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Structure and superconductivity in the 1144 type compounds of AeAFe₄As₄ (Ae = Ca, Sr, A = K, Rb, Cs)¹

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The Fe-based superconductors discovered in 2008 have attracted significant research interest, because of their rich material variety as well as their high superconducting transition temperatures (T_c). A large number of related Fe-based superconductors with various types of crystal structures have been found to date. Here, we report new-structure-type Fe-based superconductors AeAFe₄As₄ (Ae = Ca, Sr, A = K, Rb, or Cs), which can be regarded as hybrid phases between AeFe₂As₂ and AFe₂As₂. Unlike solid solutions such as (Ba_{1-x}K_x)Fe₂As₂ and (Sr_{1-x}Na_x)Fe₂As₂, the Ae and A do not occupy crystallographically equivalent sites, owing to large differences between their ionic radii. Rather, the Ae and A layers are inserted alternately between the Fe₂As₂ layers in the *c*-axis direction in AeAFe₄As₄ (AeA1144). The ordering of the Ae and A layers causes a change in space group from I4/mmm to P4/mmm, which is clearly apparent in powder X-ray diffraction patterns. AeA1144 is the first known structure among not only Fe-based superconductors, but also other materials. The AeA1144 is formed as a stoichiometric compound. Therefore, each AeA1144 has its own T_c of approximately 31–36 K.

¹This study has been done in collaboration with IMRA Material RD Co., Ltd.