

Supporting Information

Stabilization of an all - metal antiaromatic molecule (Al_4Li_4) using BH and C as caps

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1.Free Al₄Li₄ (C_{2h}) [Singlet]

#RB3LYP/6-311++G(d,p)

13	1.124431000	0.727277000	1.273706000
13	-1.124431000	-0.727277000	1.273706000
13	-1.124431000	-0.727277000	-1.273706000
13	1.124431000	0.727277000	-1.273706000
3	-1.124431000	1.808411000	0.000000000
3	-3.426711000	-0.346587000	0.000000000
3	3.426711000	0.346587000	0.000000000
3	1.124431000	-1.808411000	0.000000000

E = -999.9330848 Hartree

Frequency Analysis:

Number of imaginary frequencies = 0

Lowest Frequency in cm⁻¹ = 88

2. Al₄Li₄BH (C_{2v}) [Singlet]

#RB3LYP/6-311++G(d,p)

13	-1.332720000	1.310654000	0.240000000
13	1.332720000	1.310654000	0.240000000
13	1.332720000	-1.310654000	0.240000000
13	-1.332720000	-1.310654000	0.240000000
3	0.000000000	-2.755478000	-1.562343000
3	1.715470000	0.000000000	-2.087023000
3	0.000000000	2.755478000	-1.562343000
3	-1.715470000	0.000000000	-2.087023000
5	0.000000000	0.000000000	1.369781000
1	0.000000000	0.000000000	2.567312000

E = -1025.4052233 Hartree

Frequency Analysis:

Number of imaginary frequencies = 0

Lowest Frequency in cm^{-1} = 69

3.Al₄Li₄BH (C_{4v}) [Singlet]

#b3lyp/6-311++g**

13	0.000000000	1.867652000	0.246329000
13	1.867652000	0.000000000	0.246329000
13	0.000000000	-1.867652000	0.246329000
13	-1.867652000	0.000000000	0.246329000
3	-1.642361000	-1.642361000	-1.852685000
3	1.642361000	-1.642361000	-1.852685000
3	1.642361000	1.642361000	-1.852685000
3	-1.642361000	1.642361000	-1.852685000
5	0.000000000	0.000000000	1.370912000
1	0.000000000	0.000000000	2.568551000

E = -1025.403747 Hartree

Frequency Analysis:

Number of imaginary frequencies = 1

Lowest Frequency in cm^{-1} = -67

4. Al₄Li₄C (C_{2v}) [Singlet]

#b3lyp/6-311++g**

13	-1.313650000	1.299248000	0.323484000
13	1.313650000	1.299248000	0.323484000
13	1.313650000	-1.299248000	0.323484000
13	-1.313650000	-1.299248000	0.323484000
3	0.000000000	-2.637286000	-1.669908000
3	1.581938000	0.000000000	-2.210035000
3	0.000000000	2.637286000	-1.669908000
3	-1.581938000	0.000000000	-2.210035000
6	0.000000000	0.000000000	1.076415000

E = -1038.0347987 Hartree

Frequency Analysis:

Number of imaginary frequencies = 0

Lowest Frequency in cm⁻¹ = 98

5. Al₄Li₄C (C_{4v}) [Singlet]

#b3lyp/6-311++g**

13	0.000000000	1.844020000	0.329149000
13	1.844020000	0.000000000	0.329149000
13	0.000000000	-1.844020000	0.329149000
13	-1.844020000	0.000000000	0.329149000
3	-1.520476000	-1.520476000	-1.972732000
3	1.520476000	-1.520476000	-1.972732000
3	1.520476000	1.520476000	-1.972732000
3	-1.520476000	1.520476000	-1.972732000
6	0.000000000	0.000000000	1.092839000

$E = -1038.0320633$ Hartree

Frequency Analysis:

Number of imaginary frequencies = 1

Lowest Frequency in $\text{cm}^{-1} = -92$