

Impact of the Interfacial Molecular Structure Organization on the Charge Transfer State Formation and Exciton Delocalization in Merocyanine:PC₆₁BM Blends

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Synthesis of ML merocyanine

2,3,3-trimethylindolenine (5g, 31.4 mmol) and 1-iodononane (7.98 g, 31.4 mmol) were heated under an argon atmosphere to 120 °C for 24 hours. After cooling to room temperature the residue was dissolved in dichloromethane and a 1M aqueous solution of potassium hydroxide (90 ml) was added. The mixture was stirred at room temperature for 1 h and the crude product (1-heptyl-3,3-dimethyl-2-methyleneindoline) was extracted with dichloromethane. After drying the organic phase over MgSO₄ the solvent was removed under reduced pressure. The crude product was used immediately without any further purification.

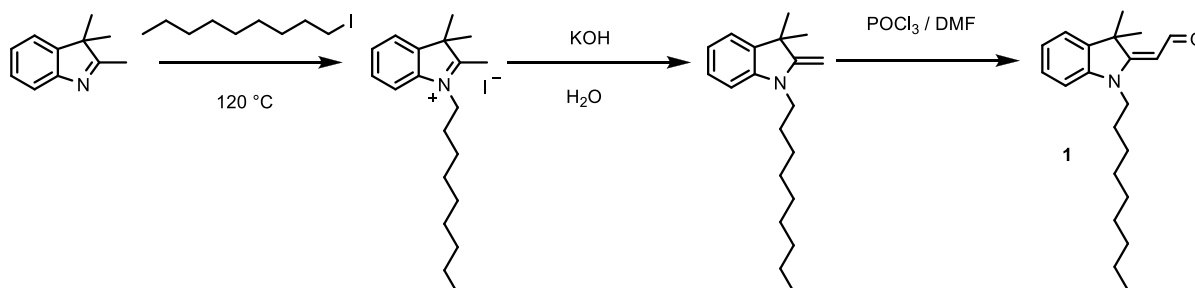


Figure S1 Synthesis of (E)-2-(3,3-dimethyl-1-nonylindolin-2-ylidene)acetaldehyde (I).

Under an argon atmosphere dry dimethylformamide (5.5 ml) was cooled to 0 °C and phosphorous oxychloride (5.37 g, 35.0 mmol) was slowly added. The crude 3,3-dimethyl-1-nonyl-2-methyleneindoline was dissolved in dry dimethylformamide (7.5 ml) and added dropwise to the POCl₃ / DMF mixture. The reaction mixture was stirred at 40 °C for 1 h and then added to water containing ice (30 ml). After adjusting the pH to 10 with a diluted sodium hydroxide solution the mixture was heated under reflux for 30 minutes. The crude product was extracted with dichloromethane, the organic phase was dried over MgSO₄ and the solvent was removed under reduced pressure.

Column chromatography on silica with toluene / ethyl acetate (5:1) as eluent yielded a red oil (7.36 g, 23.5 mmol, 75 %).

¹H NMR (acetone-d₆, 300 MHz): δ / ppm = 10.00 (1H, d, ³J = 8.5 Hz); 7.38 (1H, m); 7.27 (1H, m); 7.07 – 6.99 (2H); 5.33 (1H, d, ³J = 8.5 Hz); 3.78 (2H, t, ³J = 7.5 Hz); 1.70 (2H, m); 1.65 (6H, s); 1.50 – 1.23 (12H); 0.86 (3H, m).

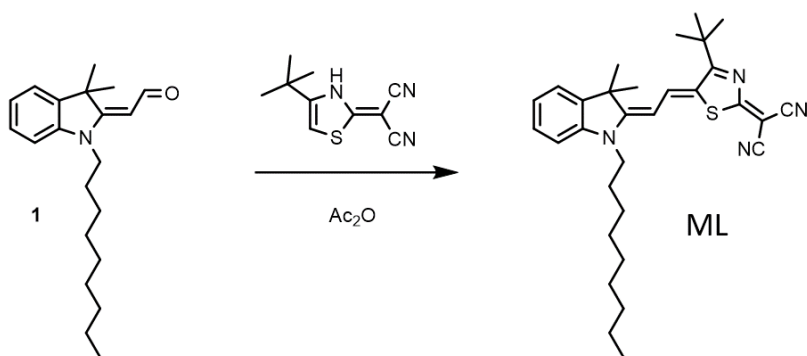


Figure S2 Synthesis of 2-((Z)-4-tert-butyl-5-((E)-2-(3,3-dimethyl-1-nonylindolin-2-ylidene)ethylidene)thiazol-2(5H)-ylidene)malononitrile (**ML**).

A mixture of **1** (1.76 g, 5.62 mmol), 2-(4-tert-butylthiazol-2(3H)-ylidene)malononitrile^[1] (1.05 g, 5.09 mmol) and acetic anhydride (6 ml) was heated to 90 °C for 1 h. After cooling to room temperature n-hexane was added and the precipitate was collected by filtration, washed with 2-propanol and n-hexane and dried in vacuo. Subsequent purification by column chromatography on silica with dichloromethane / ethyl acetate (99 : 1) as eluent yielded a blue powder (1.47 g, 2.94 mmol, 52 %).

¹H NMR (CD₂Cl₂, 500 MHz): δ / ppm = 8.33 (1H, d, ³J = 13.4 Hz); 7.45 – 7.34 (2H), 7.25 (1H, m), 7.09 (1H, m), 5.65 (1H, d, ³J = 13.4 Hz), 3.94 (2H, t, ³J = 7.3 Hz), 1.81 (2H, m), 1.69 (6H, s), 1.55 (9H, s), 1.48 – 1.21 (12H), 0.87 (3H, m). ¹³C NMR (CD₂Cl₂, 125 MHz): δ / ppm = 185.0 (C_q), 179.4 (C_q), 172.4 (C_q), 142.4 (C_q), 140.6 (C_q), 138.3 (CH), 128.9 (CH), 126.5 (C_q), 125.2 (CH), 122.5 (CH), 118.2 (C_q), 116.1 (C_q), 110.7 (CH), 99.2 (CH), 55.9 (C_q), 49.1 (C_q), 44.5 (CH₂), 38.1 (C_q), 32.1 (CH₂), 31.4 (CH₃), 29.5 (3xCH₂), 28.4 (CH₃), 27.3 (CH₂), 27.2 (CH₂), 22.9 (CH₂), 14.1 (CH₃). HR-ESI-MS (MeCN): calc. m/z = 500.29682 for C₃₁H₄₀N₄S, found m/z = 500.29739, Δ = 1.14 ppm.

Synthesis of MB merocyanine

2,3,3-trimethylindolenine (2.26 g, 14.2 mmol) and 1-iodo-2-ethylhexane (3.41 g, 14.2 mmol) were heated under an argon atmosphere to 120 °C for 24 hours. After cooling to room temperature the residue was dissolved in dichloromethane and a 1M aqueous solution of potassium hydroxide (90 ml) was added. The mixture was stirred at room temperature for 1 h and the crude product (1-(2-ethylhexyl)-3,3-dimethyl-2-methyleneindoline) was extracted with dichloromethane. After drying the organic phase over MgSO₄ the solvent was removed under reduced pressure. The crude product was used immediately without any further purification.

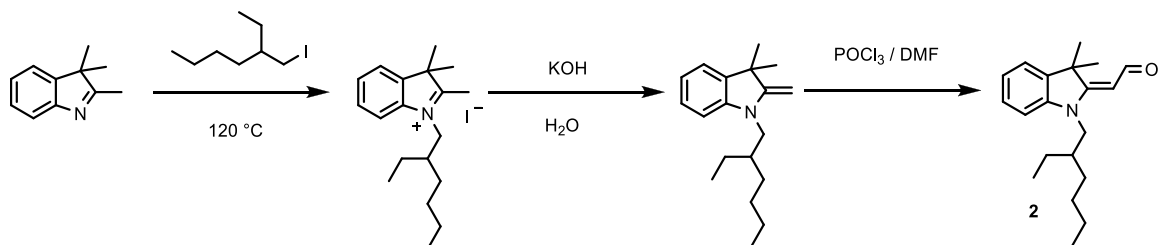


Figure S3 Synthesis of (E)-2-(3,3-dimethyl-1-(2-ethylhexyl)indolin-2-ylidene)acetaldehyde (**2**).

Under an argon atmosphere dry dimethylformamide (3.5 ml) was cooled to 0 °C and phosphorous oxychloride (2.43 g, 15.8 mmol) was slowly added. The crude 3,3-dimethyl-1-(2-ethylhexyl)-2-methyleneindoline was dissolved in dry dimethylformamide (4.5 ml) and added dropwise to the POCl₃ / DMF mixture. The reaction mixture was stirred at 40 °C for 1 h and then added to water containing ice (30 ml). After adjusting the pH to 10

with a diluted sodium hydroxide solution the mixture was heated under reflux for 30 minutes. The crude product was extracted with dichloromethane, the organic phase was dried over MgSO₄ and the solvent was removed under reduced pressure.

Column chromatography on silica with toluene / ethyl acetate (7:1) as eluent yielded a red oil (0.92 g, 3.07 mmol, 22 %).

¹H NMR (CDCl₃, 300 MHz): δ / ppm = 10.01 (1H, d, ³J = 9.0 Hz); 7.29 – 7.21 (2H); 7.05 (1H, m); 6.84 (1H, m); 5.42 (1H, d, ³J = 9.0 Hz); 3.57 (2H, d, ³J = 7.7 Hz); 1.96 (1H, m); 1.66 (6H, s); 1.41 – 1.21 (8H); 0.91 (3H, m); 0.85 (3H, m).

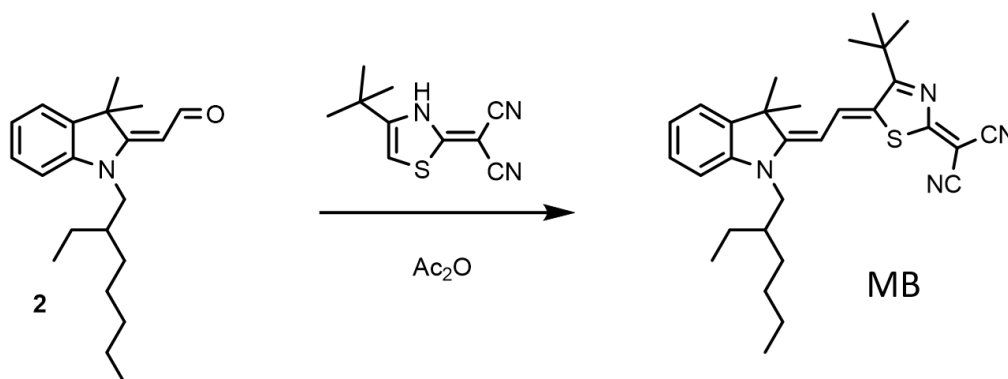


Figure S4 Synthesis of 2-((Z)-4-tert-butyl-5-((E)-2-(3,3-dimethyl-1-(2-ethylhexyl)indolin-2-ylidene)ethyldene)thiazol-2(5H)-ylidene)malononitrile (MB).

A mixture of **2** (0.92 g, 2.25 mmol), 2-(4-tert-butylthiazol-2(3H)-ylidene)malononitrile^[1] (0.42 g, 2.04 mmol) and acetic anhydride (2.3 ml) was heated to 90 °C for 1 h. After cooling to room temperature n-hexane was added and the precipitate was collected by filtration, washed with 2-propanol and n-hexane and dried in vacuo. Subsequent purification by column chromatography on silica with dichloromethane as eluent yielded a blue powder (0.59 g, 1.21 mmol, 54 %).

¹H NMR (CD₂Cl₂, 500 MHz): δ / ppm = 8.31 (1H, d, ³J = 13.4 Hz); 7.42 – 7.34 (2H), 7.24 (1H, m), 7.08 (1H, m), 5.66 (1H, d, ³J = 13.4 Hz), 3.84 (2H, m), 1.98 (1H, m), 1.69 (6H, s), 1.55 (9H, s), 1.49 – 1.25 (8H), 0.98 (3H, t, ³J = 7.4 Hz); 0.90 (3H, t, ³J = 7.2 Hz). ¹³C NMR APT (CD₂Cl₂, 125 MHz): δ / ppm = 185.0 (C_q), 179.4 (C_q), 172.9 (C_q), 143.1 (C_q), 140.6 (C_q), 138.2 (CH), 128.9 (CH), 126.7 (C_q), 125.1 (CH), 122.5 (CH), 118.0 (C_q), 116.0 (C_q), 111.0 (CH), 99.9 (CH), 55.9 (C_q), 49.1 (C_q), 48.6 (CH₂), 38.4 (CH), 31.5 (CH₃), 31.2 (CH₂), 31.1 (C_q), 29.0 (CH₂), 28.3 (CH₃), 24.7 (CH₂), 23.2 (CH₂), 14.1 (CH₃), 11.1 (CH₃). HR-ESI-MS (MeCN): calc. m/z = 486.28117 for C₃₀H₃₈N₄S, found m/z = 486.28029, Δ = 1.81 ppm.

References

[1] H. Bürckstümmer, E. V Tulyakova, M. Deppisch, M. R. Lenze, N. M. Kronenberg, M. Gsänger, M. Stolte, K. Meerholz, F. Würthner, *Angew. Chem. Int. Ed.* **2011**, *50*, 11628–11632.

Device characteristics

All solar cells were fabricated on indium–tin oxide (ITO, 125 nm) coated glass. The substrates were exposed to ozone for 3 min and transferred to the evaporation chamber to evaporate 10 nm MoO₃. After transfer to a glove box active layers of about 70 nm were spin-coated from chloroform solutions of 13 to 15 mg/mL mixed in a

ratio of 2:3 (MC to PC₆₁BM). Neat film was prepared without PC₆₁BM in the same way. The device fabrication was completed by thermal evaporation of 5 nm Ca and 120 nm Ag for solar cells or 10 nm MoO₃ and 120 nm Ag for unipolar diodes (SCLC).

The solar cell characteristics were measured using a Keithley 2425 source-measurement unit with a filtered Xe lamp, providing the AM 1.5 G solar spectrum. The intensity of the lamp was adjusted to 100 mWcm⁻².

OFETs were characterized using a semiconductor parameter analyzer (Keithley 4200). Mobilities were obtained from saturation regime curves using standard OFET models.

To further substantiate our hypothesis that molecular packing affects device performance [Table S1](#).

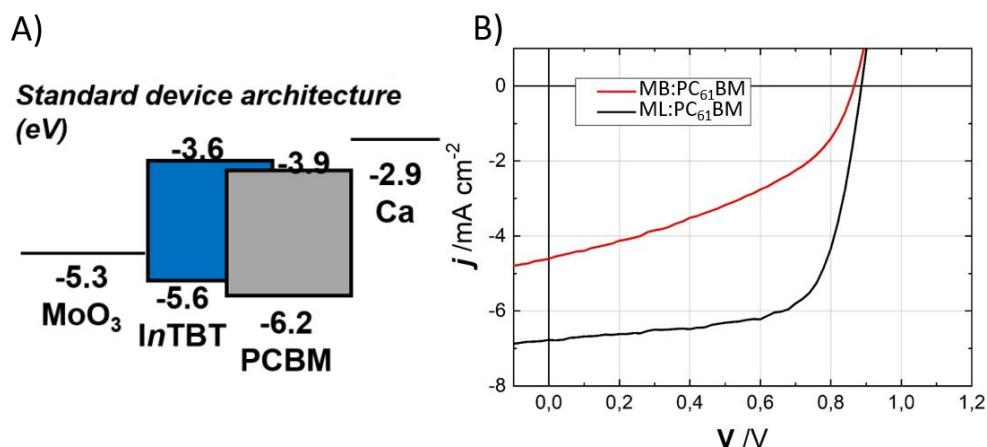


Figure S5 A) Standard solar cell architecture used for device characterization B) Voltamperic characteristics of ML and MB based devices with PC₆₁BM as the electron acceptor.

Bulk heterojunction solar cells with the same thickness of both compounds were made in a standard configuration of ITO/MoO₃/BHJ/Ca/Ag. The PCE of ML and MB under AM1.5 illumination are 4.1 % and 1.7 %, respectively. Having a closer look at the short circuit current (6.77 vs. 4.61 mA/cm²) and fill factor (0.68 vs. 0.42)) (sup info) it is apparent that ML has a higher photogeneration yield and fill factor. A higher charge generation is attributed to less pronounced CT formation among the merocyanines in ML in the presence of PC₆₁BM as suggested by theoretical modelling. That a higher fraction of H-type aggregation in ML improves charge transport is reflected in the higher FF of these devices.

Material	V _{OC} / V	j / cm ² /Vs	FF	PCE / %	μ / cm ² V ⁻¹ s ⁻¹ SCLC
ML:PC ₆₁ BM	0.87	6.77	0.68	4.09	1.5 · 10 ⁻⁵
	±0.009	±0.28	±0.013	±0.13	±0.5 · 10 ⁻⁵
MB:PC ₆₁ BM	0.87	4.61	0.42	1.66	1.4 · 10 ⁻⁷
	±0.01	±0.20	±0.01	±0.07	±0.5 · 10 ⁻⁷

Table S1. Device characteristics of merocyanine bulk heterojunction solar cells together with mobility.

Linear absorption as the function of PC₆₁BM content

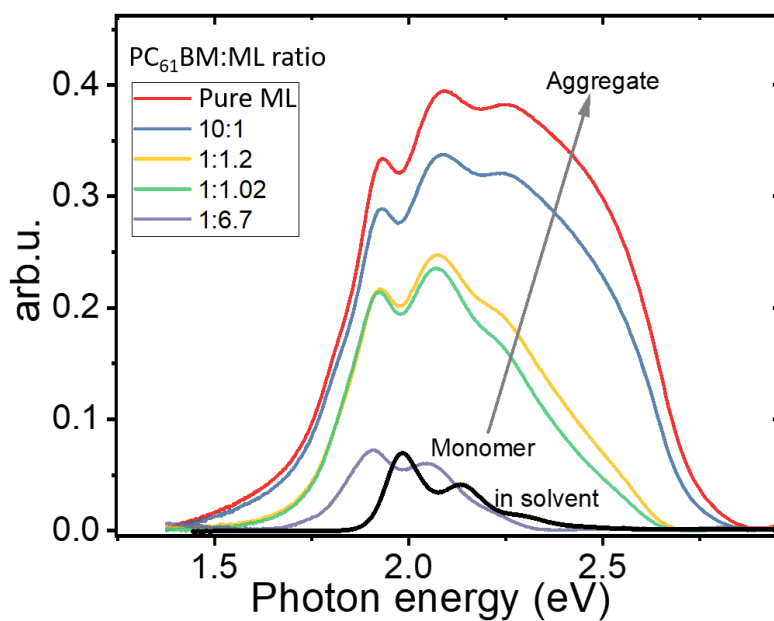


Figure S6 Absorption spectra of ML:PC₆₁BM films with varying PC₆₁BM:ML ratio. The absorption spectrum of ML, molecule, dissolved in Acetone solvent is shown in black. With increasing PC₆₁BM ratio, a reduction in spectra weights at the blue side of the spectrum was observed, hint to a reduction in H-aggregate formation. The red shift of the spectrum was attributed to the difference in local surrounding and change in dielectric constant.

DFT calculations

TDDFT calculations using TD- ω B97X-D3/6-31G* merocyanine molecules and clusters is shown below. The represented Absorption spectrum was calculated by convoluting excited states with Lorentzian function.

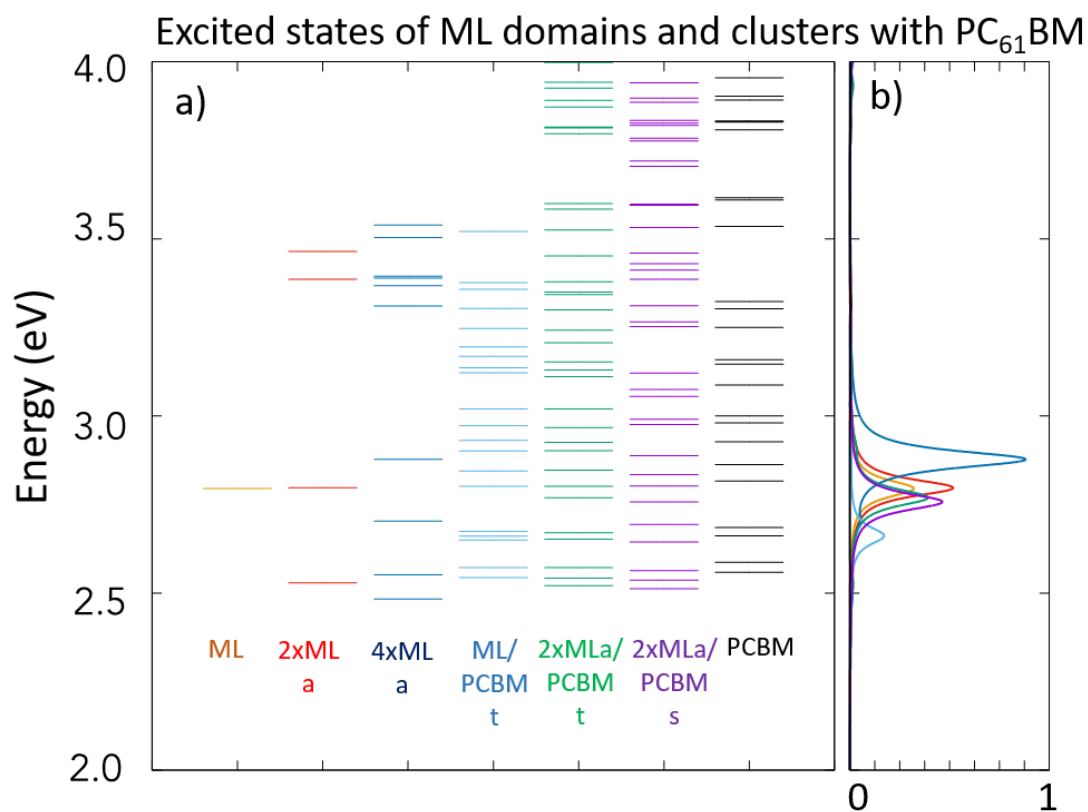


Figure S7 a) Computed TD- ω B97X-D3/6-31G* excited state vertical energies for ML molecules and cluster with PC₆₁BM; b) Absorption spectra of computed transitions, plotted using the Lorentz convolution of calculated states. 2xML a: dimer with antiparallel alignment, 4xML a: cluster of 4 antiparallel molecules, ML/PCBM t: merocyanine and PC₆₁BM cluster with PC₆₁BM on top, 2xMLa/PCBM t: two ML molecules aligned antiparallel with PC₆₁BM on top, 2xMLa/PCBM s: two ML molecules with antiparallel alignment with PC₆₁BM on the side, PCBM: spectrum of the pure PC₆₁BM.

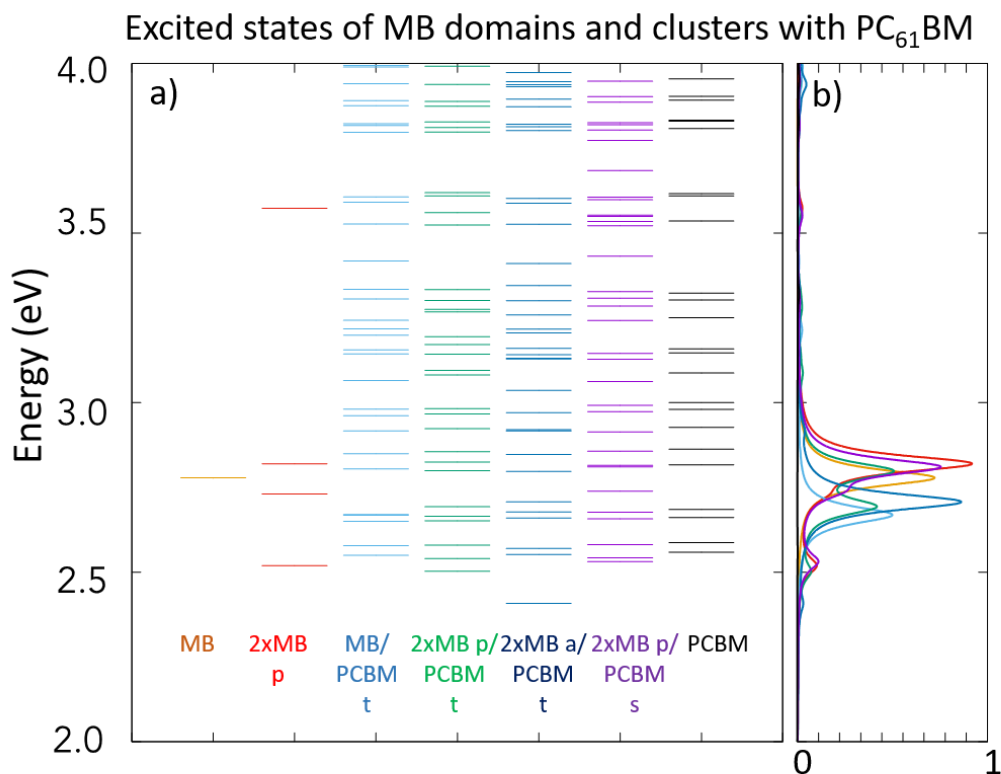


Figure S8 a) Computed TD- ω B97X-D3/6-31G* excited state vertical energies for MB molecules and cluster with PC₆₁BM; b) Absorption spectra of computed transitions, plotted using the Lorentz convolution of calculated states. 2xMB p: dimer with parallel alignment, MB/PCBM t: MB molecule and PC₆₁BM cluster with PC₆₁BM on top, 2xMB p/PCBM t: two MB molecules aligned parallel with PC₆₁BM on top, 2xMB a/PCBM t: two MB molecules with antiparallel alignment with PC₆₁BM on the top, 2xMB p/PCBM s: two MB molecules with parallel alignment with PC₆₁BM on the side, PCBM: spectrum of the pure PC₆₁BM.

Here below we reported the Cartesian coordinates of the optimized DFT structures (single molecules and structures) considered in the manuscript. The first entry in the data is Atom and three numbers represent X, Y, Z coordinates in Angstrom.

MB single molecule							
C	5.125662	0.030095	-1.175431	C	-4.260452	0.797220	-0.290565
C	3.841426	-0.449128	-0.958693	N	-4.468422	-0.523975	-0.010126
C	3.597956	-1.774943	-0.616295	C	-3.368785	-1.227526	-0.017698
C	4.648618	-2.663862	-0.486391	C	-5.281062	1.716623	-0.332302
C	5.951304	-2.205923	-0.702365	C	-6.626777	1.318967	-0.078922
C	6.179965	-0.875320	-1.042602	N	-7.728408	1.016408	0.124398
C	2.106775	-1.983738	-0.451663	C	-3.459532	-2.720632	0.285647
C	1.567473	-0.570564	-0.727906	C	-2.948235	-3.541072	-0.915773
N	2.624454	0.245273	-1.031597	C	1.601683	-2.994783	-1.498668
C	0.265629	-0.142643	-0.691705	C	1.796664	-2.452968	0.981073
C	-0.865020	-0.943877	-0.390085	C	2.573241	1.663558	-1.344828
C	-2.151297	-0.493418	-0.317366	C	2.938892	2.606393	-0.183803
S	-2.578489	1.204300	-0.588079	C	-2.655383	-3.049471	1.559729
				C	-4.925967	-3.106345	0.535360

C	-5.006824	3.081999	-0.628235
N	-4.735580	4.184611	-0.873273
H	-0.710251	-1.995743	-0.197272
H	-2.779215	-4.110177	1.802937
H	-1.584771	-2.854337	1.456393
H	-3.021446	-2.462459	2.408206
H	-4.981674	-4.178596	0.753612
H	-5.346476	-2.554287	1.379273
H	-5.548962	-2.893337	-0.336744
H	-3.087167	-4.607920	-0.710644
H	-3.513966	-3.293952	-1.819855
H	-1.888667	-3.379295	-1.130495
H	0.071695	0.903732	-0.900621
H	5.316131	1.066171	-1.433717
H	7.195850	-0.529232	-1.205540
H	6.787792	-2.889717	-0.602414
H	4.468406	-3.702238	-0.220808
H	2.320028	-3.394060	1.178369
H	2.133317	-1.715183	1.713845
H	0.728959	-2.624154	1.138227
H	2.100280	-3.957584	-1.347309
H	0.523158	-3.157790	-1.424325
H	1.825982	-2.649455	-2.511844
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H	3.254469	1.832377	-2.187152
C	2.781749	4.053011	-0.681282
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H	3.122572	5.069155	1.224992
H	4.571105	4.890881	0.225384
H	3.175417	4.131878	-1.703788
H	1.711336	4.291975	-0.745307
C	2.108608	2.329004	1.084067
C	2.737742	1.318158	2.046841
C	1.768891	0.863957	3.137903
C	2.428976	-0.028298	4.187236
H	1.705875	-0.368264	4.935358
H	2.880472	-0.916945	3.729615
H	3.227397	0.509098	4.711314
H	1.953894	3.266642	1.631245
H	1.104628	1.990995	0.798980
H	3.627821	1.771105	2.505910
H	3.101988	0.439376	1.500220
H	1.333800	1.744439	3.628822
H	0.930365	0.332409	2.666857
H	3.999690	2.447754	0.060449

ML single molecule

C	2.102622	-3.598767	-0.321244
S	1.063195	-2.208840	-0.586617
C	2.395583	-1.154851	-0.084762
C	3.538470	-1.990133	0.243671
N	3.358567	-3.276184	0.110188
C	2.275682	0.203763	-0.041903
C	1.114216	0.935198	-0.399237
C	4.901122	-1.492444	0.718317
C	4.754049	-0.736104	2.054082
C	1.697708	-4.896299	-0.524184
C	0.375212	-5.173837	-0.972593
N	-0.713160	-5.350910	-1.337933
C	5.833666	-2.691580	0.950852
C	5.540712	-0.591167	-0.357239
C	2.591925	-5.981451	-0.287378
N	3.303594	-6.878690	-0.100371
H	3.143982	0.756124	0.288926
H	5.746082	-0.447894	2.417889
H	4.153717	0.173667	1.971285
H	4.288931	-1.376412	2.810485
H	6.808975	-2.325786	1.290538
H	5.431078	-3.370318	1.706611
H	5.975931	-3.270466	0.035111
H	6.543802	-0.295356	-0.031802
H	5.637997	-1.131617	-1.304323
H	4.970704	0.321273	-0.551137
C	0.970515	2.296600	-0.323257
C	1.961914	3.340718	0.211535
N	-0.164829	2.942687	-0.726940
C	-0.093753	4.318643	-0.462908
C	1.153120	4.616318	0.079511
H	0.267430	0.359281	-0.759254
C	3.229483	3.423855	-0.659376
C	2.307643	3.091524	1.690886
C	1.473390	5.919452	0.410674
C	0.524157	6.923596	0.199073
C	-0.723157	6.608660	-0.333020
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H	-2.035675	5.062049	-1.076014
H	-1.456213	7.394551	-0.485929
H	0.758670	7.951424	0.455594
H	2.445137	6.162571	0.832468
H	2.910919	3.922111	2.071235
H	1.399068	3.023902	2.295817
H	2.878420	2.169517	1.828792
H	3.847079	4.264346	-0.326758

H	3.833969	2.515197	-0.591541	C	5.247121	1.239497	-0.421323
H	2.970024	3.585089	-1.709476	C	6.625405	-1.940174	0.222047
C	-1.342597	2.290780	-1.270198	C	8.013993	-1.843908	-0.084628
C	-2.277055	1.752845	-0.186019	N	9.150172	-1.790266	-0.313265
C	-3.469941	1.002265	-0.775324	C	5.576460	2.655598	-0.875667
C	-4.406967	0.443888	0.295392	C	4.763710	3.022685	-2.131144
C	-5.595067	-0.320627	-0.287502	C	-0.152894	3.150222	-0.908364
C	-6.528019	-0.886985	0.782535	C	0.865986	3.980228	1.261660
C	-7.715453	-1.654226	0.201714	C	-0.590705	-0.455928	2.223643
C	-8.648075	-2.224064	1.270909	C	-0.159934	-0.599632	3.696265
C	-9.831373	-2.988800	0.680574	C	5.288634	3.642893	0.274199
H	-10.482960	-3.386231	1.465588	C	7.068571	2.743781	-1.229629
H	-10.437593	-2.339692	0.038021	C	6.092405	-3.184740	0.663081
H	-9.488401	-3.832336	0.070574	N	5.595466	-4.169467	1.029060
H	-1.013873	1.486536	-1.936712	H	2.708659	2.449626	-0.284360
H	-1.862636	3.016365	-1.902865	H	5.587384	4.651449	-0.031019
H	-1.710230	1.087163	0.476877	H	4.231833	3.676489	0.553200
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H	-3.106157	0.176667	-1.402908	H	7.700004	2.501915	-0.371172
H	-3.838882	-0.220699	0.960891	H	7.324138	2.047875	-2.032598
H	-4.774672	1.267850	0.923178	H	5.069689	4.013972	-2.482149
H	-6.164920	0.343718	-0.952799	H	4.956255	2.306329	-2.935765
H	-5.224297	-1.141560	-0.916870	H	3.684995	3.055226	-1.962524
H	-6.898477	-0.066574	1.413889	H	1.669862	-0.159825	0.999567
H	-5.956749	-1.550936	1.446468	H	-3.021798	0.591747	3.120447
H	-8.287896	-0.991026	-0.462782	H	-4.678967	2.427834	3.244884
H	-7.344477	-2.473881	-0.429747	H	-4.261093	4.589226	2.117290
H	-9.017454	-1.404705	1.902301	H	-2.157981	4.947232	0.837499
H	-8.075290	-2.887218	1.932714	H	0.438718	4.976158	1.106402
2xMB cluster				H	0.955570	3.812638	2.338662
C	-2.835017	1.532596	2.613375	H	1.868880	3.977018	0.827694
C	-1.668950	1.757407	1.892146	H	-0.521487	4.162727	-1.104484
C	-1.415436	2.974445	1.262198	H	0.811195	3.036351	-1.411637
C	-2.344700	3.995817	1.328432	H	-0.847389	2.438048	-1.362836
C	-3.527263	3.792603	2.048494	H	0.030937	-1.086009	1.584267
C	-3.760468	2.575957	2.684896	H	-1.610846	-0.833032	2.104966
C	-0.047560	2.924502	0.609002	C	-0.577800	-2.003088	4.173499
C	0.397766	1.492828	0.944553	C	-0.578351	-2.171322	5.692130
N	-0.597883	0.888086	1.677666	H	-0.903128	-3.178706	5.970454
C	1.571290	0.862326	0.651708	H	0.414830	-2.016883	6.124756
C	2.741374	1.428678	0.071666	H	-1.262001	-1.455260	6.162330
C	3.928312	0.764670	-0.016160	H	-1.587456	-2.226599	3.802954
S	4.085477	-0.923373	0.489241	H	0.088661	-2.748120	3.716598
C	5.792726	-0.855326	0.099374	C	1.346854	-0.364468	3.909362
N	6.213544	0.369697	-0.331788	C	1.776668	1.099879	4.034239
				C	3.288093	1.279485	3.892315
				C	3.715908	2.744624	3.887298

C	3.222117	-4.253885	-1.061077	H	9.410655	-6.242676	-1.436861
N	4.333030	-4.435039	-0.771309	H	7.735926	-6.774043	-1.221480
C	-2.379887	-1.673983	-2.364158	H	4.355162	2.156952	0.975399
C	-1.958434	0.261499	-0.853068	H	5.468660	3.500215	0.846830
C	0.949984	-5.047295	-1.540649	H	4.985114	1.928255	-1.687862
N	0.203986	-5.934477	-1.611095	H	6.482687	2.638995	-1.122700
H	0.362256	1.743775	-1.580898	H	6.804424	0.796757	0.498545
H	-2.452901	0.738565	-3.549265	H	5.176906	0.204960	0.211906
H	-0.822803	1.319734	-3.198533	H	5.743242	-0.368381	-2.129414
H	-1.046050	-0.117634	-4.205110	H	7.392761	0.199759	-1.897177
H	-3.389015	-1.289773	-2.550443	H	7.786882	-1.529867	-0.166980
H	-2.057393	-2.252795	-3.233259	H	6.101997	-2.036602	-0.240514
H	-2.420342	-2.358819	-1.512917	H	8.012753	-2.212293	-2.622731
H	-2.993509	0.576767	-1.024848	H	6.353056	-2.801549	-2.553057
H	-1.942084	-0.389374	0.027016	H	8.685276	-3.829661	-0.856730
H	-1.379846	1.156128	-0.609218	H	7.008868	-4.355262	-0.681530
C	2.598838	3.154085	-0.791475	H	8.656663	-4.647263	-3.244189
C	1.666712	4.299807	-1.186907	H	6.995208	-5.182328	-3.019851
N	3.750375	3.668212	-0.291728	C	-1.618269	3.291050	2.429227
C	3.731039	5.077496	-0.306744	S	-2.620852	1.854474	2.367264
C	2.509542	5.503884	-0.818294	C	-1.187790	0.876461	2.718095
H	3.212048	1.147771	-0.586211	C	-0.059164	1.758327	2.869508
C	0.370422	4.286379	-0.358069	N	-0.310928	3.037574	2.713011
C	1.374331	4.286122	-2.698174	C	-1.229428	-0.493962	2.755568
C	2.229565	6.854645	-0.908305	C	-2.374536	-1.277356	2.512310
C	3.198107	7.771154	-0.492928	C	1.367481	1.340253	3.219849
C	4.422424	7.328270	0.000721	C	1.885648	0.216214	2.294422
C	4.711919	5.966550	0.102922	C	-2.106554	4.559721	2.190598
H	5.670051	5.634624	0.488413	C	-3.476482	4.747937	1.858016
H	5.167282	8.051121	0.318130	N	-4.599776	4.851869	1.578855
H	2.992130	8.834694	-0.549861	C	2.298201	2.554507	3.072310
H	1.270586	7.200243	-1.283098	C	1.390187	0.869221	4.688085
H	0.790047	5.172420	-2.964248	C	-1.245324	5.692735	2.238394
H	2.301511	4.299037	-3.278696	N	-0.549879	6.622877	2.246688
H	0.800168	3.400943	-2.987892	H	-0.295161	-0.996623	2.959655
H	-0.189295	5.208291	-0.540378	H	2.980589	0.234414	2.273429
H	-0.276586	3.443449	-0.619486	H	1.604363	-0.783307	2.637850
H	0.589328	4.233554	0.710910	H	1.527716	0.338715	1.269251
C	4.817905	2.848977	0.261128	H	3.312905	2.266078	3.369685
C	5.610624	2.060694	-0.797984	H	2.322894	2.902592	2.034816
C	6.037329	0.684593	-0.279958	H	1.974028	3.393020	3.691361
C	6.536974	-0.253051	-1.377348	H	2.407746	0.569375	4.961779
C	6.926377	-1.631847	-0.843900	H	1.077336	1.674335	5.360605
C	7.254722	-2.636052	-1.947480	H	0.727169	0.013426	4.851765
C	7.742627	-3.978065	-1.404230	C	-2.388308	-2.649356	2.363041
C	7.947400	-5.027671	-2.495900	C	-1.210303	-3.628343	2.421565
C	8.447148	-6.362473	-1.946537	N	-3.520119	-3.341140	2.076251
H	8.579550	-7.101271	-2.744168	C	-3.248368	-4.709500	1.871370

C -1.894557 -4.938002 2.088318
H -3.308615 -0.745560 2.362041
C -0.572023 -3.680503 3.820781
C -0.173650 -3.316429 1.327922
C -1.371097 -6.207666 1.930384
C -2.228224 -7.245956 1.559295
C -3.582218 -7.001129 1.347429
C -4.118881 -5.720986 1.497083
H -5.171825 -5.539025 1.309706
H -4.234792 -7.815009 1.047869
H -1.831716 -8.245444 1.417372
H -0.310455 -6.395063 2.069842
H 0.605376 -4.084652 1.335744
H -0.640237 -3.324755 0.339509
H 0.306793 -2.344188 1.470086
H 0.175740 -4.479109 3.847868
H -0.070258 -2.742912 4.077639
H -1.323661 -3.888983 4.587648
C -4.812441 -2.734679 1.800602
C -4.890842 -2.188759 0.374319
C -6.193357 -1.445128 0.090095
C -6.208562 -0.824172 -1.306694
C -7.495738 -0.064179 -1.621647
C -7.484489 0.577873 -3.008694
C -8.767155 1.344163 -3.329869
C -8.753307 1.991115 -4.715132
C -10.039036 2.754772 -5.026922
H -10.003606 3.208476 -6.022730
H -10.909414 2.089313 -4.992256
H -10.205381 3.556730 -4.298587
H -4.989850 -1.943824 2.536373
H -5.581484 -3.491814 1.974815
H -4.044946 -1.511238 0.210143
H -4.763297 -3.019021 -0.331799
H -7.046941 -2.128503 0.199484
H -6.332828 -0.651882 0.837961
H -5.353938 -0.138778 -1.400805
H -6.053971 -1.612077 -2.057513
H -8.352169 -0.748639 -1.542967
H -7.652327 0.714519 -0.862385
H -7.325043 -0.200345 -3.768801
H -6.626175 1.260759 -3.083738
H -9.626600 0.662407 -3.256486
H -8.926364 2.120830 -2.568592
H -8.592910 1.214652 -5.475218
H -7.894977 2.672479 -4.786203

2xMB:PC₆₁BM (PC₆₁BM on the side) cluster

C -4.389469 -3.428727 2.798151
C -5.327061 -2.552211 2.266288
C -6.673006 -2.895128 2.152871
C -7.106569 -4.145107 2.553784
C -6.179068 -5.047101 3.086869
C -4.840038 -4.684591 3.210126
C -7.445032 -1.713593 1.598494
C -6.318860 -0.692598 1.375481
N -5.133310 -1.254301 1.789102
C -6.393830 0.586213 0.905684
C -7.567797 1.338855 0.623973
C -7.550721 2.668514 0.324300
S -6.033371 3.561074 0.152000
C -6.955221 5.025391 -0.124361
N -8.306770 4.852119 -0.044797
C -8.650704 3.613437 0.172203
C -6.362989 6.235535 -0.392228
C -7.143316 7.411488 -0.590868
N -7.752458 8.387338 -0.742314
C -10.130483 3.276640 0.304975
C -10.542282 2.215732 -0.732716
C -8.158910 -2.086349 0.289344
C -8.454262 -1.225827 2.656781
C -3.818718 -0.639041 1.767954
C -3.330843 0.013324 3.076061
C -10.414272 2.782373 1.738688
C -10.965913 4.540597 0.052199
C -4.943857 6.319142 -0.472295
N -3.782759 6.322465 -0.522876
H -8.530911 0.850203 0.686605
H -11.488436 2.602036 1.854028
H -9.890209 1.853516 1.980592
H -10.114641 3.535616 2.475105
H -12.028726 4.291057 0.145758
H -10.725898 5.330596 0.768032
H -10.784286 4.937810 -0.949613
H -11.621399 2.042308 -0.662258
H -10.322274 2.564926 -1.746079
H -10.048027 1.251248 -0.595842
H -5.460030 1.132992 0.840336
H -3.347480 -3.150298 2.913372
H -4.127244 -5.387956 3.630069
H -6.506749 -6.028977 3.413150
H -8.153675 -4.422417 2.465745
H -9.164139 -2.028970 2.879549
H -7.948677 -0.950624 3.586713

H	-9.025662	-0.362294	2.306973	C	1.119075	0.377152	0.924437
H	-8.917231	-2.850670	0.489945	C	1.873297	-0.559113	1.729945
H	-8.656977	-1.228846	-0.170837	C	2.608466	-0.106986	2.814747
H	-7.452016	-2.487520	-0.441753	C	3.934939	-0.636200	3.063433
H	-3.789509	0.085756	0.951926	C	4.480755	-1.587056	2.208632
H	-3.124197	-1.432071	1.479829	C	3.710324	-2.056817	1.075442
C	-1.820026	0.273083	2.927573	C	2.439290	-1.557301	0.842428
C	-1.097936	0.565762	4.240828	C	2.020252	-1.244205	-0.509889
H	-0.026247	0.704260	4.068624	C	2.885737	-1.455802	-1.570789
H	-1.470506	1.473619	4.725171	C	4.211836	-1.986918	-1.326860
H	-1.219651	-0.264531	4.945912	C	4.621127	-2.275366	-0.029698
H	-1.342114	-0.600451	2.465288	C	5.122761	-1.330778	-2.226501
H	-1.667261	1.106044	2.227477	C	6.394912	-0.998411	-1.782017
C	-4.084640	1.309477	3.423804	C	6.977520	0.277563	-2.139116
C	-5.435029	1.124477	4.121644	C	7.784927	0.733052	-1.038459
C	-6.277316	2.400147	4.112651	C	7.786222	2.071499	-0.712361
C	-7.673658	2.196388	4.694362	C	7.695870	2.504648	0.695149
H	-8.244332	3.130577	4.696279	C	7.610065	1.579474	1.711954
H	-8.236287	1.465275	4.101555	C	6.667475	1.789972	2.778048
H	-7.628501	1.827168	5.725752	C	5.897503	2.943070	2.838062
H	-3.453895	1.933411	4.067889	C	4.508681	2.867802	3.249493
H	-4.219493	1.894626	2.503177	C	3.757562	3.808083	2.443439
H	-5.264960	0.793619	5.155796	C	2.480456	3.483831	2.012135
H	-6.005073	0.325880	3.638826	C	2.073309	3.798861	0.658603
H	-5.752592	3.190873	4.664799	C	2.960088	4.422614	-0.205579
H	-6.368558	2.757222	3.078982	C	4.293876	4.759169	0.244284
H	-3.475596	-0.712661	3.890813	C	4.685264	4.460302	1.539446
C	13.159274	0.100958	-1.805789	C	6.007586	3.923120	1.790114
C	12.333317	0.569846	-0.629116	C	6.880364	3.695481	0.733177
C	11.091953	-0.287232	-0.415248	C	6.468487	4.011234	-0.619013
C	10.261598	0.202674	0.769579	C	5.208117	4.534017	-0.858991
C	8.978210	-0.601141	0.954517	C	4.434874	4.070347	-1.994927
C	7.766837	0.113743	1.500693	C	3.047202	3.997193	-1.589723
C	7.860496	-0.357051	-0.025338	C	2.243816	2.965440	-2.050346
C	6.832599	-1.343018	-0.457068	C	2.791856	1.960578	-2.938243
C	5.956806	-1.953020	0.411859	C	2.211338	0.680883	-2.580200
C	5.869462	-1.520611	1.818767	C	2.982917	-0.470563	-2.630464
C	6.663119	-0.499605	2.291027	C	4.370280	-0.393105	-3.038142
C	6.086485	0.512827	3.133868	C	4.925535	0.829398	-3.376432
C	4.760318	0.442463	3.537810	C	4.120786	2.032630	-3.327989
C	3.953538	1.646709	3.591836	C	4.961358	3.111353	-2.845271
C	2.619886	1.305592	3.142401	C	6.284271	2.572855	-2.598840
C	1.899159	2.203796	2.368671	C	6.260469	1.170962	-2.922537
C	1.131756	1.729180	1.236017	C	7.021971	3.006982	-1.504208
C	1.241402	2.714644	0.178782	C	9.204165	-2.014437	1.419727
C	1.325851	2.308072	-1.142996	C	9.350309	-3.057788	0.505656
C	1.308593	0.896578	-1.468830	C	9.624018	-4.348357	0.948097
C	1.206312	-0.048692	-0.459864	C	9.751795	-4.606799	2.309545

C	-4.851484	-2.470829	1.300978	H	-6.117209	0.341094	2.844241
C	-4.941604	-2.123181	2.646784	H	-3.644530	-0.592672	-1.187076
C	-5.545740	-2.984831	3.544054	H	-4.733466	-1.941620	-1.319360
C	-6.042293	-4.208426	3.081685	C	-2.167294	-2.140006	-2.543570
C	-5.928014	-4.548944	1.735890	C	-1.251614	-3.171964	-3.197163
C	-4.251320	-0.790477	2.866500	H	-0.966997	-2.852845	-4.204507
C	-3.807187	-0.438788	1.439194	H	-0.326957	-3.314420	-2.628811
N	-4.179162	-1.465570	0.603483	H	-1.750703	-4.144595	-3.278575
C	-3.135003	0.667008	0.997663	H	-3.042832	-1.984662	-3.190891
C	-2.656861	1.760922	1.770584	H	-1.651283	-1.170668	-2.487114
C	-2.038282	2.849775	1.228349	C	-1.508648	-2.463019	-0.098136
S	-1.875728	3.042841	-0.520037	C	-1.625049	-3.486706	1.033861
C	-0.960770	4.507206	-0.250622	C	-0.472864	-3.432521	2.036754
N	-0.797643	4.825795	1.064894	C	-0.688412	-4.374436	3.219171
C	-1.368730	3.972349	1.870158	H	0.144526	-4.323176	3.927583
C	-0.398892	5.233940	-1.273759	H	-1.608563	-4.121004	3.760169
C	0.427102	6.362542	-1.003578	H	-0.780614	-5.413502	2.882522
N	1.132924	7.262879	-0.808842	H	-0.558588	-2.637126	-0.613063
C	-1.257978	4.198513	3.371120	H	-1.434326	-1.450697	0.318843
C	-2.663858	4.329346	3.987499	H	-1.676413	-4.495564	0.599231
C	-5.224030	0.237464	3.464720	H	-2.566816	-3.353038	1.577134
C	-3.023464	-0.987941	3.778699	H	0.469637	-3.678252	1.532023
C	-3.837826	-1.593201	-0.798532	H	-0.354389	-2.403549	2.402314
C	-2.647156	-2.518582	-1.131660	H	-3.019076	-3.553589	-1.169295
C	-0.471486	3.042128	4.019847	C	12.035344	-3.732934	-1.858475
C	-0.492305	5.503509	3.635120	C	11.592693	-2.501574	-1.101446
C	-0.552671	4.789952	-2.616452	C	10.279558	-2.715286	-0.358966
N	-0.696124	4.361597	-3.687507	C	9.844618	-1.459325	0.393814
H	-2.764804	1.731727	2.846792	C	8.497766	-1.631712	1.088740
H	-0.401368	3.213842	5.099412	C	7.606640	-0.420835	1.216208
H	-0.932420	2.062911	3.862903	C	7.265018	-1.626296	0.223137
H	0.546120	2.998322	3.619422	C	5.989411	-2.342619	0.497583
H	-0.417795	5.661589	4.716823	C	5.220976	-2.116823	1.617219
H	0.516320	5.464690	3.215431	C	5.535353	-1.006294	2.534879
H	-1.003636	6.359443	3.187664	C	6.603951	-0.173436	2.290064
H	-2.571721	4.565180	5.053031	C	6.445971	1.246931	2.449381
H	-3.217798	5.143215	3.509105	C	5.254883	1.789855	2.911884
H	-3.266156	3.421524	3.902940	C	4.741996	3.016926	2.332792
H	-2.903698	0.711723	-0.061117	C	3.300721	2.897421	2.250100
H	-5.239801	-3.956780	-0.225154	C	2.627628	3.416202	1.154190
H	-6.310919	-5.502931	1.385403	C	1.556761	2.658408	0.543296
H	-6.508184	-4.899003	3.777256	C	1.629301	2.855174	-0.889555
H	-5.620428	-2.724780	4.596560	C	1.321674	1.819456	-1.753874
H	-3.346953	-1.371836	4.751571	C	0.941486	0.525820	-1.221839
H	-2.322268	-1.704686	3.342682	C	0.883313	0.332102	0.151193
H	-2.490616	-0.048273	3.947598	C	1.191588	1.424125	1.054930
H	-5.534924	-0.091511	4.461869	C	1.900067	0.879750	2.194041
H	-4.775022	1.228570	3.563043	C	2.931202	1.597705	2.779103

C	4.143768	0.918749	3.190080	H	11.511570	-1.676081	-1.819853
C	4.282522	-0.450180	2.989390	H	12.398704	-2.219402	-0.412656
C	3.202031	-1.196844	2.378008	H	9.502230	-3.001055	-1.077283
C	2.039693	-0.548585	1.991807	H	10.385258	-3.556957	0.332925
C	1.410575	-0.882340	0.729997	H	9.803693	-0.614542	-0.301358
C	1.960986	-1.860635	-0.081387	H	10.586166	-1.197094	1.158951
C	3.167853	-2.547619	0.328160	H	7.963010	-4.308969	1.107082
C	3.783821	-2.217399	1.530138	H	8.138511	-5.871417	3.015625
C	3.971489	-2.763923	-0.845195	H	8.796194	-5.028835	5.256297
C	5.350784	-2.636716	-0.756078	H	9.286367	-2.615112	5.569955
C	6.086830	-1.974565	-1.812042	H	9.110449	-1.057689	3.654520
C	7.192012	-1.267085	-1.221400	H	14.639124	-4.276537	-3.680249
C	7.535876	-0.025960	-1.710613	H	12.995986	-4.908298	-4.022056
C	7.848391	1.086817	-0.793345	H	13.880193	-5.480614	-2.589241
C	7.802550	0.907398	0.571534	O	13.201447	-3.516310	-2.489403
C	7.180891	1.910868	1.393826	O	11.436990	-4.781325	-1.906282
C	6.692675	3.087937	0.843772	C	-9.594841	-5.168183	-0.478323
C	5.443890	3.650390	1.321030	C	-8.901754	-4.095022	-1.020235
C	4.741322	4.198057	0.178544	C	-8.557026	-4.044832	-2.367987
C	3.362985	4.081873	0.096149	C	-8.893809	-5.087034	-3.210966
C	2.743459	3.735611	-1.165799	C	-9.584859	-6.183444	-2.686633
C	3.521538	3.526897	-2.292511	C	-9.929158	-6.216596	-1.337999
C	4.961450	3.643974	-2.204657	C	-7.830514	-2.745358	-2.649298
C	5.559089	3.972160	-0.998028	C	-7.802100	-2.107485	-1.252711
C	6.765700	3.287680	-0.579800	N	-8.441530	-2.938095	-0.375993
C	7.320682	2.296173	-1.379907	C	-7.297090	-0.891983	-0.878426
C	6.693833	1.957333	-2.640722	C	-6.638945	0.055878	-1.700468
C	5.544155	2.616207	-3.045457	C	-6.252826	1.289956	-1.262480
C	4.461019	1.873359	-3.662331	S	-6.614840	1.831774	0.380691
C	3.211660	2.433266	-3.194199	C	-5.640431	3.258110	0.091753
C	2.133719	1.601035	-2.933028	N	-5.185564	3.366939	-1.189339
C	2.257318	0.171794	-3.131767	C	-5.488511	2.331429	-1.927283
C	1.520034	-0.493577	-2.073618	C	-5.341545	4.162414	1.083266
C	2.015686	-1.664239	-1.515566	C	-4.512557	5.293070	0.833879
C	3.265048	-2.222272	-1.990789	N	-3.823329	6.214136	0.678289
C	3.968109	-1.585502	-2.999264	C	-5.005313	2.291802	-3.372379
C	3.454655	-0.363757	-3.584477	C	-3.983288	1.148362	-3.541385
C	4.581935	0.506499	-3.856694	C	-6.422507	-3.026971	-3.202678
C	5.789317	-0.179490	-3.440290	C	-8.646399	-1.886161	-3.633882
C	5.411184	-1.463230	-2.911617	C	-8.614012	-2.737906	1.054575
C	6.822702	0.527932	-2.837967	C	-9.962418	-2.154741	1.513963
C	8.530958	-2.582164	2.254905	C	-6.198017	2.104744	-4.331491
C	8.257311	-3.939312	2.085362	C	-4.309915	3.615610	-3.723044
C	8.354633	-4.817323	3.160549	C	-5.794105	3.924445	2.410551
C	8.724695	-4.344736	4.416067	N	-6.166213	3.672233	3.482636
C	9.000228	-2.991106	4.592311	H	-6.406950	-0.205247	-2.724489
C	8.903938	-2.115986	3.516188	H	-5.839724	2.160331	-5.364612
C	13.703524	-4.620758	-3.240315	H	-6.708803	1.145491	-4.209659

H	-6.937807	2.898914	-4.187870	N	2.950740	-2.190366	-0.718201
H	-3.962275	3.576897	-4.760423	C	2.903035	1.410191	-0.129226
H	-4.992035	4.462888	-3.612547	C	2.522704	2.550406	-0.857794
H	-3.444933	3.800265	-3.084109	C	3.795160	-1.288154	1.389505
H	-3.583302	1.165182	-4.560320	C	2.780705	-0.847528	2.461823
H	-3.139493	1.278622	-2.854652	C	2.074582	-2.867537	-2.857974
H	-4.417752	0.158821	-3.367399	C	1.531011	-2.489113	-4.115139
H	-7.428980	-0.610544	0.159141	N	1.095198	-2.131014	-5.131687
H	-9.879730	-5.196890	0.568065	C	4.126470	-2.769733	1.624501
H	-10.471845	-7.069841	-0.943162	C	5.096945	-0.474432	1.508087
H	-9.857858	-7.009748	-3.334629	C	2.192422	-4.249078	-2.534768
H	-8.628767	-5.058079	-4.264606	N	2.290395	-5.379623	-2.290014
H	-8.727132	-2.404946	-4.594549	H	3.167650	1.519912	0.913659
H	-9.657496	-1.714240	-3.254533	H	3.236266	-0.947258	3.452903
H	-8.177054	-0.913716	-3.808381	H	2.454810	0.190055	2.346735
H	-6.504357	-3.578192	-4.144830	H	1.891137	-1.482872	2.433451
H	-5.866229	-2.106914	-3.404694	H	4.554900	-2.888403	2.625951
H	-5.840115	-3.638941	-2.507308	H	3.235301	-3.396221	1.543472
H	-7.785328	-2.127023	1.425716	H	4.851452	-3.135906	0.891654
H	-8.473660	-3.719464	1.514752	H	5.581738	-0.692995	2.465878
C	-10.031214	-2.316047	3.044476	H	5.791558	-0.739990	0.704772
C	-11.432646	-2.147427	3.629117	H	4.941708	0.606243	1.462162
H	-11.420095	-2.298213	4.712977	C	2.317475	3.815735	-0.348659
H	-11.841361	-1.149375	3.443142	C	2.450079	4.305136	1.093862
H	-12.125857	-2.877841	3.196520	N	1.937440	4.851039	-1.138703
H	-9.657617	-3.311356	3.320415	C	1.760111	6.029168	-0.387017
H	-9.343161	-1.595123	3.507800	C	2.069657	5.763935	0.943292
C	-10.168619	-0.688191	1.096267	H	2.324273	2.402747	-1.913176
C	-10.665108	-0.472199	-0.336023	C	3.899543	4.175736	1.595205
C	-10.535220	0.981849	-0.787502	C	1.455419	3.593577	2.029046
C	-10.993344	1.201510	-2.227024	C	1.996090	6.772648	1.885528
H	-10.907103	2.253562	-2.516413	C	1.596640	8.047223	1.476757
H	-10.383416	0.613902	-2.923542	C	1.275665	8.292178	0.144141
H	-12.038496	0.900110	-2.362608	C	1.351327	7.281777	-0.816062
H	-10.888960	-0.216527	1.774849	H	1.093758	7.483330	-1.850430
H	-9.228973	-0.140278	1.254389	H	0.962449	9.286110	-0.159436
H	-11.714197	-0.792287	-0.403367	H	1.538643	8.851769	2.202244
H	-10.111389	-1.107404	-1.033886	H	2.251088	6.582477	2.924090
H	-11.109422	1.628227	-0.110770	H	1.537714	4.015644	3.035497
H	-9.486202	1.291666	-0.689771	H	0.427585	3.730753	1.683355
H	-10.763641	-2.764630	1.069152	H	1.651245	2.519408	2.094380
				H	4.002540	4.688431	2.556025
				H	4.190619	3.130509	1.738551
				H	4.602220	4.632911	0.894263
				C	1.793949	4.749289	-2.582976
				C	0.540996	3.979474	-3.025856
				C	0.732045	3.303633	-4.387447
				C	-0.347766	2.264396	-4.679727
2xML:PC ₆₁ BM t (PC ₆₁ BM on top) cluster							
C	2.467306	-1.899523	-1.955914				
S	2.392220	-0.186952	-2.307101				
C	2.928140	0.140682	-0.651787				
C	3.209007	-1.116089	-0.007727				

C	-0.156946	1.501533	-5.988659	C	-3.421917	2.578094	2.087950
C	-1.136247	0.334950	-6.108986	C	-4.345833	2.855742	1.087009
C	-0.974669	-0.482122	-7.387153	C	-3.918490	2.879206	-0.297257
C	-1.877402	-1.715205	-7.408520	C	-2.596886	2.621238	-0.623576
C	-1.724648	-2.542831	-8.682853	C	-2.284304	1.793818	-1.771230
H	-2.377480	-3.422200	-8.671417	C	-3.303070	1.274590	-2.553860
H	-1.975112	-1.950464	-9.571148	C	-4.684241	1.555045	-2.218135
H	-0.692354	-2.893154	-8.796116	C	-4.988793	2.335176	-1.108173
H	2.694102	4.251151	-2.962526	C	-5.453086	0.367467	-2.480633
H	1.810646	5.760776	-2.993590	C	-6.486413	0.022710	-1.620520
H	0.317728	3.209572	-2.279318	C	-6.679027	-1.359580	-1.236898
H	-0.327212	4.648187	-3.039678	C	-7.149378	-1.393127	0.122724
H	0.771261	4.056637	-5.186421	C	-6.687359	-2.374332	0.972092
H	1.708524	2.795014	-4.397639	C	-6.280291	-2.046007	2.351796
H	-0.343173	1.536321	-3.860158	C	-6.357046	-0.752782	2.819932
H	-1.338976	2.738230	-4.663958	C	-5.264208	-0.214616	3.585298
H	-0.266822	2.182510	-6.844646	C	-4.169818	-0.998450	3.922933
H	0.867250	1.104922	-6.031344	C	-2.833651	-0.435109	3.882188
H	-2.168213	0.709455	-6.033382	C	-1.938521	-1.458770	3.383171
H	-0.985088	-0.332891	-5.251475	C	-0.898164	-1.112654	2.534496
H	-1.184636	0.147946	-8.264264	C	-0.594281	-1.943072	1.386919
H	0.070182	-0.807876	-7.469813	C	-1.343640	-3.082510	1.135745
H	-2.925112	-1.404004	-7.293076	C	-2.432691	-3.439779	2.019289
H	-1.637143	-2.336735	-6.536514	C	-2.724052	-2.648573	3.119342
C	-12.508683	-2.388904	0.615801	C	-4.103035	-2.358571	3.457589
C	-11.422431	-2.045242	1.609709	C	-5.133978	-2.862580	2.674132
C	-10.498584	-0.944457	1.103584	C	-4.825718	-3.691440	1.526904
C	-9.406069	-0.611911	2.118054	C	-3.508202	-3.977779	1.207860
C	-8.428630	0.438441	1.600109	C	-3.076268	-3.963349	-0.176609
C	-6.993045	0.356970	2.057468	C	-1.740953	-3.406270	-0.221562
C	-7.429768	0.003449	0.559961	C	-1.372554	-2.575199	-1.267837
C	-6.831213	0.857280	-0.502228	C	-2.320513	-2.266749	-2.319615
C	-6.084779	1.982736	-0.237426	C	-2.131840	-0.880459	-2.700709
C	-5.681272	2.309638	1.142403	C	-3.224346	-0.092302	-3.029914
C	-6.044743	1.497910	2.193389	C	-4.557514	-0.655828	-2.985986
C	-5.073265	1.167853	3.200875	C	-4.739427	-1.978066	-2.617054
C	-3.795560	1.709865	3.172392	C	-3.597954	-2.803369	-2.277828
C	-2.650657	0.887709	3.516065	C	-3.985010	-3.669947	-1.180857
C	-1.562748	1.252670	2.631858	C	-5.365103	-3.379928	-0.846375
C	-0.705337	0.272921	2.150452	C	-5.826343	-2.339061	-1.726710
C	-0.284446	0.296840	0.765741	C	-5.778757	-3.383790	0.480306
C	-0.214293	-1.071979	0.293993	C	-9.025763	1.813187	1.465436
C	-0.599687	-1.380431	-0.999954	C	-9.609623	2.229903	0.269289
C	-1.071924	-0.334858	-1.882627	C	-10.215043	3.479544	0.179035
C	-1.143658	0.973084	-1.431174	C	-10.239778	4.324318	1.284634
C	-0.738424	1.299373	-0.078400	C	-9.659719	3.914120	2.482368
C	-1.636868	2.317928	0.421025	C	-9.056750	2.664404	2.570735
C	-2.041487	2.296848	1.747103	C	-14.361373	-3.764023	0.219830

S	-6.886963	-0.324576	-1.628571	C	-7.117844	-4.920938	-1.415385
C	-5.147945	-0.236561	-1.299040	C	-8.447892	-4.163568	-1.394200
C	-4.720729	1.125220	-1.480162	C	-8.968331	-3.809125	-2.785831
N	-5.663432	1.981888	-1.804851	C	-10.258812	-2.990655	-2.744490
C	-4.437021	-1.341130	-0.893141	C	-10.724387	-2.529211	-4.124741
C	-5.021199	-2.594074	-0.638624	C	-12.037525	-1.748993	-4.079822
C	-3.296545	1.640849	-1.312208	C	-12.479952	-1.236907	-5.450437
C	-2.358299	0.928313	-2.304574	C	-13.790806	-0.454548	-5.393330
C	-8.043095	2.118871	-2.170054	H	-14.086364	-0.092128	-6.383740
C	-9.294088	1.448140	-2.239681	H	-14.604976	-1.079831	-5.008065
N	-10.294302	0.857181	-2.275582	H	-13.696640	0.413245	-4.730875
C	-3.257246	3.147252	-1.612284	H	-6.854925	-4.187602	0.616408
C	-2.827359	1.430535	0.140470	H	-6.749274	-5.930140	0.493921
C	-8.008020	3.536601	-2.294545	H	-6.426258	-4.406177	-2.091750
N	-8.003903	4.696342	-2.357228	H	-7.253076	-5.927547	-1.826418
H	-3.371812	-1.219317	-0.745442	H	-9.203047	-4.743465	-0.845963
H	-1.370008	1.394710	-2.263027	H	-8.317898	-3.227932	-0.828755
H	-2.227851	-0.135117	-2.086209	H	-8.194871	-3.234471	-3.315348
H	-2.731992	1.020610	-3.329545	H	-9.127509	-4.726112	-3.370333
H	-2.231449	3.511078	-1.485307	H	-11.052024	-3.584743	-2.268179
H	-3.581717	3.361495	-2.633633	H	-10.110638	-2.105815	-2.110233
H	-3.910409	3.707034	-0.937415	H	-10.832724	-3.399571	-4.788766
H	-1.837893	1.880734	0.273300	H	-9.944542	-1.894856	-4.569155
H	-3.520063	1.910583	0.838794	H	-12.827081	-2.389377	-3.659394
H	-2.744081	0.378035	0.425501	H	-11.922166	-0.898860	-3.395914
C	-4.362192	-3.752337	-0.279426	H	-12.585204	-2.083793	-6.142769
C	-2.865559	-3.986354	-0.086846	H	-11.690314	-0.595975	-5.864629
N	-5.029812	-4.905131	-0.024889	C	11.961201	2.920606	-1.671303
C	-4.140477	-5.952295	0.293209	C	10.997713	2.710844	-0.525266
C	-2.841370	-5.456263	0.273818	C	10.372410	1.321521	-0.538419
H	-6.099740	-2.647255	-0.731243	C	9.390998	1.132518	0.616776
C	-2.333177	-3.156463	1.094768	C	8.693842	-0.223734	0.576181
C	-2.075214	-3.734800	-1.382444	C	7.277183	-0.306707	1.088885
C	-1.775865	-6.281815	0.580060	C	7.626437	-0.422838	-0.467936
C	-2.032485	-7.618973	0.890881	C	7.251165	-1.709489	-1.115514
C	-3.337576	-8.105317	0.890588	C	6.788033	-2.801164	-0.417027
C	-4.420345	-7.276625	0.590308	C	6.467198	-2.696583	1.018024
H	-5.431818	-7.668938	0.591888	C	6.623488	-1.504097	1.687838
H	-3.522494	-9.147311	1.131947	C	5.596742	-1.060036	2.591315
H	-1.210175	-8.281283	1.139902	C	4.481649	-1.844143	2.851732
H	-0.760076	-5.895988	0.590128	C	3.175454	-1.229356	2.977541
H	-1.039015	-4.056657	-1.246322	C	2.209095	-2.116325	2.365814
H	-2.501196	-4.300102	-2.216669	C	1.145521	-1.590056	1.648270
H	-2.063515	-2.675453	-1.653023	C	0.757879	-2.197448	0.393471
H	-1.323947	-3.488116	1.347620	C	0.360393	-1.143010	-0.516775
H	-2.289034	-2.088103	0.858729	C	0.663842	-1.243234	-1.866410
H	-2.955209	-3.287417	1.982989	C	1.369690	-2.405587	-2.368737
C	-6.481180	-5.003050	-0.015373	C	1.751339	-3.413273	-1.494985

C	1.434639	-3.309988	-0.083029	C	10.703070	-2.794055	2.507855
C	2.542551	-3.859350	0.668113	C	9.822120	-1.761808	2.205335
C	2.922697	-3.275141	1.865413	C	13.431589	4.445423	-2.667797
C	4.328715	-3.102906	2.171817	H	10.228747	3.491438	-0.585737
C	5.297467	-3.507816	1.261372	H	11.538373	2.896252	0.411133
C	4.894598	-4.117933	0.010408	H	9.852408	1.170658	-1.491686
C	3.551159	-4.294231	-0.279236	H	11.162840	0.565555	-0.495018
C	3.056915	-4.026382	-1.616456	H	8.649577	1.937854	0.598512
C	3.929980	-3.604277	-2.606244	H	9.913155	1.212394	1.578453
C	5.337031	-3.431966	-2.305177	H	10.104487	-1.772195	-1.174255
C	5.810294	-3.674883	-1.020797	H	11.676838	-3.604568	-0.641721
C	5.805465	-2.277079	-3.023549	H	12.057966	-4.269471	1.719421
C	6.724222	-1.427776	-2.422692	H	10.863047	-3.081221	3.542672
C	6.584702	0.006393	-2.561021	H	9.292552	-1.246653	3.002817
C	7.027345	0.626113	-1.339734	H	13.771488	5.463197	-2.478242
C	6.343421	1.717138	-0.850003	H	12.941831	4.380542	-3.642614
C	6.019115	1.822582	0.585848	H	14.274724	3.750355	-2.648364
C	6.393522	0.831172	1.465647	O	12.509054	4.145925	-1.621024
C	5.454235	0.373643	2.454634	O	12.217337	2.110616	-2.530144
C	4.203500	0.961496	2.583832	C	-2.388832	-1.088612	4.030778
C	3.038813	0.140704	2.847111	S	-2.466674	0.655695	3.882828
C	1.929090	0.693157	2.099567	C	-4.190098	0.515307	3.509114
C	1.000340	-0.153072	1.512320	C	-4.550429	-0.877749	3.529429
C	0.519118	0.121548	0.173899	N	-3.571379	-1.715170	3.789308
C	0.980459	1.232582	-0.517675	C	-4.961645	1.606876	3.198644
C	1.949816	2.113934	0.096652	C	-4.486544	2.926344	3.081309
C	2.413964	1.852520	1.376460	C	-5.955569	-1.444745	3.337097
C	3.821552	2.016734	1.682859	C	-6.653270	-0.876590	2.080771
C	4.709919	2.421913	0.694211	C	-1.227146	-1.757441	4.365016
C	4.220874	2.689556	-0.641331	C	-0.078999	-1.022010	4.763996
C	2.876090	2.540755	-0.932711	N	0.822095	-0.375215	5.111871
C	2.467484	1.942500	-2.186703	C	-5.871196	-2.972732	3.194903
C	1.302211	1.125823	-1.928728	C	-6.779439	-1.106004	4.596663
C	1.142040	-0.082505	-2.590465	C	-1.162905	-3.178715	4.338453
C	2.141364	-0.525874	-3.540100	N	-1.080487	-4.335931	4.281266
C	2.282431	-1.962497	-3.402828	H	-6.004713	1.413527	2.994835
C	3.533464	-2.549763	-3.519843	H	-7.393702	-1.594612	1.713267
C	4.696509	-1.726551	-3.779263	H	-7.201215	0.048759	2.281980
C	4.561965	-0.354860	-3.911838	H	-5.943560	-0.686207	1.272186
C	3.256795	0.260360	-3.789751	H	-6.885938	-3.381454	3.127763
C	3.423959	1.523552	-3.097651	H	-5.325264	-3.247849	2.287206
C	4.831859	1.688459	-2.796240	H	-5.359417	-3.432978	4.041931
C	5.529572	0.532228	-3.293403	H	-7.794713	-1.503287	4.488735
C	5.224578	2.253637	-1.588670	H	-6.328941	-1.551655	5.489320
C	9.600062	-1.386081	0.879957	H	-6.851207	-0.024868	4.755405
C	10.274868	-2.057081	-0.139741	C	-5.223284	4.005040	2.635708
C	11.158315	-3.089227	0.160930	C	-6.694345	4.044599	2.205680
C	11.372672	-3.460583	1.484847	N	-4.687422	5.242094	2.483599

C	-5.623790	6.142948	1.935093
C	-6.839043	5.488544	1.772246
H	-3.434684	3.089704	3.293000
C	-7.640081	3.722001	3.376073
C	-6.953128	3.133455	0.992748
C	-7.919666	6.157253	1.228055
C	-7.764576	7.495358	0.859321
C	-6.541355	8.137587	1.031205
C	-5.441793	7.468091	1.571381
H	-4.487870	7.972900	1.681393
H	-6.431718	9.174366	0.729387
H	-8.598388	8.031203	0.418798
H	-8.866242	5.649972	1.067031
H	-7.986874	3.262773	0.658734
H	-6.299548	3.397790	0.157720
H	-6.801880	2.074919	1.220941
H	-8.675568	3.880921	3.059559
H	-7.543880	2.682443	3.703193
H	-7.440074	4.371475	4.233273
C	-3.277584	5.568367	2.631222
C	-2.487271	5.227588	1.367317
C	-1.007218	5.589989	1.466865
C	-0.268649	5.366395	0.146888
C	1.206394	5.762648	0.195465
C	1.873413	5.720278	-1.178655
C	3.378340	5.979495	-1.132352
C	4.076754	5.710663	-2.465436
C	5.594176	5.856528	-2.379444
H	6.071167	5.656351	-3.344391
H	5.877429	6.868032	-2.065905
H	6.010323	5.152514	-1.648835
H	-2.882126	5.044431	3.506224
H	-3.206882	6.635847	2.858081
H	-2.595007	4.157080	1.157260
H	-2.943799	5.757011	0.520944
H	-0.905922	6.644834	1.759730
H	-0.531035	4.999980	2.262024
H	-0.345378	4.307411	-0.140773
H	-0.773939	5.937162	-0.645158
H	1.304668	6.772252	0.618975
H	1.738965	5.087021	0.879848
H	1.392418	6.451112	-1.843738
H	1.692213	4.736528	-1.632424
H	3.567181	7.015589	-0.817738
H	3.829352	5.341272	-0.360116
H	3.679053	6.389648	-3.231317
H	3.829027	4.694335	-2.801122