

Supporting Information

Prediction and Characterization of Novel Polynuclear Superalkali Cations

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Table S1. Fragmentation products and ZPVE-corrected dissociation energies (in kcal/mol) of the O_2Li_3^+ cations, obtained at the MP2/6-311+G(3df) level.

Isomer	$\text{O}_2\text{Li}_3^+ \rightarrow \text{O}_2\text{Li}_2^+ + \text{Li}^+$	$\text{O}_2\text{Li}_3^+ \rightarrow \text{Li}_3^+ + \text{O}_2$
A	30.1	134.2
B	-82.0	22.1

Table S2. Fragmentation products and ZPVE-corrected dissociation energies (in kcal/mol) of the CO_4Li_3^+ cations, obtained at the MP2/6-311+G(3df) level.

Isomer	$\text{CO}_4\text{Li}_3^+ \rightarrow \text{Li}_2\text{CO}_4 + \text{Li}^+$	$\text{CO}_4\text{Li}_3^+ \rightarrow \text{Li}_3\text{CO}_2^+ + \text{O}_2$	$\text{CO}_4\text{Li}_3^+ \rightarrow \text{Li}_3\text{O}_2^+ + \text{CO}_2$
A	67.6	112.1	11.8
B	66.5	111.1	10.8
C	64.6	109.1	8.8
D	57.6	102.2	1.9
E	55.4	99.9	-0.4
F	22.3	66.9	-33.4
G	24.0	68.6	-31.7

Table S3. Fragmentation products and ZPVE-corrected dissociation energies (in kcal/mol) of the $C_2O_4Li_3^+$ cations, obtained at the MP2/6-311+G(3df) level.

Isomer	$C_2O_4Li_3^+ \rightarrow Li_2C_2O_4 + Li^+$	$C_2O_4Li_3^+ \rightarrow Li_3C_2O_2^+ + O_2$	$C_2O_4Li_3^+ \rightarrow Li_3CO_2^+ + CO_2$
A	59.4	255.3	49.9
B	54.5	250.4	45.0
C	39.7	235.6	30.1
D	23.2	219.1	13.7
E	23.1	218.9	13.5
F	19.8	215.7	10.3

Table S4. Fragmentation products and ZPVE-corrected dissociation energies (in kcal/mol) of the $C_2O_6Li_3^+$ cations, obtained at the MP2/6-311+G(3df) level.

Isomer	$C_2O_6Li_3^+ \rightarrow Li_2C_2O_6 + Li^+$	$C_2O_6Li_3^+ \rightarrow Li_3C_2O_4^+ + O_2$	$C_2O_6Li_3^+ \rightarrow Li_3CO_4^+ + CO_2$
A	52.8	67.7	8.5
B	48.1	63.0	3.9
C	48.4	63.3	4.1
D	48.0	62.8	3.7
E	46.4	61.3	2.1
F	41.1	56.0	-3.1
G	38.9	53.8	-5.4
H	34.9	49.8	-9.4
I	30.4	45.3	-13.9

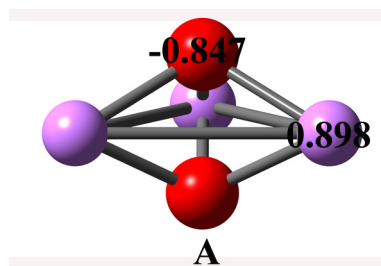


Figure S1. The NBO charges of the O_2Li_3^+ cations.

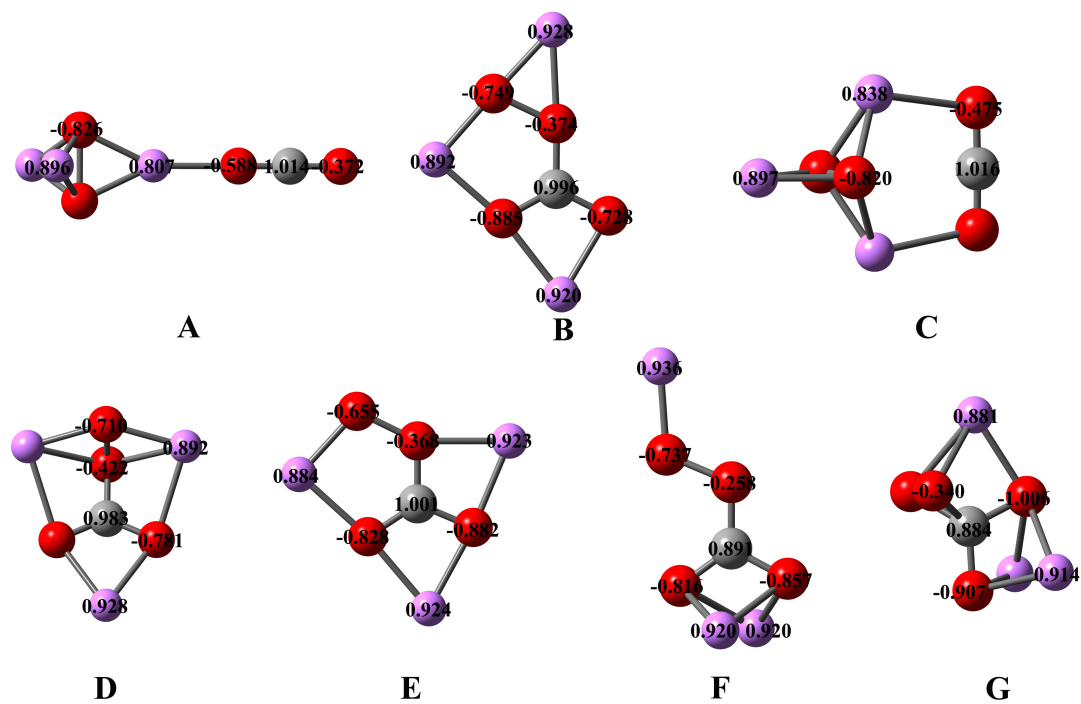


Figure S2. The NBO charges of the CO_4Li_3^+ cations.

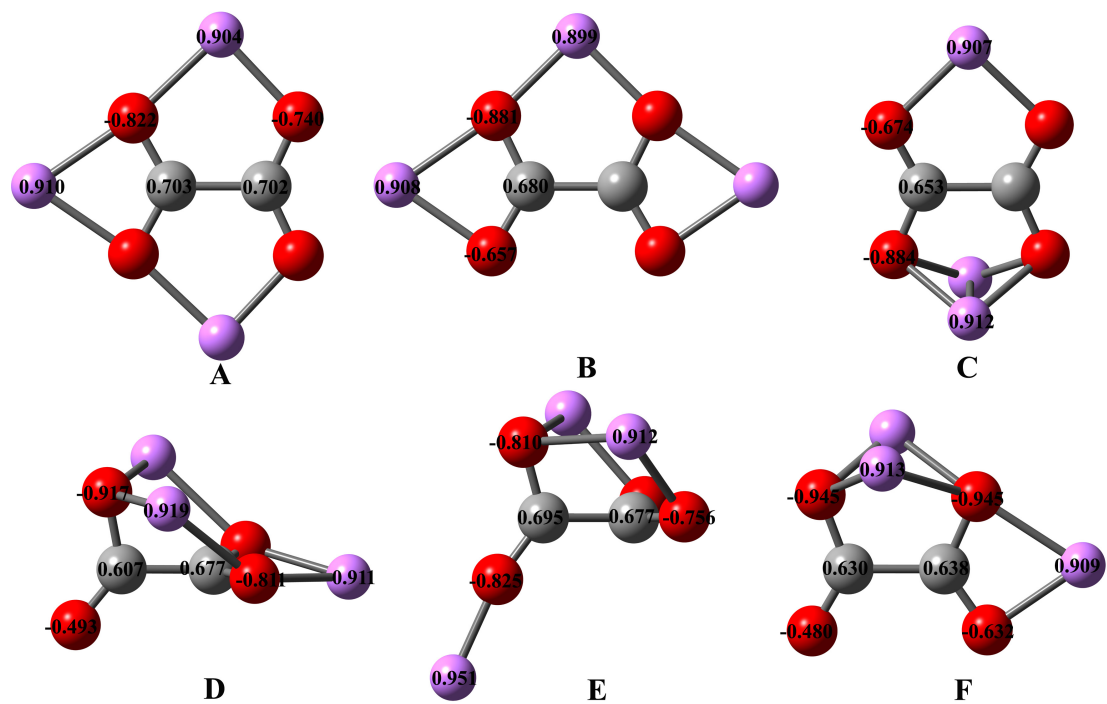


Figure S3. The NBO charges of the $C_2O_4Li_3^+$ cations.

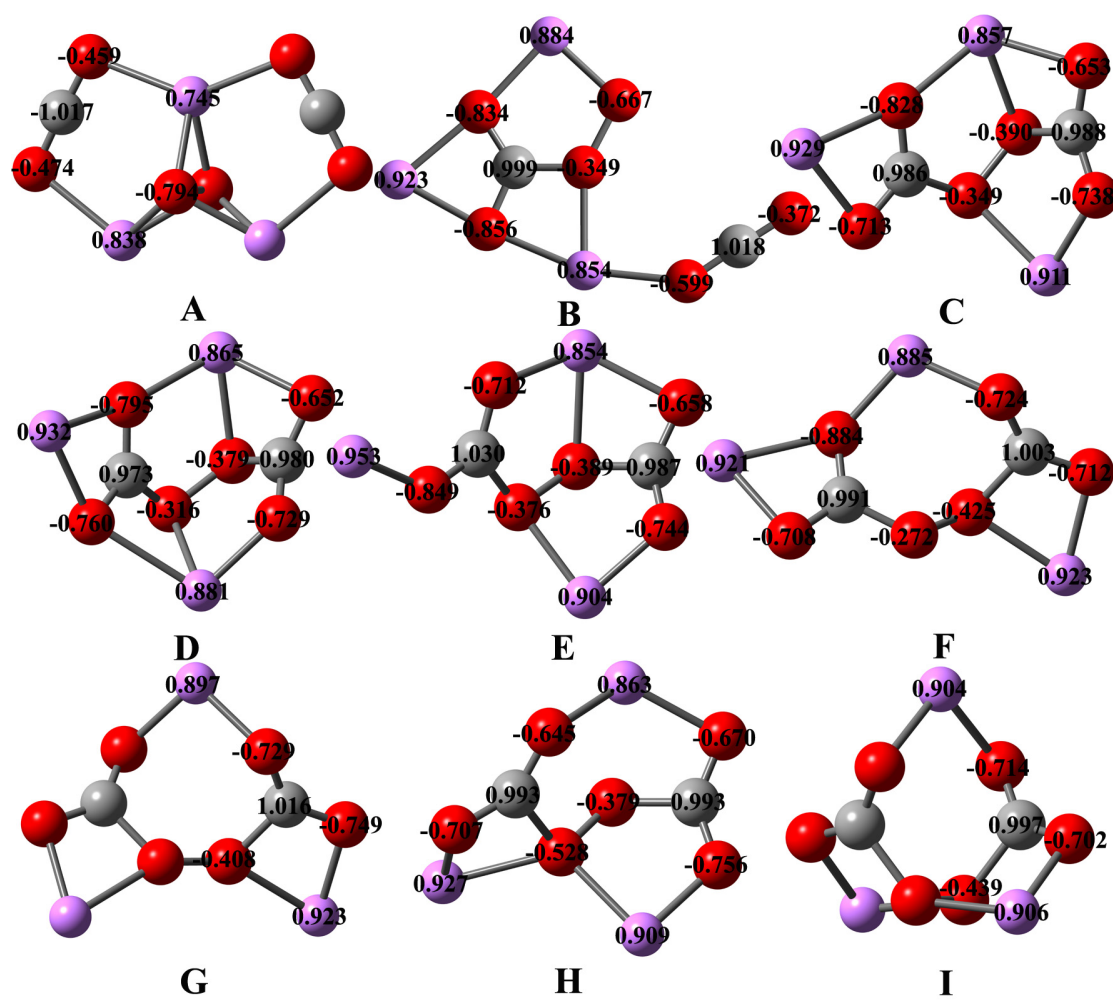


Figure S4. The NBO charges of the $C_2O_6Li_3^+$ cations