5a

host with R = H, E = -1294.861740 hartree

O	-3.868224	0.137809	-3.755453
O	3.868207	-0.137814	-3.755443
N	-3.415751	-0.070301	-1.495132
H	-2.650069	-0.121865	-0.832764
N	-1.730054	-0.322932	-3.066458
H	-1.237421	-0.948728	-2.438763
N	3.415750	0.070310	-1.495119
H	2.650072	0.121881	-0.832748
N	1.730048	0.322961	-3.066436
H	1.237433	0.948773	-2.438741
C	0.000004	0.000000	1.919346
H	0.000005	-0.000007	0.833918
C	-1.222995	0.065067	2.609260
C	-1.211628	0.064284	4.019859
H	-2.151612	0.114218	4.560629
C	-0.000001	0.000016	4.707631
C	1.211629	-0.064260	4.019864
H	2.151612	-0.114187	4.560637
C	1.223000	-0.065058	2.609265
C	-2.449469	0.131524	1.883575
C	-3.503221	0.197329	1.273044
C	-4.706105	0.273675	0.514059
C	-4.669233	0.152279	-0.904664
C	-5.863507	0.239389	-1.634018
H	-5.829555	0.157729	-2.711823
C	-7.073208	0.438145	-0.968261
H	-7.987594	0.502604	-1.552267
C	-7.122944	0.555273	0.424754
C	-5.943218	0.472537	1.156669
H	-5.955472	0.563315	2.238802
C	-3.086671	-0.083948	-2.840267
C	2.449476	-0.131523	1.883583
C	3.503228	-0.197334	1.273053
C	4.706109	-0.273687	0.514064
C	4.669233	-0.152285	-0.904658
C	5.863503	-0.239403	-1.634017
H	5.829547	-0.157739	-2.711821
C	7.073205	-0.438172	-0.968266
H	7.987588	-0.502637	-1.552275
C	7.122946	-0.555304	0.424749
C	5.943223	-0.472561	1.156669
H	5.955481	-0.563343	2.238802
C	3.086663	0.083957	-2.840253
H	1.539244	0.519685	-4.041864

H	8.070070	-0.710474	0.933409
H	-8.070068	0.710433	0.933418
H	-1.539253	-0.519658	-4.041887
H	-0.000002	0.000022	5.794338

5a•NO3

Nitrate complex with truncated receptor, E = -1575.23377

C	-1.127905	-4.006671	0.111508
C	-1.168823	-2.596879	0.069679
C	0.095178	-4.670895	0.147528
H	0.009478	-0.784667	0.034467
C	1.287938	-3.952828	0.141427
H	0.119022	-5.757607	0.180388
H	2.243942	-4.467340	0.168370
C	1.267463	-2.542423	0.098427
C	0.033917	-1.868454	0.064061
C	2.504229	-1.830945	0.093548
C	3.601173	-1.302132	0.094041
C	4.918943	-0.764148	0.111935
C	7.556220	0.168456	0.161184
C	5.182015	0.618457	-0.123014
C	5.994629	-1.638576	0.365781
C	7.306983	-1.187564	0.392308
C	6.519262	1.060343	-0.091942
H	5.765549	-2.685745	0.541465
H	8.121449	-1.879349	0.590184
H	6.710111	2.108574	-0.270108
H	8.576847	0.544566	0.177944
N	4.107926	1.464770	-0.381296
H	3.183144	1.040822	-0.360948
C	4.155609	2.838814	-0.655827
N	2.937467	3.358660	-0.981675
H	2.897491	4.366229	-0.982035
H	2.069606	2.854908	-0.793765
O	5.187957	3.509174	-0.639602
N	-0.039313	1.898934	0.036083
O	-1.015545	1.244494	0.502331
O	-0.058953	3.151301	0.037168
O	0.956662	1.275942	-0.431490
H	-2.060282	-4.563459	0.116559
C	-2.434601	-1.939930	0.027251
C	-3.551040	-1.455679	-0.016186
C	-4.886628	-0.968173	-0.086714
C	-7.551927	-0.135733	-0.245167
C	-5.920768	-1.887857	-0.352878
C	-5.206406	0.409084	0.105992

C	-6.556950	0.799938	0.019244
C	-7.247048	-1.486895	-0.433581
H	-5.647471	-2.929549	-0.494908
H	-6.794575	1.843723	0.163083
H	-8.029030	-2.212757	-0.640608
H	-8.584084	0.202757	-0.304706
N	-4.171730	1.299029	0.378633
H	-3.232405	0.908323	0.396802
C	-4.276051	2.674520	0.629187
N	-3.088387	3.239599	0.992319
H	-2.199232	2.762092	0.836637
H	-3.080846	4.247911	0.970618
O	-5.329037	3.308868	0.564018

5b

host with R = nitro, E = -1499.368112 hartree

O	3.892887	-0.168778	-4.295727
O	-3.892887	0.168778	-4.295727
N	3.429147	0.083141	-2.042024
H	2.658060	0.142626	-1.387157
N	1.755147	0.326517	-3.627641
H	1.270281	0.976921	-3.019132
N	-3.429147	-0.083141	-2.042024
H	-2.658060	-0.142626	-1.387157
N	-1.755147	-0.326517	-3.627641
H	-1.270281	-0.976921	-3.019132
C	0.000000	0.000000	1.383739
H	0.000000	0.000000	0.298789
C	1.226594	-0.059592	2.069640
C	1.222418	-0.060000	3.477825
H	2.146298	-0.105807	4.040319
C	0.000000	0.000000	4.139910
C	-1.222418	0.060000	3.477825
H	-2.146298	0.105807	4.040319
C	-1.226594	0.059592	2.069640
C	2.451659	-0.119281	1.343793
C	3.504084	-0.180614	0.731018
C	4.709051	-0.253350	-0.023081
C	4.678061	-0.136783	-1.442391
C	5.877120	-0.223971	-2.163963
H	5.850106	-0.147628	-3.242303
C	7.082908	-0.416572	-1.489882
H	8.000707	-0.480829	-2.068420
C	7.126300	-0.527360	-0.095798
C	5.942978	-0.445318	0.629034
H	5.949033	-0.531429	1.711531

C	3.108027	0.077224	-3.390592
C	-2.451659	0.119281	1.343793
C	-3.504084	0.180614	0.731018
C	-4.709051	0.253350	-0.023081
C	-4.678061	0.136783	-1.442391
C	-5.877120	0.223971	-2.163963
H	-5.850106	0.147628	-3.242303
C	-7.082908	0.416572	-1.489882
H	-8.000707	0.480829	-2.068420
C	-7.126300	0.527360	-0.095798
C	-5.942978	0.445318	0.629034
H	-5.949033	0.531429	1.711531
C	-3.108027	-0.077224	-3.390592
H	-1.570869	-0.500396	-4.608806
H	-8.071169	0.677226	0.418252
H	8.071169	-0.677226	0.418252
H	1.570869	0.500396	-4.608806
N	0.000000	0.000000	5.619944
O	1.088642	-0.056821	6.190746
O	-1.088642	0.056821	6.190746

5d

host with R = fluoro, E = -1394.102086 hartree

O	-3.870891	0.144543	-3.760643
O	3.870876	-0.144545	-3.760633
N	-3.416277	-0.073890	-1.501672
H	-2.649224	-0.127853	-0.841288
N	-1.733331	-0.326528	-3.076095
H	-1.242910	-0.957807	-2.452116
N	3.416276	0.073897	-1.501661
H	2.649227	0.127867	-0.841273
N	1.733326	0.326555	-3.076075
H	1.242921	0.957848	-2.452097
C	0.000003	-0.000000	1.913295
H	0.000004	-0.000007	0.828696
C	-1.223045	0.065734	2.604207
C	-1.220226	0.065807	4.014146
H	-2.143880	0.115630	4.579638
C	-0.000000	0.000015	4.671236
C	1.220227	-0.065784	4.014149
H	2.143879	-0.115600	4.579645
C	1.223049	-0.065726	2.604211
C	-2.449696	0.131900	1.880422
C	-3.502053	0.196638	1.267737
C	-4.704628	0.272647	0.509129
C	-4.668306	0.150757	-0.909647

C	-5.863388	0.238895	-1.637708
H	-5.830842	0.157371	-2.715535
C	-7.072007	0.438533	-0.970604
H	-7.986850	0.503678	-1.553767
C	-7.120928	0.555555	0.422623
C	-5.940951	0.472112	1.153504
H	-5.952093	0.562833	2.235620
C	-3.088797	-0.083602	-2.847877
C	2.449702	-0.131900	1.880429
C	3.502059	-0.196643	1.267745
C	4.704631	-0.272658	0.509134
C	4.668306	-0.150763	-0.909642
C	5.863384	-0.238908	-1.637707
H	5.830835	-0.157381	-2.715534
C	7.072004	-0.438558	-0.970608
H	7.986845	-0.503708	-1.553774
C	7.120930	-0.555584	0.422618
C	5.940956	-0.472134	1.153503
H	5.952101	-0.562859	2.235620
C	3.088789	0.083611	-2.847864
H	1.543852	0.518868	-4.052698
H	8.067609	-0.711219	0.931827
H	-8.067607	0.711181	0.931836
H	-1.543860	-0.518841	-4.052719
F	-0.000002	0.000022	6.028266

5e

host with R = t-butyl, E = -1452.120263 hartree

O	3.876760	-4.574042	-0.083402
O	-3.879773	-4.608298	0.087879
N	3.410110	-2.313328	-0.251356
H	2.641902	-1.651807	-0.262468
N	1.716588	-3.886289	-0.428960
H	1.190640	-3.253546	-1.021678
N	-3.420262	-2.345676	0.249727
H	-2.654558	-1.681230	0.259754
N	-1.721103	-3.913167	0.425442
H	-1.193460	-3.276440	1.012292
C	-0.014753	1.054408	0.001724
H	-0.008845	-0.030822	0.002434
C	1.199935	1.760523	0.006924
C	1.175132	3.167080	0.006106
H	2.123881	3.693451	0.009511
C	-0.031189	3.885540	0.000409
C	-1.227365	3.159328	-0.004769
H	-2.184211	3.666656	-0.009041

C	-1.233132	1.747205	-0.004332
C	2.438306	1.050782	0.012869
C	3.500103	0.450889	0.025950
C	4.709156	-0.302371	0.040958
C	4.671359	-1.720619	-0.086031
C	5.870648	-2.446423	-0.059685
H	5.836058	-3.523942	-0.145168
C	7.086416	-1.777424	0.084614
H	8.004784	-2.358468	0.102011
C	7.136962	-0.384934	0.206444
C	5.952113	0.343367	0.183908
H	5.965268	1.425096	0.279639
C	3.083242	-3.658767	-0.257959
C	-2.465047	1.026658	-0.010313
C	-3.522900	0.419700	-0.023426
C	-4.728036	-0.339664	-0.039154
C	-4.684117	-1.757901	0.086215
C	-5.880391	-2.488727	0.059531
H	-5.841172	-3.566142	0.144164
C	-7.099037	-1.824820	-0.083986
H	-8.014896	-2.409802	-0.101770
C	-7.155555	-0.432459	-0.204632
C	-5.973840	0.300840	-0.181427
H	-5.991527	1.382600	-0.276036
C	-3.088732	-3.690011	0.258160
H	-1.518266	-4.885876	0.623323
H	-8.109516	0.074793	-0.316685
H	8.088748	0.126272	0.319008
H	1.517322	-4.860242	-0.624476
C	0.005174	5.426185	-0.000500
C	-1.404378	6.047848	-0.004902
H	-1.982430	5.762916	0.882230
H	-1.977067	5.762127	-0.895248
H	-1.319509	7.140483	-0.005181
C	0.747243	5.923554	1.263959
H	0.236210	5.593243	2.175939
H	0.783791	7.020097	1.272979
H	1.778439	5.556255	1.305837
C	0.754192	5.921354	-1.261702
H	0.247451	5.590355	-2.175819
H	1.785141	5.552746	-1.297763
H	0.791960	7.017849	-1.272008

5g
host with R = dimethylamino, E = -1428.833032 hartree

O	3.811243	4.349636	-0.101976

O	-3.885195	4.391065	0.089319
N	3.406771	2.079031	0.092770
H	2.654501	1.402219	0.158058
N	1.701782	3.613108	0.421123
H	1.251138	2.970671	1.063728
N	-3.402439	2.132033	-0.054666
H	-2.631522	1.473738	-0.074557
N	-1.721163	3.717734	-0.247696
H	-1.177824	3.076689	-0.814902
C	0.018992	-1.270665	0.007299
H	0.023927	-0.187417	-0.042117
C	1.226544	-1.986144	-0.033572
C	1.218397	-3.390154	0.020728
H	2.168762	-3.905852	-0.019395
C	0.006142	-4.109791	0.126837
C	-1.200228	-3.373422	0.154626
H	-2.155921	-3.876389	0.220955
C	-1.195465	-1.968976	0.100227
C	2.463763	-1.279240	-0.131419
C	3.519373	-0.675231	-0.221001
C	4.713640	0.095376	-0.319887
C	4.662063	1.511593	-0.175540
C	5.842760	2.259352	-0.284755
H	5.796259	3.335306	-0.185252
C	7.055525	1.613667	-0.527654
H	7.959933	2.211025	-0.608905
C	7.120153	0.223436	-0.667263
C	5.952959	-0.526343	-0.562903
H	5.977555	-1.606719	-0.671118
C	3.055002	3.416669	0.133917
C	-2.427629	-1.247625	0.138370
C	-3.484043	-0.639760	0.180089
C	-4.692453	0.113534	0.227720
C	-4.659841	1.533448	0.118749
C	-5.860566	2.255710	0.173042
H	-5.829529	3.334092	0.098958
C	-7.072447	1.582367	0.329079
H	-7.991550	2.161242	0.368572
C	-7.117914	0.188521	0.435568
C	-5.931739	-0.536203	0.384334
H	-5.940736	-1.619118	0.466483
C	-3.084380	3.479644	-0.075275
H	-1.529155	4.689578	-0.459177
H	-8.066511	-0.326463	0.557945
H	8.069334	-0.269721	-0.856637
H	1.500209	4.582229	0.637884

N	0.002011	-5.493691	0.211039
C	1.234420	-6.230512	-0.026342
H	1.039569	-7.297425	0.096601
H	2.007635	-5.951783	0.699710
H	1.635890	-6.066759	-1.039430
C	-1.259116	-6.214845	0.131230
H	-1.935537	-5.917226	0.941514
H	-1.064785	-7.283092	0.243145
H	-1.778563	-6.057705	-0.828183

6a

1,3-ethynylbenzene, E = -384.555499

C	0.000000	0.000000	2.062309
C	0.000000	0.000000	-0.733900
C	-1.211213	0.000000	1.370926
C	1.211213	0.000000	1.370926
C	1.220480	0.000000	-0.037914
C	-1.220480	0.000000	-0.037914
H	-2.154029	0.000000	1.909337
H	2.154029	0.000000	1.909337
H	0.000000	0.000000	-1.818971
C	-2.459312	0.000000	-0.754752
C	-3.511642	0.000000	-1.355668
C	2.459312	0.000000	-0.754752
C	3.511642	0.000000	-1.355668
H	-4.436832	0.000000	-1.888100
H	0.000000	0.000000	3.149015
H	4.436832	0.000000	-1.888100

6b

1,3-ethynyl-5-nitrobenzene, E = -589.061789

C	0.000000	0.000000	1.048499
C	0.000000	0.000000	-1.702482
C	1.217249	0.000000	0.386263
C	-1.217249	0.000000	0.386263
C	-1.216738	0.000000	-1.012030
C	1.216738	0.000000	-1.012030
H	2.142615	0.000000	0.947742
H	-2.142615	0.000000	0.947742
H	0.000000	0.000000	-2.786667
C	2.454598	0.000000	-1.733366
H	4.415424	0.000000	-2.881053
C	3.494121	0.000000	-2.342732
C	-2.454598	0.000000	-1.733366
H	-4.415424	0.000000	-2.881053
C	-3.494121	0.000000	-2.342732

N	0.000000	0.000000	2.520752
O	1.082001	0.000000	3.084643
O	-1.082001	0.000000	3.084643

6c
1,3-ethynyl-5-chlorobenzene, E = -844.149553

C	0.000000	0.000000	1.296439
C	0.000000	0.000000	-1.487216
C	-1.216478	0.000000	0.619073
C	1.216478	0.000000	0.619073
C	1.218524	0.000000	-0.789044
C	-1.218524	0.000000	-0.789044
H	-2.152514	0.000000	1.165958
H	2.152514	0.000000	1.165958
H	0.000000	0.000000	-2.571678
C	-2.459630	0.000000	-1.501018
H	-4.439096	0.000000	-2.630693
C	-3.512311	0.000000	-2.100474
C	2.459630	0.000000	-1.501018
H	4.439096	0.000000	-2.630693
C	3.512311	0.000000	-2.100474
Cl	0.000000	0.000000	3.054360

6d
1,3-ethynyl-5-fluorobenzene, E = -483.795928

C	0.000000	0.000000	1.663503
C	0.000000	0.000000	-1.102146
C	-1.219734	0.000000	1.002923
C	1.219734	0.000000	1.002923
C	1.220242	0.000000	-0.405104
C	-1.220242	0.000000	-0.405104
H	-2.146600	0.000000	1.565615
H	2.146600	0.000000	1.565615
H	0.000000	0.000000	-2.186469
C	-2.459401	0.000000	-1.120155
C	2.459401	0.000000	-1.120155
H	4.434175	0.000000	-2.257730
C	3.509380	0.000000	-1.724289
H	-4.434175	0.000000	-2.257730
C	-3.509380	0.000000	-1.724289
F	0.000000	0.000000	3.020845

6e
1,3-ethynyl-5-t-butylbenzene, E = -541.812968

C	-0.734185	-0.034409	0.000000
C	2.106352	-0.000205	0.000000

C	-0.007262	-0.023133	-1.198568
C	-0.007262	-0.023133	1.198568
C	1.400481	-0.007082	1.211651
C	1.400481	-0.007082	-1.211651
H	-0.518628	-0.030687	-2.153832
H	-0.518628	-0.030687	2.153832
H	3.191181	0.008148	0.000000
C	2.104353	-0.002706	-2.458534
C	2.104353	-0.002706	2.458534
H	3.216894	0.002632	4.448146
C	2.694394	0.000634	3.517287
H	3.216894	0.002632	-4.448146
C	2.694394	0.000634	-3.517287
C	-2.276321	-0.001630	0.000000
C	-2.858318	-0.704600	-1.246951
H	-2.608018	-0.183724	-2.177226
H	-3.952432	-0.728347	-1.178738
H	-2.501915	-1.738671	-1.327783
C	-2.858318	-0.704600	1.246951
H	-2.608018	-0.183724	2.177226
H	-2.501915	-1.738671	1.327783
H	-3.952432	-0.728347	1.178738
C	-2.735317	1.477991	0.000000
H	-2.365023	2.007126	-0.886034
H	-2.365023	2.007126	0.886034
H	-3.831489	1.538592	0.000000

6f

1,3-ethynyl-5-methoxybenzene, E = -499.081559

C	0.778517	-1.045949	0.000000
C	-1.095568	1.044758	0.000000
C	1.219193	0.280230	0.000000
C	-0.593189	-1.334497	0.000000
C	-1.531822	-0.293997	0.000000
C	0.275708	1.329614	0.000000
H	2.273368	0.528084	0.000000
H	-0.914602	-2.370665	0.000000
H	-1.819312	1.852090	0.000000
C	0.730184	2.686923	0.000000
H	1.457197	4.847074	0.000000
C	1.119808	3.834443	0.000000
C	-2.932761	-0.590898	0.000000
H	-5.163809	-1.054975	0.000000
C	-4.118914	-0.837522	0.000000
O	1.606759	-2.131064	0.000000
C	3.013507	-1.916626	0.000000

H	3.332833	-1.371034	-0.897322
H	3.463024	-2.910910	0.000000
H	3.332833	-1.371034	0.897322

6g

1,3-ethynyl-5-(N,N-dimethyl)aminobenzene, E = -518.526079

C	-1.000144	-0.077149	0.000000
C	1.846627	0.000962	0.000000
C	-0.269773	-0.045123	-1.208544
C	-0.269773	-0.045123	1.208544
C	1.134164	-0.012220	1.208825
C	1.134164	-0.012220	-1.208825
H	-0.777033	-0.046201	-2.164306
H	-0.777033	-0.046201	2.164306
H	2.930199	0.028336	0.000000
C	1.838002	0.012645	-2.456523
C	1.838002	0.012645	2.456523
H	2.957963	0.050159	4.441502
C	2.431147	0.032724	3.513380
H	2.957963	0.050159	-4.441502
C	2.431147	0.032724	-3.513380
N	-2.388557	-0.147280	0.000000
C	-3.111134	0.065165	1.245439
H	-2.937958	1.066721	1.672857
H	-2.829287	-0.682856	1.995677
H	-4.181030	-0.047990	1.058199
C	-3.111134	0.065165	-1.245439
H	-2.937958	1.066721	-1.672857
H	-4.181030	-0.047990	-1.058199
H	-2.829287	-0.682856	-1.995677