Supporting information for:

PCBM-CG: A place for tired LaTeXto rest

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Abstract

Abstract. EPSRC gave us some money so we did our best to do great science, and these are our conclusions.

Lambdas

Some mobs

Coarse Graining

C60 has 90 bonds between the 60 atoms. 30 of these are 6,6 coordinating (1.37 A long - along two hexagonal facets) and have more double-bond like character. The remaining 60 bonds are 5,6 coordinating (1.448 A long). PCBM is formed by 4+2 cycloaddition. These sidechains are believed (ref - that synth paper) to wholly coordinate with the 6,6 bonds.

The 8 unique bis isomers, and 45 tris isomers, have been identified and their point group derived in previous work (ref, Hirsch?). However we did not find a computationally readable list of structures which would be directly useful in constructing our coarse grained model.

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Table S1: Inner sphere reorganisation energies of Mono, Bis and Tris PC−60BM fullerenes. All units meV.

Isomer	λ_{neut}	λ_{ion}	λ_{tot}
mono	77.91	77.49	155.40
bis-C1	111.52	182.64	294.16
bis-C2	108.54	158.89	267.43
bis-C3	81.38	83.31	164.69
bis-E1	88.82	89.49	178.31
bis-T1	138.30	151.32	289.62
bis-T2	80.30	80.93	161.23
bis-T3	125.77	166.20	291.97
bis-T4	87.66	95.56	183.22
tris-E,E,E	108.42	105.41	213.84
tris-E,E,T1(1)	99.51	100.82	200.33
tris-E,E,T1(2)	94.62	98.86	193.49
tris-E,T3,T2	93.97	92.93	186.90
tris-E,T4,T2	98.54	106.46	205.00
tris-E,T4,T3	100.51	100.06	200.56
tris-T3,T3,T3	137.97	173.63	311.60
tris-T4,T3,T3	200.30	226.34	426.64
tris-T4,T4,T2	149.22	148.26	297.48
tris-T4,T4,T4	136.01	166.56	302.57

Table S2: Inner sphere reorganisation energies of Mono, Bis and Tris Methano fullerenes. All units meV.

Isomer	λ_{neut}	λ_{ion}	λ_{tot}
mono	68.80	68.83	137.63
bis-c1	70.42	70.57	140.99
bis-c2	70.45	73.48	143.93
bis-c3	78.69	72.39	151.08
bis-e1	69.79	74.79	144.58
bis-t1	69.37	69.01	138.38
bis-t2	78.85	79.53	158.38
bis-t3	75.42	72.98	148.40
bis-t4	70.03	68.63	138.66
tris-EEE	105.49	78.63	184.12
tris-EET1-1	76.11	76.12	152.22
tris-EET1-2	72.66	72.96	145.62
tris-ET3T2	73.33	75.39	148.72
tris-ET4T2	75.29	72.51	147.80
tris-ET4T3	76.80	73.70	150.50
tris-T3T3T3	82.08	75.01	157.09
tris-T4T3T3	77.78	78.22	155.99
tris-T4T4T2	74.82	74.58	149.40
tris-T4T4T4	0.00	0.00	0.00
c70-mono	92.31	87.75	180.07
c70-bis-4158	98.25	96.06	194.31
c70-bis-5657	87.27	89.48	176.75
c70-bis-6768	96.07	96.10	192.17

Table S3: Simulated mobility by Time of Flight (using the ToFET code), with varying energetic disorder. Units are cm^2/Vs

σ	$0. \times 10^{-3}$	56×10^{-3}	121×10^{-3}
M	4.40×10^{-3}	2.72×10^{-3}	0.837×10^{-3}
B	2.27×10^{-3}	1.30×10^{-3}	0.329×10^{-3}
B-E1	1.88×10^{-3}	1.09×10^{-3}	0.277×10^{-3}
T	1.20×10^{-3}	0.589×10^{-3}	0.126×10^{-3}
T-EEE	0.623×10^{-3}	0.429×10^{-3}	0.0854×10^{-3}

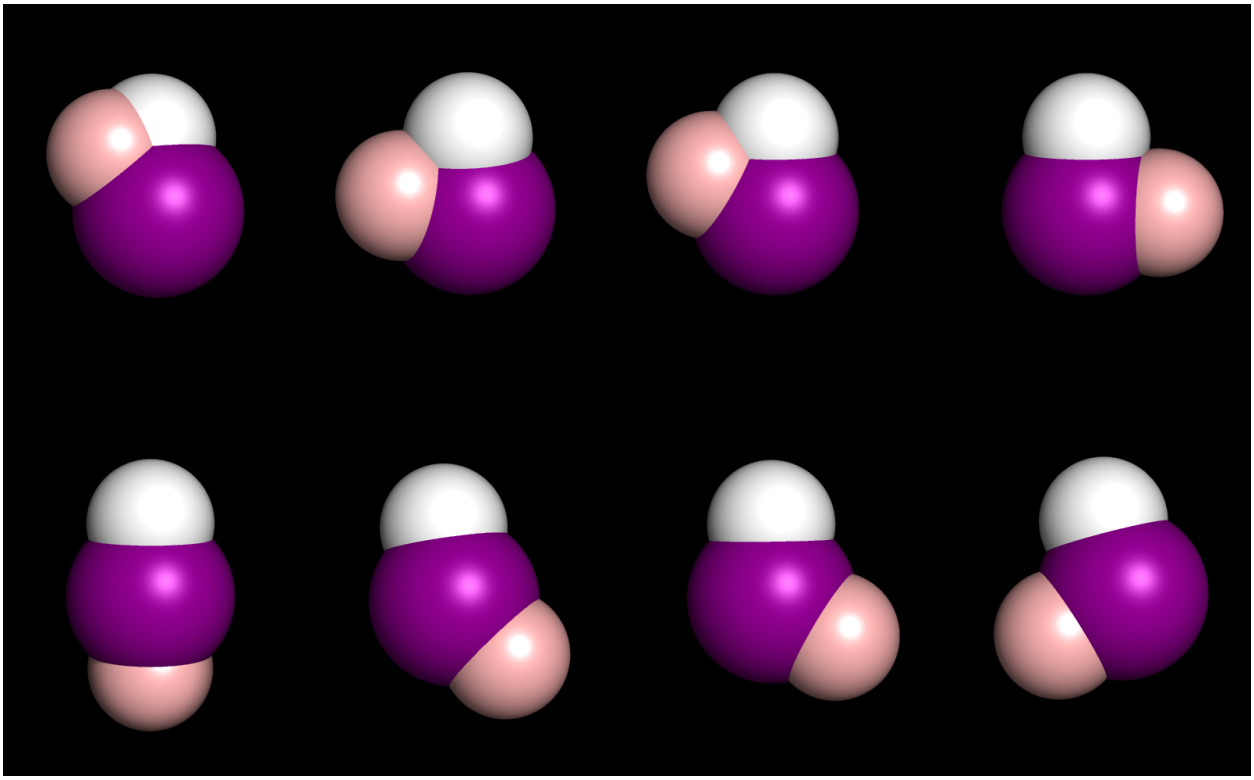

Figure S1: The 8 unique bis isomers, at the coarse grain level.

The bis isomers can be enumerated (identified) by hand and are defined in our coarse grain model simply as the internal angle between the two sidechains. Of the 9 unique isomers, two are equitorial, which for our coarse grain model results in equivalent 90-degree angles.

Identifying unique tris isomers is much more difficult, so we developed a computational method to directly enumerate the isomers and calculate the coarse-grain specification of angles between the three sidechains.

First we read in the coorinates of a C60 molecule with (0,0,0) defined as the centre of the fullerene. We then identify the 6,6 bonds by spacing ($<$1.4A) between atoms. The midpoint of these bonds, and thus the attachment point of the sidechains, was found by averaging the cartessian positions of the two bonded atoms.

We can then enumerate over all possible permutations of these bonds (30 options, 3 selections leading to 24360 permutations, which can be immediately simplified by inspection to 812 permutations by taking 2 selections of 29 options if we choose the first location for the

first sidechain). Three inter-sidechain angles are then generated (arcos of the dot production) from these sets of 3 coordinates (a,b;a,c;b,c).

As the order in which we specify the inter-sidechain angles does not matter, we are free to rearrange. By reordering these angles in ascending order, we can identify degenerate configurations by direct comparison.

The newly calculated set of three angles is compared against a list of uniquely defined isomers, and either appended to this list if found to be unique, or discarded and the degeneracy counter of that (already identified) isomer incremented.

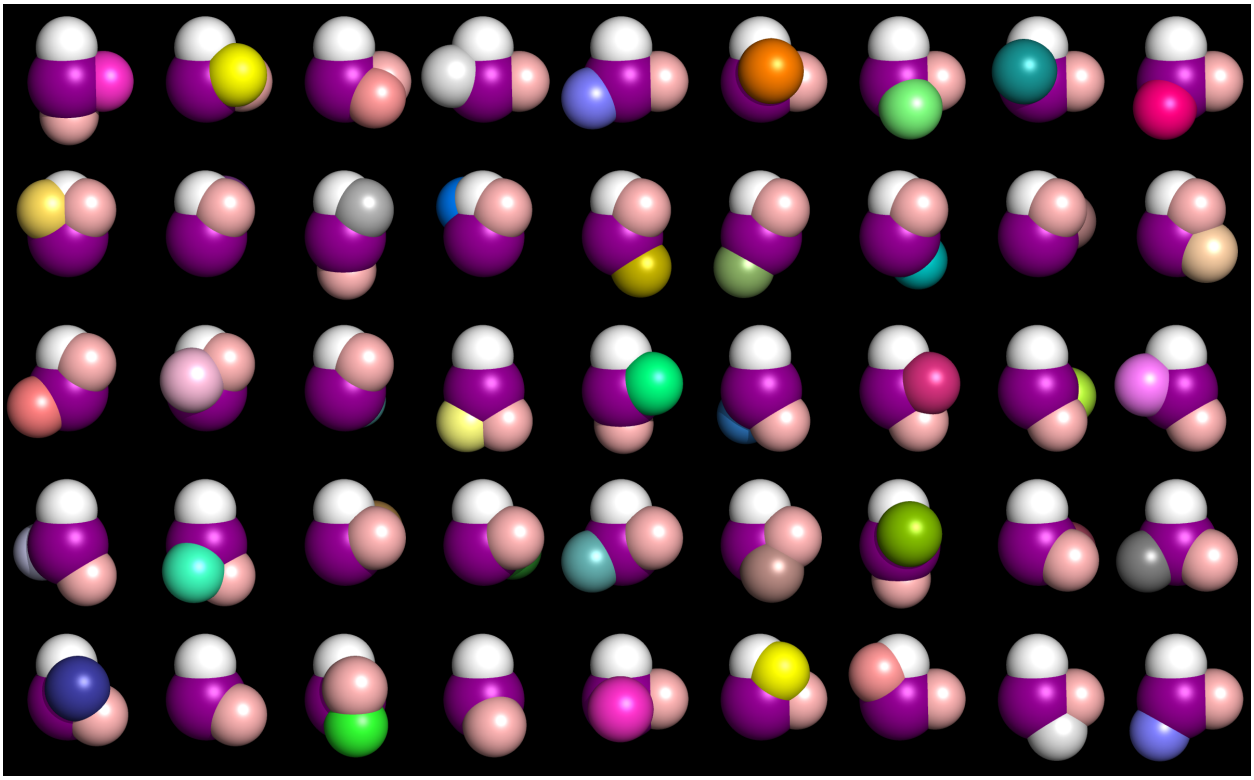

Figure S2: The 45 unique bis isomers, at the coarse grain level, as generated automatically by the method described here.

With a simple bit of trigonometry and enumeration we directly discover the 45 unique tris isomers and their symmetry derived degeneracy, and can directly generate the angle specification suitable for an empirical force field specificaiton, and a relaxed set of coarse grain coordinates for visualisation and the generation of a dense initial structure for molecular

dynamics.

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Supporting Information Available

The data set and analysis codes, TrendyName, are available as a source code repository on GitHub.[S1] This material is available free of charge via the Internet at `http://pubs.acs.org/`.

References

(S1) WMD-Bath/StarryNight. `https://github.com/WMD-Bath/StarryNight`.