C Journal of Carbon Research

MDPI

Supplementary Material

Conformational Analysis of [60]PCBM from DFT Simulations of Electronic Energies, Bond Strain and the ^{13}C NMR Spectrum: Input Geometry Determination and Ester Bond Rotation Dynamics

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Table S1. The relevant bond angles for each of the 24 [60]PCBM conformers, their mean absolute difference from those of a powder XRD study (from Ref. 16 and given in parentheses) and their relative calculated total electronic energies. These values are plotted in Figure 3 of the paper.

Conf.	F1,C61,C4 (116.6°)	Ph1,C61,C4 (115.5°)	C61,C4,C3 (114.4°)	C4,C3,C2 (110.9°)	C3,C2,C1 (113.6°)	C2,C1,O (110.8°)	C1,O,Me (116.0°)	C2,C1=O (125.0°)	O,C1=O (123.3°)	MAD bond angle	Relative electr. energy (kJ/mol)
aaa-aa	124.2°	107.6°	122.5°	110.9°	112.2°	111.6°	115.6°	125.6°	123.5°	2.9°	11.3
aaa-sa	124.2°	107.6°	122.3°	110.3°	116.1°	112.6°	115.7°	124.0°	123.4°	3.4°	14.8
aaa-as	124.2°	107.6°	122.4°	110.3°	111.8°	117.7°	121.4°	123.6°	118.6°	4.7°	41.0
aaa-ss	124.3°	107.6°	122.1°	109.2°	124.5°	124.8°	126.9°	118.1°	117.1°	8.3°	67.3
aas-aa	125.2°	106.9°	121.0°	117.3°	121.3°	108.8°	115.6°	128.6°	122.6°	5.2°	41.1
aas-sa	125.2°	106.7°	121.2°	118.4°	126.0°	115.9°	115.6°	121.4°	122.7°	6.0°	50.0
aas-as	125.2°	106.8°	120.7°	118.0°	121.0°	115.9°	122.8°	126.6°	117.5°	6.4°	72.7
aas-ss	125.2°	106.4°	121.3°	122.9°	138.1°	129.9°	129.4°	114.3°	129.4°	12.3°	143.5
asa-aa	129.4°	103.3°	135.5°	125.0°	111.7°	110.2°	115.7°	126.4°	123.4°	7.1°	84.8
asa-sa	129.4°	103.2°	135.6°	124.6°	115.7°	113.6°	115.5°	123.2°	123.2°	7.5°	92.5
asa-as	129.2°	103.5°	135.9°	125.7°	110.5°	117.3°	121.4°	124.1°	118.5°	8.8°	106.6
asa-ss	129.9°	102.7°	135.7°	121.9°	125.0°	125.8°	126.6°	117.3°	116.9°	12.2°	153.7
						0.0					
saa-aa	116.7°	116.3°	115.4°	110.7°	113.0°	110.8°	115.6°	125.7°	123.5°	0.6°	4.6
saa-sa	116.7°	116.2°	115.4°	110.5°	116.8°	112.8°	115.5°	123.9°	123.3°	1.0°	29.3
saa-as	116.7°	116.3°	115.4°	110.7°	112.4°	117.7°	121.5°	123.8°	121.5°	1.9°	59.2
saa-ss	116.9°	115.9°	114.7°	110.1°	124.6°	124.8°	126.9°	118.2°	117.1°	5.7°	
						25.5					
sas-aa	116.2°	117.1°	114.2°	117.6°	120.8°	108.9°	115.6°	128.5°	122.6°	2.8°	33.0
sas-sa	115.9°	117.3°	114.7°	118.5°	125.5°	115.7°	115.9°	121.5°	122.8°	3.5°	57.6
sas-as	116.2°	117.2°	113.9°	118.2°	120.6°	116.0°	122.8°	126.5°	117.5°	4.1°	124.3
sas-ss	115.8°	117.3°	114.6°	123.0°	137.6°	129.9°	129.7°	114.3°	115.7°	10.1°	
						43.8					
ssa-aa	115.4°	120.0°	125.3°	122.8°	111.2°	110.5°	115.6°	126.3°	123.2°	3.6°	50.3
ssa-sa	115.3°	120.1°	125.4°	122.6°	115.3°	113.6°	115.5°	123.4°	123.0°	4.0°	67.3
ssa-as	115.3°	120.4°	125.4°	122.4°	111.0°	117.1°	121.2°	124.4°	118.5°	5.1°	112.5
ssa-ss	115.1°	120.3°	126.1°	121.3°	123.8°	125.9°	127.2	117.5°	116.6°	8.9°	11.3