Supplementary data

Prediction and characterization of a new kind of alkali-superhalogen species with considerable stability: $M\text{BeX}_3$ ($M = \text{Li, Na}$; $X = \text{F, Cl, Br}$)

Song-Hua Cui, Ying Li, Fang-Fang Wang, Di Wu,* Zhi-Ru Li

State Key Laboratory of Theoretical and Computational Chemistry, Institute of Theoretical Chemistry, Jilin University, Changchun, 130023, China    Email: wud@mail.jlu.edu.cn

Figure S1. The optimized geometries (bond lengths in Å, bond angles in degrees), the Laplacian of the electron density at a bond critical point $\nabla^2 \rho(r)$ (au.) of the NaBeX$_3$ ($X = \text{F, Cl, Br}$) species.