Electronic Supplementary Material for PCCP

Supporting Information for

Experimental and Theoretical Study of the Rotational Reorientation Dynamics of 7-Animocoumarins Derivatives in Polar Solvents: Hydrogen-Bonding Effects

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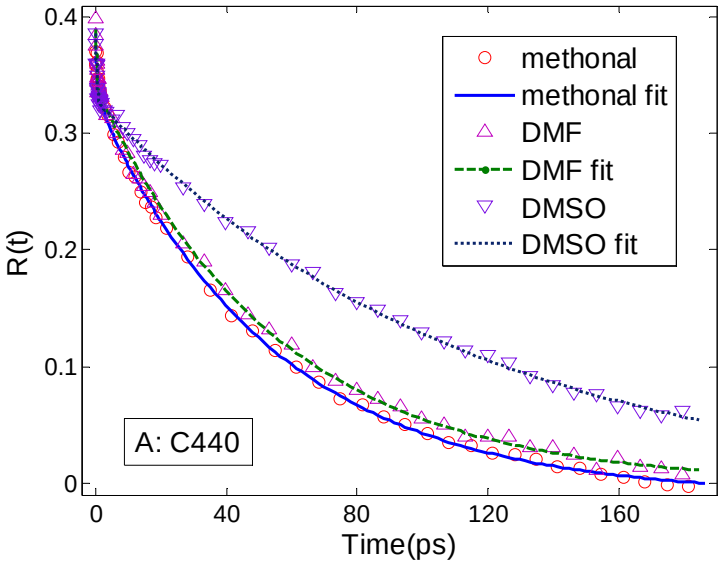
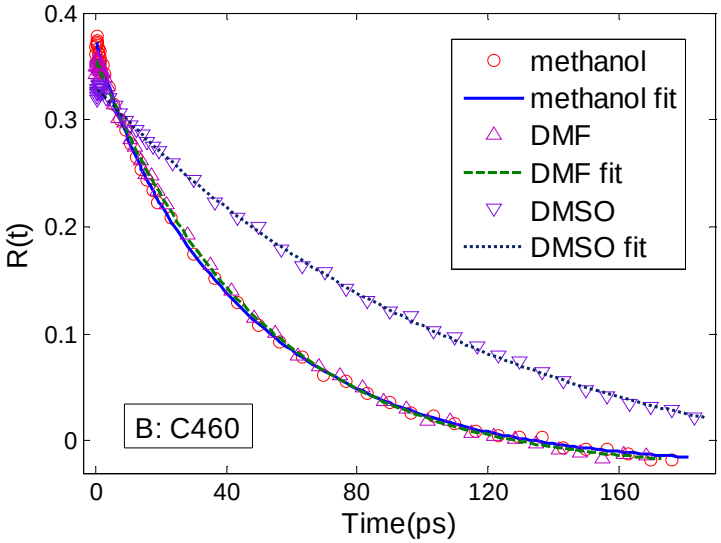

methonal
methonal fit
DMF
DMF fit
DMSO
DMSO fit
A: C440
R(t)
Time(ps)
0
0.1
0.2
0.3
0.4
0
40
80
120
160


methanol
methanol fit
DMF
DMF fit
DMSO
DMSO fit
B: C460
R(t)
Time(ps)
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0.1
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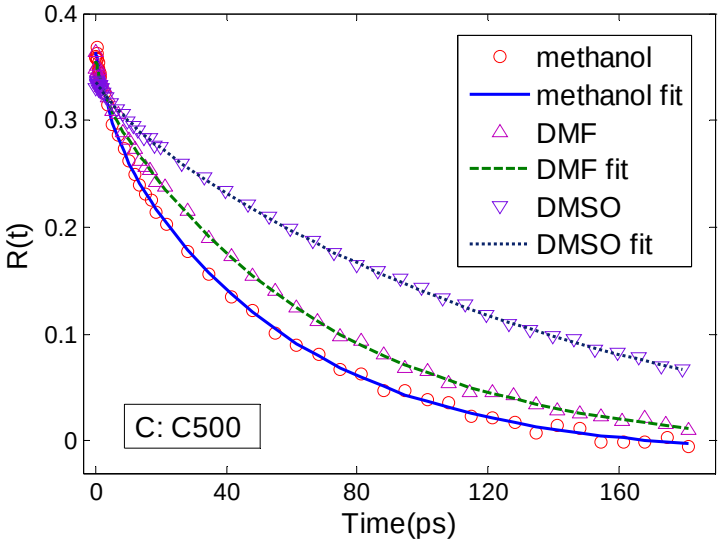
0.3
0.4
0
40
80
120
160


methanol
methanol fit
DMF
DMF fit
DMSO
DMSO fit
C: C500
R(t)
Time(ps)
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0.2
0.3
0.4
0
40
80
120
160

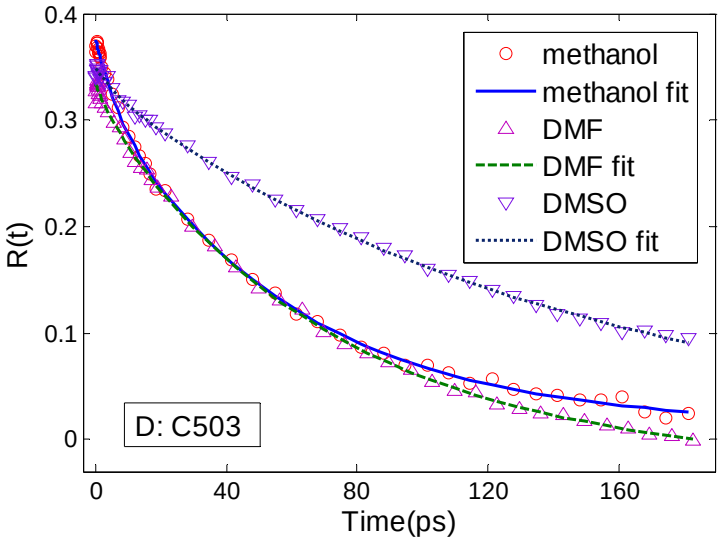
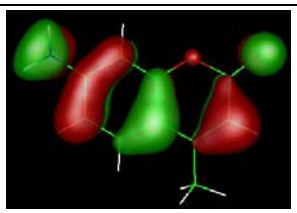
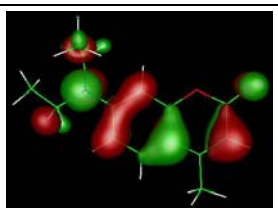
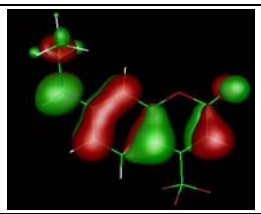
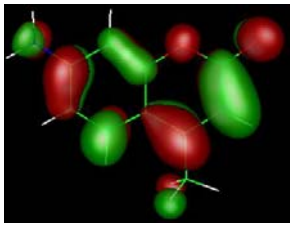
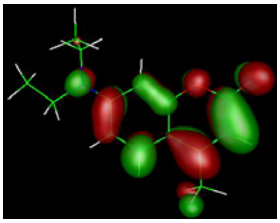
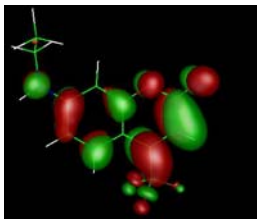
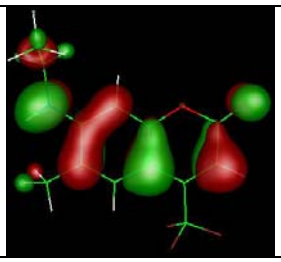
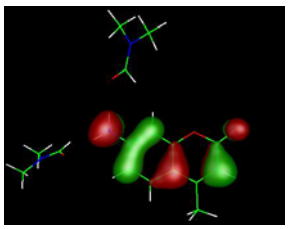
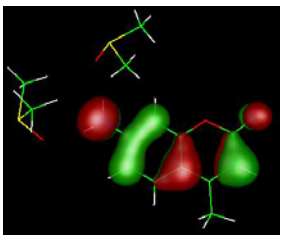
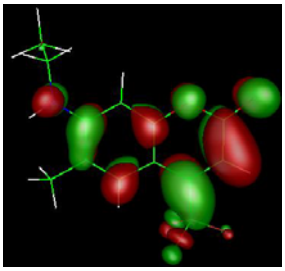
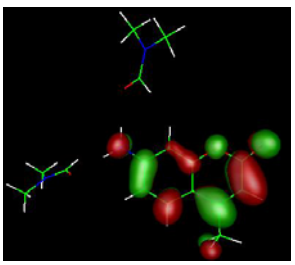
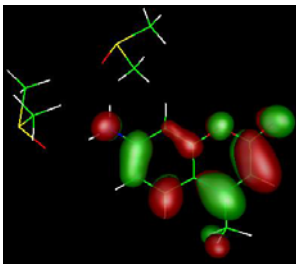
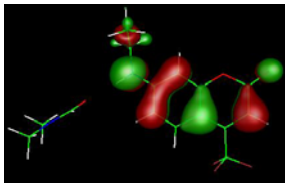
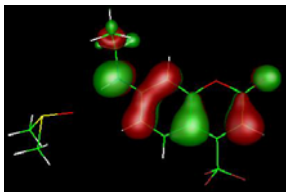
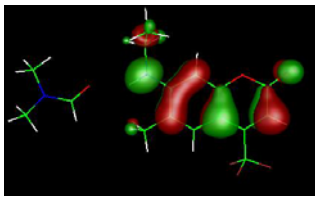
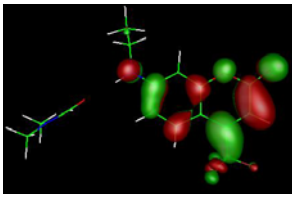
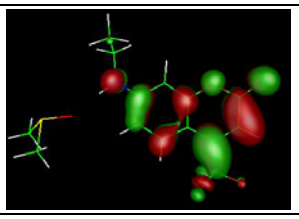
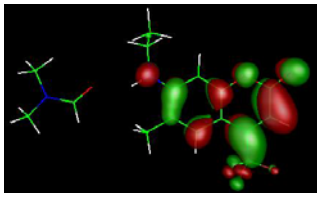
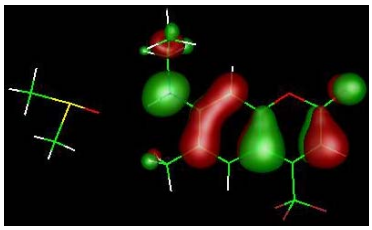
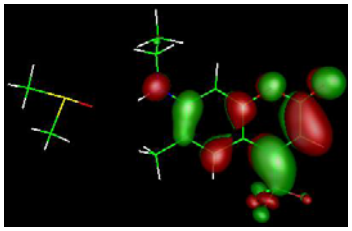
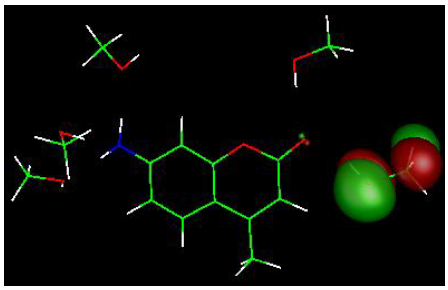
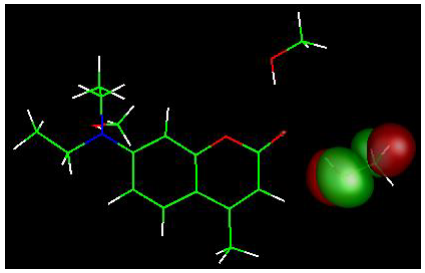
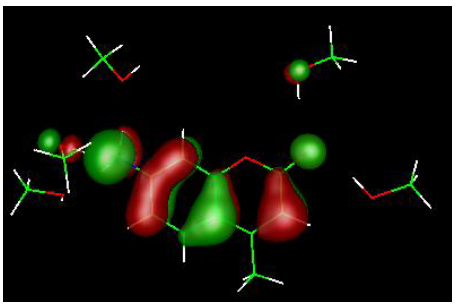
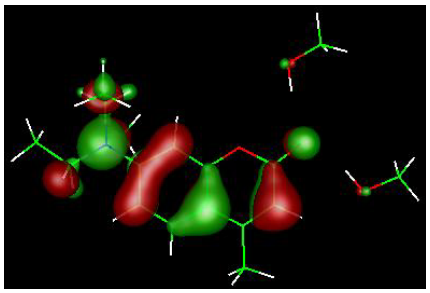
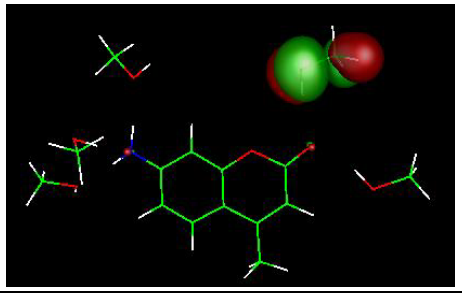
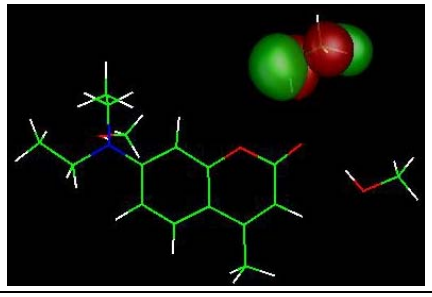


Figure S1: Experimental and simulated anisotropy decays of C440, C460, C500, and C503 in DMF, DMSO, and methanol.

	C440	C460	C500
HOMO			
LUMO			
	C503	C440-$(DMF)_2$	C440-$(DMSO)_2$
HOMO			
LUMO			

	C500-DMF	C500-DMSO	C503-DMF
HOMO			
LUMO			

	HOMO	LUMO
C503-DMSO		

	C440-(Meth)$_5$	C460-(Meth)$_4$
HOMO-2		
HOMO-1		
HOMO		

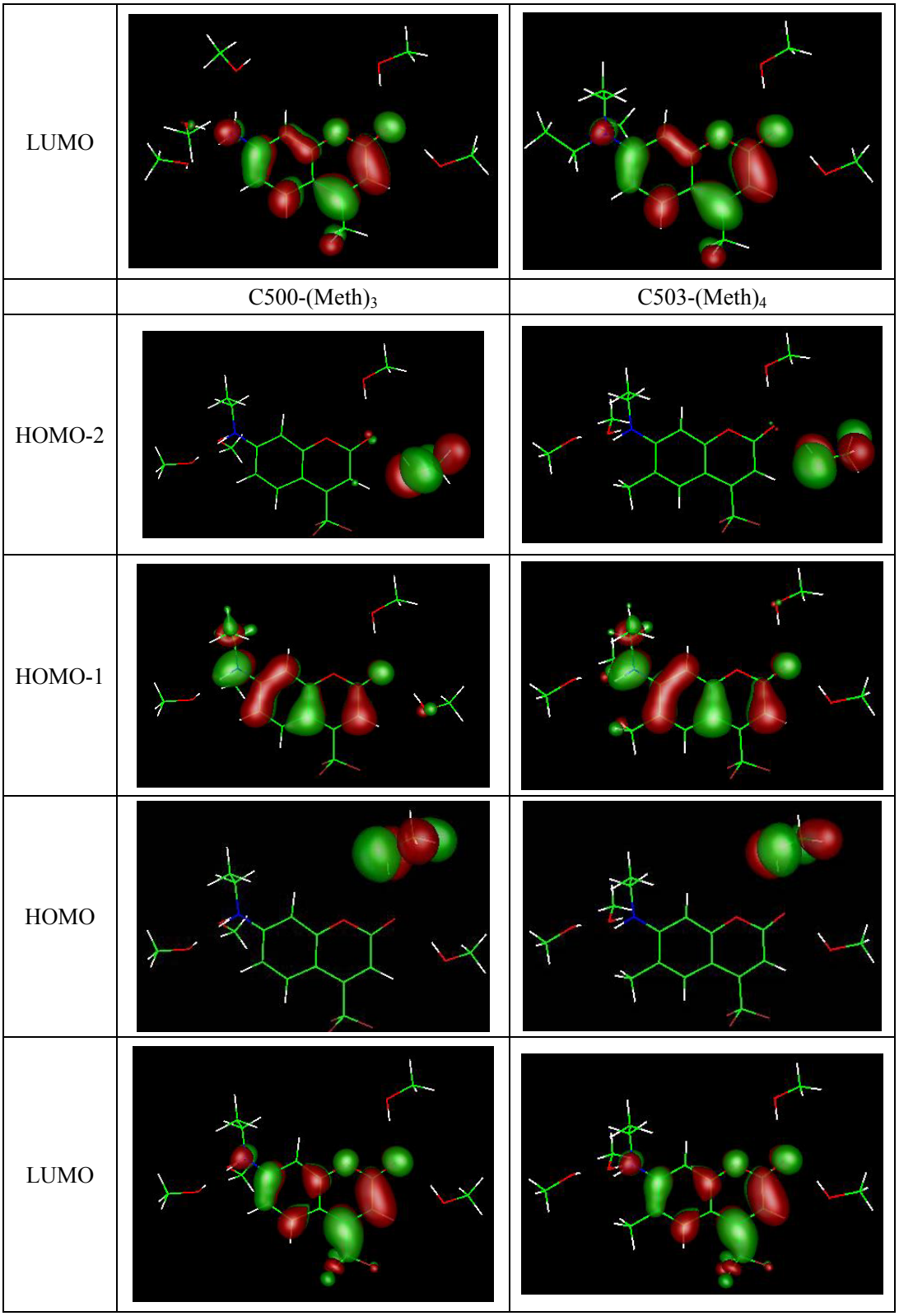


Figure S2. Frontier molecular orbitals (MOs) of all of the isolated coumarins and coumarin-solvent complexes under study.

Table S1: Calculated electronic excitation energies (eV) and corresponding oscillator strengths (in the parenthesis) of the low-lying electronically excited states for all the isolated coumarins and hydrogen-bonded coumarin-solvent complexes under study, together with dominant contributions of the orbital transitions for these electronic states (H, HOMO; L, LUMO; H-1, HOMO-1; H-2, HOMO-2).

	C440	C440-$(DMF)_2$	C440-$(DMSO)_2$	C460	C500
S1	3.5(0.24) H→L 86.6%	3.2 (0.25) H→L 85.9%	3.2 (0.26) H→L 88.1%	3.2(0.25) H→L 88.3%	3.1(0.24) H→L 88.3%
S2	3.8(0.00)	3.3 (0.00)	3.6 (0.00)	3.8(0.04)	3.6(0.04)
S3	3.9(0.02)	3.4 (0.00)	3.7 (0.00)	3.8(0.00)	3.7(0.00)
S4	4.4(0.04)	3.9(0.04)	3.8(0.00)	4.2(0.08)	4.2(0.02)
S5	4.8(0.04)	3.9(0.00)	3.9(0.04)	4.6(0.09)	4.5(0.08)
	C500-DMF	C500-DMSO	C503	C503-DMF	C503-DMSO
S1	2.9 (0.26) H→L 89.3%	2.9 (0.26) H→L 89.4%	3.1(0.25) H→L 88.9%	2.9(0.28) H→L 89.4%	2.9(0.28) H→L 89.6%
S2	3.4(0.00)	3.6(0.04)	3.5(0.03)	3.4(0.00)	3.4(0.03)
S3	3.6(0.05)	3.7(0.00)	3.6 (0.00)	3.5(0.03)	3.7(0.00)
S4	3.7(0.00)	3.7(0.00)	4.2(0.03)	3.7(0.00)	3.7(0.00)
S5	4.1(0.02)	3.8(0.00)	4.5(0.07)	4.1(0.00)	3.8(0.00)

	C440-$(Meth)_5$	C460-$(Meth)_3$	C500-$(Meth)_4$	C503-$(Meth)_4$
S1	2.5(0.00) H→L 98.9%	2.4(0.00) H→L 99.7%	2.1(0.00) H→L 99.9%	2.1(0.00) H→L 99.8%
S2	2.9(0.00) H-2→L 99.9%	2.7(0.00) H-2→L 99.3%	2.4(0.00) H-2→L 98.9%	2.4(0.00) H-2→L 100.0%
S3	3.3(0.28) H-1→L 87.2%	3.1(0.25) H-1→L 88.2%	3.0(0.27) H-1→L 88.7%	3.0(0.29) H-1→L 89.6%
S4	3.4(0.00)	3.2(0.00)	3.4(0.00)	3.3(0.00)
S5	3.8(0.00)	3.7(0.00)	3.6(0.00)	3.4(0.03)

Table S2: Calculated torsions between amino group and the coumarin ring plane for all the isolated coumarins and hydrogen-bonded coumarin-solvent complexes under study (for definition of α and β, see Figure 3).

	C440		C440-$(DMF)_2$		C440-$(DMSO)_2$		C440-$(Meth)_5$	
	S0	S1	S0	S1	S0	S1	S0	S3
α	-19.9	1.5	-11.9	-6.8	3.6	-5.4	19.7	11.3
β	21.6	-1.0	7.1	-3.1	1.2	13.6	-23.4	11.9
	C460		C460-$(Meth)_2$		C500		C500-DMF	
	S0	S1	S0	S3	S0	S1	S0	S1
α	-15.3	91.3	-15.6	-96.4	-8.7	-11.5	-1.5	-0.0
β	6.2	88.1	5.4	-81.9	8.9	3.3	5.7	7.1
	C500-DMSO		C500-$(Meth)_4$		C503		C503-DMF	
	S0	S1	S0	S3	S0	S1	S0	S1
α	-0.8	11.3	-18.9	-19.0	-7.7	-8.0	-3.5	-5.0
β	3.2	17.3	16.4	-12.5	9.7	5.3	3.8	3.1
	C503-DMSO		C503-$(Meth)_3$		C460-$(Meth)_3$		C503-$(Meth)_4$	
	S0	S1	S0	S3	S0	S3	S0	S3
α	-4.8	-2.1	-2.2	-8.0	-21.2	-	-19.2	-
β	7.0	7.6	-4.9	-6.2	11.9	-	18.2	-

Table S3: All the optimized geometric coordinates of isolated coumarins and hydrogen-bonded coumarin-solvent complexes involved here (see the following 8 pages).

C440/S0

Energy = -591.9414541561

C	-2.5966833	0.3708770	0.0058240
C	-2.4287335	-1.0367303	0.0062574
C	-1.1603438	-1.5906989	0.0095654
C	0.0028130	-0.7884483	0.0013360
C	-0.1868291	0.6164527	-0.0005525
C	-1.4569488	1.1902905	0.0018114
C	1.3543460	-1.2976692	-0.0018514
C	2.3953829	-0.4103054	-0.0068261
C	2.2176657	1.0256436	0.0001260
O	0.8704626	1.4838267	0.0021425
O	3.0853035	1.8745056	0.0040143
C	1.6079044	-2.7804974	-0.0038733
N	-3.8661202	0.9226571	-0.0496879
H	-3.3084347	-1.6833258	0.0050168
H	-1.0578768	-2.6764875	0.0127312
H	-1.5397911	2.2780721	0.0012407
H	3.4313949	-0.7483612	-0.0115274
H	2.6835735	-2.9941381	-0.0073610
H	1.1596319	-3.2582398	-0.8888753
H	1.1648812	-3.2600677	0.8823252
H	-3.9631856	1.8977501	0.2140710
H	-4.6401939	0.3361272	0.2443018

C440/S1

Energy = -591.9197070409

C	-2.6646955	0.3323962	-0.0007803
C	-2.4898991	-1.0456726	-0.0010630
C	-1.1698828	-1.5521827	0.0000262
C	0.0010506	-0.7746681	-0.0001130
C	-0.1652651	0.6191590	0.0001852
C	-1.5054034	1.1760728	-0.0004410
C	1.3789542	-1.3223850	0.0003606
C	2.4484390	-0.4222517	-0.0001836
C	2.3847257	0.9744271	-0.0000074
O	0.8052634	1.4987805	0.0003741
O	3.1437889	1.9125088	-0.0002618
C	1.5847867	-2.7988846	0.0002792
N	-3.8878118	0.9608495	0.0031749
H	-3.3425984	-1.7236474	-0.0010430
H	-1.0556683	-2.6382602	-0.0000241
H	-1.5981825	2.2635684	0.0010535
H	3.4704778	-0.8087219	-0.0003065
H	2.6553399	-3.0439778	0.0006011
H	1.1342128	-3.2909523	-0.8850104
H	1.1336817	-3.2911057	0.8852036
H	-3.9560723	1.9713939	-0.0168469
H	-4.7494928	0.4271149	-0.0088263

C460/S0

Energy = -749.2256214687

C	-1.3962287	-0.2588295	-0.1350899
C	-0.9526811	-1.5999169	0.0728039
C	0.3960043	-1.9036988	0.1556147
C	1.3987421	-0.9166127	0.0551319
C	0.9495806	0.4144277	-0.1262107
C	-0.3996952	0.7422708	-0.2110223
C	2.8182296	-1.1608976	0.1365288
C	3.6775677	-0.1004693	0.0351528
C	3.2363137	1.2654216	-0.1472612
O	1.8304060	1.4603432	-0.2208978
O	3.9331577	2.2559653	-0.2427014
C	3.3397456	-2.5592431	0.3258456
N	-2.7429406	0.0474095	-0.2733861
C	-3.1828861	1.4425550	-0.1653228
C	-3.7372121	-1.0184665	-0.0647201
C	-3.2406315	1.9782747	1.2713405
C	-5.1497855	-0.6829241	-0.5393429
H	-1.6693620	-2.4096518	0.1824031
H	0.6864082	-2.9431293	0.3150785
H	-0.6405736	1.7941132	-0.3425475
H	4.7576225	-0.2352410	0.0889299
H	4.4358159	-2.5671290	0.3648694
H	3.0197752	-3.2167115	-0.4971734
H	2.9592901	-3.0018075	1.2595365
H	-4.1705311	1.5199636	-0.6349739
H	-2.5202200	2.0646368	-0.7818203
H	-3.7684109	-1.3210875	1.0007181
H	-3.3978222	-1.8971127	-0.6313187
H	-2.2571098	1.9197478	1.7573112
H	-3.9558813	1.4065504	1.8803777
H	-3.5607741	3.0306826	1.2736932
H	-5.7702668	-1.5857979	-0.4485968
H	-5.1591023	-0.3754093	-1.5947615
H	-5.6302915	0.1020152	0.0601258

C460/S1

Energy = -749.1951219120

C	-1.3281358	-0.1499956	-0.0368088
C	-0.9882349	-1.4771947	-0.2454611
C	0.3745901	-1.8120002	-0.3012844
C	1.4021893	-0.8498921	-0.1472019
C	0.9947787	0.5043142	0.0652582
C	-0.3578945	0.8500674	0.1203513
C	2.8093296	-1.1434416	-0.1938132
C	3.7192292	-0.0799566	-0.0206699
C	3.3578063	1.2640075	0.1919083
O	1.8794630	1.5197622	0.2241349
O	4.0287921	2.2722081	0.3573434
C	3.2843890	-2.5484196	-0.4184630
N	-2.7393731	0.2644062	-0.0022214
C	-3.4627108	0.2204561	1.2573887
C	-3.3736585	0.6057086	-1.2659699
C	-4.0563080	-1.1780113	1.5267394
C	-4.7346217	1.2835333	-1.2005949
H	-1.7464421	-2.2479957	-0.3884983
H	0.6471273	-2.8527922	-0.4745409
H	-0.6185804	1.8956395	0.2876782
H	4.7927240	-0.2688335	-0.0468455
H	4.3820513	-2.5879421	-0.4270103
H	2.9329987	-2.9647424	-1.3810282
H	2.9365544	-3.2433843	0.3684729
H	-4.2592521	0.9743004	1.2390322
H	-2.7367375	0.4745617	2.0379673
H	-3.4234916	-0.3440302	-1.8315887
H	-2.6335988	1.2104583	-1.8110265
H	-3.2646275	-1.9333143	1.5772295
H	-4.7807336	-1.4632564	0.7526664
H	-4.5747410	-1.1485178	2.4920153
H	-5.0694999	1.4854457	-2.2263134
H	-4.6865702	2.2469422	-0.6755962
H	-5.4988260	0.6555342	-0.7240816

C500/S0

Energy = -968.4507864100

C	-2.4812637	-0.8147493	-0.2488719
C	-1.5259076	-1.8685798	-0.1652541
C	-0.1762350	-1.6021610	-0.0817666
C	0.3162644	-0.2724239	-0.0679496
C	-0.6480440	0.7660765	-0.1479942
C	-2.0148718	0.5128390	-0.2293180
C	1.6947272	0.1254911	0.0171923
C	2.0513691	1.4440957	0.0242318
C	1.0673391	2.5051266	-0.0528140
O	-0.2849694	2.0865903	-0.1379450
O	1.2809016	3.6987060	-0.0512420
C	2.7833074	-0.9301768	0.1014661
F	2.7675131	-1.7527146	-0.9887183
F	2.6260862	-1.7240667	1.2015302
F	4.0265819	-0.3937371	0.1749609
N	-3.8111899	-1.1268459	-0.3753591
C	-4.9115737	-0.1700727	-0.3246177
C	-5.2867374	0.2901671	1.0899654
H	-1.8725296	-2.9041029	-0.1784138
H	0.5217435	-2.4355493	-0.0205379
H	-2.6894533	1.3652706	-0.2812612
H	3.0888894	1.7621595	0.0882008
H	-4.0516362	-2.1061994	-0.2609106
H	-5.7755827	-0.6479072	-0.8089934
H	-4.6497710	0.6937352	-0.9545320
H	-4.4356776	0.7695694	1.5924473
H	-5.6113090	-0.5603717	1.7064523
H	-6.1120894	1.0160341	1.0492299

C500/S1

Energy = -968.4382418598

C	-2.4857560	-0.8253095	-0.2886849
C	-1.5566253	-1.8776873	-0.2173646
C	-0.1965680	-1.5805595	-0.1273627
C	0.3039235	-0.2639879	-0.0962914
C	-0.6177240	0.7752348	-0.1621327
C	-2.0232513	0.5050142	-0.2666712
C	1.7598184	0.1203690	0.0101727
C	2.0544902	1.4698902	0.0263261
C	1.0969989	2.5257788	-0.0509078
O	-0.3185834	2.0862049	-0.1442021
O	1.2621317	3.7336294	-0.0478292
C	2.7989329	-0.9095449	0.1143405
F	2.8035335	-1.7934998	-0.9660428
F	2.6289689	-1.7493806	1.2171082
F	4.0543228	-0.4005600	0.2045245
N	-3.8526933	-1.0879700	-0.4056349
C	-4.9354004	-0.1291025	-0.2826483
C	-5.3031059	0.2055154	1.1761755
H	-1.8930801	-2.9151332	-0.2329141
H	0.5092048	-2.4087359	-0.0723725
H	-2.6896428	1.3626744	-0.3407274
H	3.0879453	1.8064488	0.1039862
H	-4.1090570	-2.0729974	-0.3811676
H	-5.8053682	-0.5589153	-0.7996941
H	-4.6616608	0.7874485	-0.8241343
H	-4.4470470	0.6479297	1.7024751
H	-5.6203436	-0.6941632	1.7207484
H	-6.1322840	0.9268658	1.1882855

C503/S0

Energy = -1007.780629991

C	-2.4128888	-0.4786276	-0.2187858
C	-1.5450529	-1.6192355	-0.1308959
C	-0.1785982	-1.4170968	-0.0550324
C	0.4089700	-0.1275877	-0.0579721
C	-0.4744544	0.9769178	-0.1473372
C	-1.8533317	0.8122153	-0.2197333
C	1.8132991	0.1698587	0.0179585
C	2.2636464	1.4598759	0.0098450
C	1.3591224	2.5887708	-0.0781830
O	-0.0189959	2.2693648	-0.1550587
O	1.6607780	3.7637249	-0.0924930
C	2.8239826	-0.9593531	0.1128634
F	2.7464276	-1.7927680	-0.9667821
F	2.6154411	-1.7271269	1.2233488
F	4.1029690	-0.5126938	0.1763912
N	-3.7666835	-0.6784279	-0.3341955
C	-4.7795487	0.3718257	-0.3089931
C	-5.1061654	0.9045659	1.0922224
C	-2.1213858	-3.0114998	-0.1329607
H	0.4664870	-2.2929589	0.0102558
H	-2.4705566	1.7067602	-0.2766414
H	3.3216930	1.7027046	0.0669231
H	-4.0947817	-1.6284116	-0.1991929
H	-5.6844865	-0.0445694	-0.7751067
H	-4.4486446	1.1908444	-0.9655934
H	-4.2142914	1.3223702	1.5786764
H	-5.5010238	0.1039960	1.7340752
H	-5.8652240	1.6983135	1.0316600
H	-2.6932413	-3.2185348	-1.0535118
H	-2.7979372	-3.1820905	0.7227393
H	-1.3239359	-3.7618194	-0.0671838

C503/S1

Energy = -1007.768348073

C	-2.4159515	-0.4877299	-0.2458540
C	-1.5728581	-1.6221241	-0.1826066
C	-0.1957145	-1.3941159	-0.1047258
C	0.3995361	-0.1159474	-0.0823290
C	-0.4422133	0.9857703	-0.1451417
C	-1.8612275	0.8076830	-0.2351331
C	1.8797339	0.1601930	0.0111231
C	2.2717675	1.4856531	-0.0072866
C	1.3919593	2.6070671	-0.0950390
O	-0.0505761	2.2747795	-0.1454190
O	1.6497170	3.7987725	-0.1276673
C	2.8414146	-0.9392089	0.1346419
F	2.7825660	-1.8431327	-0.9296048
F	2.6127718	-1.7463939	1.2522628
F	4.1304767	-0.5213123	0.2156244
N	-3.7994155	-0.6464328	-0.3371949
C	-4.8022753	0.4013374	-0.2653666
C	-5.1372486	0.8390158	1.1732975
C	-2.1427728	-3.0177081	-0.2000550
H	0.4573850	-2.2660379	-0.0551707
H	-2.4715629	1.7067018	-0.3026947
H	3.3277861	1.7479845	0.0501380
H	-4.1337047	-1.6053593	-0.2678554
H	-5.7056029	0.0148497	-0.7589337
H	-4.4591157	1.2631960	-0.8550375
H	-4.2473131	1.2383344	1.6775045
H	-5.5229401	-0.0036250	1.7631240
H	-5.9065842	1.6235396	1.1480374
H	-2.7102210	-3.2302974	-1.1232239
H	-2.8124122	-3.2130785	0.6568370
H	-1.3365568	-3.7593630	-0.1448503

C440-$(DMF)_2$/S0

Energy = -1089.194146589

C	-0.2180613	-0.5115540	0.0798091
C	-0.2933449	-1.8672812	0.5170231
C	0.8411853	-2.6530619	0.5755721
C	2.1177427	-2.1590246	0.2104485
C	2.1748705	-0.8091133	-0.2269757
C	1.0443862	-0.0048881	-0.3007287
C	3.3399148	-2.9155740	0.2523718
C	4.5134411	-2.3126247	-0.1242095
C	4.5910501	-0.9399686	-0.5639676
O	3.3618364	-0.2292599	-0.6002059
O	5.5869201	-0.3273819	-0.9037865
C	3.3319658	-4.3519607	0.7038200
N	-1.3364623	0.2635840	0.0143204
H	-1.2622172	-2.2710975	0.8153215
H	0.7511770	-3.6848909	0.9192534
H	1.1450780	1.0163963	-0.6678309
H	5.4608873	-2.8506345	-0.1053287
H	4.3430622	-4.7766607	0.6771757
H	2.6833312	-4.9666898	0.0606380
H	2.9470988	-4.4435555	1.7313982
H	-1.2431303	1.2728958	-0.1372354
H	-2.2240847	-0.0910568	0.3826557
C	0.0956219	3.6906116	0.3894743
H	0.6944724	3.0865702	1.1042859
O	-0.8406399	3.2122099	-0.2588145
N	0.5174704	4.9810343	0.3232548
C	-0.1372933	5.9290353	-0.5685572
H	-0.5374680	6.7809827	0.0029890
H	0.5758137	6.3096710	-1.3165296
H	-0.9571925	5.4090977	-1.0762152
C	1.6507515	5.4518730	1.1057645
H	2.0421195	4.6270036	1.7149203
H	2.4568806	5.8130612	0.4478273
H	1.3498381	6.2732973	1.7752534
C	-4.7291859	-0.9245502	-0.2934651
H	-4.3500558	-0.6617278	-1.3047903
O	-4.0297407	-0.8273404	0.7188155
N	-6.0201594	-1.3521535	-0.3172570
C	-6.6927960	-1.7423020	0.9151898
H	-7.5799896	-1.1125622	1.0854100
H	-7.0121748	-2.7949685	0.8632343
H	-5.9875699	-1.6136973	1.7436965
C	-6.7712153	-1.4371125	-1.5602648
H	-6.1353863	-1.1118015	-2.3938967
H	-7.0983772	-2.4716647	-1.7510718
H	-7.6623412	-0.7902571	-1.5248429

C440-$(DMF)_2$/S1

C	-0.3018436	-0.5000338	0.2099456
C	-0.4777514	-1.8568683	0.5338356
C	0.6436148	-2.6995597	0.5082659
C	1.9447832	-2.2666151	0.1779987
C	2.1143703	-0.9175711	-0.1414769
C	0.9907888	-0.0318414	-0.1370308
C	3.1609984	-3.1501687	0.1476608
C	4.3614167	-2.5365834	-0.1572368
C	4.5534555	-1.1599471	-0.4613003
O	3.2816587	-0.3424464	-0.4592569
O	5.5624430	-0.5151958	-0.7260513
C	3.0200607	-4.5971441	0.4551032
N	-1.3271270	0.4204175	0.1964257
H	-1.4608309	-2.2338947	0.8124542
H	0.5032405	-3.7514129	0.7649331
H	1.1472810	1.0085074	-0.4207041
H	5.2814030	-3.1258725	-0.1789829
H	3.9881589	-5.1115116	0.3833709
H	2.3154205	-5.1078845	-0.2341546
H	2.6198304	-4.7768281	1.4752742
H	-1.1149715	1.4195283	0.0442257
H	-2.2999425	0.1296167	0.3835965
C	0.3597533	3.7423662	0.4735771
H	0.8544305	3.2552659	1.3400954
O	-0.5544070	3.1964827	-0.1595606
N	0.8701670	4.9681507	0.2059174
C	0.3592340	5.7593765	-0.9074110
H	-0.0168228	6.7285891	-0.5456773
H	1.1563580	5.9417436	-1.6444991
H	-0.4558140	5.2010158	-1.3800556
C	1.9716711	5.5201908	0.9835568
H	2.2533472	4.8127968	1.7737528
H	2.8494016	5.6959951	0.3427048
H	1.6784230	6.4736593	1.4496550
C	-4.7962939	-0.7361138	-0.3993254
H	-4.4302390	-0.7310199	-1.4480312
O	-4.0791354	-0.4092007	0.5537623
N	-6.0893448	-1.1345707	-0.3014680
C	-6.7468789	-1.2081202	0.9981790
H	-7.6242722	-0.5435933	1.0214255
H	-7.0779348	-2.2380201	1.2022667
H	-6.0288546	-0.8952497	1.7638157
C	-6.8622614	-1.5080549	-1.4774362
H	-6.2379989	-1.4041811	-2.3742721
H	-7.2022864	-2.5530233	-1.4049919
H	-7.7453537	-0.8591399	-1.5860347

C440-$(DMSO)_2$/S0

Energy = -1698.600595732

C	0.2157155	-0.8673079	-0.2630775
C	0.7935117	-2.1157227	-0.6404757
C	2.1635877	-2.2911554	-0.6207512
C	3.0514369	-1.2562053	-0.2349771
C	2.4611198	-0.0213055	0.1420560
C	1.0856804	0.1726260	0.1349193
C	4.4849072	-1.3670418	-0.1941814
C	5.2289670	-0.2836067	0.2002355
C	4.6462526	0.9806556	0.5809482
O	3.2258221	1.0484070	0.5336575
O	5.2279665	1.9894013	0.9347763
C	5.1602665	-2.6560766	-0.5792403
N	-1.1296664	-0.6795943	-0.2875050
H	0.1357906	-2.9302336	-0.9478637
H	2.5744799	-3.2577830	-0.9165990
H	0.6872530	1.1327834	0.4636714
H	6.3168830	-0.3270118	0.2435659

H 6.2503463 -2.5685322 -0.4932386
H 4.9181849 -2.9371242 -1.6159063
H 4.8297010 -3.4854014 0.0651110
H -1.5295977 0.2377498 -0.0694363
H -1.7861536 -1.4227842 -0.5568756
C -1.3252190 3.1053269 -1.8254606
H -1.8539234 2.4901572 -2.5622467
H -1.1338137 4.1050840 -2.2369341
H -0.3927850 2.6144344 -1.5208889
C -1.2774568 4.1757619 0.7252241
H -1.0870499 5.1682936 0.2961117
H -1.7746275 4.2757208 1.6966145
H -0.3479905 3.6031990 0.8288592
O -2.5881281 1.8369401 0.2361066
S -2.4498755 3.2573407 -0.3677273
C -5.1596942 -0.5469587 -0.0056761
H -5.5338798 -0.5095970 -1.0355739
H -5.9816498 -0.3467346 0.6951505
H -4.3348604 0.1663424 0.1310205
C -3.8612885 -2.0149852 1.9452510
H -4.6753904 -1.7705758 2.6404006
H -3.3905885 -2.9613608 2.2350638
H -3.1137676 -1.2137982 1.9039328
O -3.3707154 -2.4981084 -0.7013905
S -4.5670991 -2.2805982 0.2544800

C440-(DMSO)2/S1

Energy = -1698.588869008

C 0.1315505 -1.0878770 -0.6101329
C 0.7205011 -2.3575208 -0.7178288
C 2.1033157 -2.4690115 -0.4970034
C 2.9373370 -1.3783372 -0.1742688
C 2.3414421 -0.1187261 -0.0677956
C 0.9415875 0.0262092 -0.2870151
C 4.4185643 -1.4703873 0.0662636
C 5.0691112 -0.2878768 0.3639104
C 4.4756429 1.0020912 0.4709125
O 2.9865640 1.0206115 0.2307302
O 4.9554531 2.1025249 0.7234189
C 5.0941421 -2.7907760 -0.0307469
N -1.2094177 -0.8273615 -0.8138362
H 0.1173857 -3.2294397 -0.9672391
H 2.5594435 -3.4569994 -0.5817283
H 0.4940630 1.0136778 -0.1827547
H 6.1467790 -0.2938263 0.5440420
H 6.1703391 -2.6980420 0.1691884
H 4.9770122 -3.2518320 -1.0334363
H 4.6811223 -3.5296902 0.6869076
H -1.5487686 0.1302319 -0.6362070
H -1.9275203 -1.5724682 -0.8629577
C -1.0588981 3.6128292 -1.6421684
H -1.6641502 3.3171808 -2.5065144
H -0.8354175 4.6866627 -1.6895021
H -0.1363346 3.0217829 -1.5975553
C -0.8033971 3.7017220 1.1138396
H -0.5856526 4.7760553 1.0510128
H -1.2401790 3.4657140 2.0906842
H 0.1030660 3.1080253 0.9448115
O -2.3051175 1.7499429 -0.0743165
S -2.0876819 3.2871538 -0.1450612
C -5.1378873 -0.3441098 -0.1368901
H -5.5142082 -0.4204422 -1.1637225
H -5.9436989 -0.0047121 0.5280810
H -4.2700380 0.3287198 -0.0875533
C -3.8977943 -1.6096420 1.9857670
H -4.6884636 -1.2520821 2.6584660
H -3.4524108 -2.5285644 2.3834193
H -3.1290388 -0.8430063 1.8310194
O -3.4814413 -2.4800485 -0.5688806
S -4.6487862 -2.0568779 0.3569116

C440-(Meth)5/S0

Energy = -1170.858366966

C -1.7576555 -0.4780276 -0.5850992
C -1.7996958 -1.8958079 -0.5000365
C -0.6403026 -2.6244015 -0.3099968
C 0.6227030 -1.9958941 -0.1912283
C 0.6377653 -0.5822563 -0.2804419
C -0.5156120 0.1699833 -0.4689085
C 1.8745662 -2.6823997 0.0000271
C 3.0310102 -1.9480494 0.0868189
C 3.0366939 -0.5152475 -0.0181671
O 1.8142750 0.1233237 -0.1891446
O 4.0289566 0.2205195 0.0302688
C 1.9148865 -4.1816008 0.1054327
N -2.9262409 0.2514313 -0.7264600
H -2.7628664 -2.4009398 -0.5883532
H -0.6995457 -3.7116243 -0.2505345
H -0.4400186 1.2557482 -0.5296470
H 4.0057742 -2.4169337 0.2270071
H 2.9421972 -4.5361126 0.2497843
H 1.5121397 -4.6523490 -0.8044036
H 1.3037703 -4.5354613 0.9499031
H -2.8180925 1.2218896 -1.0506360
H -3.7310142 -0.2469617 -1.1293728
C -3.1987319 3.9774347 -0.2064221
H -3.8395140 3.3396885 0.4152368
H -3.7968600 4.8161421 -0.5986436
H -2.3787627 4.3729551 0.4146010
O -2.7038929 3.1428931 -1.2745337
H -2.0809585 3.6594371 -1.8123255
C -6.5541420 -0.7711306 -0.7427237
H -6.1801915 -0.2687582 0.1585092
H -7.1581301 -1.6454857 -0.4494842
H -7.1845788 -0.0642191 -1.3062894
O -5.3930121 -1.1694086 -1.5028879
H -5.6881304 -1.5442519 -2.3490285
C 5.0962519 3.5645696 -0.4667218
H 5.0586271 4.6557820 -0.5935376
H 5.5246627 3.1302202 -1.3902843
H 5.7887918 3.3446805 0.3684301
O 3.7693982 3.1195717 -0.2125603
H 3.7998316 2.1430689 -0.1085716
C -4.1269086 0.7516543 2.8631521
H -3.1600929 1.2273087 3.1075162
H -4.0310417 -0.3363344 3.0315649
H -4.8838760 1.1397049 3.5575643
O -4.5676496 1.0616461 1.5402081
H -3.8954838 0.7245058 0.8970449
C 7.5448455 -1.0434482 0.5156459
H 7.5173724 -0.5659410 1.5128723
H 8.2270525 -1.9029481 0.5712565
H 7.9678910 -0.3178417 -0.2041220
O 6.2722770 -1.5361835 0.1079973
H 5.6383462 -0.7839930 0.0748478

C440-(Meth)5/S1

Energy = -1170.846783835

C -1.7441757 -0.5807952 -0.6753396
C -1.8130587 -1.9823801 -0.6230213
C -0.6307208 -2.6999828 -0.4096143
C 0.6339783 -2.0916354 -0.2446874
C 0.6898192 -0.7004222 -0.3130029
C -0.4930556 0.0673826 -0.5103590
C 1.9186106 -2.8356461 -0.0094598
C 3.0612212 -2.0620796 0.0577491
C 3.0946330 -0.6472276 -0.0498986
O 1.8178616 0.0292595 -0.2058648
O 4.0731009 0.1338248 -0.0199385
C 1.8985728 -4.3149668 0.1375882
N -2.8537898 0.2263548 -0.8562395
H -2.7676997 -2.4924642 -0.7449627
H -0.6859725 -3.7890095 -0.3698848
H -0.4177887 1.1550152 -0.5351953
H 4.0413240 -2.5251552 0.1966681
H 2.9080242 -4.7012338 0.3297555
H 1.5101620 -4.8263932 -0.7662680
H 1.2469780 -4.6424322 0.9730315
H -2.7086271 1.2348322 -1.0398660
H -3.7537165 -0.1978442 -1.1438374
C -3.0422430 3.9651000 -0.2006130
H -3.6869367 3.3656970 0.4538004
H -3.6545535 4.7222002 -0.7152848
H -2.2740442 4.4642831 0.4098026
O -2.4496277 3.0451055 -1.1438443
H -1.8344961 3.5296972 -1.7192920
C -6.5505971 -0.6117650 -0.6869758
H -6.1855933 -0.0527095 0.1836012
H -7.0387460 -1.5384368 -0.3461062
H -7.2773223 0.0085039 -1.2348699
O -5.3908791 -0.9029155 -1.4980902
H -5.6717889 -1.3552006 -2.3103407
C 4.8709808 3.5052437 -0.4985689
H 4.7417368 4.5901156 -0.6283860
H 5.3345167 3.1053145 -1.4209243
H 5.5834239 3.3469860 0.3341695
O 3.5902749 2.9468293 -0.2391488
H 3.7095119 1.9725077 -0.1356126
C -4.1807577 0.8088375 2.9473421
H -3.2291480 1.2611027 3.2747145
H -4.1442157 -0.2765323 3.1422986
H -4.9934849 1.2412966 3.5440897
O -4.4759958 1.1023661 1.5745511
H -3.7706980 0.7149789 1.0153531
C 7.4888294 -0.7665134 0.6058837
H 7.1843874 -0.6241058 1.6605771
H 8.3443075 -1.4573622 0.5915103
H 7.8367341 0.2102643 0.2181754
O 6.4631183 -1.3385506 -0.1948437
H 5.6776255 -0.7393391 -0.1603204

C460-(Meth)3/S0

Energy = -1096.571804896

C -2.0019864 -0.4148180 0.4421052

C	-1.9887833	-1.8402569	0.4811225
C	-0.8095297	-2.5523783	0.3404283
C	0.4365658	-1.9129427	0.1671768
C	0.4101801	-0.4993423	0.1497088
C	-0.7594726	0.2382738	0.2889033
C	1.7059968	-2.5809380	0.0172012
C	2.8381803	-1.8227599	-0.1383269
C	2.8018044	-0.3844920	-0.1507352
O	1.5640494	0.2315313	-0.0013565
O	3.7678623	0.3721188	-0.2845475
C	1.7834849	-4.0817139	0.0269003
N	-3.1986393	0.3079871	0.5103225
C	-3.1385322	1.7333256	0.8938797
C	-4.4277637	-0.4298680	0.8943637
C	-2.8452674	1.9772516	2.3779999
C	-5.7190873	0.3740100	0.7612275
H	-2.9107402	-2.3967496	0.6258802
H	-0.8496340	-3.6417334	0.3756614
H	-0.6647770	1.3210981	0.2670073
H	3.8246252	-2.2727134	-0.2577346
H	2.8189144	-4.4213530	-0.0922255
H	1.1819925	-4.5132897	-0.7879990
H	1.3913237	-4.4917467	0.9704153
H	-4.0961008	2.1853053	0.6110183
H	-2.3885180	2.2294075	0.2647106
H	-4.3286630	-0.8246995	1.9234734
H	-4.5062872	-1.2947621	0.2220639
H	-1.8822167	1.5390055	2.6743054
H	-3.6290832	1.5454528	3.0170118
H	-2.8032001	3.0570290	2.5810573
H	-6.5649008	-0.3051242	0.9389919
H	-5.8280757	0.7885671	-0.2504905
H	-5.7961886	1.1863843	1.4965143
C	4.4043110	3.8386580	0.3895779
H	4.2417769	4.9246044	0.4365945
H	5.3562981	3.6615877	-0.1464623
H	4.5207118	3.4675701	1.4259338
O	3.2838185	3.2704964	-0.2782327
H	3.4249533	2.3000999	-0.3230313
C	-3.4518669	0.7354350	-3.4533482
H	-2.9014058	-0.2061883	-3.6282625
H	-2.7248819	1.5665603	-3.4229156
H	-4.1242454	0.9016771	-4.3049677
O	-4.2690844	0.6792216	-2.2816694
H	-3.6942972	0.5285917	-1.5007755
C	7.3344837	-0.7908466	-0.7788022
H	8.0372074	-1.6344398	-0.8135554
H	7.3787789	-0.2685156	-1.7525467
H	7.6793877	-0.0919284	0.0056383
O	6.0424492	-1.3242649	-0.5031033
H	5.3988252	-0.5820496	-0.4544840

C460-(Meth)2/S0

Energy = -980.7927729870

C	-2.4498948	-0.3216147	0.0903915
C	-2.4324902	-1.7508511	0.1051879
C	-1.2551580	-2.4588818	-0.0593603
C	-0.0100996	-1.8169101	-0.2389378
C	-0.0399941	-0.4017392	-0.2382518
C	-1.2058276	0.3328387	-0.0721734
C	1.2586674	-2.4785550	-0.4005702
C	2.3891122	-1.7162791	-0.5592024
C	2.3493197	-0.2798848	-0.5585564
O	1.1121568	0.3325551	-0.3960529
O	3.3141061	0.4807567	-0.6897155
C	1.3466191	-3.9792821	-0.3965031
N	-3.6303945	0.3905932	0.2145573
C	-3.5818149	1.8254961	0.5229407
C	-4.8789088	-0.3436074	0.4864896
C	-3.2753812	2.1409980	1.9929208
C	-6.1573785	0.4706811	0.3009000
H	-3.3501465	-2.3117657	0.2620117
H	-1.2935949	-3.5488624	-0.0367931
H	-1.1091435	1.4154776	-0.0783540
H	3.3756856	-2.1636600	-0.6854291
H	2.3840692	-4.3096586	-0.5261923
H	0.7411406	-4.4144705	-1.2062989
H	0.9678249	-4.3946848	0.5502239
H	-4.5449759	2.2630067	0.2359161
H	-2.8415766	2.2986559	-0.1355517
H	-4.8610758	-0.7759482	1.5061649
H	-4.9198198	-1.1897212	-0.2139944
H	-2.3124858	1.7098788	2.2995172
H	-4.0552459	1.7401574	2.6565529
H	-3.2263483	3.2287412	2.1476555
H	-7.0168084	-0.2061690	0.4072613
H	-6.2085916	0.9209126	-0.7005895
H	-6.2750349	1.2645742	1.0504026
C	3.9545240	3.9315913	-0.0088100
H	3.7984686	5.0186518	0.0365885
H	4.9142080	3.7489777	-0.5291990
H	4.0522599	3.5592452	1.0291781
O	2.8418259	3.3709545	-0.6946761
H	2.9749583	2.3986078	-0.7336251
C	6.8680322	-0.6866392	-1.1785437
H	7.5674580	-1.5320103	-1.2330027
H	6.8543891	-0.1905403	-2.1665317
H	7.2596486	0.0325238	-0.4352378
O	5.5955752	-1.2102722	-0.8112401
H	4.9457734	-0.4717435	-0.7832464

C460-(Meth)2/S3

Energy = -980.7610000453

C	-2.1908318	-0.2633108	0.5481064
C	-2.2456179	-1.6065381	0.9186953
C	-1.0868951	-2.3879486	0.8585069
C	0.1593875	-1.8572672	0.4351959
C	0.1662810	-0.4815941	0.0708973
C	-0.9803620	0.3038514	0.1183048
C	1.3826361	-2.5975232	0.3520105
C	2.5401755	-1.9076698	-0.0883139
C	2.5331321	-0.5621233	-0.4407036
O	1.3156019	0.1548337	-0.3511213
O	3.4939538	0.1638865	-0.8460145
C	1.4269752	-4.0512735	0.7143698
N	-3.3742192	0.5762012	0.5732030
C	-3.7646519	1.2135742	1.8216544
C	-4.2976980	0.5234834	-0.5525296
C	-4.7613643	0.3913250	2.6627898
C	-4.8753089	1.8809522	-0.9681908
H	-3.1878377	-2.0558009	1.2353226
H	-1.1428852	-3.4387661	1.1423119
H	-0.9166108	1.3515955	-0.1748420
H	3.4948185	-2.4259164	-0.1663656
H	2.4385792	-4.4567944	0.5815901
H	0.7431730	-4.6556078	0.0913254
H	1.1332097	-4.2301489	1.7644270
H	-4.2052802	2.1961253	1.5913410
H	-2.8447128	1.3844658	2.3949073
H	-5.1288359	-0.1705316	-0.3093854
H	-3.7462769	0.0686847	-1.3844943
H	-4.3301070	-0.5767591	2.9467086
H	-5.7001317	0.2164560	2.1193115
H	-4.9985943	0.9447155	3.5818030
H	-5.4804543	1.7491749	-1.8753890
H	-4.0713625	2.5945724	-1.1945111
H	-5.5265617	2.3169964	-0.1986863
C	3.5972899	3.4833527	-0.5366672
H	3.6837118	4.5314148	-0.8529784
H	4.5246817	3.1911755	-0.0084833
H	2.7660531	3.3933246	0.1872756
O	3.3772829	2.6895759	-1.6860067
H	3.3226795	1.7257161	-1.3877167
C	6.3458029	0.2394061	-2.5422038
H	7.2648649	-0.1494818	-3.0008016
H	5.5454125	0.2802817	-3.3038895
H	6.5337059	1.2791237	-2.2113625
O	6.0007754	-0.6019203	-1.4575480
H	5.0664160	-0.3672894	-1.1718530

C500-DMF/S0

Energy = -1217.079130983

C	-0.8076007	1.1882879	-0.3674644
C	-0.6863837	-0.2354695	-0.3958208
C	0.5394944	-0.8495121	-0.2728390
C	1.7344752	-0.0996648	-0.1088134
C	1.5992984	1.3147003	-0.0837130
C	0.3687334	1.9511043	-0.2045289
C	3.0608354	-0.6273379	0.0301689
C	4.1417735	0.1974238	0.1858777
C	4.0053467	1.6377344	0.2177523
O	2.6865749	2.1358081	0.0741932
O	4.8955146	2.4523821	0.3536553
C	3.2841517	-2.1285275	0.0057431
F	2.8546359	-2.6828914	-1.1669481
F	2.6041179	-2.7556544	1.0122333
F	4.5911670	-2.4668493	0.1451731
N	-2.0406594	1.7498990	-0.5166942
C	-2.3152453	3.1793274	-0.4969938
C	-2.4229251	3.7828983	0.9110012
H	-1.5877779	-0.8340804	-0.5354123
H	0.5889883	-1.9369681	-0.3052653
H	0.3511156	3.0386270	-0.1650175
H	5.1525420	-0.1877744	0.2923046
H	-2.8493830	1.1173592	-0.5553345
H	-3.2593540	3.3305329	-1.0401524
H	-1.5375107	3.7021715	-1.0767796
H	-1.4944840	3.6384384	1.4804875
H	-3.2431400	3.3147526	1.4735963
H	-2.6219206	4.8633974	0.8507911
C	-4.9752227	-0.5757815	0.3764082
H	-4.5809793	-0.5352596	1.4146343
O	-4.4345196	0.0219796	-0.5609376

N	-6.0899775	-1.3429725	0.2750827
C	-6.7536896	-1.5216979	-1.0113243
H	-6.7705288	-2.5869207	-1.2886699
H	-7.7897743	-1.1528156	-0.9623147
H	-6.1974162	-0.9550491	-1.7658098
C	-6.6594371	-2.0163856	1.4337548
H	-6.0547892	-1.7916697	2.3219113
H	-7.6910606	-1.6760364	1.6149411
H	-6.6720305	-3.1073223	1.2837392

C500-DMF/S1

Energy = -1217.066968693

C	0.6076379	0.8812094	-0.4566343
C	0.7209872	-0.5250328	-0.4903192
C	1.9767245	-1.1155158	-0.3600685
C	3.1590299	-0.3701304	-0.1880523
C	3.0435145	1.0145691	-0.1513360
C	1.7701018	1.6544404	-0.2891401
C	4.5494859	-0.9458049	-0.0414602
C	5.5834054	-0.0494317	0.1126160
C	5.4424215	1.3763029	0.1436232
O	4.0709046	1.8776905	0.0053365
O	6.3060673	2.2309700	0.2705157
C	4.7645765	-2.3965446	-0.0514513
F	4.3121240	-3.0106141	-1.2214126
F	4.0594802	-3.0637225	0.9541479
F	6.0687593	-2.7508843	0.0911799
N	-0.6390112	1.4888728	-0.5883928
C	-0.8935840	2.9125954	-0.5714961
C	-1.0116157	3.5098586	0.8468448
H	-0.1682356	-1.1372645	-0.6364141
H	2.0443982	-2.2024275	-0.3972079
H	1.7539110	2.7423365	-0.2593241
H	6.6085037	-0.4024566	0.2234787
H	-1.4660341	0.8643490	-0.5958870
H	-1.8362835	3.0744131	-1.1144723
H	-0.1018663	3.4335687	-1.1315723
H	-0.0850153	3.3567907	1.4158638
H	-1.8388207	3.0439923	1.3993366
H	-1.2049109	4.5901179	0.7783947
C	-3.5096853	-0.7915111	0.3232578
H	-3.1129902	-0.7795593	1.3599912
O	-2.9941968	-0.1317614	-0.5906474
N	-4.5912960	-1.5932492	0.1877049
C	-5.2467867	-1.7471162	-1.1072610
H	-5.2354305	-2.8034820	-1.4154708
H	-6.2917892	-1.4063420	-1.0497019
H	-4.7036346	-1.1440429	-1.8424112
C	-5.1407694	-2.3294446	1.3189144
H	-4.5467987	-2.1193965	2.2175513
H	-6.1832182	-2.0297278	1.5069765
H	-5.1161626	-3.4128931	1.1260157

C500-DMSO/S0

Energy = -1521.781377618

C	-0.8505024	1.1251767	-0.2904396
C	-0.6861085	-0.2945780	-0.2798579
C	0.5631220	-0.8643171	-0.1860723
C	1.7391034	-0.0722543	-0.0936252
C	1.5592776	1.3372307	-0.1065718
C	0.3048416	1.9305585	-0.1977537
C	3.0860725	-0.5529856	0.0097162
C	4.1454323	0.3096977	0.0943899
C	3.9638967	1.7451042	0.0835286
O	2.6252387	2.1967030	-0.0200061
O	4.8323216	2.5914160	0.1534951
C	3.3569208	-2.0462589	0.0263586
F	2.9027257	-2.6541058	-1.1101199
F	2.7356857	-2.6598234	1.0783492
F	4.6786632	-2.3389300	0.1268058
N	-2.1069444	1.6408165	-0.4052300
C	-2.4303838	3.0589144	-0.4317652
C	-2.5094747	3.7131032	0.9553921
H	-1.5764643	-0.9201252	-0.3617097
H	0.6473689	-1.9501154	-0.1863555
H	0.2531432	3.0177523	-0.1914467
H	5.1714472	-0.0402078	0.1728600
H	-2.8876749	0.9739714	-0.4283770
H	-3.3975499	3.1574891	-0.9460574
H	-1.6924452	3.5859999	-1.0584203
H	-1.5560087	3.6234963	1.4937907
H	-3.2896448	3.2374382	1.5664885
H	-2.7501764	4.7827729	0.8625559
C	-5.2196654	-2.0480953	1.4301855
H	-4.5742012	-1.6174237	2.2039782
H	-6.1669927	-2.3826815	1.8729216
H	-4.7034477	-2.8689927	0.9175803
C	-6.5042006	-1.7169245	-0.9948084
H	-7.4366778	-2.0623764	-0.5296834
H	-6.7266913	-1.0622783	-1.8448619
H	-5.8782960	-2.5582654	-1.3165313
O	-4.1972365	-0.3981686	-0.4736884
S	-5.5498416	-0.6971577	0.2134667

C500-DMSO/S1

Energy = -1521.765770282

C	-0.9313068	1.1308422	-0.5137657
C	-0.7204840	-0.2384269	-0.7771647
C	0.5581873	-0.7764125	-0.6283515
C	1.6630689	-0.0080504	-0.2195421
C	1.4563823	1.3484639	0.0053758
C	0.1572576	1.9315983	-0.1313606
C	3.0672747	-0.5290790	-0.0058837
C	4.0579969	0.4125466	0.1479992
C	3.8349543	1.8256246	0.2574419
O	2.4300318	2.2384185	0.3040313
O	4.6559394	2.7257026	0.3493765
C	3.3377592	-1.9701687	0.0291784
F	3.0374053	-2.6215435	-1.1737902
F	2.5564334	-2.6465350	0.9637778
F	4.6341883	-2.2696908	0.3067185
N	-2.2174986	1.6701101	-0.6051105
C	-2.5488698	3.0757528	-0.5600186
C	-2.8399519	3.6040438	0.8614000
H	-1.5544206	-0.8577872	-1.1074576
H	0.7066071	-1.8350072	-0.8415013
H	0.0636571	2.9975987	0.0692684
H	5.1026303	0.1137215	0.2359601
H	-3.0038731	0.9925779	-0.5927764
H	-3.4443920	3.2181064	-1.1853058
H	-1.7345168	3.6546707	-1.0197912
H	-1.9617395	3.4905837	1.5108866
H	-3.6787464	3.0596261	1.3154815
H	-3.1045767	4.6702914	0.8126886
C	-4.3077440	-2.6482153	0.6148330
H	-3.2717878	-2.5203539	0.9486049
H	-4.8599769	-3.2673007	1.3339090
H	-4.3345382	-3.0811252	-0.3925765
C	-6.6877076	-1.4540957	-0.1375046
H	-7.2144383	-2.0947197	0.5817020
H	-7.2494302	-0.5271807	-0.2983137
H	-6.5210775	-1.9701068	-1.0907667
O	-4.3317592	-0.2101665	-0.5877076
S	-5.0541796	-0.9623269	0.5615357

C500-(Meth)4/S0

Energy = -1431.587287901

C	-1.6888835	-0.1396368	0.4428503
C	-1.6376734	-1.5618711	0.5305757
C	-0.4414369	-2.2387562	0.4286590
C	0.7858595	-1.5488432	0.2429538
C	0.7101768	-0.1350715	0.1672851
C	-0.4856809	0.5667602	0.2683633
C	2.0902854	-2.1356654	0.1209744
C	3.2060388	-1.3615906	-0.0540449
C	3.1041791	0.0745964	-0.1185361
O	1.8378341	0.6309280	-0.0058493
O	4.0367597	0.8659202	-0.2688561
C	2.2474415	-3.6468987	0.1818636
F	1.5315963	-4.2578236	-0.8085304
F	1.7924651	-4.1444040	1.3688818
F	3.5328274	-4.0433593	0.0476310
N	-2.9226033	0.4837219	0.4793076
C	-3.0853907	1.9184957	0.7426019
C	-2.8076881	2.3281479	2.1935460
H	-2.5703564	-2.1101749	0.6763750
H	-0.4415199	-3.3251285	0.5010929
H	-0.4483237	1.6527064	0.2050352
H	4.2091485	-1.7778216	-0.1488775
H	-3.6921308	-0.1097821	0.8311702
H	-4.1199308	2.1713415	0.4695472
H	-2.4392598	2.4804782	0.0517984
H	-1.7771485	2.0876333	2.4882842
H	-3.4902158	1.8116510	2.8834338
H	-2.9521708	3.4112310	2.3173664
C	-6.4657627	-1.5013173	1.2529184
H	-6.3295547	-1.6772878	2.3274913
H	-6.9957089	-2.3687974	0.8247087
H	-7.0926462	-0.6026082	1.1207622
O	-5.1651239	-1.3422613	0.6769774
H	-5.2477934	-1.1534203	-0.2921528
C	4.5164634	4.4242909	0.2246009
H	4.2769745	5.4964947	0.2445460
H	5.4402640	4.2940997	-0.3703457
H	4.7280170	4.1035493	1.2622493
O	3.3980381	3.7512131	-0.3440844
H	3.6034538	2.7925524	-0.3590485
C	-4.3265736	-0.8406009	-3.0770610
H	-3.5834532	-1.6500813	-2.9889568
H	-3.9296079	-0.0570096	-3.7422615
H	-5.2407066	-1.2473193	-3.5258736
O	-4.6935682	-0.3020913	-1.7966360
H	-3.8970706	0.0739426	-1.3575559
C	7.4724619	-0.3894333	-1.1752845

H	8.0037427	0.5193834	-0.8376152
H	7.1410026	-0.2301003	-2.2180029
H	8.1871786	-1.2229250	-1.1675804
O	6.3992513	-0.7428451	-0.3044953
H	5.7428626	-0.0121938	-0.3080776

C500-(Meth)4/S3

Energy = -1431.572922614

C	-1.5697693	-0.0104676	0.7827003
C	-1.5909556	-1.4218044	0.7916646
C	-0.4101187	-2.1309695	0.5774572
C	0.8265294	-1.4961187	0.3528568
C	0.8350573	-0.1082359	0.3500865
C	-0.3533303	0.6536640	0.5594404
C	2.1557420	-2.1866979	0.1384200
C	3.2643445	-1.3865017	0.0162845
C	3.2165192	0.0445818	0.0234367
O	1.9422421	0.6562245	0.1751212
O	4.1667611	0.8390654	-0.1001122
C	2.2381649	-3.6581250	0.0913294
F	1.4407689	-4.2026628	-0.9098558
F	1.7741377	-4.2607392	1.2547921
F	3.4961541	-4.1186809	-0.1147308
N	-2.7558565	0.7129361	0.9378557
C	-2.8488663	2.1153517	1.2767059
C	-2.5698343	2.4182891	2.7645562
H	-2.5313667	-1.9453831	0.9583179
H	-0.4463847	-3.2197555	0.5986974
H	-0.2685907	1.7380457	0.5083222
H	4.2624327	-1.8110349	-0.1060236
H	-3.6397196	0.1736299	0.8546827
H	-3.8668038	2.4368970	1.0164026
H	-2.1536448	2.7009995	0.6525077
H	-1.5628100	2.0862900	3.0499392
H	-3.3012884	1.9136285	3.4095076
H	-2.6400561	3.5019424	2.9358030
C	-6.3271812	-1.1303119	0.7254108
H	-6.2962850	-1.0882662	1.8213840
H	-6.5976530	-2.1570797	0.4269862
H	-7.1064642	-0.4361844	0.3682593
O	-5.0271897	-0.7693960	0.2458612
H	-5.0229001	-0.7538655	-0.7460275
C	4.3163005	4.4227289	0.2313003
H	3.9467970	5.4581318	0.2511338
H	5.2825614	4.4176297	-0.3084349
H	4.5062656	4.1081003	1.2747227
O	3.3255894	3.6282657	-0.4111598
H	3.6184866	2.6909178	-0.3587844
C	-4.9061794	-1.5058723	-3.4963551
H	-4.1040195	-2.2578783	-3.4348784
H	-4.9163149	-1.0575834	-4.5014548
H	-5.8706772	-1.9954140	-3.3214051
O	-4.7697890	-0.4897949	-2.4807818
H	-3.9414521	-0.0061310	-2.6411723
C	7.3952974	-0.2163412	-1.3213454
H	7.6816723	0.8491096	-1.3953855
H	6.8313064	-0.4834146	-2.2349531
H	8.3174635	-0.8134963	-1.3071401
O	6.6796391	-0.5079647	-0.1253721
H	5.8752680	0.0597419	-0.1065729

C503-DMF/S0

Energy = -1256.407140059

C	-0.6777625	0.8025487	-0.1644279
C	-0.3764386	-0.6013699	-0.0608581
C	0.9445758	-1.0045092	-0.0052096
C	2.0318988	-0.0945156	-0.0452683
C	1.7051627	1.2816575	-0.1518031
C	0.3901308	1.7242686	-0.2050665
C	3.4264724	-0.4265684	0.0120107
C	4.3897871	0.5444474	-0.0369252
C	4.0561701	1.9485577	-0.1485414
O	2.6742865	2.2519110	-0.1979223
O	4.8335893	2.8805542	-0.2016659
C	3.8564589	-1.8770484	0.1313591
F	3.4154701	-2.6229855	-0.9256028
F	3.3563537	-2.4592644	1.2623049
F	5.2052383	-2.0226847	0.1784926
N	-1.9781918	1.2088553	-0.2410488
C	-2.4159274	2.5982027	-0.2976034
C	-2.4321421	3.3045306	1.0650903
C	-1.4920146	-1.6123087	-0.0211799
H	1.1510802	-2.0718115	0.0729459
H	0.2172985	2.7962004	-0.2766397
H	5.4500302	0.3090511	0.0055365
H	-2.7289362	0.5188626	-0.1649574
H	-3.4283253	2.5884087	-0.7239843
H	-1.7794923	3.1493386	-1.0086197
H	-1.4341435	3.3152798	1.5243021
H	-3.1191393	2.7950734	1.7550531
H	-2.7666065	4.3466740	0.9519092
H	-2.1128819	-1.5669767	-0.9316628
H	-2.1658276	-1.4461891	0.8354926
H	-1.0886597	-2.6296747	0.0602025
C	-5.4193650	-0.9590363	-0.2028685
H	-5.0259527	-1.9616526	-0.4780276
O	-4.6854353	0.0242068	-0.0671289
N	-6.7683839	-0.9622935	-0.0412572
C	-7.4765594	0.2591908	0.3219429
H	-8.2060052	0.5266465	-0.4581457
H	-8.0118488	0.1235375	1.2743794
H	-6.7408352	1.0636792	0.4269414
C	-7.5546978	-2.1735120	-0.2258011
H	-6.8891657	-3.0052095	-0.4909080
H	-8.0923910	-2.4346826	0.6992005
H	-8.2917984	-2.0420473	-1.0335825

C503-DMF/S1

Energy = -1256.395105824

C	-0.7139476	0.8001715	-0.1570314
C	-0.4323743	-0.5873453	-0.0583286
C	0.9101853	-0.9754288	-0.0153222
C	1.9954293	-0.0790713	-0.0596783
C	1.7031343	1.2740697	-0.1575198
C	0.3472050	1.7232024	-0.2122388
C	3.4564215	-0.4610980	0.0012632
C	4.3722736	0.5640667	-0.0947304
C	4.0468672	1.9531329	-0.2255185
O	2.6158774	2.2696498	-0.2253440
O	4.7993426	2.9106184	-0.3273159
C	3.8621460	-1.8602239	0.1652871
F	3.4002881	-2.6917088	-0.8602991
F	3.3389380	-2.4526688	1.3169950
F	5.2093569	-2.0302209	0.2192582
N	-2.0293762	1.2566502	-0.2139694
C	-2.4434392	2.6450022	-0.2261578
C	-2.4550704	3.2972513	1.1715238
C	-1.5405925	-1.6064462	-0.0058881
H	1.1247323	-2.0420006	0.0603648
H	0.1834221	2.7950376	-0.3074029
H	5.4413235	0.3543492	-0.0683611
H	-2.8014295	0.5782321	-0.1354357
H	-3.4579996	2.6624775	-0.6470197
H	-1.7937482	3.2189701	-0.9046739
H	-1.4517878	3.2892899	1.6180513
H	-3.1393597	2.7609535	1.8420608
H	-2.7923762	4.3405050	1.0889071
H	-2.1637966	-1.5871531	-0.9170022
H	-2.2146106	-1.4488702	0.8530220
H	-1.1227025	-2.6171065	0.0841457
C	-5.3246618	-0.8834500	-0.2862952
H	-4.8702923	-1.8013874	-0.7150942
O	-4.6548124	0.1244482	-0.0263923
N	-6.6597202	-1.0074676	-0.0909684
C	-7.4379391	0.0920120	0.4687737
H	-8.2141045	0.4125004	-0.2428693
H	-7.9244818	-0.2225259	1.4046056
H	-6.7588661	0.9267342	0.6715183
C	-7.3676642	-2.2353604	-0.4290504
H	-6.6585159	-2.9679948	-0.8349346
H	-7.8467323	-2.6659468	0.4637888
H	-8.1444060	-2.0407562	-1.1847354

C503-DMSO/S0

Energy = -1561.109006776

C	-0.7061859	0.7121537	-0.1224990
C	-0.3501423	-0.6764489	0.0102851
C	0.9867100	-1.0258744	0.0516450
C	2.0376600	-0.0766156	-0.0318709
C	1.6562719	1.2825477	-0.1686867
C	0.3240570	1.6725631	-0.2084302
C	3.4447076	-0.3526021	0.0071186
C	4.3686694	0.6530768	-0.0847968
C	3.9793658	2.0396925	-0.2256110
O	2.5858283	2.2879188	-0.2593836
O	4.7183635	2.9999323	-0.3173153
C	3.9333578	-1.7818602	0.1521507
F	3.5041269	-2.5685906	-0.8799586
F	3.4763041	-2.3570924	1.3047327
F	5.2878239	-1.8738699	0.1782805
N	-2.0236144	1.0673489	-0.1891920
C	-2.5103463	2.4394066	-0.2504021
C	-2.5133936	3.1660167	1.1019767
C	-1.4238803	-1.7288518	0.0893450
H	1.2354808	-2.0819587	0.1542121
H	0.1092042	2.7349510	-0.3039921
H	5.4377850	0.4593312	-0.0569933
H	-2.7468108	0.3584409	-0.0370428
H	-3.5339121	2.3905192	-0.6479913
H	-1.9159131	3.0018175	-0.9881445
H	-1.5030956	3.2207813	1.5297449
H	-3.1584385	2.6399829	1.8194101
H	-2.8901032	4.1933200	0.9851407
H	-2.0487604	-1.7394178	-0.8188312

H	-2.1087706	-1.5639240	0.9364345
H	-0.9787207	-2.7254994	0.2034229
C	-7.2123008	-0.2017387	0.8737167
H	-7.1093093	0.8291342	1.2306555
H	-8.2084516	-0.3514333	0.4371876
H	-7.0206234	-0.9075533	1.6912038
C	-6.2529289	-2.2291035	-0.7368144
H	-7.2613276	-2.3497219	-1.1538763
H	-5.5038837	-2.5631444	-1.4634586
H	-6.1392512	-2.7775697	0.2063684
O	-4.5655497	-0.3695411	0.3076609
S	-5.9225451	-0.4366666	-0.4287181

C503-DMSO/S1

Energy = -1561.096940516

C	-0.7420675	0.8120678	-0.1580578
C	-0.4509455	-0.5774274	-0.1684142
C	0.8936990	-0.9591255	-0.1309336
C	1.9710894	-0.0542196	-0.0831106
C	1.6694657	1.3005147	-0.0842958
C	0.3119669	1.7437864	-0.1261634
C	3.4339852	-0.4293422	-0.0154028
C	4.3426104	0.6018960	-0.1051231
C	4.0058762	1.9937353	-0.1752721
O	2.5783040	2.3034483	-0.0902836
O	4.7518583	2.9565929	-0.2763287
C	3.8473023	-1.8283003	0.1289973
F	3.4255130	-2.6424602	-0.9297435
F	3.2946120	-2.4492854	1.2491860
F	5.1943479	-1.9879217	0.2171661
N	-2.0613261	1.2609367	-0.1885946
C	-2.4845565	2.6454018	-0.1479621
C	-2.5382339	3.2314962	1.2780377
C	-1.5517571	-1.6044668	-0.2174449
H	1.1160441	-2.0268052	-0.1401830
H	0.1411541	2.8185894	-0.1397985
H	5.4133889	0.3988831	-0.1025128
H	-2.8298260	0.5766578	-0.0998209
H	-3.4903358	2.6756503	-0.5898627
H	-1.8223246	3.2524898	-0.7834113
H	-1.5470620	3.2095284	1.7505591
H	-3.2364507	2.6587667	1.9023730
H	-2.8825635	4.2749220	1.2353506
H	-2.1804604	-1.4972287	-1.1177767
H	-2.2236981	-1.5389917	0.6552290
H	-1.1274432	-2.6163985	-0.2307829
C	-6.9089447	-0.5248205	-1.2447024
H	-6.4856178	-0.2101335	-2.2051853
H	-7.6116501	-1.3542557	-1.3979260
H	-7.3902332	0.3231979	-0.7423968
C	-6.4533576	-1.4369803	1.3258897
H	-7.1645899	-2.2528138	1.1423137
H	-5.7254042	-1.7382040	2.0874468
H	-6.9655877	-0.5159961	1.6298426
O	-4.6473457	0.1601590	0.0857009
S	-5.4919604	-1.1038457	-0.2135808

C503-(Meth)4/S0

Energy = -1470.915002970

C	-1.4087711	-0.3871623	0.4013211
C	-1.2238750	-1.8104162	0.3537656
C	0.0566949	-2.3169564	0.2115904
C	1.2037592	-1.4894352	0.1155811
C	0.9815570	-0.0929211	0.1684928
C	-0.2860444	0.4544345	0.3138853
C	2.5642952	-1.9229275	-0.0374990
C	3.5911887	-1.0218899	-0.1236807
C	3.3376534	0.3962570	-0.0642280
O	2.0207189	0.8038226	0.0875707
O	4.1837981	1.2897104	-0.1329846
C	2.8838339	-3.4075635	-0.1071120
F	2.2493025	-4.0015762	-1.1604671
F	2.4735229	-4.0555252	1.0235212
F	4.2061454	-3.6504805	-0.2484879
N	-2.6918903	0.1302989	0.4723078
C	-2.9667234	1.5203088	0.8702908
C	-2.6825269	1.8202081	2.3459104
C	-2.4091501	-2.7354768	0.4441880
H	0.1802368	-3.3989482	0.1777545
H	-0.3721778	1.5386034	0.3509238
H	4.6323829	-1.3197738	-0.2481857
H	-3.4345928	-0.5138046	0.7746437
H	-4.0297675	1.6916612	0.6532173
H	-2.3945145	2.1965856	0.2177766
H	-1.6300595	1.6367926	2.6016882
H	-3.3102825	1.1941625	2.9954544
H	-2.9067099	2.8736075	2.5680067
H	-3.1212154	-2.5682143	-0.3796607
H	-2.9682104	-2.5970657	1.3840089
H	-2.0850158	-3.7826882	0.4021453
C	4.4521731	4.8726283	-0.4566572
H	4.1557079	5.9302683	-0.4242439
H	4.7192977	4.6264833	-1.5020669
H	5.3593412	4.7557382	0.1664551
O	3.3520441	4.1092229	0.0259234
H	3.6118869	3.1637718	0.0018565
C	-6.5245178	-1.6518292	0.9442180
H	-6.5467678	-1.7402238	2.0379480
H	-6.3739531	-2.6580214	0.5155610
H	-7.5040720	-1.2688167	0.6097039
O	-5.4624630	-0.7553137	0.6088870
H	-5.4037865	-0.6650283	-0.3736088
C	-4.5812483	0.4411265	-3.0636382
H	-3.7098641	0.3625444	-3.7335178
H	-4.7485108	1.5019300	-2.8121056
H	-5.4632470	0.0636834	-3.5949102
O	-4.4167500	-0.3732213	-1.8931655
H	-3.6255510	-0.0754544	-1.3874927
C	7.8911170	0.4329265	-0.3840127
H	8.6336354	-0.3411772	-0.6194584
H	7.9670628	0.6646196	0.6944570
H	8.1533102	1.3427387	-0.9545148
O	6.6123534	-0.0833722	-0.7462058
H	5.9290560	0.5919390	-0.5419349

C503-(Meth)3/S0

Energy = -1355.127791449

C	-1.9495044	-0.3686524	0.1786898
C	-1.7654995	-1.7916911	0.0475889
C	-0.4941474	-2.2913295	-0.1614944
C	0.6554253	-1.4630258	-0.2459486
C	0.4389096	-0.0698701	-0.1018152
C	-0.8184315	0.4724194	0.1140512
C	2.0050310	-1.8887742	-0.4680097
C	3.0349084	-0.9856509	-0.5385306
C	2.7890342	0.4247858	-0.3937548
O	1.4806641	0.8263675	-0.1663004
O	3.6347693	1.3219834	-0.4490195
C	2.3157279	-3.3673120	-0.6330327
F	1.6513373	-3.8989776	-1.7023236
F	1.9332555	-4.0823925	0.4674143
F	3.6331252	-3.6068492	-0.8237202
N	-3.2041775	0.1373294	0.3567946
C	-3.5164452	1.5516197	0.5419480
C	-3.2817205	2.0569489	1.9712986
C	-2.9466493	-2.7200468	0.1487105
H	-0.3762230	-3.3701422	-0.2596377
H	-0.8966642	1.5528012	0.2160452
H	4.0696870	-1.2783157	-0.7157890
H	-4.0082920	-0.4912393	0.3206234
H	-4.5745438	1.6730292	0.2723208
H	-2.9358462	2.1523925	-0.1772042
H	-2.2340935	1.9306979	2.2765858
H	-3.9125208	1.5097918	2.6857855
H	-3.5287768	3.1263843	2.0419848
H	-3.7143658	-2.4993496	-0.6104514
H	-3.4392831	-2.6422167	1.1321880
H	-2.6321681	-3.7625293	0.0139266
C	3.8121316	4.8926704	-0.7927366
H	3.5051968	5.9465403	-0.7372347
H	3.9547967	4.6362473	-1.8598624
H	4.7903341	4.7975961	-0.2835895
O	2.7916232	4.1202538	-0.1709152
H	3.0571502	3.1770640	-0.2250802
C	-7.0031892	-1.5594437	0.7131733
H	-6.6517429	-1.6033255	1.7504625
H	-7.1405924	-2.5887343	0.3433989
H	-7.9710887	-1.0327745	0.6931927
O	-5.9979404	-0.8503502	-0.0328933
H	-6.2888073	-0.7898626	-0.9582686
C	7.2751833	0.4419756	-0.5606268
H	8.0523009	-0.2867674	-0.8277970
H	7.1903147	0.4639308	0.5417874
H	7.6095098	1.4387697	-0.9024583
O	6.0692906	0.0273052	-1.1977325
H	5.3551999	0.6571457	-0.9538853

C503-(Meth)3/S3

Energy = -1355.116509710

C	-1.9473157	-0.3792426	0.1520519
C	-1.7882175	-1.7864197	0.0445145
C	-0.4969038	-2.2811832	-0.1588887
C	0.6524496	-1.4717467	-0.2567116
C	0.4735417	-0.1041911	-0.1332263
C	-0.8201308	0.4585184	0.0694436
C	2.0647873	-1.9580644	-0.4871759
C	3.0520385	-1.0028420	-0.5444176
C	2.8096883	0.3999167	-0.4046140
O	1.4666547	0.8202010	-0.1919488
O	3.6468334	1.3214802	-0.4401073
C	2.3505308	-3.3955223	-0.6282444
F	1.6579021	-3.9803233	-1.6843234
F	1.9474294	-4.1334584	0.4822463
F	3.6631959	-3.6654210	-0.8225616

N	-3.2126452	0.1850375	0.3121807
C	-3.4898718	1.5853497	0.5697827
C	-3.2560401	2.0040644	2.0353959
C	-2.9682323	-2.7169910	0.1507862
H	-0.3768224	-3.3616951	-0.2423783
H	-0.8855953	1.5432633	0.1307514
H	4.0974014	-1.2685661	-0.7185253
H	-4.0384772	-0.4249379	0.2540923
H	-4.5426214	1.7464015	0.3020682
H	-2.8785632	2.2135961	-0.0979625
H	-2.2122073	1.8377058	2.3319507
H	-3.9067258	1.4349618	2.7123491
H	-3.4834726	3.0733397	2.1506488
H	-3.7185607	-2.5390855	-0.6376625
H	-3.4876689	-2.6197432	1.1191352
H	-2.6382948	-3.7592533	0.0587731
C	3.7355587	4.8363510	-0.7885335
H	3.4221455	5.8884141	-0.7267238
H	3.8536358	4.5786901	-1.8584929
H	4.7277990	4.7498236	-0.3056193
O	2.7396099	4.0548322	-0.1395069
H	3.0229829	3.1140720	-0.1932051
C	-6.8797005	-1.5081568	0.7623751
H	-6.5389648	-1.4304446	1.8010051
H	-6.8923000	-2.5706749	0.4714188
H	-7.8990847	-1.0966236	0.6946440
O	-5.9521951	-0.7457440	-0.0356357
H	-6.2407447	-0.7879938	-0.9630895
C	7.2254781	0.4557543	-0.5111075
H	8.0159214	-0.2608444	-0.7744236
H	7.0559113	0.3916213	0.5799149
H	7.5957346	1.4722826	-0.7429434
O	6.0709077	0.1121288	-1.2705015
H	5.3300966	0.7005906	-0.9956650