Electronic Supplementary Material (ESI) for RSC Advances.

A time dependent DFT study of the efficiency of polymers for organic photovoltaics at the interface with PCBM

–

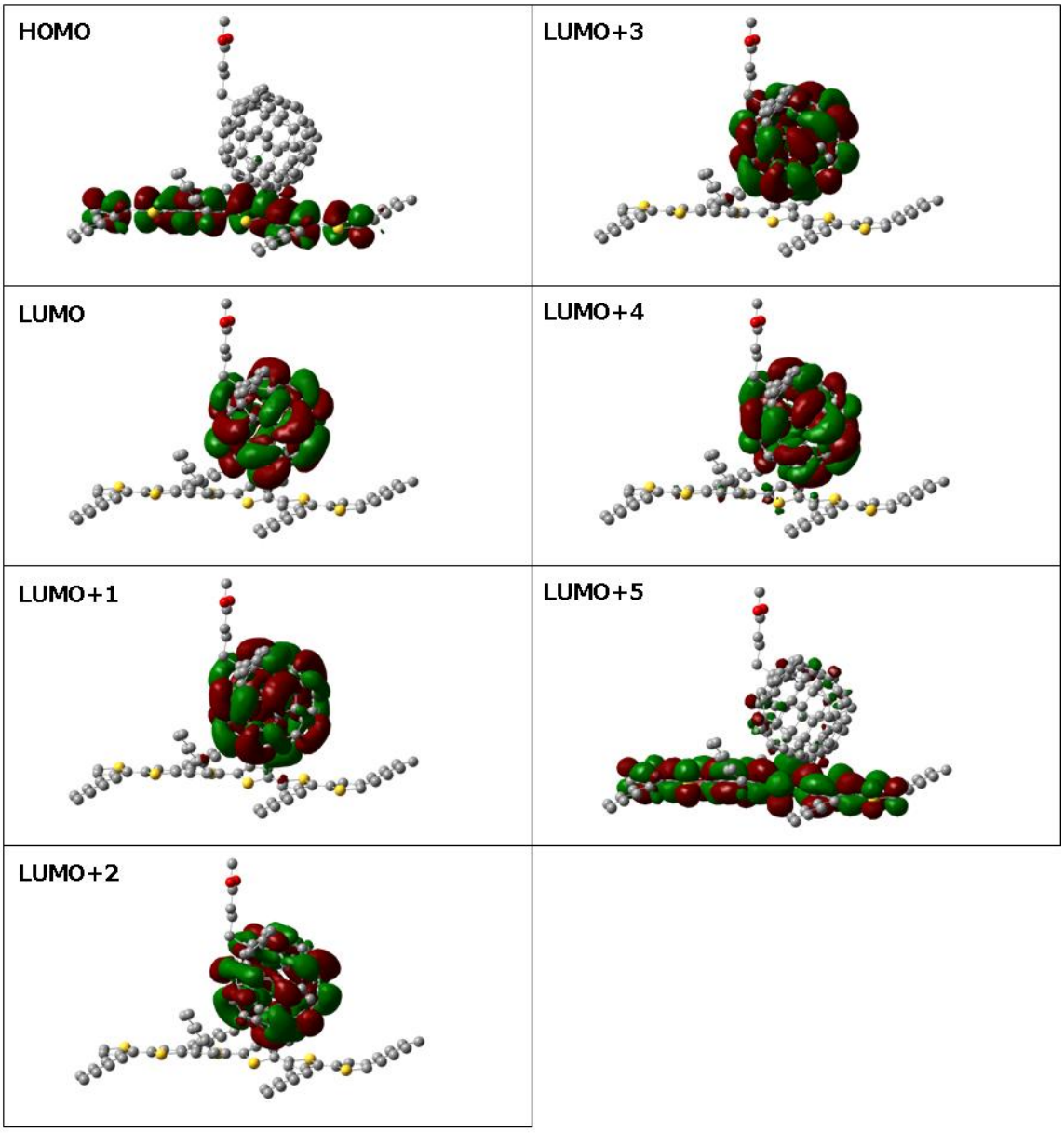
Supplementary information.

N. Van den Brande[a,b], G. Van Lier[a], F. Da Pieve[a], G. Van Assche[b], B. Van Mele[b], F. De Proft[a], P. Geerlings[a]

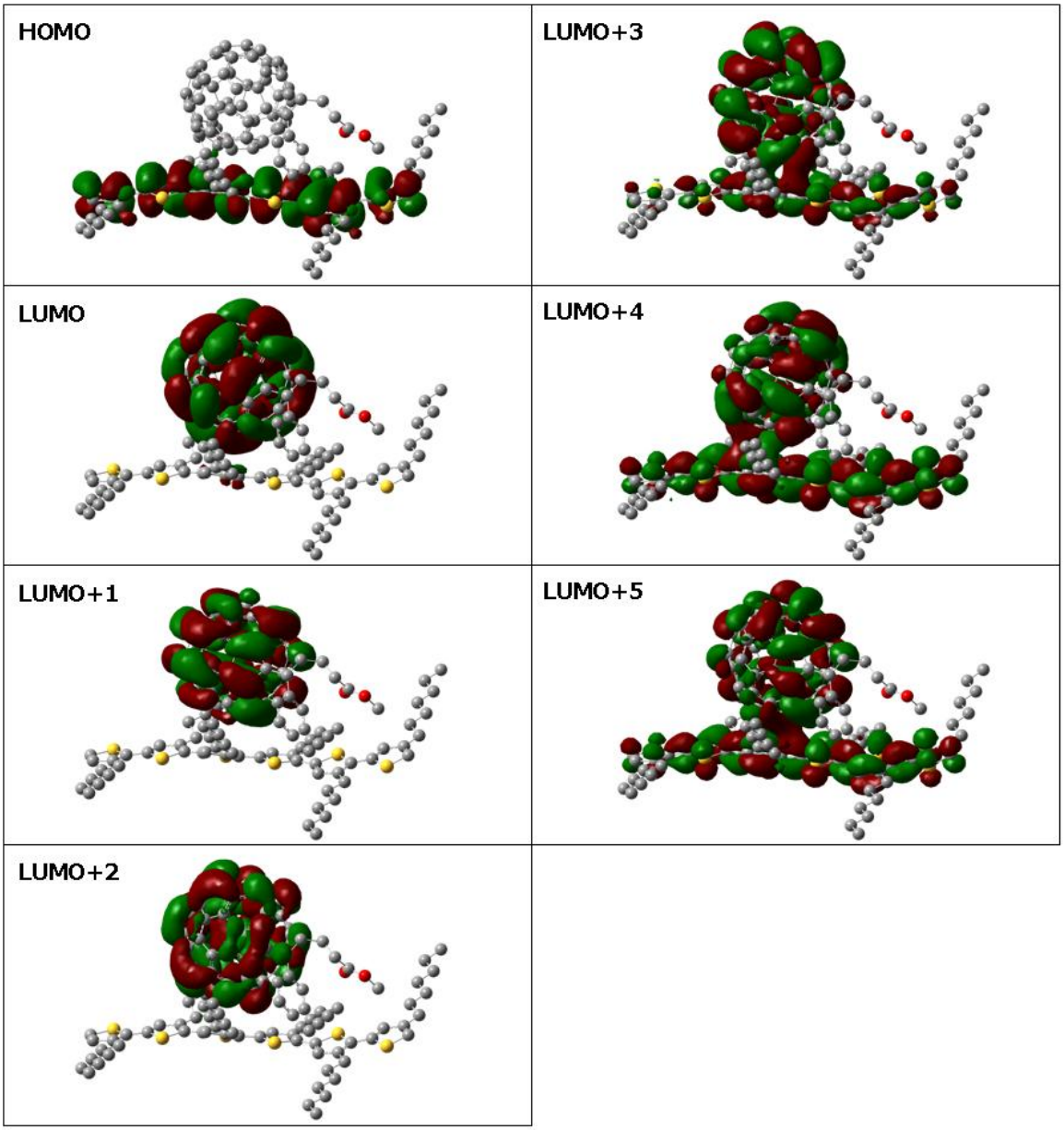
This supplementary information contains the coordinates of the geometry optimized systems used for the charge transfer study, visualizations of the most important molecular orbitals for all the systems studied and more detailed excitation tables mentioning the molecular orbital contributions.

Figure 1. Visualizations of the most important molecular orbitals for the three P3HT/PCBM configurations.

A configuration



B configuration



C configuration

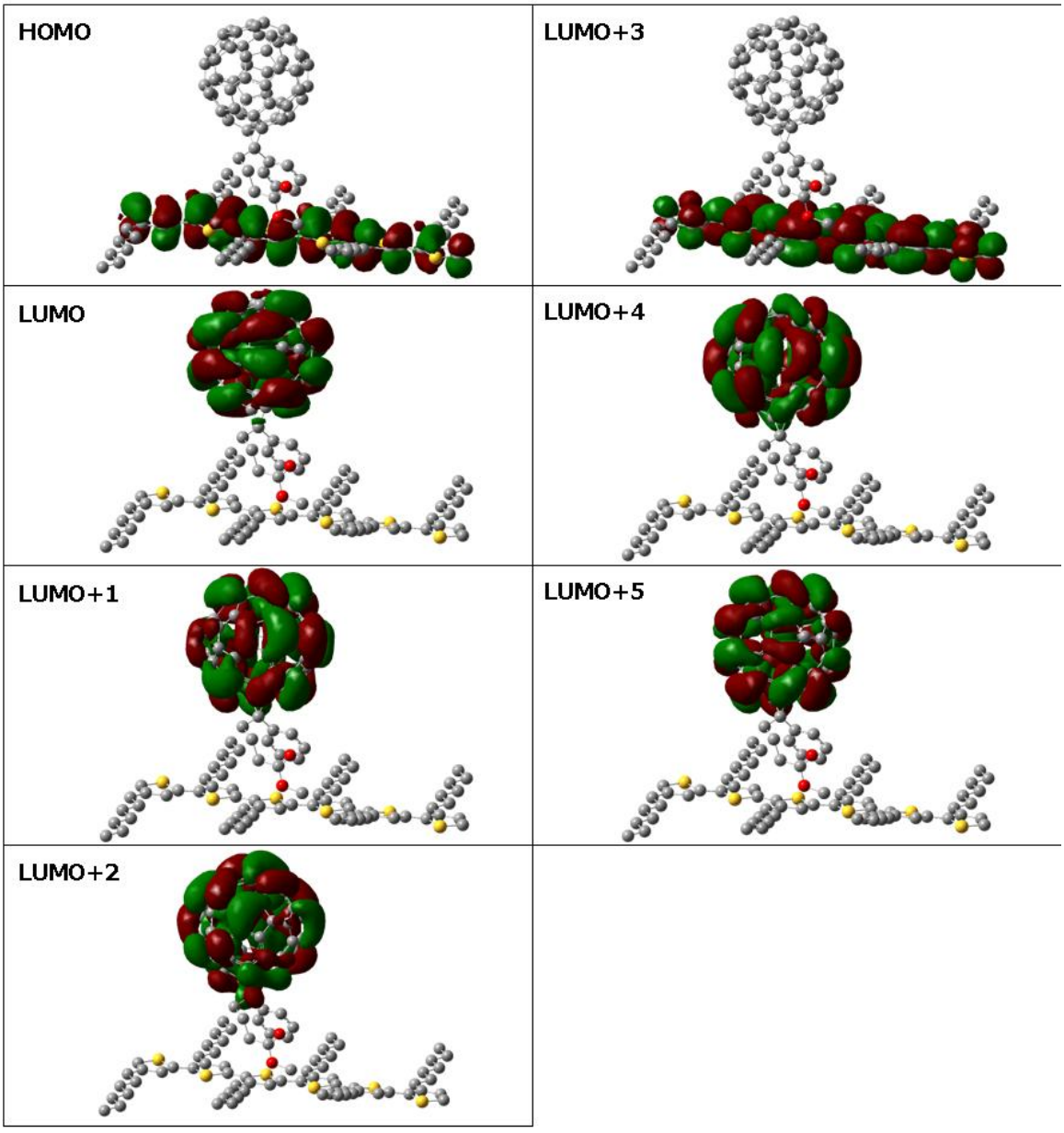


Table 1. Characteristics of the first singlet excitations for the three configurations of P3HT/PCBM with largest orbital contributions.

P3HT/PCBM A

Excitation	Excitation energy (eV)	Λ	*f*	Major MO involved in the transition ((r,s) operator)[46]
$S_{1,P3HT}$	2.86	0.80	2.07	HOMO → LUMO (-0.66568)
S_1	2.15	0.11	$8.60.10^{-4}$	HOMO → LUMO (0.62614)
S_2	2.21	0.15	$4.75.10^{-2}$	HOMO → LUMO+1 (0.65617)
S_3	2.40	0.12	$7.09.10^{-3}$	HOMO → LUMO+2 (0.61812)
S_4	2.62	0.62	$5.15.10^{-3}$	HOMO-2 → LUMO (-0.66338)
S_5	2.67	0.74	$1.53.10^{-4}$	HOMO-2 → LUMO+1 (-0.61680)
S_6	2.74	0.58	$3.19.10^{-6}$	HOMO-3 → LUMO (0.55872)
S_7	2.77	0.70	$5.24.10^{-5}$	HOMO-4 → LUMO (0.58967)
S_8	2.91	0.54	$5.27.10^{-4}$	HOMO-5 → LUMO+1 (-0.51774) HOMO-6 → LUMO+1 (-0.32626)
S_9	2.93	0.74	1.72	HOMO → LUMO+5 (0.61299)
S_{10}	2.94	0.65	$1.31.10^{-1}$	HOMO-4 → LUMO+1 (0.38497) HOMO-2 → LUMO+2 (-0.33414)

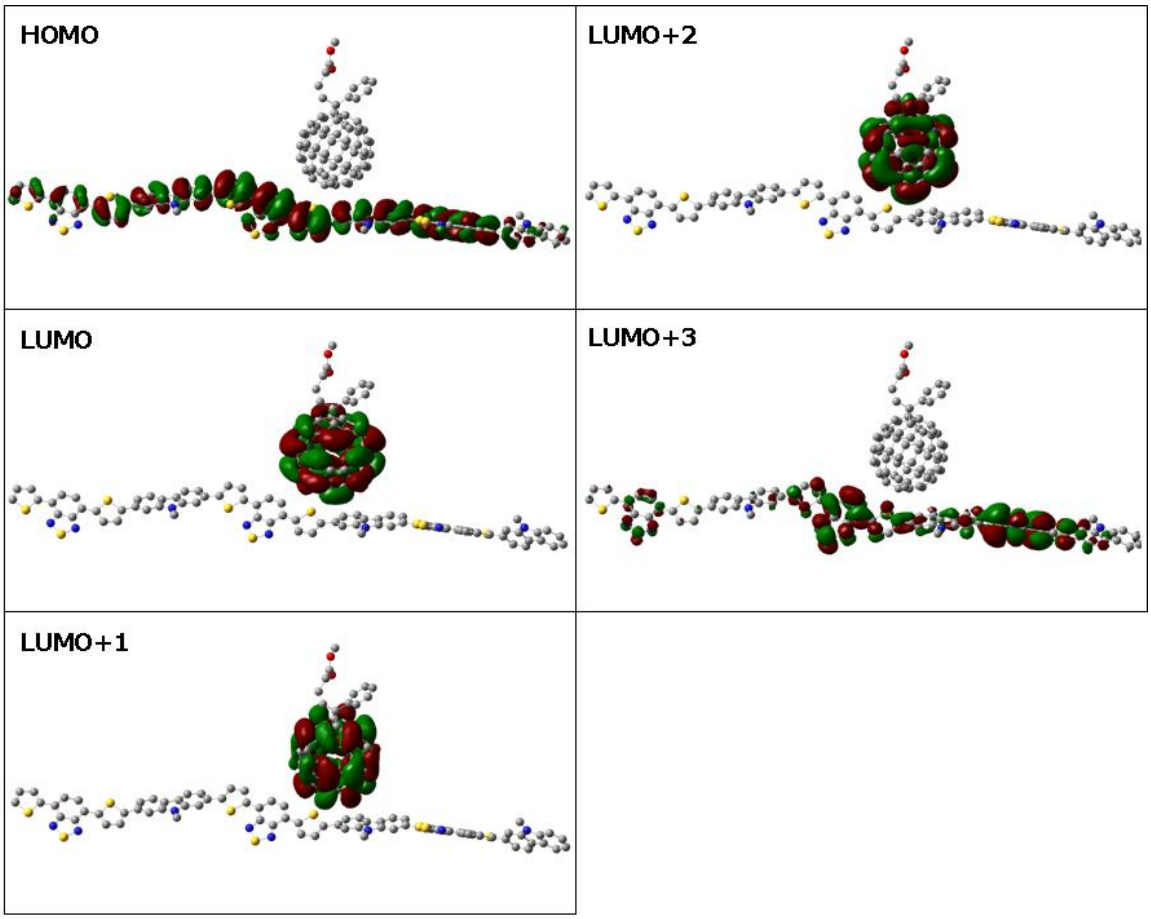
P3HT/PCBM B

Excitation	Excitation energy (eV)	Λ	*f*	Major MO involved in the transition ((r,s) operator)[46]
$S_{1,P3HT}$	2.86	0.80	2.07	HOMO → LUMO (-0.66568)
S_1	2.26	0.15	$2.62.10^{-2}$	HOMO → LUMO (0.67784)
S_2	2.42	0.09	$7.02.10^{-3}$	HOMO → LUMO+1 (0.68804)
S_3	2.58	0.13	$4.25.10^{-2}$	HOMO → LUMO+2 (0.66116)
S_4	2.64	0.63	$1.82.10^{-3}$	HOMO-2 → LUMO (0.65589)
S_5	2.66	0.75	$2.14.10^{-5}$	HOMO-2 → LUMO+1 (0.62006)
S_6	2.74	0.61	$6.12.10^{-4}$	HOMO-3 → LUMO (-0.61122)
S_7	2.77	0.67	$1.06.10^{-3}$	HOMO-4 → LUMO (0.67116)
S_8	2.87	0.65	$6.85.10^{-4}$	HOMO-5 → LUMO+1 (0.46133) HOMO-3 → LUMO+1(0.37047)
S_9	2.92	0.62	$1.18.10^{-1}$	HOMO-5 → LUMO+1 (0.36157) HOMO-4 → LUMO+1 (-0.33123) HOMO-3 → LUMO+2 (0.30481)
S_{10}	2.93	0.54	1.49	HOMO → LUMO+4 (0.44532) HOMO → LUMO+5 (0.33591)

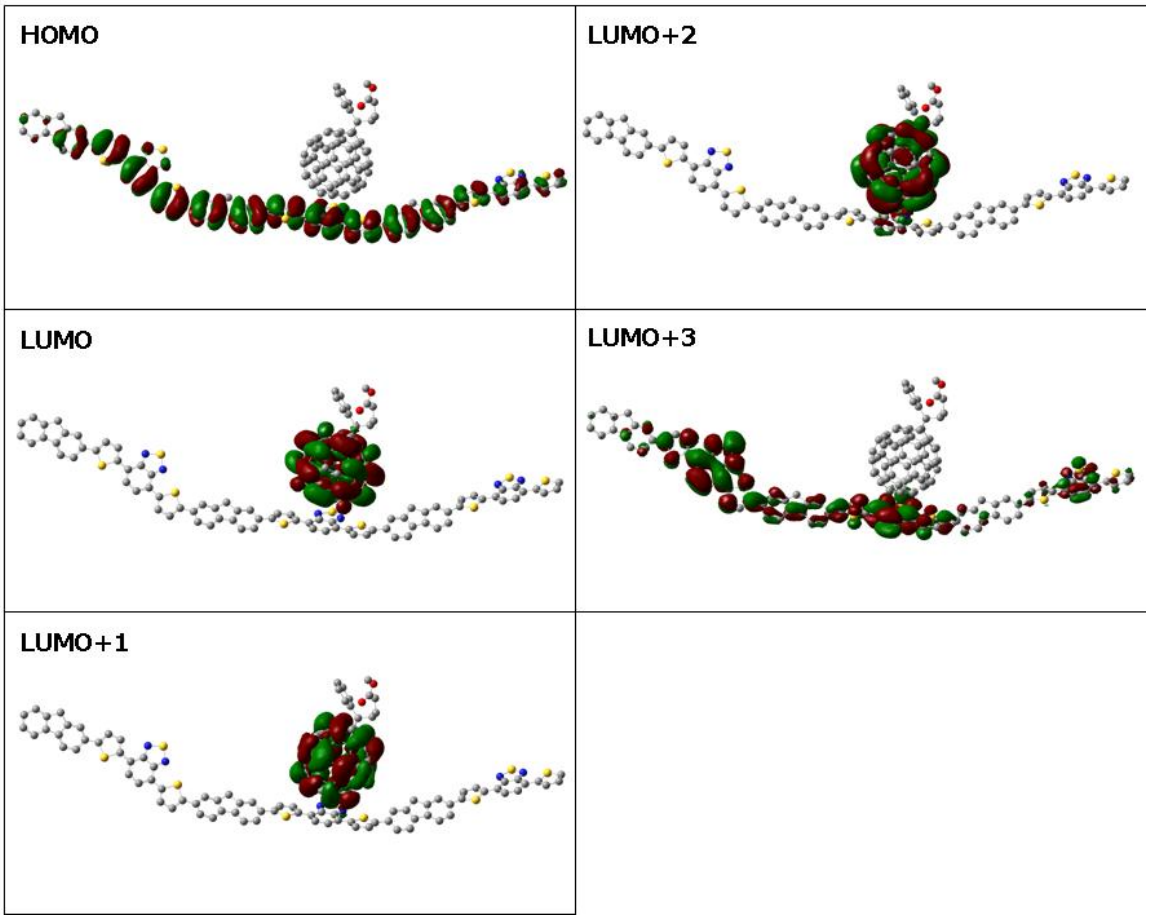
P3HT/PCBM C				
Excitation	**Excitation energy (eV)**	**Λ**	***f***	**Major MO involved in the transition ((r,s) operator)[46]**
$S_{1,P3HT}$	2.86	0.80	2.07	HOMO → LUMO (-0.66568)
S_1	2.63	0.63	$6.27.10^{-1}$	HOMO-2 → LUMO (0.66874)
S_2	2.67	0.76	$7.58.10^{-1}$	HOMO-2 → LUMO+1 (0.62874)
S_3	2.69	0.00	$3.70.10^{-3}$	HOMO → LUMO (0.70277)
S_4	2.76	0.77	$7.66.10^{-1}$	HOMO-3 → LUMO (-0.65627)
S_5	2.77	0.66	$6.64.10^{-1}$	HOMO-4 → LUMO (0.65974)
S_6	2.78	0.00	$3.17.10^{-3}$	HOMO → LUMO+1 (0.70056)
S_7	2.80	0.79	$7.89.10^{-1}$	HOMO → LUMO+3 (-0.66329)
S_8	2.90	0.71	$7.09.10^{-1}$	HOMO-5 → LUMO+1 (-0.52993) HOMO-4 → LUMO+1 (0.41929)
S_9	2.94	0.69	$6.94.10^{-1}$	HOMO-3 → LUMO+1 (-0.50012) HOMO-2 → LUMO+2 (0.35640)
S_{10}	3.01	0.67	2.16	HOMO-5 → LUMO (-0.49323) HOMO-3 → LUMO+2 (-0.41945)

Figure 2. Visualizations of the most important molecular orbitals for the PCDTBT/PCBM, APFO3/PCBM, MDMO-PPV/PCBM, PCPDTBT/PCBM and PBDTTPD/PCBM systems

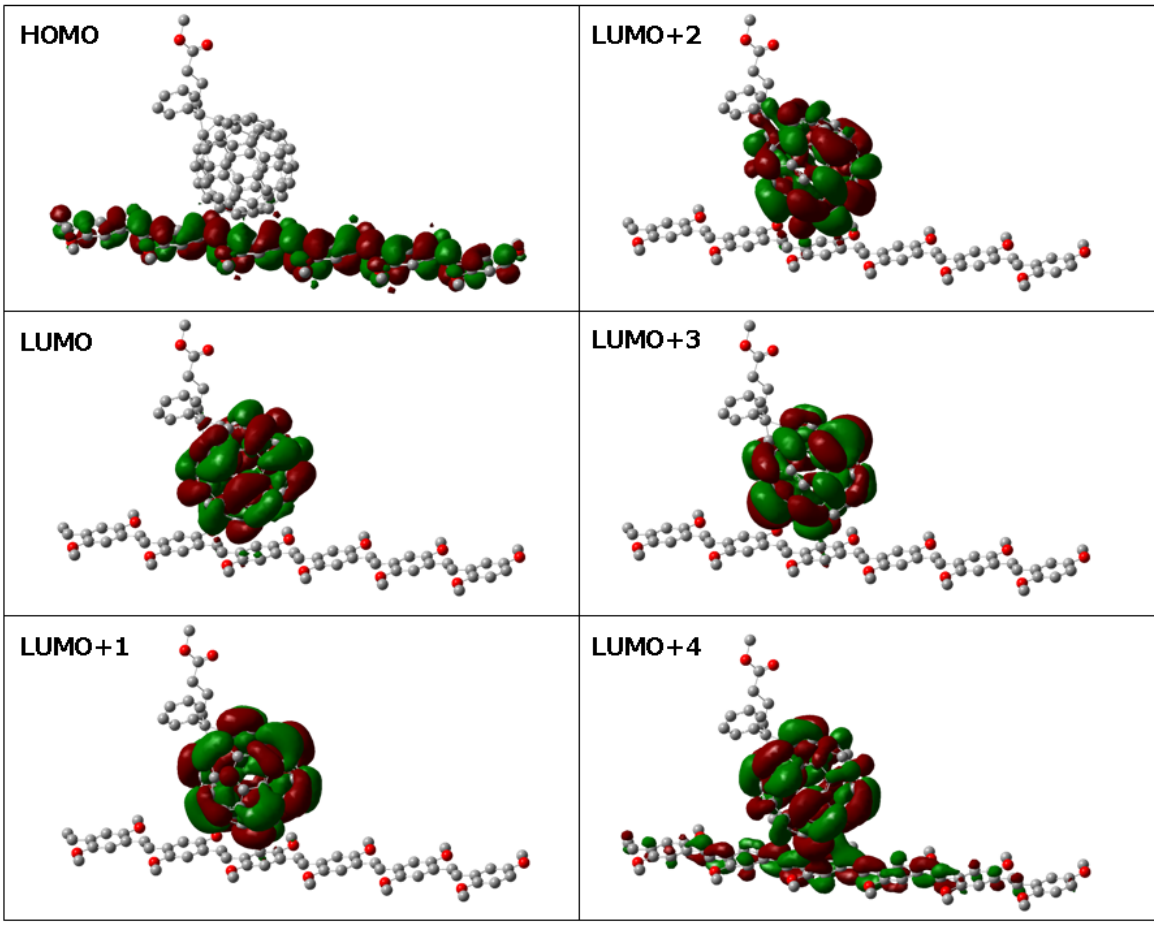
PCDTBT/PCBM



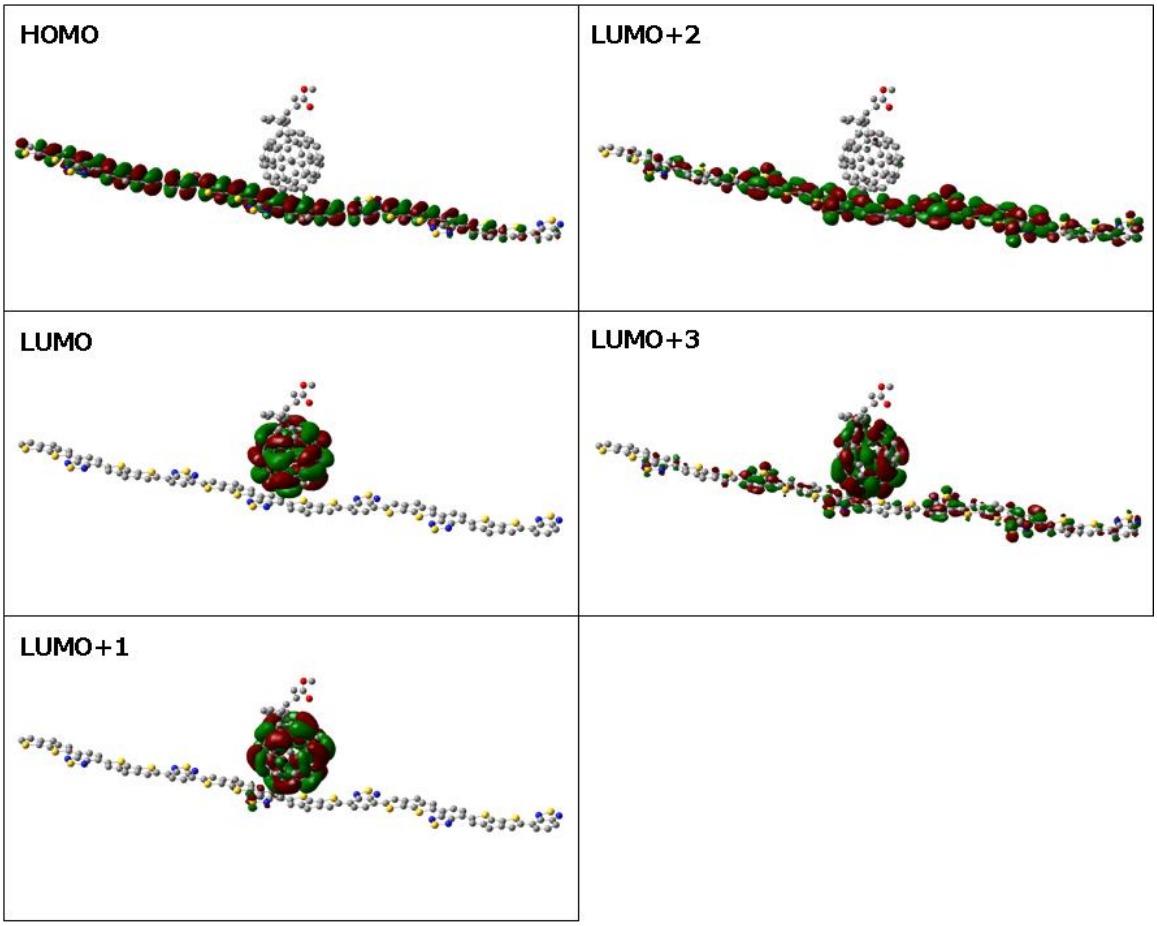
APFO3/PCBM



MDMO-PPV/PCBM



PCPDTBT/PCBM



PBDTTPD/PCBM

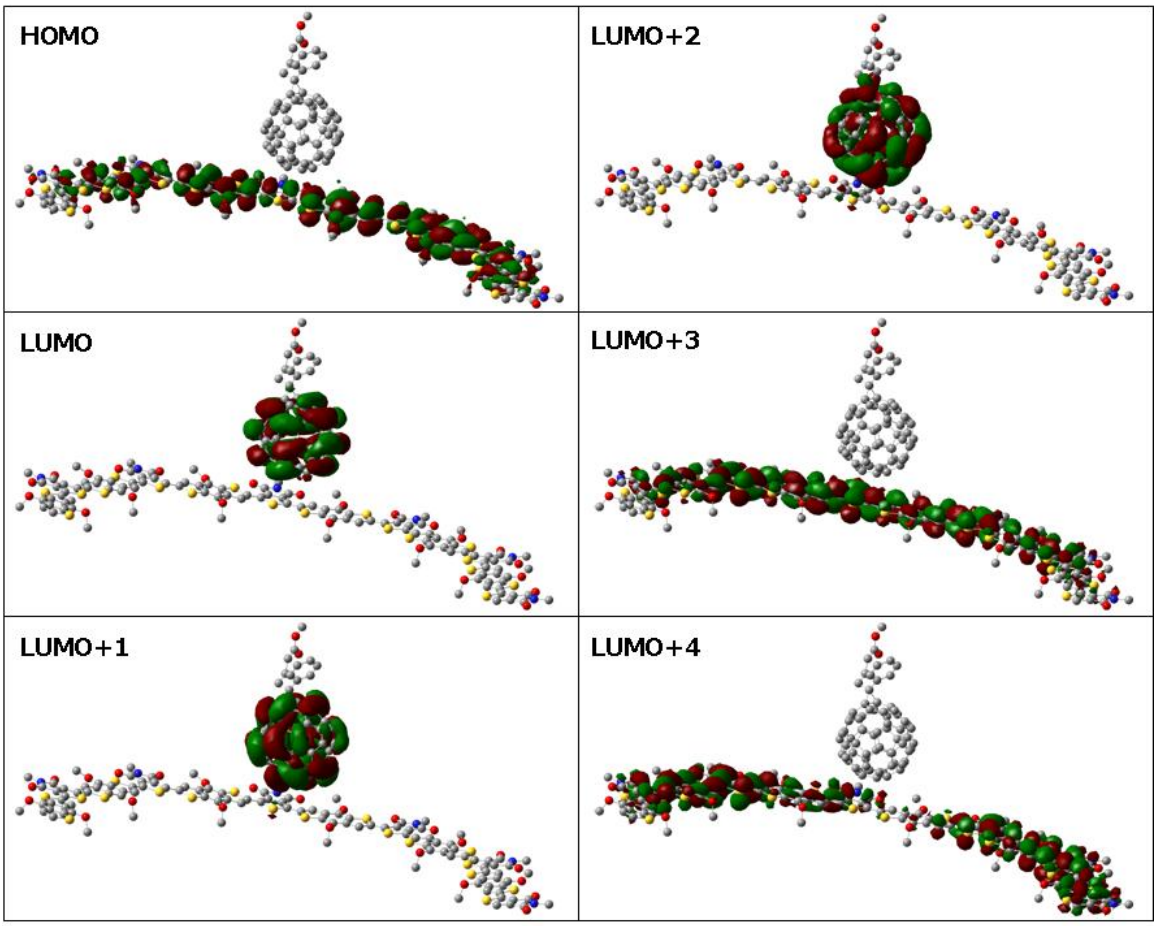


Table 2. Characteristics of the first singlet excitations for the PCDTBT/PCBM, APFO3/PCBM, MDMO-PPV/PCBM, PCPDTBT/PCBM and PBDTTPD/PCBM systems.

PCDTBT/PCBM

Excitation	Excitation energy (eV)	Λ	*f*	Major MO involved in the transition ((r,s) operator)[46]
$S_{1,PCDTBT}$	2.47	0.54	2.59	HOMO → LUMO (-0.42401) HOMO → LUMO+2 (-0.39441)
S_1	2.49	0.60	3.21	HOMO → LUMO+3 (0.440397)
S_2	2.59	0.59	$2.20.10^{-1}$	HOMO-1 → LUMO+3 (0.42108) HOMO → LUMO+4 (-0.38386)
S_3	2.63	0.55	$2.40.10^{-3}$	HOMO-8 → LUMO (0.62656)
S_4	2.67	0.68	$3.69.10^{-5}$	HOMO-8 → LUMO+1 (0.58875)
S_5	2.72	0.14	$1.57.10^{-1}$	HOMO → LUMO (-0.41212) HOMO → LUMO+1 (-0.40577)
S_6	2.74	0.50	$3.30.10^{-1}$	HOMO-2 → LUMO+4 (-0.34020)
S_7	2.74	0.08	$1.02.10^{-2}$	HOMO → LUMO (0.42009) HOMO → LUMO+1 (-0.45680)
S_8	2.76	0.65	$1.89.10^{-4}$	HOMO-9 → LUMO+1 (0.66440)
S_9	2.77	0.71	$8.26.10^{-6}$	HOMO-10 → LUMO+1 (0.67243)
S_{10}	2.90	0.08	$1.79.10^{-3}$	HOMO → LUMO+2 (-0.60923)

APFO3/PCBM

Excitation	Excitation energy (eV)	Λ	*f*	Major MO involved in the transition ((r,s) operator)[46]
$S_{1,APFO3}$	2.45	0.54	2.56	HOMO → LUMO (-0.42075) HOMO → LUMO+2 (0.38831)
S_1	2.48	0.55	2.83	HOMO → LUMO+3 (-0.42185)
S_2	2.59	0.53	$2.82.10^{-1}$	HOMO-1 → LUMO+3 (-0.40453) HOMO → LUMO+4 (-0.30974)
S_3	2.62	0.60	$6.96.10^{-3}$	HOMO-3 → LUMO (0.63208)
S_4	2.64	0.13	$8.93.10^{-2}$	HOMO → LUMO (-0.38563) HOMO → LUMO+1 (-0.36294)
S_5	2.67	0.73	$6.86.10^{-3}$	HOMO-3 → LUMO+1 (0.60466)
S_6	2.70	0.18	$2.48.10^{-1}$	HOMO → LUMO (-0.39357) HOMO → LUMO+1 (0.33490)
S_7	2.74	0.53	$3.89.10^{-1}$	HOMO-2 → LUMO+4 (-0.33973)
S_8	2.76	0.61	$1.37.10^{-4}$	HOMO-6 → LUMO (0.64596)
S_9	2.76	0.73	$6.69.10^{-5}$	HOMO-7 → LUMO (0.66607)
S_{10}	2.85	0.26	$4.71.10^{-2}$	HOMO → LUMO+2 (-0.48117)

MDMO-PPV/PCBM

Excitation	Excitation energy (eV)	Λ	*f*	Major MO involved in the transition ((r,s) operator)[46]
$S_{1,MDMO-PPV}$	2.72	0.78	4.61	HOMO → LUMO (0.61519)
S_1	2.07	0.11	$9.56.10^{-3}$	HOMO → LUMO (-0.46173)
				HOMO → LUMO+1 (-0.41724)
S_2	2.10	0.10	$3.22.10^{-2}$	HOMO → LUMO (0.41403)
				HOMO → LUMO+1 (-0.47034)
S_3	2.32	0.12	$2.34.10^{-2}$	HOMO → LUMO+2 (0.61858)
S_4	2.62	0.47	$7.72.10^{-3}$	HOMO-6 → LUMO (0.54592)
S_5	2.65	0.52	$1.97.10^{-3}$	HOMO-6 → LUMO+1 (-0.50164)
S_6	2.70	0.59	4.02	HOMO → LUMO+4 (-0.51153)
S_7	2.73	0.18	$2.84.10^{-1}$	HOMO-1 → LUMO (0.58371)
S_8	2.76	0.67	$2.40.10^{-3}$	HOMO-7 → LUMO (0.64017)
S_9	2.77	0.52	$2.42.10^{-3}$	HOMO-8 → LUMO (-0.55389)
				HOMO-1 → LUMO+1 (-0.30634)
S_{10}	2.77	0.74	$6.51.10^{-3}$	HOMO-1 → LUMO+1 (0.53058)
				HOMO-8 → LUMO (-0.30374)

PCPDTBT/PCBM

Excitation	Excitation energy (eV)	Λ	*f*	Major MO involved in the transition ((r,s) operator)[46]
$S_{1,PCPDTBT}$	1.85	0.68	6.49	HOMO → LUMO (-0.50977)
S_1	1.86	0.60	6.30	HOMO → LUMO+2 (-0.45164)
S_2	2.05	0.59	$1.81.10^{-2}$	HOMO → LUMO+3 (0.40289)
				HOMO-1 → LUMO+2 (-0.37112)
S_3	2.26	0.50	$5.09.10^{-1}$	HOMO → LUMO+5 (-0.30622)
				HOMO → LUMO+1 (-0.30463)
S_4	2.32	0.21	$2.54.10^{-2}$	HOMO → LUMO (0.48131)
S_5	2.34	0.36	$2.87.10^{-2}$	HOMO → LUMO (0.34056)
				HOMO → LUMO+1 (0.32043)
S_6	2.43	0.54	$4.48.10^{-2}$	HOMO-1 → LUMO+5 (-0.28721)
S_7	2.52	0.50	$7.78.10^{-2}$	HOMO → LUMO+4 (-0.32948)
S_8	2.62	0.51	$4.74.10^{-2}$	HOMO → LUMO+7 (0.30587)
				HOMO → LUMO+4 (-0.29724)
S_9	2.63	0.56	$6.18.10^{-3}$	HOMO-6 → LUMO (-0.62455)
S_{10}	2.68	0.67	$8.41.10^{-4}$	HOMO-6 → LUMO+1 (-0.55426)

PBDTTPD/PCBM				
Excitation	**Excitation energy (eV)**	**Λ**	***f***	**Major MO involved in the transition ((r,s) operator)[46]**
$S_{1,PBDTTPD}$	2.27	0.28	$3.10.10^{-2}$	HOMO-3 → LUMO (-0.47846)
$S_{2,PBDTTPD}$	2.81	0.56	$5.98.10^{-1}$	HOMO → LUMO+1 (-0.54131)
S_1	2.56	0.66	3.85	HOMO → LUMO+3 (-0.44998)
S_2	2.63	0.48	$7.43.10^{-3}$	HOMO-8 → LUMO (0.59253)
S_3	2.67	0.59	$7.99.10^{-3}$	HOMO-8 → LUMO+1 (0.54779)
S_4	2.70	0.63	2.87	HOMO → LUMO+4 (-0.37217) HOMO-1 → LUMO+3 (0.36991)
S_5	2.73	0.17	$8.42.10^{-2}$	HOMO → LUMO+1 (0.42291)
S_6	2.75	0.35	$3.24.10^{-3}$	HOMO-12 → LUMO (0.33568)
S_7	2.75	0.64	$4.58.10^{-3}$	HOMO-11 → LUMO (0.54596)
S_8	2.79	0.37	$6.15.10^{-3}$	HOMO-12 → LUMO (-0.44543) HOMO → LUMO (0.36690)
S_9	2.83	0.54	$3.09.10^{-3}$	HOMO → LUMO+5 (0.29940) HOMO-2 → LUMO+3 (0.29884)
S_{10}	2.90	0.49	$8.50.10^{-2}$	HOMO-13 → LUMO+1 (-0.34975)

Coordinates and final energies obtained after geometry optimization for all the systems studied using the PBE0 exchange-correlation functional in combination with the 3-21G* basis set.

P3HT/PCBM A configuration

Total energy: -7817.3188374 A.U.

C	-1.16378	3.20664	-0.00177
C	-0.65272	3.30298	1.27934
S	0.11978	3.28936	-1.1659
C	0.76014	3.41599	1.34029
H	-1.28507	3.25419	2.15564
C	1.33793	3.40294	0.07189
C	1.54247	3.48132	2.62787
H	2.37251	2.76153	2.57189
H	1.98928	4.48182	2.73766

C	0.71536	3.16357	3.8844
H	-0.07266	3.9184	4.0151
H	0.229	2.18651	3.75791
C	1.59647	3.12909	5.14209
H	2.38021	2.3686	5.01057
H	2.09832	4.10035	5.26462
C	0.79083	2.80958	6.41014
H	0.29326	1.83647	6.286
H	0.00242	3.56549	6.5412
C	1.67097	2.77174	7.66846
H	2.45973	2.01634	7.5369
H	2.17011	3.74433	7.79258
C	0.87024	2.44956	8.93952
H	0.08192	3.20443	9.06887
H	0.37183	1.4782	8.81347
C	1.76519	2.41491	10.18717
H	2.25483	3.38548	10.33476
H	1.18473	2.18295	11.08756
H	2.5465	1.65287	10.07657
C	2.72057	3.38783	-0.32055
C	3.21749	3.04814	-1.56837
S	4.02956	3.7765	0.75258
C	4.62935	3.08076	-1.66935
H	2.57237	2.75314	-2.38476
C	5.22855	3.46989	-0.47316
C	5.39041	2.6996	-2.91532
H	6.01713	3.54701	-3.23364
H	6.07086	1.86722	-2.67657
C	4.4991	2.27178	-4.09242
H	3.87709	1.41897	-3.78639

H	3.829	3.09827	-4.36752
C	5.33633	1.86927	-5.31577
H	5.96965	2.71577	-5.61954
H	6.00599	1.04163	-5.03939
C	4.46234	1.43768	-6.50298
H	3.79641	2.26671	-6.78435
H	3.82407	0.59609	-6.19598
C	5.29722	1.02124	-7.72336
H	5.93814	1.86132	-8.02961
H	5.96216	0.19128	-7.44192
C	4.42723	0.58961	-8.9139
H	3.78551	-0.24751	-8.60508
H	3.76451	1.42013	-9.19463
C	5.2776	0.17287	-10.12311
H	5.93353	-0.66582	-9.8587
H	4.64826	-0.13593	-10.96575
H	5.90859	1.00723	-10.45337
C	6.61687	3.62607	-0.13316
C	7.12576	4.06071	1.07914
S	7.92084	3.26524	-1.22576
C	8.53922	4.10355	1.14549
H	6.48819	4.34471	1.90588
C	9.13017	3.69193	-0.0472
C	9.30973	4.54065	2.36704
H	9.96797	3.71931	2.69068
H	9.96097	5.38723	2.09969
C	8.42863	4.95774	3.55526
H	7.77658	5.78983	3.25499
H	7.78652	4.11583	3.84962
C	9.27605	5.39085	4.76122

H	9.9321	4.56068	5.0616
H	9.9238	6.23001	4.46785
C	8.41202	5.81275	5.9592
H	7.76342	4.97411	6.25239
H	7.75592	6.64308	5.65902
C	9.25685	6.2459	7.16682
H	9.91288	5.41576	7.46798
H	9.90695	7.08361	6.87384
C	8.39641	6.67038	8.36689
H	7.74155	7.49955	8.06423
H	7.7466	5.83301	8.65733
C	9.25649	7.09922	9.56488
H	9.90001	7.9445	9.29116
H	8.63377	7.40298	10.41421
H	9.90037	6.27252	9.88944
H	-4.12971	0.7577	-3.47888
C	-3.16949	0.47532	-3.02592
C	-2.42273	1.72901	-2.53064
H	-3.3847	-0.17207	-2.16511
C	-2.33482	-0.29999	-4.05576
C	-3.15978	2.48422	-1.45299
H	-2.23033	2.395	-3.38594
H	-1.4478	1.41092	-2.13983
H	-2.13624	0.34058	-4.92769
H	-1.36488	-0.55463	-3.60648
C	-3.02038	-1.5956	-4.51434
C	-4.5726	2.59175	-1.40151
C	-2.55474	3.11471	-0.37216
H	-3.98254	-1.35533	-4.99053
H	-3.23683	-2.21748	-3.63308

C	-2.15001	-2.39877	-5.49253
C	-5.05996	3.28606	-0.30705
H	-5.22515	2.14534	-2.14065
S	-3.73775	3.84152	0.67679
H	-1.91449	-1.77696	-6.36896
H	-1.19651	-2.64629	-5.00289
C	-2.8275	-3.69626	-5.95881
C	-6.44278	3.53959	-0.00117
H	-3.07325	-4.308	-5.07932
H	-3.77535	-3.44929	-6.45729
C	-1.93199	-4.49886	-6.91426
S	-7.65102	3.09693	-1.17443
C	-7.03017	4.08838	1.13567
H	-0.99159	-4.77002	-6.41832
H	-2.42559	-5.42029	-7.24456
H	-1.68761	-3.9029	-7.80229
C	-8.95265	3.62115	-0.1472
C	-8.44256	4.12546	1.03754
C	-6.25692	4.57903	2.33506
C	-10.34069	3.51127	-0.50607
H	-9.07853	4.51431	1.82176
H	-5.59528	3.77335	2.68895
H	-5.60839	5.41547	2.03103
C	-7.13522	5.04259	3.5079
S	-11.54484	3.94567	0.67467
C	-10.93674	3.08761	-1.69165
H	-7.77648	5.8737	3.18256
H	-7.78848	4.21728	3.8239
C	-6.28523	5.50158	4.70233
C	-12.85412	3.56745	-0.40607

C	-12.35016	3.12661	-1.61847
C	-10.16972	2.63842	-2.91104
H	-5.63879	4.67317	5.02749
H	-5.62762	6.3247	4.38627
C	-7.14596	5.96678	5.88647
H	-12.99132	2.83341	-2.43921
H	-9.47966	3.4395	-3.21803
H	-9.55119	1.76638	-2.647
C	-11.05189	2.26365	-4.11242
H	-7.80454	5.14398	6.20155
H	-7.79217	6.79597	5.56254
C	-6.29786	6.42333	7.08306
H	-11.72346	1.44	-3.83262
H	-11.67405	3.12463	-4.39413
C	-10.20515	1.83491	-5.32051
H	-5.65023	5.59485	7.40632
H	-5.63926	7.2466	6.76885
C	-7.15455	6.88745	8.27099
H	-9.53603	2.65969	-5.60632
H	-9.57051	0.98286	-5.03555
C	-11.06869	1.44068	-6.52824
H	-7.80072	7.71529	7.9467
H	-7.8132	6.06459	8.58229
C	-6.29105	7.33809	9.45844
H	-11.70674	2.29064	-6.81188
H	-11.73521	0.61341	-6.24301
C	-10.22315	1.01595	-7.7384
H	-5.63874	8.16954	9.16394
H	-6.91132	7.66982	10.29906
H	-5.65588	6.51349	9.80479

H	-9.55923	1.84437	-8.02662
H	-9.58095	0.16929	-7.45374
C	-11.08256	0.61363	-8.94683
H	-11.7447	-0.21436	-8.65709
H	-11.7251	1.45952	-9.22861
C	-10.22148	0.19398	-10.14741
H	-9.58548	-0.65981	-9.88262
H	-10.8434	-0.0936	-11.00295
H	-9.56999	1.01987	-10.45854
C	-0.85773	-1.32278	0.04165
C	-0.71681	-1.18206	1.41467
C	0.0618	-0.6347	-0.85438
C	-1.14758	-2.62809	-0.52829
C	-0.86299	-2.34206	2.28101
C	0.33945	-0.34534	1.95826
C	0.33724	-1.51686	-1.97559
C	1.0738	0.16213	-0.33684
C	-1.27678	-3.74025	0.29752
C	-0.41236	-2.74691	-1.76809
C	-1.13179	-3.58894	1.73493
C	0.09816	-2.21664	3.36664
C	1.21609	0.30964	1.10266
C	0.84457	-0.98721	3.16424
C	1.60638	-1.56312	-2.5334
C	2.40831	0.1084	-0.91668
C	-0.70663	-5.01731	-0.08773
C	0.14898	-3.96877	-2.11699
C	-0.46336	-4.77275	2.24899
C	0.73614	-3.34459	3.86161
C	2.63758	0.34696	1.41073

C	2.20002	-0.94012	3.46352
C	2.19054	-2.8431	-2.90492
C	2.66737	-0.73073	-1.99228
C	3.37313	0.22353	0.16322
C	-0.02662	-5.13421	-1.2811
C	-0.19645	-5.66689	1.13737
C	1.47964	-4.01849	-2.6975
C	0.44524	-4.65203	3.29501
C	2.15668	-3.29594	4.1756
C	3.11758	-0.25963	2.56259
C	2.87133	-2.12218	3.97811
C	3.60325	-2.80479	-2.60154
C	3.90423	-1.50091	-2.03343
C	4.55357	-0.50279	0.12125
C	1.14505	-6.02795	-1.47444
C	0.9675	-6.40488	1.11283
C	2.1382	-5.21599	-2.22769
C	1.67862	-5.40443	3.25504
C	2.74133	-4.57251	3.80044
C	4.35686	-1.02041	2.52237
C	4.20468	-2.1716	3.39591
C	4.22547	-3.94503	-2.10249
C	4.82324	-1.38783	-1.00091
C	5.05486	-1.14341	1.32862
C	1.70212	-6.73925	-0.13824
C	1.1665	-7.53893	-1.30774
C	1.93459	-6.23906	2.17512
C	3.48	-5.17619	-1.9167
C	4.01157	-4.61898	3.24675
C	4.76217	-3.39205	3.03973

C	5.18967	-3.82311	-1.02199
C	5.4836	-2.57744	-0.48616
C	5.63383	-2.42108	0.95329
C	3.13361	-6.47562	0.1689
C	2.1645	-8.27426	-2.14913
C	-0.18078	-8.22608	-1.10931
C	3.26499	-6.28555	1.59438
C	3.9892	-5.82156	-0.68993
C	4.28229	-5.49984	2.12059
C	5.49294	-3.52026	1.78704
C	5.03665	-4.97593	-0.15006
C	3.17172	-9.04937	-1.5693
C	2.03093	-8.25037	-3.54033
H	-0.85944	-7.52657	-0.60984
H	-0.60374	-8.43745	-2.10103
C	-0.08699	-9.51756	-0.27767
C	5.19489	-4.82767	1.22425
H	3.28074	-9.06365	-0.48996
C	4.03219	-9.797	-2.37235
C	2.89126	-8.99577	-4.34232
H	1.25592	-7.63768	-3.99041
H	0.63449	-9.3831	0.53792
H	-1.05395	-9.70867	0.20286
C	0.29106	-10.75167	-1.10072
C	3.89266	-9.77233	-3.7591
H	4.81132	-10.39639	-1.91436
H	2.78328	-8.96895	-5.42108
H	-0.42428	-10.91853	-1.91668
H	1.27832	-10.64039	-1.56233
C	0.30564	-11.97801	-0.22908

H	4.56358	-10.3521	-4.38334
O	0.59012	-13.09417	-0.97287
O	0.09992	-12.01944	0.97778
C	0.62887	-14.34343	-0.20492
H	-0.33414	-14.52776	0.27914
H	0.85342	-15.11642	-0.93878
H	1.40217	-14.29722	0.56684
H	-13.89764	3.66113	-0.136
H	10.17369	3.59825	-0.31727

P3HT/PCBM B configuration

Total energy: -7817.3280444 A.U.

C	-0.34255	2.53034	0.03434
C	0.14683	2.58104	1.32922
S	0.96396	2.65943	-1.10102
C	1.55233	2.72125	1.4207
H	-0.4964	2.48618	2.19348
C	2.14851	2.79445	0.16448
C	2.31222	2.74887	2.72434
H	2.93688	1.84428	2.79353
H	2.99342	3.61281	2.7301
C	1.41728	2.80769	3.97264
H	0.76781	3.69244	3.91837
H	0.77354	1.91722	4.00196
C	2.24984	2.86457	5.26222
H	2.91028	1.98595	5.30658
H	2.89278	3.75672	5.2422
C	1.37105	2.89993	6.52161
H	0.72694	2.00843	6.53886
H	0.71066	3.77865	6.47983

C	2.20038	2.95015	7.81356
H	2.86187	2.07203	7.85438
H	2.84472	3.84171	7.79823
C	1.32468	2.98145	9.07561
H	0.66491	3.85946	9.03387
H	0.67997	2.0915	9.08744
C	2.16877	3.02762	10.35785
H	2.80676	3.92006	10.36461
H	1.53462	3.0523	11.25152
H	2.81727	2.1451	10.42133
C	3.53553	2.91963	-0.19742
C	4.04106	3.27562	-1.4364
S	4.83414	2.51819	0.88276
C	5.45483	3.21372	-1.53419
H	3.40025	3.58011	-2.25339
C	6.04223	2.81481	-0.33573
C	6.22721	3.53574	-2.79014
H	6.89157	4.39309	-2.59948
H	6.87273	2.6807	-3.04378
C	5.34775	3.85396	-4.00985
H	4.68414	3.00119	-4.21199
H	4.71633	4.72713	-3.79495
C	6.19469	4.13855	-5.2592
H	6.86073	4.99093	-5.06036
H	6.83237	3.26797	-5.47202
C	5.33096	4.44683	-6.49146
H	4.69213	5.31676	-6.27917
H	4.66489	3.59406	-6.69047
C	6.175	4.73151	-7.74286
H	6.83929	5.58607	-7.54642

H	6.81673	3.86325	-7.95399
C	5.31368	5.03497	-8.97839
H	4.65206	4.17945	-9.1743
H	4.67053	5.90012	-8.76446
C	6.17157	5.32131	-10.21957
H	6.80922	4.45948	-10.45232
H	5.54682	5.53196	-11.09516
H	6.82107	6.18794	-10.04513
C	7.42528	2.62249	0.00992
C	7.91215	2.20192	1.2365
S	8.74514	2.8723	-1.0956
C	9.32048	2.06224	1.29752
H	7.26129	1.98247	2.07266
C	9.92801	2.38216	0.08561
C	10.0652	1.60877	2.53038
H	10.7536	0.79453	2.25833
H	10.68473	2.43921	2.90354
C	9.15591	1.12767	3.67252
H	8.49685	1.94813	3.98913
H	8.51939	0.30614	3.31393
C	9.97149	0.64782	4.88257
H	10.626	-0.18117	4.57596
H	10.62035	1.46516	5.23051
C	9.07484	0.18597	6.04103
H	8.4265	-0.63254	5.69513
H	8.41878	1.0152	6.34441
C	9.88513	-0.28845	7.2568
H	10.53964	-1.11989	6.95611
H	10.53602	0.52902	7.60111
C	8.99029	-0.74468	8.41928

H	8.33453	0.08605	8.71547
H	8.34216	-1.56266	8.07474
C	9.81484	-1.21109	9.62817
H	10.44974	-0.39596	9.99689
H	9.16716	-1.5396	10.44909
H	10.4653	-2.0488	9.34777
H	-3.00411	1.54178	-4.29368
C	-2.224	0.8808	-3.89113
C	-1.44998	1.59412	-2.77122
H	-2.71259	-0.01076	-3.47662
C	-1.27448	0.45487	-5.02153
C	-2.2724	1.94278	-1.55711
H	-0.99847	2.51094	-3.18198
H	-0.61986	0.94136	-2.46003
H	-0.79988	1.34741	-5.45606
H	-0.47216	-0.16514	-4.59527
C	-1.98787	-0.33283	-6.12992
C	-3.684	1.83388	-1.48418
C	-1.71987	2.36941	-0.34974
H	-2.78616	0.28554	-6.56616
H	-2.46517	-1.22139	-5.69108
C	-1.0221	-0.77338	-7.24047
C	-4.21757	2.15962	-0.2492
H	-4.29697	1.48404	-2.30447
S	-2.95565	2.64947	0.83768
H	-0.55077	0.11482	-7.68723
H	-0.21707	-1.38043	-6.79834
C	-1.71658	-1.58576	-8.344
C	-5.61144	2.17221	0.11869
H	-2.18866	-2.47082	-7.89506

H	-2.51948	-0.97847	-8.78479
C	-0.73406	-2.02177	-9.44084
S	-6.79993	2.35596	-1.13796
C	-6.21374	2.02786	1.36449
H	0.06581	-2.64034	-9.01493
H	-1.2394	-2.60441	-10.21963
H	-0.27221	-1.14589	-9.91308
C	-8.11916	2.21837	-0.0129
C	-7.62749	2.05551	1.27125
C	-5.46538	1.83728	2.66027
C	-9.50456	2.29184	-0.39528
H	-8.2758	1.94336	2.13062
H	-4.52246	1.3154	2.45216
H	-5.20752	2.8189	3.08749
C	-6.22841	1.01212	3.7123
S	-10.71626	2.24902	0.85386
C	-10.09076	2.38637	-1.65485
H	-7.15645	1.52247	4.00396
H	-6.50095	0.04374	3.27091
C	-5.36755	0.77711	4.96319
C	-12.01587	2.34763	-0.29602
C	-11.50589	2.41574	-1.58109
C	-9.31414	2.4321	-2.9477
H	-4.40978	0.33299	4.65704
H	-5.14317	1.74067	5.44372
C	-6.0448	-0.15817	5.97532
H	-12.14237	2.46982	-2.45453
H	-8.67657	3.33	-2.95588
H	-8.64175	1.56158	-2.99361
C	-10.18823	2.44062	-4.21193

H	-6.28094	-1.11009	5.4773
H	-6.9955	0.2837	6.30865
C	-5.15402	-0.43823	7.19489
H	-10.83004	1.5485	-4.21931
H	-10.84079	3.3249	-4.20321
C	-9.33298	2.45832	-5.48797
H	-4.21004	-0.88856	6.85288
H	-4.90188	0.51112	7.69044
C	-5.82185	-1.37749	8.21067
H	-8.68805	3.34924	-5.48167
H	-8.67383	1.57781	-5.49498
C	-10.18792	2.46	-6.7642
H	-6.76681	-0.9293	8.5489
H	-6.07197	-2.32449	7.71223
C	-4.91572	-1.65185	9.41994
H	-10.84649	3.34107	-6.75967
H	-10.83406	1.56975	-6.76907
C	-9.3336	2.47245	-8.04078
H	-4.67325	-0.71554	9.93775
H	-5.40043	-2.32482	10.13665
H	-3.97546	-2.11484	9.09591
H	-8.68804	3.3632	-8.03763
H	-8.67291	1.59284	-8.04408
C	-10.18396	2.46952	-9.32044
H	-10.82885	1.57953	-9.32115
H	-10.84386	3.34842	-9.31565
C	-9.31408	2.48069	-10.58615
H	-8.66291	1.59819	-10.61093
H	-9.92983	2.47833	-11.49292
H	-8.67754	3.37392	-10.60552

C	-2.7533	-7.29676	0.44311
C	-2.63934	-7.3719	1.82334
C	-3.81962	-6.50633	-0.15537
C	-1.56274	-7.14155	-0.37761
C	-1.32768	-7.29462	2.44939
C	-3.58316	-6.66447	2.67113
C	-3.28523	-5.86223	-1.3435
C	-4.7187	-5.82664	0.65449
C	-0.30938	-7.05542	0.22033
C	-1.89041	-6.25742	-1.47302
C	-0.19366	-7.13514	1.66641
C	-1.4653	-6.54812	3.69092
C	-4.59822	-5.90846	2.10133
C	-2.85703	-6.15517	3.82619
C	-3.67224	-4.57095	-1.66783
C	-5.12682	-4.47207	0.31307
C	0.67808	-6.10956	-0.2654
C	-0.94724	-5.3387	-1.91451
C	0.86433	-6.23108	2.0861
C	-0.45697	-5.68544	4.09499
C	-4.93193	-4.60521	2.65427
C	-3.18084	-4.9141	4.35694
C	-2.68575	-3.61119	-2.14011
C	-4.61482	-3.85766	-0.8217
C	-5.25657	-3.71776	1.54796
C	0.37044	-5.28232	-1.32358
C	1.41575	-5.59168	0.9057
C	-1.35286	-3.98592	-2.25478
C	0.73654	-5.52771	3.27911
C	-0.79572	-4.38469	4.65351

C	-4.2413	-4.12059	3.75509
C	-2.12548	-4.00756	4.77984
C	-3.01444	-2.31433	-1.59468
C	-4.20869	-2.46074	-0.77602
C	-4.86825	-2.38557	1.59033
C	0.88394	-3.89482	-1.45708
C	1.81258	-4.27279	0.96152
C	-0.28912	-3.08322	-1.88041
C	1.13075	-4.13776	3.33041
C	0.18831	-3.42533	4.18039
C	-3.83913	-2.72327	3.80492
C	-2.53378	-2.65184	4.44103
C	-1.98884	-1.46826	-1.18453
C	-4.3309	-1.74223	0.40374
C	-4.14058	-1.87875	2.74462
C	1.68816	-3.32704	-0.18059
C	2.34231	-3.47007	-1.53902
C	1.63199	-3.52806	2.18772
C	-0.59959	-1.85562	-1.33726
C	-0.19945	-2.13454	3.85518
C	-1.59199	-1.73769	3.98597
C	-2.12371	-0.70821	0.04713
C	-3.26886	-0.83708	0.82102
C	-3.15482	-0.92384	2.26916
C	1.14841	-2.07259	0.40916
C	2.59576	-2.20169	-2.29807
C	3.38796	-4.57552	-1.66658
C	1.22726	-2.1758	1.84739
C	0.13715	-1.33594	-0.16648
C	0.33603	-1.49092	2.66471

C	-1.90971	-0.8491	2.87817
C	-0.81763	-0.64603	0.67818
C	3.30421	-1.14595	-1.71743
C	2.15702	-2.0975	-3.62161
H	2.95783	-5.51056	-1.29116
H	3.60819	-4.72164	-2.73227
C	4.66876	-4.25262	-0.87511
C	-0.71303	-0.69892	2.06401
H	3.68573	-1.23851	-0.7052
C	3.56492	0.00685	-2.4579
C	2.41787	-0.9449	-4.36036
H	1.59951	-2.91698	-4.06468
H	4.39016	-3.75059	0.05992
H	5.16548	-5.19082	-0.60035
C	5.66976	-3.35309	-1.62329
C	3.11777	0.11013	-3.77482
H	4.10099	0.83294	-2.00485
H	2.06883	-0.86958	-5.38501
H	6.46945	-3.91933	-2.10713
H	5.14967	-2.77366	-2.39844
C	6.28233	-2.34303	-0.68586
H	3.31712	1.01322	-4.34273
O	7.51416	-1.95608	-1.11846
O	5.75138	-1.878	0.32177
C	8.15434	-0.90475	-0.31059
H	8.28172	-1.24387	0.72092
H	9.11625	-0.72701	-0.78842
H	7.5464	0.00222	-0.30665
H	-13.05878	2.37359	-0.00909
H	10.97092	2.3562	-0.20132

P3HT/PCBM C configuration

Total energy: -7817.3262286 A.U.

C	-0.8125	3.2948	-0.00861
C	-0.30649	3.17055	1.27377
S	0.49646	3.42863	-1.14954
C	1.10729	3.17019	1.3557
H	-0.94352	3.06142	2.14127
C	1.70274	3.30092	0.10356
C	1.86863	3.01243	2.6491
H	2.51675	2.12495	2.57272
H	2.52909	3.8818	2.79143
C	0.97287	2.85984	3.88795
H	0.36408	3.76689	4.01227
H	0.29314	2.00771	3.76198
C	1.79533	2.62791	5.16513
H	2.42873	1.73793	5.02618
H	2.46549	3.48126	5.34461
C	0.88858	2.40868	6.38697
H	0.2046	1.57832	6.16302
H	0.27578	3.30858	6.54704
C	1.68145	2.10371	7.66596
H	2.29007	1.20006	7.51017
H	2.37712	2.93062	7.87256
C	0.77169	1.89231	8.886
H	0.16922	2.79777	9.04517
H	0.07287	1.07077	8.67428
C	1.57571	1.57566	10.15558
H	2.26857	2.39487	10.38426
H	0.91663	1.43236	11.0196

H	2.16465	0.66041	10.01802
C	3.09027	3.32101	-0.27159
C	3.5986	3.37909	-1.55859
S	4.39525	3.26754	0.8776
C	5.01234	3.38105	-1.63558
H	2.96119	3.41512	-2.43224
C	5.60401	3.32382	-0.37559
C	5.78258	3.43058	-2.93208
H	6.43478	4.31777	-2.93156
H	6.43995	2.54933	-2.99387
C	4.90227	3.47001	-4.19125
H	4.25403	2.5828	-4.21342
H	4.25635	4.35865	-4.16124
C	5.75068	3.50495	-5.47144
H	6.40101	4.39181	-5.45344
H	6.4042	2.6206	-5.49775
C	4.88813	3.53413	-6.74219
H	4.23639	4.41998	-6.71918
H	4.23514	2.64904	-6.75749
C	5.73433	3.56056	-8.02389
H	6.38713	4.44595	-8.01081
H	6.38771	2.67579	-8.04582
C	4.87536	3.58516	-9.29755
H	4.22235	2.70122	-9.30752
H	4.22358	4.46981	-9.27476
C	5.73659	3.60792	-10.56897
H	6.37842	2.71937	-10.61263
H	5.11444	3.62634	-11.47114
H	6.38209	4.49487	-10.5787
C	6.99095	3.30083	0.00172

C	7.49755	3.2506	1.29001
S	8.29794	3.32764	-1.14575
C	8.91104	3.23333	1.36848
H	6.85876	3.22909	2.16306
C	9.50456	3.27265	0.10884
C	9.68059	3.1827	2.66534
H	10.30532	2.27589	2.67953
H	10.36472	4.04419	2.7118
C	8.80022	3.18854	3.92506
H	8.17339	4.09119	3.93033
H	8.133	2.31535	3.91134
C	9.64763	3.15552	5.20597
H	10.28312	2.25775	5.19922
H	10.31578	4.02909	5.22162
C	8.78434	3.15544	6.47658
H	8.1198	2.27894	6.46412
H	8.14413	4.04993	6.48046
C	9.62934	3.13226	7.75915
H	10.27186	2.23926	7.75542
H	10.29287	4.00964	7.77274
C	8.76933	3.13006	9.03237
H	8.12589	4.02107	9.03288
H	8.10801	2.25237	9.01796
C	9.62932	3.11061	10.30469
H	10.28108	3.99232	10.3399
H	9.00637	3.10822	11.2065
H	10.26473	2.21656	10.32398
H	-3.58839	4.37459	-4.14604
C	-2.9091	3.51215	-4.1957
C	-2.02771	3.4775	-2.93719

H	-3.52279	2.60151	-4.23825
C	-2.06314	3.60689	-5.47448
C	-2.79505	3.35643	-1.64351
H	-1.41615	4.39278	-2.91068
H	-1.33142	2.62867	-3.02281
H	-1.44338	4.51474	-5.43623
H	-1.38012	2.74596	-5.52134
C	-2.9276	3.63556	-6.74394
C	-4.20768	3.2856	-1.56784
C	-2.19951	3.28585	-0.38631
H	-3.60288	4.50299	-6.70477
H	-3.55657	2.73361	-6.77437
C	-2.08413	3.7067	-8.02573
C	-4.71258	3.1618	-0.28455
H	-4.84697	3.31234	-2.44024
S	-3.40592	3.13281	0.86469
H	-1.45328	4.60752	-7.99745
H	-1.40931	2.83875	-8.06437
C	-2.94554	3.73294	-9.29771
C	-6.09908	3.09258	0.08914
H	-3.57945	2.83542	-9.32068
H	-3.6161	4.60291	-9.26018
C	-2.08728	3.79402	-10.56985
S	-7.30571	3.39196	-1.12997
C	-6.69221	2.79548	1.31387
H	-1.42777	2.91943	-10.62916
H	-2.71141	3.81464	-11.47061
H	-1.45979	4.69387	-10.56616
C	-8.61176	3.10737	-0.01825
C	-8.10603	2.80666	1.23589

C	-5.92227	2.47564	2.57164
C	-9.99831	3.20382	-0.38546
H	-8.74666	2.58316	2.07867
H	-5.20384	1.66926	2.356
H	-5.33413	3.35714	2.87169
C	-6.79833	2.04587	3.75959
S	-11.20279	3.14319	0.87102
C	-10.59206	3.33344	-1.63878
H	-7.47745	2.86536	4.03262
H	-7.41177	1.18181	3.46938
C	-5.94325	1.67012	4.97889
C	-12.51015	3.27381	-0.26878
C	-12.00463	3.36993	-1.555
C	-9.82486	3.41658	-2.93553
H	-5.27382	0.84122	4.70455
H	-5.31044	2.52559	5.25903
C	-6.78913	1.24761	6.18902
H	-12.64415	3.46443	-2.42259
H	-9.21071	4.33081	-2.93589
H	-9.13113	2.5641	-2.99698
C	-10.70738	3.42213	-4.19389
H	-7.43111	0.40099	5.90504
H	-7.45054	2.07719	6.47851
C	-5.92212	0.84477	7.39157
H	-11.33501	2.52016	-4.20448
H	-11.37372	4.29587	-4.17321
C	-9.86164	3.46497	-5.4756
H	-5.25795	0.01734	7.09924
H	-5.28065	1.69163	7.67816
C	-6.75888	0.41284	8.60566

H	-9.22521	4.36204	-5.46271
H	-9.19439	2.5909	-5.49907
C	-10.72656	3.47552	-6.74504
H	-7.42127	1.23964	8.89783
H	-7.40057	-0.43138	8.31713
C	-5.8753	0.01012	9.79545
H	-11.38965	4.353	-6.72578
H	-11.36817	2.58208	-6.75419
C	-9.88299	3.50582	-8.0284
H	-5.24282	0.85113	10.10539
H	-6.48161	-0.29788	10.65493
H	-5.22032	-0.82583	9.52058
H	-9.23956	4.39812	-8.02004
H	-9.22032	2.62794	-8.04804
C	-10.74447	3.51635	-9.30058
H	-11.38886	2.62606	-9.30546
H	-11.40482	4.39467	-9.28041
C	-9.88585	3.54198	-10.57371
H	-9.23547	2.65954	-10.61475
H	-10.5098	3.55047	-11.47479
H	-9.24902	4.43512	-10.58848
C	5.59577	-8.05992	-0.65051
C	5.17052	-9.24428	-0.0672
C	5.36872	-7.82737	-2.06972
C	5.41129	-6.79781	0.04769
C	4.53892	-9.22266	1.24376
C	4.50091	-10.25196	-0.87099
C	5.04219	-6.42213	-2.2455
C	4.72492	-8.78851	-2.83654
C	4.79623	-6.77388	1.29526

C	5.06772	-5.79329	-0.93337
C	4.35252	-8.01677	1.90376
C	3.48544	-10.22685	1.25217
C	4.28143	-10.0293	-2.22293
C	3.45896	-10.85954	-0.0551
C	4.08953	-6.04128	-3.17785
C	3.72537	-8.38874	-3.81591
C	3.83948	-5.73484	1.62839
C	4.13208	-4.81882	-0.61346
C	3.11131	-7.75501	2.61327
C	2.30027	-9.98097	1.92953
C	3.00925	-10.39877	-2.8239
C	2.24712	-11.21562	-0.63026
C	3.11607	-5.01115	-2.84672
C	3.41514	-7.04641	-3.98239
C	2.66511	-9.38383	-3.80732
C	3.52985	-4.76559	0.6995
C	2.78126	-6.35042	2.45635
C	3.134	-4.41931	-1.59034
C	2.11075	-8.72084	2.63035
C	1.029	-10.35713	1.32794
C	2.01668	-10.97818	-2.04705
C	1.00339	-10.9586	0.07715
C	1.84948	-5.37245	-3.44165
C	2.02864	-6.63316	-4.14423
C	1.34361	-8.98911	-3.96297
C	2.18194	-4.15373	0.56889
C	1.4645	-5.96469	2.32036
C	1.90696	-4.11582	-0.89122
C	0.73292	-8.31882	2.45997

C	0.05718	-9.32742	1.65717
C	0.63033	-10.57007	-2.21414
C	0.00351	-10.55833	-0.90229
C	0.67118	-5.12291	-2.74501
C	1.01871	-7.58363	-4.13398
C	0.30166	-9.5968	-3.14748
C	1.0258	-4.81905	1.47693
C	1.43936	-3.36947	1.63338
C	0.43016	-6.97472	2.28626
C	0.69891	-4.47622	-1.44649
C	-0.8946	-8.94654	0.72426
C	-0.92367	-9.57556	-0.58576
C	-0.38572	-6.12098	-2.7379
C	-0.21995	-7.31871	-3.41756
C	-0.66671	-8.56598	-2.81496
C	-0.15615	-5.32001	0.7252
C	0.48129	-2.32936	1.13985
C	2.2229	-3.00188	2.88952
C	-0.56637	-6.57616	1.30777
C	-0.35737	-5.09342	-0.61847
C	-1.21917	-7.53895	0.54842
C	-1.26691	-8.5542	-1.56469
C	-1.01126	-6.10539	-1.42602
C	-0.86759	-2.36641	1.49581
C	0.97676	-1.23576	0.42023
H	2.86915	-3.84206	3.16501
H	2.87649	-2.15258	2.64751
C	1.29705	-2.65265	4.0699
C	-1.45003	-7.29676	-0.85717
H	-1.25076	-3.19499	2.07966

C	-1.71402	-1.31774	1.13315
C	0.13283	-0.18619	0.06811
H	2.02623	-1.21037	0.14196
H	0.43253	-3.32732	4.07699
H	1.83846	-2.82303	5.00805
C	0.78525	-1.20279	4.03444
C	-1.21705	-0.22614	0.42484
H	-2.76049	-1.35346	1.41642
H	0.52188	0.66896	-0.47288
H	1.35182	-0.5441	4.70215
H	0.86758	-0.78364	3.02307
C	-0.67067	-1.11678	4.39922
H	-1.86889	0.59744	0.15565
O	-1.03744	0.20791	4.53303
O	-1.45738	-2.04338	4.54002
C	-2.4688	0.46943	4.74146
H	-2.95759	-0.44882	5.07558
H	-2.5381	1.25582	5.49307
H	-2.89979	0.80443	3.79412
H	-13.55412	3.27293	0.01545
H	10.54853	3.27352	-0.17539

PCDTBT/PCBM

Total energy: -10032.5786444 A.U.

C	8.16378	-1.91699	-4.4939
C	6.81485	-1.7497	-4.76418
C	5.87129	-2.31606	-3.90589
C	6.31134	-3.04687	-2.7665
C	7.66245	-3.23144	-2.50184
H	8.90524	-1.45259	-5.1334

H	6.49643	-1.17571	-5.62759
H	7.996	-3.83321	-1.66366
C	3.4397	-1.8204	-4.71931
C	2.10629	-2.04672	-4.41376
C	1.73209	-2.7951	-3.27347
C	2.71496	-3.32216	-2.42515
C	4.05015	-3.09954	-2.73867
C	4.42824	-2.34805	-3.88801
H	3.71018	-1.24822	-5.59997
H	1.32919	-1.6662	-5.06775
H	2.42395	-3.86932	-1.53627
C	0.32205	-3.0234	-2.96622
C	-0.25127	-4.11977	-2.35473
S	-0.88295	-1.84267	-3.35971
C	-1.65512	-4.01163	-2.20871
H	0.32035	-4.98876	-2.0572
C	-2.16376	-2.82523	-2.70652
H	-2.29755	-4.76257	-1.77354
C	-3.89687	-1.10351	-3.16456
C	-5.22501	-0.63401	-3.19823
C	-3.53651	-2.3663	-2.71722
C	-6.30585	-1.39357	-2.77931
H	-5.39409	0.36974	-3.56884
C	-4.61754	-3.18632	-2.26341
C	-5.98216	-2.69637	-2.29898
N	-4.53443	-4.43893	-1.77472
N	-6.8754	-3.58944	-1.84062
S	-6.04876	-4.9328	-1.4031
H	-3.11853	-0.42546	-3.50087
C	-7.6707	-0.91033	-2.82131

C	-8.09589	0.32706	-3.27888
S	-9.03325	-1.86094	-2.29724
C	-9.49311	0.50834	-3.20002
H	-7.421	1.08589	-3.65077
C	-10.14747	-0.59096	-2.67958
H	-9.9997	1.42241	-3.47871
C	-13.86641	-0.16501	-3.08416
C	-14.34677	-0.95929	-2.04212
C	-13.42439	-1.64395	-1.20173
C	-12.0526	-1.54007	-1.3954
C	-11.58207	-0.73686	-2.44298
H	-14.55579	0.3545	-3.74089
H	-11.34934	-2.0453	-0.74259
C	-16.95633	-0.92015	-1.95218
C	-18.04455	-1.41755	-1.25139
C	-17.87122	-2.28201	-0.14602
C	-16.58203	-2.65111	0.26162
C	-15.4946	-2.15334	-0.44483
C	-15.66822	-1.28408	-1.55973
H	-17.10649	-0.26385	-2.80244
H	-19.05153	-1.1678	-1.56842
H	-16.45196	-3.28989	1.12717
C	-19.02873	-2.80532	0.57583
C	-19.14905	-4.01599	1.22662
S	-20.49571	-1.89129	0.70993
C	-20.41731	-4.21038	1.824
H	-18.35924	-4.75513	1.23759
C	-21.27934	-3.14624	1.63117
H	-20.72169	-5.09008	2.3713
C	-23.41502	-1.88507	1.80132

C	-24.74449	-1.71472	2.23911
C	-22.64432	-3.00067	2.09102
C	-25.41325	-2.65422	3.00544
H	-25.25452	-0.80238	1.95466
C	-23.29286	-4.00327	2.8801
C	-24.66071	-3.82166	3.32629
N	-22.76951	-5.17398	3.29274
N	-25.11872	-4.8541	4.05488
S	-23.91411	-5.95574	4.16078
H	-22.98018	-1.09087	1.20253
C	-26.78172	-2.47602	3.45499
C	-27.59937	-1.38797	3.20155
S	-27.62663	-3.65661	4.41983
C	-28.88916	-1.50704	3.77852
H	-27.28624	-0.53112	2.62082
H	-29.66296	-0.7574	3.68753
C	8.60123	-2.66104	-3.37266
C	-12.4985	-0.05993	-3.28159
H	-12.11384	0.52288	-4.11038
C	27.17746	-5.5591	3.21835
C	26.00309	-5.65988	2.48021
C	24.81148	-5.1992	3.0402
C	24.81477	-4.63499	4.34651
C	25.9908	-4.54023	5.08775
H	28.11164	-5.91369	2.79792
H	26.01099	-6.09062	1.48469
H	25.99577	-4.12482	6.08871
C	22.81345	-5.53181	1.3883
C	21.44631	-5.33837	1.25365
C	20.68359	-4.7579	2.29247

C	21.30602	-4.36195	3.48386
C	22.67487	-4.5598	3.61517
C	23.44361	-5.14873	2.57167
H	23.38311	-5.98636	0.58507
H	20.94028	-5.66357	0.35082
H	20.7236	-3.8901	4.26642
C	19.2411	-4.5756	2.14475
C	18.27589	-4.6173	3.12968
S	18.52291	-4.26363	0.59822
C	16.96432	-4.40631	2.64204
H	18.50583	-4.83337	4.16442
C	16.91732	-4.20244	1.27477
H	16.06664	-4.40985	3.24216
C	15.8473	-3.77505	-0.92879
C	14.73673	-3.53598	-1.76226
C	15.758	-3.96001	0.44315
C	13.43677	-3.46541	-1.2867
H	14.92161	-3.4021	-2.8212
C	14.43451	-3.89188	0.98401
C	13.29522	-3.64695	0.12049
N	14.07789	-4.03354	2.27534
N	12.12768	-3.61172	0.78459
S	12.45344	-3.8682	2.36795
H	16.82541	-3.81432	-1.39803
C	12.2957	-3.22691	-2.1458
C	12.31615	-3.06423	-3.52228
S	10.66524	-3.09384	-1.54695
C	11.04078	-2.84455	-4.08368
H	13.22098	-3.1158	-4.11244
C	10.03257	-2.83724	-3.13906

H	10.86061	-2.73365	-5.14428
N	23.52061	-4.24519	4.66975
N	5.1986	-3.49969	-2.06972
N	-14.13556	-2.34688	-0.23768
C	23.11219	-3.63194	5.92203
H	22.27465	-2.95266	5.73683
H	22.81115	-4.38182	6.66373
H	23.9424	-3.04355	6.32339
C	5.22983	-4.28952	-0.84971
H	4.36674	-4.03169	-0.22859
H	5.21443	-5.36528	-1.06217
H	6.13574	-4.04736	-0.28676
C	-13.55177	-3.17491	0.80456
H	-14.18945	-3.14247	1.69303
H	-13.43702	-4.216	0.47964
H	-12.57136	-2.7739	1.07722
C	4.95182	4.57773	-1.4976
C	4.79504	3.45779	-2.30082
C	-1.29581	3.57178	1.2487
C	-1.479	2.4473	0.45714
C	3.78346	1.61746	1.67958
C	2.52821	1.41478	2.23208
C	0.95526	5.58575	-3.29759
C	-0.30071	5.38446	-2.74616
C	2.52131	6.02633	2.1648
C	1.86781	6.94421	1.01373
C	1.599	0.30214	-2.03028
C	1.03514	1.09116	-3.0216
C	5.11336	4.43064	-0.06093
C	4.1579	5.77028	-1.74182

C	4.7829	2.12994	-1.70519
C	3.82679	3.47152	-3.3874
C	-0.32421	3.55411	2.32913
C	-1.27964	4.89538	0.64782
C	-0.69002	1.24903	0.7008
C	-1.64597	2.59042	-0.98128
C	4.40266	2.93295	1.74147
C	4.11698	1.02994	0.39218
C	1.82901	2.51881	2.87273
C	1.54109	0.61653	1.52439
C	1.94304	6.38376	-2.58716
C	1.65428	4.48553	-3.9414
C	-0.63123	5.97096	-1.45561
C	-0.92036	4.07119	-2.80809
C	3.77262	5.31855	1.7821
C	1.63145	4.97342	2.72062
C	2.60006	6.96002	-0.28069
C	0.45867	6.62025	0.66184
C	3.01518	0.41837	-1.72295
C	0.88306	0.07745	-0.78488
C	1.86003	2.0394	-3.7542
C	-0.2703	1.6977	-2.81534
C	5.11552	3.15968	0.50507
C	3.243	5.78643	-2.78955
C	4.94033	1.98541	-0.33504
C	3.06991	4.60931	-3.62569
C	0.42027	2.40371	2.56883
C	-1.45208	5.03124	-0.72551
C	0.23679	1.2288	1.73252
C	-1.63287	3.8522	-1.55772

C	3.73138	3.98869	2.34528
C	3.1755	0.26794	-0.28551
C	2.41571	3.77638	2.92342
C	1.85667	0.05651	0.29465
C	1.63076	6.93467	-1.35099
C	1.06415	3.23084	-4.00101
C	0.31475	6.72501	-0.77314
C	-0.25416	3.01922	-3.42133
C	4.43311	5.53305	0.59223
C	0.29323	4.8645	2.40983
C	3.8332	6.37434	-0.46364
C	-0.30719	5.70741	1.35514
C	3.80189	1.32791	-2.41541
C	-0.3614	0.6583	-0.58488
C	3.21084	2.15774	-3.4559
C	-0.95383	1.48732	-1.62517
H	2.92091	9.64908	0.70162
C	3.7396	9.40415	1.37016
C	3.61552	8.33808	2.26614
C	4.89081	10.19047	1.38008
C	4.65007	8.06762	3.16605
C	5.92332	9.91553	2.27602
H	4.9794	11.01846	0.685
C	5.8006	8.85351	3.1715
H	4.55472	7.23181	3.85207
H	6.82049	10.52498	2.27594
H	6.60146	8.63389	3.869
C	2.35409	7.52936	2.32253
C	1.27635	8.01005	3.29003
H	0.51843	7.22563	3.39043

H	1.73606	8.14802	4.27773
C	0.60235	9.30822	2.80846
H	0.50403	9.27678	1.71616
H	-0.41329	9.3579	3.21889
C	1.36084	10.5929	3.18906
H	0.96593	11.06636	4.09158
H	2.42168	10.36727	3.36584
C	1.32749	11.58933	2.06015
O	1.4844	12.8629	2.52742
O	1.21835	11.33336	0.86299
C	1.5408	13.89774	1.48686
H	0.62772	13.88649	0.88612
H	1.64333	14.83525	2.03127
H	2.39611	13.72994	0.82673
C	27.16711	-5.00496	4.50784
H	28.09407	-4.94078	5.06731
C	-29.03977	-2.68536	4.46574
H	-29.91886	-3.02279	4.99515

APFO3/PCBM

Total energy: -9867.5857796 A.U.

C	-11.48446	-4.85359	2.37881
C	-10.12406	-5.10713	2.50895
C	-9.25003	-4.63147	1.53276
C	-9.74746	-3.90258	0.43099
C	-11.10136	-3.65911	0.29763
H	-12.17029	-5.18774	3.14935
H	-9.75208	-5.65755	3.3666
H	-11.48747	-3.12464	-0.56533
C	-6.84818	-5.35217	2.22472

C	-5.50888	-5.30924	1.85424
C	-5.09549	-4.65919	0.676
C	-6.06113	-4.03874	-0.14247
C	-7.3936	-4.09007	0.21924
C	-7.79636	-4.74385	1.40479
H	-7.14564	-5.86222	3.13469
H	-4.76593	-5.80638	2.47
H	-5.74585	-3.50573	-1.03334
C	-8.60422	-3.50186	-0.48664
H	-8.5251	-2.41	-0.57215
H	-8.72884	-3.92848	-1.49064
C	-3.68761	-4.62827	0.29157
C	-3.15548	-4.53262	-0.97865
S	-2.42416	-4.72417	1.47583
C	-1.74107	-4.54619	-0.99957
H	-3.76774	-4.49048	-1.86938
C	-1.17835	-4.65532	0.25941
H	-1.1289	-4.48984	-1.88731
C	0.65533	-4.83352	1.92775
C	2.0112	-4.8512	2.30871
C	0.22291	-4.70386	0.61583
C	3.0505	-4.75047	1.3978
H	2.2367	-4.93562	3.36489
C	1.26113	-4.60844	-0.36362
C	2.65433	-4.64375	0.03288
N	1.11059	-4.47548	-1.69573
N	3.50167	-4.54473	-1.00486
S	2.60127	-4.40182	-2.36257
H	-0.08636	-4.91219	2.71642
C	4.44168	-4.6981	1.79106

C	4.93648	-4.72175	3.08659
S	5.74634	-4.55153	0.64765
C	6.34166	-4.62067	3.15476
H	4.30434	-4.78986	3.96138
C	6.93114	-4.51409	1.90945
H	6.90017	-4.58284	4.08029
C	10.67359	-4.8032	2.22149
C	11.08982	-4.08115	1.10416
C	10.13667	-3.50348	0.23761
C	8.78336	-3.63641	0.48545
C	8.35344	-4.36417	1.61287
H	11.39707	-5.26035	2.88816
H	8.04877	-3.16349	-0.15967
C	13.69182	-4.08949	1.1002
C	14.8186	-3.64437	0.41774
C	14.70702	-2.87171	-0.75335
C	13.42643	-2.54452	-1.24287
C	12.30616	-2.99431	-0.57069
C	12.42986	-3.76664	0.60545
H	13.80027	-4.68643	1.99943
H	15.80622	-3.915	0.77786
H	13.33399	-1.91967	-2.12507
C	10.83817	-2.76524	-0.89013
H	10.58967	-1.69573	-0.88221
H	10.57095	-3.1844	-1.86914
C	15.89603	-2.40983	-1.46377
C	16.03299	-2.15087	-2.81234
S	17.38735	-2.11006	-0.63067
C	17.33198	-1.72192	-3.17447
H	15.23077	-2.30082	-3.52234

C	18.20146	-1.6499	-2.10134
H	17.65186	-1.47735	-4.17644
C	20.36167	-1.23799	-0.94246
C	21.7175	-0.85267	-0.90712
C	19.59389	-1.25398	-2.09683
C	22.41727	-0.45019	-2.0321
H	22.22282	-0.87811	0.05072
C	20.27423	-0.84924	-3.28907
C	21.66884	-0.45422	-3.24537
N	19.76007	-0.78135	-4.53231
N	22.15514	-0.10434	-4.44852
S	20.94376	-0.26509	-5.53592
H	19.90288	-1.53805	-0.00552
C	23.81198	-0.05085	-1.99236
C	24.62432	0.00173	-0.87251
S	24.70063	0.44109	-3.40883
C	25.94535	0.43211	-1.15557
H	24.2853	-0.25818	0.12098
H	26.72003	0.5353	-0.40844
C	-11.99367	-4.13792	1.27803
C	9.31224	-4.94446	2.46505
H	8.97324	-5.53273	3.3106
C	-30.68689	1.55678	-2.35681
C	-29.47868	0.87359	-2.21864
C	-28.29297	1.6047	-2.21234
C	-28.31558	3.00963	-2.34345
C	-29.51952	3.68367	-2.4802
H	-31.61968	1.00337	-2.3638
H	-29.46564	-0.20662	-2.11806
H	-29.54342	4.76398	-2.58082

C	-26.34528	-0.09894	-1.92026
C	-24.96393	-0.22596	-1.81963
C	-24.12046	0.89922	-1.87228
C	-24.68914	2.179	-2.02946
C	-26.06105	2.30471	-2.13949
C	-26.89793	1.16913	-2.08331
H	-26.97722	-0.97972	-1.88142
H	-24.52083	-1.21223	-1.72301
H	-24.04691	3.05351	-2.03511
C	-26.90015	3.56089	-2.30495
H	-26.76087	4.24769	-1.45947
H	-26.65064	4.08904	-3.23483
C	-22.67059	0.75561	-1.7727
C	-21.69736	1.56746	-2.31895
S	-21.94943	-0.55496	-0.89527
C	-20.37977	1.13287	-2.04096
H	-21.92868	2.42814	-2.93197
C	-20.33535	-0.01978	-1.27761
H	-19.47728	1.61759	-2.38239
C	-19.26894	-1.9049	-0.05687
C	-18.1557	-2.6333	0.40721
C	-19.1729	-0.74565	-0.81279
C	-16.84686	-2.25908	0.14693
H	-18.34606	-3.52515	0.99195
C	-17.83968	-0.31469	-1.1041
C	-16.69813	-1.06986	-0.62546
N	-17.47531	0.7721	-1.81171
N	-15.52094	-0.53115	-0.98501
S	-15.84111	0.81737	-1.8553
H	-20.25447	-2.28254	0.19709

C	-15.70327	-3.01323	0.61681
C	-15.73221	-4.18581	1.35586
S	-14.05752	-2.53181	0.31199
C	-14.45139	-4.68974	1.66442
H	-16.64852	-4.67639	1.65465
C	-13.43071	-3.90466	1.16281
H	-14.2814	-5.61314	2.20142
C	-0.43911	3.55854	0.23576
C	-0.97665	2.31259	0.52334
C	5.90223	1.22927	1.6409
C	5.39093	-0.02626	1.93416
C	2.21821	1.04817	-2.38326
C	3.49261	0.57979	-2.10244
C	1.43266	2.92677	4.27641
C	2.70679	2.45849	4.55773
C	3.94698	4.86381	-0.45667
C	3.76434	5.29874	1.08185
C	1.23018	-1.5611	1.15059
C	1.07425	-1.18717	2.47712
C	0.37937	3.74625	-0.95075
C	0.11427	4.38019	1.29947
C	-0.71414	1.18506	-0.3593
C	-0.9794	1.82012	1.89294
C	5.89874	1.71775	0.27199
C	5.63298	2.35332	2.52297
C	4.8398	-0.85462	0.87178
C	4.57513	-0.22059	3.12371
C	1.94202	2.47658	-2.34545
C	1.05401	0.35621	-1.85592
C	4.55396	1.51745	-1.76626

C	3.66848	-0.60299	-1.27712
C	1.25866	4.11059	3.44817
C	0.37066	1.99208	3.94279
C	3.87102	3.15124	4.02574
C	2.98383	1.03226	4.52153
C	2.6907	4.51558	-1.17408
C	4.8624	3.71609	-0.69123
C	2.36493	5.29026	1.58592
C	4.53953	4.49703	2.06744
C	0.39995	-0.95662	0.12101
C	2.56386	-1.74934	0.60099
C	0.08173	-0.18834	2.83909
C	2.24359	-0.98449	3.31914
C	0.61823	2.66996	-1.79966
C	0.09775	3.91372	2.61008
C	0.06441	1.36079	-1.49302
C	-0.45489	2.60277	2.91099
C	5.38303	0.91938	-0.74411
C	4.86261	2.16327	3.66492
C	4.83847	-0.39322	-0.43654
C	4.31754	0.84946	3.96766
C	2.95266	3.37031	-2.01488
C	1.21904	-0.77367	-1.06682
C	4.28754	2.87944	-1.71946
C	2.55742	-1.26467	-0.77039
C	2.36985	4.76408	2.93074
C	0.63378	0.62985	3.90628
C	3.70505	4.27538	3.22736
C	1.97119	0.13812	4.20269
C	1.43528	4.68956	-0.63428

C	5.63467	3.14418	0.29683
C	1.26805	5.08787	0.77825
C	5.46895	3.54407	1.70983
C	-0.54406	0.00084	0.465
C	3.68003	-1.54845	1.40084
C	-0.70823	0.39369	1.85695
C	3.51633	-1.15905	2.793
H	3.03147	8.07708	1.59812
C	2.85389	8.2251	0.5381
C	3.44676	7.36991	-0.39545
C	2.08454	9.30336	0.10273
C	3.26267	7.60323	-1.76129
C	1.8985	9.53067	-1.26039
H	1.62974	9.96517	0.83191
C	2.49145	8.67993	-2.19306
H	3.71474	6.92961	-2.48262
H	1.29336	10.36623	-1.59501
H	2.34855	8.85106	-3.25441
C	4.33477	6.24534	0.04634
C	5.82544	6.55233	0.16002
H	6.37026	5.60942	0.27784
H	6.15831	7.00672	-0.78265
C	6.13621	7.47131	1.35581
H	5.48178	7.20027	2.19345
H	7.1672	7.29504	1.68496
C	5.95087	8.97178	1.06414
H	6.88806	9.4734	0.81024
H	5.25739	9.10907	0.22273
C	5.32463	9.67257	2.24105
O	5.65577	10.99754	2.25445

O	4.5782	9.16978	3.07803
C	5.03031	11.7771	3.33053
H	5.28284	11.35356	4.30596
H	5.43545	12.7817	3.21894
H	3.9425	11.77697	3.22005
C	26.12468	0.70311	-2.48894
H	27.0304	1.0454	-2.96796
C	-30.70875	2.94782	-2.48621
H	-31.65793	3.46179	-2.59237

MDMO-PPV/PCBM

Total energy: -6087.9913658 A.U.

C	21.35774	0.64091	-0.79824
C	22.72434	0.5917	-0.58129
C	23.26534	0.13017	0.62573
C	22.36663	-0.27547	1.6411
C	20.99843	-0.20122	1.43341
C	20.45767	0.24821	0.22133
H	23.40572	0.89729	-1.3642
H	20.31656	-0.51581	2.21238
O	20.78323	1.04302	-1.98698
C	21.66826	1.43371	-3.06699
H	22.32384	0.60632	-3.3645
H	21.00808	1.69604	-3.89474
H	22.27853	2.30283	-2.79056
C	24.69008	0.0018	0.86566
H	24.93719	-0.34504	1.86378
C	25.66527	0.25857	-0.03194
H	25.41526	0.59645	-1.03249
O	22.944	-0.74573	2.80373

H	27.59026	1.54871	-3.93514
C	28.25941	1.25053	-3.12684
O	27.3897	0.89953	-2.02423
H	28.86776	0.39541	-3.44808
H	28.92068	2.08713	-2.86721
C	27.97964	0.47211	-0.8495
C	29.34914	0.37079	-0.66569
C	27.09264	0.13166	0.19866
C	29.90262	-0.06782	0.54523
H	30.02309	0.63505	-1.4699
C	27.646	-0.3099	1.40888
C	29.01499	-0.41307	1.59177
C	31.33113	-0.18355	0.78
H	26.97174	-0.57574	2.21239
O	29.60496	-0.84456	2.76568
H	31.58103	-0.54498	1.77225
C	32.30555	0.11716	-0.10323
H	32.05603	0.48291	-1.09407
C	33.73402	0.00608	0.1341
C	34.62391	0.37982	-0.89999
C	34.28542	-0.45086	1.33939
C	35.99337	0.2933	-0.70847
O	34.03665	0.82382	-2.07073
C	35.6545	-0.53803	1.53061
H	33.60948	-0.74028	2.13322
C	36.54477	-0.16167	0.49746
H	36.66939	0.58333	-1.50206
C	34.91087	1.22292	-3.1529
O	36.24158	-0.98271	2.70134
C	37.97309	-0.26315	0.7402

H	35.53809	0.38899	-3.49324
H	34.24485	1.53358	-3.95917
H	35.55454	2.06286	-2.86167
H	38.22082	-0.63053	1.73083
H	1.05239	1.48461	-4.03225
C	1.71607	1.18518	-3.21981
O	0.83874	0.78427	-2.1409
H	2.35336	0.35522	-3.55102
H	2.34995	2.03293	-2.92963
C	1.42299	0.35249	-0.96396
C	2.79191	0.28063	-0.76359
C	3.34034	-0.16229	0.44815
H	3.46987	0.5731	-1.55461
C	1.07874	-0.46903	1.27782
C	2.44744	-0.54155	1.47794
C	4.76821	-0.24785	0.69967
H	0.40085	-0.75971	2.0696
O	3.03144	-0.97336	2.65492
H	5.01403	-0.60492	1.69453
C	5.7464	0.07154	-0.17266
H	5.50082	0.42573	-1.16865
C	7.1742	-0.00669	0.0821
C	8.06758	0.36585	-0.94954
C	7.72174	-0.42972	1.30137
C	9.43621	0.31018	-0.74268
O	7.48416	0.77576	-2.13453
C	9.09033	-0.48609	1.50803
H	7.04345	-0.71633	2.09425
C	9.98372	-0.11125	0.4771
H	10.11458	0.59811	-1.53505

C	8.36222	1.17044	-3.21514
O	9.67356	-0.89637	2.69302
C	11.41118	-0.17946	0.73569
H	9.00833	0.34199	-3.53282
H	7.69919	1.45305	-4.0341
H	8.98722	2.02765	-2.9336
H	11.65595	-0.52584	1.73459
C	12.39021	0.14422	-0.13411
H	12.14613	0.49106	-1.13302
H	14.34679	1.54534	-3.98559
C	15.00907	1.27121	-3.16321
O	14.13011	0.87329	-2.08427
H	15.66298	0.44678	-3.47519
H	15.62578	2.13469	-2.88253
C	14.71208	0.46724	-0.89742
C	16.08003	0.42683	-0.68293
C	13.81742	0.08123	0.12843
C	16.62502	0.00741	0.53876
H	16.75944	0.72392	-1.47098
C	14.3627	-0.34081	1.34886
C	15.7308	-0.38263	1.56294
C	18.0513	-0.04569	0.80572
H	13.68345	-0.63944	2.13639
O	16.31238	-0.79161	2.74878
H	18.29367	-0.40269	1.80157
C	19.03252	0.3042	-0.05157
H	18.79204	0.66326	-1.04694
C	2.15385	-1.37379	3.73361
H	1.51726	-0.54342	4.06528
H	1.51917	-2.22084	3.44306

H	2.81725	-1.67428	4.54589
C	8.79555	-1.29564	3.77189
H	8.1486	-0.46895	4.09251
H	8.17139	-2.15233	3.48693
H	9.45858	-1.5808	4.58997
C	15.43434	-1.21736	3.81776
H	14.77313	-0.40445	4.14432
H	14.82536	-2.08003	3.51862
H	16.09713	-1.50215	4.63611
C	22.06223	-1.22514	3.84847
H	21.41233	-0.42525	4.22537
H	21.44528	-2.06096	3.49625
H	22.72398	-1.56668	4.64556
C	28.73291	-1.21843	3.85873
H	28.11894	-0.37205	4.19247
H	28.07655	-2.05357	3.58235
H	29.40029	-1.52726	4.66455
C	35.36696	-1.37671	3.78484
H	34.74147	-0.54051	4.12286
H	34.72141	-2.21624	3.4964
H	36.03255	-1.68636	4.59186
C	21.25248	-8.26565	0.43597
C	20.35107	-7.29321	0.84364
C	23.42901	-4.19473	-4.68946
C	22.53667	-3.20584	-4.3017
C	24.08276	-4.77868	0.69798
C	24.51621	-3.96127	-0.33354
C	19.24423	-7.49649	-3.51503
C	19.68236	-6.67853	-4.54482
C	24.82539	-8.02224	-2.49318

C	23.71075	-8.65471	-3.46925
C	20.12184	-3.00613	-0.51217
C	19.15886	-3.54776	-1.34911
C	22.68082	-8.05716	0.60692
C	21.04724	-8.97366	-0.8162
C	20.83328	-6.05624	1.43799
C	19.19882	-6.97437	0.01327
C	24.57503	-4.51202	-3.85413
C	22.94139	-5.43089	-5.27727
C	22.74001	-2.48554	-3.05242
C	21.10627	-3.40926	-4.47638
C	24.29692	-6.21572	0.62735
C	22.77881	-4.55454	1.30259
C	25.19119	-4.54025	-1.48411
C	23.67618	-2.87459	-0.80987
C	20.09019	-8.57967	-3.03635
C	18.56825	-6.92033	-2.36446
C	20.98814	-6.90274	-5.14755
C	19.4653	-5.24281	-4.47888
C	24.48323	-8.02014	-1.04581
C	25.22843	-6.62487	-2.8027
C	22.47873	-9.14029	-2.79063
C	23.22843	-7.75357	-4.55282
C	20.54521	-3.73381	0.67443
C	21.28796	-2.3406	-1.07173
C	18.57209	-4.8429	-1.0442
C	19.31253	-3.45438	-2.79323
C	23.14009	-6.87835	1.18635
C	19.93788	-8.67748	-1.60274
C	22.19597	-5.85383	1.60275

C	18.99838	-7.65054	-1.18116
C	24.77364	-3.81889	-2.66504
C	21.57438	-5.61824	-5.45533
C	23.83588	-2.78589	-2.25181
C	20.63689	-4.58689	-5.04071
C	24.93248	-6.77029	-0.47683
C	21.97404	-3.52131	0.84458
C	25.39017	-5.91297	-1.55555
C	22.43259	-2.65548	-0.23335
C	21.34081	-8.78616	-3.60512
C	18.36233	-5.54927	-2.29733
C	21.79945	-7.93109	-4.6864
C	18.82238	-4.69068	-3.37902
C	23.36898	-8.64305	-0.52804
C	24.80976	-5.94264	-3.92436
C	22.34241	-9.21696	-1.42179
C	23.7837	-6.51985	-4.81793
C	19.98949	-4.97263	0.96446
C	21.43919	-2.25776	-2.45035
C	18.97696	-5.54079	0.08531
C	20.4298	-2.83012	-3.32955
H	23.52416	-11.4741	-3.54261
C	24.3489	-11.6109	-2.85105
C	25.21809	-10.5465	-2.59896
C	24.53841	-12.83769	-2.21643
C	26.27394	-10.72064	-1.70017
C	25.59581	-13.00746	-1.32385
H	23.85948	-13.659	-2.41804
C	26.46213	-11.94543	-1.06464
H	26.94077	-9.88903	-1.49436

H	25.74159	-13.96125	-0.82889
H	27.28199	-12.07076	-0.3659
C	25.09785	-9.25209	-3.34342
C	26.04018	-9.06867	-4.52857
H	25.93593	-8.04393	-4.90111
H	27.07019	-9.17789	-4.16186
C	25.77511	-10.05207	-5.68192
H	24.69395	-10.17682	-5.82271
H	26.15398	-9.62222	-6.61682
C	26.43206	-11.42106	-5.48779
H	27.51066	-11.31797	-5.30656
H	26.01697	-11.95274	-4.6257
C	26.24386	-12.27233	-6.7142
O	26.81199	-13.50739	-6.53371
O	25.67373	-11.94972	-7.74943
C	26.68399	-14.40993	-7.68262
H	27.16748	-13.98148	-8.56492
H	27.17843	-15.32971	-7.37266
H	25.63084	-14.58865	-7.91638
C	38.95449	0.05547	-0.13838
H	38.70706	0.41972	-1.11357
H	39.98032	-0.05759	0.1441
C	0.53027	-0.0247	0.06653
H	-0.53027	0.0247	-0.06653

PCPDTBT/PCBM

Total energy: -14096.5601445 A.U.

C	-33.68361	-1.45461	-0.69847
C	-34.11026	-1.82407	-1.97085
C	-35.51944	-1.76834	-2.10953

C	-36.12725	-1.35982	-0.94488
S	-34.99322	-1.04102	0.32504
H	-36.06582	-2.01276	-3.01027
C	-29.78557	-1.72039	-0.67106
C	-30.36639	-2.06267	-1.89071
C	-31.7646	-1.95834	-1.87155
C	-32.24892	-1.53542	-0.63369
S	-31.00728	-1.26409	0.50854
H	-29.79004	-2.3734	-2.75151
C	-32.91541	-2.18132	-2.83896
H	-32.96139	-3.2246	-3.17732
H	-32.8411	-1.52175	-3.71329
C	-28.37487	-1.72277	-0.36124
C	-27.88478	-1.35314	0.92662
C	-27.397	-2.08042	-1.28024
C	-26.46962	-1.35364	1.24467
C	-26.02356	-2.08342	-0.97823
H	-27.69167	-2.37323	-2.2807
C	-25.50039	-1.73174	0.26067
H	-25.34047	-2.38003	-1.7682
N	-28.65618	-0.97409	1.95851
N	-26.22968	-0.97176	2.51349
S	-27.66852	-0.64691	3.22221
C	-21.62224	-1.96995	0.37715
C	-22.04751	-1.54414	1.63738
C	-23.44259	-1.41582	1.73195
C	-24.08561	-1.74386	0.54249
S	-22.92964	-2.21486	-0.69728
H	-24.00335	-1.10347	2.60083
C	-17.73113	-2.21034	0.4912

C	-18.30678	-1.79264	1.69163
C	-19.70292	-1.71524	1.62282
C	-20.19456	-2.07542	0.36453
S	-18.95697	-2.50837	-0.73343
H	-17.72575	-1.55703	2.57278
C	-20.8486	-1.34296	2.54838
H	-20.77235	-0.30174	2.88728
H	-20.89351	-2.00464	3.423
C	-16.3229	-2.39041	0.23262
C	-15.83957	-2.82378	-1.03768
C	-15.33994	-2.15811	1.18681
C	-14.42591	-3.0056	-1.30568
C	-13.9683	-2.3322	0.93358
H	-15.62994	-1.82612	2.17634
C	-13.45126	-2.75168	-0.28742
H	-13.2807	-2.12206	1.74698
N	-16.61662	-3.10314	-2.09646
N	-14.19275	-3.4181	-2.56607
S	-15.63542	-3.55759	-3.32582
C	-9.57269	-2.99968	-0.27445
C	14.53836	-2.47921	-0.35585
C	-10.00589	-3.36569	-1.55117
C	14.10741	-2.69247	-1.66757
C	-11.40173	-3.32042	-1.69133
C	12.71032	-2.76465	-1.78131
C	-12.03816	-2.91867	-0.52059
C	12.07094	-2.60615	-0.55522
S	-10.8742	-2.59891	0.75929
S	13.23373	-2.36477	0.74282
H	-11.96797	-3.55777	-2.58014

H	12.14518	-2.92517	-2.68788
C	-5.67988	-3.22347	-0.26797
C	18.43567	-2.36882	-0.42406
C	-6.26323	-3.56667	-1.48835
C	17.8546	-2.57225	-1.67614
C	-7.65982	-3.47961	-1.46217
C	16.45602	-2.60524	-1.62317
C	-8.14423	-3.06808	-0.21644
C	15.96835	-2.42586	-0.32512
S	-6.89905	-2.78907	0.92182
S	17.21247	-2.21695	0.8294
H	-5.68697	-3.86454	-2.35359
H	18.43335	-2.69224	-2.58173
C	-8.8118	-3.70758	-2.42571
C	15.30492	-2.78948	-2.59721
H	-8.85134	-4.74922	-2.76954
H	15.34883	-3.76676	-3.09485
H	-8.74819	-3.04221	-3.29632
H	15.28791	-1.9977	-3.35721
C	-4.26883	-3.20553	0.03208
C	19.84798	-2.29029	-0.13702
C	-3.77779	-2.8435	1.32186
C	20.33737	-2.08561	1.18719
C	-3.2906	-3.53114	-0.89976
C	20.82867	-2.40907	-1.11381
C	-2.36195	-2.82375	1.63068
C	21.75488	-2.01148	1.48406
C	-1.9157	-3.5049	-0.60887
C	22.20433	-2.3379	-0.8327
H	-3.58676	-3.81602	-1.90196

H	20.53408	-2.56503	-2.1445
C	-1.39291	-3.15876	0.63242
C	22.72719	-2.14303	0.44085
H	-1.23119	-3.77526	-1.40691
H	22.88974	-2.44315	-1.66797
N	-4.54836	-2.48749	2.36224
N	19.56312	-1.94361	2.27496
N	-2.11942	-2.45322	2.90244
N	21.99383	-1.815	2.79457
S	-3.55767	-2.15521	3.62246
S	20.55161	-1.73393	3.56332
C	2.48525	-3.00521	0.65209
C	26.61281	-2.07138	0.47688
C	2.05846	-2.81028	1.97045
C	26.18479	-1.88059	1.79206
C	0.66598	-2.86194	2.10763
C	24.78641	-1.88442	1.92036
C	0.0234	-3.09772	0.89318
C	24.14442	-2.0785	0.70135
S	1.18022	-3.27691	-0.41724
S	25.30519	-2.25645	-0.60849
H	0.10203	-2.70386	3.01513
H	24.22303	-1.75675	2.83322
C	6.37278	-2.72518	0.64739
C	30.51139	-1.99935	0.51032
C	5.79626	-2.54916	1.90557
C	29.93457	-1.82191	1.76595
C	4.40051	-2.65619	1.87863
C	28.53411	-1.85246	1.72608
C	3.91212	-2.91538	0.59445

C	28.04489	-2.05429	0.433
S	5.1505	-3.01978	-0.5802
S	29.28657	-2.20542	-0.73219
H	6.37516	-2.35033	2.79696
H	30.51541	-1.67576	2.66639
C	3.2551	-2.56444	2.87149
C	27.3845	-1.72352	2.71059
H	3.20338	-1.57023	3.33368
H	27.38465	-0.74448	3.20681
H	3.33432	-3.32828	3.6555
H	27.41314	-2.51394	3.47164
C	7.7825	-2.68841	0.33836
C	31.92845	-2.01882	0.20875
C	8.26714	-2.86608	-0.99105
C	32.40232	-2.198	-1.12774
C	8.76418	-2.48465	1.29986
C	32.90665	-1.8665	1.17867
C	9.68191	-2.83741	-1.30731
C	33.81688	-2.21457	-1.43055
C	10.13734	-2.45661	1.00044
C	34.29405	-1.88344	0.87824
H	8.47242	-2.3427	2.33338
H	32.6129	-1.7283	2.21213
C	10.65621	-2.6285	-0.27831
C	34.76781	-2.05289	-0.39778
H	10.82402	-2.29292	1.82513
H	34.9941	-1.75684	1.69676
N	7.49087	-3.07462	-2.06663
N	31.62648	-2.36433	-2.21195
N	9.917	-3.02617	-2.61954

N	34.06868	-2.39421	-2.74657
S	8.47457	-3.21952	-3.3674
S	32.62604	-2.52676	-3.50301
H	-37.18456	-1.22992	-0.76863
H	35.82396	-2.06634	-0.63004
C	0.93139	4.46675	3.29974
C	1.10101	3.10656	3.51348
C	0.07596	3.376	-3.45651
C	0.24182	2.01118	-3.27029
C	-2.75578	2.98391	1.19427
C	-2.92817	2.76417	-0.16361
C	4.10711	3.68477	0.21248
C	3.93384	3.46547	-1.14524
C	-0.64954	6.76817	-0.39041
C	0.93648	6.92905	-0.61631
C	0.32549	-0.25491	0.61907
C	1.69329	-0.11896	0.42411
C	-0.37056	4.99281	2.92434
C	1.94673	5.22871	2.59282
C	-0.02512	2.199	3.3507
C	2.29487	2.43545	3.02034
C	-1.11578	4.04186	-2.95779
C	1.20264	4.27873	-3.28866
C	-0.77454	1.24341	-2.56745
C	1.54479	1.47897	-2.89881
C	-2.3603	4.29899	1.67561
C	-2.07946	1.99121	2.01323
C	-2.71125	3.84967	-1.10821
C	-2.43289	1.54071	-0.77373
C	3.60811	4.90894	0.82118

C	3.89422	2.60102	1.15813
C	3.25438	4.4594	-1.96219
C	3.54095	2.15127	-1.62797
C	-1.05454	6.26373	0.94945
C	-1.34567	5.88826	-1.36598
C	1.78793	6.54974	0.54239
C	1.4958	6.18119	-1.77469
C	-0.29909	0.30363	1.80852
C	-0.58992	-0.06718	-0.49516
C	2.4992	0.58864	1.40773
C	2.20777	0.21547	-0.89488
C	-1.44842	4.12428	2.78315
C	3.09367	4.58859	2.1334
C	-1.2709	2.69702	2.99652
C	3.26746	3.16051	2.34594
C	-2.09149	3.3041	-2.29497
C	2.44977	3.76809	-2.94475
C	-1.91524	1.87517	-2.0924
C	2.62243	2.33883	-2.74055
C	-2.14444	5.33209	0.77249
C	-1.6029	0.82416	1.43186
C	-2.32522	5.10259	-0.65031
C	-1.78303	0.5942	0.00584
C	2.94932	5.8523	0.04279
C	3.51741	1.34618	0.69961
C	2.77032	5.62406	-1.38027
C	3.33614	1.11633	-0.72613
C	-0.17128	6.08603	1.99164
C	-0.7374	5.36035	-2.48439
C	1.28376	6.23467	1.78464

C	0.71778	5.51012	-2.69355
C	0.46922	0.97311	2.75005
C	-0.10014	0.2457	-1.75481
C	1.90543	1.11962	2.54493
C	1.33479	0.39185	-1.95949
H	2.18047	9.37758	0.35616
C	1.26231	9.64082	0.87074
C	0.04915	9.07491	0.46741
C	1.28162	10.58913	1.89262
C	-1.13762	9.46417	1.09505
C	0.09658	10.97246	2.51962
H	2.22563	11.02743	2.19806
C	-1.11461	10.40994	2.11772
H	-2.07592	9.01365	0.78687
H	0.11633	11.70537	3.31888
H	-2.03893	10.70291	2.60349
C	-0.00408	8.11368	-0.6818
C	-0.23778	8.71442	-2.06562
H	-0.4707	7.90436	-2.76517
H	-1.11963	9.3669	-2.01506
C	0.99283	9.4873	-2.57492
H	1.90119	8.96086	-2.257
H	0.98921	9.48536	-3.67143
C	1.07643	10.94147	-2.07531
H	0.68684	11.66156	-2.79927
H	0.50045	11.05363	-1.14627
C	2.49625	11.31002	-1.73441
O	2.69173	12.6576	-1.84273
O	3.38174	10.54208	-1.36472
C	4.03222	13.11728	-1.45764

H	4.79534	12.62075	-2.06246
H	4.02169	14.19103	-1.63876
H	4.22361	12.89766	-0.40374

PBDTTPD/PCBM

Total energy: -16490.5332364 A.U.

C	19.74024	14.54945	1.39616
C	21.14744	14.67782	1.56111
C	21.73534	15.88616	1.90738
C	20.89121	16.98185	2.10666
C	19.48216	16.84889	1.94969
C	18.8935	15.64781	1.58755
C	19.37349	13.21909	1.05162
C	20.44967	12.37043	0.95306
H	18.34276	12.92022	0.90873
C	21.25827	18.31619	2.49296
C	20.181	19.13401	2.61555
S	18.66334	18.34553	2.28561
H	22.28055	18.61019	2.68249
H	20.18764	20.17559	2.90258
S	21.98048	13.17881	1.29397
O	23.10952	16.02111	2.0641
O	17.52164	15.50984	1.41689
C	23.83502	16.16532	0.78662
H	23.51358	17.07079	0.26019
H	24.88746	16.23963	1.06264
H	23.67647	15.29099	0.14599
C	17.04061	16.01337	0.1152
H	17.49096	15.44708	-0.70744
H	15.96029	15.86492	0.13199

H	17.27322	17.07747	-0.00154
C	20.38312	10.9713	0.63519
S	18.82673	10.20003	0.37002
C	19.53302	8.62836	0.06054
C	21.36808	10.02746	0.4858
C	20.90228	8.72434	0.16643
C	22.83698	9.99411	0.56363
C	22.06818	7.83275	0.03473
O	22.16069	6.62656	-0.22743
O	23.65797	10.87812	0.80979
N	23.17512	8.65485	0.28199
C	24.54779	8.17689	0.25738
H	24.79546	7.77846	-0.73085
H	25.18215	9.03678	0.48619
H	24.69255	7.39327	1.00685
C	15.81178	3.85717	-1.31841
C	17.07752	3.22317	-1.32215
C	18.26735	3.89451	-1.04463
C	18.17493	5.26787	-0.74986
C	16.88318	5.89439	-0.74754
C	15.71114	5.22467	-1.02521
C	14.76899	2.9334	-1.59736
C	15.22973	1.65408	-1.81463
H	13.72364	3.21537	-1.60596
C	19.1997	6.22083	-0.46517
C	18.72113	7.4874	-0.24334
S	16.97112	7.58671	-0.36453
H	20.26301	6.02483	-0.42439
S	16.98006	1.53159	-1.68161
O	19.38988	3.11666	-1.11016

O	14.48626	5.88445	-1.02008
C	20.62096	3.49335	-0.42002
H	20.41001	3.85465	0.59217
H	21.19864	2.56933	-0.37142
H	21.18364	4.25052	-0.97221
C	14.10371	6.39193	-2.35428
H	14.01382	5.56834	-3.07106
H	13.13763	6.8775	-2.21091
H	14.84147	7.11516	-2.71839
C	14.40326	0.51409	-2.10162
S	12.65726	0.69046	-2.18837
C	12.39143	-1.00443	-2.535
C	14.72014	-0.80041	-2.3352
C	13.60764	-1.6488	-2.57627
C	15.94934	-1.60686	-2.40862
C	14.10631	-3.01603	-2.80857
O	13.52004	-4.07864	-3.05145
O	17.13226	-1.29815	-2.26609
N	15.49858	-2.91146	-2.69555
C	16.40139	-4.03961	-2.85558
H	16.30109	-4.46947	-3.85649
H	17.4133	-3.65265	-2.71236
H	16.18477	-4.81067	-2.11041
C	6.58871	-3.03464	-3.37984
C	7.31758	-4.24209	-3.50158
C	8.70411	-4.31256	-3.3728
C	9.38545	-3.1095	-3.10831
C	8.63008	-1.89468	-2.98446
C	7.25998	-1.8319	-3.11636
C	5.19251	-3.25682	-3.51923

C	4.88024	-4.57846	-3.74887
H	4.46069	-2.46451	-3.42416
C	10.78266	-2.85287	-2.96109
C	11.07325	-1.53294	-2.72367
S	9.63985	-0.51882	-2.6602
H	11.57816	-3.58319	-3.02805
S	6.30225	-5.61329	-3.79762
O	9.22789	-5.56448	-3.53652
O	6.58136	-0.62295	-2.99908
C	10.54511	-5.91725	-3.01408
H	10.68153	-5.53389	-1.99728
H	10.5493	-7.00796	-3.00298
H	11.35063	-5.55269	-3.657
C	6.37458	0.04559	-4.30071
H	5.77543	-0.58306	-4.96852
H	5.84138	0.96829	-4.06842
H	7.33537	0.27183	-4.77573
C	3.55087	-5.09851	-3.91345
S	2.16588	-4.03017	-3.78885
C	1.00737	-5.319	-4.03291
C	3.09824	-6.37491	-4.13455
C	1.68706	-6.50264	-4.21137
C	3.69795	-7.71188	-4.2688
C	1.35808	-7.92635	-4.40792
O	0.2769	-8.51231	-4.54231
O	4.87273	-8.07877	-4.2551
N	2.59753	-8.57802	-4.42251
C	2.7405	-10.01933	-4.5513
H	2.15999	-10.37664	-5.40569
H	3.80449	-10.22004	-4.6979

H	2.39394	-10.51873	-3.64073
C	-5.05444	-4.09114	-3.55325
C	-5.07309	-5.49206	-3.7648
C	-3.91754	-6.25033	-3.93681
C	-2.69091	-5.56374	-3.89855
C	-2.68581	-4.14744	-3.673
C	-3.83355	-3.4022	-3.50552
C	-6.36613	-3.58011	-3.36005
C	-7.33736	-4.55371	-3.43375
H	-6.56265	-2.53681	-3.14747
C	-1.36475	-6.05598	-4.08117
C	-0.40352	-5.08291	-3.97042
S	-1.07539	-3.49463	-3.63908
H	-1.08732	-7.08162	-4.28595
S	-6.67344	-6.15284	-3.74866
O	-4.11517	-7.58965	-4.13751
O	-3.77907	-2.02765	-3.29822
C	-3.14112	-8.56786	-3.64355
H	-2.73518	-8.2604	-2.67378
H	-3.71252	-9.49042	-3.53084
H	-2.32492	-8.72457	-4.35303
C	-3.85306	-1.2555	-4.55605
H	-4.79589	-1.45358	-5.07763
H	-3.79885	-0.20879	-4.25419
H	-3.01228	-1.5048	-5.2125
C	-8.74638	-4.33598	-3.25429
S	-9.35293	-2.72984	-2.88002
C	-11.02048	-3.25601	-2.80289
C	-9.81008	-5.20139	-3.3079
C	-11.07545	-4.60785	-3.0593

C	-10.00779	-6.63799	-3.56083
C	-12.10756	-5.65608	-3.15157
O	-13.33697	-5.61861	-3.01191
O	-9.20509	-7.53614	-3.81333
N	-11.40079	-6.8269	-3.45195
C	-12.03634	-8.12195	-3.63211
H	-12.74822	-8.08547	-4.46189
H	-11.23735	-8.8339	-3.85338
H	-12.56253	-8.41909	-2.72021
C	-15.44691	0.90132	-1.5176
C	-16.21207	-0.28421	-1.62664
C	-15.65513	-1.53156	-1.90682
C	-14.25929	-1.58575	-2.0822
C	-13.49826	-0.37297	-1.96856
C	-14.05648	0.85688	-1.6955
C	-16.26559	2.01692	-1.19324
C	-17.5977	1.68796	-1.07433
H	-15.86626	3.01028	-1.03156
C	-13.4069	-2.68838	-2.39624
C	-12.08332	-2.34287	-2.50319
S	-11.79866	-0.63296	-2.21658
H	-13.71576	-3.71412	-2.54929
S	-17.90168	-0.02231	-1.35413
O	-16.56451	-2.54852	-1.98347
O	-13.26667	1.99912	-1.60884
C	-16.16253	-3.9497	-1.93675
H	-15.47909	-4.13908	-1.10244
H	-17.09557	-4.49271	-1.78158
H	-15.69959	-4.27327	-2.87276
C	-13.18226	2.73527	-2.88735

H	-14.17565	3.06357	-3.21221
H	-12.54643	3.59721	-2.68132
H	-12.73185	2.10899	-3.66507
C	-18.65361	2.60545	-0.74483
S	-18.29347	4.3006	-0.45494
C	-19.96347	4.71614	-0.13586
C	-20.00405	2.41502	-0.59248
C	-20.73689	3.58291	-0.25392
C	-20.94251	1.285	-0.6908
C	-22.16004	3.21976	-0.12942
O	-23.16226	3.89051	0.14964
O	-20.75869	0.09725	-0.95595
N	-22.20286	1.84714	-0.40284
C	-23.42913	1.06629	-0.38872
H	-24.13155	1.44449	-1.13726
H	-23.14697	0.03727	-0.62473
H	-23.89791	1.11125	0.59861
C	-21.43295	10.61172	1.1296
C	-22.69662	9.98619	1.24909
C	-22.89103	8.61708	1.06847
C	-21.75718	7.84451	0.75393
C	-20.48194	8.49506	0.64072
C	-20.29827	9.84938	0.81791
C	-21.51976	12.00681	1.39073
C	-22.79951	12.41721	1.68437
H	-20.65642	12.65997	1.38116
C	-21.6383	6.44821	0.47685
C	-20.35619	6.05606	0.18596
S	-19.20641	7.3835	0.24469
H	-22.44335	5.72508	0.47096

S	-23.96063	11.0967	1.65896
O	-24.18643	8.20656	1.21131
O	-19.04089	10.4299	0.67963
C	-24.52906	6.80715	1.44369
H	-23.89082	6.367	2.21717
H	-25.56331	6.83597	1.78884
H	-24.46279	6.21277	0.52869
C	-18.78427	10.91436	-0.69274
H	-19.51526	11.67935	-0.97664
H	-17.78045	11.34014	-0.66464
H	-18.82492	10.08629	-1.40868
C	-23.19352	13.76714	1.99544
S	-22.00292	15.06054	2.01693
C	-23.17237	16.26164	2.43911
H	-22.89103	17.29499	2.57617
C	-24.41938	14.29786	2.30717
C	-24.4026	15.69805	2.55518
C	-25.80319	13.81377	2.46533
C	-25.77943	16.14247	2.87852
O	-26.23123	17.24769	3.15676
O	-26.284	12.68679	2.3488
N	-26.54351	14.95899	2.80143
C	-27.9751	14.93106	3.05057
H	-28.27013	15.9545	3.29541
H	-28.51101	14.58709	2.16091
H	-28.20363	14.26234	3.88569
C	-0.79586	-6.32482	4.55421
C	-1.31078	-5.71445	3.42027
C	4.16158	-9.29839	0.78952
C	3.66845	-8.69945	-0.36022

C	2.9906	-4.45156	3.01054
C	3.98642	-5.04948	2.25351
C	-1.1381	-9.95456	1.91995
C	-0.14217	-10.55359	1.16389
C	3.24216	-8.47338	5.25011
C	2.28888	-9.75052	5.00216
C	0.57433	-5.44363	-0.65754
C	-0.24934	-6.53744	-0.87751
C	0.48696	-5.90471	5.09326
C	-0.90675	-7.76415	4.72344
C	-0.56248	-4.65501	2.76032
C	-1.95697	-6.51594	2.39139
C	4.80231	-8.49326	1.81524
C	3.40686	-10.35228	1.44769
C	3.78367	-7.25955	-0.53988
C	2.38571	-9.12042	-0.90417
C	2.62582	-5.0081	4.30485
C	1.77264	-3.98176	2.37115
C	4.6663	-6.23464	2.75344
C	3.81741	-5.20744	0.81857
C	-0.96534	-9.79517	3.35604
C	-1.8216	-8.77273	1.42187
C	1.07771	-11.02216	1.80609
C	0.2219	-10.00024	-0.12948
C	2.5385	-7.18198	5.46958
C	4.23627	-8.20118	4.179
C	0.82966	-9.46025	5.01347
C	2.52933	-10.48669	3.73061
C	0.32323	-4.55675	0.46672
C	2.01461	-5.57047	-0.81742

C	-1.36266	-6.80088	0.02027
C	0.3297	-7.81609	-1.26138
C	1.19505	-4.88322	4.46796
C	-1.53815	-8.52729	3.74627
C	0.66137	-4.25075	3.27237
C	-2.06844	-7.88896	2.55185
C	4.92042	-7.11869	1.63806
C	2.18828	-10.76298	0.91802
C	4.39563	-6.48812	0.43747
C	1.66393	-10.12902	-0.28122
C	3.26831	-6.14542	4.77693
C	1.60779	-4.13536	1.00189
C	4.3124	-6.77109	3.98417
C	2.65413	-4.76114	0.20709
C	0.20395	-10.23201	3.96591
C	-1.47503	-8.24134	0.18727
C	1.24753	-10.86044	3.17483
C	-0.42736	-8.86888	-0.60536
C	1.17229	-7.07523	5.60889
C	4.45592	-9.04499	3.11213
C	0.29768	-8.24216	5.37444
C	3.58026	-10.21265	2.88173
C	-0.73696	-4.80901	1.32646
C	2.56895	-6.78932	-1.18325
C	-1.5999	-5.95881	1.09812
C	1.70438	-7.93965	-1.40462
H	1.04557	-10.89132	7.27646
C	1.50889	-10.18647	7.95879
C	2.60938	-9.43857	7.53273
C	1.0099	-10.02654	9.25064

C	3.20067	-8.52463	8.40925
C	1.60573	-9.11678	10.12285
H	0.15566	-10.61098	9.57433
C	2.70075	-8.36353	9.69914
H	4.04814	-7.93548	8.07285
H	1.21561	-8.99124	11.12682
H	3.16269	-7.6497	10.37226
C	3.2279	-9.66852	6.18788
C	4.45589	-10.57301	6.16047
H	4.87814	-10.55844	5.14992
H	5.20916	-10.14056	6.8333
C	4.14965	-12.02806	6.55891
H	3.17667	-12.33223	6.15373
H	4.89035	-12.69128	6.09586
C	4.16962	-12.26596	8.07109
H	5.1494	-12.0241	8.50154
H	3.4312	-11.63692	8.5814
C	3.85808	-13.70547	8.37839
O	4.00343	-13.95444	9.71866
O	3.51263	-14.56529	7.577
C	3.70503	-15.33414	10.11772
H	4.35637	-16.03674	9.59074
H	3.88641	-15.36048	11.19143
H	2.66566	-15.58514	9.88847