

Supplementary Information

Nonlinear Optical Switch Induced by External Electric Field: Inorganic

Alkaline-earth Alkalide

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Contents

Table S1 The geometrical parameters of $\text{Mg}(\text{NH}_3)_6\text{Na}_2$S2

Table S2 The geometrical parameters of $\text{Ca}(\text{NH}_3)_6\text{Na}_2$S2

Table S3 Natural population analysis charge on Na atoms $Q_{\text{Na}2}$ of $\text{M}(\text{NH}_3)_6\text{Na}_2$S2

Table S1 The geometrical parameters of $\text{Mg}(\text{NH}_3)_6\text{Na}_2$ at CAM-B3LYP/6-311++G(2d,2p) level.

$EEF(10^{-4}\text{a.u.})$	L(Å)	R1(Å)	R2(Å)	R3(Å)	R4(Å)
0	10.10361	3.08437	2.23366	2.23366	3.08437
10	10.11344	3.11612	2.23702	2.23044	3.06126
20	10.14431	3.16033	2.24019	2.22726	3.04605
30	10.20107	3.22046	2.24352	2.22412	3.03839
40	10.29523	3.30597	2.24697	2.22103	3.03893
50	10.45748	3.44346	2.25036	2.21807	3.05122
58	10.72265	3.64835	2.25277	2.21669	3.08731
60	10.83510	3.72813	2.25316	2.21694	3.10810
63	11.09980	3.92423	2.25397	2.27720	3.15295

Table S2 The geometrical parameters of $\text{Ca}(\text{NH}_3)_6\text{Na}_2$ at CAM-B3LYP/6-311++G(2d,2p) level.

$EEF(10^{-4}\text{a.u.})$	L(Å)	R1(Å)	R2(Å)	R3(Å)	R4(Å)
0	10.29636	3.09707	2.53116	2.53116	3.09707
10	10.30591	3.12976	2.53577	2.52669	3.07383
20	10.33623	3.17493	2.54055	2.52235	3.05868
30	10.39296	3.23711	2.54542	2.51811	3.05105
40	10.48970	3.32271	2.55054	2.51392	3.05153
50	10.67081	3.47586	2.55582	2.50967	3.06415
53	10.77546	3.53633	2.55669	2.50903	3.08164
60	11.13142	3.60012	2.55296	2.51768	3.23702
68	11.89544	3.74149	2.54774	2.53691	3.70137

Table S3 Natural population analysis charge on Na atoms Q_{Na_2} of $\text{M}(\text{NH}_3)_6\text{Na}_2$ at CAM-B3LYP/6-311++G(2d,2p) level.

$\text{Mg}(\text{NH}_3)_6\text{Na}_2$		$\text{Ca}(\text{NH}_3)_6\text{Na}_2$	
$EEF(10^{-4}\text{a.u.})$	Q_{Na_2}	$EEF(10^{-4}\text{a.u.})$	Q_{Na_2}
0	-0.776	0	-0.904
10	-0.772	10	-0.900
20	-0.761	20	-0.787
30	-0.735	30	-0.859
40	-0.717	40	-0.837
50	-0.695	50	-0.811
58	-0.698	53	-0.822
60	-0.717	60	-0.941
63	-0.747	68	-1.055