Conjugate Acene Fused Buckybowls: Evaluating Their Suitability for p-type, Ambipolar and n-type Air Stable Organic Semiconductors

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We have found typographical errors in the reorganization energy data in Table 3 and Figure 5. This effect the text as follows:

Page 5045, right column, line 20: "The λ_+values clustered in the range of 0.01 eV to 0.03 eV" is incorrect and should read "The λ_+values clustered in the range of 0.01 eV to 0.25eV'.
Page 5045, right column, line 22: "The λ_+ values are lower in boron doped compounds by 0.08 eV to 0.18 eV compared to undoped bowls" is incorrect and should read "The λ_+ values are lower in boron doped compounds by 0.02 eV to 0.11 eV compared to undoped bowls". However, none of the changes mentioned here alter the concepts and interpretations of the results of the manuscript.

The Table 3 and Figure 5 should read as follows.

Table 3: Energies of HOMO, LUMO orbitals, HOMO-LUMO orbital energy gap (HLG) and reorganization energies λ_+ (hole transport), λ_- (electron transport) of boron and nitrogen doped acene fused buckybowls at B3LYP/6-311+G(d)// B3LYP/6-31G level of theory (all values are given in eV).

Str.	HOMO	LUMO	HLG	λ_+	λ_-
Cor-B1-Cor-B	-5.17	-4.90	-0.27	0.08	0.19
Cor-B2-Cor-B	-5.11	-4.87	-0.24	0.07	0.07
Cor-B3-Cor-B	-5.06	-4.83	-0.23	0.05	0.04
Cor-B4-Cor-B	-4.98	-4.77	-0.21	0.01	0.09
Cor-B5-Cor-B	-4.93	-4.73	-0.20	0.08	0.06
Sum-B1-Cor-B	-4.98	-4.61	-0.37	0.07	0.09
Sum-B1-Sum-B	-4.81	-4.35	-0.46	0.07	0.08
Sum-B2-Cor-B	-4.91	-4.58	-0.32	0.10	0.08
Sum-B2-Sum-B	-4.73	-4.33	-0.40	0.07	0.07
Sum-B3-Cor-B	-4.84	-4.55	-0.29	0.06	0.07
Sum-B3-Sum-B	-4.67	-4.31	-0.36	0.06	0.06
Sum-B4-Cor-B	-4.77	-4.44	-0.33	0.07	0.05
Sum-B4-Sum-B	-4.61	-4.29	-0.32	0.06	0.06
Sum-B5-Cor-B	-4.74	-4.38	-0.36	0.08	0.06
Sum-B5-Sum-B	-4.55	-4.27	-0.28	0.06	0.10
Cor-B1-Cor-N	-3.34	-3.01	-0.34	0.14	0.09
Cor-B2-Cor-N	-3.34	-3.05	-0.29	0.12	0.06
Cor-B3-Cor-N	-3.35	-3.09	-0.26	0.09	0.03
Cor-B4-Cor-N	-3.38	-3.14	-0.24	0.10	0.03
Cor-B5-Cor-N	-3.40	-3.18	-0.22	0.09	0.14
Sum-B1-Cor-N	-3.13	-2.71	-0.42	0.25	0.22
Sum-B1-Sum-N	-2.95	-2.44	-0.52	0.14	0.11
Sum-B2-Cor-N	-3.15	-2.77	-0.38	0.14	0.11
Sum-B2-Sum-N	-3.00	-2.51	-0.49	0.12	0.12
Sum-B3-Cor-N	-3.19	-2.83	-0.36	0.10	0.06
Sum-B3-Sum-N	-3.05	-2.59	-0.46	0.10	0.12
Sum-B4-Cor-N	-3.30	-2.91	-0.39	0.09	0.14
Sum-B4-Sum-N	-3.10	-2.69	-0.41	0.09	0.12
Sum-B5-Cor-N	-3.25	-2.93	-0.31	0.07	0.09
Sum-B5-Sum-N	-3.14	-2.77	-0.37	0.05	0.10

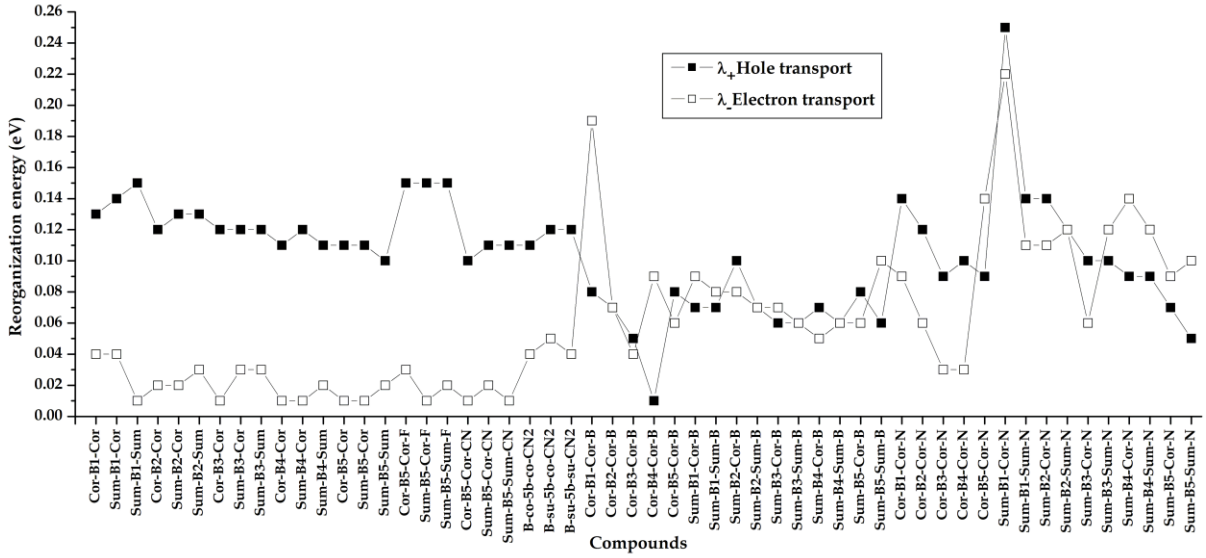

Figure 5: The reorganization energy, hole transport (λ_+) and electron transport (λ_-) of acene fused buckybowls and there boron and nitrogen doped bowls at B3LYP/6-311+G(d)//B3LYP/6-31G level of theory.