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Electronic Supporting Information

Theoretical investigations on the structures, electronic and optical properties of neutral and anionic M_2-doped B_{24} clusters (M=Li, Na, K)

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Table S1 Cartesian coordinates for the lowest energy structures of $M_2B_{24}^{0/-}$ (M=Li, Na, K) clusters.

Li_2B_{24}

0 1

B	0.80335100	1.93946200	1.49262800
B	-0.80335100	1.93946200	1.49262800
B	-1.93946200	0.80335100	1.49262800
B	-1.93946200	-0.80335100	1.49262800
B	-0.80335100	-1.93946200	1.49262800
B	0.80335100	-1.93946200	1.49262800
B	1.93946200	-0.80335100	1.49262800
B	1.93946200	0.80335100	1.49262800
B	0.80335100	1.93946200	-1.49262800
B	1.93946200	0.80335100	-1.49262800
B	1.93946200	-0.80335100	-1.49262800
B	0.80335100	-1.93946200	-1.49262800
B	-0.80335100	-1.93946200	-1.49262800
B	-1.93946200	-0.80335100	-1.49262800
B	-1.93946200	0.80335100	-1.49262800
B	-0.80335100	1.93946200	-1.49262800
B	0.00000000	2.22563500	0.00000000
B	-1.57376200	1.57376200	0.00000000
B	-2.22563500	0.00000000	0.00000000
B	-1.57376200	-1.57376200	0.00000000
B	0.00000000	-2.22563500	0.00000000
B	1.57376200	-1.57376200	0.00000000
B	2.22563500	0.00000000	0.00000000
B	1.57376200	1.57376200	0.00000000
Li	0.00000000	0.00000000	2.55459300
Li	0.00000000	0.00000000	-2.55459300

Na_2B_{24}

0 1

B	1.93945200	0.80335100	1.49083600
B	0.80335100	1.93945200	1.49083600
B	-0.80335100	1.93945200	1.49083600
B	-1.93945200	0.80335100	1.49083600
B	-1.93945200	-0.80335100	1.49083600
B	-0.80335100	-1.93945200	1.49083600
B	0.80335100	-1.93945200	1.49083600
B	1.93945200	-0.80335100	1.49083600
B	1.93945200	0.80335100	-1.49083600

B	1.93945200	-0.80335100	-1.49083600
B	0.80335100	-1.93945200	-1.49083600
B	-0.80335100	-1.93945200	-1.49083600
B	-1.93945200	-0.80335100	-1.49083600
B	-1.93945200	0.80335100	-1.49083600
B	-0.80335100	1.93945200	-1.49083600
B	0.80335100	1.93945200	-1.49083600
B	1.57636800	1.57636800	0.00000000
B	0.00000000	2.22930300	0.00000000
B	-1.57636800	1.57636800	0.00000000
B	-2.22930300	0.00000000	0.00000000
B	-1.57636800	-1.57636800	0.00000000
B	0.00000000	-2.22930300	0.00000000
B	1.57636800	-1.57636800	0.00000000
B	2.22930300	0.00000000	0.00000000
Na	0.00000000	0.00000000	3.16963500
Na	0.00000000	0.00000000	-3.16963500

K_2B_{24}
0 1

B	1.93755500	0.80252600	1.49168400
B	0.80252600	1.93755500	1.49168400
B	-0.80252600	1.93755500	1.49168400
B	-1.93755500	0.80252600	1.49168400
B	-1.93755500	-0.80252600	1.49168400
B	-0.80252600	-1.93755500	1.49168400
B	0.80252600	-1.93755500	1.49168400
B	1.93755500	-0.80252600	1.49168400
B	1.93755500	0.80252600	-1.49168400
B	1.93755500	-0.80252600	-1.49168400
B	0.80252600	-1.93755500	-1.49168400
B	-0.80252600	-1.93755500	-1.49168400
B	-1.93755500	-0.80252600	-1.49168400
B	-1.93755500	0.80252600	-1.49168400
B	-0.80252600	1.93755500	-1.49168400
B	0.80252600	1.93755500	-1.49168400
B	1.57734100	1.57734100	0.00000000
B	0.00000000	2.23064100	0.00000000
B	-1.57734100	1.57734100	0.00000000
B	-2.23064100	0.00000000	0.00000000
B	-1.57734100	-1.57734100	0.00000000
B	0.00000000	-2.23064100	0.00000000
B	1.57734100	-1.57734100	0.00000000

B	2.23064100	0.00000000	0.00000000
K	0.00000000	0.00000000	3.64319400
K	0.00000000	0.00000000	-3.64319400

$Li_2B_{24}^-$

-1 2

B	0.068110000	0.203771000	-1.553902000
B	-1.329026000	0.806732000	-1.004834000
B	1.546317000	0.431178000	-0.863027000
B	0.217625000	1.690435000	-0.805795000
B	0.885102000	-1.151768000	-1.213843000
B	-0.864971000	-0.033113000	1.774034000
B	1.268017000	-1.511327000	0.739700000
B	0.740861000	-0.359044000	1.788010000
B	-0.350297000	-1.580381000	1.304978000
B	-1.814481000	0.846928000	0.857479000
B	-1.854288000	-0.942026000	0.832574000
B	2.047185000	0.062044000	0.995918000
Li	0.249382000	1.825007000	1.781149000
B	0.197068000	-2.599157000	-0.224692000
Li	-1.318907000	-1.355147000	-1.917904000
B	-1.405489000	-2.440446000	0.102550000
B	-2.878808000	-0.107635000	-0.436278000
B	2.589200000	-1.168430000	-0.464324000
B	-1.554797000	2.424287000	-0.203506000
B	2.516746000	1.641691000	0.040229000
B	1.332627000	2.762839000	0.023301000
B	-0.123330000	3.155128000	-0.025260000
B	1.738583000	-2.517004000	-0.594467000
B	-2.741963000	-1.705808000	-0.312960000
B	-2.808402000	1.496860000	-0.396176000
B	3.220125000	0.312328000	-0.277653000

$Na_2B_{24}^-$

-1 2

B	0.69393600	1.57006900	2.49121900
B	0.58264800	2.85498200	1.51784200
B	0.50331500	3.40573900	0.00000000
B	0.58264800	2.85498200	-1.51784200
B	0.69393600	1.57006900	-2.49121900
B	0.75318500	0.02107300	-2.93002100
B	0.78247900	-1.57774200	-2.68138400
B	0.90276900	-2.74571200	-1.56374700

B	0.95746400	-3.14474000	0.00000000
B	0.90276900	-2.74571200	1.56374700
B	0.78247900	-1.57774200	2.68138400
B	0.75318500	0.02107300	2.93002100
B	-0.83164500	2.25211600	2.21762300
B	-0.93696400	3.04997400	0.80215600
B	-0.93696400	3.04997400	-0.80215600
B	-0.83164500	2.25211600	-2.21762300
B	-0.75237400	0.80659900	-2.92448800
B	-0.72568200	-0.81207600	-2.76985700
B	-0.63808700	-2.25193500	-2.07428600
B	-0.51850300	-3.26120500	-0.80442200
B	-0.51850300	-3.26120500	0.80442200
B	-0.63808700	-2.25193500	2.07428600
B	-0.72568200	-0.81207600	2.76985700
B	-0.75237400	0.80659900	2.92448800
Na	1.71445500	0.82564800	0.00000000
Na	-1.75277500	-0.85895900	0.00000000

$K_2B_{24}^-$

-1 2

K	0.00000000	0.00000000	-1.93856000
K	0.00000000	0.00000000	1.95291100
B	0.00000000	3.20987900	-0.70074100
B	-2.63047500	1.51870500	-0.77164000
B	-2.77983700	-1.60494000	-0.70074100
B	0.00000000	-3.03741100	-0.77164000
B	2.77983700	-1.60494000	-0.70074100
B	2.63047500	1.51870500	-0.77164000
B	-0.80408500	-3.07992000	0.71220200
B	-2.95489400	-0.78259500	0.76029500
B	-2.26524600	2.23631800	0.71220200
B	0.79970000	2.95031000	0.76029500
B	3.06933200	0.84360200	0.71220200
B	2.15519400	-2.16771600	0.76029500
B	0.80408500	-3.07992000	0.71220200
B	2.95489400	-0.78259500	0.76029500
B	2.26524600	2.23631800	0.71220200
B	-0.79970000	2.95031000	0.76029500
B	-3.06933200	0.84360200	0.71220200
B	-2.15519400	-2.16771600	0.76029500
B	1.53967000	2.70644400	-0.74539400
B	3.11368400	-0.01982800	-0.74539400

B	1.57401400	-2.68661600	-0.74539400
B	-1.57401400	-2.68661600	-0.74539400
B	-3.11368400	-0.01982800	-0.74539400
B	-1.53967000	2.70644400	-0.74539400

Table S2 Theretical vertical detachment energy (VDE) for the lowest and low-lying energy structrures of $M_2B_{24}^-$ (M=Li, Na, K) clusters

	$Li_2B_{24}^-$			$Na_2B_{24}^-$			$K_2B_{24}^-$		
	1a	2a	3a	1a	2a	3a	1a	2a	3a
VDE(eV)	2.45	1.68	2.50	2.57	2.02	2.54	2.44	2.75	2.22

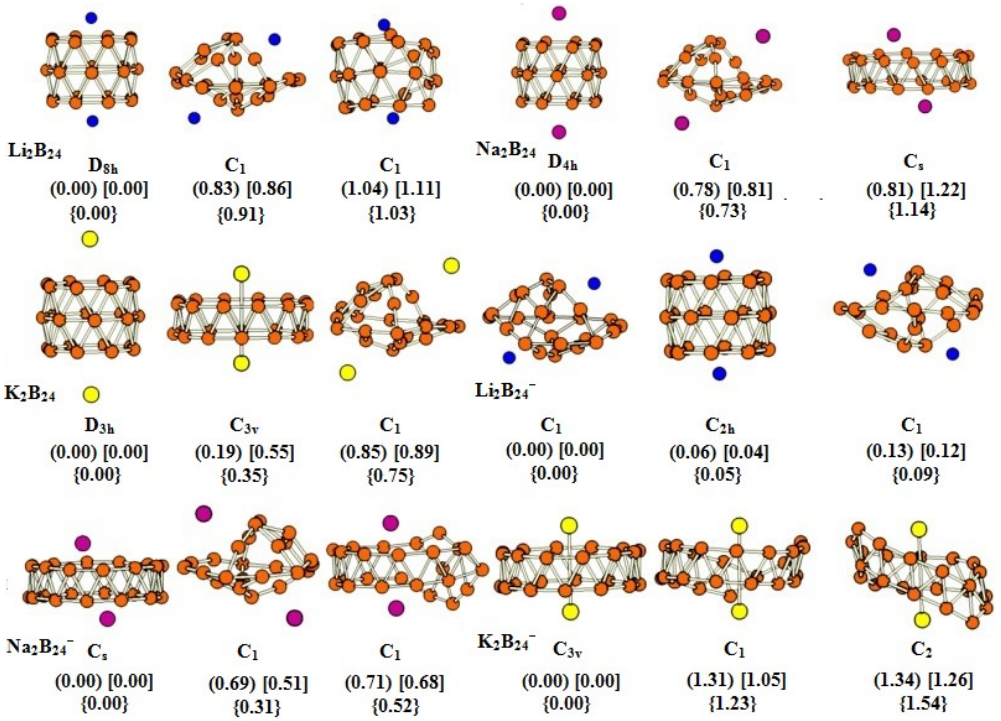

Figure S1 Geometrical structures of the lowest and low-lying isomers of $M_2B_{24}^{0/-}$ (M=Li, Na, K) clusters at PBE0/6-311+G(d) (in parentheses), PBE0-D3/6-311+G(d) (in square brakets) and CCSD(T)/def2-TZVP//PBE0/6-311+G(d) (in braces) levels along with the point group symmetry, and relative energy (eV). The orange, blue, pink and yellow balls are B, Li, Na and K atoms, respectively.

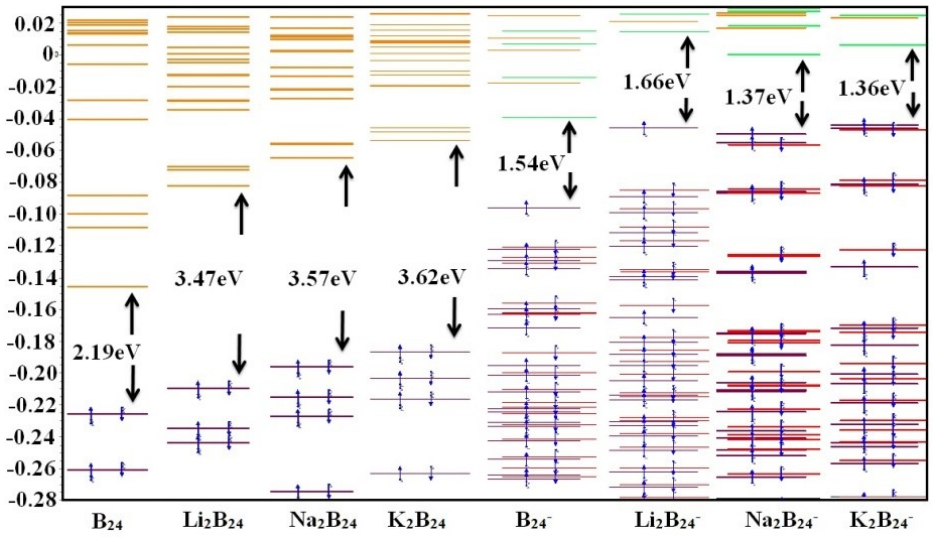

Figure S2 Molecular orbital energy levels of the lowest energy structures of $M_2B_{24}^{0/-}$ (M=Li, Na, K) clusters

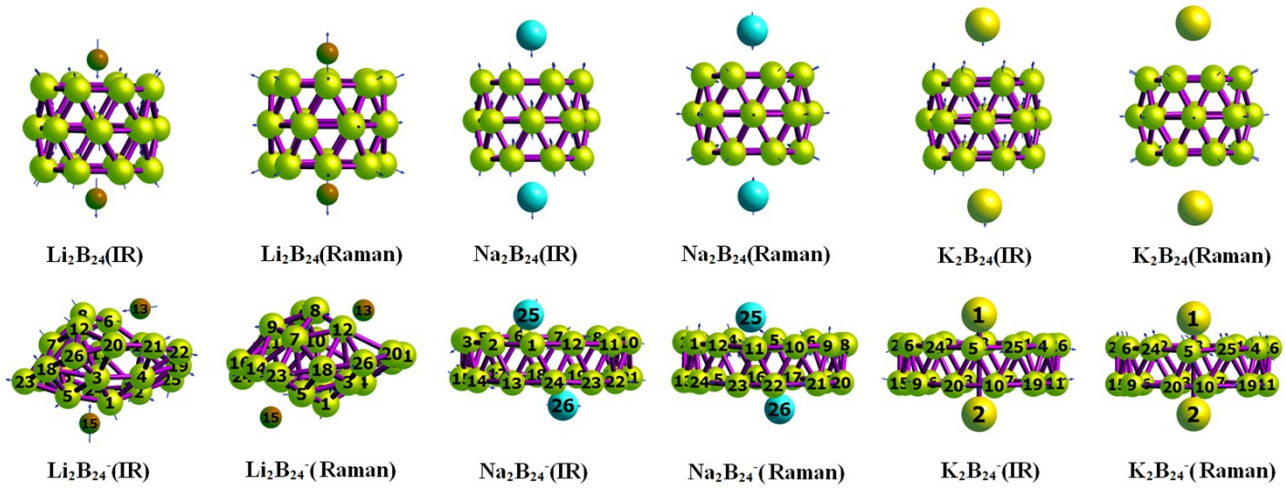

Figure S3 The vibrational modes of stongest peaks for the lowest energy structures of $M_2B_{24}^{0/-}$ (M=Li, Na, K) clusters.