

Supporting Information

Ab Initio Investigation on a New Class of Binuclear Superalkali

Cations $M_2Li_{2k+1}^+$ ($F_2Li_3^+$, $O_2Li_5^+$, $N_2Li_7^+$ and $C_2Li_9^+$)

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Table S1. Symmetry Point Group, Relative Energies E_{rel} (in kcal/mol), the Lowest Vibrational Frequencies (ν_1 , in cm^{-1}) of the F_2Li_3 species.

Isomer	Symmetry	E_{rel}	ν_1
1A	C_{2v}	0.00	136
1B	C_s	0.14	61
1C	D_{3h}	10.65	218

Table S2. Symmetry Point Group, Relative Energies E_{rel} (in kcal/mol), the Lowest Vibrational Frequencies (ν_1 , in cm^{-1}) of the O_2Li_5 species.

Isomer	Symmetry	E_{rel}	ν_1
2A	D_{3h}	0.00	52
2B	C_{2v}	4.57	68
2C	C_{2v}	18.56	36
2D	C_s	114.36	113
2E	C_s	24.31	15
2F	C_{2v}	130.95	30

Table S3. Symmetry Point Group, Relative Energies E_{rel} (in kcal/mol), the Lowest Vibrational Frequencies (ν_1 , in cm^{-1}) of the N_2Li_7 species.

Isomer	Symmetry	E_{rel}	ν_1
3A	C_{2v}	0.00	29
3B	C_{3v}	8.38	99
3C	C_s	21.84	97
3D	C_s	26.33	75
3E	C_2	34.19	80
3F	C_{5v}	64.09	41
3G	C_s	47.10	97

Table S4. Symmetry Point Group, Relative Energies E_{rel} (in kcal/mol), the Lowest Vibrational Frequencies (ν_1 , in cm^{-1}) of the C_2Li_9 species.

Isomer	Symmetry	E_{rel}	ν_1
4A	C_2	0.00	56
4B	C_1	4.55	66
4C	C_s	9.38	72
4D	D_{3h}	30.90	90
4E	C_s	27.30	19

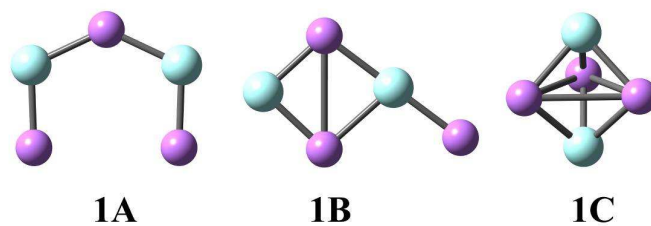


Figure S1. Three equilibrium structures of binuclear superalkali F_2Li_3 . Color legend: F, cyan; Li, purple.

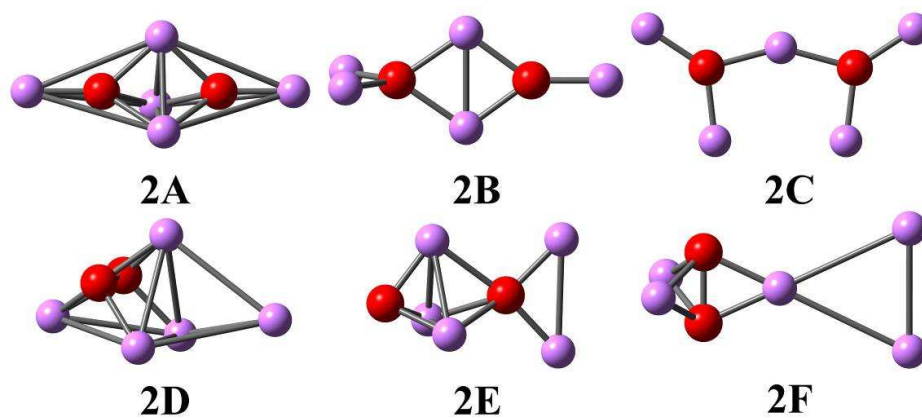


Figure S2. Six equilibrium structures of binuclear superalkali O_2Li_5 . Color legend: O, red; Li, purple.

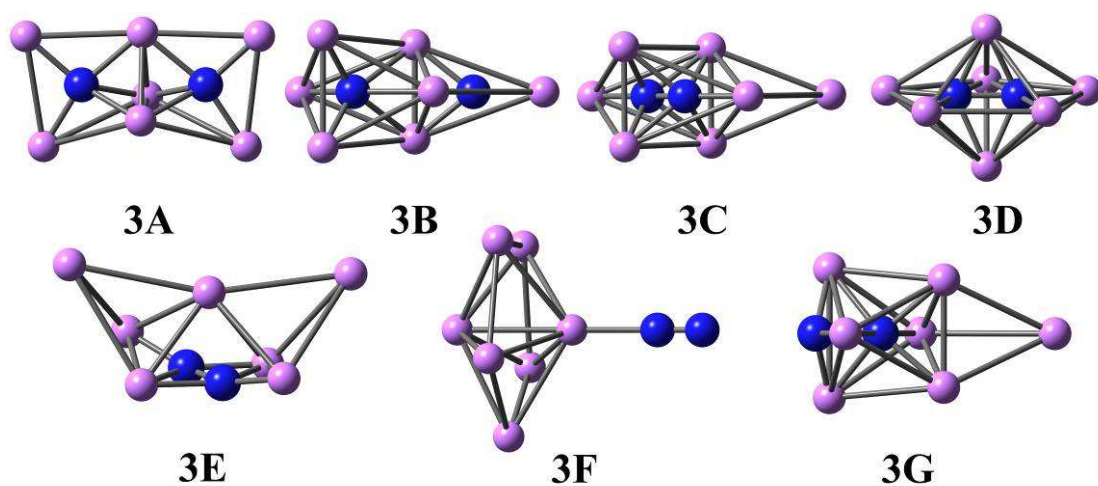


Figure S3. Seven equilibrium structures of binuclear superalkali N_2Li_7 . Color legend: N, blue; Li, purple.

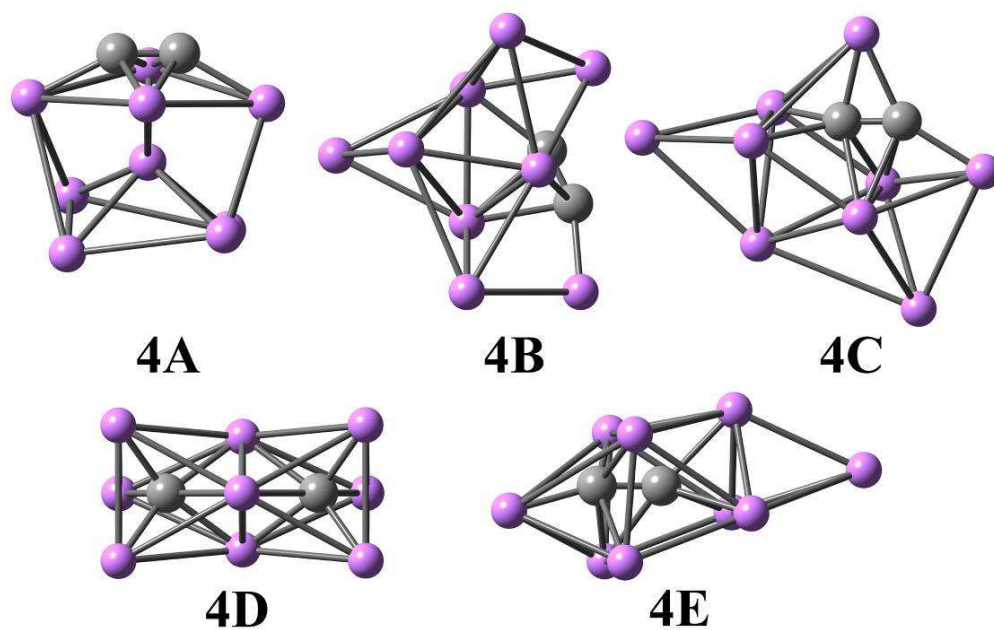


Figure S4. Five equilibrium structures of binuclear superalkali C_2Li_9 . Color legend: C, gray; Li, purple.