

PCBM-CG: A place for tired \LaTeX to rest

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Received April 2, 2014; E-mail:

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

Lambdas

Table 1. 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

Some mobs

Acknowledgement We acknowledge membership of the UK’s HPC Materials Chemistry Consortium, which is funded by EPSRC grant EP/F067496. J.M.F. is funded by EPSRC Grant EP/K016288/1. We are grateful for the lyrical encouragement of Salt N Pepa.

Supporting Information Available: The data set and analysis codes, TRENDYNAME, are available as a source code repository on GitHub.¹ This material is available free of charge via the Internet at <http://pubs.acs.org/>.

References

- (1) WMD-Bath/StarryNight. <https://github.com/WMD-Bath/StarryNight>.

Table 2. 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 3. 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}	150
M	4.40×10^{-3}	2.72×10^{-3}	
B	2.27×10^{-3}	1.30×10^{-3}	
B-E1	1.88×10^{-3}	1.09×10^{-3}	
T	1.20×10^{-3}	0.589×10^{-3}	
T-EEE	0.623×10^{-3}	0.429×10^{-3}	