Supplementary Information

to the

Comment on "Fullerene-based materials for solar cell applications: design of novel acceptors for efficient polymer solar cells – a DFT study" by A. Mohajeri and A. Omidvar, *Phys. Chem. Chem. Phys.*, 2015, 17, 22367

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The PBE/3ζ density functional theory method (Priroda program) has been chosen for the study because it is successfully used for theoretical studies of thermodynamics and kinetics of fullerene reactions, IR and NMR spectra, and especially the measured mean polarizabilities of fullerenes and their derivatives (Ref. 4).

After standard DFT-optimizations and vibration modes solving (to prove that all the stationary points, respective to the molecules under study, are minima of the potential energy surfaces), the components of polarizability tensors α have been calculated in terms of the finite field approach as the second order derivatives of the total energy *E* with respect to the homogeneous external electric field *F*:

$$\alpha_{ij} = -\frac{\partial^2 E}{\partial F_i \partial F_j}$$

Tensors α have been calculated in the arbitrary coordinate system and then diagonalized. Their eigenvalues α_{ii} (*i* = *x*, *y*, and *z*) allow calculating the mean polarizability α and its anisotropy a^2 :

$$\alpha = \frac{1}{3} \left(\alpha_{xx} + \alpha_{yy} + \alpha_{zz} \right)$$
$$a^{2} = \frac{1}{2} \left(\left(\alpha_{yy} - \alpha_{xx} \right)^{2} + \left(\alpha_{zz} - \alpha_{yy} \right)^{2} + \left(\alpha_{zz} - \alpha_{xx} \right)^{2} \right)$$

We have studied the bisadducts from the Troshin group's study and served the numeration of compounds of the original paper (Ref. 20).

Number of	Computational data of this work						Experiment from Ref. 20
compound	Eigenvalues of α tensor			α (Å ³)	a² (Å ⁶)	LUMO	V _{oc} (mV)
					(eV)		
	α _{xx} (A ³)	α _{γγ} (A ³)	α _{zz} (A ³)				
1	102.09	96.67	126.07	108.27	734.58	-4.183	640
2	104.79	98.20	128.22	110.40	746.71	-4.176	640
3	101.27	95.94	125.35	107.52	736.39	-4.203	600
4	99.06	94.05	121.83	104.98	657.67	-4.200	600
5	118.45	113.29	155.44	129.06	1585.83	-4.100	610
6	99.99	95.38	123.39	106.25	676.36	-4.197	407
7	102.17	97.00	125.88	108.35	711.61	-4.186	362
8	105.74	97.98	127.14	110.29	684.00	-4.188	585
9	104.13	98.35	128.53	110.34	769.88	-4.182	640
10	106.75	100.12	130.52	112.46	766.77	-4.184	620
11	145.66	100.91	105.55	117.37	1816.32	-4.206	600
12	103.90	96.89	130.39	110.40	936.08	-4.159	350
13	116.43	112.17	152.35	126.98	1460.99	-4.112	620
14	118.60	113.65	155.16	129.14	1541.73	-4.105	560
15	120.85	115.09	157.75	131.23	1607.90	-4.102	660
16	122.82	116.61	160.40	133.28	1684.33	-4.100	640
17	100.72	96.92	124.86	107.50	688.72	-4.225	600
18	103.57	97.66	127.77	109.67	763.21	-4.202	600
19	104.88	100.47	129.24	111.53	720.48	-4.222	600
20	119.45	114.42	157.56	130.48	1668.89	-4.120	590
21	121.65	115.97	159.89	132.51	1711.95	-4.121	590
22	103.18	97.55	127.64	109.45	767.57	-4.171	600
23	98.32	94.67	122.90	105.30	707.50	-4.173	620
24	102.31	96.84	126.96	108.70	772.32	-4.190	580
25	99.17	93.43	119.81	104.14	577.29	-4.211	320
26	98.27	92.37	118.85	103.16	580.02	-4.219	580
27	125.02	97.68	95.37	106.02	815.87	-4.223	340

Computational and experimental data associated with Figure 1

Numeration of compounds (Ref. 20)

Note: structures 5, 13–16, 20, 21 are the C₇₀ derivatives; the others are the C₆₀ adducts.

