Electronic Supplementary Material (ESI) for Energy & Environmental Science

On-line Supporting Information

Controlling dye aggregation, injection energetics and catalytic recombination in organic sensitizer based dye cells using a single electrolyte additive

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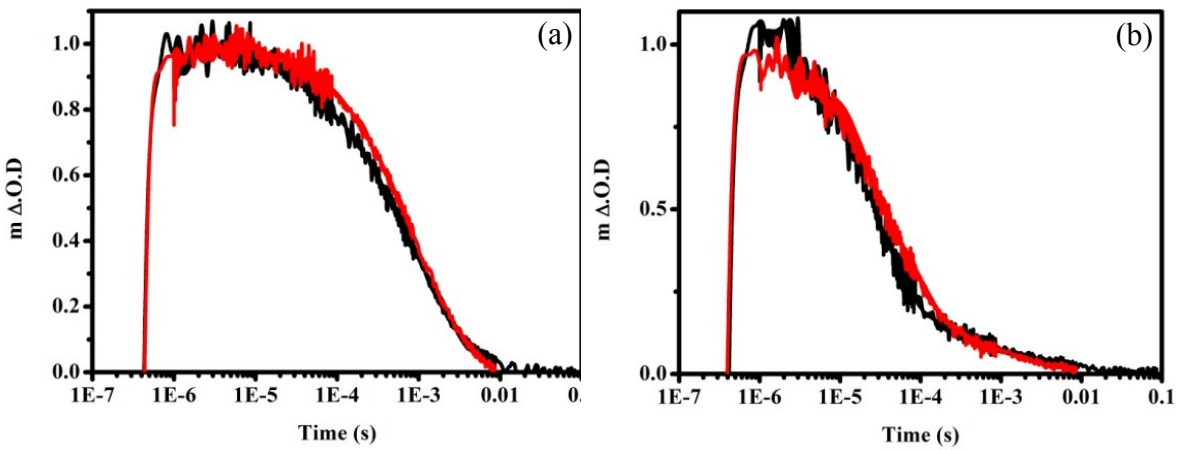
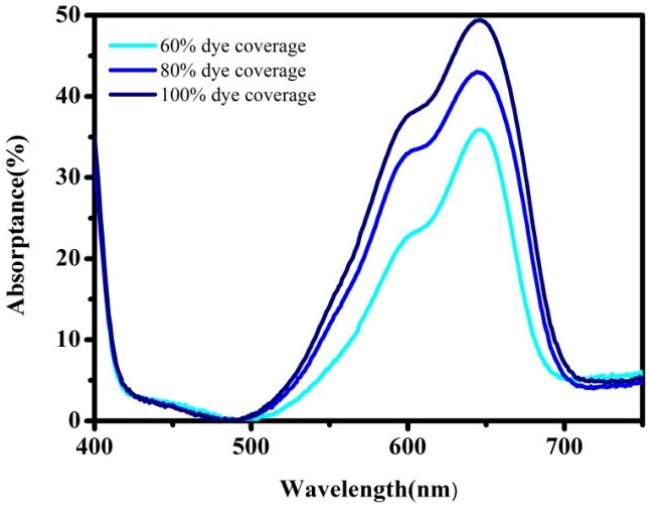
Transient Absorption kinetics

Figure S1: Normalized Transient Absorption kinetics (TAS) for DSC devices recorded under 1sun AM 1.5G simulated illumination in ACN only (black) and 1:1 ACN:bromobenzene (red) in the absence (a) and presence of iodide/tri-iodide (b). Kinetics were recorded at 800 nm following excitation at 600 nmshow the Electron lifetime as a function of photo-voltage.



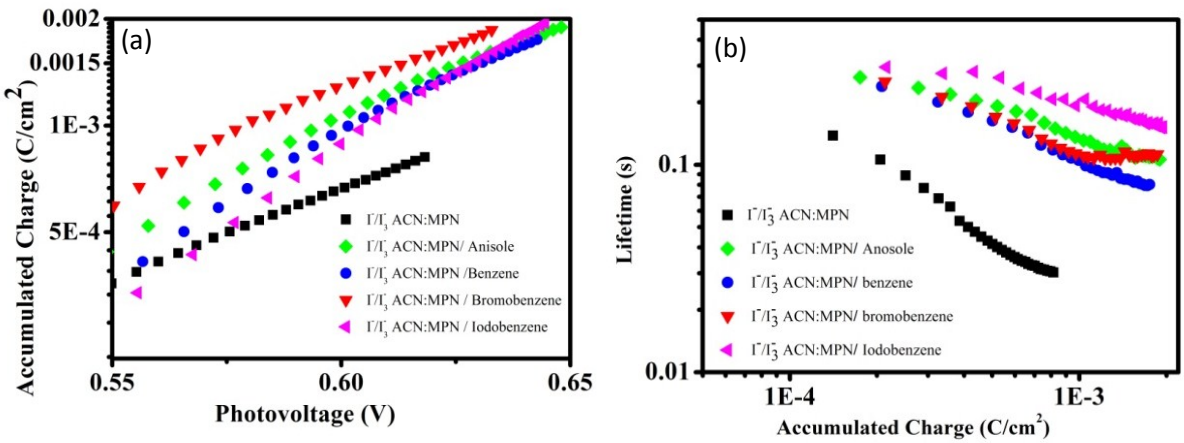
Absorption spectra

Figure S2: Absorption spectra of mesoporouse TiO_2 electrodes sensitized by SQ-1 dye for different dye coverage: 4h (100% =dark Blue), 2h (80% =turquiose), 10 min (60%=light blue).



Charge Extraction and Transient Photovoltage

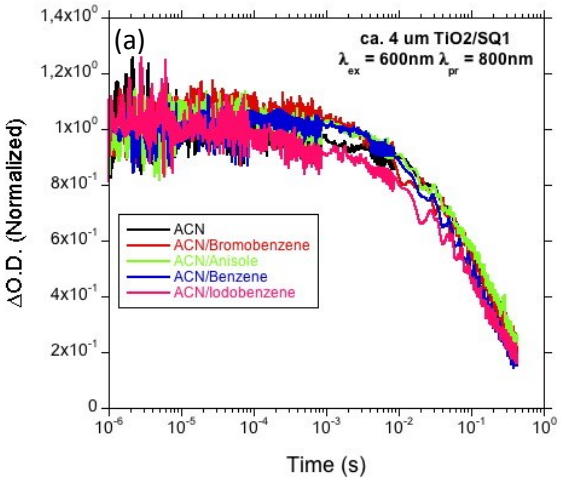
(a) Accumulated charge as a function of the photo-voltage for the reference cell containing I^-/I_3^- in ACN (black) and the samples cell with I^-/I_3^- in ACN and anisole (green),benzene (blue), bromobenzene (red) and Iodobenzene(pink). (b) Electron lifetime as a function of charge for the reference cell and the samples cells.

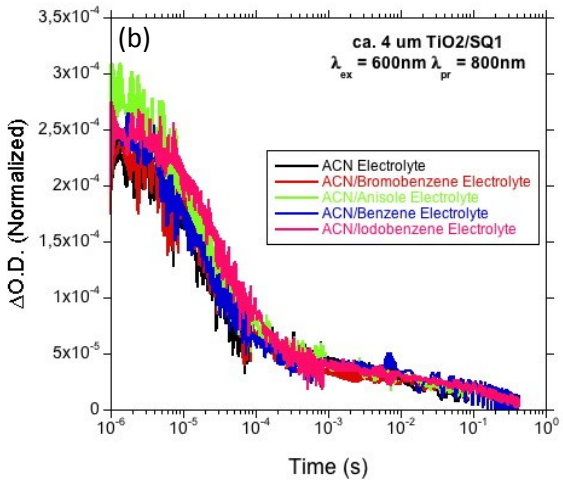


Transient absorption

Below are the TAS data recorded of TiO_2/SQ1 films in a cuvette containing electrolyte solutions with different benzene additives in the absence (a) and presence (b) of the I^-/I_3^- red/ox couple. As you can see the kinetics are identical.

These were recorded under lower light conditions than those in the paper (1 sun). Moreover, in the paper the cells were sealed. Below are films only.





Computational Information

Optimized geometries of the SQ-1 bromobenzene complexes:

UPBE1PBE

1

C	-6.60648	2.53546	-1.86691
C	-5.82167	1.44773	-2.23871
C	-4.58735	1.31386	-1.61094
C	-4.12900	2.21306	-0.64752
C	-4.91418	3.28954	-0.28516
C	-6.16200	3.44759	-0.90175
C	-2.76459	1.78689	-0.16773
C	-2.54236	0.53097	-0.99175
N	-3.60616	0.32282	-1.78963
C	-1.45575	-0.36209	-1.02069
C	-0.26400	-0.37619	-0.32878
C	0.57184	0.32957	0.67669
C	1.66058	-0.66063	0.49028
C	0.81141	-1.38064	-0.49886
O	0.47363	1.31674	1.38404
O	0.90500	-2.37423	-1.19718
C	2.88535	-0.61119	1.10681
C	4.02562	-1.43850	0.99992
C	4.27461	-2.66663	0.14427
C	5.68928	-3.01236	0.53452

C	6.15355	-2.08429	1.46537
N	5.12353	-1.15532	1.71053
C	7.43210	-2.13603	2.01041
C	8.25518	-3.17673	1.58558
C	7.80677	-4.11827	0.65518
C	6.51838	-4.04218	0.12070
C	-6.98384	4.61629	-0.48665
O	-6.63453	5.42352	0.34476
O	-8.15897	4.68468	-1.13094
C	-3.74139	-0.77993	-2.72699
C	-2.78678	1.47040	1.33989
C	-1.71010	2.86307	-0.49363
C	3.30704	-3.81490	0.48503
C	4.20071	-2.30928	-1.35483
C	5.25915	-0.03491	2.62780
H	5.24637	0.90936	2.07661
H	-7.57688	2.68210	-2.32805
H	-6.18107	0.75001	-2.98702
H	-4.60296	4.01791	0.45823
H	-1.54009	-1.20229	-1.70863
H	2.96647	0.23152	1.79145
H	7.79493	-1.41097	2.73078
H	9.26079	-3.25430	1.98621
H	8.47068	-4.91858	0.34381
H	6.18012	-4.77848	-0.60280
H	-3.73036	-1.73497	-2.19531
H	-2.92852	-0.75793	-3.45721
H	-4.68684	-0.68543	-3.25597
H	-3.07766	2.37341	1.88439
H	-1.79480	1.17425	1.68452
H	-3.51382	0.68556	1.56866
H	-1.98656	3.79114	0.01491
H	-1.66697	3.06438	-1.56786
H	-0.72655	2.56242	-0.12948
H	2.28768	-3.55965	0.19069
H	3.34300	-4.05489	1.55048
H	3.60648	-4.70208	-0.08058
H	3.17551	-2.07401	-1.64509
H	4.52416	-3.17596	-1.93831
H	4.86048	-1.47128	-1.59783
H	6.20434	-0.12123	3.15879
H	4.44554	-0.05031	3.35657
H	-8.62262	5.46899	-0.80069
C	0.94921	-2.52495	3.76249
C	0.36333	-3.65832	3.20998
C	-1.00382	-3.64461	2.94152
C	-1.76669	-2.51495	3.23216
C	-1.16009	-1.39223	3.79223
C	0.20689	-1.38891	4.06267
Br	2.79392	-2.56649	4.19905
H	0.95919	-4.54112	3.00371
H	-1.47132	-4.52763	2.51588
H	-2.83526	-2.51689	3.03831
H	-1.74986	-0.51279	4.03393
H	0.68104	-0.52068	4.50767

2

C	-6.72110	2.44846	-1.65282
C	-5.91762	1.41242	-2.11950
C	-4.66262	1.27301	-1.53573
C	-4.20133	2.11674	-0.52477
C	-5.00540	3.14241	-0.06823
C	-6.27389	3.30561	-0.63951
C	-2.81215	1.69912	-0.11358
C	-2.57813	0.51355	-1.03266
N	-3.65894	0.32759	-1.81168
C	-1.46705	-0.34180	-1.15687
C	-0.25700	-0.37061	-0.49927
C	0.58421	0.27891	0.54019
C	1.66865	-0.70449	0.29967
C	0.82616	-1.35164	-0.74378
O	0.48847	1.22281	1.30408
O	0.92545	-2.29176	-1.51201
C	2.87045	-0.73167	0.96250
C	3.98723	-1.58996	0.85108
C	4.22899	-2.77718	-0.06310
C	5.61859	-3.18690	0.35324
C	6.07786	-2.32437	1.34747
N	5.06695	-1.38120	1.61353
C	7.33848	-2.43947	1.92362
C	8.14750	-3.47653	1.46473
C	7.70306	-4.35400	0.47157
C	6.43340	-4.21431	-0.09398
C	-7.11469	4.41994	-0.12476
O	-6.76309	5.18123	0.74795
O	-8.30999	4.49592	-0.73011
C	-3.79287	-0.71417	-2.81686
C	-2.78261	1.27375	1.36746
C	-1.79815	2.82730	-0.38813
C	3.21847	-3.91360	0.18240
C	4.21402	-2.33755	-1.54183
C	5.20601	-0.32061	2.59862
H	5.28613	0.64975	2.10055
H	-7.70796	2.59770	-2.07667
H	-6.27902	0.75727	-2.90428
H	-4.69333	3.82691	0.71538
H	-1.55018	-1.13591	-1.89777
H	2.95101	0.06689	1.69827
H	7.69599	-1.76574	2.69447
H	9.13965	-3.60133	1.88667
H	8.35621	-5.15245	0.13356
H	6.09889	-4.89940	-0.86778
H	-3.73965	-1.70118	-2.35008
H	-3.00382	-0.62002	-3.56712
H	-4.75642	-0.61254	-3.31059
H	-3.08369	2.12557	1.98390
H	-1.77330	0.98601	1.66545
H	-3.47869	0.45209	1.55903
H	-2.08465	3.70642	0.19606
H	-1.79297	3.10832	-1.44522

H	-0.79625	2.52990	-0.07471
H	2.21710	-3.61506	-0.13238
H	3.21077	-4.21652	1.23223
H	3.51212	-4.77723	-0.42130
H	3.20589	-2.05428	-1.84878
H	4.52847	-3.18179	-2.16201
H	4.90653	-1.50954	-1.71908
H	6.10320	-0.49742	3.18721
H	4.34753	-0.32534	3.27298
H	-8.78488	5.24287	-0.33553
C	4.28400	-2.71003	5.27909
C	4.23136	-1.61192	6.13092
C	5.23747	-1.45002	7.08171
C	6.27531	-2.37587	7.17313
C	6.30470	-3.47343	6.31455
C	5.30413	-3.65126	5.36028
Br	2.89267	-2.95410	4.01041
H	3.40943	-0.90580	6.06861
H	5.20086	-0.60077	7.75766
H	7.05252	-2.24931	7.92048
H	7.10314	-4.20573	6.39126
H	5.31342	-4.51170	4.69947

3

C	-6.65808	2.42211	-1.80299
C	-5.90497	1.28856	-2.09203
C	-4.62912	1.22056	-1.54059
C	-4.09871	2.22753	-0.73430
C	-4.85499	3.34765	-0.44925
C	-6.14472	3.43904	-0.98687
C	-2.70165	1.85291	-0.31210
C	-2.54909	0.49866	-0.97513
N	-3.66618	0.20187	-1.66006
C	-1.46741	-0.40624	-0.96974
C	-0.22654	-0.34291	-0.37928
C	0.69535	0.47441	0.45717
C	1.74076	-0.57241	0.35303
C	0.81734	-1.39098	-0.47711
O	0.66913	1.55312	1.02101
O	0.84292	-2.47342	-1.03570
C	2.99204	-0.50364	0.92013
C	4.07971	-1.40178	0.90315
C	4.22600	-2.76117	0.24394
C	5.63251	-3.13076	0.64202
C	6.18073	-2.10868	1.41552
N	5.21479	-1.09154	1.54709
C	7.47102	-2.16255	1.93264
C	8.21710	-3.30302	1.64386
C	7.68484	-4.33801	0.87004
C	6.38592	-4.25917	0.36217
C	-6.94704	4.64213	-0.63953
O	-6.57968	5.50155	0.13165
O	-8.13246	4.68017	-1.26565
C	-3.87543	-1.01101	-2.43452
C	-2.59548	1.75561	1.22233

C	-1.67467	2.85385	-0.88200
C	3.21047	-3.76929	0.81694
C	4.10056	-2.65424	-1.28875
C	5.44362	0.13510	2.29363
H	5.35592	1.00200	1.63394
H	-7.65912	2.52101	-2.20785
H	-6.31913	0.50729	-2.71972
H	-4.48287	4.15232	0.17642
H	-1.60892	-1.33122	-1.52743
H	3.14100	0.42253	1.47390
H	7.89878	-1.36789	2.53417
H	9.22879	-3.38537	2.02791
H	8.29054	-5.21432	0.66172
H	5.98152	-5.06917	-0.23801
H	-3.83363	-1.88864	-1.78436
H	-3.11672	-1.09598	-3.21635
H	-4.85556	-0.96982	-2.90367
H	-2.83180	2.73312	1.65237
H	-1.57948	1.49644	1.52350
H	-3.30266	1.02327	1.62276
H	-1.90267	3.85101	-0.49574
H	-1.72317	2.89172	-1.97445
H	-0.66520	2.59015	-0.56287
H	2.19513	-3.51017	0.51288
H	3.27400	-3.82024	1.90768
H	3.43625	-4.76189	0.41695
H	3.07878	-2.40301	-1.57728
H	4.34264	-3.62543	-1.72967
H	4.79726	-1.91444	-1.69330
H	6.44669	0.11520	2.71285
H	4.72354	0.22078	3.11125
H	-8.58392	5.48844	-0.97901
C	-2.87520	5.63130	2.25423
C	-1.82621	5.26572	3.09198
C	-2.11770	4.72526	4.34270
C	-3.44134	4.56511	4.74949
C	-4.47871	4.94756	3.90132
C	-4.20265	5.49345	2.64826
Br	-2.48626	6.42859	0.58243
H	-0.79830	5.40331	2.77294
H	-1.30374	4.43974	5.00274
H	-3.66320	4.15260	5.72917
H	-5.51253	4.83695	4.21544
H	-5.00773	5.80473	1.98899

4

C	-6.29728	2.55000	-1.80071
C	-5.52138	1.46352	-2.19360
C	-4.29483	1.29933	-1.55784
C	-3.83497	2.16747	-0.56709
C	-4.61172	3.24295	-0.18372
C	-5.85132	3.43154	-0.80803
C	-2.48063	1.71222	-0.08567
C	-2.26037	0.48335	-0.94927
N	-3.32196	0.30346	-1.75555

C	-1.17508	-0.41153	-1.00645
C	0.00790	-0.46129	-0.30262
C	0.82741	0.18342	0.75679
C	1.88582	-0.84237	0.58506
C	1.06490	-1.48419	-0.47936
O	0.73210	1.14709	1.49545
O	1.16041	-2.44576	-1.22093
C	3.05571	-0.89757	1.30251
C	4.13484	-1.80915	1.27222
C	4.35168	-3.04278	0.41547
C	5.68262	-3.52631	0.93147
C	6.11863	-2.68260	1.95066
N	5.16768	-1.65739	2.11021
C	7.30791	-2.88399	2.64314
C	8.07506	-3.98378	2.26629
C	7.65919	-4.83676	1.23929
C	6.45722	-4.61425	0.56327
C	-6.66300	4.59980	-0.37182
O	-6.31053	5.38395	0.47995
O	-7.83258	4.69633	-1.02270
C	-3.46498	-0.77732	-2.71745
C	-2.52877	1.34238	1.41023
C	-1.41093	2.78768	-0.35825
C	3.25702	-4.09666	0.67820
C	4.43100	-2.68054	-1.07995
C	5.33275	-0.57980	3.07132
H	5.06408	0.37333	2.61442
H	-7.26134	2.72012	-2.26704
H	-5.88094	0.79061	-2.96418
H	-4.29961	3.94767	0.58174
H	-1.25665	-1.22267	-1.72877
H	3.12656	-0.09196	2.03173
H	7.63785	-2.23435	3.44646
H	9.00929	-4.18066	2.78257
H	8.27828	-5.68641	0.96826
H	6.14121	-5.28448	-0.23103
H	-3.42495	-1.74418	-2.20956
H	-2.67276	-0.72437	-3.46873
H	-4.42665	-0.68603	-3.21680
H	-2.82216	2.22783	1.98134
H	-1.54473	1.02887	1.76202
H	-3.26387	0.55534	1.60165
H	-1.68302	3.69890	0.18195
H	-1.35221	3.02873	-1.42355
H	-0.43532	2.46244	0.00621
H	2.29327	-3.75624	0.29678
H	3.17732	-4.33089	1.74374
H	3.52085	-5.01588	0.14749
H	3.45818	-2.35252	-1.44963
H	4.71790	-3.57422	-1.64174
H	5.18414	-1.90931	-1.26046
H	6.37995	-0.52969	3.36372
H	4.71473	-0.75808	3.95619
H	-8.28979	5.47797	-0.67750
C	7.63745	-0.51291	-1.43627

C	8.44764	-1.63524	-1.56151
C	8.61407	-2.20390	-2.82318
C	7.98778	-1.64705	-3.93662
C	7.18973	-0.51402	-3.79056
C	7.00665	0.06079	-2.53441
Br	7.43819	0.30715	0.26230
H	8.94220	-2.05537	-0.69202
H	9.24656	-3.07994	-2.93322
H	8.13123	-2.08819	-4.91821
H	6.70806	-0.06869	-4.65604
H	6.39531	0.94905	-2.41404

UB3LYP-D

1

C	-6.66243	2.42779	-1.72812
C	-5.88143	1.33291	-2.10583
C	-4.62898	1.21069	-1.50512
C	-4.15078	2.12597	-0.56194
C	-4.92791	3.20797	-0.19234
C	-6.19633	3.35846	-0.78221
C	-2.77320	1.70811	-0.10701
C	-2.56471	0.43608	-0.91386
N	-3.64597	0.21611	-1.69346
C	-1.47663	-0.45329	-0.93098
C	-0.28249	-0.43725	-0.23946
C	0.56858	0.30459	0.73561
C	1.64906	-0.70412	0.58277
C	0.78882	-1.45550	-0.37916
O	0.48945	1.32405	1.40615
O	0.86443	-2.47755	-1.04652
C	2.87206	-0.64101	1.20587
C	4.00408	-1.47798	1.11653
C	4.24758	-2.70327	0.25080
C	5.66102	-3.06360	0.63883
C	6.13020	-2.14892	1.58590
N	5.10689	-1.20733	1.83382
C	7.40736	-2.22281	2.14073
C	8.22381	-3.27182	1.70638
C	7.76857	-4.19983	0.75740
C	6.47883	-4.10114	0.21525
C	-7.01251	4.53447	-0.35987
O	-6.64594	5.35585	0.45664
O	-8.21249	4.59551	-0.98155
C	-3.79457	-0.90711	-2.62022
C	-2.75712	1.42075	1.41136
C	-1.72450	2.78403	-0.47939
C	3.27886	-3.86252	0.57559
C	4.16761	-2.32937	-1.24999
C	5.23494	-0.10016	2.78276
H	5.17877	0.85368	2.24974
H	-7.64347	2.56430	-2.16744
H	-6.25375	0.62141	-2.83381
H	-4.59288	3.94073	0.53464
H	-1.56137	-1.31657	-1.58862
H	2.95113	0.21369	1.87430

H	7.76910	-1.50984	2.87284
H	9.22559	-3.36693	2.11218
H	8.42498	-5.00372	0.44019
H	6.12969	-4.82178	-0.51802
H	-3.81976	-1.84959	-2.06471
H	-2.95524	-0.91997	-3.32088
H	-4.72279	-0.79043	-3.17629
H	-3.02465	2.34109	1.93997
H	-1.76062	1.11704	1.72779
H	-3.48841	0.64737	1.66936
H	-1.98840	3.71372	0.03452
H	-1.72629	2.97152	-1.55805
H	-0.73091	2.47979	-0.14950
H	2.25704	-3.59161	0.31239
H	3.34443	-4.13430	1.63178
H	3.57151	-4.72640	-0.02982
H	3.14296	-2.07420	-1.52326
H	4.47523	-3.19897	-1.83902
H	4.83962	-1.49684	-1.48237
H	6.19470	-0.17455	3.29020
H	4.42860	-0.16208	3.51878
H	-8.67659	5.38384	-0.65233
C	1.01436	-2.33751	3.43830
C	0.44537	-3.29324	2.59772
C	-0.84635	-3.07645	2.11080
C	-1.55628	-1.93021	2.48136
C	-0.97455	-0.99735	3.34370
C	0.32171	-1.19227	3.82614
Br	2.77844	-2.62714	4.12577
H	0.99799	-4.18193	2.31829
H	-1.29049	-3.80786	1.44279
H	-2.56016	-1.76560	2.10294
H	-1.51951	-0.10709	3.63847
H	0.77912	-0.46550	4.48780

2

C	-6.77734	2.33692	-1.92368
C	-5.94796	1.27502	-2.29120
C	-4.71032	1.18838	-1.65426
C	-4.29159	2.10764	-0.68704
C	-5.11666	3.15750	-0.32796
C	-6.37148	3.27136	-0.95362
C	-2.91527	1.73059	-0.19452
C	-2.63334	0.48641	-1.02144
N	-3.68702	0.23239	-1.82649
C	-1.50291	-0.35135	-1.03865
C	-0.32698	-0.29981	-0.31830
C	0.45030	0.43722	0.72130
C	1.57269	-0.53058	0.59051
C	0.79192	-1.26829	-0.45013
O	0.30137	1.42472	1.42665
O	0.94343	-2.25419	-1.15750
C	2.74562	-0.46686	1.30307
C	3.88284	-1.30438	1.29541
C	4.16776	-2.55257	0.47773

C	5.54760	-2.91771	0.96810
C	5.97478	-1.97045	1.90145
N	4.94117	-1.02164	2.07047
C	7.22293	-2.02174	2.51498
C	8.05572	-3.08582	2.15849
C	7.64352	-4.05032	1.22798
C	6.38020	-3.97196	0.62314
C	-7.23958	4.41451	-0.54459
O	-6.92409	5.24212	0.28676
O	-8.42438	4.43814	-1.19751
C	-3.77277	-0.88881	-2.76411
C	-2.94842	1.40264	1.31773
C	-1.89603	2.85371	-0.50107
C	3.15566	-3.68590	0.75794
C	4.20942	-2.21012	-1.03343
C	5.03284	0.11991	2.98196
H	5.06571	1.05111	2.40817
H	-7.74887	2.44586	-2.39089
H	-6.27273	0.56192	-3.04013
H	-4.82868	3.89191	0.41717
H	-1.52927	-1.19407	-1.72724
H	2.77054	0.38079	1.98469
H	7.54232	-1.29255	3.24923
H	9.03556	-3.16723	2.61728
H	8.31264	-4.86560	0.97176
H	6.06464	-4.71741	-0.10055
H	-3.69549	-1.83405	-2.21916
H	-2.96258	-0.82222	-3.49595
H	-4.72916	-0.84893	-3.28160
H	-3.27368	2.29806	1.85655
H	-1.95377	1.13199	1.67237
H	-3.65885	0.59577	1.52531
H	-2.21397	3.75947	0.02468
H	-1.86490	3.06840	-1.57427
H	-0.90437	2.57937	-0.14079
H	2.16848	-3.42176	0.37787
H	3.10118	-3.90243	1.82736
H	3.49520	-4.58276	0.22990
H	3.21586	-1.93761	-1.39048
H	4.53893	-3.10061	-1.57784
H	4.92015	-1.40098	-1.23114
H	5.93574	0.02107	3.57998
H	4.16394	0.12049	3.64461
H	-8.92456	5.20689	-0.87495
C	4.45131	-2.84776	4.79938
C	5.18767	-1.99420	5.61995
C	6.47460	-2.37796	6.01147
C	7.00637	-3.59809	5.58427
C	6.25080	-4.43942	4.76180
C	4.96050	-4.07326	4.37107
Br	2.66142	-2.35827	4.32818
H	4.75837	-1.06126	5.96915
H	7.05031	-1.72772	6.66367
H	8.00262	-3.89552	5.89646
H	6.65820	-5.38848	4.42814

H	4.36518	-4.72864	3.74537

3

C	-6.71106	2.52722	-1.77612
C	-5.94231	1.41762	-2.13569
C	-4.67730	1.30987	-1.55654
C	-4.17379	2.25708	-0.66112
C	-4.94343	3.34622	-0.29999
C	-6.22367	3.48006	-0.86172
C	-2.78584	1.86041	-0.22943
C	-2.60818	0.55057	-0.97257
N	-3.70281	0.30025	-1.71867
C	-1.51600	-0.34077	-0.97691
C	-0.29875	-0.27529	-0.33409
C	0.58565	0.52340	0.57092
C	1.65456	-0.50337	0.45495
C	0.76971	-1.30311	-0.44366
O	0.53125	1.57987	1.18370
O	0.82648	-2.36167	-1.05329
C	2.88647	-0.42958	1.06810
C	3.98760	-1.30989	1.04257
C	4.16204	-2.63498	0.31857
C	5.56326	-3.01776	0.73041
C	6.08776	-2.03111	1.57000
N	5.10773	-1.02487	1.73269
C	7.37026	-2.10325	2.11323
C	8.13281	-3.22742	1.78116
C	7.62192	-4.22829	0.94068
C	6.32858	-4.12927	0.40746
C	-7.03992	4.64614	-0.41646
O	-6.70496	5.41134	0.46761
O	-8.20366	4.76842	-1.09322
C	-3.87852	-0.86480	-2.58876
C	-2.72212	1.67555	1.30463
C	-1.74825	2.90037	-0.72302
C	3.13863	-3.68311	0.81750
C	4.07422	-2.45097	-1.21561
C	5.30553	0.17225	2.55266
H	5.24373	1.06596	1.92491
H	-7.70162	2.65339	-2.19707
H	-6.33378	0.68302	-2.83003
H	-4.59038	4.08230	0.40800
H	-1.61866	-1.23993	-1.58198
H	2.99853	0.47417	1.66449
H	7.77564	-1.33538	2.76234
H	9.13663	-3.32391	2.18153
H	8.23779	-5.08911	0.70111
H	5.93700	-4.90559	-0.24278
H	-3.88890	-1.77948	-1.98849
H	-3.05959	-0.91116	-3.31157
H	-4.82274	-0.77102	-3.12175
H	-2.97801	2.62631	1.77779
H	-1.71551	1.40016	1.61790
H	-3.44087	0.91613	1.63040
H	-1.99540	3.86858	-0.28511

H	-1.78552	2.99586	-1.81344
H	-0.74575	2.61759	-0.40281
H	2.12759	-3.40403	0.52043
H	3.19776	-3.79683	1.90486
H	3.37867	-4.64559	0.35497
H	3.06346	-2.17050	-1.51211
H	4.31804	-3.40622	-1.69098
H	4.79311	-1.69967	-1.55831
H	6.28727	0.12605	3.01945
H	4.53794	0.21781	3.33020
H	-8.67413	5.54143	-0.73763
C	-2.82522	5.43898	1.87312
C	-1.57935	5.00694	2.32996
C	-1.50992	4.27409	3.51816
C	-2.67184	3.99270	4.24364
C	-3.91071	4.44264	3.77546
C	-3.99574	5.17813	2.58834
Br	-2.92473	6.48780	0.27735
H	-0.68058	5.22954	1.76558
H	-0.54407	3.92552	3.87073
H	-2.61241	3.42854	5.16938
H	-4.81745	4.23408	4.33552
H	-4.95315	5.52961	2.21745

4

C	-6.66928	2.37843	-1.69150
C	-5.85771	1.32391	-2.11569
C	-4.59825	1.21769	-1.52641
C	-4.14126	2.11039	-0.55171
C	-4.94895	3.15303	-0.13636
C	-6.22494	3.28644	-0.71324
C	-2.74868	1.71796	-0.12094
C	-2.50177	0.49502	-0.98943
N	-3.58439	0.26428	-1.76106
C	-1.37511	-0.34566	-1.07005
C	-0.17240	-0.31427	-0.39587
C	0.64831	0.39341	0.63205
C	1.75702	-0.57831	0.43772
C	0.93575	-1.28506	-0.59171
O	0.53044	1.36424	1.36573
O	1.05251	-2.25632	-1.32555
C	2.95074	-0.55486	1.12442
C	4.08027	-1.39698	1.05039
C	4.34715	-2.59800	0.15889
C	5.73761	-2.99099	0.59677
C	6.15888	-2.14240	1.62509
N	5.13869	-1.19260	1.85564
C	7.38722	-2.28428	2.27013
C	8.20570	-3.33047	1.83940
C	7.80433	-4.18321	0.80087
C	6.56393	-4.01871	0.16976
C	-7.07319	4.42170	-0.24395
O	-6.72413	5.22615	0.59651
O	-8.28017	4.46601	-0.85324
C	-3.70841	-0.83279	-2.72326

C	-2.72504	1.35146	1.38260
C	-1.73861	2.84662	-0.43777
C	3.34636	-3.74050	0.46585
C	4.30799	-2.21549	-1.33722
C	5.23677	-0.12897	2.85832
H	5.12408	0.84523	2.37465
H	-7.65667	2.50194	-2.12024
H	-6.21229	0.63124	-2.87014
H	-4.63165	3.86735	0.61640
H	-1.43239	-1.17226	-1.77599
H	2.99848	0.26216	1.84231
H	7.71140	-1.62580	3.06774
H	9.17137	-3.47558	2.30860
H	8.46737	-4.97908	0.47970
H	6.26173	-4.67802	-0.63753
H	-3.62759	-1.79195	-2.20368
H	-2.91732	-0.75675	-3.47464
H	-4.67763	-0.76938	-3.21381
H	-3.02453	2.23403	1.95639
H	-1.71875	1.06757	1.69095
H	-3.43086	0.54236	1.59694
H	-2.03347	3.73899	0.12309
H	-1.74836	3.08899	-1.50548
H	-0.73459	2.56110	-0.12336
H	2.33823	-3.45802	0.16112
H	3.36434	-3.99842	1.52975
H	3.64611	-4.62204	-0.10940
H	3.29115	-1.96759	-1.64172
H	4.64520	-3.07728	-1.92141
H	4.98581	-1.38321	-1.53983
H	6.21197	-0.18084	3.33798
H	4.45338	-0.25557	3.61109
H	-8.76574	5.22762	-0.49347
C	9.51068	-1.95188	-0.99759
C	9.55650	-3.09002	-1.80269
C	8.60168	-3.24898	-2.81148
C	7.61668	-2.27778	-3.01112
C	7.59516	-1.13829	-2.20101
C	8.53929	-0.96870	-1.18524
Br	10.85085	-1.69811	0.33269
H	10.33184	-3.83358	-1.65289
H	8.63903	-4.12966	-3.44596
H	6.88216	-2.39874	-3.80151
H	6.84959	-0.36606	-2.36666
H	8.53438	-0.07985	-0.56372

UB3LYP-D+BSSE

1

C(Fragment=1)	-6.72055	2.40608	-1.74165
C(Fragment=1)	-5.92394	1.33259	-2.14721
C(Fragment=1)	-4.66739	1.21666	-1.55406
C(Fragment=1)	-4.19936	2.11796	-0.59264
C(Fragment=1)	-4.99154	3.17943	-0.19621
C(Fragment=1)	-6.26477	3.32281	-0.77730
C(Fragment=1)	-2.81155	1.71404	-0.15598

C(Fragment=1)	-2.58712	0.46391	-0.99237
N(Fragment=1)	-3.66863	0.24314	-1.77013
C(Fragment=1)	-1.48508	-0.40886	-1.03263
C(Fragment=1)	-0.28673	-0.38384	-0.35034
C(Fragment=1)	0.55578	0.35290	0.63699
C(Fragment=1)	1.63267	-0.66074	0.49684
C(Fragment=1)	0.78729	-1.40043	-0.48652
O(Fragment=1)	0.47098	1.37147	1.30820
O(Fragment=1)	0.86876	-2.41854	-1.15910
C(Fragment=1)	2.83081	-0.63151	1.17130
C(Fragment=1)	3.95731	-1.47814	1.09973
C(Fragment=1)	4.21221	-2.69100	0.21961
C(Fragment=1)	5.60984	-3.07443	0.64053
C(Fragment=1)	6.05535	-2.19290	1.62952
N(Fragment=1)	5.03785	-1.24200	1.86311
C(Fragment=1)	7.30810	-2.30341	2.23280
C(Fragment=1)	8.12598	-3.35133	1.79929
C(Fragment=1)	7.69606	-4.24348	0.80490
C(Fragment=1)	6.42927	-4.11113	0.21787
C(Fragment=1)	-7.09700	4.47685	-0.32632
O(Fragment=1)	-6.73936	5.28594	0.50622
O(Fragment=1)	-8.30027	4.53290	-0.94196
C(Fragment=1)	-3.80535	-0.86361	-2.71853
C(Fragment=1)	-2.78083	1.39386	1.35622
C(Fragment=1)	-1.78592	2.81670	-0.51458
C(Fragment=1)	3.22435	-3.83938	0.53229
C(Fragment=1)	4.16313	-2.30853	-1.27852
C(Fragment=1)	5.14848	-0.16977	2.85323
H(Fragment=1)	4.93710	0.79275	2.38055
H(Fragment=1)	-7.70545	2.53695	-2.17397
H(Fragment=1)	-6.28806	0.63205	-2.88977
H(Fragment=1)	-4.66467	3.90146	0.54507
H(Fragment=1)	-1.56368	-1.26490	-1.70039
H(Fragment=1)	2.89367	0.20436	1.86455
H(Fragment=1)	7.64848	-1.62166	3.00380
H(Fragment=1)	9.10892	-3.47459	2.24192
H(Fragment=1)	8.35365	-5.04695	0.48906
H(Fragment=1)	6.09858	-4.80575	-0.54829
H(Fragment=1)	-3.81528	-1.81687	-2.18118
H(Fragment=1)	-2.96874	-0.85096	-3.42235
H(Fragment=1)	-4.73737	-0.74902	-3.26864
H(Fragment=1)	-3.05392	2.29954	1.90671
H(Fragment=1)	-1.77893	1.09399	1.66119
H(Fragment=1)	-3.50378	0.60879	1.60220
H(Fragment=1)	-2.06175	3.73009	0.02177
H(Fragment=1)	-1.80261	3.02721	-1.58887
H(Fragment=1)	-0.78363	2.52401	-0.20126
H(Fragment=1)	2.20896	-3.55678	0.25648
H(Fragment=1)	3.27248	-4.10590	1.59129
H(Fragment=1)	3.51546	-4.70974	-0.06444
H(Fragment=1)	3.14717	-2.03999	-1.56965
H(Fragment=1)	4.47034	-3.17836	-1.86755
H(Fragment=1)	4.84931	-1.48300	-1.49375
H(Fragment=1)	6.16136	-0.15586	3.25067
H(Fragment=1)	4.43758	-0.35476	3.66402

H(Fragment=1)	-8.77505	5.30677	-0.59418
C(Fragment=2)	1.21935	-2.43120	3.60350
C(Fragment=2)	0.58552	-3.32666	2.74206
C(Fragment=2)	-0.65892	-2.98258	2.20848
C(Fragment=2)	-1.25990	-1.76401	2.53754
C(Fragment=2)	-0.61244	-0.88568	3.40947
C(Fragment=2)	0.63483	-1.21214	3.94736
Br(Fragment=2)	2.92744	-2.88053	4.32203
H(Fragment=2)	1.05051	-4.27164	2.48911
H(Fragment=2)	-1.15257	-3.67321	1.53160
H(Fragment=2)	-2.22454	-1.49985	2.11753
H(Fragment=2)	-1.06471	0.06670	3.66532
H(Fragment=2)	1.13847	-0.52930	4.62242

2

C(Fragment=1)	-6.78377	2.28975	-1.88549
C(Fragment=1)	-5.94958	1.23224	-2.25476
C(Fragment=1)	-4.70287	1.16257	-1.63367
C(Fragment=1)	-4.27992	2.09387	-0.67995
C(Fragment=1)	-5.10971	3.13950	-0.31926
C(Fragment=1)	-6.37367	3.23639	-0.92914
C(Fragment=1)	-2.89321	1.73429	-0.20359
C(Fragment=1)	-2.61251	0.48322	-1.02055
N(Fragment=1)	-3.67318	0.21436	-1.81124
C(Fragment=1)	-1.47854	-0.35006	-1.03868
C(Fragment=1)	-0.29324	-0.28202	-0.33544
C(Fragment=1)	0.49762	0.47712	0.67781
C(Fragment=1)	1.61559	-0.49784	0.55875
C(Fragment=1)	0.82274	-1.25460	-0.45894
O(Fragment=1)	0.35736	1.48059	1.36187
O(Fragment=1)	0.96362	-2.25595	-1.14665
C(Fragment=1)	2.79028	-0.43217	1.26988
C(Fragment=1)	3.92190	-1.27744	1.27301
C(Fragment=1)	4.19767	-2.53740	0.46999
C(Fragment=1)	5.57829	-2.90357	0.95805
C(Fragment=1)	6.00653	-1.95732	1.89219
N(Fragment=1)	4.97462	-1.00665	2.06072
C(Fragment=1)	7.25718	-2.00770	2.50163
C(Fragment=1)	8.09045	-3.07021	2.14074
C(Fragment=1)	7.67545	-4.03533	1.21220
C(Fragment=1)	6.40984	-3.95816	0.61171
C(Fragment=1)	-7.24685	4.37511	-0.51841
O(Fragment=1)	-6.92843	5.21213	0.30230
O(Fragment=1)	-8.43988	4.38283	-1.15654
C(Fragment=1)	-3.76130	-0.91539	-2.73839
C(Fragment=1)	-2.89943	1.42452	1.31260
C(Fragment=1)	-1.88945	2.86306	-0.54003
C(Fragment=1)	3.17424	-3.65059	0.79293
C(Fragment=1)	4.22523	-2.23037	-1.04741
C(Fragment=1)	5.06541	0.12515	2.98444
H(Fragment=1)	5.12418	1.06166	2.42142
H(Fragment=1)	-7.76249	2.38562	-2.34038
H(Fragment=1)	-6.27799	0.50918	-2.99247
H(Fragment=1)	-4.81872	3.88307	0.41555
H(Fragment=1)	-1.51171	-1.20615	-1.71033

H(Fragment=1)	2.82247	0.42552	1.93853
H(Fragment=1)	7.57996	-1.27624	3.23224
H(Fragment=1)	9.07338	-3.14915	2.59334
H(Fragment=1)	8.34486	-4.84925	0.95248
H(Fragment=1)	6.09347	-4.70316	-0.11210
H(Fragment=1)	-3.69709	-1.85629	-2.18402
H(Fragment=1)	-2.94450	-0.86263	-3.46371
H(Fragment=1)	-4.71252	-0.87145	-3.26501
H(Fragment=1)	-3.22330	2.32361	1.84605
H(Fragment=1)	-1.89706	1.16602	1.65440
H(Fragment=1)	-3.59960	0.61442	1.54133
H(Fragment=1)	-2.20764	3.77202	-0.01997
H(Fragment=1)	-1.87775	3.06514	-1.61608
H(Fragment=1)	-0.88953	2.60237	-0.19269
H(Fragment=1)	2.19031	-3.38971	0.40272
H(Fragment=1)	3.11534	-3.82121	1.87089
H(Fragment=1)	3.50425	-4.57253	0.30348
H(Fragment=1)	3.23080	-1.95654	-1.40060
H(Fragment=1)	4.54010	-3.13571	-1.57577
H(Fragment=1)	4.94101	-1.43238	-1.27026
H(Fragment=1)	5.95364	0.00600	3.60055
H(Fragment=1)	4.18450	0.13059	3.63012
H(Fragment=1)	-8.94303	5.14960	-0.83382
C(Fragment=2)	4.32679	-2.80346	4.87685
C(Fragment=2)	5.12256	-2.01512	5.70925
C(Fragment=2)	6.41330	-2.45244	6.02442
C(Fragment=2)	6.89817	-3.65910	5.51303
C(Fragment=2)	6.08685	-4.43128	4.67737
C(Fragment=2)	4.79544	-4.00945	4.35335
Br(Fragment=2)	2.55984	-2.22429	4.45615
H(Fragment=2)	4.73651	-1.08967	6.12309
H(Fragment=2)	7.03087	-1.85098	6.68521
H(Fragment=2)	7.89792	-3.99685	5.76694
H(Fragment=2)	6.45480	-5.36861	4.27227
H(Fragment=2)	4.16418	-4.61417	3.71259

3

C(Fragment=1)	-6.72344	2.49077	-1.74935
C(Fragment=1)	-5.95667	1.37449	-2.08998
C(Fragment=1)	-4.68255	1.28745	-1.52819
C(Fragment=1)	-4.16714	2.26091	-0.66764
C(Fragment=1)	-4.93141	3.36297	-0.33190
C(Fragment=1)	-6.22341	3.47353	-0.87434
C(Fragment=1)	-2.77818	1.86776	-0.23267
C(Fragment=1)	-2.60311	0.54637	-0.95752
N(Fragment=1)	-3.70825	0.27686	-1.68117
C(Fragment=1)	-1.50932	-0.34314	-0.96310
C(Fragment=1)	-0.28935	-0.27885	-0.32562
C(Fragment=1)	0.59305	0.51085	0.58809
C(Fragment=1)	1.66378	-0.51325	0.46202
C(Fragment=1)	0.77953	-1.30552	-0.44402
O(Fragment=1)	0.53539	1.55995	1.21307
O(Fragment=1)	0.83654	-2.35899	-1.06226
C(Fragment=1)	2.89484	-0.44512	1.07749
C(Fragment=1)	3.99815	-1.32259	1.04124

C(Fragment=1)	4.17722	-2.63629	0.29782
C(Fragment=1)	5.58017	-3.01966	0.70330
C(Fragment=1)	6.10082	-2.04408	1.55808
N(Fragment=1)	5.11684	-1.04432	1.73630
C(Fragment=1)	7.38356	-2.11960	2.10028
C(Fragment=1)	8.15044	-3.23562	1.75113
C(Fragment=1)	7.64340	-4.22545	0.89538
C(Fragment=1)	6.34973	-4.12324	0.36355
C(Fragment=1)	-7.03771	4.65366	-0.46329
O(Fragment=1)	-6.68819	5.46264	0.37477
O(Fragment=1)	-8.21999	4.73435	-1.11411
C(Fragment=1)	-3.89477	-0.90846	-2.52120
C(Fragment=1)	-2.72404	1.69216	1.30388
C(Fragment=1)	-1.73491	2.90313	-0.71916
C(Fragment=1)	3.15862	-3.69588	0.78238
C(Fragment=1)	4.08694	-2.43033	-1.23335
C(Fragment=1)	5.31041	0.14098	2.57438
H(Fragment=1)	5.25629	1.04359	1.95867
H(Fragment=1)	-7.72153	2.60100	-2.15655
H(Fragment=1)	-6.35641	0.61952	-2.75715
H(Fragment=1)	-4.56301	4.13094	0.33634
H(Fragment=1)	-1.61351	-1.24299	-1.56686
H(Fragment=1)	3.00504	0.45157	1.68471
H(Fragment=1)	7.78601	-1.36007	2.76093
H(Fragment=1)	9.15463	-3.33436	2.15005
H(Fragment=1)	8.26257	-5.08014	0.64272
H(Fragment=1)	5.96118	-4.89101	-0.29856
H(Fragment=1)	-3.88300	-1.80954	-1.90091
H(Fragment=1)	-3.09312	-0.96423	-3.26257
H(Fragment=1)	-4.85198	-0.83422	-3.03350
H(Fragment=1)	-2.98250	2.64608	1.76959
H(Fragment=1)	-1.71853	1.41885	1.62327
H(Fragment=1)	-3.44501	0.93570	1.63153
H(Fragment=1)	-1.97635	3.87111	-0.27477
H(Fragment=1)	-1.76771	3.00432	-1.80905
H(Fragment=1)	-0.73461	2.61370	-0.39715
H(Fragment=1)	2.14599	-3.41623	0.49136
H(Fragment=1)	3.22019	-3.82630	1.86771
H(Fragment=1)	3.40165	-4.65004	0.30441
H(Fragment=1)	3.07500	-2.14840	-1.52435
H(Fragment=1)	4.33273	-3.37789	-1.72287
H(Fragment=1)	4.80314	-1.67207	-1.56618
H(Fragment=1)	6.28779	0.08564	3.04928
H(Fragment=1)	4.53624	0.17759	3.34573
H(Fragment=1)	-8.68692	5.52109	-0.78508
C(Fragment=2)	-2.76695	5.54326	1.91459
C(Fragment=2)	-1.56771	5.02988	2.41265
C(Fragment=2)	-1.59352	4.25469	3.57522
C(Fragment=2)	-2.80184	3.99368	4.22804
C(Fragment=2)	-3.99271	4.51136	3.70904
C(Fragment=2)	-3.98641	5.29174	2.54801
Br(Fragment=2)	-2.74328	6.60274	0.33163
H(Fragment=2)	-0.63152	5.23012	1.90361
H(Fragment=2)	-0.66281	3.85115	3.96224
H(Fragment=2)	-2.81600	3.39309	5.13227

H(Fragment=2)	-4.93733	4.31516	4.20782
H(Fragment=2)	-4.91020	5.68746	2.13882

4

C(Fragment=1)	-6.72928	2.31291	-1.72898
C(Fragment=1)	-5.87309	1.30926	-2.18745
C(Fragment=1)	-4.62608	1.21056	-1.57102
C(Fragment=1)	-4.22248	2.06387	-0.53919
C(Fragment=1)	-5.07438	3.05596	-0.08972
C(Fragment=1)	-6.33974	3.17955	-0.69157
C(Fragment=1)	-2.82821	1.69394	-0.09460
C(Fragment=1)	-2.52045	0.52691	-1.01869
N(Fragment=1)	-3.57671	0.30223	-1.82768
C(Fragment=1)	-1.36409	-0.27091	-1.11610
C(Fragment=1)	-0.17989	-0.23802	-0.41007
C(Fragment=1)	0.59184	0.43951	0.67469
C(Fragment=1)	1.73481	-0.48732	0.46108
C(Fragment=1)	0.96402	-1.16192	-0.62708
O(Fragment=1)	0.42540	1.36711	1.45344
O(Fragment=1)	1.13243	-2.08646	-1.40964
C(Fragment=1)	2.91148	-0.46025	1.17644
C(Fragment=1)	4.06524	-1.26821	1.09584
C(Fragment=1)	4.37591	-2.44088	0.18112
C(Fragment=1)	5.76020	-2.82418	0.64566
C(Fragment=1)	6.15364	-1.97546	1.68391
N(Fragment=1)	5.10907	-1.05256	1.91697
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C(Fragment=1)	8.23056	-3.11161	1.89512
C(Fragment=1)	7.85184	-3.97015	0.85163
C(Fragment=1)	6.61140	-3.83188	0.21699
C(Fragment=1)	-7.23659	4.25960	-0.18377
O(Fragment=1)	-6.93471	5.02782	0.70732
O(Fragment=1)	-8.42965	4.29781	-0.82014
C(Fragment=1)	-3.64228	-0.74682	-2.84744
C(Fragment=1)	-2.82651	1.25204	1.38868
C(Fragment=1)	-1.84889	2.86929	-0.32804
C(Fragment=1)	3.38246	-3.60539	0.41145
C(Fragment=1)	4.38637	-2.00603	-1.30287
C(Fragment=1)	5.17004	-0.00429	2.93855
H(Fragment=1)	5.01565	0.97301	2.47339
H(Fragment=1)	-7.70902	2.42866	-2.17706
H(Fragment=1)	-6.18537	0.64880	-2.98802
H(Fragment=1)	-4.79944	3.73816	0.70811
H(Fragment=1)	-1.37596	-1.05803	-1.86792
H(Fragment=1)	2.91931	0.32668	1.92865
H(Fragment=1)	7.68662	-1.43087	3.13751
H(Fragment=1)	9.20398	-3.23228	2.35695
H(Fragment=1)	8.54136	-4.73961	0.52374
H(Fragment=1)	6.33138	-4.48969	-0.59901
H(Fragment=1)	-3.50625	-1.72579	-2.37930
H(Fragment=1)	-2.85931	-0.58712	-3.59452
H(Fragment=1)	-4.61580	-0.71290	-3.33238
H(Fragment=1)	-3.16862	2.09427	1.99819
H(Fragment=1)	-1.81837	0.98644	1.70706
H(Fragment=1)	-3.50915	0.41043	1.54506

H(Fragment=1)	-2.18670	3.72149	0.26979
H(Fragment=1)	-1.84100	3.16595	-1.38196
H(Fragment=1)	-0.84394	2.59967	-0.00260
H(Fragment=1)	2.38242	-3.32765	0.07741
H(Fragment=1)	3.36396	-3.89795	1.46628
H(Fragment=1)	3.71683	-4.46343	-0.17999
H(Fragment=1)	3.37965	-1.74833	-1.63245
H(Fragment=1)	4.74576	-2.84682	-1.90356
H(Fragment=1)	5.06853	-1.16477	-1.45465
H(Fragment=1)	6.14917	-0.02560	3.41254
H(Fragment=1)	4.39672	-0.17601	3.69304
H(Fragment=1)	-8.94919	5.02243	-0.43248
C(Fragment=2)	9.81559	-2.57136	-1.25307
C(Fragment=2)	9.50079	-3.58068	-2.16390
C(Fragment=2)	8.38043	-3.42904	-2.98666
C(Fragment=2)	7.58537	-2.28324	-2.89907
C(Fragment=2)	7.92043	-1.28096	-1.98381
C(Fragment=2)	9.03627	-1.41740	-1.15544
Br(Fragment=2)	11.32566	-2.77679	-0.11730
H(Fragment=2)	10.12242	-4.46671	-2.23504
H(Fragment=2)	8.13882	-4.20899	-3.70295
H(Fragment=2)	6.72019	-2.16777	-3.54423
H(Fragment=2)	7.31763	-0.37977	-1.91632
H(Fragment=2)	9.29920	-0.64007	-0.44673