The Effects of Sidearm Length and Structure of p-Substituted Phenyl Derivatives on their Binding to the Host Cyclobis(paraquat-p-phenylene)

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Supporting Information

Guest 3, First Minimization

SPARTAN SEMIEMPIRICAL PROGRAM: IBM Release 4.0.2b
Calculation started: Thu Apr 4 09:54:51 1996
Run type: Geometry optimization
Model: RHF/PM3
Number of shells: 154
100 S shells
54 P shells
Number of basis functions: 262
Number of electrons: 270
Use of molecular symmetry disabled
Molecular charge: 4
Spin multiplicity: 1

Point Group = C1 Order = 1 Nsymop = 1
This system has 294 degrees of freedom

Convergence on Energy - difference below .5000D-03 kcal/mol

Cycle no: 92 Heat of formation = 909.954 rmsG = .0000 rmsD = .0001

Cartesian Coordinates (Angstroms)

Atom	X	Y	Z
C 1	2.9499211	.0449630	-4.9246452
N 2	3.4809689	.2266733	-3.5266312
C 3	4.0317364	.4818268	-.7984141
C 4	3.9211994	-.8610995	-2.8113168
C 5	3.4428307	1.4678610	-2.9308032
C 6	3.7219694	1.6084913	-1.5752504
C 7	4.2086735	-.7439982	-1.4528065
H 8	4.0102631	-1.8374671	-3.3252464
H 9	3.1712102	2.3428924	-3.5508279
H 10	3.6741497	2.6056468	-1.1009853
H 11	4.5280140	-1.6373455	-.8830270
C 12	4.0400719	.5579001	.6708193
H 13	3.1557562	.9622476	-5.5232891
H 14	3.5091931	-.7755380	-5.4307840
C 15	1.4779258	-.2535037	-4.8883684
N 16	3.5442593	.6055312	3.4223830
H 17	-.6443409	-2.2748962	5.0020637
C 18	3.7862083	1.7673332	1.3326830
C 19	3.5333346	1.7777079	2.7021700
H 20	1.7848107	-1.8391038	4.9466935
C 21	4.1793579	-.6037497	1.4451097

H 22	3.7576024	2.7119481	.7589547
H 23	3.3031783	2.7222713	3.2312383
C 24	3.0435518	.5846708	4.8436922
H 25	3.2840403	1.5548139	5.3370274
C 26	-1.2672326	-.8061368	-4.8334067
C 27	.5480920	.7871951	-4.9675632
C 28	1.0265083	-1.5739770	-4.8381832
C 29	-.3388461	-1.8488636	-4.8134251
C 30	-.8158293	.5126390	-4.9396085
H 31	.8862091	1.8258372	-5.0859592
H 32	1.7425787	-2.4078343	-4.8344344
H 33	-.6763042	-2.8941962	-4.8008081
H 34	-1.5336684	1.3385883	-5.0369474
C 35	-2.7398126	-1.1012019	-4.8077042
H 36	-3.3051919	-.3614163	-5.4203120
H 37	-2.9565288	-2.0955344	-5.2620000
N 38	-3.2489303	-1.0733656	-3.3892065
C 39	-3.7484426	-.9267008	-.6401553
C 40	-3.2327887	-2.2181412	-2.6262137
C 41	-3.6396872	.1181894	-2.8229575
C 42	-3.8969786	.2024094	-1.4573066
C 43	-3.4881414	-2.1583218	-1.2591788
H 44	-2.9976601	-3.1796292	-3.1207634
H 45	-3.7252200	1.0081571	-3.4748319
H 46	-4.1826628	1.1712873	-1.0084986
H 47	-3.4648071	-3.0830568	-.6537709
C 48	-3.7398948	-.8072216	.8267429
H 49	-3.2115582	.3851205	5.4841818
C 50	-3.7255545	.4495935	1.4472228
C 51	-3.6195975	-1.9483358	1.6345592
H 52	-3.2259978	-2.7177702	3.6346625
C 53	-3.4528014	.5454816	2.8103365
H 54	-3.8788908	1.4029103	.8644150
H 55	-3.7131119	-2.9533077	1.1837134
C 56	-3.3457022	-1.8236834	2.9932564
H 57	-3.4006944	1.5355380	3.3047526
C 58	-2.6702658	-.4385935	4.9639439
N 59	-3.2043514	-.5783704	3.5618841
H 60	-2.8962840	-1.3615488	5.5463876
C 61	-1.1912436	-.1755259	4.9304343
C 62	3.9235818	-.5688228	2.8122357
H 63	1.0218864	2.4187609	4.9769952
H 64	3.5967408	-.1911601	5.4220722
C 65	1.5651024	.3187172	4.8696342
C 66	-.7101069	1.1358652	4.9573648
C 67	-.2846332	-1.2389719	4.9378318
C 68	1.0848202	-.9932070	4.9071934
C 69	.6608002	1.3819353	4.9270704
H 70	-1.4066198	1.9831184	5.0288591
H 71	4.0059979	-1.4826961	3.4310792
H 72	4.4649562	-1.5561916	.9597202
C 73	-.1898204	.7449790	-1.3715749
C 74	-.5291941	1.9294316	-.7365108
H 75	.5174535	-1.1849576	1.3702903
H 76	-.8295347	2.8196249	-1.3142835
H 77	-.0792238	.9521577	2.5202928
C 78	.1773640	-.3754681	-.6089188
H 79	-.2017064	.6919183	-2.4712857
C 80	-.5020004	2.0015128	.6634966
C 81	-.1170066	.8863747	1.4219856
C 82	.2205771	-.3002482	.7859741
O 83	.5326809	-1.4895372	-1.3460959
O 84	-.7680895	3.1334949	1.3988046
C 85	.4829609	-2.7492876	-.6767067
C 86	1.3939736	-3.7199470	-1.4444572
H 87	-.5685582	-3.0929584	-.7054878
H 88	.7790110	-2.6623276	.3914475
O 89	2.7207281	-3.5396970	-1.0080469
H 90	1.3674924	-3.5283793	-2.5370348
H 91	1.0511999	-4.7579353	-1.2744876
H 92	-1.4305681	4.1904024	-.3065225
H 93	-3.4844919	5.0706245	1.1896509
H 94	-1.0818061	5.0673592	1.2261179
C 95	-3.0219844	4.0663353	1.2221841
H 96	-3.1286887	3.6752756	2.2525712
O 97	-3.7214191	3.1631135	.3878423
H 98	-4.4373587	3.6551952	.0047678
H 99	3.1096994	-4.4035847	-.9568344
C 100	-1.5487954	4.1610715	.7981065

Heat of Formation: 909.954 kcal/mol

Guest 3, Second Minimization

SPARTAN SEMIEMPIRICAL PROGRAM: IBM Release 3.1.7
Calculation started: Sat Jul 22 22:38:19 1995
Run type: Geometry optimization
Model: RHF/PM3
Number of shells: 154
100 S shells
54 P shells
Number of basis functions: 262
Number of electrons: 270
Use of molecular symmetry disabled
Molecular charge: 4
Spin multiplicity: 1

Point Group = C1 Order = 1 Nsymop = 1
This system has 294 degrees of freedom

Convergence on Energy - difference below .5000D-03 kcal/mol

Cycle no: 42 Heat of formation = 915.000 rmsG = .0000 rmsD = .0001

Cartesian Coordinates (Angstroms)

Atom	X	Y	Z
C 1	4.8133096	2.9960830	.0738930
N 2	3.4088198	3.5020323	-.1293693
C 3	.6720855	3.9689741	-.4485097
C 4	2.6482829	3.8895290	.9496352
C 5	2.8494612	3.4722340	-1.3865434
C 6	1.4893225	3.7071083	-1.5581955
C 7	1.2850564	4.1335833	.8014403
H 8	3.1395095	3.9869397	1.9368589
H 9	3.5032331	3.2400582	-2.2488406
H 10	1.0445913	3.6571584	-2.5699364
H 11	.6769172	4.4268896	1.6774347
C 12	-.7930449	3.9397373	-.5751127
H 13	5.4494095	3.3087960	-.7864367
H 14	5.2617318	3.4825483	.9708592
C 15	4.8024310	1.5013228	.2230403
N 16	-3.5171218	3.3404502	-.7335520
H 17	-5.3856302	-1.1524916	1.7270622
C 18	-1.3965251	3.6717054	-1.8109071
C 19	-2.7539608	3.3698299	-1.8771564
H 20	-5.4140801	1.3016141	1.4789636
C 21	-1.6171415	4.0512751	.5546575
H 22	-.7894610	3.6547746	-2.7357427
H 23	-3.2290381	3.1136196	-2.8462212
C 24	-4.9048371	2.7575076	-.7790455
H 25	-5.3912938	3.0286619	-1.7447835
C 26	4.8316514	-1.2845699	.5110217
C 27	5.0033166	.6804093	-.8892092
C 28	4.6559788	.9223768	1.4861755
C 29	4.6708055	-.4617939	1.6293526
C 30	5.0169136	-.7049592	-.7464578
H 31	5.1868096	1.1204981	-1.8793799
H 32	4.5601089	1.5535236	2.3803391
H 33	4.5763930	-.8973978	2.6348283
H 34	5.2107796	-1.3336174	-1.6267602
C 35	4.8838128	-2.7777352	.6716908
H 36	5.4988483	-3.2453046	-.1316745
H 37	5.3804593	-3.0546858	1.6303375
N 38	3.4925731	-3.3546773	.6441879
C 39	.7692349	-3.9643827	.5035304
C 40	2.7231227	-3.3274137	1.7841101
C 41	2.9521511	-3.8124251	-.5360954
C 42	1.5978366	-4.1268799	-.6162380
C 43	1.3672919	-3.6352824	1.7277959
H 44	3.1955818	-3.0187888	2.7378461
H 45	3.6108232	-3.9083521	-1.4206973
H 46	1.1669971	-4.4726819	-1.5741766
H 47	.7550352	-3.5780052	2.6472179
C 48	-.6954907	-4.0004195	.3733728
H 49	-5.2645107	-3.4970913	-1.0985526
C 50	-1.3028329	-4.1906448	-.8758252
C 51	-1.5180408	-3.7168471	1.4737336

H 52	-3.5345459	-3.2310113	2.1440496
C 53	-2.6641705	-3.9441574	-1.0363725
H 54	-.6913999	-4.5053924	-1.7420790
H 55	-1.0786305	-3.6477999	2.4863863
C 56	-2.8765212	-3.4809309	1.2902064
H 57	-3.1505796	-4.0608126	-2.0240452
C 58	-4.8276797	-3.0185275	-.1915799
N 59	-3.4285321	-3.5307789	.0304135
H 60	-5.4773635	-3.3355025	.6570144
C 61	-4.8120842	-1.5228828	-.3338049
C 62	-2.9713605	3.7415493	.4653803
H 63	-4.4020779	.8869445	-2.7112154
H 64	-5.5322890	3.2245157	.0149763
C 65	-4.8473867	1.2642549	-.6170245
C 66	-4.5563008	-.9369623	-1.5770525
C 67	-5.1203336	-.7081125	.7572914
C 68	-5.1367882	.6785060	.6168559
C 69	-4.5750945	.4465141	-1.7181721
H 70	-4.3739971	-1.5638734	-2.4606693
H 71	-3.6269491	3.7961127	1.3554648
H 72	-1.1822212	4.3542474	1.5251001
O 73	-.4618700	.6347211	2.7985702
C 74	-.1926800	.2370910	1.5001110
C 75	.1918512	-.2926809	-1.2032149
C 76	1.1048145	.0670593	1.0039252
C 77	-1.2980840	.1387712	.6426406
C 78	-1.1058764	-.1267031	-.7061834
C 79	1.2961412	-.1925697	-.3477808
H 80	1.9747062	.1351728	1.6759664
H 81	-2.3164712	.2733839	1.0337417
H 82	-1.9716447	-.2034225	-1.3892528
H 83	2.3159523	-.3197164	-.7402686
O 84	.4438814	-.6870174	-2.5105213
C 85	-.0502230	-.2399345	3.8428117
C 86	.0744727	.2374841	-3.5245493
H 87	.7738636	-.0508350	-4.3303385
H 88	.3105716	1.2775162	-3.2206879
C 89	-1.3975509	.0924925	-3.9684495
C 90	1.3511249	.0869808	4.3932640
H 91	-.1458563	-1.3021212	3.5418665
H 92	-.8300451	-.0220655	4.5961375
H 93	-1.4978543	-.6258237	-4.8028782
O 94	-1.9369397	1.3481421	-4.2875722
H 95	-2.0433780	-.2639437	-3.1367553
H 96	1.7832131	.9890723	3.9201028
O 97	2.2397004	-.9690879	4.1049211
H 98	1.3022685	.2739704	5.4820379
H 99	2.5427677	-1.2992053	4.9411240
H 100	-1.8375466	1.4772455	-5.2228730

Heat of Formation: 915.000 kcal/mol

Guest 4, First Minimization

SPARTAN SEMIEMPIRICAL PROGRAM: IBM Release 3.1.7
Calculation started: Sun Jul 23 14:06:55 1995
Run type: Geometry optimization
Model: RHF/PM3
Number of shells: 174
114 S shells
60 P shells
Number of basis functions: 294
Number of electrons: 306
Use of molecular symmetry disabled
Molecular charge: 4
Spin multiplicity: 1

Point Group = C1 Order = 1 Nsymop = 1
This system has 336 degrees of freedom

Convergence on Energy - difference below .5000D-03 kcal/mol

Cycle no: 110 Heat of formation = 815.645 rmsG = .0000 rmsD = .0001

Cartesian Coordinates (Angstroms)

Atom	X	Y	Z

C	1	4.8065742	2.8637894	.0490938
N	2	3.4055980	3.3875849	-.1315114
C	3	.6748035	3.8975099	-.4270420
C	4	2.6452395	3.7143456	.9678877
C	5	2.8493221	3.4367398	-1.3890468
C	6	1.4917810	3.6960282	-1.5492148
C	7	1.2851506	3.9775642	.8325306
H	8	3.1364262	3.7439630	1.9589836
H	9	3.5011330	3.2481644	-2.2633262
H	10	1.0472581	3.7133790	-2.5630244
H	11	.6761560	4.2203876	1.7227559
C	12	-.7895945	3.8923454	-.5595208
H	13	5.4218869	3.1254982	-.8424213
H	14	5.2892614	3.3806939	.9102848
C	15	4.7715940	1.3777558	.2613078
N	16	-3.5177688	3.3372705	-.7772782
H	17	-5.4013650	-1.1257180	1.6473402
C	18	-1.3894396	3.7310769	-1.8138534
C	19	-2.7506216	3.4482892	-1.9112219
H	20	-5.3894608	1.3302240	1.4059383
C	21	-1.6173128	3.9215304	.5733706
H	22	-.7811745	3.7892940	-2.7391934
H	23	-3.2073133	3.2791185	-2.9206959
C	24	-4.9136611	2.7811980	-.8636286
H	25	-5.3676561	3.0655989	-1.8407384
C	26	4.7410900	-1.3926419	.6652112
C	27	4.8406221	.5065037	-.8295298
C	28	4.7325343	.8556195	1.5554437
C	29	4.7166169	-.5221250	1.7564207
C	30	4.8253114	-.8703078	-.6286833
H	31	4.9418476	.9009920	-1.8497267
H	32	4.7410266	1.5248282	2.4267512
H	33	4.7037219	-.9155419	2.7905420
H	34	4.9148276	-1.5417863	-1.4936480
C	35	4.7493422	-2.8789457	.8873855
H	36	5.4048255	-3.3868643	.1433076
H	37	5.1743650	-3.1287249	1.8880688
N	38	3.3518869	-3.4291349	.7894407
C	39	.6343676	-4.0094727	.5211227
C	40	2.5528639	-3.4725907	1.9039966
C	41	2.8461161	-3.7988523	-.4384940
C	42	1.4962569	-4.0972977	-.5835912
C	43	1.1964390	-3.7695977	1.7798586
H	44	3.0021123	-3.2453450	2.9228438
H	45	3.5334553	-3.8346858	-1.3050527
H	46	1.0935435	-4.3734728	-1.5751087
H	47	.5575308	-3.7779555	2.6819220
C	48	-.8252165	-4.0312050	.3428258
H	49	-5.3648807	-3.4678671	-1.2050265
C	50	-1.3928142	-4.1352472	-.9352762
C	51	-1.6822331	-3.8173635	1.4322143
H	52	-3.7160408	-3.3609812	2.0691647
C	53	-2.7467643	-3.8724566	-1.1223755
H	54	-.7540090	-4.3949433	-1.7997723
H	55	-1.2743128	-3.8188026	2.4599529
C	56	-3.0332761	-3.5609466	1.2216704
H	57	-3.2024673	-3.9195862	-2.1297591
C	58	-4.9340135	-2.9954746	-.2922135
N	59	-3.5442783	-3.5259116	-.0555055
H	60	-5.5982195	-3.3042462	.5478316
C	61	-4.8971019	-1.5001483	-.4308298
C	62	-2.9728607	3.6353131	.4530715
H	63	-4.5046968	.9095025	-2.8119903
H	64	-5.5531027	3.2558055	-.0840699
C	65	-4.8875203	1.2869238	-.7060919
C	66	-4.6662646	-.9159667	-1.6790894
C	67	-5.1573013	-.6829906	.6715806
C	68	-5.1515123	.7034116	.5350504
C	69	-4.6634189	.4685038	-1.8165041
H	70	-4.5163219	-1.5433679	-2.5685203
H	71	-3.6335265	3.6239573	1.3404436
H	72	-1.1837278	4.1430262	1.5655911
O	73	-.7842597	.2133513	2.8620530
C	74	-.3995322	.0054048	1.5518863
C	75	.1519586	-.2445636	-1.1668605
C	76	.9256517	-.1200325	1.1195466
C	77	-1.4484139	.0130679	.6190857
C	78	-1.1732812	-.1174257	-.7347200
C	79	1.2002264	-.2386373	-.2372673
H	80	1.7521797	-.1237466	1.8446547
H	81	-2.4907710	.1185912	.9552422

H 82	-1.9973273	-.1333416	-1.4707242
H 83	2.2432919	-.3342425	-.5763631
O 84	.5121132	-.4956938	-2.4817128
C 85	-.1389198	-.5464187	3.8754652
C 86	-.0310404	.3640742	-3.4731267
H 87	.7322984	.2679151	-4.2666927
H 88	-.0343083	1.4177132	-3.1269439
C 89	-1.4233683	-.0808067	-3.9708408
C 90	1.0997055	.1549039	4.4698748
H 91	.0867818	-1.5733958	3.5252446
H 92	-.9557848	-.6077413	4.6183762
H 93	-1.3468433	-.7577373	-4.8422667
O 94	-2.2481093	1.0327998	-4.2240445
H 95	-1.9925559	-.6051888	-3.1745773
H 96	1.3496713	1.0840250	3.9258811
O 97	2.2529490	-.6473296	4.3038805
H 98	.9191118	.4306736	5.5277687
C 99	2.7000431	-1.3056403	5.4898993
C 100	-2.2011551	1.5464067	-5.5577621
H 101	-1.2185180	1.3677986	-6.0357758
C 102	-2.5264787	3.0463156	-5.4762216
H 103	-2.9684523	1.0044215	-6.1409611
O 104	-1.3868353	3.7971471	-5.1375500
H 105	-3.2419666	3.2651971	-4.6519681
H 106	-2.9849445	3.3920217	-6.4218358
H 107	-1.0099986	4.1195475	-5.9464872
C 108	4.0322984	-1.9884646	5.1506099
H 109	1.9333109	-2.0301984	5.8250962
H 110	2.8470418	-.5665684	6.3018837
H 111	4.6377083	-1.3963455	4.4317615
O 112	3.8477077	-3.2149791	4.4793701
H 113	4.6352320	-2.1295892	6.0681682
H 114	3.7248989	-3.8869011	5.1400934

Heat of Formation: 815.645 kcal/mol

Guest 4, Second Minimization

SPARTAN SEMIEMPIRICAL PROGRAM: IBM Release 4.0.2b
Calculation started: Tue Mar 19 17:47:01 1996
Run type: Geometry optimization
Model: RHF/PM3
Number of shells: 174
114 S shells
60 P shells
Number of basis functions: 294
Number of electrons: 306
Use of molecular symmetry disabled
Molecular charge: 4
Spin multiplicity: 1

Point Group = C1 Order = 1 Nsymop = 1
This system has 336 degrees of freedom

Convergence on Energy - difference below .5000D-03 kcal/mol

Cycle no: 333 Heat of formation = 816.092 rmsG = .0000 rmsD = .0001

Cartesian Coordinates (Angstroms)

Atom	X	Y	Z
C 1	3.0063373	.1318772	-4.8303420
N 2	3.5324195	.3514237	-3.4366681
C 3	4.0812563	.6583472	-.7133865
C 4	4.0762399	-.6893568	-2.7263193
C 5	3.3909506	1.5863794	-2.8396271
C 6	3.6662193	1.7535360	-1.4876237
C 7	4.3653333	-.5435902	-1.3695836
H 8	4.2384351	-1.6822661	-3.2114109
H 9	3.0365306	2.4310959	-3.4591355
H 10	3.5344239	2.7419690	-1.0120954
H 11	4.7667915	-1.4108522	-.8056042
C 12	4.0856715	.7282252	.7554693
H 13	3.2166064	1.0334967	-5.4505478
H 14	3.5670311	-.7024390	-5.3106132
C 15	1.5339922	-.1654547	-4.7989315

N	16	3.5804527	.7343487	3.5033731
H	17	-.5895225	-2.2099134	5.0498819
C	18	3.7691755	1.9198265	1.4222280
C	19	3.5130130	1.9093206	2.7905756
H	20	1.8361282	-1.7523929	5.0173134
C	21	4.2818651	-.4309359	1.5216831
H	22	3.6902651	2.8636300	.8525258
H	23	3.2313747	2.8365124	3.3249170
C	24	3.0734997	.6828925	4.9213103
H	25	3.3015966	1.6466977	5.4322824
C	26	-1.2118626	-.7214110	-4.7689073
C	27	.6034910	.8706243	-4.9207215
C	28	1.0833033	-1.4842246	-4.7146684
C	29	-.2818432	-1.7606228	-4.7005103
C	30	-.7603834	.5946470	-4.9054765
H	31	.9418757	1.9063413	-5.0613961
H	32	1.7998139	-2.3160134	-4.6690809
H	33	-.6171798	-2.8056169	-4.6511798
H	34	-1.4775916	1.4163025	-5.0360904
C	35	-2.6842062	-1.0203193	-4.7659803
H	36	-3.2408725	-.2824021	-5.3882265
H	37	-2.8885670	-2.0153704	-5.2239387
N	38	-3.2200790	-.9970412	-3.3582787
C	39	-3.7516499	-.8316627	-.6169003
C	40	-3.1607748	-2.1297334	-2.5796030
C	41	-3.6876618	.1774361	-2.8156571
C	42	-3.9677337	.2718345	-1.4543347
C	43	-3.4341026	-2.0600749	-1.2175670
H	44	-2.8685668	-3.0838648	-3.0564191
H	45	-3.8176331	1.0506546	-3.4821038
H	46	-4.3343009	1.2403942	-1.0477035
H	47	-3.3770649	-2.9740083	-.5988911
C	48	-3.7240177	-.7063443	.8496171
H	49	-3.1807513	.4185548	5.5215573
C	50	-3.6175580	.5469519	1.4663578
C	51	-3.6675450	-1.8509202	1.6607066
H	52	-3.3125782	-2.6410413	3.6589474
C	53	-3.3365175	.6275088	2.8289154
H	54	-3.7143435	1.5150547	.8957018
H	55	-3.8189868	-2.8496811	1.2127663
C	56	-3.3794794	-1.7420462	3.0175856
H	57	-3.2225677	1.6138981	3.3193000
C	58	-2.6313787	-.3914465	4.9887575
N	59	-3.1611807	-.5066775	3.5837903
H	60	-2.8525309	-1.3267223	5.5526278
C	61	-1.1543847	-.1157954	4.9692699
C	62	4.0192152	-.4162814	2.8880563
H	63	1.0352406	2.4983113	5.0250958
H	64	3.6310446	-.0975221	5.4887672
C	65	1.5976585	.4029060	4.9337758
C	66	-.6850543	1.2000348	4.9954384
C	67	-.2386741	-1.1709186	4.9881316
C	68	1.1290401	-.9129806	4.9702761
C	69	.6832776	1.4583578	4.9776378
H	70	-1.3897126	2.0412982	5.0556247
H	71	4.1429991	-1.3295635	3.5004897
H	72	4.6170508	-1.3673807	1.0310841
C	73	-.1812287	.5405406	-1.3142103
C	74	-.3879059	1.7683280	-.7063556
H	75	.5518526	-1.3437961	1.4521072
H	76	-.6484674	2.6605768	-1.2995490
H	77	.1557231	.8628821	2.5560015
C	78	.1271689	-.5845537	-.5306179
H	79	-.2561136	.4538623	-2.4090920
C	80	-.2855057	1.8818667	.6871669
C	81	.0592459	.7671119	1.4636389
C	82	.2686070	-.4635079	.8548052
O	83	.2454984	-1.7594809	-1.2420722
O	84	-.4359457	3.0564797	1.3924616
C	85	.6063438	-2.9357622	-.5187536
C	86	1.3998105	-3.8488780	-1.4618741
H	87	-.3368939	-3.4270646	-.2143496
H	88	1.1751005	-2.6999437	.4064475
O	89	2.6475503	-3.2248222	-1.7187958
H	90	.8834288	-3.9893716	-2.4317693
H	91	1.5199353	-4.8449794	-.9913156
C	92	3.6998007	-4.0978900	-2.0971625
C	93	4.4381677	-4.7113858	-.8993848
H	94	4.3367561	-3.3937091	-2.6762655
H	95	3.3458430	-4.8917675	-2.7820459
H	96	5.1240801	-5.5038104	-1.2529758

H 97	3.7310550	-5.1691054	-.1810989
O 98	5.1401224	-3.7013085	-.2072600
H 99	6.0033198	-4.0530876	-.0322934
C 100	-1.1575789	4.1192496	.7806057
H 101	-1.0156839	4.1388119	-.3213994
H 102	-.6502760	4.9984126	1.2184689
C 103	-2.6432812	4.1092949	1.1696659
H 104	-3.0438035	5.1419220	1.1227933
H 105	-2.7987027	3.7358871	2.1999730
O 106	-3.3468085	3.2127383	.3156649
C 107	-4.5206626	3.7332618	-.2959640
H 108	-4.3084329	4.6907029	-.8082037
C 109	-5.7110849	3.8834093	.6600250
H 110	-4.6987595	2.9505685	-1.0642436
H 111	-6.5338991	4.4109718	.1398022
H 112	-5.4369960	4.4806096	1.5523294
O 113	-6.1087448	2.5939317	1.0719354
H 114	-7.0178191	2.6635546	1.3338223

Heat of Formation: 816.092 kcal/mol