

Influence of the solvents in the morphology of Langmuir and Langmuir-Schaefer films of PCBM and PCBM-based oligomers and polymers

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Supplementary Information

Complementary calculations were carried out under an implicit model of the solvent (PCM model) making it possible to implicitly average the degrees of freedom of the solvent and to treat the electrostatic interactions (generally dominant in the solvation) for the C₆₀, PCBM, OPCBMMB and PPCBMB systems. These new calculations show that neither the volumes nor the calculated surfaces are considerably modified whatever the considered solvent, as shown in Tables S1, S2 and S3.

Table S1: Area and volume values of OPCBMMB and PPCBMB monomers in solution in chloroform extracted from the theoretical DFT/PCM model

Materials	Structural parameters (Å)			Area in different orientations (Å ²)			Volume (Å ³)
	X	Y	Z	X.Y	Y.Z	X.Z	X.Y.Z
OPCBMMB	17.10	18.40	11.00	314.6	202.4	188.1	3461.0
PPCBMB	20.21	18.66	13.74	377.1	256.4	277.7	5181.6
C ₆₀	7.07	7.03	6.65	49.7	46.8	47.0	330.5
PCBM	14.80	9.85	6.96	145.8	68.6	103.0	1014.6

Table S2: Area and volume values of OPCBMMB and PPCBMB monomers in solution in toluene extracted from the theoretical DFT/PCM model

Materials	Structural parameters (Å)			Area in different orientations (Å ²)			Volume (Å ³)
	X	Y	Z	X.Y	Y.Z	X.Z	X.Y.Z
OPCBMMB	17.19	18.37	10.99	315.8	201.9	188.9	3470.4
PPCBMB	20.19	18.62	13.70	375.9	255.1	276.6	5150.3
C ₆₀	7.06	7.05	6.94	49.8	48.9	49.0	345.2
PCBM	14.80	9.84	6.96	145.6	68.5	103.0	1013.6

Table S3: Area and volume values of OPCBMMB and PPCBMB monomers in solution in xylene extracted from the theoretical DFT/PCM model

Materials	Structural parameters (Å)			Area in different orientations (Å ²)			Volume (Å ³)
	X	Y	Z	X.Y	Y.Z	X.Z	X.Y.Z
OPCBMMB	17.11	18.41	10.98	315.0	202.1	187.9	3458.7
PPCBMB	20.19	18.62	13.70	375.9	255.1	276.6	5150.3
C ₆₀	7.09	6.97	6.78	49.4	47.3	48.1	335.0
PCBM	14.80	9.85	6.96	145.8	68.6	103.0	1014.6

Computational Details

Optimisations of geometries and energies were determined at the DFT (Density Functional Theory) level using the B3LYP exchange-correlation functional with the 6-31G* basis set. Calculations were performed using Gaussian 09 program package.ⁱ

PCBM (*singlet*) B3LYP-6-31G* E= -2902.723357 u.a.

	X	Y	Z
C	-4.286121	2.471941	1.093775
C	-3.787332	2.282616	-0.198613
C	-3.895019	3.320950	-1.129730
C	-4.491513	4.529837	-0.776070
C	-4.987590	4.712133	0.516122
C	-4.884853	3.680476	1.449638
C	-3.200323	0.962943	-0.619108
C	-4.208159	0.007471	-1.256040
C	-5.230044	-0.522420	-0.248643
C	-6.201670	-1.510531	-0.888543
C	-7.210452	-2.051478	0.102939
O	-8.061811	-2.913239	-0.496927
C	-9.057757	-3.486662	0.364740
C	-1.800333	0.988316	-1.185174
C	-2.138936	0.357678	0.263652
C	-1.473317	1.019043	1.422694
C	-0.741008	2.188762	1.313186
C	-0.431564	2.766396	-0.010035
C	-0.867422	2.152959	-1.172528
C	-1.831965	-1.094732	0.418264
C	-1.422645	-1.901814	-0.631294
C	-1.110245	-1.323724	-1.954919
C	-1.220107	0.039302	-2.178669

C	-0.177125	0.724259	-2.905716
C	0.038459	2.020830	-2.288650
C	-1.266261	-1.300550	1.731608
C	-1.048706	-0.003816	2.347534
C	0.046867	0.195145	3.191005
C	0.798359	1.426066	3.097122
C	0.415791	2.395599	2.164375
C	1.432210	3.093312	1.394084
C	0.910234	3.316117	0.055577
C	1.770045	3.234307	-1.044422
C	1.322613	2.569130	-2.247047
C	0.899190	0.024962	-3.456284
C	0.998768	-1.402311	-3.248617
C	0.016791	-2.058086	-2.499745
C	0.404719	-3.079107	-1.540854
C	-0.478965	-2.978524	-0.390990
C	0.026401	-3.209915	0.892121
C	-0.377400	-2.348545	1.980679
C	0.771247	-2.138620	2.849758
C	0.978817	-0.894061	3.441843
C	2.316888	-0.328114	3.500288
C	2.204793	1.107887	3.286429
C	3.176708	1.778291	2.544158
C	2.782026	2.796607	1.581500
C	3.671944	2.699421	0.433570
C	3.175832	2.914546	-0.852006
C	3.594646	2.049063	-1.945462
C	2.446013	1.835358	-2.810861
C	2.239075	0.590786	-3.403108
C	2.402797	-1.731301	-3.061307
C	3.170764	-0.497944	-3.157004
C	4.272727	-0.295369	-2.325184
C	4.656284	-1.318459	-1.365796
C	3.921673	-2.501709	-1.276327
C	2.771567	-2.710482	-2.139006
C	5.111587	-0.651913	-0.155239
C	4.818265	-1.197350	1.094425
C	4.056705	-2.433534	1.188903
C	3.615393	-3.071310	0.028669
C	4.406824	-0.331284	2.188713
C	4.300325	1.045556	1.986301
C	4.606530	1.615093	0.681334
C	5.006279	0.783803	-0.366030
C	4.489084	1.004818	-1.706770
C	3.393913	-1.032652	2.960822
C	3.177177	-2.332747	2.342399
C	1.892362	-2.874827	2.288683
C	1.431224	-3.537751	1.077088
C	2.276174	-3.631583	-0.028598
C	1.750287	-3.402675	-1.366416
O	-7.265346	-1.766416	1.279554
H	-4.198731	1.673088	1.823542
H	-5.267316	3.815325	2.457198
H	-5.448906	5.655261	0.794594
H	-4.564193	5.330320	-1.506745
H	-3.499165	3.180593	-2.131861
H	-8.586340	-4.049858	1.174450
H	-9.686780	-2.704516	0.797951
H	-9.648638	-4.147545	-0.269734
H	-6.753625	-1.048712	-1.717620

H	-5.668596	-2.363845	-1.328312
H	-5.791873	0.305230	0.195184
H	-4.707410	-1.016641	0.578305
H	-3.683371	-0.832758	-1.720280
H	-4.715075	0.546022	-2.066854

PCBM xylene (*singlet*) B3LYP-6-31G* E= -2902.727044 u.a.

	X	Y	Z
C	-4.280709	2.476743	1.094921
C	-3.786520	2.283885	-0.198904
C	-3.897367	3.319544	-1.133025
C	-4.491957	4.530029	-0.780293
C	-4.982960	4.716374	0.513703
C	-4.877540	3.686906	1.449865
C	-3.200791	0.962973	-0.618005
C	-4.209376	0.007203	-1.253291
C	-5.231812	-0.519374	-0.244574
C	-6.201282	-1.510047	-0.883540
C	-7.214061	-2.049420	0.103674
O	-8.054893	-2.919772	-0.493931
C	-9.058746	-3.495095	0.360461
C	-1.801189	0.987390	-1.184864
C	-2.139059	0.358527	0.265088
C	-1.472102	1.020775	1.422637
C	-0.739877	2.190422	1.311774
C	-0.431059	2.766447	-0.012357
C	-0.867691	2.151446	-1.173785
C	-1.831884	-1.093628	0.421030
C	-1.423325	-1.902085	-0.627696
C	-1.111569	-1.325643	-1.952084
C	-1.221274	0.037114	-2.177144
C	-0.178514	0.720877	-2.905606
C	0.037709	2.018013	-2.290116
C	-1.265369	-1.298230	1.734205
C	-1.047185	-0.000926	2.348531
C	0.048697	0.198777	3.191440
C	0.800398	1.429434	3.095800
C	0.417504	2.397876	2.161996
C	1.433651	3.094436	1.390353
C	0.910952	3.315826	0.051902
C	1.770216	3.232797	-1.048467
C	1.321940	2.566282	-2.250033
C	0.897321	0.020848	-3.456250
C	0.996770	-1.406190	-3.247002
C	0.015065	-2.060721	-2.496624
C	0.403369	-3.080733	-1.536797
C	-0.479702	-2.978603	-0.386607
C	0.026215	-3.209008	0.896496
C	-0.376822	-2.346285	1.984261
C	0.772378	-2.135523	2.852416
C	0.980553	-0.890336	3.443004
C	2.318780	-0.324631	3.500007
C	2.206851	1.111171	3.284571
C	3.178567	1.780547	2.541060

C	2.783577	2.797826	1.577455
C	3.672824	2.699140	0.429166
C	3.176013	2.912918	-0.856392
C	3.594035	2.046053	-1.949080
C	2.444898	1.831678	-2.813643
C	2.237350	0.586453	-3.404322
C	2.400804	-1.735249	-3.059934
C	3.168976	-0.502155	-3.157425
C	4.271503	-0.298886	-2.326486
C	4.655376	-1.320963	-1.366152
C	3.920547	-2.503952	-1.274956
C	2.769946	-2.713526	-2.136789
C	5.111484	-0.653143	-0.156601
C	4.818761	-1.197097	1.093867
C	4.056956	-2.432997	1.190144
C	3.614845	-3.071976	0.030869
C	4.408076	-0.329694	2.187387
C	4.301735	1.046940	1.983442
C	4.607357	1.614926	0.677654
C	5.006397	0.782357	-0.368979
C	4.488453	1.001935	-1.709674
C	3.395426	-1.029987	2.960829
C	3.178064	-2.330701	2.343974
C	1.893069	-2.872524	2.291539
C	1.431110	-3.536775	1.080971
C	2.275504	-3.632076	-0.025047
C	1.748950	-3.404582	-1.362828
O	-7.280216	-1.754839	1.279293
H	-4.191752	1.679954	1.826771
H	-5.256292	3.824662	2.458391
H	-5.442679	5.660498	0.791286
H	-4.567378	5.328272	-1.513061
H	-3.507058	3.176022	-2.136835
H	-8.592709	-4.052904	1.176612
H	-9.697154	-2.713812	0.780498
H	-9.638519	-4.162007	-0.277345
H	-6.750340	-1.049979	-1.715318
H	-5.665958	-2.364017	-1.318766
H	-5.794138	0.310556	0.194345
H	-4.708694	-1.010245	0.584175
H	-3.686128	-0.835082	-1.715240
H	-4.715686	0.544197	-2.065140

PCBM toluene (*singlet*) B3LYP-6-31G* E= -2902.727024 u.a.

	X	Y	Z
C	-4.280700	2.476808	1.094915
C	-3.786503	2.283961	-0.198911
C	-3.897296	3.319650	-1.133001
C	-4.491828	4.530153	-0.780241
C	-4.982828	4.716487	0.513754
C	-4.877473	3.686986	1.449886
C	-3.200819	0.963052	-0.618028
C	-4.209354	0.007278	-1.253387
C	-5.231756	-0.519400	-0.244701

C	-6.201143	-1.510181	-0.883670
C	-7.213901	-2.049513	0.103618
O	-8.054709	-2.919961	-0.493868
C	-9.058553	-3.495159	0.360621
C	-1.801187	0.987442	-1.184878
C	-2.139097	0.358539	0.265057
C	-1.472141	1.020752	1.422632
C	-0.739903	2.190391	1.311804
C	-0.431067	2.766455	-0.012303
C	-0.867687	2.151492	-1.173753
C	-1.831938	-1.093624	0.420970
C	-1.423350	-1.902040	-0.627777
C	-1.111574	-1.325566	-1.952144
C	-1.221276	0.037193	-2.177184
C	-0.178496	0.720971	-2.905609
C	0.037727	2.018085	-2.290080
C	-1.265433	-1.298263	1.734145
C	-1.047245	-0.000978	2.348506
C	0.048628	0.198695	3.191433
C	0.800339	1.429349	3.095834
C	0.417466	2.397817	2.162051
C	1.433626	3.094394	1.390440
C	0.910948	3.315825	0.051989
C	1.770225	3.232821	-1.048369
C	1.321961	2.566342	-2.249961
C	0.897341	0.020948	-3.456254
C	0.996777	-1.406097	-3.247041
C	0.015060	-2.060641	-2.496692
C	0.403342	-3.080684	-1.536891
C	-0.479744	-2.978579	-0.386708
C	0.026153	-3.209021	0.896394
C	-0.376892	-2.346327	1.984179
C	0.772298	-2.135600	2.852354
C	0.980474	-0.890430	3.442979
C	2.318705	-0.324735	3.500016
C	2.206789	1.111071	3.284618
C	3.178517	1.780462	2.541135
C	2.783546	2.797769	1.577552
C	3.672806	2.699108	0.429274
C	3.176014	2.912925	-0.856284
C	3.594047	2.046087	-1.948988
C	2.444921	1.831747	-2.813574
C	2.237373	0.586540	-3.404289
C	2.400806	-1.735171	-3.059963
C	3.168989	-0.502082	-3.157413
C	4.271503	-0.298844	-2.326450
C	4.655360	-1.320951	-1.366144
C	3.920516	-2.503934	-1.274988
C	2.769927	-2.713478	-2.136841
C	5.111455	-0.653168	-0.156565
C	4.818703	-1.197151	1.093879
C	4.056891	-2.433049	1.190116
C	3.614792	-3.071994	0.030817
C	4.408014	-0.329777	2.187421
C	4.301684	1.046863	1.983513
C	4.607325	1.614879	0.677743
C	5.006381	0.782341	-0.368906
C	4.488458	1.001960	-1.709602
C	3.395352	-1.030083	2.960830
C	3.177989	-2.330780	2.343934

C	1.892990	-2.872594	2.291470
C	1.431044	-3.536807	1.080880
C	2.275451	-3.632084	-0.025131
C	1.748917	-3.404548	-1.362914
O	-7.280007	-1.754805	1.279220
H	-4.191817	1.679977	1.826727
H	-5.256232	3.824731	2.458411
H	-5.442497	5.660628	0.791361
H	-4.567200	5.328424	-1.512985
H	-3.506977	3.176135	-2.136808
H	-8.592506	-4.053141	1.176651
H	-9.696720	-2.713781	0.780845
H	-9.638551	-4.161889	-0.277171
H	-6.750189	-1.050202	-1.715495
H	-5.665717	-2.364146	-1.318784
H	-5.794178	0.310458	0.194220
H	-4.708628	-1.010247	0.584050
H	-3.686050	-0.834952	-1.715366
H	-4.715682	0.544281	-2.065227

PCBM chloroform (*singlet*) B3LYP-6-31G* E= -2902.729043 u.a.

	X	Y	Z
C	-4.276108	2.480435	1.096571
C	-3.786131	2.284237	-0.198496
C	-3.900290	3.317406	-1.135232
C	-4.493730	4.529000	-0.783569
C	-4.980206	4.718966	0.511873
C	-4.871679	3.691778	1.450500
C	-3.201130	0.962500	-0.616257
C	-4.210068	0.006358	-1.250401
C	-5.232449	-0.519016	-0.240954
C	-6.202695	-1.508518	-0.880588
C	-7.216578	-2.048794	0.104362
O	-8.055422	-2.919047	-0.493641
C	-9.062345	-3.496607	0.357089
C	-1.801876	0.986138	-1.183978
C	-2.138868	0.358963	0.266954
C	-1.470714	1.022313	1.423059
C	-0.738651	2.191923	1.310604
C	-0.430738	2.766490	-0.014436
C	-0.868170	2.149922	-1.174776
C	-1.831588	-1.092982	0.424300
C	-1.423733	-1.902611	-0.623718
C	-1.112869	-1.327743	-1.948924
C	-1.222604	0.034716	-2.175413
C	-0.180288	0.717474	-2.905386
C	0.036521	2.015208	-2.291510
C	-1.264084	-1.296181	1.737249
C	-1.045303	0.001747	2.349919
C	0.051072	0.202333	3.191980
C	0.802833	1.432795	3.094427
C	0.419383	2.400181	2.159738
C	1.435045	3.095766	1.386621
C	0.911441	3.315701	0.048301

C	1.769960	3.231422	-1.052569
C	1.320760	2.563537	-2.253041
C	0.895064	0.016792	-3.456137
C	0.994549	-1.410003	-3.245296
C	0.013313	-2.063484	-2.493379
C	0.402229	-3.082428	-1.532669
C	-0.480048	-2.978878	-0.382011
C	0.026636	-3.208118	0.901004
C	-0.375583	-2.344111	1.988048
C	0.774266	-2.132384	2.855106
C	0.982983	-0.886568	3.444185
C	2.321300	-0.320929	3.499611
C	2.209361	1.114642	3.282583
C	3.180661	1.783100	2.537668
C	2.785110	2.799310	1.573177
C	3.673528	2.699220	0.424408
C	3.175829	2.911589	-0.861053
C	3.593003	2.043406	-1.953028
C	2.443274	1.828221	-2.816587
C	2.235171	0.582324	-3.405644
C	2.398648	-1.738952	-3.058684
C	3.166880	-0.506066	-3.158121
C	4.270043	-0.301977	-2.328216
C	4.654486	-1.322992	-1.366990
C	3.919597	-2.505802	-1.273964
C	2.768393	-2.716277	-2.134765
C	5.111485	-0.653848	-0.158514
C	4.819586	-1.196346	1.092778
C	4.057711	-2.432047	1.190974
C	3.614725	-3.072297	0.032725
C	4.409715	-0.327655	2.185581
C	4.303360	1.048754	1.980123
C	4.608157	1.615225	0.673489
C	5.006399	0.781421	-0.372459
C	4.487509	0.999499	-1.713030
C	3.397531	-1.026974	2.960500
C	3.179597	-2.328331	2.345233
C	1.894520	-2.870105	2.294302
C	1.431654	-3.535727	1.084842
C	2.275309	-3.632328	-0.021644
C	1.747874	-3.406335	-1.359321
O	-7.285216	-1.754190	1.280898
H	-4.184875	1.685632	1.830308
H	-5.246980	3.832264	2.459935
H	-5.438969	5.663809	0.788493
H	-4.572037	5.325093	-1.518325
H	-3.514303	3.171064	-2.140266
H	-8.598254	-4.054274	1.174273
H	-9.704131	-2.716301	0.773466
H	-9.638196	-4.164332	-0.283113
H	-6.750893	-1.046631	-1.711797
H	-5.667519	-2.362171	-1.316339
H	-5.793773	0.312022	0.197313
H	-4.708824	-1.010293	0.587309
H	-3.687494	-0.836778	-1.711349
H	-4.716339	0.542399	-2.062692

C₆₀ (singlet) B3LYP-6-31G* E= -2286.490447 u.a.

	X	Y	Z
C	1.200991	3.341882	-0.060487
C	1.140084	3.097584	1.311336
C	2.064756	2.156155	1.924163
C	3.012398	1.498131	1.140043
C	3.075534	1.752621	-0.291027
C	2.189044	2.655458	-0.878561
C	1.345589	1.429447	2.959379
C	1.603776	0.074863	3.167704
C	2.591964	-0.611708	2.349739
C	3.281437	0.084952	1.357283
C	0.504216	-0.845829	3.412147
C	-0.808435	-0.373761	3.437670
C	-1.077487	1.039206	3.220088
C	-0.023260	1.921788	2.986372
C	-1.868674	-1.137112	2.797542
C	-1.572784	-2.340955	2.158717
C	-0.204079	-2.833049	2.131940
C	0.812551	-2.101392	2.745322
C	2.102842	-1.956784	2.088633
C	-2.304167	1.149410	2.445558
C	-2.793474	-0.195796	2.184364
C	-3.384509	-0.497190	0.957569
C	-3.075982	-1.752938	0.290768
C	-2.189066	-2.655591	0.878876
C	-1.200890	-3.342318	0.061206
C	0.025785	-3.452389	0.835608
C	1.263006	-3.313990	0.206031
C	2.322972	-2.549724	0.845676
C	-2.425955	2.138036	1.469296
C	-1.326553	3.059011	1.225541
C	-0.150371	2.952931	1.967899
C	3.510920	-0.533612	0.060539
C	3.041947	-1.823486	-0.189689
C	-3.041957	1.823684	0.189286
C	-3.511237	0.533684	-0.061250
C	-3.281809	-0.085116	-1.357881
C	-3.012488	-1.498076	-1.140234
C	-2.064568	-2.156190	-1.923939
C	-1.139798	-3.097478	-1.310588
C	0.150157	-2.953204	-1.967199
C	1.326392	-3.058710	-1.224774
C	2.426154	-2.137917	-1.469643
C	3.384445	0.497176	-0.958329
C	-0.025775	3.452442	-0.834948
C	-1.263053	3.313949	-0.205641
C	-2.323162	2.550426	-0.845807
C	-2.102478	1.956932	-2.088572
C	-2.591887	0.611638	-2.350189
C	-1.604058	-0.074955	-3.167856
C	-1.346041	-1.430022	-2.959404
C	0.023178	-1.922333	-2.986190
C	1.077549	-1.039573	-3.220301
C	2.304760	-1.149705	-2.446664

C	2.793144	0.195787	-2.185052
C	1.573219	2.341249	-2.158598
C	1.869293	1.137606	-2.798503
C	0.808284	0.374021	-3.437476
C	-0.504018	0.845911	-3.411718
C	-0.812529	2.101653	-2.744807
C	0.204156	2.833273	-2.130970

C₆₀ xylene (*singlet*) B3LYP-6-31G* E= -2286.490889 u.a.

	X	Y	Z
C	3.192563	-0.399102	-1.504282
C	3.066355	-1.600711	-0.807353
C	2.090796	-2.591252	-1.236266
C	1.282173	-2.339497	-2.344509
C	1.414027	-1.086142	-3.071462
C	2.349040	-0.136451	-2.660193
C	1.523481	-3.208110	-0.046954
C	0.170948	-3.547492	-0.015050
C	-0.672588	-3.285072	-1.171157
C	-0.128654	-2.693699	-2.311240
C	-0.615180	-3.292166	1.182286
C	-0.016326	-2.707792	2.298264
C	1.394387	-2.353528	2.264838
C	2.148097	-2.598474	1.117078
C	-0.720926	-1.677914	3.046281
C	-1.995252	-1.274777	2.647416
C	-2.619997	-1.884337	1.483428
C	-1.944384	-2.871625	0.766256
C	-1.979928	-2.867331	-0.688274
C	1.561801	-1.104773	2.992356
C	0.254437	-0.687115	3.475177
C	-0.084824	0.665694	3.487494
C	-1.414038	1.086165	3.071472
C	-2.348964	0.136487	2.660157
C	-3.192585	0.399112	1.504260
C	-3.359952	-0.849761	0.776871
C	-3.393808	-0.845430	-0.617490
C	-2.689286	-1.875526	-1.365517
C	2.475863	-0.152425	2.541850
C	3.262066	-0.407864	1.344584
C	3.101705	-1.605131	0.647207
C	-0.868626	-1.659210	-3.017656
C	-2.122036	-1.258833	-2.554872
C	2.121961	1.258783	2.554898
C	0.868641	1.659203	3.017741
C	0.128607	2.693678	2.311304
C	-1.282145	2.339557	2.344565
C	-2.090754	2.591364	1.236218
C	-3.066258	1.600702	0.807245
C	-3.101649	1.605174	-0.647206
C	-3.262095	0.407832	-1.344576
C	-2.475829	0.152385	-2.541828
C	0.084828	-0.665748	-3.487631
C	3.359961	0.849882	-0.776889

C	3.393775	0.845533	0.617471
C	2.689296	1.875494	1.365516
C	1.979863	2.867257	0.688189
C	0.672493	3.285103	1.171119
C	-0.170929	3.547437	0.015095
C	-1.523436	3.208063	0.046990
C	-2.147930	2.598390	-1.117119
C	-1.394442	2.353546	-2.264831
C	-1.561776	1.104769	-2.992333
C	-0.254434	0.687117	-3.475157
C	1.995174	1.274723	-2.647361
C	0.720879	1.677868	-3.046251
C	0.016372	2.707919	-2.298256
C	0.615099	3.292137	-1.182361
C	1.944330	2.871612	-0.766193
C	2.620014	1.884313	-1.483358

C₆₀ toluene (*singlet*) B3LYP-6-31G* E= -2286.490883 u.a.

	X	Y	Z
C	3.129876	-0.672289	-1.538339
C	2.844194	-1.904046	-0.949563
C	1.754213	-2.719971	-1.462440
C	0.995332	-2.270712	-2.543049
C	1.293512	-0.985927	-3.157179
C	2.338240	-0.203616	-2.665420
C	1.101043	-3.360516	-0.331119
C	-0.284025	-3.525110	-0.327152
C	-1.075704	-3.056646	-1.454444
C	-0.449465	-2.442577	-2.538937
C	-1.042732	-3.276694	0.889176
C	-0.385023	-2.873764	2.051335
C	1.059678	-2.701799	2.047062
C	1.787070	-2.940121	0.881067
C	-0.959411	-1.831350	2.888066
C	-2.167734	-1.234776	2.528080
C	-2.853866	-1.655089	1.315936
C	-2.303094	-2.654404	0.513727
C	-2.323541	-2.518487	-0.934736
C	1.378291	-1.553217	2.881295
C	0.130419	-1.015129	3.400935
C	-0.033140	0.363732	3.532640
C	-1.293520	0.985950	3.157191
C	-2.338159	0.203645	2.665387
C	-3.129897	0.672303	1.538318
C	-3.448476	-0.476401	0.704189
C	-3.467847	-0.345930	-0.684339
C	-2.893552	-1.388533	-1.521085
C	2.411001	-0.690266	2.514879
C	3.169778	-0.938819	1.298621
C	2.864446	-2.040059	0.498920
C	-1.044104	-1.263988	-3.150565
C	-2.240474	-0.748135	-2.652467
C	2.240393	0.748092	2.652489
C	1.044117	1.263971	3.150649

C	0.449415	2.442556	2.538999
C	-0.995297	2.270762	2.543110
C	-1.754156	2.720079	1.462402
C	-2.844098	1.904033	0.949454
C	-2.864386	2.040094	-0.498915
C	-3.169810	0.938789	-1.298616
C	-2.410973	0.690220	-2.514860
C	0.033138	-0.363775	-3.532782
C	3.448501	0.476520	-0.704196
C	3.467828	0.346037	0.684329
C	2.893558	1.388501	1.521082
C	2.323468	2.518429	0.934645
C	1.075614	3.056692	1.454408
C	0.284038	3.525050	0.327192
C	-1.101004	3.360459	0.331151
C	-1.786915	2.940021	-0.881116
C	-1.059731	2.701823	-2.047054
C	-1.378267	1.553208	-2.881273
C	-0.130416	1.015128	-3.400915
C	2.167648	1.234727	-2.528029
C	0.959357	1.831308	-2.888039
C	0.385084	2.873883	-2.051318
C	1.042650	3.276684	-0.889253
C	2.303039	2.654393	-0.513666
C	2.853878	1.655057	-1.315868

C₆₀ chloroform (*singlet*) B3LYP-6-31G* E= -2286.49117 u.a.

	X	Y	Z
C	0.159527	1.563144	3.185137
C	-0.693362	2.427065	2.498405
C	-2.030749	1.988397	2.130073
C	-2.459860	0.703786	2.463414
C	-1.570114	-0.197420	3.179636
C	-0.288056	0.223248	3.532980
C	-2.340830	2.542176	0.820825
C	-3.066866	1.788115	-0.101014
C	-3.514595	0.448127	0.246697
C	-3.217379	-0.082577	1.501821
C	-2.678936	1.782775	-1.503224
C	-1.580490	2.531433	-1.925702
C	-0.822871	3.317564	-0.964084
C	-1.195031	3.323035	0.380118
C	-0.642500	1.969066	-2.885181
C	-0.841608	0.681259	-3.382602
C	-1.987294	-0.099615	-2.941845
C	-2.886739	0.439528	-2.022174
C	-3.403467	-0.385343	-0.940661
C	0.583382	3.241407	-1.329418
C	0.694824	2.407829	-2.516618
C	1.777751	1.540733	-2.660756
C	1.570123	0.197406	-3.179646
C	0.288107	-0.223239	-3.532896
C	-0.159517	-1.563183	-3.185120
C	-1.565724	-1.486781	-2.819806

C	-2.061009	-2.277538	-1.783050
C	-2.999131	-1.715128	-0.823581
C	1.559413	3.173266	-0.335333
C	1.171369	3.178897	1.066885
C	-0.176804	3.251906	1.416942
C	-2.796038	-1.469810	1.623896
C	-2.689185	-2.268829	0.485640
C	2.689122	2.268820	-0.485717
C	2.796054	1.469878	-1.623948
C	3.217350	0.082595	-1.501894
C	2.459934	-0.703764	-2.463431
C	2.030849	-1.988447	-2.129992
C	0.693367	-2.427061	-2.498250
C	0.176877	-3.251873	-1.416881
C	-1.171392	-3.178893	-1.066902
C	-1.559421	-3.173193	0.335331
C	-1.777860	-1.540774	2.660860
C	1.565836	1.486705	2.819837
C	2.061090	2.277453	1.783055
C	2.999096	1.715140	0.823577
C	3.403337	0.385280	0.940669
C	3.514565	-0.448227	-0.246727
C	3.066824	-1.788042	0.100996
C	2.340801	-2.542089	-0.820808
C	1.195015	-3.322939	-0.379979
C	0.822875	-3.317601	0.964034
C	-0.583367	-3.241357	1.329403
C	-0.694824	-2.407795	2.516587
C	0.841555	-0.681264	3.382489
C	0.642450	-1.969053	2.885109
C	1.580622	-2.531454	1.925722
C	2.678865	-1.782868	1.503227
C	2.886728	-0.439535	2.022079
C	1.987309	0.099659	2.941797

OPCBMMB (*singlet*) B3LYP-6-31G* E= -5003.821242 u.a.

	X	Y	Z
C	4.223059	0.669651	-0.905037
C	-2.787948	-0.665432	-0.981064
C	4.042869	1.454885	0.510350
C	-3.287781	0.002302	0.280894
C	3.513254	0.633843	1.634413
C	-2.821941	1.478535	0.287798
C	3.336908	-0.738829	1.556863
C	-2.473754	2.173409	-0.855358
C	3.502589	-1.450052	0.272961
C	-2.307869	1.470050	-2.145475
C	3.838612	-0.768135	-0.883844
C	-2.464096	0.097785	-2.196373
C	3.488744	1.252545	-2.062265
C	-2.136046	-1.864378	-1.014097
C	2.807394	2.456663	-2.002469
C	-1.793554	-2.686022	0.213133
C	2.636442	3.168454	-0.720985

C	-1.800679	-1.747650	1.436005
C	3.159783	2.655984	0.459209
C	-2.471992	-0.549043	1.468588
C	2.568620	1.431928	2.375097
C	-2.159748	1.785217	1.518677
C	1.517485	0.836366	3.081090
C	-1.221228	2.826252	1.601334
C	1.346073	-0.596733	3.022511
C	-0.873916	3.562955	0.408166
C	2.234001	-1.363368	2.261781
C	-1.487407	3.227945	-0.804394
C	1.721954	-2.446290	1.438466
C	-0.702856	3.181420	-2.030518
C	2.498265	-2.497075	0.223195
C	-1.216884	2.102868	-2.861271
C	1.859814	-2.818304	-0.980964
C	-0.335139	1.332261	-3.627273
C	2.198521	-2.089172	-2.182682
C	-0.515233	-0.107585	-3.697529
C	3.151344	-1.070680	-2.117878
C	-1.566807	-0.709177	-2.997171
C	2.939721	0.166941	-2.845770
C	-1.346475	-1.936740	-2.256016
C	1.788757	0.336136	-3.616109
C	-0.100960	-2.532942	-2.260086
C	0.795518	-0.725799	-3.689942
C	0.995959	-1.915487	-2.980899
C	1.093150	1.605843	-3.579680
C	0.440443	-3.100784	-1.003902
C	1.586906	2.634749	-2.774023
C	-0.296542	-3.064969	0.160549
C	0.667540	3.439589	-1.988534
C	0.346011	-2.706489	1.390970
C	1.314497	3.766936	-0.726189
C	-0.577631	-1.902975	2.176134
C	0.555147	3.836055	0.444996
C	-0.082926	-0.874256	2.985355
C	1.084471	3.270178	1.667550
C	-0.786684	0.384668	3.022555
C	-0.010577	2.644260	2.387847
C	0.200118	1.451744	3.079184
C	2.348421	2.670935	1.654022
C	-1.936764	0.540673	2.240142
C	5.381766	1.281863	-0.158558
C	6.347594	0.312867	0.471151
C	6.964711	-0.662385	-0.319619
C	7.878432	-1.554476	0.239003
C	8.186866	-1.477877	1.598331
C	7.582061	-0.502350	2.391652
C	6.665670	0.387296	1.830654
H	6.183331	1.134473	2.453107
H	7.816587	-0.436535	3.450100
H	8.893165	-2.176874	2.036973
H	8.339228	-2.314741	-0.384555
H	6.711111	-0.734211	-1.373558
C	6.032195	2.529767	-0.751975
C	6.589524	3.464753	0.322685
C	7.190526	4.731987	-0.279585
C	7.734068	5.671350	0.776459
O	7.705552	5.480063	1.972838

O	8.266427	6.777370	0.209995
C	8.806835	7.736033	1.132928
H	8.029443	8.094985	1.812567
H	9.612539	7.289918	1.721957
H	9.186811	8.552395	0.518385
H	8.005316	4.496169	-0.976613
H	6.446661	5.282066	-0.871015
H	7.348697	2.949274	0.919171
H	5.788956	3.741966	1.017969
H	5.305535	3.070234	-1.366226
H	6.832813	2.203546	-1.428068
C	-4.838964	-0.152291	0.433345
H	-5.135401	0.296249	1.385833
H	-5.070117	-1.218533	0.471939
C	-5.539715	0.534962	-0.709555
C	-5.823088	-0.131926	-1.910927
C	-6.311655	0.592460	-3.005075
C	-6.468169	1.974654	-2.929081
C	-6.164676	2.649590	-1.744414
C	-5.748677	1.912875	-0.633633
O	-5.580982	-1.483608	-1.943793
H	-6.538935	0.085946	-3.935955
H	-6.798184	2.545641	-3.790777
O	-6.247102	4.015541	-1.747317
H	-5.512153	2.415463	0.295621
C	-5.229437	-2.056988	-3.204386
C	-5.439179	4.691363	-0.778329
C	-5.130959	6.099459	-1.257536
C	-4.734938	-3.475805	-2.969905
C	-4.050080	6.737747	-0.378815
H	-4.778908	6.042509	-2.295248
H	-6.043180	6.709445	-1.262037
H	-5.953158	4.711697	0.193237
H	-4.499571	4.140536	-0.647327
H	-4.450202	-1.441772	-3.675523
H	-6.100825	-2.069919	-3.874468
C	-4.217139	-4.111705	-4.266740
H	-3.945672	-3.444099	-2.213889
H	-5.554482	-4.075121	-2.551980
H	-3.300824	-3.594000	-4.580165
H	-4.950880	-3.940384	-5.067146
C	-3.966284	-5.624556	-4.165945
C	-3.706682	8.177282	-0.777462
C	-2.477259	8.746339	-0.038557
H	-3.534345	8.224734	-1.862451
H	-4.584366	8.808348	-0.586386
C	-1.154750	8.629366	-0.812183
H	-1.234760	9.222386	-1.735510
H	-0.357786	9.100835	-0.219517
C	-0.712849	7.208594	-1.182787
H	-4.372004	6.728517	0.673270
H	-3.148088	6.114231	-0.421212
H	-2.377542	8.248195	0.936646
H	-2.642534	9.808347	0.182341
C	-2.855330	-6.054135	-3.196054
H	-3.056710	-5.642439	-2.198476
H	-2.897482	-7.145662	-3.078655
C	-1.440217	-5.666458	-3.639384
H	-3.727094	-6.010212	-5.166664
H	-4.905424	-6.110514	-3.867510

H	-1.468372	6.736186	-1.823799
C	0.635929	7.197645	-1.906785
H	0.598293	7.813208	-2.814140
H	0.925296	6.184429	-2.200474
H	1.429932	7.600937	-1.266339
C	-0.354949	-6.124978	-2.658091
C	1.066870	-5.870165	-3.164329
H	-1.243990	-6.105781	-4.628657
H	-1.365044	-4.579167	-3.766233
H	-0.494939	-5.604203	-1.701791
H	-0.483336	-7.196214	-2.447447
H	1.816909	-6.168525	-2.423350
H	1.224511	-4.809371	-3.387464
H	1.262732	-6.433377	-4.084725
H	-0.649917	6.590110	-0.276940
C	-2.712586	-3.940885	0.381831
H	-2.625830	-4.533659	-0.532746
H	-3.745308	-3.595753	0.463472
C	-2.309121	-4.769387	1.572222
C	-2.828563	-4.493048	2.847828
C	-2.353072	-5.194378	3.959650
C	-1.356775	-6.157560	3.807868
C	-0.837751	-6.446634	2.544514
C	-1.328905	-5.753230	1.434777
O	-3.793493	-3.523172	2.907178
H	-2.747275	-4.988114	4.948130
H	-0.970487	-6.697185	4.666260
O	0.104711	-7.440994	2.469540
H	-0.944162	-5.960777	0.443109
C	-4.057906	-2.890533	4.158871
C	1.150528	-7.313197	1.499986
C	2.169402	-6.244428	1.884726
C	-4.914467	-1.672009	3.858393
C	3.318785	-6.147392	0.874438
H	1.666020	-5.274433	1.973688
H	2.560606	-6.489317	2.880793
H	1.622023	-8.300223	1.477504
H	0.741541	-7.126923	0.498337
H	-3.108402	-2.594597	4.627292
H	-4.570888	-3.586546	4.838461
C	-5.261249	-0.825137	5.088470
H	-4.363085	-1.069411	3.132505
H	-5.835150	-1.998089	3.358297
H	-4.359143	-0.661732	5.695996
H	-5.967386	-1.373580	5.725237
C	-5.853743	0.540066	4.693718
C	4.459528	-5.241813	1.360110
C	5.732711	-5.237366	0.494915
H	4.091639	-4.215003	1.474677
H	4.738352	-5.575434	2.369524
C	5.711838	-4.394761	-0.790341
H	5.472202	-3.354611	-0.535627
H	6.737306	-4.375460	-1.189059
C	4.776961	-4.869329	-1.909530
H	3.723695	-7.152627	0.683437
H	2.923400	-5.789650	-0.082421
H	6.000264	-6.274977	0.244203
H	6.553810	-4.855379	1.116357
C	-4.785794	1.517745	4.177620
H	-4.210885	1.908436	5.029357

H	-4.063755	0.968743	3.565072
C	-5.326103	2.684418	3.343782
H	-6.377969	0.979569	5.550701
H	-6.616454	0.384311	3.916220
H	3.734655	-4.706113	-1.619515
C	5.038502	-4.146444	-3.233193
H	4.939357	-3.061739	-3.112951
H	4.328283	-4.458710	-4.007297
H	6.051375	-4.350770	-3.601914
C	-6.200251	3.678727	4.113791
C	-6.673025	4.840466	3.236065
H	-4.478127	3.224382	2.898753
H	-5.907460	2.281531	2.501092
H	-7.071729	3.159350	4.533531
H	-5.632698	4.068627	4.970474
H	-5.819592	5.393358	2.823165
H	-7.289750	5.549884	3.798887
H	-7.270733	4.476460	2.391084
H	4.893485	-5.953018	-2.052684

OPCBMMB xylene (*singlet*) B3LYP-6-31G* E= -5003.828565 u.a.

	X	Y	Z
C	4.214666	0.735263	-0.903936
C	-2.772689	-0.722781	-0.988418
C	4.017592	1.524640	0.507125
C	-3.286838	-0.057169	0.268989
C	3.499285	0.700170	1.633836
C	-2.846563	1.426988	0.269192
C	3.347139	-0.675768	1.563248
C	-2.508005	2.121984	-0.876745
C	3.528263	-1.390663	0.283468
C	-2.326790	1.414873	-2.162822
C	3.855087	-0.708777	-0.875973
C	-2.458735	0.039770	-2.206776
C	3.472475	1.299038	-2.065415
C	-2.099756	-1.910333	-1.013840
C	2.770182	2.491399	-2.013648
C	-1.745681	-2.719602	0.218366
C	2.583859	3.206624	-0.736328
C	-1.771818	-1.774951	1.436209
C	3.113385	2.709409	0.447571
C	-2.464048	-0.588159	1.461245
C	2.539075	1.485262	2.368357
C	-2.192687	1.751457	1.499906
C	1.496923	0.875120	3.075306
C	-1.272756	2.809143	1.579208
C	1.350675	-0.561061	3.023849
C	-0.935533	3.545633	0.382954
C	2.253569	-1.315843	2.268857
C	-1.540311	3.193739	-0.829158
C	1.762547	-2.411909	1.450138
C	-0.752194	3.154560	-2.053217
C	2.542467	-2.455316	0.236942
C	-1.245346	2.062945	-2.879553

C	1.912470	-2.794106	-0.966818
C	-0.348500	1.303836	-3.639547
C	2.241199	-2.065261	-2.171506
C	-0.503266	-0.139289	-3.702661
C	3.175887	-1.029868	-2.109802
C	-1.545688	-0.755577	-3.001331
C	2.944301	0.200051	-2.844545
C	-1.305838	-1.975200	-2.253420
C	1.792475	0.345057	-3.618598
C	-0.050103	-2.549428	-2.251571
C	0.818083	-0.734454	-3.689045
C	1.037572	-1.916715	-2.973216
C	1.074716	1.602578	-3.590342
C	0.498295	-3.101368	-0.991432
C	1.548518	2.643969	-2.788695
C	-0.242039	-3.072779	0.171060
C	0.613402	3.436767	-2.009562
C	0.391424	-2.696460	1.400912
C	1.251690	3.781833	-0.747524
C	-0.547875	-1.905003	2.179765
C	0.488404	3.843835	0.421586
C	-0.073160	-0.863679	2.984835
C	1.024739	3.293685	1.648214
C	-0.798977	0.382921	3.014037
C	-0.060929	2.652459	2.369341
C	0.168951	1.467306	3.067279
C	2.298980	2.716410	1.640385
C	-1.949692	0.514741	2.228172
C	5.360745	1.371825	-0.158279
C	6.341863	0.422508	0.478052
C	6.980988	-0.542060	-0.308727
C	7.909088	-1.415967	0.255559
C	8.209788	-1.331739	1.616574
C	7.582922	-0.366385	2.405779
C	6.652343	0.505268	1.838993
H	6.153841	1.244270	2.458450
H	7.811327	-0.294561	3.465131
H	8.927206	-2.016483	2.059508
H	8.387917	-2.167578	-0.364889
H	6.734765	-0.619292	-1.363989
C	5.990440	2.627705	-0.757359
C	6.526580	3.579489	0.313483
C	7.108392	4.851550	-0.297277
C	7.631818	5.812093	0.748909
O	7.604909	5.633033	1.949132
O	8.143275	6.920671	0.173276
C	8.666776	7.904168	1.082725
H	7.883491	8.255443	1.759102
H	9.485288	7.483072	1.671951
H	9.026325	8.720087	0.456055
H	7.929867	4.622254	-0.988315
H	6.357145	5.382437	-0.896565
H	7.291863	3.080132	0.915981
H	5.717246	3.847681	1.002176
H	5.256705	3.151665	-1.377276
H	6.799290	2.312433	-1.428402
C	-4.835497	-0.237706	0.420252
H	-5.141013	0.206573	1.371672
H	-5.048868	-1.307508	0.459959
C	-5.546419	0.437047	-0.723970

C	-5.815943	-0.233217	-1.927184
C	-6.312874	0.484435	-3.022246
C	-6.493593	1.864093	-2.944440
C	-6.207077	2.541836	-1.756928
C	-5.780542	1.810882	-0.646219
O	-5.554803	-1.580966	-1.960872
H	-6.528031	-0.024107	-3.954870
H	-6.830499	2.429126	-3.807595
O	-6.316230	3.906867	-1.755374
H	-5.555863	2.315760	0.284643
C	-5.183549	-2.147703	-3.221341
C	-5.522622	4.594063	-0.779082
C	-5.247517	6.013014	-1.245409
C	-4.668856	-3.558567	-2.983585
C	-4.184586	6.668750	-0.357545
H	-4.890167	5.974782	-2.282233
H	-6.173719	6.601617	-1.245916
H	-6.037153	4.592581	0.191842
H	-4.571139	4.062952	-0.654586
H	-4.410283	-1.519080	-3.683724
H	-6.049082	-2.172557	-3.897740
C	-4.129253	-4.184398	-4.276488
H	-3.886956	-3.515915	-2.220298
H	-5.482691	-4.171988	-2.575069
H	-3.218042	-3.652264	-4.580446
H	-4.858287	-4.023286	-5.083060
C	-3.856601	-5.693350	-4.173947
C	-3.869977	8.117231	-0.747597
C	-2.657850	8.709409	0.001578
H	-3.691738	8.173372	-1.831217
H	-4.762227	8.728121	-0.558607
C	-1.327206	8.620067	-0.761840
H	-1.411896	9.212496	-1.685126
H	-0.544395	9.106088	-0.162028
C	-0.854738	7.208741	-1.130591
H	-4.511666	6.647015	0.692536
H	-3.269761	6.064320	-0.399529
H	-2.555817	8.211822	0.976847
H	-2.846119	9.767636	0.222279
C	-2.747709	-6.106220	-3.194467
H	-2.960623	-5.692409	-2.200132
H	-2.777732	-7.197685	-3.072847
C	-1.334077	-5.704093	-3.629486
H	-3.602976	-6.075095	-5.172604
H	-4.790964	-6.193033	-3.883421
H	-1.595251	6.723258	-1.779194
C	0.500617	7.224113	-1.842217
H	0.458631	7.837728	-2.750767
H	0.812896	6.216339	-2.131638
H	1.280387	7.644150	-1.194967
C	-0.251645	-6.142787	-2.636197
C	1.171409	-5.873751	-3.131498
H	-1.124693	-6.147895	-4.614039
H	-1.271538	-4.616756	-3.762922
H	-0.406380	-5.617713	-1.684611
H	-0.368479	-7.214100	-2.419668
H	1.918003	-6.158219	-2.381537
H	1.318102	-4.812395	-3.359879
H	1.382211	-6.440363	-4.046550
H	-0.788341	6.590106	-0.225093

C	-2.643769	-3.989203	0.391406
H	-2.548017	-4.583793	-0.520954
H	-3.682020	-3.661182	0.472591
C	-2.225137	-4.805983	1.584923
C	-2.744425	-4.530902	2.861574
C	-2.251447	-5.216521	3.975934
C	-1.239048	-6.163714	3.825516
C	-0.722311	-6.452852	2.561191
C	-1.230061	-5.775136	1.449139
O	-3.727017	-3.580026	2.919643
H	-2.643805	-5.010126	4.965038
H	-0.840056	-6.689283	4.687002
O	0.235696	-7.434047	2.485256
H	-0.845917	-5.982705	0.457265
C	-3.992893	-2.938156	4.169079
C	1.282652	-7.285233	1.516467
C	2.282518	-6.200835	1.905987
C	-4.877914	-1.741560	3.863830
C	3.428161	-6.081198	0.893706
H	1.762966	-5.239624	1.998512
H	2.680184	-6.442825	2.900245
H	1.770470	-8.264052	1.491351
H	0.870843	-7.102253	0.515874
H	-3.044788	-2.618025	4.623259
H	-4.484189	-3.637557	4.860194
C	-5.228133	-0.889339	5.089283
H	-4.347521	-1.135158	3.125487
H	-5.797705	-2.091869	3.378697
H	-4.321770	-0.697633	5.681848
H	-5.911739	-1.448069	5.741294
C	-5.859761	0.456415	4.688579
C	4.554595	-5.158111	1.379452
C	5.826387	-5.132395	0.512619
H	4.170575	-4.137334	1.495518
H	4.840375	-5.488624	2.387961
C	5.788339	-4.296233	-0.776563
H	5.524790	-3.260597	-0.527266
H	6.813714	-4.255436	-1.173601
C	4.866341	-4.797141	-1.895077
H	3.849026	-7.078946	0.698850
H	3.024029	-5.726895	-0.060667
H	6.113603	-6.165777	0.266109
H	6.640391	-4.731788	1.131720
C	-4.824316	1.454026	4.145431
H	-4.241875	1.863259	4.983231
H	-4.102402	0.916706	3.522461
C	-5.406555	2.602756	3.314731
H	-6.380827	0.892683	5.549109
H	-6.630232	0.273773	3.924750
H	3.820025	-4.654270	-1.608879
C	5.116096	-4.076703	-3.222462
H	4.992780	-2.993742	-3.108716
H	4.415162	-4.409268	-3.996755
H	6.134483	-4.260982	-3.586648
C	-6.288695	3.581504	4.095481
C	-6.803753	4.727368	3.220617
H	-4.579573	3.159434	2.850841
H	-5.994467	2.181713	2.485600
H	-7.140136	3.044497	4.533613
H	-5.714402	3.988874	4.939439

H	-5.970626	5.298193	2.790966
H	-7.427603	5.424588	3.790954
H	-7.406653	4.344927	2.387448
H	5.006212	-5.878959	-2.031431

OPCBMMB toluene (*singlet*) B3LYP-6-31G* E= -5003.828118 u.a.

	X	Y	Z
C	4.205237	0.772419	-0.913300
C	-2.768484	-0.751480	-0.971442
C	4.006004	1.560264	0.498428
C	-3.283921	-0.090426	0.288142
C	3.499733	0.731196	1.627205
C	-2.857597	1.397769	0.286474
C	3.360252	-0.646120	1.557426
C	-2.529971	2.095630	-0.860946
C	3.543273	-1.359528	0.277118
C	-2.347040	1.390035	-2.147642
C	3.859341	-0.674903	-0.883696
C	-2.466184	0.013744	-2.190960
C	3.453345	1.328928	-2.072033
C	-2.084547	-1.932902	-0.999312
C	2.740043	2.514618	-2.017816
C	-1.718159	-2.738047	0.232006
C	2.551816	3.228359	-0.739953
C	-1.748558	-1.793208	1.449565
C	3.090436	2.736390	0.442039
C	-2.451759	-0.613313	1.477187
C	2.534929	1.507356	2.365204
C	-2.202348	1.728745	1.514625
C	1.501224	0.887589	3.076183
C	-1.292132	2.795054	1.590217
C	1.368312	-0.549894	3.025518
C	-0.966369	3.534352	0.392541
C	2.275425	-1.296304	2.267291
C	-1.572313	3.176478	-0.817225
C	1.791702	-2.397140	1.450641
C	-0.788534	3.144541	-2.044288
C	2.567417	-2.433453	0.234489
C	-1.274485	2.048161	-2.868577
C	1.936123	-2.778450	-0.966800
C	-0.373394	1.297339	-3.631821
C	2.253440	-2.046881	-2.172889
C	-0.514788	-0.147225	-3.694123
C	3.178567	-1.002701	-2.114894
C	-1.548718	-0.773218	-2.988856
C	2.932607	0.224834	-2.848987
C	-1.294631	-1.990453	-2.241707
C	1.776583	0.358782	-3.618755
C	-0.033515	-2.552698	-2.244333
C	0.812157	-0.729893	-3.685365
C	1.045457	-1.909911	-2.970127
C	1.047107	1.609502	-3.587998
C	0.524795	-3.099007	-0.986030
C	1.514087	2.655498	-2.788308

C	-0.211382	-3.077059	0.179284
C	0.574493	3.439650	-2.005804
C	0.423141	-2.694503	1.406577
C	1.214250	3.791004	-0.746234
C	-0.520635	-1.911689	2.188675
C	0.454833	3.846018	0.425744
C	-0.052755	-0.865878	2.991887
C	1.000931	3.301251	1.650470
C	-0.790179	0.373763	3.023690
C	-0.075928	2.650002	2.375804
C	0.167724	1.467232	3.073073
C	2.280512	2.736015	1.637934
C	-1.945028	0.494535	2.242172
C	5.348018	1.419915	-0.172050
C	6.340438	0.480000	0.460549
C	6.985478	-0.478724	-0.328532
C	7.924200	-1.343529	0.232282
C	8.229691	-1.255899	1.592055
C	7.596844	-0.296233	2.383521
C	6.655623	0.566262	1.820236
H	6.152690	1.300754	2.441472
H	7.828896	-0.221807	3.441892
H	8.955434	-1.933581	2.032267
H	8.407684	-2.090709	-0.389896
H	6.735755	-0.558647	-1.382773
C	5.963593	2.681551	-0.773649
C	6.495498	3.638198	0.294883
C	7.063240	4.915241	-0.318643
C	7.583535	5.880382	0.724766
O	7.568658	5.699720	1.925003
O	8.079478	6.994523	0.146093
C	8.600364	7.982522	1.052104
H	7.819691	8.323652	1.736659
H	9.429606	7.570036	1.632420
H	8.944281	8.803477	0.423332
H	7.883477	4.692954	-1.013450
H	6.304644	5.439603	-0.914293
H	7.267777	3.145889	0.894287
H	5.686516	3.899221	0.986814
H	5.222699	3.198709	-1.390737
H	6.772540	2.373546	-1.447894
C	-4.830170	-0.285796	0.445715
H	-5.136175	0.155142	1.398470
H	-5.032915	-1.357619	0.485840
C	-5.552498	0.383117	-0.694515
C	-5.822978	-0.287230	-1.897431
C	-6.331763	0.428458	-2.988531
C	-6.523232	1.806574	-2.907159
C	-6.235643	2.484088	-1.719715
C	-5.797194	1.754677	-0.612991
O	-5.550675	-1.632699	-1.935377
H	-6.547683	-0.080081	-3.920973
H	-6.869235	2.370607	-3.767398
O	-6.354668	3.848017	-1.712880
H	-5.571227	2.259875	0.317637
C	-5.179093	-2.192949	-3.198622
C	-5.560833	4.534659	-0.736491
C	-5.299898	5.959394	-1.193299
C	-4.649814	-3.599352	-2.966400
C	-4.236851	6.616190	-0.306441

H	-4.948444	5.932281	-2.232516
H	-6.230670	6.540694	-1.183485
H	-6.069286	4.521095	0.237347
H	-4.604384	4.010282	-0.621768
H	-4.413873	-1.555873	-3.662796
H	-6.047046	-2.224721	-3.871580
C	-4.110685	-4.216941	-4.263402
H	-3.864782	-3.551057	-2.206576
H	-5.455910	-4.221436	-2.555611
H	-3.206106	-3.675458	-4.570657
H	-4.845284	-4.060738	-5.065860
C	-3.823489	-5.723534	-4.166017
C	-3.934133	8.069693	-0.687267
C	-2.721172	8.663656	0.059302
H	-3.762844	8.135424	-1.771458
H	-4.829066	8.673362	-0.488125
C	-1.394659	8.588445	-0.712855
H	-1.488516	9.187624	-1.630886
H	-0.611096	9.074359	-0.113929
C	-0.916073	7.182947	-1.095648
H	-4.558042	6.584407	0.745197
H	-3.318060	6.018508	-0.357725
H	-2.610240	8.159143	1.030025
H	-2.914529	9.718951	0.289395
C	-2.704676	-6.128158	-3.194395
H	-2.914608	-5.717600	-2.198061
H	-2.724269	-7.220016	-3.074203
C	-1.297581	-5.713091	-3.638268
H	-3.572531	-6.100739	-5.167064
H	-4.751387	-6.232457	-3.870859
H	-1.657407	6.698341	-1.743945
C	0.435159	7.211830	-1.814669
H	0.384721	7.833112	-2.717577
H	0.751193	6.208286	-2.114629
H	1.216330	7.630390	-1.168151
C	-0.204790	-6.143424	-2.652748
C	1.212542	-5.860305	-3.156574
H	-1.090813	-6.153813	-4.624759
H	-1.245570	-4.625069	-3.770674
H	-0.358290	-5.621281	-1.699410
H	-0.310332	-7.216078	-2.437143
H	1.966439	-6.139318	-2.411863
H	1.347962	-4.797150	-3.383692
H	1.422754	-6.423125	-4.074110
H	-0.840941	6.557538	-0.195529
C	-2.603440	-4.015868	0.410594
H	-2.507029	-4.611249	-0.501181
H	-3.644376	-3.697857	0.496998
C	-2.168936	-4.823616	1.604318
C	-2.682797	-4.543042	2.881543
C	-2.175505	-5.212669	3.999018
C	-1.154070	-6.150764	3.849841
C	-0.643209	-6.446263	2.584244
C	-1.165328	-5.783718	1.469529
O	-3.675123	-3.601785	2.932776
H	-2.563187	-5.001002	4.988837
H	-0.743467	-6.664156	4.713245
O	0.324066	-7.418607	2.509284
H	-0.785733	-5.996016	0.476918
C	-3.945796	-2.940898	4.171133

C	1.368251	-7.261788	1.538648
C	2.359684	-6.168263	1.924258
C	-4.851566	-1.766059	3.842197
C	3.499568	-6.039450	0.906603
H	1.831664	-5.211729	2.018073
H	2.763749	-6.405741	2.917032
H	1.864363	-8.236427	1.513660
H	0.953437	-7.083191	0.538561
H	-3.001671	-2.596306	4.615621
H	-4.423622	-3.633613	4.878213
C	-5.217477	-0.891659	5.047124
H	-4.332474	-1.166778	3.090096
H	-5.765360	-2.143623	3.366241
H	-4.314884	-0.666380	5.633598
H	-5.888815	-1.447575	5.714089
C	-5.877283	0.429661	4.611240
C	4.619825	-5.105205	1.384908
C	5.887924	-5.071395	0.513026
H	4.227410	-4.087378	1.499182
H	4.912824	-5.429826	2.393280
C	5.836706	-4.244586	-0.781759
H	5.561399	-3.210526	-0.538923
H	6.860632	-4.194241	-1.181388
C	4.918419	-4.764210	-1.894846
H	3.928572	-7.033617	0.711194
H	3.087436	-5.690301	-0.046242
H	6.185245	-6.103306	0.272328
H	6.699689	-4.657945	1.126622
C	-4.863560	1.433759	4.039357
H	-4.290495	1.878896	4.865217
H	-4.130032	0.894768	3.431384
C	-5.470490	2.545534	3.176157
H	-6.407064	0.878397	5.459951
H	-6.644074	0.209907	3.853538
H	3.871024	-4.631825	-1.607610
C	5.156912	-4.050145	-3.227759
H	5.020358	-2.968015	-3.121393
H	4.458767	-4.396882	-3.998381
H	6.176863	-4.224334	-3.592548
C	-6.379124	3.524546	3.925499
C	-6.920063	4.630561	3.015172
H	-4.655309	3.108633	2.699217
H	-6.045577	2.087916	2.357740
H	-7.218184	2.979363	4.377194
H	-5.818239	3.971197	4.758521
H	-6.100056	5.209605	2.571523
H	-7.563465	5.328226	3.562820
H	-7.510121	4.208746	2.191379
H	5.070851	-5.845225	-2.023956

OPCBMMB chloroform (*singlet*) B3LYP-6-31G* E= -5003.832582 u.a.

	X	Y	Z
C	4.212088	0.753260	-0.902377
C	-2.768279	-0.740296	-0.991069

C	4.009461	1.544884	0.506631
C	-3.286981	-0.074194	0.264260
C	3.493759	0.720468	1.634475
C	-2.853943	1.412104	0.261394
C	3.348715	-0.656406	1.567119
C	-2.517745	2.106184	-0.885752
C	3.534981	-1.373420	0.289214
C	-2.331394	1.396919	-2.169947
C	3.859564	-0.692422	-0.871374
C	-2.456369	0.021023	-2.210774
C	3.468234	1.310482	-2.065866
C	-2.089146	-1.924423	-1.013015
C	2.759921	2.499391	-2.017744
C	-1.732329	-2.729122	0.221411
C	2.568544	3.216575	-0.742323
C	-1.764620	-1.781765	1.437090
C	3.099254	2.724809	0.443255
C	-2.462819	-0.598400	1.458663
C	2.528853	1.502355	2.366195
C	-2.203084	1.742660	1.492043
C	1.489028	0.888627	3.073504
C	-1.288657	2.805162	1.569891
C	1.350052	-0.548400	3.025306
C	-0.953790	3.540576	0.372279
C	2.257546	-1.300337	2.272958
C	-1.555416	3.182786	-0.839626
C	1.773009	-2.400777	1.456264
C	-0.765742	3.144742	-2.062672
C	2.554486	-2.443020	0.244090
C	-1.252456	2.048769	-2.887049
C	1.927550	-2.787906	-0.959487
C	-0.350945	1.292358	-3.644238
C	2.253971	-2.060151	-2.165476
C	-0.498411	-0.151645	-3.704109
C	3.183333	-1.019900	-2.105138
C	-1.538484	-0.771592	-3.002455
C	2.946420	0.207080	-2.843004
C	-1.293412	-1.988186	-2.251503
C	1.794847	0.344445	-3.618883
C	-0.034806	-2.555913	-2.246823
C	0.825917	-0.740098	-3.687710
C	1.050489	-1.919547	-2.968837
C	1.070725	1.598391	-3.594320
C	0.514981	-3.102280	-0.984934
C	1.538348	2.643908	-2.794395
C	-0.226860	-3.074934	0.176590
C	0.598375	3.433872	-2.018210
C	0.403355	-2.692391	1.406195
C	1.233553	3.785071	-0.756304
C	-0.540748	-1.903796	2.182161
C	0.468566	3.846040	0.411794
C	-0.072196	-0.858252	2.985378
C	1.006295	3.301453	1.640271
C	-0.804348	0.384741	3.010957
C	-0.076951	2.656466	2.361729
C	0.158074	1.474060	3.062650
C	2.283444	2.730569	1.635111
C	-1.954721	0.508912	2.223393
C	5.354126	1.397324	-0.157042
C	6.339100	0.453904	0.482306

C	6.985470	-0.507345	-0.302862
C	7.916886	-1.376295	0.264045
C	8.213677	-1.290349	1.626046
C	7.579689	-0.327969	2.413564
C	6.645828	0.538761	1.844091
H	6.141989	1.275233	2.462253
H	7.805100	-0.254755	3.473454
H	8.933620	-1.971148	2.070892
H	8.401687	-2.125130	-0.355097
H	6.742984	-0.585527	-1.358877
C	5.978381	2.654862	-0.758396
C	6.508066	3.611723	0.311204
C	7.085020	4.884616	-0.302401
C	7.603019	5.851527	0.740069
O	7.585786	5.672033	1.941430
O	8.097763	6.965280	0.162482
C	8.617686	7.956724	1.066783
H	7.835457	8.300439	1.748046
H	9.446248	7.545871	1.648916
H	8.962680	8.775561	0.436053
H	7.908872	4.655888	-0.990723
H	6.332440	5.409655	-0.904859
H	7.274797	3.116938	0.915691
H	5.695641	3.877446	0.997323
H	5.243096	3.174087	-1.380317
H	6.789679	2.342350	-1.427518
C	-4.834898	-0.261606	0.415526
H	-5.142748	0.181349	1.366729
H	-5.043549	-1.332302	0.455600
C	-5.549036	0.409804	-0.728747
C	-5.815189	-0.260992	-1.932739
C	-6.315238	0.454996	-3.027629
C	-6.503036	1.833935	-2.948568
C	-6.220907	2.511938	-1.759991
C	-5.790730	1.782333	-0.649712
O	-5.549227	-1.607594	-1.967275
H	-6.527318	-0.053628	-3.960893
H	-6.842523	2.397086	-3.812042
O	-6.338279	3.876757	-1.756355
H	-5.569555	2.287503	0.281799
C	-5.171069	-2.172038	-3.228164
C	-5.547279	4.567589	-0.778546
C	-5.280207	5.988604	-1.242961
C	-4.650812	-3.580567	-2.989291
C	-4.221152	6.648752	-0.353633
H	-4.921677	5.954525	-2.279579
H	-6.209466	6.572413	-1.242120
H	-6.061791	4.561455	0.192109
H	-4.593244	4.040996	-0.655888
H	-4.399148	-1.539230	-3.686621
H	-6.034260	-2.199760	-3.906930
C	-4.103874	-4.203059	-4.280768
H	-3.871599	-3.535239	-2.223336
H	-5.463339	-4.198356	-2.584717
H	-3.193653	-3.666998	-4.580722
H	-4.830693	-4.044272	-5.089653
C	-3.825676	-5.710950	-4.177689
C	-3.914526	8.099369	-0.742097
C	-2.706433	8.697782	0.008611
H	-3.735630	8.157547	-1.825503

H	-4.810385	8.704847	-0.552864
C	-1.374444	8.615850	-0.753314
H	-1.461413	9.207785	-1.676698
H	-0.594926	9.105891	-0.152445
C	-0.894068	7.207114	-1.121677
H	-4.548728	6.623843	0.696091
H	-3.303218	6.049178	-0.396482
H	-2.602867	8.200475	0.983872
H	-2.900714	9.754953	0.229182
C	-2.718432	-6.119700	-3.194602
H	-2.934846	-5.704861	-2.201428
H	-2.745865	-7.211099	-3.071680
C	-1.304639	-5.714692	-3.626391
H	-3.567183	-6.091435	-5.175577
H	-4.759134	-6.214131	-3.890336
H	-1.631308	6.717916	-1.771187
C	0.462055	7.229647	-1.831730
H	0.417372	7.842024	-2.741011
H	0.780643	6.223331	-2.119623
H	1.238559	7.655063	-1.184002
C	-0.224156	-6.149120	-2.629160
C	1.199836	-5.877287	-3.120203
H	-1.091419	-6.159807	-4.609528
H	-1.244706	-4.627382	-3.761345
H	-0.383233	-5.623223	-1.678779
H	-0.338776	-7.220395	-2.411501
H	1.944376	-6.159383	-2.367285
H	1.344833	-4.815745	-3.349110
H	1.414783	-6.444374	-4.034031
H	-0.825499	6.588765	-0.216129
C	-2.624433	-4.002849	0.395908
H	-2.526418	-4.598066	-0.515703
H	-3.664168	-3.679663	0.477115
C	-2.201442	-4.816105	1.590432
C	-2.720847	-4.541570	2.867518
C	-2.222199	-5.222104	3.982702
C	-1.204748	-6.164287	3.832482
C	-0.689013	-6.453646	2.567705
C	-1.201784	-5.780704	1.454969
O	-3.709279	-3.597318	2.925464
H	-2.613690	-5.015674	4.972098
H	-0.802021	-6.685093	4.695219
O	0.273330	-7.431387	2.491293
H	-0.817579	-5.987887	0.463063
C	-3.974557	-2.951510	4.174513
C	1.319871	-7.277747	1.520832
C	2.314523	-6.188569	1.909621
C	-4.868170	-1.761784	3.868007
C	3.458630	-6.064180	0.896090
H	1.790711	-5.229588	2.001825
H	2.714774	-6.428405	2.903403
H	1.812221	-8.254181	1.495793
H	0.905749	-7.097073	0.521075
H	-3.026445	-2.623917	4.622765
H	-4.458388	-3.651432	4.869851
C	-5.216677	-0.906894	5.092178
H	-4.345125	-1.155196	3.124516
H	-5.788782	-2.119191	3.389626
H	-4.308247	-0.708719	5.679324
H	-5.894054	-1.467101	5.749256

C	-5.857202	0.434244	4.690230
C	4.581274	-5.135903	1.380660
C	5.851889	-5.104284	0.512256
H	4.192579	-4.116868	1.496972
H	4.869837	-5.465227	2.388775
C	5.808108	-4.269529	-0.777715
H	5.537474	-3.235385	-0.529635
H	6.833073	-4.222172	-1.174878
C	4.889236	-4.777811	-1.895520
H	3.883580	-7.060085	0.701333
H	3.051659	-5.711860	-0.057746
H	6.144040	-6.136383	0.266276
H	6.664641	-4.699137	1.130111
C	-4.829659	1.434462	4.137273
H	-4.240939	1.845810	4.969656
H	-4.111952	0.898528	3.508339
C	-5.421992	2.581224	3.311033
H	-6.374775	0.871246	5.552493
H	-6.631380	0.245374	3.931702
H	3.842009	-4.640905	-1.609716
C	5.135025	-4.057950	-3.224020
H	5.005089	-2.975583	-3.111864
H	4.436430	-4.396172	-3.998086
H	6.154731	-4.236533	-3.587342
C	-6.298508	3.558698	4.099643
C	-6.821112	4.705065	3.229932
H	-4.600553	3.139425	2.839140
H	-6.016810	2.158510	2.487651
H	-7.145972	3.020623	4.544099
H	-5.717580	3.965688	4.939240
H	-5.991677	5.277473	2.795313
H	-7.442043	5.400583	3.805604
H	-7.429044	4.322680	2.400407
H	5.035846	-5.858967	-2.030051

PPCBMB (*singlet*) B3LYP-6-31G* E= -5347.946194 u.a.

	X	Y	Z
C	5.785181	-0.809726	2.554782
C	6.441276	-1.042925	1.345374
C	7.804008	-1.371895	1.337158
C	8.504900	-1.451661	2.542899
C	7.847155	-1.200123	3.745065
C	6.484051	-0.877002	3.764746
C	5.695477	-0.910798	0.030890
C	4.591721	-1.899343	-0.143421
C	3.158293	-1.514513	-0.362185
C	2.380633	-2.897358	-0.451125
C	3.499954	-3.959924	-0.254566
N	4.748830	-3.208141	-0.115160
C	2.725583	-0.569112	0.763153
C	2.737585	0.764669	0.257048
C	2.956324	0.723227	-1.176769
C	3.096670	-0.625853	-1.605649
C	2.546310	-1.050760	-2.823064

C	1.874291	-0.086598	-3.657938
C	1.767449	1.267326	-3.269074
C	2.323220	1.689645	-1.989705
C	1.905478	1.761818	0.804431
C	1.274778	2.732220	-0.052249
C	1.520071	2.713384	-1.430941
C	0.490201	3.153207	-2.477661
C	0.578990	2.009638	-3.500945
C	1.613047	-3.099260	-1.769870
C	1.782049	-2.294994	-2.888249
C	0.660210	-2.084280	-3.789841
C	0.723909	-0.717275	-4.271949
C	-0.450713	0.014848	-4.473172
C	-0.530073	1.411843	-4.085306
C	-0.973283	3.407366	-1.888375
C	-1.131279	3.162167	-0.379474
C	-0.061790	2.973358	0.478070
C	-0.239236	2.136263	1.658930
C	0.988841	1.395170	1.867003
C	0.950118	0.070251	2.323144
C	1.836332	-0.938289	1.770329
C	1.087981	-2.187948	1.666367
C	1.257080	-3.046049	0.583411
C	0.119714	-3.621531	-0.051440
C	0.335424	-3.665331	-1.485925
C	-0.761269	-3.486981	-2.352838
C	-0.583421	-2.671113	-3.528481
C	-1.807742	-1.917956	-3.734875
C	-1.738302	-0.601742	-4.197530
C	-2.598398	0.409667	-3.627643
C	-1.868094	1.657229	-3.556641
C	-2.079861	2.519927	-2.478408
C	-1.258057	4.842084	-2.257251
N	-0.317985	5.348533	-3.026043
C	0.872840	4.506685	-3.132366
C	-2.752614	-2.292701	-2.690209
C	-3.606170	-1.324343	-2.162541
C	-3.495737	0.035893	-2.609880
C	-2.095016	-3.275149	-1.828323
C	-2.304461	-3.278576	-0.444346
C	-3.300398	-2.393998	0.224882
C	-4.035780	-1.308815	-0.727833
C	-2.598261	-1.827652	1.414675
C	-2.685965	-0.491699	1.791214
C	-3.344002	0.490468	0.925483
C	-3.908925	0.110611	-0.293119
C	-3.664799	0.905163	-1.465199
C	-1.182916	-3.409367	0.435438
C	-1.364198	-2.540980	1.578822
C	-0.246518	-1.934385	2.170240
C	-0.336941	-0.555452	2.583351
C	-1.526969	0.153703	2.389914
C	-1.473993	1.525500	1.913936
C	-2.578965	1.717621	1.007296
C	-2.378756	2.516928	-0.137906
C	-2.940803	2.108277	-1.407063
C	-4.786585	-2.404049	-0.000434
C	-5.352210	-3.551900	-0.834696
C	-5.355041	-4.878539	-0.072747
C	-5.877054	-6.024362	-0.934275

C	-5.899708	-7.346446	-0.198815
O	-6.337287	-8.342811	-1.007034
C	-6.395743	-9.638843	-0.395062
C	-2.411163	5.653034	-1.749112
C	-2.349803	5.889727	-0.244043
C	-1.183196	6.330687	0.393798
C	-1.144163	6.380587	1.790768
C	-2.263431	6.045494	2.543257
C	-3.451701	5.657364	1.913907
C	-3.477018	5.577086	0.519392
O	-0.100686	6.609479	-0.413203
C	0.898259	7.552121	0.009612
C	2.272837	6.902523	0.110072
C	2.408110	5.870705	1.232659
C	3.828298	5.308970	1.409442
C	4.404207	4.593514	0.180468
C	5.811562	4.018027	0.394202
C	5.918646	2.926468	1.466802
C	7.329792	2.340086	1.557722
O	-4.507091	5.373114	2.728237
C	-5.767293	5.103549	2.107839
C	-5.879884	3.695752	1.511720
C	-6.942407	3.647418	0.408230
C	-7.100986	2.262321	-0.218658
C	-8.084912	2.245148	-1.394208
C	-8.308362	0.856994	-2.011878
C	-7.051276	0.239689	-2.634747
C	-7.295961	-1.135863	-3.255711
C	-0.272021	6.715123	-3.530322
C	5.981134	-3.943156	0.128601
O	8.345523	-1.618480	0.096571
C	9.733043	-1.911599	-0.036735
C	10.014812	-2.094474	-1.523695
C	9.299739	-3.313112	-2.162531
C	8.400865	-2.985567	-3.368820
C	7.186254	-2.118401	-3.016903
C	6.165909	-1.917775	-4.146883
C	5.245075	-3.123383	-4.369466
C	4.244255	-2.900948	-5.504732
O	5.942952	-0.645612	4.992276
C	4.627508	-0.083225	5.097929
C	3.518981	-1.132894	5.125171
C	2.182936	-0.519607	5.560253
C	1.050061	-1.542869	5.693105
C	-0.261090	-0.901121	6.163882
C	-1.405813	-1.891957	6.422237
C	-1.962731	-2.569084	5.164952
C	-3.120191	-3.522203	5.468318
C	-5.672041	-2.011963	1.150850
C	-6.795192	-1.212596	0.919784
C	-7.668691	-0.895552	1.958455
C	-7.427128	-1.375943	3.247148
C	-6.312563	-2.180398	3.485213
C	-5.442738	-2.497642	2.441929
O	-5.574865	-7.522963	0.954949
H	-0.228022	6.649433	2.301887
H	-2.232104	6.073476	3.627133
H	-4.357071	5.221405	0.000428
H	-4.912334	3.387562	1.102386
H	-6.112706	2.973935	2.303373

H	-6.503919	5.250497	2.902207
H	-5.956745	5.866731	1.339486
H	0.602554	8.017316	0.954587
H	2.501159	6.439437	-0.858143
H	3.008662	7.708534	0.248414
H	1.708685	5.049057	1.048858
H	2.102649	6.336769	2.180368
H	-6.116617	1.911634	-0.547485
H	-7.430238	1.554292	0.552114
H	-8.702942	0.177017	-1.241651
H	-9.091927	0.926614	-2.779467
H	-7.910711	3.989632	0.803610
H	-6.669670	4.368442	-0.378709
H	-7.722905	2.931310	-2.174539
H	-9.051306	2.648197	-1.058908
H	3.723914	3.791321	-0.122072
H	4.445694	5.293218	-0.665292
H	3.804325	4.609804	2.253748
H	4.508987	6.123095	1.702919
H	-6.267967	0.151902	-1.876912
H	-8.015746	-1.081356	-4.081750
H	6.166306	3.603047	-0.560087
H	6.506413	4.833410	0.647089
H	5.633385	3.333093	2.445538
H	5.192915	2.130802	1.249984
H	7.616312	1.853525	0.616883
H	7.407194	1.593496	2.352987
H	8.066483	3.128029	1.759066
H	-6.648061	0.923252	-3.394681
H	-3.333347	5.106719	-1.967326
H	-2.464520	6.603234	-2.289380
H	-4.574227	-3.118582	2.632384
H	-6.114290	-2.563304	4.482124
H	-8.104626	-1.126290	4.059024
H	-8.537535	-0.273229	1.760927
H	-6.977551	-0.834863	-0.079162
H	-5.404704	-9.948135	-0.051788
H	-7.077175	-9.630990	0.460119
H	-6.760829	-10.313786	-1.169884
H	-6.895815	-5.821604	-1.292073
H	-5.267531	-6.149885	-1.838681
H	-5.962682	-4.796332	0.834267
H	-4.335997	-5.109748	0.257502
H	-4.774477	-3.660831	-1.756772
H	-6.372912	-3.284086	-1.134977
H	-1.169596	6.938845	-4.112311
H	0.597789	6.811824	-4.181348
H	6.002425	-4.298402	1.165266
H	6.846114	-3.310653	-0.054086
H	6.012921	-4.803928	-0.545753
H	-0.187272	7.415126	-2.695191
H	9.560115	-1.699778	2.555429
H	8.382179	-1.246059	4.687793
H	4.728527	-0.570036	2.526392
H	3.407943	-1.601975	4.139860
H	3.816462	-1.923280	5.826457
H	4.643997	0.457879	6.049295
H	4.467435	0.653083	4.299712
H	9.977697	-2.824562	0.526511
H	9.727201	-1.167871	-2.033892

H	11.100877	-2.185809	-1.643225
H	8.687858	-3.814917	-1.401939
H	10.050819	-4.048681	-2.474037
H	0.901033	-2.043333	4.729476
H	1.348860	-2.324808	6.407368
H	-1.065497	-2.662558	7.130844
H	-2.226194	-1.360023	6.925089
H	2.319186	-0.009088	6.525469
H	1.884754	0.253519	4.839923
H	-0.584672	-0.160270	5.420462
H	-0.061597	-0.342553	7.089786
H	6.667174	-2.579400	-2.169135
H	7.536673	-1.141219	-2.662867
H	8.059529	-3.930418	-3.811455
H	8.995437	-2.482978	-4.145196
H	-1.166360	-3.118635	4.649972
H	-2.814633	-4.313236	6.164631
H	-3.486809	-4.007450	4.556666
H	-3.961865	-2.987067	5.926151
H	5.533811	-1.052845	-3.906983
H	6.688652	-1.670531	-5.082406
H	5.841243	-4.024330	-4.571170
H	4.692473	-3.316172	-3.438482
H	3.631777	-2.014058	-5.311214
H	3.565893	-3.753962	-5.613836
H	4.760342	-2.754380	-6.461666
H	-2.302039	-1.799365	4.461443
H	5.258854	0.085924	-0.053255
H	6.407639	-1.011467	-0.788903
H	10.326221	-1.085322	0.378337
H	-6.364051	-1.563394	-3.640698
H	-7.700519	-1.834757	-2.512683
H	0.914374	8.341794	-0.753534
H	3.581438	-4.634455	-1.112799
H	3.338220	-4.561329	0.646787
H	1.693674	4.995660	-2.594279
H	1.157013	4.393216	-4.182084

PPCBMB xylene (*singlet*) B3LYP-6-31G* E= -5347.960959 u.a.

	X	Y	Z
C	5.803237	-0.797979	2.554007
C	6.453249	-1.039233	1.342694
C	7.816230	-1.369214	1.328523
C	8.522054	-1.446118	2.532102
C	7.870018	-1.188100	3.736184
C	6.508092	-0.861033	3.760394
C	5.702171	-0.912222	0.031182
C	4.600240	-1.905268	-0.137260
C	3.166158	-1.517621	-0.354699
C	2.387158	-2.900277	-0.437564
C	3.506658	-3.962697	-0.241615
N	4.756303	-3.208987	-0.104893
C	2.734674	-0.566983	0.767824
C	2.745643	0.763775	0.257149

C	2.960888	0.716439	-1.177657
C	3.102881	-0.632222	-1.601703
C	2.548494	-1.062431	-2.817469
C	1.874258	-0.100864	-3.653411
C	1.767227	1.254471	-3.269002
C	2.326184	1.681980	-1.991978
C	1.914919	1.764347	0.801616
C	1.283732	2.732884	-0.056129
C	1.525381	2.707079	-1.436155
C	0.493807	3.144292	-2.482721
C	0.579086	1.996039	-3.501150
C	1.616655	-3.105531	-1.754444
C	1.785834	-2.306117	-2.878079
C	0.660804	-2.098472	-3.777074
C	0.722772	-0.732983	-4.264040
C	-0.452390	-0.001076	-4.465408
C	-0.531616	1.397790	-4.083358
C	-0.968731	3.403122	-1.891599
C	-1.124693	3.161196	-0.380817
C	-0.052269	2.974539	0.474356
C	-0.228300	2.141707	1.658031
C	1.000150	1.400825	1.866528
C	0.962067	0.078288	2.328510
C	1.847039	-0.933156	1.778205
C	1.099064	-2.182737	1.682140
C	1.265801	-3.045251	0.599955
C	0.127858	-3.620287	-0.030494
C	0.340828	-3.669882	-1.466481
C	-0.759092	-3.495946	-2.332034
C	-0.582780	-2.684363	-3.511415
C	-1.807550	-1.931936	-3.717624
C	-1.739230	-0.616961	-4.184676
C	-2.597796	0.396794	-3.616224
C	-1.868174	1.644641	-3.551365
C	-2.079276	2.512583	-2.475778
C	-1.244628	4.841980	-2.260224
N	-0.306850	5.345100	-3.020261
C	0.876096	4.493613	-3.146549
C	-2.750112	-2.303842	-2.669048
C	-3.602951	-1.332363	-2.143106
C	-3.492976	0.025573	-2.594756
C	-2.091603	-3.283500	-1.806488
C	-2.298259	-3.281798	-0.419684
C	-3.292090	-2.393468	0.247565
C	-4.029522	-1.310827	-0.707167
C	-2.588793	-1.822502	1.435186
C	-2.676146	-0.483969	1.806346
C	-3.336026	0.495041	0.939874
C	-3.904153	0.110445	-0.277884
C	-3.660282	0.899339	-1.452406
C	-1.175369	-3.406751	0.457087
C	-1.354648	-2.534539	1.598954
C	-0.234372	-1.926472	2.185865
C	-0.324526	-0.545716	2.593720
C	-1.514917	0.162726	2.400337
C	-1.462622	1.532511	1.918848
C	-2.569976	1.721538	1.014228
C	-2.370580	2.516849	-0.134400
C	-2.934619	2.102660	-1.401579
C	-4.778760	-2.404670	0.024140

C	-5.345893	-3.554035	-0.807136
C	-5.349426	-4.879954	-0.044231
C	-5.877847	-6.023510	-0.905894
C	-5.911504	-7.346449	-0.173207
O	-6.363407	-8.333756	-0.978885
C	-6.434822	-9.636448	-0.376524
C	-2.406232	5.652506	-1.770761
C	-2.373577	5.873358	-0.263068
C	-1.216187	6.303085	0.399322
C	-1.205519	6.351093	1.797161
C	-2.343568	6.025097	2.525343
C	-3.520945	5.645188	1.870260
C	-3.518967	5.566759	0.475450
O	-0.112505	6.563334	-0.380897
C	0.867136	7.530368	0.041121
C	2.249715	6.897957	0.131919
C	2.389934	5.858212	1.247085
C	3.811163	5.298863	1.421917
C	4.387547	4.595625	0.185933
C	5.795917	4.018812	0.391225
C	5.904696	2.915339	1.451531
C	7.313825	2.321528	1.527971
O	-4.595770	5.365598	2.663140
C	-5.844247	5.095144	2.016131
C	-5.945576	3.681517	1.433402
C	-6.997360	3.616839	0.320575
C	-7.139534	2.223537	-0.292023
C	-8.107748	2.183397	-1.479669
C	-8.314262	0.783678	-2.076768
C	-7.043939	0.163497	-2.668608
C	-7.273727	-1.218960	-3.280076
C	-0.257420	6.711105	-3.534915
C	5.990821	-3.947661	0.129265
O	8.352827	-1.616257	0.088369
C	9.740687	-1.922206	-0.046638
C	10.021773	-2.102028	-1.533456
C	9.301437	-3.314033	-2.178514
C	8.406768	-2.975243	-3.384540
C	7.194386	-2.107170	-3.027878
C	6.186929	-1.876963	-4.163500
C	5.274817	-3.079207	-4.434401
C	4.280710	-2.823821	-5.568889
O	5.972729	-0.619684	4.990860
C	4.660741	-0.047833	5.097290
C	3.545818	-1.090419	5.133891
C	2.213518	-0.463309	5.560668
C	1.074653	-1.477665	5.709780
C	-0.231221	-0.820551	6.173986
C	-1.382943	-1.798896	6.448734
C	-1.946934	-2.490105	5.202381
C	-3.115574	-3.425150	5.520163
C	-5.663650	-2.010723	1.175566
C	-6.782366	-1.204051	0.946817
C	-7.655128	-0.885964	1.986352
C	-7.417574	-1.372969	3.273576
C	-6.307284	-2.184729	3.509513
C	-5.438136	-2.502346	2.465499
O	-5.585355	-7.527846	0.981681
H	-0.297690	6.613265	2.326768
H	-2.333786	6.052817	3.609777

H	-4.391699	5.222738	-0.063252
H	-4.972996	3.373428	1.035537
H	-6.183959	2.967463	2.230520
H	-6.598127	5.251386	2.792073
H	-6.013252	5.851098	1.236646
H	0.569729	7.979753	0.992705
H	2.485031	6.447091	-0.840301
H	2.975212	7.711011	0.280071
H	1.694800	5.034489	1.055529
H	2.079728	6.316291	2.197208
H	-6.148669	1.874100	-0.603430
H	-7.475780	1.523681	0.483106
H	-8.716484	0.114598	-1.300885
H	-9.085481	0.835565	-2.858214
H	-7.971201	3.954937	0.704931
H	-6.722205	4.331685	-0.470702
H	-7.739060	2.858763	-2.266193
H	-9.080691	2.585842	-1.163380
H	3.708024	3.795216	-0.124188
H	4.427410	5.304531	-0.652027
H	3.790541	4.593422	2.261331
H	4.489397	6.113020	1.720470
H	-6.274778	0.085658	-1.895001
H	-7.979045	-1.174192	-4.119110
H	6.150287	3.615090	-0.568176
H	6.489718	4.832277	0.652774
H	5.628439	3.314069	2.436137
H	5.174762	2.124141	1.231112
H	7.589329	1.835897	0.583479
H	7.394189	1.571987	2.320390
H	8.056211	3.105449	1.724873
H	-6.628465	0.840295	-3.428182
H	-3.324590	5.111419	-2.015127
H	-2.442215	6.607086	-2.303170
H	-4.571982	-3.127253	2.654011
H	-6.112567	-2.572185	4.505393
H	-8.093868	-1.122067	4.086004
H	-8.519688	-0.257112	1.791316
H	-6.962238	-0.821207	-0.050920
H	-5.444013	-9.962850	-0.050066
H	-7.107601	-9.625002	0.484904
H	-6.818618	-10.298083	-1.153135
H	-6.893988	-5.813072	-1.265485
H	-5.267076	-6.152755	-1.808873
H	-5.954959	-4.795701	0.863926
H	-4.329713	-5.112397	0.282709
H	-4.768680	-3.665454	-1.729168
H	-6.366519	-3.286680	-1.107610
H	-1.162687	6.937307	-4.101660
H	0.602690	6.796187	-4.199033
H	6.014181	-4.303075	1.164924
H	6.855005	-3.316131	-0.059409
H	6.013647	-4.807489	-0.545520
H	-0.153057	7.411781	-2.703367
H	9.576653	-1.696098	2.540887
H	8.410756	-1.231730	4.675899
H	4.747384	-0.554257	2.529861
H	3.433409	-1.569649	4.153622
H	3.836176	-1.874806	5.844938
H	4.682916	0.498397	6.045516

H	4.503556	0.684875	4.295543
H	9.974419	-2.838694	0.514082
H	9.741963	-1.171758	-2.041565
H	11.107322	-2.199884	-1.650221
H	8.686241	-3.817643	-1.421851
H	10.049444	-4.051122	-2.493299
H	0.920312	-1.990532	4.753407
H	1.369869	-2.250957	6.434860
H	-1.047389	-2.561698	7.168030
H	-2.198714	-1.253286	6.944539
H	2.353730	0.060452	6.518034
H	1.919401	0.300730	4.829148
H	-0.550875	-0.088132	5.420505
H	-0.025886	-0.250404	7.091502
H	6.663728	-2.580933	-2.193978
H	7.548370	-1.139198	-2.653059
H	8.064149	-3.915631	-3.835496
H	9.004533	-2.466991	-4.154736
H	-1.156432	-3.056001	4.696268
H	-2.818519	-4.208657	6.228707
H	-3.487872	-3.920084	4.616030
H	-3.951092	-2.873356	5.969350
H	5.548351	-1.022082	-3.904366
H	6.719913	-1.598865	-5.084536
H	5.878165	-3.968423	-4.663325
H	4.717139	-3.308162	-3.514978
H	3.656779	-1.951534	-5.346057
H	3.613052	-3.679747	-5.717183
H	4.802498	-2.634386	-6.515224
H	-2.276597	-1.727625	4.486550
H	5.262442	0.082976	-0.054676
H	6.410152	-1.015559	-0.791792
H	10.339565	-1.102133	0.370930
H	-6.333997	-1.647606	-3.644634
H	-7.689177	-1.911572	-2.537281
H	0.863024	8.325643	-0.715169
H	3.590180	-4.638274	-1.097874
H	3.350884	-4.562874	0.660618
H	1.706337	4.982966	-2.625397
H	1.139745	4.381507	-4.201005

PPCBMB toluene (*singlet*) B3LYP-6-31G* E= -5347.960874 u.a.

	X	Y	Z
C	5.802813	-0.798207	2.554291
C	6.452815	-1.040046	1.343093
C	7.815689	-1.370465	1.329128
C	8.521437	-1.447169	2.532753
C	7.869436	-1.188479	3.736709
C	6.507596	-0.861010	3.760740
C	5.701923	-0.913104	0.031468
C	4.599932	-1.906042	-0.137091
C	3.165910	-1.518255	-0.354639
C	2.386747	-2.900819	-0.437460
C	3.506132	-3.963359	-0.241490

N	4.755859	-3.209803	-0.104741
C	2.734518	-0.567516	0.767813
C	2.745695	0.763222	0.257069
C	2.960971	0.715786	-1.177727
C	3.102786	-0.632926	-1.601695
C	2.548383	-1.063122	-2.817456
C	1.874291	-0.101512	-3.653464
C	1.767439	1.253861	-3.269133
C	2.326413	1.681367	-1.992113
C	1.915105	1.763927	0.801473
C	1.284067	2.732513	-0.056341
C	1.525735	2.706613	-1.436362
C	0.494232	3.143886	-2.482996
C	0.579397	1.995564	-3.501342
C	1.616233	-3.106031	-1.754336
C	1.785539	-2.306707	-2.878002
C	0.660562	-2.098960	-3.777044
C	0.722728	-0.733509	-4.264080
C	-0.452333	-0.001455	-4.465518
C	-0.531376	1.397433	-4.083530
C	-0.968263	3.402923	-1.891882
C	-1.124269	3.161077	-0.381101
C	-0.051897	2.974376	0.474124
C	-0.228074	2.141626	1.657829
C	1.000272	1.400589	1.866396
C	0.961989	0.078073	2.328425
C	1.846843	-0.933516	1.778210
C	1.098689	-2.183004	1.682170
C	1.265349	-3.045599	0.600054
C	0.127326	-3.620519	-0.030398
C	0.340321	-3.670211	-1.466370
C	-0.759548	-3.496171	-2.331962
C	-0.583104	-2.684674	-3.511380
C	-1.807772	-1.932093	-3.717662
C	-1.739263	-0.617153	-4.184781
C	-2.597703	0.396751	-3.616397
C	-1.867904	1.644507	-3.551588
C	-2.078920	2.512542	-2.476061
C	-1.243846	4.841880	-2.260266
N	-0.305929	5.344979	-3.020191
C	0.876670	4.493112	-3.146978
C	-2.750410	-2.303812	-2.669091
C	-3.603124	-1.332195	-2.143219
C	-3.492951	0.025710	-2.594935
C	-2.092044	-3.283510	-1.806447
C	-2.298732	-3.281701	-0.419665
C	-3.292471	-2.393214	0.247526
C	-4.029740	-1.310537	-0.707303
C	-2.589102	-1.822286	1.435121
C	-2.676278	-0.483724	1.806204
C	-3.336008	0.495323	0.939666
C	-3.904172	0.110745	-0.278076
C	-3.660159	0.899548	-1.452632
C	-1.175872	-3.406785	0.457153
C	-1.355064	-2.534497	1.598971
C	-0.234721	-1.926540	2.185871
C	-0.324692	-0.545745	2.593635
C	-1.514974	0.162852	2.400187
C	-1.462486	1.532605	1.918639
C	-2.569794	1.721724	1.013978

C	-2.370261	2.516934	-0.134691
C	-2.934346	2.102778	-1.401858
C	-4.779138	-2.404250	0.024026
C	-5.346358	-3.553605	-0.807221
C	-5.350124	-4.879412	-0.044119
C	-5.878553	-6.023108	-0.905598
C	-5.912161	-7.345899	-0.172617
O	-6.365507	-8.333114	-0.977627
C	-6.436668	-9.635710	-0.375045
C	-2.405337	5.652537	-1.770778
C	-2.372773	5.873430	-0.263077
C	-1.215332	6.302849	0.399443
C	-1.204728	6.350750	1.797273
C	-2.342906	6.024993	2.525356
C	-3.520328	5.645407	1.870167
C	-3.518283	5.567052	0.475346
O	-0.111428	6.562671	-0.380640
C	0.868207	7.529762	0.041222
C	2.250798	6.897315	0.131686
C	2.391124	5.857595	1.246873
C	3.812299	5.298042	1.421464
C	4.388257	4.594476	0.185471
C	5.796598	4.017502	0.390498
C	5.905550	2.914356	1.451133
C	7.314577	2.320246	1.527183
O	-4.595248	5.366013	2.662977
C	-5.843742	5.095693	2.015961
C	-5.945239	3.682048	1.433292
C	-6.996962	3.617461	0.320410
C	-7.139286	2.224183	-0.292214
C	-8.107245	2.184326	-1.480073
C	-8.313897	0.784722	-2.077368
C	-7.043511	0.164276	-2.668791
C	-7.273477	-1.217988	-3.280638
C	-0.256278	6.711133	-3.534406
C	5.990278	-3.948603	0.129514
O	8.352219	-1.618351	0.089114
C	9.740476	-1.922331	-0.046078
C	10.021656	-2.101172	-1.533012
C	9.302044	-3.313336	-2.178607
C	8.407261	-2.974517	-3.384548
C	7.194409	-2.107247	-3.027533
C	6.186855	-1.876988	-4.163065
C	5.274998	-3.079369	-4.434199
C	4.280858	-2.823984	-5.568657
O	5.972262	-0.619015	4.991086
C	4.660337	-0.046964	5.097280
C	3.545333	-1.089455	5.134272
C	2.213064	-0.462164	5.560849
C	1.074126	-1.476423	5.710062
C	-0.231780	-0.819147	6.173949
C	-1.383566	-1.797397	6.448770
C	-1.947468	-2.488847	5.202512
C	-3.116046	-3.423924	5.520430
C	-5.664102	-2.010141	1.175354
C	-6.782925	-1.203678	0.946317
C	-7.655769	-0.885396	1.985721
C	-7.418203	-1.371995	3.273097
C	-6.307828	-2.183554	3.509315
C	-5.438594	-2.501378	2.465435

O	-5.584636	-7.527302	0.981872
H	-0.296841	6.612572	2.326968
H	-2.333190	6.052624	3.609792
H	-4.391036	5.223191	-0.063424
H	-4.972677	3.373820	1.035486
H	-6.183738	2.968048	2.230424
H	-6.597605	5.252057	2.791895
H	-6.012663	5.851638	1.236444
H	0.571031	7.978991	0.992948
H	2.485834	6.446369	-0.840569
H	2.976402	7.710310	0.279627
H	1.695827	5.033969	1.055496
H	2.081161	6.315776	2.197030
H	-6.148432	1.874547	-0.603424
H	-7.475836	1.524357	0.482817
H	-8.716593	0.115666	-1.301707
H	-9.084800	0.836889	-2.859108
H	-7.970785	3.955698	0.704689
H	-6.721652	4.332262	-0.470858
H	-7.738238	2.859691	-2.266448
H	-9.080184	2.586934	-1.163972
H	3.708541	3.794090	-0.124291
H	4.427988	5.303196	-0.652656
H	3.791759	4.592742	2.261003
H	4.490741	6.112134	1.719715
H	-6.274705	0.086055	-1.894856
H	-7.978514	-1.172865	-4.119884
H	6.150589	3.613409	-0.568888
H	6.490616	4.830937	0.651558
H	5.629779	3.313474	2.435719
H	5.175334	2.123266	1.231282
H	7.589484	1.834077	0.582792
H	7.395169	1.571094	2.319941
H	8.057235	3.104104	1.723300
H	-6.627496	0.841092	-3.428044
H	-3.323750	5.111556	-2.015178
H	-2.441193	6.607099	-2.303249
H	-4.572402	-3.126163	2.654162
H	-6.113104	-2.570708	4.505313
H	-8.094566	-1.120945	4.085423
H	-8.520404	-0.256715	1.790466
H	-6.962801	-0.821172	-0.051551
H	-5.445595	-9.962452	-0.049721
H	-7.108399	-9.623942	0.487201
H	-6.821640	-10.297296	-1.151116
H	-6.894649	-5.812768	-1.265346
H	-5.267679	-6.152545	-1.808492
H	-5.955752	-4.794903	0.863952
H	-4.330492	-5.111921	0.283004
H	-4.769087	-3.665189	-1.729197
H	-6.366919	-3.286135	-1.107800
H	-1.160759	6.937094	-4.102528
H	0.604851	6.796800	-4.197122
H	6.013595	-4.303884	1.165224
H	6.854571	-3.317232	-0.059230
H	6.012986	-4.808532	-0.545147
H	-0.153525	7.411639	-2.702524
H	9.575947	-1.697541	2.541646
H	8.410096	-1.231912	4.676477
H	4.747037	-0.554180	2.529987

H	3.432888	-1.568993	4.154157
H	3.835678	-1.873633	5.845555
H	4.682560	0.499657	6.045280
H	4.503238	0.685438	4.295241
H	9.975527	-2.838743	0.514225
H	9.741156	-1.170837	-2.040613
H	11.107259	-2.198249	-1.649929
H	8.687037	-3.817552	-1.422198
H	10.050477	-4.049889	-2.493630
H	0.919880	-1.989505	4.753792
H	1.369215	-2.249570	6.435348
H	-1.048104	-2.560070	7.168246
H	-2.199366	-1.251666	6.944397
H	2.353245	0.061778	6.518122
H	1.919042	0.301746	4.829155
H	-0.551310	-0.086889	5.420259
H	-0.026542	-0.248799	7.091362
H	6.663996	-2.581702	-2.193871
H	7.547870	-1.139272	-2.652227
H	8.065144	-3.914894	-3.835917
H	9.004783	-2.465620	-4.154505
H	-1.156915	-3.054780	4.696522
H	-2.818967	-4.207249	6.229164
H	-3.488250	-3.919093	4.616384
H	-3.951639	-2.872104	5.969449
H	5.548087	-1.022318	-3.903707
H	6.719730	-1.598559	-5.084062
H	5.878536	-3.968432	-4.663235
H	4.717338	-3.308571	-3.514826
H	3.656741	-1.951874	-5.345661
H	3.613380	-3.680020	-5.717123
H	4.802624	-2.634261	-6.514946
H	-2.277168	-1.726509	4.486542
H	5.262279	0.082120	-0.054514
H	6.410039	-1.016542	-0.791369
H	10.338233	-1.101606	0.371808
H	-6.333734	-1.646800	-3.644978
H	-7.689332	-1.910653	-2.538113
H	0.863887	8.325163	-0.714948
H	3.589586	-4.638927	-1.097766
H	3.350253	-4.563538	0.660724
H	1.707345	4.982142	-2.626216
H	1.139775	4.380893	-4.201567

PPCBMB chloroform (*singlet*) B3LYP-6-31G* E= -5347.969625 u.a.

	X	Y	Z
C	5.825829	-0.785299	2.540076
C	6.471440	-1.027611	1.326499
C	7.835816	-1.352744	1.306455
C	8.547181	-1.423850	2.507459
C	7.899313	-1.165215	3.713792
C	6.536368	-0.843238	3.743206
C	5.714622	-0.906628	0.017989
C	4.613591	-1.902334	-0.143244

C	3.178427	-1.514464	-0.358477
C	2.400050	-2.897736	-0.437247
C	3.521212	-3.959142	-0.244529
N	4.770213	-3.203083	-0.107953
C	2.748861	-0.562149	0.764133
C	2.757028	0.767319	0.251982
C	2.967354	0.717990	-1.183909
C	3.110178	-0.629757	-1.606509
C	2.551999	-1.062686	-2.820715
C	1.873593	-0.102114	-3.654849
C	1.766241	1.253484	-3.271694
C	2.329097	1.683332	-1.996820
C	1.927542	1.768611	0.797569
C	1.293172	2.736182	-0.058628
C	1.529354	2.707284	-1.439878
C	0.494669	3.143898	-2.484007
C	0.577051	1.994042	-3.500809
C	1.625161	-3.104657	-1.751593
C	1.791168	-2.306433	-2.877863
C	0.662092	-2.100652	-3.772593
C	0.720787	-0.735542	-4.261414
C	-0.455801	-0.004434	-4.459506
C	-0.535199	1.394938	-4.079466
C	-0.966401	3.404670	-1.888768
C	-1.117709	3.162610	-0.376231
C	-0.041193	2.977055	0.475037
C	-0.212979	2.145287	1.659977
C	1.016844	1.405443	1.865747
C	0.981307	0.083780	2.330015
C	1.865240	-0.928127	1.778392
C	1.118362	-2.178211	1.687164
C	1.282232	-3.042328	0.604367
C	0.143093	-3.617394	-0.021719
C	0.351533	-3.669100	-1.459086
C	-0.752577	-3.497943	-2.321233
C	-0.580354	-2.687404	-3.502354
C	-1.806372	-1.936254	-3.705179
C	-1.740947	-0.621414	-4.173464
C	-2.598304	0.392184	-3.602999
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