Electronic Supplementary Material (ESI) for RSC Advances.

Supporting information

First-principles study on the mechanical and electronic properties of energetic molecular perovskites $AM(ClO_4)_3$ (A = $C_6H_{14}N_2^{2+}$, $C_4H_{12}N_2^{2+}$, $C_6H_{14}N_2O^{2+}$; M = Na^+, K^+)

Qiaoli Li[a], Shenshen Li[a], Jijun Xiao[a,*]

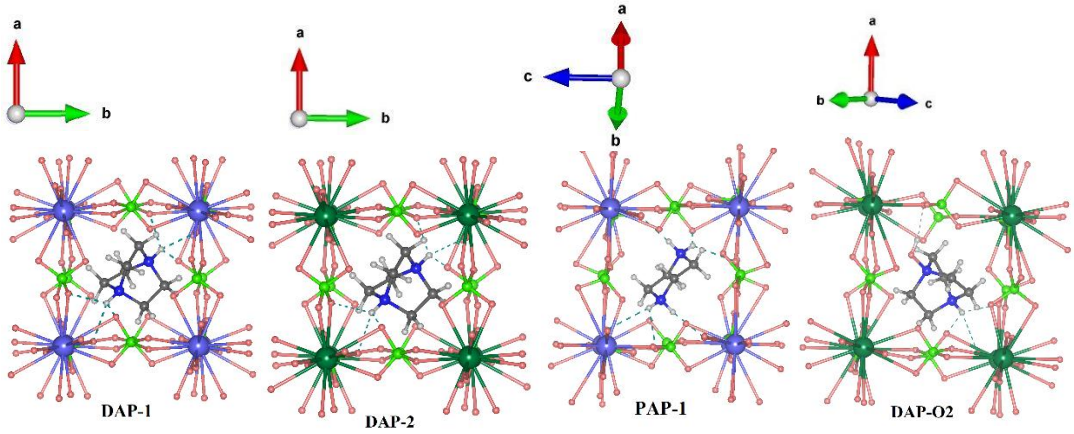

Figure S1. Cage structures of $AM(ClO_4)_3$. H atom in light grey, C atom in dark gray, N atom in blue, O atom in pink, Cl atom in green, Na atom in purple, K atom in dark green. Hydrogen bonds are represented by dashed lines.

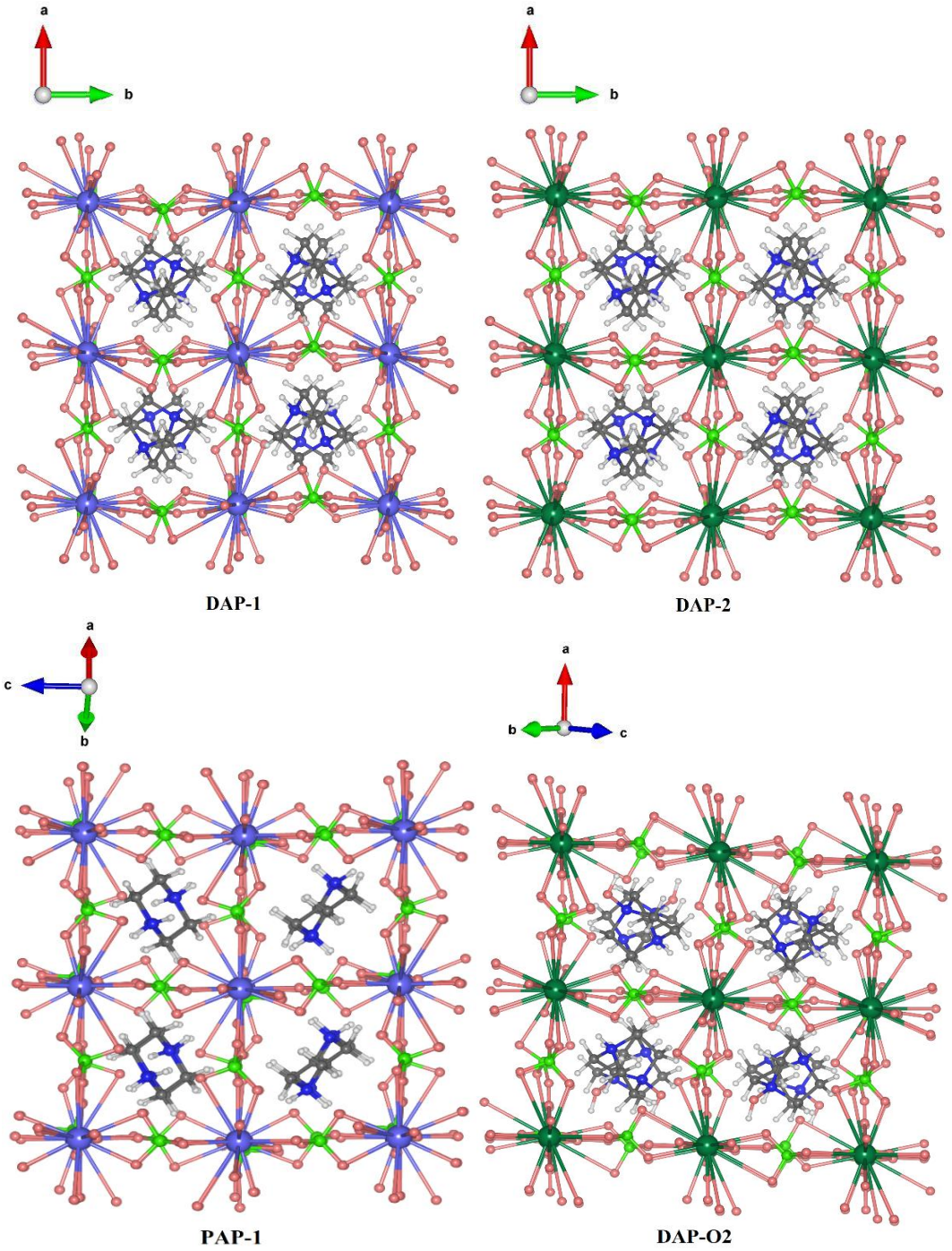

Figure S2. Packing structures of $AM(ClO_4)_3$. H atom in light grey, C atom in dark gray, N atom in blue, O atom in pink, Cl atom in green, Na atom in purple, K atom in dark green.

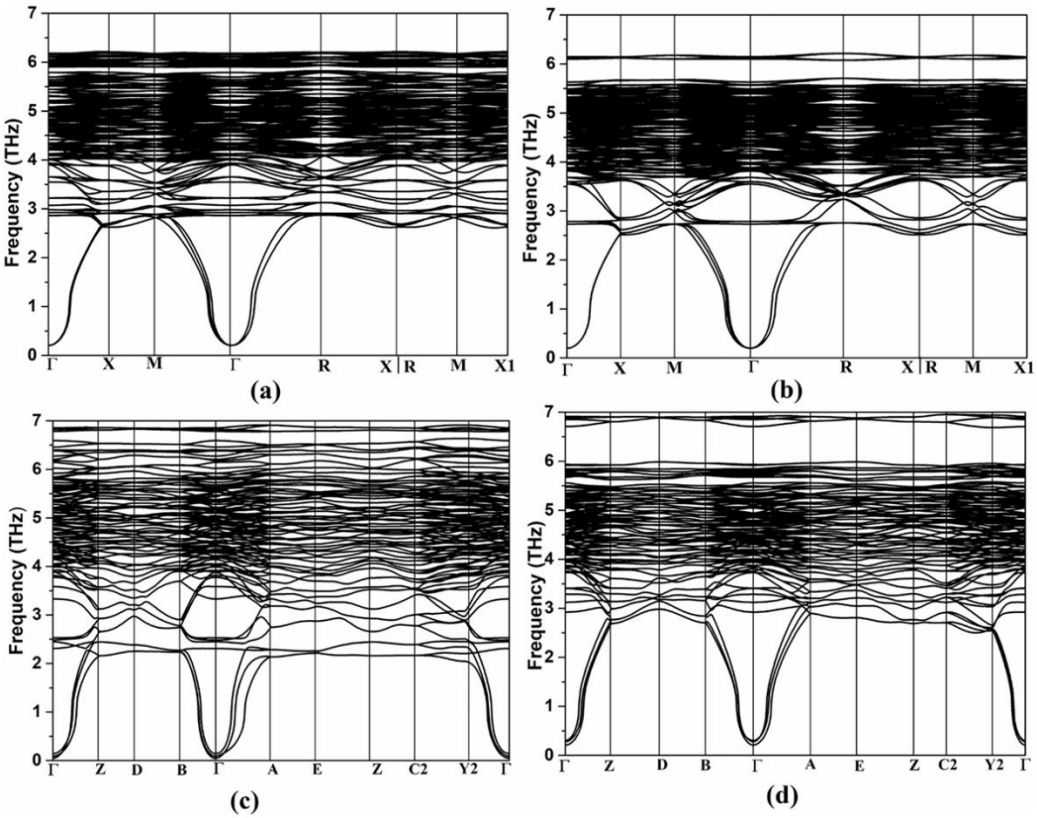

Figure S3. Phonon dispersion curves of (a) DAP-1, (b) DAP-2, (c) PAP-1 and (d) DAP-O2.