SUPPORTING INFORMATION

Electrochemical and Quantum Chemical Investigation of Tetranitrocalix[4]arenes: Molecules with Multiple Redox Centers

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Computed Structures
Neutral Nitrobenzene (1)

ENERGY = - 436.7781272 Hartrees

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.823009	1.214666	0.000033
2	6	0	-0.428821	1.224266	-0.000045
3	6	0	0.245373	0.000000	-0.000105
4	6	0	-0.428821	-1.224266	-0.000062
5	6	0	-1.823009	-1.214666	0.000015
6	6	0	-2.519067	0.000000	0.000064
7	1	0	-2.364806	2.155466	0.000072
8	1	0	0.127873	2.153362	-0.000071
9	1	0	0.127873	-2.153362	-0.000102
10	1	0	-2.364806	-2.155466	0.000038
11	1	0	-3.605231	0.000000	0.000127
12	7	0	1.710773	0.000000	-0.000210
13	8	0	2.297989	-1.087287	0.000149
14	8	0	2.297989	1.087287	0.000103

Nitrobenzene Anion Radical (2)
Energy = - 436.90394057 Hartrees

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.829416	1.209192	0.000029
2	6	0	-0.436375	1.221618	0.000025
3	6	0	0.279544	0.000000	0.000000
4	6	0	-0.436375	-1.221618	-0.000025
5	6	0	-1.829416	-1.209192	-0.000029
6	6	0	-2.542077	0.000000	-0.000001
7	1	0	-2.366757	2.155101	0.000056
8	1	0	0.113630	2.154766	0.000051
9	1	0	0.113630	-2.154766	-0.000048
10	1	0	-2.366757	-2.155101	-0.000056
11	1	0	-3.628685	0.000000	-0.000001
12	7	0	1.677643	0.000000	0.000000
13	8	0	2.322258	-1.131919	0.000068
14	8	0	2.322258	1.131919	-0.000069

Nitrobenzene Dianion (3)
Energy = - 436.97607191 Hartrees

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.837499	1.206853	-0.000025
2	6	0	0.449635	1.232637	-0.000020
3	6	0	-0.318700	0.000000	0.000000
4	6	0	0.449635	-1.232637	0.000020
5	6	0	1.837499	-1.206853	0.000026
6	6	0	2.574411	0.000000	0.000000
7	1	0	2.371723	2.158602	-0.000052

8	1	0	-0.085433	2.175728	-0.000044
9	1	0	-0.085433	-2.175728	0.000043
10	1	0	2.371723	-2.158602	0.000052
11	1	0	3.661642	0.000000	0.000001
12	7	0	-1.649838	0.000000	0.000000
13	8	0	-2.354077	-1.160445	-0.000041
14	8	0	-2.354077	1.160445	0.000040

Nitrosobenzene neutral
Energy = -361.5626649 hartrees

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.274528	1.341371	0.000000
2	6	0	0.094957	1.108643	0.000000
3	6	0	0.558796	-0.220658	0.000000
4	6	0	-0.335728	-1.303029	0.000000
5	6	0	-1.709019	-1.058565	0.000000
6	6	0	-2.174505	0.260698	0.000000
7	1	0	-1.653479	2.359284	0.000000
8	1	0	0.808905	1.925578	0.000000
9	1	0	0.061146	-2.314117	0.000000
10	1	0	-2.411572	-1.886350	0.000000
11	1	0	-3.243517	0.454631	0.000000
12	7	0	1.935922	-0.583551	0.000000
13	8	0	2.740903	0.346884	0.000000

Nitrosobenzene anion radical
Energy = -361.6948538 hartrees

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.256969	1.343852	0.000000
2	6	0	-0.111980	1.077796	0.000000
3	6	0	-0.586346	-0.261802	0.000000
4	6	0	0.376093	-1.306455	0.000000
5	6	0	1.739476	-1.028026	0.000000
6	6	0	2.197523	0.301963	0.000000
7	1	0	1.600554	2.377366	0.000000
8	1	0	-0.838909	1.883309	0.000000
9	1	0	0.020853	-2.335296	0.000000
10	1	0	2.455617	-1.847645	0.000000
11	1	0	3.262662	0.519021	0.000000
12	7	0	-1.929038	-0.630574	0.000000

Nitrosobenzene dianion
Energy = -361.7633756 hartrees

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.239190	1.350407	-0.000001
2	6	0	0.126374	1.070683	-0.000005

3	6	0	0.622894	-0.301710	-0.000004
4	6	0	-0.419034	-1.320875	0.000000
5	6	0	-1.765765	-1.005273	0.000003
6	6	0	-2.222868	0.341506	0.000003
7	1	0	-1.555180	2.396832	-0.000001
8	1	0	0.856598	1.872826	-0.000007
9	1	0	-0.106239	-2.366217	0.000000
10	1	0	-2.495076	-1.817806	0.000006
11	1	0	-3.284277	0.579660	0.000005
12	7	0	1.901256	-0.667858	-0.000007
13	8	0	2.832615	0.400161	0.000009

Tetranitrocalix[4]arene neutral species.
Energy = -2358.1639330 Hartrees

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.221381	-2.644420	-0.381722
2	6	0	-1.206609	-2.665403	1.003600
3	6	0	-0.000061	-2.705421	1.673735
4	6	0	1.206500	-2.665430	1.003624
5	6	0	1.221300	-2.644452	-0.381698
6	6	0	-0.000034	-2.690031	-1.057965
7	6	0	2.551726	2.517295	-1.112998
8	6	0	3.264967	1.222847	-0.760294
9	6	0	4.408266	1.211471	0.022525
10	6	0	4.973266	-0.000070	0.381970
11	6	0	4.408211	-1.211626	0.022619
12	6	0	3.264937	-1.223012	-0.760216
13	6	0	2.742242	-0.000085	-1.180546
14	6	0	2.551632	-2.517423	-1.112906
15	6	0	-2.551661	2.517366	-1.112941
16	6	0	-3.264928	1.222933	-0.760246
17	6	0	-4.408226	1.211568	0.022573
18	6	0	-4.973275	0.000034	0.381966
19	6	0	-4.408264	-1.211529	0.022570
20	6	0	-3.264981	-1.222926	-0.760252
21	6	0	-2.742242	0.000000	-1.180538
22	6	0	-2.551701	-2.517353	-1.112948
23	8	0	-0.000019	-2.783117	-2.440378
24	8	0	1.638557	-0.000109	-1.987767
25	8	0	-1.638550	-0.000035	-1.987747
26	6	0	1.206610	2.665468	1.003493
27	6	0	1.221378	2.644388	-0.381831
28	6	0	0.000068	2.705532	1.673629
29	6	0	-1.206493	2.665493	1.003524
30	6	0	-1.221297	2.644417	-0.381799
31	6	0	0.000032	2.689951	-1.058081
32	7	0	-0.000077	-2.768288	3.118951
33	7	0	6.184281	-0.000065	1.171554
34	7	0	0.000087	2.768505	3.118842
35	8	0	-1.080562	-2.798528	3.698002
36	8	0	1.080396	-2.798546	3.698024

37	8	0	6.673648	1.080265	1.484626
38	8	0	6.673445	-1.080383	1.484957
39	8	0	1.080577	2.798794	3.697878
40	8	0	-1.080386	2.798811	3.697907
41	7	0	-6.184294	0.000053	1.171542
42	8	0	-6.673610	1.080388	1.484676
43	8	0	-6.673497	-1.080260	1.484905
44	8	0	0.000012	2.783006	-2.440500
45	1	0	-2.118089	-2.645340	1.563420
46	1	0	2.117970	-2.645389	1.563462
47	1	0	2.379567	2.567415	-2.176431
48	1	0	3.193271	3.351194	-0.850788
49	1	0	4.861091	2.122551	0.353951
50	1	0	4.860998	-2.122699	0.354115
51	1	0	3.193148	-3.351371	-0.850779
52	1	0	2.379399	-2.567460	-2.176329
53	1	0	-3.193180	3.351282	-0.850722
54	1	0	-2.379514	2.567476	-2.176376
55	1	0	-4.861026	2.122652	0.354023
56	1	0	-4.861081	-2.122598	0.354037
57	1	0	-3.193241	-3.351283	-0.850825
58	1	0	-2.379461	-2.567405	-2.176371
59	1	0	2.118096	2.645456	1.563307
60	1	0	-2.117965	2.645504	1.563361
61	6	0	-1.788138	-0.000285	-3.430133
62	1	0	-1.303487	0.884348	-3.803666
63	1	0	-1.301727	-0.884069	-3.803357
64	1	0	-2.834172	-0.001369	-3.706962
65	6	0	-0.000001	4.111445	-3.012744
66	1	0	0.882956	4.656192	-2.708755
67	1	0	-0.000003	3.974002	-4.080272
68	1	0	-0.882967	4.656175	-2.708751
69	6	0	1.788162	0.000265	-3.430151
70	1	0	1.301495	0.883909	-3.803365
71	1	0	2.834199	0.001665	-3.706968
72	1	0	1.303776	-0.884507	-3.803705
73	6	0	-0.000016	-4.111562	-3.012614
74	1	0	-0.882976	-4.656296	-2.708613
75	1	0	-0.000016	-3.974130	-4.080142
76	1	0	0.882947	-4.656290	-2.708613

Tetranitrocalix[4]arene monoanion
Energy = -2358.2991278 Hartrees

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.264889	2.516564	0.302599
2	6	0	1.269124	1.925049	1.562665
3	6	0	0.065677	1.660676	2.231654

4	6	0	-1.156522	1.943632	1.604170
5	6	0	-1.185477	2.532703	0.344452
6	6	0	0.031975	2.865594	-0.280797
7	6	0	-2.585761	-2.110055	-1.738028
8	6	0	-3.331553	-0.943695	-1.112340
9	6	0	-4.469884	-1.137070	-0.336009
10	6	0	-5.025810	-0.054551	0.343862
11	6	0	-4.437611	1.209194	0.330549
12	6	0	-3.298430	1.426733	-0.438404
13	6	0	-2.809999	0.359352	-1.214279
14	6	0	-2.524640	2.731366	-0.363501
15	6	0	2.531346	-2.173292	-1.729440
16	6	0	3.294515	-1.013529	-1.115931
17	6	0	4.415053	-1.214308	-0.320589
18	6	0	5.014462	-0.123512	0.309444
19	6	0	4.467703	1.156519	0.233781
20	6	0	3.337816	1.384979	-0.545202
21	6	0	2.822946	0.304601	-1.294955
22	6	0	2.588364	2.704394	-0.440904
23	8	0	0.014248	3.477177	-1.522363
24	8	0	-1.730313	0.571976	-2.024749
25	8	0	1.786496	0.460477	-2.155297
26	6	0	-1.249526	-2.517235	0.361425
27	6	0	-1.260067	-2.350795	-1.020005
28	6	0	-0.037767	-2.639111	1.040210
29	6	0	1.177865	-2.549729	0.363651
30	6	0	1.196582	-2.382658	-1.017947
31	6	0	-0.030652	-2.335140	-1.708720
32	7	0	0.083419	1.065629	3.514936
33	7	0	-6.239991	-0.262128	1.132076
34	7	0	-0.041156	-2.808077	2.475210
35	8	0	1.205585	0.769197	4.051277
36	8	0	-1.023684	0.818806	4.104983
37	8	0	-6.741127	-1.386008	1.150446
38	8	0	-6.712823	0.696304	1.742209
39	8	0	-1.135573	-2.837343	3.072268
40	8	0	1.050920	-2.903945	3.069353
41	7	0	6.215320	-0.335877	1.107004
42	8	0	6.657179	-1.481345	1.210470
43	8	0	6.743911	0.638850	1.644232
44	8	0	-0.030382	-2.199761	-3.077980
45	1	0	2.199950	1.641097	2.034772
46	1	0	-2.075255	1.672625	2.107005
47	1	0	-2.389369	-1.925528	-2.793083
48	1	0	-3.210713	-3.005309	-1.680645
49	1	0	-4.917928	-2.117864	-0.245449
50	1	0	-4.861061	2.005893	0.927799
51	1	0	-3.128163	3.469775	0.171560
52	1	0	-2.343508	3.130956	-1.360501
53	1	0	3.138332	-3.079798	-1.657666
54	1	0	2.347451	-1.984679	-2.786131
55	1	0	4.830226	-2.205290	-0.192156
56	1	0	4.905918	1.960477	0.810526
57	1	0	3.218168	3.417322	0.098122
58	1	0	2.396249	3.140175	-1.419172

59	1	0	-2.173967	-2.532878	0.922905
60	1	0	2.100457	-2.588630	0.927015
61	6	0	1.939549	1.373015	-3.264076
62	1	0	1.659523	0.824599	-4.163915
63	1	0	1.280176	2.227642	-3.125732
64	1	0	2.975102	1.703921	-3.355468
65	6	0	-0.026542	-3.440993	-3.801276
66	1	0	-0.918596	-4.030571	-3.570300
67	1	0	-0.024339	-3.180183	-4.858375
68	1	0	0.866115	-4.027942	-3.566280
69	6	0	-2.057049	0.959029	-3.370041
70	1	0	-2.657148	0.189664	-3.863300
71	1	0	-2.602816	1.906121	-3.382280
72	1	0	-1.110671	1.074828	-3.892229
73	6	0	0.012838	4.911066	-1.477139
74	1	0	0.908814	5.288405	-0.974861
75	1	0	0.002322	5.254605	-2.510930
76	1	0	-0.874393	5.285916	-0.957869

Tetranitrocalix[4]arene dianion
Energy = -2358.4130037 Hartrees

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.223801	2.759598	0.503131
2	6	0	-1.200893	2.918419	-0.877084
3	6	0	0.021022	3.040956	-1.553287
4	6	0	1.231063	2.934023	-0.854025
5	6	0	1.232389	2.768190	0.526439
6	6	0	-0.001888	2.751348	1.208782
7	6	0	2.556664	-2.538792	1.248888
8	6	0	3.191537	-1.229270	0.803472
9	6	0	4.108985	-1.218616	-0.241164
10	6	0	4.597307	0.000133	-0.741500
11	6	0	4.108972	1.218650	-0.240612
12	6	0	3.191526	1.228815	0.804030
13	6	0	2.787514	-0.000356	1.362622
14	6	0	2.556654	2.538119	1.250083
15	6	0	-2.557382	-2.539513	1.207646
16	6	0	-3.199796	-1.230035	0.775483
17	6	0	-4.183301	-1.219185	-0.207520
18	6	0	-4.696602	0.000062	-0.677154
19	6	0	-4.183318	1.219070	-0.206880
20	6	0	-3.199806	1.229413	0.776122
21	6	0	-2.751373	-0.000444	1.296270
22	6	0	-2.557415	2.538665	1.208998
23	8	0	-0.017314	2.695490	2.586618
24	8	0	1.921804	-0.000593	2.434406
25	8	0	-1.789201	-0.000684	2.278957
26	6	0	1.231168	-2.933330	-0.855519
27	6	0	1.232440	-2.768516	0.525067
28	6	0	0.021155	-3.039766	-1.554906
29	6	0	-1.200787	-2.917793	-0.878651
30	6	0	-1.223748	-2.759996	0.501680

31	6	0	-0.001861	-2.752225	1.207381
32	7	0	0.033909	3.245043	-2.960838
33	7	0	5.558225	0.000365	-1.784115
34	7	0	0.034098	-3.242701	-2.962623
35	8	0	-1.061828	3.307265	-3.582235
36	8	0	1.141133	3.348453	-3.555590
37	8	0	5.972153	-1.102052	-2.241257
38	8	0	5.972058	1.102976	-2.240877
39	8	0	1.141345	-3.345628	-3.557415
40	8	0	-1.061619	-3.304494	-3.584098
41	7	0	-5.725285	0.000304	-1.660319
42	8	0	-6.166500	-1.100058	-2.086528
43	8	0	-6.166506	1.100868	-2.086003
44	8	0	-0.017346	-2.697409	2.585258
45	1	0	-2.121830	2.939661	-1.444224
46	1	0	2.160683	2.967355	-1.405618
47	1	0	2.386321	-2.539596	2.323141
48	1	0	3.242641	-3.360340	1.025677
49	1	0	4.459716	-2.144501	-0.676786
50	1	0	4.459697	2.144737	-0.675808
51	1	0	3.242615	3.359788	1.027264
52	1	0	2.386343	2.538391	2.324340
53	1	0	-3.237147	-3.361616	0.968388
54	1	0	-2.399660	-2.553474	2.284054
55	1	0	-4.565144	-2.144959	-0.616727
56	1	0	-4.565173	2.145055	-0.615599
57	1	0	-3.237211	3.360885	0.970226
58	1	0	-2.399669	2.552023	2.285409
59	1	0	2.160807	-2.966173	-1.407110
60	1	0	-2.121699	-2.938607	-1.445845
61	6	0	-2.294007	-0.000928	3.618456
62	1	0	-2.899268	-0.891630	3.813313
63	1	0	-1.425895	-0.000973	4.275670
64	1	0	-2.899383	0.889633	3.813598
65	6	0	-0.000186	-3.981467	3.222964
66	1	0	0.902417	-4.541180	2.958417
67	1	0	-0.010551	-3.794249	4.296099
68	1	0	-0.880778	-4.569591	2.945801
69	6	0	2.565790	-0.000865	3.713482
70	1	0	1.774117	-0.000889	4.461302
71	1	0	3.188722	-0.891690	3.842107
72	1	0	3.188930	0.889773	3.842386
73	6	0	-0.000160	3.979067	3.225289
74	1	0	-0.880774	4.567380	2.948595
75	1	0	-0.010487	3.791042	4.298284
76	1	0	0.902422	4.538998	2.961132

Tetranitrocalix[4]arene trianion
Energy = -2358. 5289502 Hartrees

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.223801	2.759598	0.503131
2	6	0	-1.200893	2.918419	-0.877084

3	6	0	0.021022	3.040956	-1.553287
4	6	0	1.231063	2.934023	-0.854025
5	6	0	1.232389	2.768190	0.526439
6	6	0	-0.001888	2.751348	1.208782
7	6	0	2.556664	-2.538792	1.248888
8	6	0	3.191537	-1.229270	0.803472
9	6	0	4.108985	-1.218616	-0.241164
10	6	0	4.597307	0.000133	-0.741500
11	6	0	4.108972	1.218650	-0.240612
12	6	0	3.191526	1.228815	0.804030
13	6	0	2.787514	-0.000356	1.362622
14	6	0	2.556654	2.538119	1.250083
15	6	0	-2.557382	-2.539513	1.207646
16	6	0	-3.199796	-1.230035	0.775483
17	6	0	-4.183301	-1.219185	-0.207520
18	6	0	-4.696602	0.000062	-0.677154
19	6	0	-4.183318	1.219070	-0.206880
20	6	0	-3.199806	1.229413	0.776122
21	6	0	-2.751373	-0.000444	1.296270
22	6	0	-2.557415	2.538665	1.208998
23	8	0	-0.017314	2.695490	2.586618
24	8	0	1.921804	-0.000593	2.434406
25	8	0	-1.789201	-0.000684	2.278957
26	6	0	1.231168	-2.933330	-0.855519
27	6	0	1.232440	-2.768516	0.525067
28	6	0	0.021155	-3.039766	-1.554906
29	6	0	-1.200787	-2.917793	-0.878651
30	6	0	-1.223748	-2.759996	0.501680
31	6	0	-0.001861	-2.752225	1.207381
32	7	0	0.033909	3.245043	-2.960838
33	7	0	5.558225	0.000365	-1.784115
34	7	0	0.034098	-3.242701	-2.962623
35	8	0	-1.061828	3.307265	-3.582235
36	8	0	1.141133	3.348453	-3.555590
37	8	0	5.972153	-1.102052	-2.241257
38	8	0	5.972058	1.102976	-2.240877
39	8	0	1.141345	-3.345628	-3.557415
40	8	0	-1.061619	-3.304494	-3.584098
41	7	0	-5.725285	0.000304	-1.660319
42	8	0	-6.166500	-1.100058	-2.086528
43	8	0	-6.166506	1.100868	-2.086003
44	8	0	-0.017346	-2.697409	2.585258
45	1	0	-2.121830	2.939661	-1.444224
46	1	0	2.160683	2.967355	-1.405618
47	1	0	2.386321	-2.539596	2.323141
48	1	0	3.242641	-3.360340	1.025677
49	1	0	4.459716	-2.144501	-0.676786
50	1	0	4.459697	2.144737	-0.675808
51	1	0	3.242615	3.359788	1.027264
52	1	0	2.386343	2.538391	2.324340
53	1	0	-3.237147	-3.361616	0.968388
54	1	0	-2.399660	-2.553474	2.284054
55	1	0	-4.565144	-2.144959	-0.616727
56	1	0	-4.565173	2.145055	-0.615599
57	1	0	-3.237211	3.360885	0.970226

58	1	0	-2.399669	2.552023	2.285409
59	1	0	2.160807	-2.966173	-1.407110
60	1	0	-2.121699	-2.938607	-1.445845
61	6	0	-2.294007	-0.000928	3.618456
62	1	0	-2.899268	-0.891630	3.813313
63	1	0	-1.425895	-0.000973	4.275670
64	1	0	-2.899383	0.889633	3.813598
65	6	0	-0.000186	-3.981467	3.222964
66	1	0	0.902417	-4.541180	2.958417
67	1	0	-0.010551	-3.794249	4.296099
68	1	0	-0.880778	-4.569591	2.945801
69	6	0	2.565790	-0.000865	3.713482
70	1	0	1.774117	-0.000889	4.461302
71	1	0	3.188722	-0.891690	3.842107
72	1	0	3.188930	0.889773	3.842386
73	6	0	-0.000160	3.979067	3.225289
74	1	0	-0.880774	4.567380	2.948595
75	1	0	-0.010487	3.791042	4.298284
76	1	0	0.902422	4.538998	2.961132

Tetranitrocalix[4]arene tetraanion
Energy = -2358.6444562 Hartrees

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.233963	-2.718249	-0.385992
2	6	0	-1.188738	-2.786030	1.009728
3	6	0	0.045040	-2.832138	1.690971
4	6	0	1.241964	-2.719281	0.953915
5	6	0	1.221843	-2.652873	-0.443218
6	6	0	-0.020833	-2.731188	-1.108539
7	6	0	2.589655	2.589570	-1.075818
8	6	0	3.283542	1.273126	-0.751298
9	6	0	4.374739	1.230733	0.118518
10	6	0	4.949687	-0.006492	0.490621
11	6	0	4.356475	-1.211347	0.048890
12	6	0	3.260625	-1.189455	-0.816263
13	6	0	2.788273	0.059149	-1.269091
14	6	0	2.538998	-2.475345	-1.195780
15	6	0	-2.539100	2.474395	-1.197197
16	6	0	-3.260696	1.188747	-0.816810
17	6	0	-4.356662	1.211236	0.048181
18	6	0	-4.949944	0.006679	0.490619
19	6	0	-4.374944	-1.230790	0.119431
20	6	0	-3.283609	-1.273795	-0.750177
21	6	0	-2.788237	-0.060164	-1.268693
22	6	0	-2.589764	-2.590495	-1.073768
23	8	0	-0.053605	-2.790684	-2.475256
24	8	0	1.794182	0.095449	-2.199702
25	8	0	-1.793943	-0.097070	-2.199051
26	6	0	1.188852	2.786849	1.007671
27	6	0	1.233928	2.717832	-0.387990
28	6	0	-0.044847	2.833678	1.689014
29	6	0	-1.241877	2.720146	0.952204
30	6	0	-1.221892	2.652465	-0.444873

31	6	0	0.020715	2.730135	-1.110392
32	7	0	0.079866	-2.969176	3.064488
33	7	0	6.065372	-0.039603	1.301745
34	7	0	-0.079425	2.972176	3.062393
35	8	0	-1.016586	-3.092023	3.724348
36	8	0	1.209120	-3.003531	3.677089
37	8	0	6.591662	1.057647	1.716133
38	8	0	6.587194	-1.168332	1.627523
39	8	0	1.017185	3.095456	3.721912
40	8	0	-1.208555	3.007630	3.675161
41	7	0	-6.065767	0.040288	1.301523
42	8	0	-6.587542	1.169213	1.626707
43	8	0	-6.592234	-1.056734	1.716284
44	8	0	0.053290	2.788326	-2.477177
45	1	0	-2.096860	-2.797158	1.577810
46	1	0	2.173397	-2.682203	1.480651
47	1	0	2.460815	2.692713	-2.142388
48	1	0	3.231688	3.402208	-0.751705
49	1	0	4.786686	2.135953	0.516682
50	1	0	4.755076	-2.143492	0.395089
51	1	0	3.192354	-3.312779	-0.971409
52	1	0	2.346672	-2.498368	-2.257262
53	1	0	-3.192461	3.311957	-0.973322
54	1	0	-2.346858	2.496744	-2.258710
55	1	0	-4.755312	2.143615	0.393700
56	1	0	-4.786951	-2.135738	0.518151
57	1	0	-3.231783	-3.402864	-0.748956
58	1	0	-2.461069	-2.694464	-2.140274
59	1	0	2.097039	2.798434	1.575639
60	1	0	-2.173277	2.683577	1.479048
61	6	0	-2.223784	-0.144520	-3.539832
62	1	0	-1.335500	-0.169526	-4.153180
63	1	0	-2.817007	-1.031871	-3.730727
64	1	0	-2.811127	0.731761	-3.792826
65	6	0	0.018032	4.090397	-3.016182
66	1	0	0.872162	4.672367	-2.685754
67	1	0	0.049674	3.987045	-4.091690
68	1	0	-0.892628	4.606900	-2.731443
69	6	0	2.224363	0.142054	-3.540403
70	1	0	2.817634	1.029282	-3.731760
71	1	0	2.811790	-0.734380	-3.792671
72	1	0	1.336233	0.166654	-4.153985
73	6	0	-0.018230	-4.093283	-3.012984
74	1	0	-0.872160	-4.675087	-2.681751
75	1	0	-0.050167	-3.991008	-4.088584
76	1	0	0.892603	-4.609324	-2.727957

5-nitrocalix[4]arene (distant nitro)

Energy = -1744.1862737 Hartrees

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.674921	-2.644408	-0.555104
2	6	0	1.448672	-2.665425	-1.921905
3	6	0	0.153905	-2.705455	-2.399835
4	6	0	-0.936111	-2.665443	-1.553253
5	6	0	-0.739088	-2.644432	-0.181934
6	6	0	0.571229	-2.689999	0.299799
7	6	0	-1.942167	2.517338	0.743918
8	6	0	-2.700921	1.222884	0.504355
9	6	0	-3.950397	1.211493	-0.094600
10	6	0	-4.563680	-0.000055	-0.363474
11	6	0	-3.950357	-1.211604	-0.094642
12	6	0	-2.700903	-1.222975	0.504333
13	6	0	-2.120126	-0.000040	0.839841
14	6	0	-1.942088	-2.517380	0.743935
15	6	0	3.101298	2.517391	-0.035835
16	6	0	3.752307	1.222947	-0.493331
17	6	0	4.762584	1.211559	-1.441633
18	6	0	5.266091	0.000014	-1.883106
19	6	0	4.762622	-1.211538	-1.441577
20	6	0	3.752361	-1.222912	-0.493274
21	6	0	3.299970	0.000026	0.001913
22	6	0	3.101340	-2.517328	-0.035712
23	8	0	0.782419	-2.783051	1.665988
24	8	0	-0.906071	-0.000049	1.468964
25	8	0	2.332560	0.000014	0.968267
26	6	0	-0.936201	2.665455	-1.553237
27	6	0	-0.739145	2.644408	-0.181919
28	6	0	0.153793	2.705498	-2.399842
29	6	0	1.448568	2.665471	-1.921942
30	6	0	1.674848	2.644429	-0.555143
31	6	0	0.571180	2.689983	0.299793
32	7	0	-5.881111	-0.000065	-0.958770
33	8	0	-6.412564	1.080260	-1.193427
34	8	0	-6.412414	-1.080388	-1.193732
35	8	0	0.782406	2.783072	1.665977
36	1	0	2.263922	-2.645378	-2.614409
37	1	0	-1.922413	-2.645412	-1.967264
38	1	0	-1.609558	2.567483	1.768563
39	1	0	-2.616241	3.351233	0.582781
40	1	0	-4.448542	2.122566	-0.352974
41	1	0	-4.448474	-2.122684	-0.353047
42	1	0	-2.616120	-3.351332	0.582917
43	1	0	-1.609406	-2.567392	1.768561
44	1	0	3.695224	3.351298	-0.393008
45	1	0	3.093644	2.567527	1.041415
46	1	0	5.159429	2.122633	-1.838393
47	1	0	5.159482	-2.122617	-1.838312
48	1	0	3.695301	-3.351267	-0.392752

49	1	0	3.093592	-2.567354	1.041543
50	1	0	-1.922515	2.645433	-1.967221
51	1	0	2.263808	2.645466	-2.614461
52	6	0	2.700760	-0.000202	2.370866
53	1	0	2.278868	0.884442	2.814037
54	1	0	2.277081	-0.883975	2.814044
55	1	0	3.776808	-0.001283	2.484632
56	6	0	0.869846	4.111524	2.231469
57	1	0	-0.049189	4.656267	2.065934
58	1	0	1.032946	3.974107	3.286467
59	1	0	1.696002	4.656244	1.796132
60	6	0	-0.833552	0.000361	2.917272
61	1	0	-0.295578	0.884012	3.211730
62	1	0	-1.825016	0.001771	3.350653
63	1	0	-0.297780	-0.884404	3.212457
64	6	0	0.869843	-4.111483	2.231539
65	1	0	1.695992	-4.656227	1.796221
66	1	0	1.032940	-3.974025	3.286531
67	1	0	-0.049200	-4.656215	2.066019
68	1	0	6.062602	0.000011	-2.597578
69	1	0	-0.009403	-2.751981	-3.456275
70	1	0	-0.009541	2.752052	-3.456277

11-nitrocalix[4]arene (pinched nitro)

Energy = -1744. Hartrees

Center Number	Atomic Number	Atomi Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.218647	2.613431	-1.183205
2	6	0	-1.204276	2.115241	-2.476022
3	6	0	0.002106	1.900736	-3.112472
4	6	0	1.208832	2.112813	-2.475860
5	6	0	1.224032	2.610978	-1.183043
6	6	0	0.002949	2.907186	-0.572890
7	6	0	2.549677	-1.904971	1.424127
8	6	0	3.264065	-0.836799	0.613345
9	6	0	4.407137	-1.119912	-0.116930
10	6	0	4.973201	-0.131010	-0.902997
11	6	0	4.409430	1.127634	-1.022430
12	6	0	3.266406	1.431866	-0.300645
13	6	0	2.742653	0.455111	0.546155
14	6	0	2.554463	2.765026	-0.457227
15	6	0	-2.553707	-1.899891	1.423691
16	6	0	-3.265827	-0.830284	0.612810
17	6	0	-4.409351	-1.111092	-0.117645
18	6	0	-4.973335	-0.121033	-0.903752
19	6	0	-4.407040	1.136490	-1.023055
20	6	0	-3.263509	1.438412	-0.301102
21	6	0	-2.741828	0.460582	0.545740
22	6	0	-2.548868	2.770144	-0.457571
23	8	0	0.003474	3.510080	0.674607
24	8	0	1.639214	0.757876	1.294809

25	8	0	-1.637891	0.761119	1.294555
26	6	0	1.203775	-2.831895	-0.483800
27	6	0	1.218984	-2.294718	0.793304
28	6	0	-0.003009	-3.118238	-1.090522
29	6	0	-1.209327	-2.829487	-0.484013
30	6	0	-1.223689	-2.292284	0.793089
31	6	0	-0.002200	-2.083057	1.437498
32	8	0	-0.001890	-1.652818	2.754554
33	1	0	-2.115945	1.888372	-2.987868
34	1	0	2.120111	1.884112	-2.987586
35	1	0	2.377793	-1.553925	2.429245
36	1	0	3.190334	-2.777094	1.492555
37	1	0	4.858978	-2.089297	-0.083880
38	1	0	4.862999	1.848389	-1.670309
39	1	0	3.196707	3.439971	-1.011928
40	1	0	2.382602	3.208970	0.510457
41	1	0	-3.196114	-2.770733	1.492015
42	1	0	-2.381286	-1.549183	2.428836
43	1	0	-4.863135	-2.079573	-0.084688
44	1	0	-4.859075	1.858169	-1.670978
45	1	0	-3.189679	3.446374	-1.012364
46	1	0	-2.376256	3.213754	0.510136
47	1	0	2.115109	-3.023435	-1.010469
48	1	0	-2.120949	-3.019211	-1.010841
49	6	0	-1.787040	1.300462	2.632358
50	1	0	-1.303133	0.618991	3.309425
51	1	0	-1.299659	2.259196	2.648353
52	1	0	-2.832988	1.405967	2.888646
53	6	0	-0.003016	-2.671209	3.781731
54	1	0	0.879320	-3.290979	3.703382
55	1	0	-0.002560	-2.144830	4.720577
56	1	0	-0.886602	-3.289177	3.703230
57	6	0	1.789258	1.296338	2.632867
58	1	0	1.301848	0.616647	3.309190
59	1	0	2.835377	1.397415	2.890240
60	1	0	1.305843	2.257094	2.648721
61	6	0	0.004939	4.956121	0.709008
62	1	0	-0.877585	5.348699	0.223412
63	1	0	0.005130	5.227535	1.750564
64	1	0	0.888337	5.346905	0.223556
65	1	0	-5.869829	-0.338503	-1.445881
66	1	0	0.001814	1.544432	-4.121406
67	7	0	-0.003498	-3.726353	-2.428840
68	8	0	1.051342	-3.954705	-2.951895
69	8	0	-1.058722	-3.969855	-2.944223
70	1	0	5.869337	-0.350287	-1.444992

Computation of reduction potentials.

Nitrobenzene vs nitrosobenzene: E_1. Using the data above and a published procedure[1] the absolute reduction potential of nitrobenzene was computed as 3.4235 V. From the relation[1] $1.056E_{absolute}$ -4.90, the reduction potential relative to SCE is -1.28 V. Using the same procedures, the absolute potential of nitrosobenzene is 3.597 V and the reduction potential is estimated as -1.10 vs SCE. Nitrosobenzene is predicted to have a reduction potential 0.18 V positive of that of nitrobenzene.

Nitrobenzene vs nitrosobenzene: E_2. Using the data above and the same procedures[1] the absolute second reduction potential of nitrobenzene was computed as 1.9628 V. From the relation[1] $1.056E_{absolute}$ -4.90, the second reduction potential relative to SCE is -2.827 V. Using the same procedures, the absolute potential of nitrosobenzene is 1.8646 V and the reduction potential is estimated as -2.93 V vs SCE. Nitrosobenzene is predicted to have a reduction potential 0.10 V negative of that of nitrobenzene.

11-Nitrocalix[4]arene (pinched nitro] vs the 5-nitro isomer (distant nitro). Using the data above and the same procedures, the difference between the absolute potentials of 5-nitro and 11-nitrocalix[4]arene is 0.307 V and the difference in reduction potentials is estimated as 0.32 V.