Supporting Information for

New Germanate and Mixed Cobalt Germanate Salt Inclusion Materials:
$[(Rb_6F)(Rb_4F)][Ge_{14}O_{32}]$ and
$[(Rb_6F)(Rb_{3.1}Co_{0.9}F_{0.96})][Co_{3.8}Ge_{10.2}O_{30}F_2]$
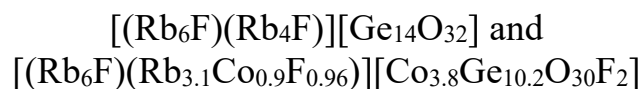
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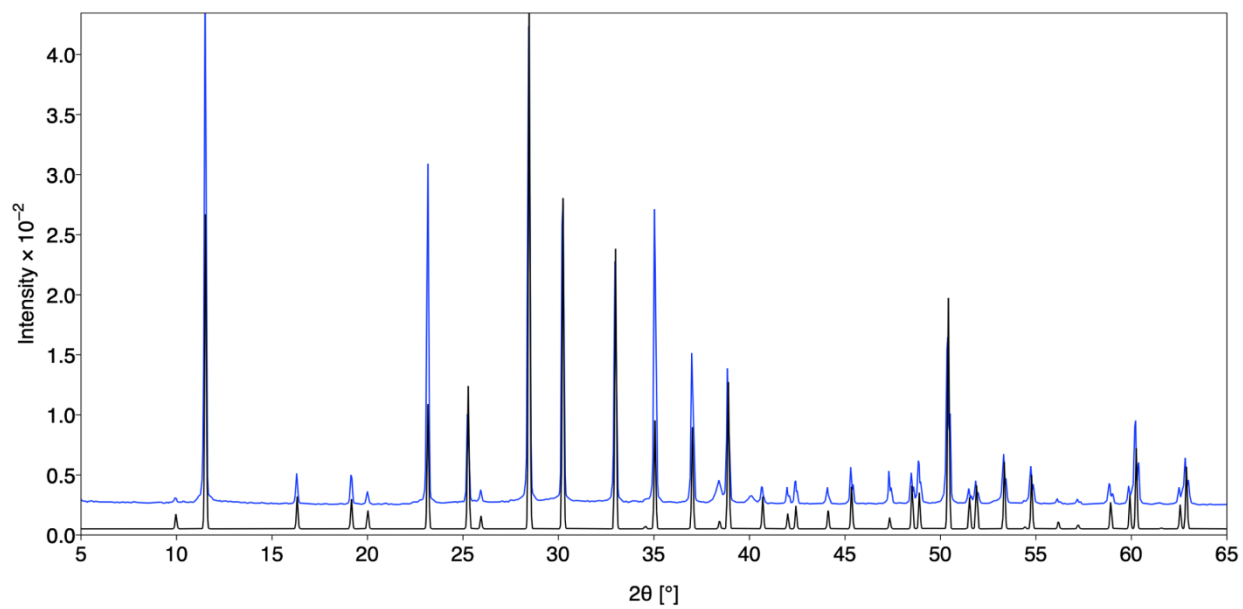
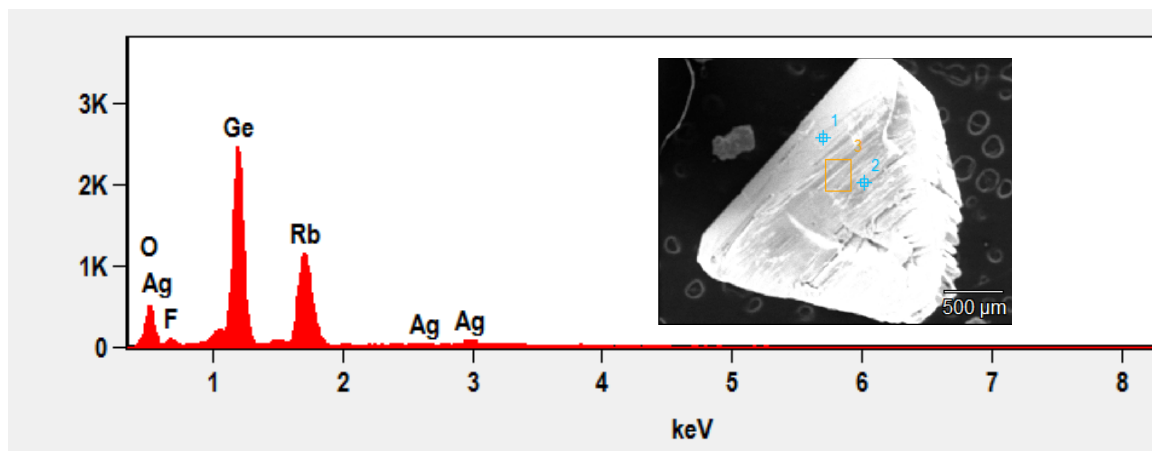Figure S1. PXRD pattern of $[(Rb_6F)(Rb_4F)][Ge_{14}O_{32}]$

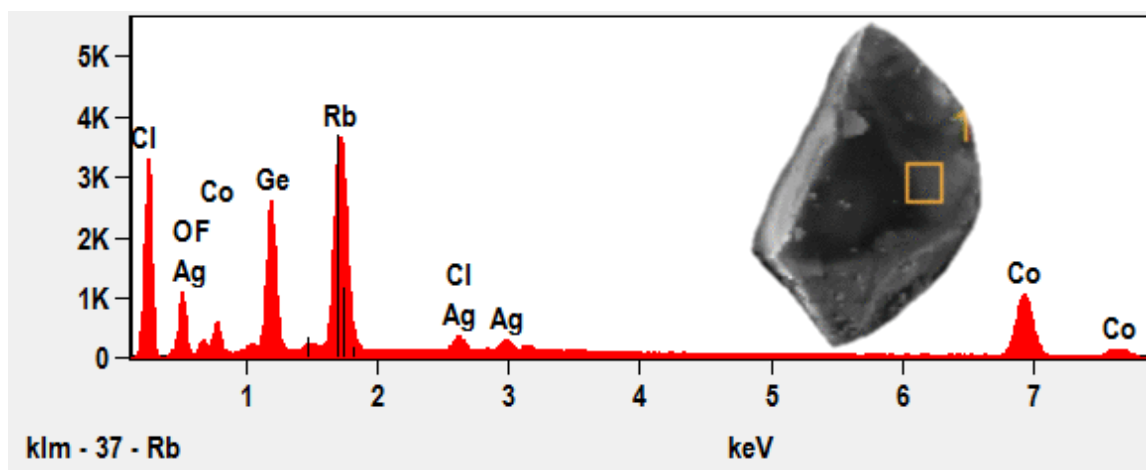Figure S2. EDS spectrum and SEM image of $[(Rb_6F)(Rb_4F)][Ge_{14}O_{32}]$.

Figure S3. EDS spectrum and SEM image of $[(Rb_6F)(Rb_{3.1}Co_{0.9}F_{0.96})][Co_{3.8}Ge_{10.2}O_{30}F_2]$.

To check if the initially used super quasirandom structure (SQS) is good enough, we generated additional SQS where the position of the atoms in the partially occupied sites was chosen completely random, oppose to using the mcsqs as for the initial SQS. The second SQS was relaxed using the same method, in both high-spin (HS) and low-spin (LS) magnetic ordering. In the case of the second SQS, the HS phase is more stable be -5.5 meV/atom compared to the LS phase. More importantly, both HS and LS phases are significantly less stable (have more positive energy) by 63 meV/atom and 73 meV/atom, respectively, compared to the respective initial SQS phases. Furthermore, the atomic positions in the second SQS are significantly distorted from the crystallographically determined atomic positions and the atomic positions in the initial SQS. This distortion of atoms gives rise to a much structured DOS compared to the DOS of the initial SQS, where impurity states in the band gap of the initial SQS can be seen (see Figure S4).
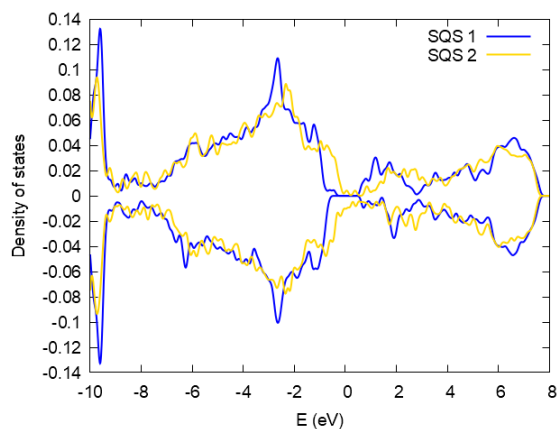

Figure S4. Density of states of the relaxed initial (SQS 1) and second (SQS 2) SQS, shown in blue and yellow, respectively.