Supplementary Information

KCaEr₂CuS₅: A New Pentanary Rare-Earth Layered Chalcogenide without Substitutional Disorder

Hui-Yi Zeng,^{a,b} Hansjürgen Mattausch,^b Arndt Simon,^b Fa-Kun Zheng,^a Zhen-Chao Dong,^{*a,c}
Guo-Cong Guo,^{*a} Jin-Shun Huang^a

a State Key Laboratory of Structural Chemistry, Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences, Fuzhou, Fujian 350002, P. R. China

b Max Planck Institute for Solid State Research, Heisenbergstrasse 1, D-70569 Stuttgart, Germany

c Hefei National Laboratory for Physical Sciences at Microscale, University of Science and Technology of China, Hefei, Anhui 230026, P. R. China

Figure S1. Optical absorption spectrum of KCaEr₂CuS₅ transformed from diffuse reflectance data.

Figure S2. Far-IR spectrum of KCaEr₂CuS₅ (600-200 cm⁻¹).

Table S1. Anisotropic displacement parameters for KCaEr₂CuS₅, $U_{12}=U_{13}=0$.

Name	U_{11}	U_{22}	U_{33}	U_{23}
Er	0.0039(3)	0.0086(3)	0.0077(3)	0.0006(5)
Cu	0.011(2)	0.012(2)	0.010(2)	0
Ca	0.002(2)	0.009(2)	0.010(2)	0.000(2)
K	0.014(3)	0.007(3)	0.033(4)	0
S(1)	0.006(3)	0.011(3)	0.008(3)	0
S(2)	0.007(2)	0.013(2)	0.011(2)	0.005(2)
S(3)	0.004(2)	0.007(2)	0.008(2)	0.001(2)

The form of the anisotropic displacement parameter is:

$$\exp[-2\pi^2\{h^2a^{*2}U_{11}+k^2b^{*2}U_{22}+l^2c^{*2}U_{33}+2hla^*b^*U_{12}+2hla^*c^*U_{13}+2klb^*c^*U_{23}\}]$$