Supplementary Material (ESI) for PCCP

The Leapfrog Principle for Boron Fullerenes: A Theortical Study of Structure and Stability of B_{112}

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SUPPLEMENTARY INFORMATIONS

Manuscript submitted to Physical Chemistry Chemical Physics
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Version: January 28, 2011

Table . Symmetries and energies of valences molecular orbitals for B_{112} isomers computed at B3LYP/SVP level.

Valence orbitals of D_2-B_{112}		Valence orbitals of T_d-B_{112}	
Mos	Energies(eV)	Mos	Energies(eV)
70 b_1	*-3.3470 eV*	*19 a_1*	*-3.238 eV*
70 b_3	*-3.529 eV*	*42 t_2*	*-3.325 eV*
70 b_2	*-3.719 eV*	*41 t_2*	*-3.529 eV*
69 b_1	-5.462 eV	24 e	-5.266 eV
73 a	-5.486 eV	7 a_2	-5.450 eV
69 b_2	-5.502 eV	29 t1	-5.682 eV
72 a	-5.584 eV	40 t2	-6.111 eV
69 b_3	-5.624 eV	23 e	-6.264 eV
71 a	-5.725 eV	28 t1	-6.431 eV
68 b_2	-5.836 eV	39 t2	-6.921 eV
70 a	-5.954 eV	18 a1	-6.968 eV
68 b_1	-6.054 eV	38 t2	-7.262 eV
68 b_3	-6.097 eV	37 t2	-7.475 eV
67 b_2	-6.326 eV	22 e	-7.489 eV
67 b_1	-6.391 eV	17 a1	-7.537 eV
67 b_3	-6.443 eV	27 t1	-7.540 eV
69 a	-6.513 eV	21 e	-7.807 eV
66 b_3	-7.046 eV	36 t2	-7.837 eV
66 b_2	-7.163 eV	26 t1	-7.929 eV
68 a	-7.165 eV	25 t1	-8.290 eV
66 b_1	-7.257 eV	20 e	-8.563 eV
67 a	-7.334 eV	24 t1	-8.773 eV
65 b_1	-7.335 eV	19 e	-8.783 eV
65 b_2	-7.354 eV	6 a2	-8.974 eV
66 a	-7.498 eV	35 t2	-9.023 eV
65 b_3	-7.525 eV	16 a1	-9.504 eV
64 b_2	-7.527 eV	34 t2	-9.592 eV
63 b_2	-7.549 eV	23 t1	-9.728 eV
64 b_3	-7.559 eV	33 t2	-10.484 eV
63 b_3	-7.586 eV	18 e	-10.511 eV
65 a	-7.595 eV	32 t2	-10.896 eV
64 b_1	-7.663 eV	17 e	-10.943 eV
64 a	-7.705 eV	31 t2	-11.220 eV

The first three orbitals are virtuals orbitals and the forth orbital is HOMO.