

## Remarkable NLO Responses of Hyperalkalized Species: Size Effect and Atomic Number Dependence

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### *Supplementary Information submitted to New Journal of Chemistry*

#### **Cartesian coordinates (X, Y, Z) of all structures considered in this study.**

Please note: Atoms are represented by respective atomic numbers.

<b>i.</b>	FLi <sub>2</sub> -F (a)			
	3	0.000000000	1.268312000	-0.107926000
	3	0.000000000	0.000000000	-2.919487000
	3	0.000000000	-1.268312000	-0.107926000
	9	0.000000000	0.000000000	1.045113000
<b>ii.</b>	FLi <sub>2</sub> -F (b)			
	3	0.000000000	1.757772000	0.000000000
	3	1.522275000	-0.878886000	0.000000000
	9	0.000000000	0.000000000	0.000000000
	3	-1.522275000	-0.878886000	0.000000000
<b>iii.</b>	FLi <sub>2</sub> -Na			
	3	0.000000000	1.287422000	-0.901972000
	3	0.000000000	-1.287422000	-0.901972000
	9	0.000000000	0.000000000	-2.027850000
	11	0.000000000	0.000000000	2.151135000
<b>iv.</b>	FLi <sub>2</sub> -K (a)			
	3	0.000000000	1.310268000	-1.657066000
	3	0.000000000	-1.310268000	-1.657066000
	9	0.000000000	0.000000000	-2.755138000
	19	0.000000000	0.000000000	1.828349000
<b>v.</b>	FLi <sub>2</sub> -K (b)			
	3	-1.391162000	1.242900000	1.433495000
	9	-1.391162000	0.261675000	0.000000000
	3	-1.391162000	1.242900000	-1.433495000
	19	1.098286000	-0.516446000	0.000000000
<b>vi.</b>	OLi <sub>3</sub> -Li (a)			
	8	0.000000000	0.000000000	0.739017000
	3	0.000000000	0.000000000	2.411121000
	3	0.000000000	1.226396000	-0.507769000
	3	0.000000000	-1.226396000	-0.507769000
	3	0.000000000	0.000000000	-3.366296000

<b>vii.</b>	OLi <sub>3</sub> -Li (b)			
	8	0.000000000	0.000000000	0.000000000
	3	1.020920000	1.020920000	1.020920000
	3	-1.020920000	-1.020920000	1.020920000
	3	1.020920000	-1.020920000	-1.020920000
	3	-1.020920000	1.020920000	-1.020920000
<b>viii.</b>	OLi <sub>3</sub> -Na (a)			
	8	0.000000000	0.000000000	-1.776472000
	3	0.000000000	0.000000000	-3.449755000
	3	0.000000000	1.245429000	-0.553262000
	3	0.000000000	-1.245429000	-0.553262000
	11	0.000000000	0.000000000	2.534601000
<b>ix.</b>	OLi <sub>3</sub> -Na (b)			
	8	0.000000000	0.000000000	-0.720612000
	3	0.000000000	1.685332000	-1.188926000
	3	1.459540000	-0.842666000	-1.188926000
	3	-1.459540000	-0.842666000	-1.188926000
	11	0.000000000	0.000000000	1.496839000
<b>x.</b>	OLi <sub>3</sub> -K (a)			
	8	0.000000000	0.000000000	-0.950014000
	3	0.000000000	0.000000000	-2.624621000
	3	0.000000000	-1.269810000	0.242503000
	3	0.000000000	1.269810000	0.242503000
	19	0.000000000	0.000000000	3.744243000
<b>xi.</b>	OLi <sub>3</sub> -K (b)			
	8	0.000000000	0.000000000	-1.201115000
	3	0.000000000	1.666593000	-1.726970000
	3	1.443312000	-0.833297000	-1.726970000
	3	-1.443312000	-0.833297000	-1.726970000
	19	0.000000000	0.000000000	1.323771000
<b>xii.</b>	NLi <sub>4</sub> -Li (a)			
	3	0.000000000	1.278959000	-0.664297000
	3	1.533450000	0.000000000	1.618977000
	3	-1.533450000	0.000000000	1.618977000
	3	0.000000000	-1.278959000	-0.664297000
	7	0.000000000	0.000000000	0.668750000
	3	0.000000000	0.000000000	-3.469777000
<b>xiii.</b>	NLi <sub>4</sub> -Li (b)			
	7	0.000000000	0.000000000	0.000000000
	3	0.000000000	0.000000000	1.924845000
	3	0.000000000	0.000000000	-1.924845000
	3	0.000000000	1.886489000	0.000000000
	3	-1.633747000	-0.943244000	0.000000000
	3	1.633747000	-0.943244000	0.000000000

<b>xiv.</b>	N <sub>Li4</sub> -Na (a)			
	3	0.000000000	1.304504000	-0.355708000
	3	-1.537575000	0.000000000	-2.604209000
	3	1.537575000	0.000000000	-2.604209000
	3	0.000000000	-1.304504000	-0.355708000
	7	0.000000000	0.000000000	-1.657652000
	11	0.000000000	0.000000000	2.669369000
<b>xv.</b>	N <sub>Li4</sub> -Na (b)			
	7	0.000000000	0.000000000	-0.662680000
	3	0.000000000	1.908310000	-0.571936000
	3	0.000000000	-1.908310000	-0.571936000
	3	1.550827000	0.000000000	-1.736283000
	3	-1.550827000	0.000000000	-1.736283000
	11	0.000000000	0.000000000	1.680734000
<b>xvi.</b>	N <sub>Li4</sub> -K			
	3	0.000000000	1.903026000	-1.125504000
	3	-1.571005000	0.000000000	-2.233977000
	3	1.571005000	0.000000000	-2.233977000
	3	0.000000000	-1.903026000	-1.125504000
	7	0.000000000	0.000000000	-1.199999000
	19	0.000000000	0.000000000	1.502994000