Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

A Novel Class of Compounds—Superalkalides: $M^+(en)_3M'_3O^-$ (M, M'= Li, Na, and K; en = Ethylenediamine) with Excellent Nonlinear Optical Properties and High Stabilities

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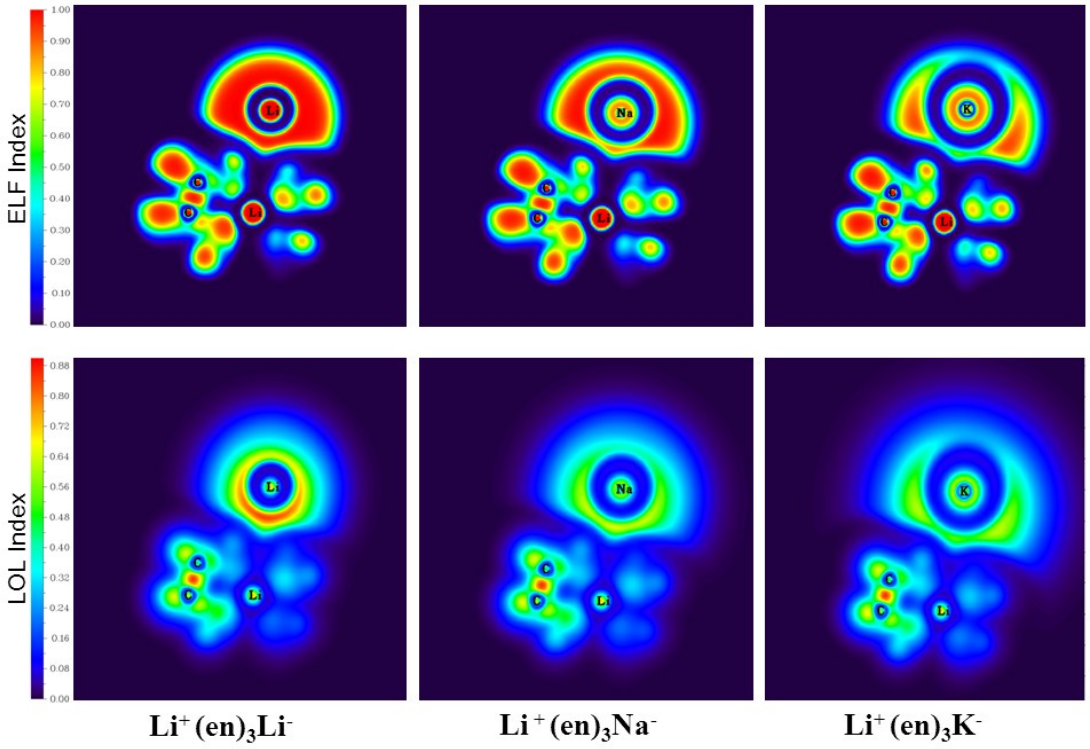
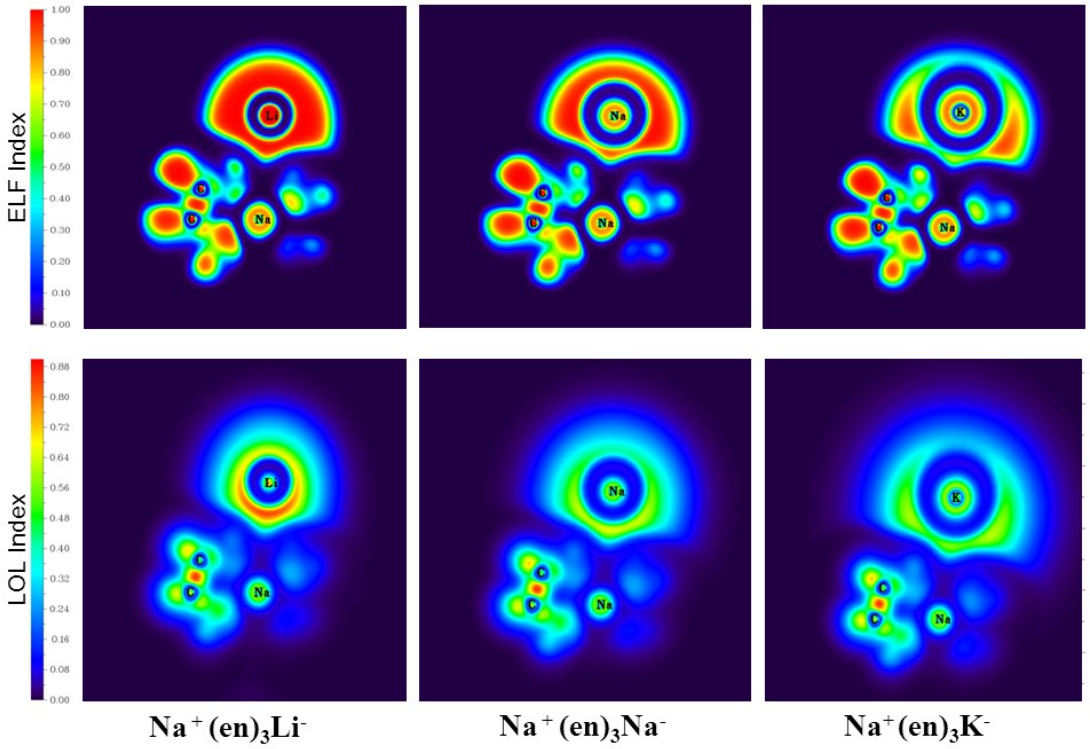
Figure S1. Cut-plane ELF and LOL of $M^+(en)_3M'^-$ and $M^+(en)_3M'_3O^-$(M, M'=Li, Na, and K) molecules.

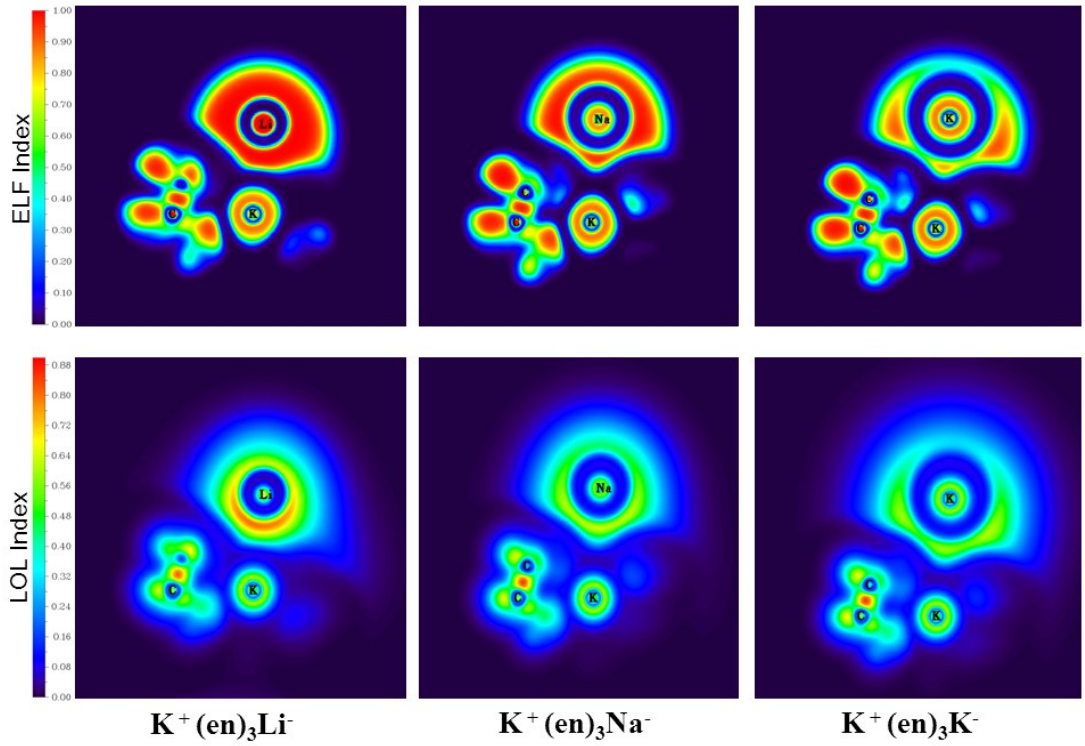
Figure S2. Crucial transition states of $M^+(en)_3M'^-$ and $M^+(en)_3M'_3O^-$ (M, M'=Li, Na, and K) molecules, where component coefficient percentage is marked.



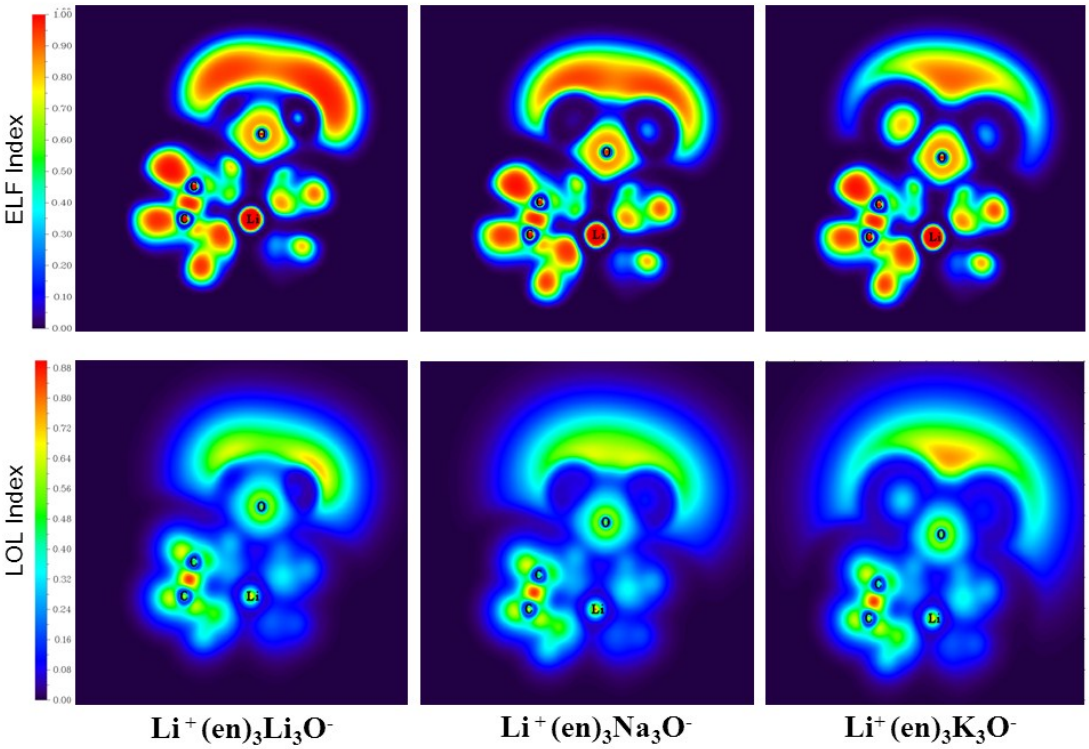
$Li^+(en)_3Li^-$ $Li^+(en)_3Na^-$ $Li^+(en)_3K^-$



$Na^+(en)_3Li^-$ $Na^+(en)_3Na^-$ $Na^+(en)_3K^-$



$K^+(en)_3Li^-$ $K^+(en)_3Na^-$ $K^+(en)_3K^-$



$Li^+(en)_3Li_3O^-$ $Li^+(en)_3Na_3O^-$ $Li^+(en)_3K_3O^-$

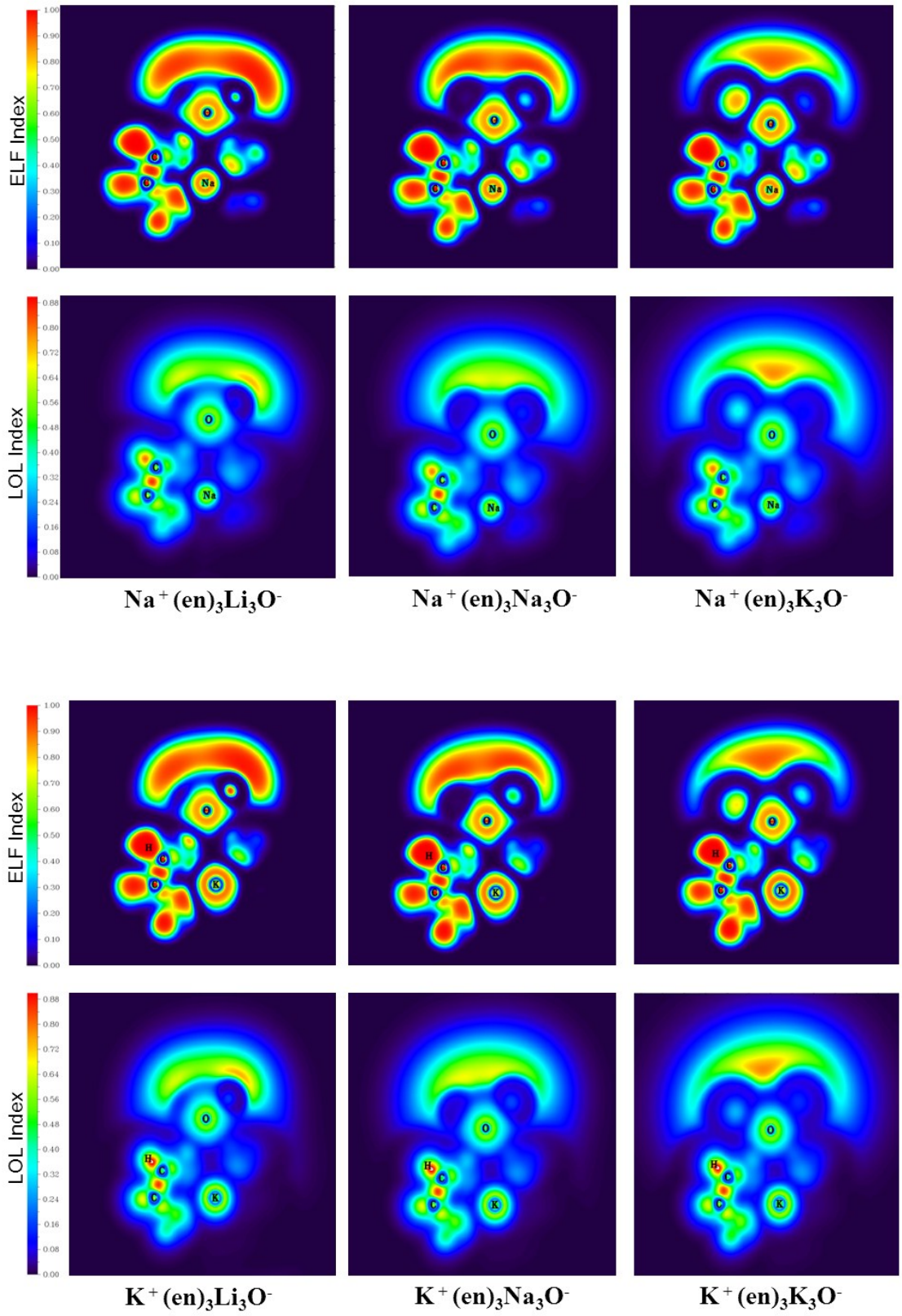


Figure S1. Cut-plane ELF and LOL of $M^{+}(en)_3M'^{-}$ and $M^{+}(en)_3M'_3O^{-}$(M, M' = Li, Na, and K) molecules.

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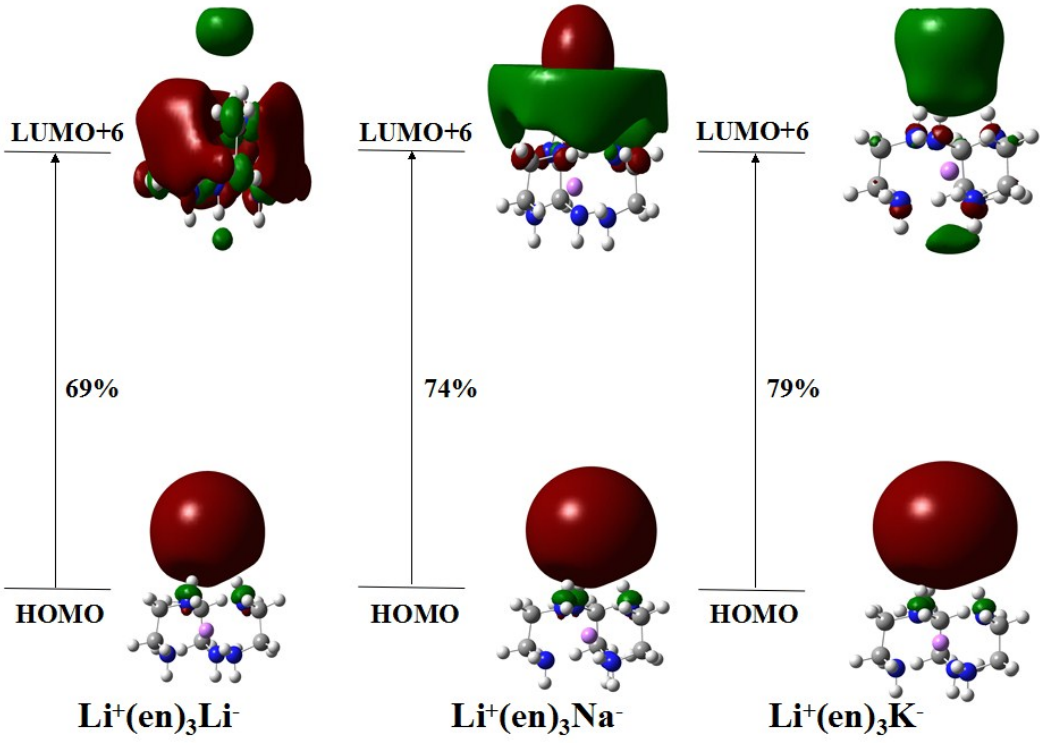
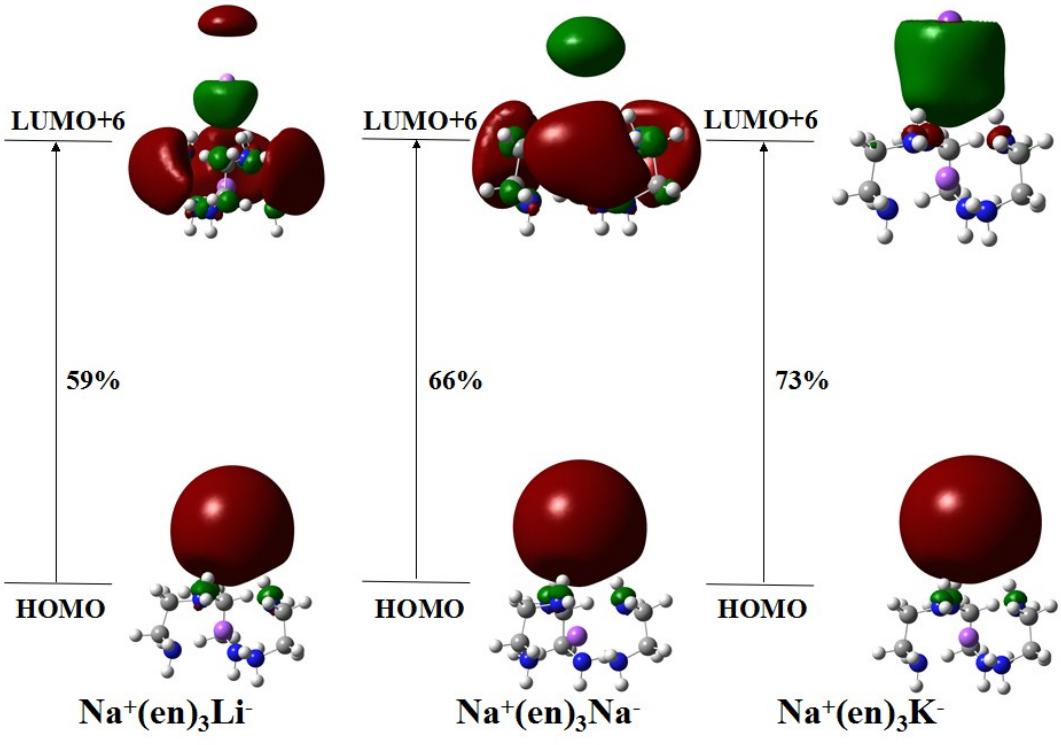
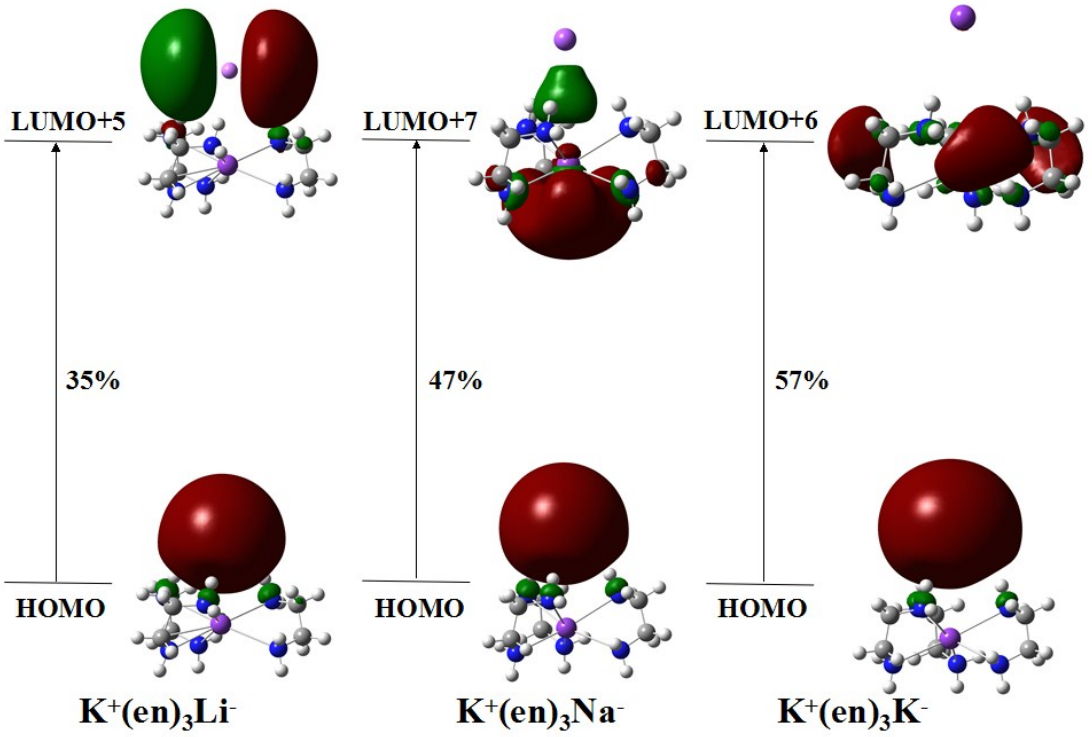
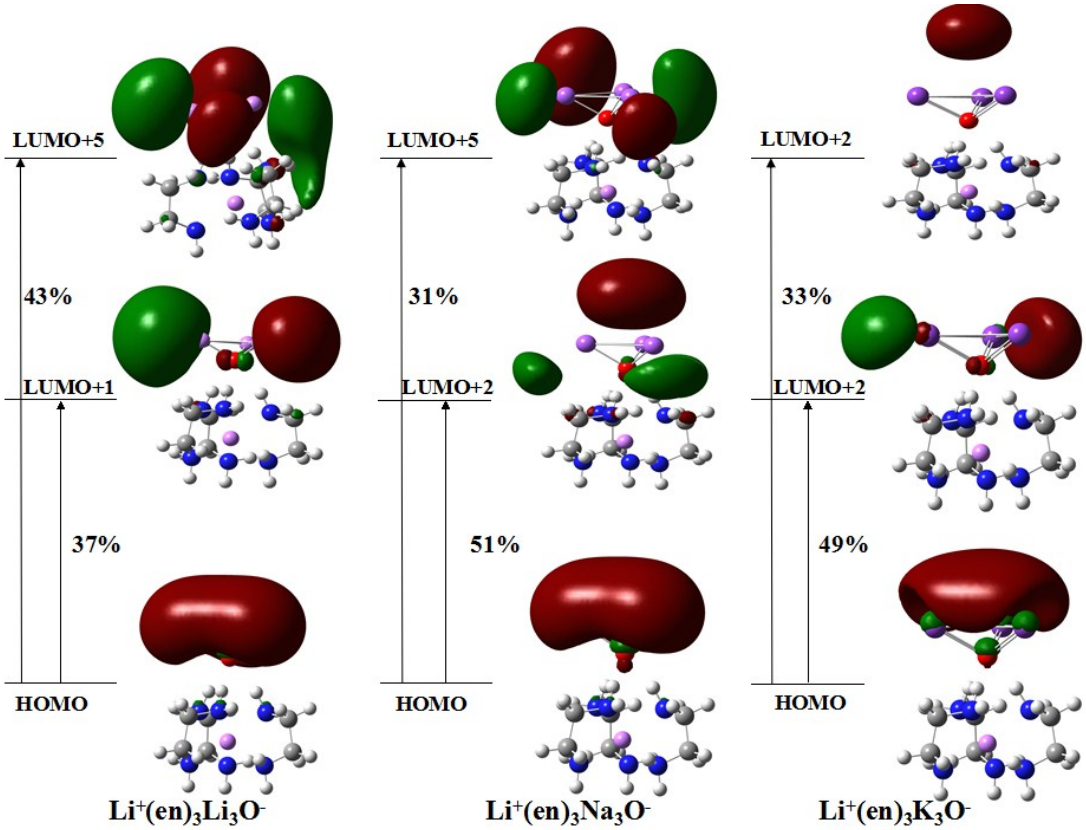


$Li^+(en)_3Li^-$ $Li^+(en)_3Na^-$ $Li^+(en)_3K^-$



$Na^+(en)_3Li^-$ $Na^+(en)_3Na^-$ $Na^+(en)_3K^-$


LUMO+5
35%
HOMO
K+(en)3Li-
LUMO+7
47%
HOMO
K+(en)3Na-
LUMO+6
57%
HOMO
K+(en)3K-


LUMO+5
43%
LUMO+1
37%
HOMO
Li+(en)3Li3O-
LUMO+5
31%
LUMO+2
51%
HOMO
Li+(en)3Na3O-
LUMO+2
33%
LUMO+2
49%
HOMO
Li+(en)3K3O-

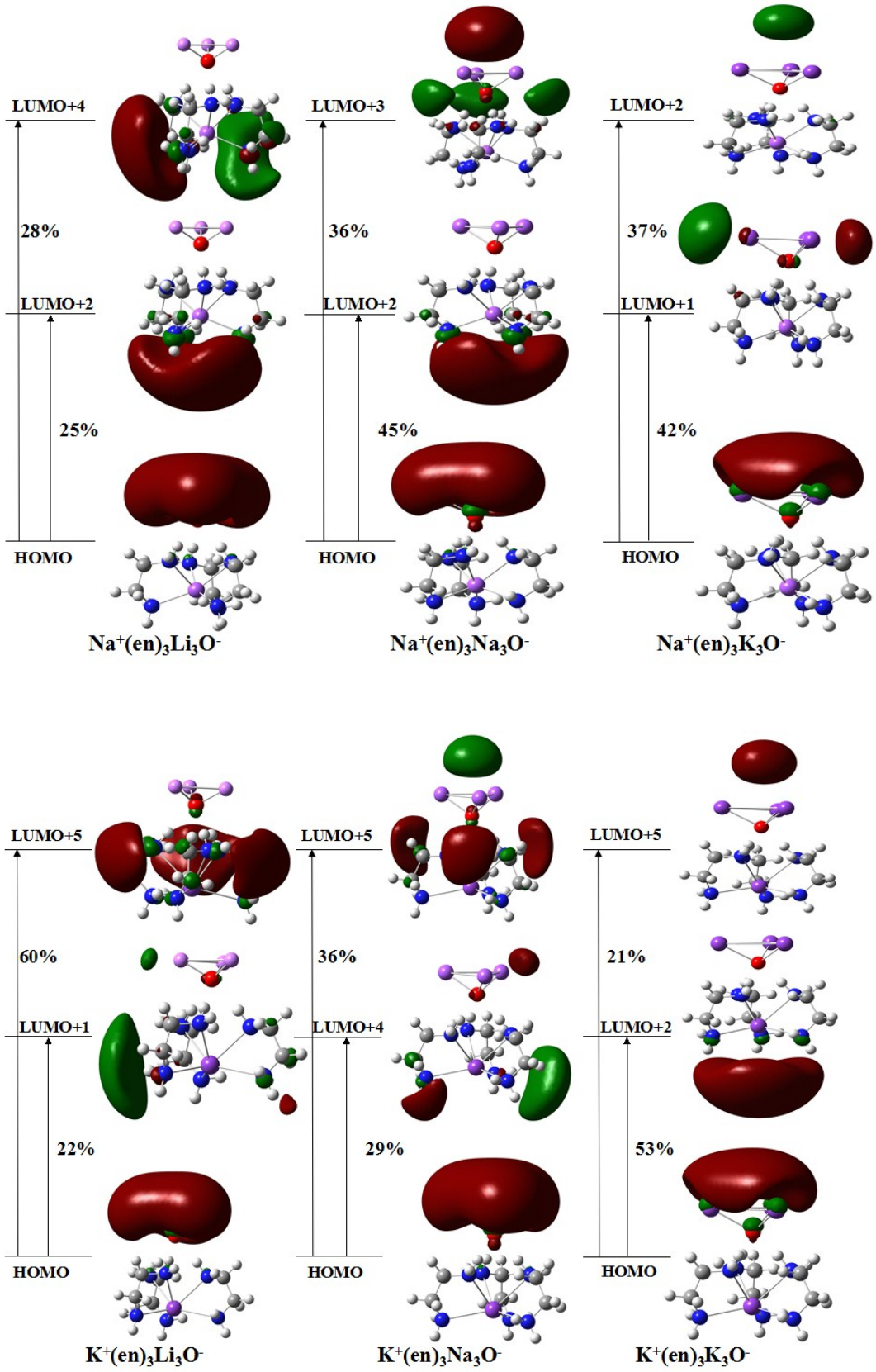


Figure S2. Crucial transition states of $M^{+}(en)_3M'^{-}$ and $M^{+}(en)_3M'_3O^{-}$ (M, M' = Li, Na, and K) molecules, where component coefficient percentage is marked. The isovalues of the corresponding MO isosurfaces are 0.02.