Journal of Organic Chemistry

SUPPORTING INFORMATION

TITLE: THEORETICAL STUDY OF ALKYL-π AND ARYL-π INTERACTIONS. RECONCILING THEORY AND EXPERIMENT

AUTHORS: Jordi Ribas[1], Elena Cubero[1], F.Javier Luque[2] and Modesto Orozco[1]

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Donor	Method	Energy	Reference
CH_4	MP2/6-31G(d)[a]	-1.3	
	MP2/6-311+G(2d,p)	-1.3	
	MP2/aug-cc-pVDZ	-1.4	
	MP2/aug-cc-pVDZ	-1.2	50
	MP2/6-311G(2d,2pd)	-1.3	
	CCSD(T)/aug-cc-pVDZ	-1.2	
	MP2/full basis + ΔCCSD(T)	-1.4	42
	GMIPp	-1.3	
C_6H_6	MP2/6-31G(d)[a]	-3.1	
	MP2/6-311+G(2d,p)	-2.8	
	MP2/aug-cc-pVDZ	-2.9	
	MP2/aug-cc-pVDZ	-3.0	45
	CCSD(T)/aug-cc-pVDZ	-2.3	
	MP2/aug(df,p)-6-311G(d,p)	-3.2	43
	MP2/aug(df,p)-6-311G(d,p) + ΔCCSD(T)	-2.5	43
	GMIPp	-2.5	

Table S1. Energy values for alkyl(CH_4)-benzene and aryl(benzene)-benzene interactions computed at different levels of theory in this work, or in previous works by other authors.

(a) MP2/6-31G(d) calculations are not corrected by BSSE

Derivatives Comp. I	E_{ele}	E_{pol}	$E_{disp-rep}$	E_{tot}(GMIPp)	E_{tot}(MP2)
Tetra-fluorinated	0.1	-0.0	-1.1	-1.1	-1.1
X=NO_2	-0.1	-0.0	-1.2	-1.3	-1.2
X=CN	-0.1	-0.0	-1.1	-1.2	-1.2
X=H	-0.2	-0.1	-1.0	-1.3	-1.3
X=CH_3	-0.2	-0.1	-1.1	-1.3	-1.4
X=OH	-0.1	-0.1	-1.1	-1.3	-1.3
X=NH_2	-0.1	-0.1	-1.1	-1.3	-1.3

Table S2. GMIPp total interaction energy and its electrostatic, polarization and dispersion-repulsion contributions for different dimers of CH_4 and benzene derivatives in the ideal gas phase conformation (see text). GMIPp results are compared with MP2/6-31G(d) estimates. All values are in kcal/mol.

Derivatives Comp.II	E_{ele}	E_{pol}	$E_{disp-rep}$	E_{tot}(GMIPp)	E_{tot}(MP2)
Tetra-fluorinated	0.3	-0.1	-1.7	-1.5	-2.2
X=NO_2	-0.3	-0.1	-1.8	-2.2	-2.7
X=CN	-0.4	-0.1	-1.7	-2.1	-2.7
X=H	-0.8	-0.2	-1.5	-2.5	-3.2
X=CH_3	-0.7	-0.2	-1.7	-2.6	-3.3
X=OH	-0.8	-0.1	-1.6	-2.6	-3.2
X=NH_2	-0.9	-0.2	-1.6	-2.7	-3.3

Table S3. GMIPp total interaction energy and its electrostatic, polarization and dispersion-repulsion contributions different dimers of C_6H_6 and benzene derivatives in the ideal gas phase conformation (see text). GMIPp results are compared with MP2/6-31G(d) estimates. All values are in kcal/mol.

Derivatives Comp. I	E_{ele}	E_{pol}	$E_{disp-rep}$	E_{tot}(GMIPp)	E_{tot}(MP2)
Tetra-fluorinated	0.0	0.0	-1.7	-1.7 (-1.2)[a]	-1.5
X=NO_2	0.0	0.0	-1.6	-1.6 (-1.2)[a]	-1.5
X=CN	0.0	0.0	-1.4	-1.4 (-1.1)[a]	-1.4
X=H	0.1	-0.1	-1.4	-1.4 (-1.0)[a]	-1.5
X=CH_3	0.1	-0.1	-1.6	-1.6 (-1.1)[a]	-1.7
X=OH	0.0	0.0	-1.6	-1.7 (-1.1)[a]	-1.7
X=NH_2	0.0	-0.1	-1.3	-1.4 (-1.0)[a]	-1.4

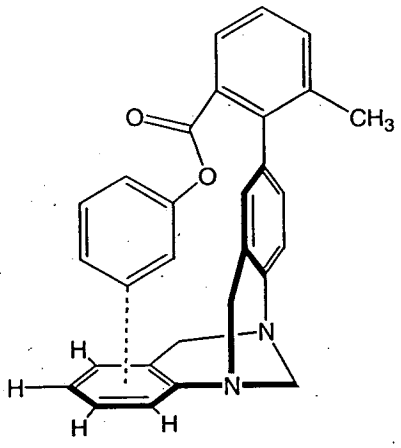
Table S4. GMIPp total interaction energy and its electrostatic, polarization and dispersion-repulsion contributions for different dimers of isopropyl (donor) and benzene (acceptor) derivatives (see text) in the conformation found in Wilcox's folding models. GMIPp results are compared with MP2/6-31G(d) estimates. All values are in kcal/mol.

(a) Numbers in parenthesis are those for a donor CH_4 group.

Derivatives Comp. II	E_{ele}	E_{pol}	$E_{disp-rep}$	E_{tot}(GMIPp)	E_{tot}(MP2)
Tetra-fluorinated	-0.4 (0.3)[a]	-0.1 (-0.0)[a]	-1.8 (-1.7)[a]	-2.2 (-1.4)[a]	-3.4 (-1.9)[a]
X=NO_2	-0.3 (0.0)[a]	-0.1 (-0.1)[a]	-2.6 (-1.9)[a]	-2.9 (-1.9)[a]	-3.0 (-2.2)[a]
X=CN	-0.2	-0.1	-1.6	-1.9	-2.3
X=H	-0.5	-0.1	-1.4	-2.0	-2.4
X=CH_3	-0.3	-0.1	-1.7	-2.1	-2.7
X=OH	-0.5	-0.1	-1.6	-2.2	-2.8
X=NH_2	-0.7	-0.2	-1.6	-2.5	-3.0

Table S5. GMIPp total interaction energy and its electrostatic, polarization and dispersion-repulsion contributions for different dimers of C_6H_6 (donor) and benzene (acceptor) derivatives (see text) in the conformation found in Wilcox's folding models. GMIPp results are compared with MP2/6-31G(d) estimates. All values are in kcal/mol.

(a) The values in parentheses is obtained by fixing the cis conformation in the T-shape orientation detected for the unmodified compound II (X=H). Otherwise a parallel stacking is obtained.



COMPOUND 1

MP2/6-31G*//oniom(mp2/6-31G(d):hf/6-31G(d))

6	4.368891	0.574038	0.862333
6	3.654553	-0.607766	0.621148
6	3.536583	-1.073376	-0.698938
6	4.099735	-0.336390	-1.750435
6	4.783094	0.848526	-1.498060
6	4.927805	1.305066	-0.183107
1	4.473484	0.931147	1.886409
1	4.014652	-0.723147	-2.762911
1	5.219635	1.407827	-2.321838
1	5.480311	2.218798	0.022898
6	3.044381	-1.414569	1.771398
1	2.489628	-0.761904	2.432114
1	3.835684	-1.868573	2.360261
7	2.873832	-2.315966	-0.988371
7	2.166706	-2.477438	1.291125
6	2.818037	-3.157965	0.189682
1	3.820335	-3.432521	0.490038
1	2.274794	-4.062005	-0.051914
6	1.519992	-2.160132	-1.514097
1	1.509421	-1.358266	-2.240362
1	1.258635	-3.072160	-2.043210
6	0.502094	-1.887824	-0.417401
6	-0.794517	-1.500832	-0.733099
6	-1.731681	-1.226186	0.248301
6	-1.349469	-1.350442	1.581695
6	-0.072582	-1.757904	1.911934
6	0.862031	-2.032103	0.920757

1	-1.068924	-1.385450	-1.768157
1	-2.061860	-1.147484	2.361455
1	0.207488	-1.885942	2.942011
6	-3.140654	-0.835798	-0.091671
6	-3.585881	0.481418	0.045481
6	-4.920828	0.807609	-0.160384
6	-5.816957	-0.165506	-0.549541
6	-5.380862	-1.469168	-0.702947
6	-4.059593	-1.825986	-0.466634
1	-5.240051	1.822675	-0.018061
1	-6.847578	0.085109	-0.724361
1	-6.083513	-2.229619	-0.994799
6	-3.650536	-3.277984	-0.597969
1	-3.169957	-3.637932	0.304541
1	-4.517653	-3.899180	-0.787926
1	-2.951534	-3.426318	-1.413921
6	-2.699743	1.633326	0.416268
8	-3.006922	2.464536	1.204547
8	-1.576614	1.658568	-0.299402
6	-0.626088	2.661947	-0.125900
6	0.686443	2.247479	0.077636
6	1.696256	3.208495	0.158230
6	1.391900	4.563135	0.017997
6	0.068595	4.957076	-0.191564
6	-0.949457	4.007353	-0.284222
1	0.906946	1.189190	0.177459
1	2.721609	2.883593	0.307415
1	2.179233	5.309983	0.081235
1	-0.176093	6.010310	-0.302927
1	-1.979418	4.307660	-0.437253

ENERGY = -1375.1627993 Hartrees

FREQUENCIES WERE NOT CALCULATED

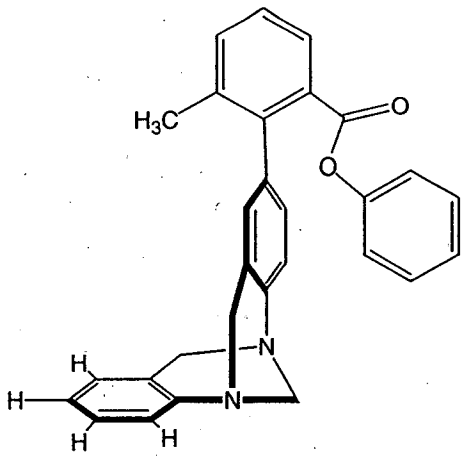
MP2/6-31G(d)//B3LYP/6-31G(d)

6	4.5292936840	0.7651773938	0.7467851128
6	3.7920931005	-0.4194309905	0.6168889948
6	3.6386760017	-0.9922729547	-0.6613844608
6	4.1775584119	-0.3435193539	-1.7830808192
6	4.8824256143	0.8484436784	-1.6409886085
6	5.0745142857	1.4002150634	-0.3683942495
1	4.6603666661	1.2016883269	1.7359997817
1	4.0568366014	-0.8055141062	-2.7595661911
1	5.3000474864	1.3373160755	-2.5171950601
1	5.6423376149	2.3192818255	-0.2489875610
6	3.1566046098	-1.0795919707	1.8365892211
1	2.5765389002	-0.3449526055	2.4042146880
1	3.9353180625	-1.4623597718	2.5116605019
7	2.9834438000	-2.2589029633	-0.8319114203

7	2.2699850331	-2.2030917372	1.4747625390
6	2.9343529295	-2.9902596107	0.4346869054
1	3.9514384717	-3.2220396645	0.7643434645
1	2.3901296216	-3.9266541011	0.2799305537
6	1.6119685122	-2.1851446652	-1.3731226911
1	1.5865764686	-1.4256666530	-2.1610738763
1	1.3804043872	-3.1483970603	-1.8498714320
6	0.5752248092	-1.8636425510	-0.3007382222
6	-0.7515854190	-1.5926393272	-0.6511734377
6	-1.7066570248	-1.2351990500	0.3057095298
6	-1.3053916607	-1.1531860464	1.6502089635
6	0.0020159722	-1.4523176493	2.0209822080
6	0.9506208023	-1.8230465428	1.0574375168
1	-1.0387767776	-1.6216022256	-1.7011381753
1	-2.0323147351	-0.8763394691	2.4094913890
1	0.2977138070	-1.4307659477	3.0666903804
6	-3.1333697443	-0.9695271036	-0.0650500499
6	-3.6858824948	0.3289441769	-0.0073552212
6	-5.0557053131	0.5343052660	-0.2299328370
6	-5.8785547757	-0.5355625743	-0.5608208656
6	-5.3359418538	-1.8181631176	-0.6422535887
6	-3.9798906013	-2.0564877465	-0.3855484913
1	-5.4496585949	1.5421472418	-0.1492058151
1	-6.9365733275	-0.3754793842	-0.7494733361
1	-5.9786342792	-2.6597735921	-0.8908335633
6	-3.4568349458	-3.4763945343	-0.4238336071
1	-2.9322815899	-3.7348930029	0.5026843731
1	-4.2782160908	-4.1860883635	-0.5627994304
1	-2.7420609787	-3.6270155037	-1.2410402730
6	-2.9009898210	1.5735442829	0.2753271660
8	-3.3416605704	2.5228836743	0.8846273401
8	-1.6690652252	1.5340840019	-0.3027267677
6	-0.7629558300	2.5918522589	-0.1940009847
6	0.5737162979	2.2181863427	-0.0562283346
6	1.5594023730	3.2048362423	-0.0239627011
6	1.2075884934	4.5533036040	-0.1261515519
6	-0.1356276159	4.9092729912	-0.2691576879
6	-1.1342635023	3.9330120251	-0.3096244260
1	0.8245584045	1.1650476230	0.0174338862
1	2.5999809626	2.9108644088	0.0750938293
1	1.9756133615	5.3218209550	-0.0982853237
1	-0.4166352321	5.9559896485	-0.3525030684
1	-2.1754485039	4.2070823164	-0.4142150667

ENERGY = -1375.1692963 Hartrees

Three lowest frequencies (cm-1): 30.05 33.95 45.75



COMPOUND 2

MP2/6-31G*//oniom(mp2/6-31G(d):hf/6-31G(d))

6	5.620224	0.406607	0.823954
6	4.509107	-0.395397	0.531475
6	4.192006	-0.652750	-0.811691
6	4.973052	-0.093124	-1.832206
6	6.059191	0.720203	-1.525844
6	6.389534	0.970434	-0.189640
1	5.871173	0.606060	1.865120
1	4.725331	-0.324212	-2.865247
1	6.658896	1.146680	-2.326192
1	7.242911	1.597271	0.056462
6	3.660804	-1.013528	1.646535
1	3.423451	-0.266737	2.392533
1	4.224446	-1.796225	2.145468
7	3.084939	-1.501734	-1.161162
7	2.423128	-1.598527	1.137523
6	2.726942	-2.365886	-0.055013
1	3.545095	-3.039804	0.161132
1	1.864707	-2.955811	-0.337310
6	1.894251	-0.769755	-1.585819
1	2.187818	0.035698	-2.245694
1	1.272024	-1.445049	-2.165938
6	1.102280	-0.223243	-0.408635
6	0.070112	0.690526	-0.608039
6	-0.659182	1.208833	0.447138
6	-0.347735	0.785562	1.738700
6	0.657919	-0.131213	1.951003

6	1.395159	-0.640713	0.883590
1	-0.152716	1.014639	-1.611048
1	-0.915857	1.157080	2.572425
1	0.875118	-0.480373	2.944555
6	-1.735309	2.222798	0.191069
6	-2.948138	1.863538	-0.403032
6	-3.893201	2.826700	-0.734687
6	-3.660361	4.152663	-0.436871
6	-2.468223	4.515094	0.163924
6	-1.493024	3.575204	0.471182
1	-4.802835	2.523658	-1.217641
1	-4.394752	4.899782	-0.677695
1	-2.281801	5.551743	0.382534
6	-0.184438	4.039173	1.075803
1	0.665338	3.670333	0.513167
1	-0.136646	5.121508	1.086646
1	-0.067318	3.692995	2.097001
6	-3.332802	0.452940	-0.734981
8	-3.845374	0.139772	-1.757650
8	-3.107650	-0.386940	0.275118
6	-3.371343	-1.748181	0.149837
6	-2.317345	-2.614657	0.421297
6	-2.549011	-3.991350	0.396755
6	-3.823922	-4.486823	0.120171
6	-4.869353	-3.598379	-0.141462
6	-4.654423	-2.219992	-0.113457
1	-1.337114	-2.205746	0.643430
1	-1.730788	-4.675297	0.607469
1	-4.001675	-5.558872	0.100823
1	-5.865316	-3.977045	-0.356055
1	-5.458376	-1.524808	-0.326548

ENERGY = -1375.1597554 Hartrees

FREQUENCIES WERE NOT CALCULATED

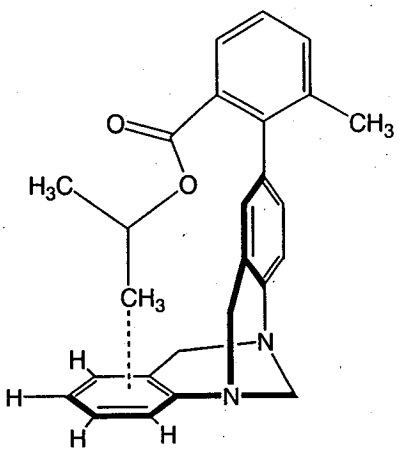
MP2/6-31G(d)//B3LYP/6-31G(d)

6	5.6361886653	0.5087168962	0.6747881398
6	4.4923471299	-0.2675737668	0.4510593986
6	4.0929447013	-0.5311959092	-0.8736756205
6	4.8209975875	0.0158680487	-1.9404314741
6	5.9419799418	0.8056367954	-1.7008920785
6	6.3606927773	1.0462405680	-0.3871221091
1	5.9490911733	0.7072256606	1.6989196440
1	4.5061519072	-0.2110886033	-2.9557723335
1	6.5007473000	1.2179926873	-2.5369512531
1	7.2430694535	1.6505655564	-0.1945295883
6	3.6769526703	-0.8092830590	1.6197025751
1	3.4784472875	-0.0134289011	2.3447411859

1	4.2386165858	-1.5915574619	2.1500766671
7	2.9698326324	-1.3812213391	-1.1583854951
7	2.3885833488	-1.3851561763	1.1877375943
6	2.6347408683	-2.2086236452	0.0007326191
1	3.4599612688	-2.8942682677	0.2147744273
1	1.7389136088	-2.7925302721	-0.2307521847
6	1.7490176379	-0.6616219465	-1.5712625933
1	2.0304928034	0.1391173582	-2.2623186473
1	1.1116016947	-1.3597342402	-2.1319220678
6	0.9824528978	-0.0877048172	-0.3849216113
6	-0.1058602160	0.7674651829	-0.5862462187
6	-0.8138382472	1.3263917329	0.4838070090
6	-0.3917530894	1.0269476906	1.7905128944
6	0.6733382463	0.1603425630	2.0091023284
6	1.3589007696	-0.4196829918	0.9302380997
1	-0.4074477018	1.0098293918	-1.6043574990
1	-0.9363504231	1.4351937452	2.6375442241
1	0.9623587952	-0.1147883600	3.0203026933
6	-1.9902576925	2.2107752039	0.2192113355
6	-3.1526955685	1.7078532940	-0.4080857571
6	-4.1997684934	2.5675849215	-0.7701966032
6	-4.1279128522	3.9217893084	-0.4664594858
6	-2.9933430432	4.4221899161	0.1723402790
6	-1.9155735026	3.5933493643	0.5074950226
1	-5.0635776610	2.1510878283	-1.2779287574
1	-4.9450267698	4.5868892064	-0.7315032003
1	-2.9273887752	5.4841334149	0.3977663225
6	-0.6783351282	4.2038497512	1.1306119993
1	0.2306053939	3.8866483966	0.6082052365
1	-0.7301598469	5.2963999808	1.0980998673
1	-0.5570583535	3.9081219535	2.1791805892
6	-3.3784590120	0.2634821633	-0.7401591526
8	-3.9423619254	-0.1120441937	-1.7445102157
8	-2.9433016913	-0.5563590222	0.2549410837
6	-2.9789354838	-1.9495259939	0.1692668657
6	-1.9578024347	-2.5954391531	0.8700023753
6	-1.9232202111	-3.9889749898	0.9012399301
6	-2.9030589864	-4.7327302004	0.2374657343
6	-3.9218895186	-4.0705788335	-0.4496875382
6	-3.9754758590	-2.6742905360	-0.4888975171
1	-1.2085682193	-1.9963158847	1.3770989708
1	-1.1277920769	-4.4915171683	1.4453385912
1	-2.8736341440	-5.8187899246	0.2576322544
1	-4.6900694437	-4.6405586160	-0.9658476269
1	-4.7593248336	-2.1638832715	-1.0297928951

ENERGY = -1375.1666345 Hartrees

Three lowest frequencies (cm-1): 29.42 31.52 38.03



COMPOUND 3

MP2/6-31G*//oniom(mp2/6-31G(d):hf/6-31G(d))

6	4.206635	1.086670	0.994078
6	3.655340	-0.133616	0.581048
6	3.543234	-0.398532	-0.793831
6	3.960472	0.563787	-1.724232
6	4.483540	1.780488	-1.298071
6	4.613208	2.044948	0.069742
1	4.299587	1.292414	2.059956
1	3.886669	0.332285	-2.783894
1	4.805621	2.516924	-2.030183
1	5.033743	2.988430	0.408931
6	3.195731	-1.183283	1.596944
1	2.615040	-0.714571	2.380033
1	4.058683	-1.642639	2.069688
7	3.016406	-1.650263	-1.267547
7	2.403721	-2.239023	0.971896
6	3.081327	-2.667181	-0.236349
1	4.114856	-2.882596	-0.000321
1	2.621644	-3.572379	-0.610450
6	1.635966	-1.558431	-1.736285
1	1.526270	-0.678573	-2.355981
1	1.438730	-2.418858	-2.369320
6	0.644829	-1.518722	-0.584859
6	-0.678906	-1.142747	-0.797439
6	-1.589938	-1.065562	0.239597
6	-1.164021	-1.409193	1.521408
6	0.136287	-1.803666	1.744914
6	1.055967	-1.850657	0.699913

1	-0.992955	-0.880058	-1.794096
1	-1.854421	-1.355563	2.343981
1	0.458460	-2.081900	2.732425
6	-2.997023	-0.617150	-0.024856
6	-3.292357	0.721982	-0.300955
6	-4.585385	1.106741	-0.635714
6	-5.601804	0.175305	-0.659199
6	-5.317933	-1.148670	-0.376356
6	-4.028733	-1.565249	-0.071986
1	-4.778009	2.136226	-0.869938
1	-6.605269	0.473673	-0.903783
1	-6.109074	-1.877007	-0.408539
6	-3.765863	-3.035621	0.177677
1	-3.471250	-3.224230	1.204338
1	-4.657213	-3.618189	-0.022674
1	-2.970165	-3.409446	-0.456530
6	-2.284008	1.837383	-0.267704
8	-2.298305	2.727696	-1.061065
8	-1.453889	1.753069	0.748762
6	-0.398225	2.707395	0.966022
6	0.627332	2.701205	-0.166251
6	-0.949044	4.088221	1.294473
1	0.221015	3.121620	-1.083324
1	-1.391825	4.558214	0.427940
1	0.977359	1.686834	-0.360057
1	-1.697066	4.019076	2.077398
1	1.494915	3.292939	0.133880
1	-0.141239	4.717020	1.656463
1	0.072778	2.304174	1.851666

ENERGY = -1262.3661426 Hartrees

FREQUENCIES WERE NOT CALCULATED

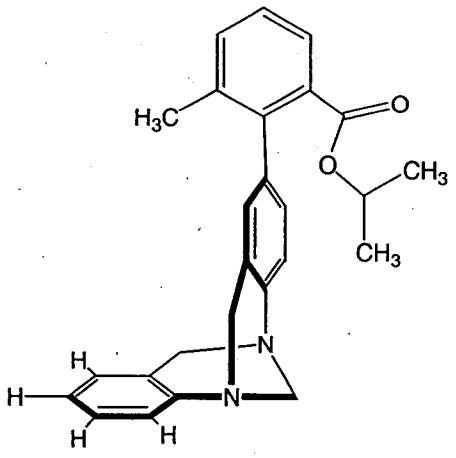
MP2/6-31G(d)//B3LYP/6-31G(d)

6	4.2291723568	1.2205836401	0.9747411454
6	3.6870174554	-0.0114958973	0.5872953844
6	3.5525172567	-0.2972137384	-0.7859534823
6	3.9293130750	0.6639532924	-1.7358920959
6	4.4476428727	1.8921761634	-1.3339915170
6	4.6082872140	2.1714176847	0.0283080378
1	4.3377793310	1.4409907837	2.0359152870
1	3.8298736931	0.4204059155	-2.7906021041
1	4.7405365532	2.6253920446	-2.0809585891
1	5.0235164872	3.1236731431	0.3478160598
6	3.2332144741	-1.0286777474	1.6289530262
1	2.6233452270	-0.5395786010	2.3950688000
1	4.1020748853	-1.4645035751	2.1426729862
7	3.0576840543	-1.5682538776	-1.2377674545

7	2.4515382359	-2.1334398446	1.0366779813
6	3.1459010862	-2.5728223178	-0.1755717400
1	4.1963615900	-2.7564281713	0.0692825460
1	2.6994978028	-3.5039710968	-0.5369548560
6	1.6599895658	-1.5342264408	-1.7131181785
1	1.5250430679	-0.6544052046	-2.3497888093
1	1.4967028156	-2.4159311736	-2.3491725178
6	0.6599129051	-1.5138486940	-0.5632585265
6	-0.6834901582	-1.1931239309	-0.7895464623
6	-1.6059413751	-1.1061566433	0.2568228783
6	-1.1685870476	-1.3947680824	1.5592504964
6	0.1580664502	-1.7334895761	1.8002777187
6	1.0864431608	-1.7876504617	0.7495761924
1	-1.0099710273	-0.9635938946	-1.8030072799
1	-1.8706758414	-1.3310056709	2.3865249803
1	0.4952595783	-1.9680510924	2.8068356722
6	-3.0165892947	-0.6857447241	-0.0221905905
6	-3.3481360098	0.6654382034	-0.2732358761
6	-4.6584495113	1.0180480976	-0.6299212513
6	-5.6521161862	0.0492248807	-0.7029739481
6	-5.3334171264	-1.2834225151	-0.4401356801
6	-4.0282433234	-1.6690405566	-0.1118268505
1	-4.8716879564	2.0605241460	-0.8419151509
1	-6.6689185208	0.3261529173	-0.9682106800
1	-6.1063395502	-2.0461237258	-0.5054602267
6	-3.7155871448	-3.1323597765	0.1149356809
1	-3.3711867820	-3.3221736323	1.1380489137
1	-4.6013962179	-3.7500210728	-0.0627877313
1	-2.9173151718	-3.4787451877	-0.5514454695
6	-2.3783507630	1.8140013028	-0.1988895281
8	-2.5166186242	2.8309938092	-0.8545973441
8	-1.3969951972	1.6073179241	0.6929619036
6	-0.3147991076	2.5777044864	0.8544313346
6	0.4966450065	2.7410957635	-0.4284295660
6	-0.8253428263	3.8895848222	1.4452882514
1	-0.0762352093	3.2628183372	-1.1980305949
1	-1.4314438859	4.4378020793	0.7212606667
1	0.8055526418	1.7624605041	-0.8079050589
1	-1.4277362876	3.6975087009	2.3398060209
1	1.4054157153	3.3131071742	-0.2106666721
1	0.0288653963	4.5121431168	1.7365984037
1	0.3074154264	2.0697806572	1.5978628616

ENERGY = -1262.3730685 Hartrees

Three lowest frequencies (cm-1): 28.16 30.02 40.84



COMPOUND 4

MP2/6-31G*//oniom(mp2/6-31G(d):hf/6-31G(d))

6	5.257820	0.843777	1.096379
6	4.308808	-0.098987	0.679338
6	4.120502	-0.310261	-0.695618
6	4.864227	0.431673	-1.623567
6	5.786029	1.380764	-1.193883
6	5.988727	1.587802	0.174763
1	5.408781	1.008449	2.162608
1	4.721049	0.235579	-2.683316
1	6.358732	1.948392	-1.923235
1	6.714424	2.321194	0.517191
6	3.502984	-0.916482	1.692995
1	3.103021	-0.268348	2.461321
1	4.153805	-1.632943	2.185500
7	3.185963	-1.294372	-1.171765
7	2.409344	-1.652309	1.064645
6	2.903541	-2.278169	-0.145818
1	3.804335	-2.830182	0.087130
1	2.165166	-2.973914	-0.522423
6	1.922007	-0.727026	-1.634888
1	2.124076	0.157194	-2.224714
1	1.452303	-1.449303	-2.296683
6	0.981253	-0.392019	-0.488131
6	-0.167446	0.357078	-0.708288
6	-1.041621	0.670746	0.318334
6	-0.747989	0.212381	1.599346
6	0.381315	-0.548019	1.832115
6	1.255317	-0.854431	0.796326

1	-0.384312	0.701652	-1.705545
1	-1.412264	0.442771	2.413498
1	0.591523	-0.921970	2.818198
6	-2.261686	1.512651	0.078097
6	-3.545139	0.958397	0.025689
6	-4.663608	1.774183	-0.104248
6	-4.517369	3.139759	-0.222141
6	-3.250448	3.693204	-0.180786
6	-2.119023	2.904696	-0.019065
1	-5.637133	1.322970	-0.114796
1	-5.380698	3.770037	-0.336863
1	-3.137257	4.760110	-0.259905
6	-0.761820	3.571221	0.068671
1	-0.129724	3.311216	-0.773340
1	-0.870915	4.649184	0.080373
1	-0.232021	3.277239	0.967481
6	-3.842626	-0.512766	0.102197
8	-4.807524	-0.936226	0.660691
8	-2.976939	-1.252377	-0.556767
6	-3.069568	-2.686613	-0.603069
6	-2.923718	-3.316172	0.781561
6	-4.305304	-3.146536	-1.364122
1	-2.041139	-2.920696	1.285729
1	-4.368885	-2.638221	-2.320517
1	-3.797482	-3.136743	1.403203
1	-4.230602	-4.212806	-1.554904
1	-5.211165	-2.957232	-0.806095
1	-2.792883	-4.395029	0.669563
1	-2.193174	-2.938122	-1.184133

ENERGY = -1262.3626285 Hartrees

FREQUENCIES WERE NOT CALCULATED

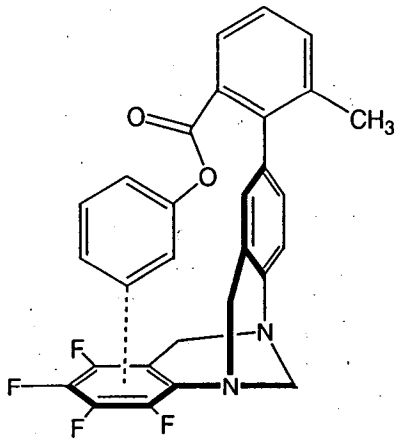
MP2/6-31G(d)//B3LYP/6-31G(d)

6	5.3649762463000	0.5861652888000	1.1296251921000
6	4.3410872073000	-0.2575614032000	0.6809882485000
6	4.1047155830000	-0.3680039864000	-0.7030021312000
6	4.8684520504000	0.3908548607000	-1.6019627633000
6	5.8672602893000	1.2426032661000	-1.1386311139000
6	6.1260547820000	1.3349900590000	0.2339718134000
1	5.5528834236000	0.6678987494000	2.1992994446000
1	4.6800962550000	0.2796695784000	-2.6668787888000
1	6.4563595839000	1.8197877066000	-1.8465984920000
1	6.9134143839000	1.9880361865000	0.6008143126000
6	3.4833699440000	-1.0396441022000	1.6698609311000
1	3.1253134327000	-0.3796461624000	2.4664645426000
1	4.0794415135000	-1.8276887341000	2.1523088832000
7	3.1143298373000	-1.2719126698000	-1.2196837741000

7	2.3178657248000	-1.6786618744000	1.0277701341000
6	2.7687014866000	-2.2885094488000	-0.2246830922000
1	3.6440760258000	-2.9113307986000	-0.0173382480000
1	1.9734193132000	-2.9211228614000	-0.6307042898000
6	1.8657292569000	-0.6182432114000	-1.6588531004000
1	2.1214458412000	0.2959688999000	-2.2037789388000
1	1.3644976637000	-1.2859258412000	-2.3744238574000
6	0.9323035782000	-0.2979047746000	-0.4965854481000
6	-0.2127428965000	0.4782916669000	-0.6970332424000
6	-1.0846020372000	0.7853091944000	0.3511676048000
6	-0.7702762728000	0.3228316458000	1.6394223371000
6	0.3587131593000	-0.4631160201000	1.8548613105000
6	1.2090246419000	-0.7965550549000	0.7919007215000
1	-0.4431386759000	0.8364501002000	-1.6993440994000
1	-1.4334799154000	0.5563595652000	2.4686091506000
1	0.5771746992000	-0.8575828056000	2.8441072541000
6	-2.3311325524000	1.5853167201000	0.1235578480000
6	-3.5994757261000	0.9699194679000	0.0302745407000
6	-4.7607298605000	1.7501394809000	-0.0740214834000
6	-4.6720421843000	3.1360907160000	-0.1311853482000
6	-3.4201531970000	3.7483086303000	-0.0603969630000
6	-2.2477663699000	2.9956745443000	0.0792195150000
1	-5.7206978363000	1.2457367796000	-0.1138844898000
1	-5.5711241664000	3.7390383571000	-0.2261548754000
1	-3.3470165628000	4.8329969948000	-0.0983006718000
6	-0.9142567419000	3.7011480385000	0.1987956812000
1	-0.2463187328000	3.4512318911000	-0.6336743717000
1	-1.0494608540000	4.7871112851000	0.2084380483000
1	-0.3886487236000	3.4129226763000	1.1163200386000
6	-3.8283610702000	-0.5164821733000	0.0387695488000
8	-4.8327904444000	-1.0248204756000	0.5022347152000
8	-2.8387515315000	-1.1925329305000	-0.5689571993000
6	-2.8555712207000	-2.6534130123000	-0.6199856904000
6	-2.7892497028000	-3.2667183280000	0.7770123710000
6	-4.0062577004000	-3.1721173359000	-1.4801020481000
1	-1.9633119117000	-2.8258418437000	1.3444529652000
1	-4.0163289848000	-2.6651783869000	-2.4511180926000
1	-3.7220160291000	-3.1102880954000	1.3228719991000
1	-3.8708320927000	-4.2454511491000	-1.6580516947000
1	-4.9682067770000	-3.0141491116000	-0.9886361507000
1	-2.6081908719000	-4.3444975770000	0.6899105568000
1	-1.9104445355000	-2.8524921956000	-1.1353089531000

ENERGY = -1262.3697052 Hartrees

Three lowest frequencies (cm-1): 26.76 28.63 34.22



COMPOUND 5

MP2/6-31G*//oniom(mp2/6-31G(d):hf/6-31G(d))

6	-3.430483	-0.295277	-1.243353
6	-2.662925	-1.350979	-0.763106
6	-2.513050	-1.500219	0.628236
6	-3.134722	-0.577389	1.477400
6	-3.864585	0.492211	0.972671
6	-4.055628	0.610531	-0.399903
9	-3.557870	-0.111841	-2.580753
9	-2.987859	-0.670723	2.816576
9	-4.422070	1.389129	1.804020
9	-4.764529	1.640874	-0.901344
6	-1.934214	-2.303603	-1.717124
1	-1.450120	-1.736799	-2.498085
1	-2.647535	-2.966441	-2.194230
7	-1.773538	-2.586638	1.182361
7	-0.951833	-3.107509	-1.002314
6	-1.570396	-3.633543	0.197016
1	-2.519079	-4.083347	-0.062681
1	-0.939523	-4.395082	0.633517
6	-0.466911	-2.189476	1.708055
1	-0.578005	-1.298717	2.309314
1	-0.125906	-2.978906	2.370051
6	0.533583	-1.957479	0.588386
6	1.713237	-1.266905	0.828226
6	2.602990	-0.970192	-0.189589
6	2.314786	-1.424465	-1.473239
6	1.162591	-2.144348	-1.722961
6	0.256281	-2.402303	-0.702801

1	1.912175	-0.901192	1.820741
1	2.996480	-1.215158	-2.278448
1	0.954966	-2.510713	-2.712259
6	3.840907	-0.156010	0.057851
6	3.841537	1.230572	-0.125496
6	5.015220	1.963257	-0.003602
6	6.189640	1.330227	0.347550
6	6.192159	-0.037956	0.550764
6	5.038360	-0.796737	0.398881
1	4.992704	3.021958	-0.180409
1	7.097297	1.895367	0.458018
1	7.110121	-0.529896	0.819927
6	5.099878	-2.296670	0.593649
1	4.826054	-2.826648	-0.312132
1	6.101477	-2.603052	0.870436
1	4.421994	-2.625928	1.373395
6	2.618279	2.026866	-0.471462
8	2.600999	2.892874	-1.279782
8	1.571423	1.695371	0.286577
6	0.324694	2.278027	0.085370
6	-0.401385	2.028709	-1.076413
6	-1.690896	2.550185	-1.187122
6	-2.254428	3.281299	-0.136510
6	-1.513311	3.508123	1.023606
6	-0.218744	2.997225	1.143932
1	0.046714	1.457703	-1.883440
1	-2.269495	2.360005	-2.087620
1	-3.264467	3.669656	-0.225753
1	-1.946179	4.071579	1.846152
1	0.374719	3.159635	2.038867

ENERGY = -1771.2161483 Hartrees

FREQUENCIES WERE NOT CALCULATED

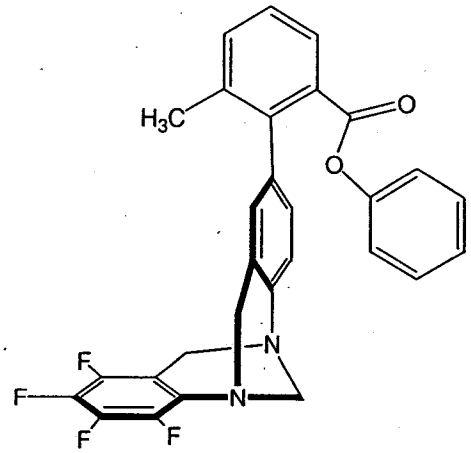
MP2/6-31G(d)//B3LYP/6-31G(d)

6	-0.0896904338000	-0.2465287600000	-0.0085041879000
6	-0.0107798014000	-0.1133511503000	1.3736943202000
6	1.2565429245000	-0.1642416902000	1.9892568908000
6	2.3869606501000	-0.3882281720000	1.1927149868000
6	2.2831239391000	-0.5450920238000	-0.1860489558000
6	1.0325800876000	-0.4668939481000	-0.7988050871000
6	-1.2718326179000	0.0295931217000	2.2188644965000
1	-2.0157319265000	-0.7097767402000	1.9104968425000
1	-1.7247950309000	1.0182681099000	2.0672995785000
7	1.4129170802000	0.0240892378000	3.3931947092000
7	-0.9839477319000	-0.1394984549000	3.6541748405000
6	0.2140313019000	0.6381288340000	3.9717276013000
1	0.0928632218000	1.6518819135000	3.5792180159000

1	0.3436433850000	0.6905106958000	5.0560719125000
6	1.6953261082000	-1.2218867712000	4.1379527372000
1	2.4559205646000	-1.7911828797000	3.5968688626000
1	2.1373227037000	-0.9392338855000	5.1032350998000
6	0.4372789289000	-2.0566575854000	4.3443085160000
6	0.5265094059000	-3.3813160442000	4.7822279079000
6	-0.6059156491000	-4.1904588188000	4.9145093206000
6	-1.8621722225000	-3.6352351177000	4.6235916096000
6	-1.9733901356000	-2.3095794285000	4.2129826860000
6	-0.8317074535000	-1.5096109448000	4.0667712357000
1	1.5083736035000	-3.8089838779000	4.9780452231000
1	-2.7553719959000	-4.2458281453000	4.7274257975000
1	-2.9491011133000	-1.8723798612000	4.0168972219000
6	-0.4937495719000	-5.6137648625000	5.3691610127000
6	-0.6244826650000	-6.7035056375000	4.4781262489000
6	-0.6027398508000	-8.0219230590000	4.9608750467000
6	-0.4162884617000	-8.2726859499000	6.3142562562000
6	-0.2728616834000	-7.2015618263000	7.1962215349000
6	-0.3196592732000	-5.8759415040000	6.7481612131000
1	-0.7278172712000	-8.8323791629000	4.2507521981000
1	-0.3867186185000	-9.2941772173000	6.6832962941000
1	-0.1358359259000	-7.3923655095000	8.2582344724000
6	-0.2083688804000	-4.7486561309000	7.7520494373000
1	-1.0556869388000	-4.0581229500000	7.6751627029000
1	-0.1790145300000	-5.1421637266000	8.7726628390000
1	0.6971926299000	-4.1511587242000	7.5957557452000
6	-0.7922465573000	-6.5933480013000	2.9924312119000
8	-1.3248154510000	-7.4424441567000	2.3134673213000
8	-0.2285042131000	-5.4629181134000	2.4788558862000
6	-0.2973192222000	-5.2202955411000	1.1025372266000
6	-0.8627232744000	-4.0115767801000	0.7047068772000
6	-0.8684314091000	-3.6746547487000	-0.6507366919000
6	-0.3133937754000	-4.5452460015000	-1.5918637889000
6	0.2487957545000	-5.7550025840000	-1.1739376453000
6	0.2637054561000	-6.1008833988000	0.1785791355000
1	-1.2787642619000	-3.3523580324000	1.4596332307000
1	-1.2965824148000	-2.7277001151000	-0.9657358166000
1	-0.3143925695000	-4.2799917394000	-2.6455168054000
1	0.6835602405000	-6.4345803113000	-1.9020913409000
1	0.6974939764000	-7.0364872556000	0.5126229449000
9	3.6029768015000	-0.4673698770000	1.7597923581000
9	3.3777295789000	-0.7563380858000	-0.9260516176000
9	0.9179277531000	-0.6237090749000	-2.1238124295000
9	-1.3026842656000	-0.2280261422000	-0.6069743463000

ENERGY = -1771.2208135 Hartrees

Three lowest frequencies (cm-1) 23.77 38.57 42.41



COMPOUND 6

MP2/6-31G*//oniom(mp2/6-31G(d):hf/6-31G(d))

6	-4.828329	-0.088784	-1.101184
6	-3.676965	-0.793673	-0.762657
6	-3.373294	-0.983508	0.597632
6	-4.221062	-0.431512	1.563860
6	-5.348885	0.296618	1.203960
6	-5.668569	0.460471	-0.141653
9	-5.138565	0.094119	-2.406645
9	-3.947188	-0.572869	2.877593
9	-6.147508	0.820588	2.149684
9	-6.768054	1.149681	-0.496513
6	-2.744512	-1.357149	-1.841257
1	-2.539817	-0.597246	-2.580969
1	-3.232871	-2.180230	-2.351027
7	-2.245919	-1.754333	1.004431
7	-1.496112	-1.836206	-1.263546
6	-1.791953	-2.610390	-0.076070
1	-2.554391	-3.341294	-0.309197
1	-0.904771	-3.133964	0.251828
6	-1.118744	-0.946980	1.472340
1	-1.484443	-0.167525	2.125928
1	-0.480383	-1.587240	2.072207
6	-0.330320	-0.356081	0.314727
6	0.626118	0.631604	0.539331
6	1.352219	1.192007	-0.496070
6	1.116340	0.737163	-1.793069
6	0.187005	-0.250977	-2.030398
6	-0.547481	-0.802963	-0.982906

1	0.791027	0.978347	1.545754
1	1.684604	1.142047	-2.610734
1	0.030580	-0.622559	-3.027165
6	2.343901	2.282584	-0.214391
6	3.561717	2.014054	0.416454
6	4.423288	3.045104	0.770047
6	4.102414	4.349600	0.458828
6	2.905371	4.622021	-0.178240
6	2.011002	3.612089	-0.508933
1	5.338234	2.811285	1.280492
1	4.772687	5.149213	0.717068
1	2.650221	5.641423	-0.407765
6	0.690597	3.977109	-1.154412
1	-0.147067	3.557126	-0.609460
1	0.567997	5.053081	-1.180463
1	0.625626	3.612682	-2.173905
6	4.040009	0.636657	0.766019
8	4.550991	0.366935	1.801478
8	3.897251	-0.223021	-0.242725
6	4.266800	-1.558634	-0.106127
6	3.292859	-2.507484	-0.400136
6	3.633291	-3.861168	-0.365445
6	4.936608	-4.252252	-0.056181
6	5.900610	-3.282290	0.227636
6	5.576785	-1.925610	0.189608
1	2.288908	-2.178898	-0.648061
1	2.878294	-4.609080	-0.594082
1	5.199290	-5.306483	-0.028815
1	6.918166	-3.579437	0.467567
1	6.317317	-1.168210	0.419640

ENERGY = -1771.2085847 Hartrees

FREQUENCIES WERE NOT CALCULATED

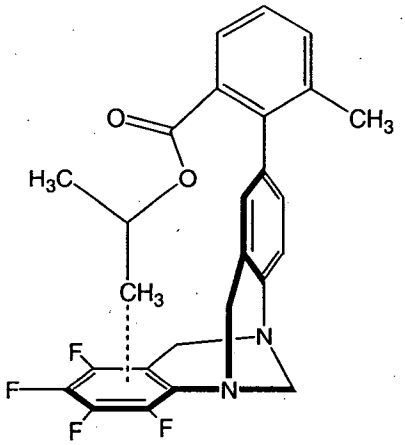
MP2/6-31G(d)//B3LYP/6-31G(d)

6	0.0043192708000	0.1934206935000	0.1004730804000
6	0.0023383935000	0.0749555505000	1.4872832025000
6	1.2340505146000	-0.0059197849000	2.1686837147000
6	2.4190013092000	-0.0209793973000	1.4212259023000
6	2.4001757937000	0.0699087913000	0.0329012800000
6	1.1828202223000	0.1903363689000	-0.6388198146000
6	-1.3101545671000	-0.0068658826000	2.2583686861000
1	-1.9720394841000	-0.7428260166000	1.7935787673000
1	-1.8339594891000	0.9576931614000	2.2272573888000
7	1.3003948553000	-0.0347454479000	3.5916904152000
7	-1.0886538672000	-0.3756410743000	3.6666980889000
6	0.0335432487000	0.4126768652000	4.1777899128000
1	-0.1334096614000	1.4665202703000	3.9369685186000

1	0.0975835226000	0.3009104850000	5.2635446976000
6	1.6262871406000	-1.3595461865000	4.1611403229000
1	2.4406941861000	-1.8019723867000	3.5808043040000
1	2.0108747991000	-1.2017640794000	5.1777683382000
6	0.4126324741000	-2.2805463531000	4.1887225653000
6	0.5540769682000	-3.6334962556000	4.5152162184000
6	-0.5387238476000	-4.5072575196000	4.5317303010000
6	-1.8024938909000	-4.0007846022000	4.1844069960000
6	-1.9659402259000	-2.6539872057000	3.8796098806000
6	-0.8697381505000	-1.7782012586000	3.8949955366000
1	1.5432533623000	-4.0187439128000	4.7578926143000
1	-2.6679266846000	-4.6573864594000	4.2038015780000
1	-2.9532552290000	-2.2527747740000	3.6650990512000
6	-0.3428734275000	-5.9400808010000	4.9138839055000
6	0.0610029305000	-6.2974422106000	6.2201567573000
6	0.3629648875000	-7.6302483437000	6.5354423473000
6	0.2187134599000	-8.6249236789000	5.5755818886000
6	-0.1980729747000	-8.2821198335000	4.2893415806000
6	-0.4676765181000	-6.9540086384000	3.9362006647000
1	0.6991339368000	-7.8645042590000	7.5402732765000
1	0.4368857429000	-9.6602266870000	5.8223797363000
1	-0.2968224036000	-9.0561526035000	3.5317075789000
6	-0.8466806855000	-6.6304090821000	2.5067338060000
1	-0.2370204960000	-5.8134866670000	2.1057828217000
1	-0.7112064505000	-7.5062567621000	1.8650104488000
1	-1.8927519633000	-6.3139858778000	2.4202637317000
6	0.2111519695000	-5.3301194391000	7.3555893592000
8	1.0815359766000	-5.4145115243000	8.1940556919000
8	-0.7841156685000	-4.4017471663000	7.3654535198000
6	-0.8381964441000	-3.3530640654000	8.2864532410000
6	-1.4283588403000	-2.1855104082000	7.7974218448000
6	-1.5849596459000	-1.0893672050000	8.6450691465000
6	-1.1556038836000	-1.1595780038000	9.9734714316000
6	-0.5776940123000	-2.3383531578000	10.4486438138000
6	-0.4164508072000	-3.4487808650000	9.6149216639000
1	-1.7563861780000	-2.1561709570000	6.7635760537000
1	-2.0439596311000	-0.1805630665000	8.2645446418000
1	-1.2732687410000	-0.3041010417000	10.6331541804000
1	-0.2451658662000	-2.4038268446000	11.4814019680000
1	0.0387565273000	-4.3571238205000	9.9829174875000
9	-1.1711410106000	0.2786261092000	-0.5561469837000
9	1.1587925988000	0.2910176123000	-1.9743312365000
9	3.5462460481000	0.0635329228000	-0.6587236322000
9	3.6057126337000	-0.1259914164000	2.0434411814000

ENERGY = -1771.2157408 Hartrees

Three lowest frequencies (cm-1): 31.45 31.76 40.00



COMPOUND 7

MP2/6-31G*//oniom(mp2/6-31G(d):hf/6-31G(d))

6	-3.664590	0.280587	-1.152302
6	-2.958170	-0.846525	-0.743017
6	-2.822009	-1.098540	0.634767
6	-3.378681	-0.194185	1.545938
6	-4.053310	0.942560	1.115775
6	-4.211895	1.180551	-0.247222
9	-3.806920	0.535163	-2.475033
9	-3.250123	-0.392370	2.874324
9	-4.576635	1.798854	2.009410
9	-4.873582	2.272903	-0.671110
6	-2.319425	-1.799164	-1.760490
1	-1.795798	-1.230543	-2.514422
1	-3.092665	-2.368405	-2.264395
7	-2.151219	-2.261041	1.114195
7	-1.402351	-2.724931	-1.109718
6	-2.044033	-3.265291	0.070482
1	-3.029132	-3.624901	-0.194427
1	-1.468626	-4.096043	0.454046
6	-0.811163	-1.982104	1.632249
1	-0.849591	-1.116149	2.277812
1	-0.516534	-2.823495	2.250968
6	0.188715	-1.774517	0.507041
6	1.434262	-1.205235	0.760435
6	2.350347	-0.978644	-0.249813
6	2.016114	-1.366256	-1.546379
6	0.796486	-1.947823	-1.811153
6	-0.132670	-2.145206	-0.792859

1	1.678619	-0.911974	1.767779
1	2.712757	-1.199124	-2.347896
1	0.546820	-2.257988	-2.809999
6	3.665980	-0.327269	0.060110
6	3.748319	1.040867	0.338160
6	4.955858	1.613375	0.719144
6	6.097350	0.842341	0.786267
6	6.024191	-0.508935	0.500260
6	4.823280	-1.112447	0.150438
1	4.985255	2.660111	0.954391
1	7.035383	1.286216	1.066753
1	6.912892	-1.111549	0.565637
6	4.790117	-2.605331	-0.101571
1	4.551366	-2.834898	-1.134404
1	5.753689	-3.047754	0.120891
1	4.045374	-3.095468	0.515311
6	2.587048	1.992825	0.257592
8	2.426102	2.866367	1.052444
8	1.830928	1.794734	-0.801372
6	0.669969	2.597731	-1.081402
6	-0.409814	2.438724	-0.011366
6	1.040943	4.045180	-1.372565
1	-0.118585	2.898914	0.930151
1	1.359922	4.564002	-0.480000
1	-0.623715	1.382424	0.158737
1	1.837330	4.088073	-2.108037
1	-1.329274	2.915331	-0.359985
1	0.176839	4.558154	-1.783266
1	0.312477	2.143503	-1.995013

ENERGY = -1658.4149536 Hartrees

FREQUENCIES WERE NOT CALCULATED

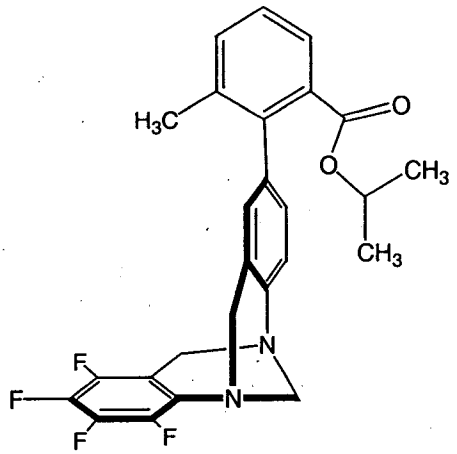
MP2/6-31G(d)//B3LYP/6-31G(d)

6	0.0118368239000	-0.0071536221000	0.0292632355000
6	-0.0012804099000	0.0151088475000	1.4207312800000
6	1.1974851958000	-0.0478193836000	-0.6977084195000
9	-1.1582364119000	-0.0292189460000	-0.6420599978000
6	1.2259305151000	0.0352945357000	2.1147905176000
6	2.4115499186000	-0.0564973393000	-0.0099803613000
9	1.1832664532000	-0.0884842750000	-2.0366790015000
6	-1.3180047438000	-0.0248896219000	2.1887522002000
6	2.4187871000000	-0.0099688072000	1.3808184148000
9	3.5634495542000	-0.0945206763000	-0.6899438969000
7	1.2802689533000	0.1172428174000	3.5363497621000
7	-1.1028388444000	-0.2862046518000	3.6231808348000
9	3.6013039150000	-0.0154895748000	2.0188811073000
6	-0.0056975020000	0.5661275312000	4.0809678857000

6	1.6343815098000	-1.1601540178000	4.1929690025000
6	-0.8427691535000	-1.6690661935000	3.9275565300000
6	0.4558958642000	-2.1254371133000	4.2228703792000
6	-1.9116241935000	-2.5770031660000	3.9343689118000
6	0.6496718289000	-3.4812468788000	4.5130390771000
6	-1.6969332265000	-3.9228019035000	4.2079317799000
6	-0.4059881424000	-4.3970840034000	4.4895296317000
6	-0.1435128337000	-5.8509446238000	4.7384929559000
6	0.4298986942000	-6.6781323525000	3.7465621513000
6	-0.4066459849000	-6.3923653034000	6.0172926902000
6	0.7560001584000	-8.0109644271000	4.0387863227000
6	-0.0999687279000	-7.7348082750000	6.2702245090000
6	-0.9901527507000	-5.5377661857000	7.1216200457000
6	0.7438859111000	-6.2415595258000	2.3414950300000
6	0.4822485845000	-8.5427245474000	5.2931691452000
8	1.6397611631000	-6.7411631699000	1.6857073254000
8	-0.0971640437000	-5.2958670136000	1.8909337135000
6	0.0779919787000	-4.7149860970000	0.5602623541000
6	1.4094341748000	-3.9775945045000	0.4358053578000
6	-0.1719039366000	-5.7437925386000	-0.5398326164000
1	-1.9680338034000	-0.8004001814000	1.7753188327000
1	-1.8513885393000	0.9290104884000	2.0827395057000
1	-0.1999620358000	1.5951875959000	3.7650201152000
1	0.0551100349000	0.5357372994000	5.1721331121000
1	2.4886412356000	-1.5998088035000	3.6709020748000
1	1.9726662605000	-0.9264440279000	5.2116870941000
1	-2.9123609629000	-2.2075045432000	3.7257797515000
1	1.6563825736000	-3.8393218950000	4.7231820579000
1	-2.5299998033000	-4.6201282132000	4.1835732769000
1	1.2201434020000	-8.6100905735000	3.2624709073000
1	-0.3082384688000	-8.1450511684000	7.2558669469000
1	-1.9899180832000	-5.1680391561000	6.8664653535000
1	-1.0691114716000	-6.1081106422000	8.0521709284000
1	-0.3706887076000	-4.6541824079000	7.3140014787000
1	0.7241750772000	-9.5789179273000	5.5134192065000
1	-0.7325176273000	-3.9794308880000	0.5484516376000
1	2.2508918159000	-4.6732814195000	0.4378232696000
1	1.5281330688000	-3.2682753010000	1.2611547577000
1	1.4220651856000	-3.4122178546000	-0.5031280309000
1	0.6316780523000	-6.4816295010000	-0.5798864618000
1	-1.1221214345000	-6.2613396769000	-0.3699912876000
1	-0.2313741189000	-5.2312067703000	-1.5070275108000

ENERGY = -1658.4220213 Hartrees

Three lowest frequencies (cm-1): 28.21 32.00 37.29



COMPOUND 8

MP2/6-31G*//oniom(mp2/6-31G(d):hf/6-31G(d))

6	-4.510347	0.149944	-1.244226
6	-3.479655	-0.676649	-0.806482
6	-3.272047	-0.826990	0.576510
6	-4.086683	-0.116560	1.464519
6	-5.089796	0.728894	1.005764
6	-5.317616	0.856312	-0.362268
9	-4.728894	0.297059	-2.572478
9	-3.899312	-0.217277	2.797437
9	-5.858473	1.404161	1.877774
9	-6.298113	1.659971	-0.812456
6	-2.576776	-1.416082	-1.800814
1	-2.236399	-0.731880	-2.563961
1	-3.144406	-2.195920	-2.296446
7	-2.277126	-1.711791	1.084305
7	-1.433334	-2.020003	-1.130861
6	-1.886621	-2.679726	0.075028
1	-2.726395	-3.318638	-0.162864
1	-1.093185	-3.293444	0.478127
6	-1.078421	-1.029292	1.572734
1	-1.371357	-0.174300	2.165844
1	-0.560398	-1.711561	2.238970
6	-0.161835	-0.610344	0.434464
6	0.901824	0.252931	0.664598
6	1.754809	0.645917	-0.352342
6	1.527940	0.151311	-1.633523
6	0.485237	-0.721001	-1.876624
6	-0.368189	-1.106193	-0.850605

1	1.068098	0.624195	1.661757
1	2.177469	0.442097	-2.439929
1	0.329678	-1.121146	-2.862483
6	2.879399	1.609235	-0.101988
6	4.211240	1.188096	-0.021232
6	5.237907	2.115097	0.118945
6	4.951358	3.459912	0.217863
6	3.636051	3.881263	0.147825
6	2.593659	2.979986	-0.023931
1	6.251795	1.765588	0.152244
1	5.743882	4.175787	0.340280
1	3.413615	4.931729	0.212459
6	1.177715	3.504677	-0.142192
1	0.560287	3.190248	0.692259
1	1.177256	4.587794	-0.163514
1	0.696738	3.151457	-1.047238
6	4.659473	-0.245468	-0.075198
8	5.680239	-0.570600	-0.598565
8	3.851786	-1.067325	0.560098
6	4.095290	-2.483430	0.627439
6	4.065653	-3.136785	-0.753524
6	5.345582	-2.802032	1.435390
1	3.164179	-2.842300	-1.292362
1	5.321468	-2.281333	2.386860
1	4.936418	-2.870397	-1.347520
1	5.377724	-3.868379	1.636981
1	6.245174	-2.522599	0.905879
1	4.046589	-4.222421	-0.632994
1	3.231027	-2.821979	1.182009

ENERGY = -1658.411706 Hartrees

FREQUENCIES WERE NOT CALCULATED

MP2/6-31G(d)//B3LYP/6-31G(d)

6	-0.0003194791000	0.0146043596000	0.0173110110000
6	-0.0025274196000	0.0177799239000	1.4093092145000
6	1.1796765299000	-0.0259299410000	-0.7187677027000
9	-1.1758233111000	0.0165065972000	-0.6445260832000
6	1.2297497887000	0.0246921928000	2.0941118171000
6	2.3983191736000	-0.0587199740000	-0.0395204547000
9	1.1560675060000	-0.0426841342000	-2.0580341368000
6	-1.3142414126000	-0.0220028413000	2.1856940715000
6	2.4164599698000	-0.0271871827000	1.3512777684000
9	3.5458536532000	-0.0986158245000	-0.7279451770000
7	1.2941009458000	0.1204189294000	3.5141952605000
7	-1.0901492286000	-0.2523287072000	3.6228723275000
9	3.6041162276000	-0.0494888669000	1.9808007475000
6	0.0180668804000	0.5967771140000	4.0572064914000

6	1.6405963298000	-1.1464027173000	4.1926701401000
6	-0.8501810435000	-1.6251009237000	3.9814434566000
6	0.4439139989000	-2.0838480676000	4.3004948560000
6	-1.9330059412000	-2.5105828040000	4.0586791661000
6	0.6120079978000	-3.4023512664000	4.7335121298000
6	-1.7439164264000	-3.8246610272000	4.4782273661000
6	-0.4681421907000	-4.2821117107000	4.8451186725000
6	-0.2867412695000	-5.6847584273000	5.3413541383000
6	-0.6090060146000	-6.0494323010000	6.6675887629000
6	0.1432918373000	-6.6843350012000	4.4393595728000
6	-0.5302623594000	-7.3901587340000	7.0727795318000
6	0.2448387146000	-8.0091096431000	4.8809300356000
6	0.4749488230000	-6.3475418220000	3.0017823698000
6	-1.0583435131000	-5.0878822051000	7.7327916525000
6	-0.0934516786000	-8.3671342894000	6.1860998957000
8	-1.8162117630000	-5.4088468314000	8.6295581902000
8	-0.4888328585000	-3.8768368086000	7.6094706150000
6	-0.8391125432000	-2.7936094814000	8.5272325939000
6	-2.3137237893000	-2.4140261588000	8.4117352881000
6	-0.3768801424000	-3.0908331824000	9.9521765967000
1	-1.9581117243000	-0.8130592096000	1.7916347829000
1	-1.8590575429000	0.9234987517000	2.0629928012000
1	-0.1653476361000	1.6215623664000	3.7214657534000
1	0.0838079718000	0.5874123627000	5.1486637591000
1	2.4635379010000	-1.6212779528000	3.6512577734000
1	2.0235044328000	-0.8959999141000	5.1915809299000
1	-2.9280079343000	-2.1452124246000	3.8175549575000
1	1.6068112462000	-3.7480096424000	5.0096656535000
1	-2.5952726805000	-4.4963130161000	4.5528240016000
1	-0.8130537715000	-7.6397042597000	8.0901353564000
1	0.5806543633000	-8.7718952715000	4.1820528176000
1	1.3207679551000	-5.6538498503000	2.9314652659000
1	0.7330604820000	-7.2513146828000	2.4415431266000
1	-0.3690322137000	-5.8624026308000	2.4981672198000
1	-0.0200858535000	-9.4031683107000	6.5054056228000
1	-0.2335283466000	-1.9764783545000	8.1221008949000
1	-2.5801869134000	-2.2448115191000	7.3633888619000
1	-2.9568960514000	-3.1950919968000	8.8224088921000
1	-2.4917491446000	-1.4842795876000	8.9646786441000
1	0.6752564457000	-3.3954032537000	9.9572764832000
1	-0.4712976177000	-2.1833794150000	10.5601112248000
1	-0.9766700767000	-3.8828294233000	10.4044375825000

ENERGY = -1658.4188754 Hartrees

Three lowest frequencies (cm-1): 26.73 29.06 34.57