

《稀土掺杂硼团簇 REB_n^- ($RE = La, Sc; n = 6, 8$) 的几何及电子结构*》的补充材料

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补充材料 A: REB_n^- ($RE = La, Sc; n = 6, 8$) 低能异构体的笛卡尔坐标

Suppl. A: Cartesian coordinates of the low-lying isomers of the REB_n^- ($RE = La, Sc; n = 6, 8$) clusters

表 S1 PBE1PBE/La/SDD/B/6-311+G* 计算水平下, LaB_6^- 低能异构体的笛卡尔坐标

Table S1. Cartesian coordinates of the low-lying isomers of the LaB_6^- clusters at the PBE1PBE/La/SDD/B/6-311+G* level.

Cluster	Atoms	X	Y	Z
LaB_6^- -I	B	-1.79113700	0.48102800	0.74105200
	B	-0.82430700	1.80550800	0.30725200
	B	-1.68074300	1.11063700	-0.82050800
	B	-1.68010300	-1.11079500	0.82070600
	B	-0.82417500	-1.80548100	-0.30755400
	B	-1.79159100	-0.48118100	-0.74073200
	La	0.75368900	0.00002500	-0.00001900
LaB_6^- -II	B	0.75876600	1.61491200	0.59962500
	B	2.07612700	1.39743800	-0.19616000
	B	2.07480900	-1.39785400	-0.19663700
	B	2.69236200	-0.00041300	-0.61748300
	B	0.75803600	-1.61500500	0.60014200
	B	1.51396400	-0.00007400	0.58976100
	La	-0.86614600	0.00008700	-0.06835500
LaB_6^- -III	B	-3.16743800	-0.00000400	-0.00042100
	B	-0.86809400	-1.61523400	0.00033200
	B	-2.41615400	-1.41485000	0.00023600
	B	-1.49439100	-0.00000200	0.00104100
	B	-0.86810400	1.61523300	0.00015600
	B	-2.41616500	1.41484600	0.00044100
	La	0.98511800	0.00000100	-0.00015700
LaB_6^- -IV	B	1.48923500	0.80265400	-1.00699900
	B	1.48923300	0.80281400	1.00682600
	B	1.17566100	1.94387600	-0.00018600
	B	1.48924200	-0.80295600	1.00696400
	B	1.17493000	-1.94396500	0.00012000
	B	1.48910800	-0.80312100	-1.00696400
	La	-0.72872000	0.00006100	0.00002100

表 S2 PBE1PBE/Sc/SDD/B/6-311+G*计算水平下, ScB_6^- 低能异构体的笛卡尔坐标

 Table S2. Cartesian coordinates of the low-lying isomers of the ScB_6^- clusters at the PBE1PBE/Sc/SDD/B/6-311+G* level.

Cluster	Atoms	X	Y	Z
ScB_6^- -I	B	-1.02779800	1.11481300	0.81541100
	B	-0.14281100	1.75174700	-0.31553900
	B	-0.14103400	-1.75185200	0.31527200
	B	-1.15598600	0.47335000	-0.75272600
	B	-1.02699400	-1.11561900	-0.81534200
	B	-1.15520800	-0.47446600	0.75302500
	Sc	1.10710200	0.00048300	-0.00002400
ScB_6^- -II	B	-0.03208500	1.57760300	0.24921900
	B	-2.25721600	0.00004200	-0.29542600
	B	-1.53907900	1.41004400	-0.08333200
	B	-1.53912300	-1.41015900	-0.08313200
	B	-0.72342900	-0.00007100	0.39151400
	B	-0.03206500	-1.57735400	0.24906700
	Sc	1.45785700	-0.00002500	-0.10188300
ScB_6^- -III	B	0.00000000	0.69908500	0.00000000
	B	0.00232000	2.36646400	0.00000000
	B	1.57669300	0.05427000	0.00000000
	B	-1.41396400	1.60737700	0.00000000
	B	1.41681800	1.60400800	0.00000000
	B	-1.57724600	0.05787700	0.00000000
	Sc	-0.00110000	-1.52121000	0.00000000
ScB_6^- -IV	B	-1.90177500	-0.46205000	0.00000700
	B	1.90186100	-0.46193600	-0.00000400
	B	0.80411200	-0.84817200	1.02925600
	B	-0.80405500	-0.84823600	-1.02930900
	B	-0.80403600	-0.84823600	1.02930500
	B	0.80409800	-0.84812300	-1.02927600
	Sc	-0.00004900	1.02779600	0.00000500

 表 S3 PBE1PBE/La/SDD/B/6-311+G*计算水平下, LaB_8^- 低能异构体的笛卡尔坐标

 Table S3. Cartesian coordinates of the low-lying isomers of the LaB_8^- clusters at the PBE1PBE/La/SDD/B/6-311+G* level.

Cluster	Atoms	X	Y	Z
LaB_8^- -I	B	1.41808900	-0.08250400	-1.62638400
	B	1.41974700	-0.08228300	1.62617500
	B	1.06905700	1.33224500	-0.98082000
	B	1.51596600	-1.40474400	-0.79501400
	B	0.02362900	2.06774300	0.00005600
	B	1.51694900	-1.40437600	0.79453300
	B	1.86844000	0.02498100	-0.00034000
	B	1.06972400	1.33219300	0.97998200
	La	-0.86856200	-0.15642600	0.00015900
	B	0.00000000	0.00000000	-1.70483500

LaB ₈ ⁻ -II	B	0.00000000	1.77532500	-1.39330500
	B	1.38800500	1.10689700	-1.39330500
	B	0.77028500	-1.59951300	-1.39330500
	B	-0.77028500	1.59951300	-1.39330500
	B	-1.38800500	1.10689700	-1.39330500
	B	-1.73081400	-0.39504700	-1.39330500
	B	1.73081400	-0.39504700	-1.39330500
	La	0.00000000	0.00000000	1.00508500
LaB ₈ ⁻ -III	B	-1.21551000	-0.00004000	-0.63044800
	B	-0.72551800	1.77502100	-0.25846100
	B	-1.23187500	0.77340000	0.99631000
	B	-2.28005100	1.46148900	-0.31053700
	B	-2.28009300	-1.46149400	-0.31044600
	B	-0.72544600	-1.77491800	-0.25862900
	B	-2.86301300	-0.00000900	-0.03637300
	B	-1.23174800	-0.77348900	0.99640900
La	1.10116300	0.00000300	-0.01647600	
LaB ₈ ⁻ -IV	B	0.71300000	-0.02715800	1.29738700
	B	2.23870100	-0.22371700	0.89627600
	B	2.43475000	-1.29829500	-0.47981600
	B	3.13040400	0.12116200	-0.53360200
	B	2.30776000	1.42025700	-0.14849700
	B	1.27051500	0.08404500	-0.63441400
	B	0.97013200	-1.43913300	0.16651700
	B	0.71240300	1.54129300	0.11079000
La	-1.20856700	-0.01565400	-0.05917900	

 表 S4 PBE1PBE/Sc/SDD/B/6-311+G*计算水平下, ScB₈⁻ 低能异构体的笛卡尔坐标

 Table S4. Cartesian coordinates of the low-lying isomers of the ScB₈⁻ clusters at the PBE1PBE/Sc/SDD/B/6-311+G* level.

Cluster	Atoms	X	Y	Z
ScB ₈ ⁻ -I	B	-0.63675500	-1.77085200	-0.12114200
	B	-0.65938400	-1.00452800	-1.46461800
	B	-0.64339900	1.64588800	-0.65089800
	B	-0.68514200	-1.20691800	1.30537400
	B	-1.04527800	-0.00438000	-0.00114900
	B	-0.67488600	0.50990800	-1.69911800
	B	-0.70046800	1.53974400	0.88078600
	B	-0.62860300	0.26932100	1.74961300
Sc	1.35093200	0.00519400	0.00027400	
ScB ₈ ⁻ -II	B	-1.68054500	0.33763600	-0.78894900
	B	-0.66754600	-0.50324200	1.62649200
	B	1.81259000	-0.79322400	-0.00009600
	B	-0.89408500	-0.93610900	-0.00014300
	B	-0.66752500	-0.50277200	-1.62665000
	B	-1.68057000	0.33740900	0.78904500
	B	0.65372600	-1.12859100	-1.04129800

	B	0.65372500	-1.12888700	1.04101000
	Sc	0.58815000	1.02804300	0.00014000
ScB ₈ ⁻ -III	B	0.00000000	2.02629800	-0.44509600
	B	2.02629800	0.00000000	-0.44509600
	B	-1.43280900	-1.43280900	-0.44509600
	B	0.00000000	-2.02629800	-0.44509600
	B	1.43280900	1.43280900	-0.44509600
	B	-2.02629800	0.00000000	-0.44509600
	B	1.43280900	-1.43280900	-0.44509600
	B	-1.43280900	1.43280900	-0.44509600
	Sc	0.00000000	0.00000000	0.84780100
ScB ₈ ⁻ -IV	B	0.47014200	-0.77097200	0.98835100
	B	0.51052700	-0.00003200	-0.64452300
	B	-0.04200900	-1.70612600	-0.34097300
	B	1.52622600	1.46078100	-0.29652000
	B	0.47018700	0.77093200	0.98833100
	B	-0.04200800	1.70609000	-0.34096100
	B	2.09765400	0.00001500	0.05136400
	B	1.52622500	-1.46074400	-0.29652900
	Sc	-1.55165300	0.00001400	-0.02584300

补充材料 B: REB_n⁻ (RE = La, Sc; n = 6, 8) 团簇低能异构体的对称性, 相对能和第一垂直拆分能

Suppl. B: Symmetry, relative energies, and first VDE of low-lying isomers of REB_n⁻ (RE = La, Sc; n = 6, 8)

表 S5 REB_n⁻ (RE = La, Sc; n = 6, 8) 团簇低能异构体的对称性, 相对能和第一垂直拆分能 (VDE)

Table S5. Symmetry, relative energies, and first VDE of low-lying isomers of REB_n⁻ (RE = La, Sc; n = 6, 8).

Cluster	Isomers	Sym.	ΔE /eV	VDE/eV
LaB ₆ ⁻	I	C ₂	0.00	1.74
	II	C _s	0.06	1.89
	III	C _{2v}	0.19	2.36
	IV	C _{2v}	0.86	1.66
ScB ₆ ⁻	I	C ₂	0.00	2.08
	II	C ₂	0.03	1.92
	III	C _{2v}	0.05	1.91
	IV	C _{2v}	0.57	1.93
LaB ₈ ⁻	I	C _s	0.00	2.29
	II	C _{7v}	0.43	1.24
	III	C _s	1.40	2.04
	IV	C ₁	1.52	2.02
ScB ₈ ⁻	I	C _{7v}	0.00	1.91
	II	C _s	0.30	2.45
	III	C _{8v}	1.22	1.71
	IV	C _s	1.54	3.22