1.623881
35	1	0	-4.971129	0.232043	-0.421652

6b radical cation

E(UB+HF-LYP) = -630.535902931

Zero-point correction= 0.311847

1	6	0	1.026415	-2.919091	-0.038024
2	6	0	1.163750	-1.406219	-0.024094
3	6	0	1.410344	1.476046	-0.016286
4	6	0	0.002417	-0.527235	-0.031559
5	6	0	2.437591	-0.830881	0.002143
6	6	0	2.539534	0.596126	0.015158
7	6	0	0.131052	0.908609	-0.059900
8	16	0	-1.584356	-1.347355	0.028684
9	6	0	3.721272	-1.641072	0.023835
10	8	0	3.760691	1.209769	0.049574
11	6	0	-1.070906	1.843616	-0.106177
12	6	0	1.637526	2.973084	-0.001986
13	1	0	1.463614	-3.359082	0.867126
14	1	0	1.555246	-3.346155	-0.898782
15	1	0	-0.006952	-3.261730	-0.096445
16	1	0	4.317019	-1.431454	0.925065
17	1	0	4.345579	-1.433556	-0.858194
18	1	0	3.532515	-2.713883	0.023592
19	1	0	2.683666	3.208456	0.193944
20	1	0	1.024309	3.462209	0.763719
21	1	0	1.371424	3.422507	-0.969019
22	1	0	4.532145	0.603613	0.064074
23	1	0	-1.279617	2.207131	0.911196
24	6	0	-2.354010	1.267453	-0.729304
25	1	0	-0.794234	2.733422	-0.680385
26	6	0	-2.951100	0.063465	0.016147
27	1	0	-2.171442	0.992329	-1.776738
28	1	0	-3.119402	2.056134	-0.738512
29	6	0	-3.323616	0.351619	1.484501
30	6	0	-4.129915	-0.562140	-0.753377
31	1	0	-2.478193	0.709447	2.080105
32	1	0	-3.727754	-0.541001	1.973968
33	1	0	-4.104847	1.123890	1.501888
34	1	0	-4.490062	-1.481182	-0.276744
35	1	0	-3.869276	-0.786387	-1.793356
36	1	0	-4.961697	0.154538	-0.758499

6c antioxidant

E(RB+HF-LYP) = -629.899686744 (LANL2DZ)

E(ROB+HF-LYP) = -630.091906239 (LANL2DZdp)

Zero-point correction= 0.309637

Thermal correction to Enthalpy= 0.328559

1	6	0	0.976367	-2.808949	0.028321
2	6	0	1.296850	-1.322502	-0.001348
3	6	0	1.786181	1.488652	-0.034146
4	6	0	0.219794	-0.388753	-0.049751
5	6	0	2.629104	-0.842124	0.021752
6	6	0	2.837076	0.558457	0.018097
7	6	0	0.449921	1.006670	-0.088568
8	34	0	-1.589404	-1.188083	-0.074026
9	6	0	3.861474	-1.737379	0.049021
10	8	0	4.144054	1.093090	0.059210
11	6	0	-0.661042	2.054758	-0.149958
12	6	0	2.104465	2.974365	-0.030485
13	1	0	1.861836	-3.440022	0.116994
14	1	0	0.443959	-3.117470	-0.883106
15	1	0	0.319371	-3.047876	0.876250
16	1	0	4.433579	-1.615235	0.982852
17	1	0	4.536335	-1.514540	-0.792219
18	1	0	3.616017	-2.796378	-0.028080
19	1	0	3.167963	3.131164	0.156295
20	1	0	1.533594	3.507497	0.740942
21	1	0	1.860943	3.441885	-0.995787
22	1	0	4.823131	0.396132	0.145100
23	1	0	-0.807536	2.479350	0.855974
24	6	0	-2.022788	1.611550	-0.714934
25	1	0	-0.311526	2.891448	-0.766735
26	6	0	-2.731780	0.492098	0.074175
27	1	0	-1.903620	1.288868	-1.758343
28	1	0	-2.689159	2.490213	-0.723156

29	6	0	-2.944305	0.857290	1.559518
30	6	0	-4.082350	0.141394	-0.587629
31	1	0	-1.998838	0.987282	2.095234
32	1	0	-3.509527	0.071493	2.074551
33	1	0	-3.516338	1.795911	1.634754
34	1	0	-4.555407	-0.726663	-0.109924
35	1	0	-3.959930	-0.079416	-1.654442
36	1	0	-4.771355	0.993301	-0.488325

6c phenoxyl radical

E(ROB+HF-LYP) = -629.460717047

Thermal correction to Enthalpy= 0.316089

1	6	0	1.084299	-2.791433	-0.008002
2	6	0	1.360049	-1.296314	-0.014508
3	6	0	1.775993	1.544405	-0.025925
4	6	0	0.258951	-0.367727	-0.038794
5	6	0	2.671431	-0.814832	0.010590
6	6	0	2.912880	0.627680	0.016084
7	6	0	0.464245	1.048454	-0.067799
8	34	0	-1.507497	-1.190725	-0.026822
9	6	0	3.885206	-1.721899	0.042699
10	8	0	4.126965	1.090568	0.055330
11	6	0	-0.679955	2.061507	-0.106209
12	6	0	2.084443	3.027351	-0.017993
13	1	0	2.007923	-3.372143	-0.013925
14	1	0	0.497219	-3.094326	-0.886498
15	1	0	0.510892	-3.087903	0.881782
16	1	0	4.790287	-1.111440	0.065283
17	1	0	3.927581	-2.372792	-0.841327
18	1	0	3.882986	-2.371152	0.928917
19	1	0	3.157528	3.171123	0.123673
20	1	0	1.546349	3.551966	0.782843
21	1	0	1.800200	3.505257	-0.967261
22	1	0	-0.859699	2.439241	0.912328
23	6	0	-2.012666	1.592212	-0.718447
24	1	0	-0.345947	2.932110	-0.681680
25	6	0	-2.720615	0.452131	0.039827
26	1	0	-1.853156	1.284561	-1.761160
27	1	0	-2.700836	2.452781	-0.739722
28	6	0	-3.020318	0.809623	1.511985
29	6	0	-4.019721	0.041558	-0.687288
30	1	0	-2.110653	0.995135	2.091360
31	1	0	-3.567642	-0.001394	2.006655
32	1	0	-3.644665	1.715615	1.551935
33	1	0	-4.487197	-0.836690	-0.223357
34	1	0	-3.835600	-0.185507	-1.743724
35	1	0	-4.741727	0.869381	-0.634119

6c radical cation

E(UB+HF-LYP) = -629.656860005

Zero-point correction= 0.310521

1	6	0	1.137431	-2.831733	-0.043130
2	6	0	1.338139	-1.324962	-0.027310
3	6	0	1.733468	1.537571	-0.005670
4	6	0	0.222151	-0.393140	-0.018872
5	6	0	2.641401	-0.814469	-0.015368
6	6	0	2.815526	0.603803	0.002789
7	6	0	0.424405	1.034464	-0.037474
8	34	0	-1.518398	-1.171634	0.069289
9	6	0	3.883967	-1.687781	-0.013273
10	8	0	4.069010	1.154441	0.024314
11	6	0	-0.723894	2.037900	-0.046599
12	6	0	2.039616	3.021507	0.025037
13	1	0	1.632468	-3.278945	-0.913633
14	1	0	0.090606	-3.136805	-0.087627
15	1	0	1.568645	-3.293688	0.853716
16	1	0	4.496855	-1.515603	0.884363
17	1	0	4.510116	-1.501894	-0.898816
18	1	0	3.644206	-2.750263	-0.022152
19	1	0	3.101540	3.195841	0.198490
20	1	0	1.473959	3.529935	0.814436
21	1	0	1.776050	3.501138	-0.927874
22	1	0	4.806495	0.507832	0.024916
23	1	0	-0.932928	2.348726	0.988281
24	6	0	-2.029631	1.593689	-0.731483
25	1	0	-0.381929	2.943383	-0.555783
26	6	0	-2.793631	0.458051	-0.029245
27	1	0	-1.827508	1.312062	-1.773845
28	1	0	-2.707597	2.459166	-0.766561
29	6	0	-3.231680	0.797619	1.411369
30	6	0	-3.988037	-0.031210	-0.875009
31	1	0	-2.395794	1.070424	2.062843
32	1	0	-3.763341	-0.039732	1.876946
33	1	0	-3.925587	1.649096	1.373194
34	1	0	-4.489034	-0.896493	-0.424502
35	1	0	-3.692168	-0.291448	-1.897352
36	1	0	-4.726994	0.779441	-0.933937

6d antioxidant

E(RB+HF-LYP) = -628.719583029 (LANL2DZ)

E(ROB+HF-LYP) = -628.903216052 (LANL2DZdp)

Zero-point correction= 0.308878

Thermal correction to Enthalpy= 0.327965

1	6	0	-1.244897	-2.765279	0.245330
2	6	0	-1.520813	-1.275701	0.098419
3	6	0	-2.063988	1.528373	-0.146671
4	6	0	-0.470897	-0.343368	-0.118537
5	6	0	-2.856674	-0.802000	0.164830
6	6	0	-3.092263	0.586591	0.056600
7	6	0	-0.735146	1.046727	-0.250433
8	52	0	1.556888	-1.025427	-0.337280
9	6	0	-4.051793	-1.731550	0.333020
10	8	0	-4.403642	1.102103	0.140531
11	6	0	0.415967	2.016383	-0.476680
12	6	0	-2.414421	3.003702	-0.260062
13	1	0	-1.859891	-3.216951	1.031802
14	1	0	-0.199529	-2.951444	0.513233
15	1	0	-1.448517	-3.311824	-0.687607
16	1	0	-4.825042	-1.533908	-0.425978
17	1	0	-4.519466	-1.629523	1.325420
18	1	0	-3.774437	-2.780338	0.218412
19	1	0	-3.489146	3.144780	-0.135049
20	1	0	-2.130324	3.411062	-1.239839
21	1	0	-1.901107	3.601138	0.505688
22	1	0	-5.060979	0.403595	0.327045
23	1	0	0.884624	1.808473	-1.451750
24	6	0	1.502736	1.927089	0.631697
25	1	0	0.041649	3.041596	-0.522929
26	6	0	2.566015	0.820864	0.427625
27	1	0	1.006459	1.786888	1.601402
28	1	0	2.043662	2.886250	0.685083
29	6	0	3.612296	1.244166	-0.631293
30	6	0	3.269079	0.494511	1.765113
31	1	0	3.141179	1.550854	-1.571702
32	1	0	4.314070	0.431400	-0.859404
33	1	0	4.199067	2.093745	-0.247113
34	1	0	4.033159	-0.283964	1.644402
35	1	0	2.553944	0.152052	2.521174
36	1	0	3.770395	1.398476	2.148306

6d phenoxyl radical

E(ROB+HF-LYP) = -628.270865988

Thermal correction to Enthalpy= 0.315506

1	6	0	-1.266074	-2.736964	0.072829
2	6	0	-1.575982	-1.249202	0.032345
3	6	0	-2.069261	1.587114	-0.093956
4	6	0	-0.507281	-0.297873	-0.102284
5	6	0	-2.896378	-0.794780	0.120096
6	6	0	-3.174279	0.641297	0.068798
7	6	0	-0.753832	1.112076	-0.180552
8	52	0	1.473085	-1.060601	-0.212566
9	6	0	-4.083068	-1.725598	0.271165

10	8	0	-4.396679	1.073673	0.159127
11	6	0	0.402544	2.083176	-0.385986
12	6	0	-2.428215	3.058154	-0.174246
13	1	0	-0.606085	-2.983572	0.916478
14	1	0	-0.759386	-3.066132	-0.846729
15	1	0	-2.170425	-3.339316	0.173842
16	1	0	-4.169530	-2.412498	-0.582081
17	1	0	-4.999255	-1.134596	0.331580
18	1	0	-4.005359	-2.338357	1.179662
19	1	0	-3.509569	3.168542	-0.069374
20	1	0	-2.127787	3.498031	-1.135198
21	1	0	-1.942252	3.640991	0.620465
22	1	0	0.795890	1.968267	-1.408104
23	6	0	1.563609	1.915895	0.627688
24	1	0	0.030728	3.107886	-0.318569
25	6	0	2.587987	0.808078	0.288224
26	1	0	1.144885	1.738048	1.627724
27	1	0	2.126650	2.862132	0.682436
28	6	0	3.469258	1.196155	-0.922552
29	6	0	3.482244	0.505863	1.513192
30	1	0	2.874175	1.440416	-1.808611
31	1	0	4.158525	0.387602	-1.196861
32	1	0	4.075797	2.077826	-0.662360
33	1	0	4.206469	-0.292249	1.304594
34	1	0	2.889141	0.208406	2.384996
35	1	0	4.052781	1.410095	1.777973

6d radical cation

E(UB+HF-LYP) = -628.479701795

Zero-point correction= 0.309810

1	6	0	-1.309377	-2.775742	0.027311
2	6	0	-1.544710	-1.273887	0.008455
3	6	0	-2.025687	1.574800	-0.084256
4	6	0	-0.462317	-0.320721	-0.100378
5	6	0	-2.860237	-0.794565	0.101650
6	6	0	-3.073816	0.614956	0.057170
7	6	0	-0.706261	1.098564	-0.157171
8	52	0	1.492039	-1.057445	-0.179074
9	6	0	-4.071825	-1.699504	0.248519
10	8	0	-4.342921	1.132776	0.137070
11	6	0	0.435255	2.090752	-0.347048
12	6	0	-2.383465	3.047724	-0.159136
13	1	0	-1.584247	-3.207895	0.998138
14	1	0	-0.270574	-3.060229	-0.160816
15	1	0	-1.912408	-3.276709	-0.738414
16	1	0	-4.744406	-1.620511	-0.618887
17	1	0	-4.649271	-1.458152	1.153754
18	1	0	-3.797713	-2.750391	0.334843
19	1	0	-3.462284	3.185904	-0.088858
20	1	0	-2.047365	3.492587	-1.104063
21	1	0	-1.919036	3.614910	0.657741
22	1	0	-5.055589	0.465580	0.226201
23	1	0	0.799936	2.028793	-1.383490
24	6	0	1.622566	1.918261	0.631867
25	1	0	0.049824	3.104403	-0.231935
26	6	0	2.641176	0.820446	0.258086
27	1	0	1.241012	1.745283	1.647033
28	1	0	2.185317	2.863392	0.664844
29	6	0	3.465101	1.167957	-1.003338
30	6	0	3.571939	0.484427	1.445141
31	1	0	2.842480	1.415635	-1.869290
32	1	0	4.139477	0.352857	-1.291748
33	1	0	4.090492	2.043700	-0.778294
34	1	0	4.284702	-0.313849	1.204357
35	1	0	3.016725	0.197439	2.345163
36	1	0	4.160209	1.381397	1.687797