Supplementary

Exploring The Effect Of External Dopant On Electride Characteristics Of Bimetallic Sandwich Complexes Based On $B_4N_4H_8$ Ligand, $M_2(B_4N_4H_8)_2Ca_2$ (M=Na and K)

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Table S1. Computed WBI index of the studied complexes

$Na_2(B_4N_4H_8)_2Ca_2$	Bond	Ca_{18}-B_{22}	Ca_{18}-N_{28}	Ca_{17}-B_{25}	Ca_{17}-N_{34}	Na_{36}-B_{20}	Na_{36}-N_{27}	Na_{35}-B_{23}	Na_{35}-N_{33}
	WBI	0.0401	0.0242	0.0402	0.0242	0.0114	0.0121	0.0113	0.0121
$NaK(B_4N_4H_8)\ Ca_2$	Bond	Ca_{18}-B_{21}	Ca_{18}-N_{30}	Ca_{17}-B_{28}	Ca_{17}-N_{33}	K_{19}-B_{23}	K_{19}-N_{32}	Na_{20}-B_{26}	Na_{20}-N_{33}
	WBI	0.0390	0.0251	0.0396	0.0240	0.0144	0.0092	0.0114	0.0121
$K_2(B_4N_4H_8)_2Ca_2$	Bond	Ca_{18}-B_{22}	Ca_{18}-N_{28}	Ca_{17}-B_{25}	Ca_{17}-N_{34}	K_{19}-B_{20}	K_{19}-N_{29}	K_{36}-N_{32}	K_{36}-B_{26}
	WBI	0.0386	0.0249	0.0385	0.0248	0.0145	0.0092	0.0092	0.0145

Table S2. Important geometrical parameters (Å) of the optimized complexes at MN15functional

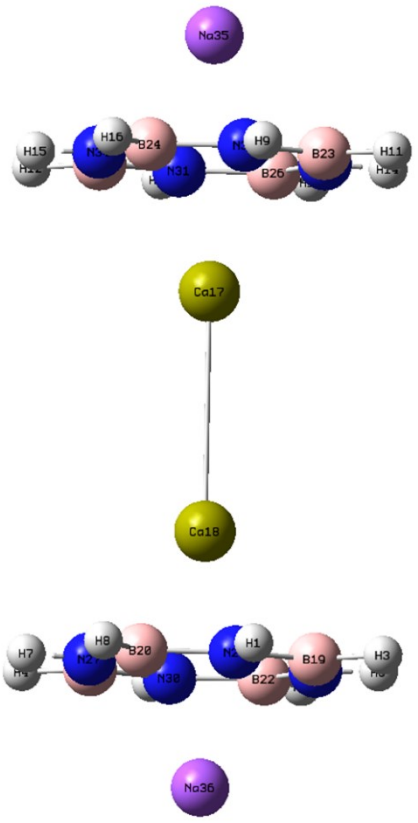
Molecules	Bond length (Å)					
	B-N	B-H	N-H	Ca-Ca	Na -B/Na-N K-B/K-N	Ca-B/ Ca-N
MN15/ 6-31+G(d,p)						
$Na_2(B_4N_4H_8)_2Ca_2$	1.45	1.19	1.01	3.57	2.69/2.56	2.84/2.74
$NaK(B_4N_4H_8)\ Ca_2$	1.45	1.19	1.01	3.57	2.69/2.56	2.85/2.74
					2.98/2.89	2.84/2.72
$K_2(B_4N_4H_8)_2Ca_2$	1.45	1.19	1.01	3.58	2.98/2.89	2.85/2.73
MN15/ def2-TZVPP						
$Na_2(B_4N_4H_8)_2Ca_2$	1.45	1.19	1.01	3.62	2.71/2.57	2.74/2.66
$NaK(B_4N_4H_8)\ Ca_2$	1.45	1.19	1.01	3.62	2.71/2.57	2.74/2.66
					2.99/2.88	2.74/2.64
$K_2(B_4N_4H_8)_2Ca_2$	1.45	1.19	1.01	3.62	2.99/2.88	2.74/2.65

Molecules	B-N	B-H	N-H	Ca-Ca	Na -B/Na-N K-B/K-N	Ca-B/ Ca-N
$Na_2(B_4N_4H_8)_2Ca_2$	1.45	1.19	1.01	3.67	2.66/2.54	2.82/2.72
$NaK(B_4N_4H_8)\ Ca_2$	1.45	1.19	1.01	3.68	2.66/2.54 2.96/2.86	2.82/2.72 2.96/2.86
$K_2(B_4N_4H_8)_2Ca_2$	1.45	1.19	1.01	3.68	2.96/2.86	2.86/2.70

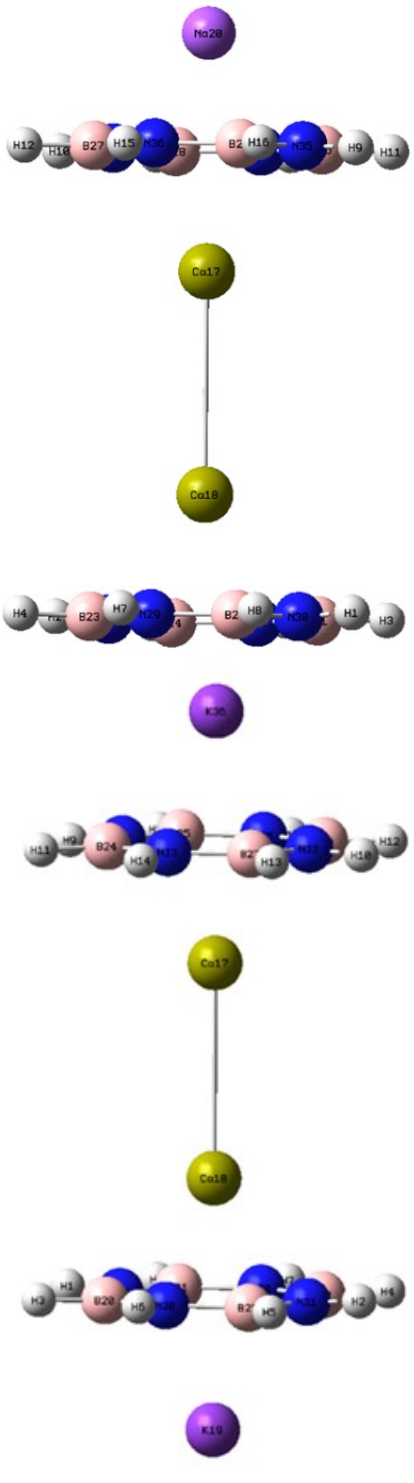
Table S3. Important geometrical parameters (Å) of the optimized complexes at M06-2X/6-31+G(d,p) level

Table S4 Computed aromaticity value of the complexes (1000*AV1245, as performed in Multiwfn)

Molecules	values
$Na_2(B_4N_4H_8)_2Ca_2$	2.43
$NaK(B_4N_4H_8)\ Ca_2$	2.05
$K_2(B_4N_4H_8)_2Ca_2$	1.52



$Na_2(B_4N_4H_8)_2Ca_2$



$NaK(B_4N_4H_8)_2C$

Fig S1: Optimized structure with levels and numbering on atoms