Electronic Supplementary Material (ESI) for Dalton Transactions.

Thermoelectric properties of (Ba,K)Cd_2As_2 crystallized in the $CaAl_2Si_2$-type structure

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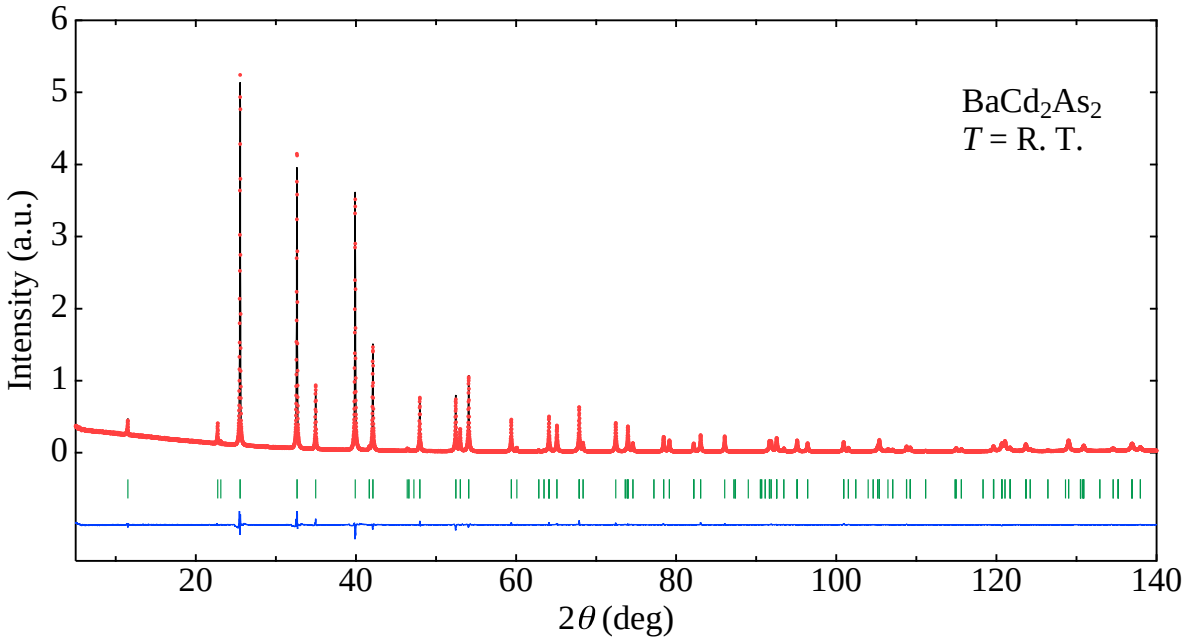

FIG. S1. Observed (red dots) and calculated (solid black line) x-ray powder diffraction patterns for $BaCd_2As_2$ at room temperature. Vertical bars show the calculated positions of the diffraction peaks for $BaCd_2As_2$. The solid line at the bottom indicates the difference between observations and calculations.

Atom	Site	g	x	y	z	B (Å^2)
$BaCd_2As_2$						
a = 4.5142(5) Å, c = 7.6905(7) Å, R_{wp} = 5.46 %						
Ba	1a	1	0	0	0	0.21(2)
Cd	2d	1	1/3	2/3	0.62892(6)	0.59(2)
As	2d	1	1/3	2/3	0.2632(1)	0.34(2)
$Ba_{0.99}K_{0.01}Cd_2As_2$						
a = 4.5146(4) Å, c = 7.6930(5) Å, R_{wp} = 5.22 %						
Ba	1a	0.99	0	0	0	0.10(2)
K	1a	0.01	0	0	0	B_{Ba}
Cd	2d	1	1/3	2/3	0.62885(6)	0.40(2)
As	2d	1	1/3	2/3	0.26271(9)	0.18(2)
$Ba_{0.98}K_{0.02}Cd_2As_2$						
a = 4.5151(4) Å, c = 7.6980(5) Å, R_{wp} = 5.40 %						
Ba	1a	0.98	0	0	0	0.16(2)
K	1a	0.02	0	0	0	B_{Ba}
Cd	2d	1	1/3	2/3	0.62895(6)	0.44(2)
As	2d	1	1/3	2/3	0.26266(9)	0.23(2)
$Ba_{0.97}K_{0.03}Cd_2As_2$						
a = 4.5143(4) Å, c = 7.7021(5) Å, R_{wp} = 5.45 %						
Ba	1a	0.97	0	0	0	0.25(2)
K	1a	0.03	0	0	0	B_{Ba}
Cd	2d	1	1/3	2/3	0.62910(6)	0.57(2)
As	2d	1	1/3	2/3	0.26270(9)	0.36(2)
$Ba_{0.96}K_{0.04}Cd_2As_2$						
a = 4.5138(4) Å, c = 7.7061(5) Å, R_{wp} = 5.77 %						
Ba	1a	0.96	0	0	0	0.38(2)
K	1a	0.04	0	0	0	B_{Ba}
Cd	2d	1	1/3	2/3	0.62890(6)	0.72(2)
As	2d	1	1/3	2/3	0.2626(1)	0.45(2)
$Ba_{0.92}K_{0.08}Cd_2As_2$						
a = 4.5119(4) Å, c = 7.7129(5) Å, R_{wp} = 6.56 %						
Ba	1a	0.92	0	0	0	0.35(2)
K	1a	0.08	0	0	0	B_{Ba}
Cd	2d	1	1/3	2/3	0.62966(7)	0.80(2)
As	2d	1	1/3	2/3	0.2637(1)	0.62(2)

FIG. S2. Atomic parameters for $Ba_{1-x}K_xCd_2As_2$ (space group $P\bar{3}m1$) determined by Rietveld refinements. The quantities g and B are the site occupancy and the isotropic atomic displacement parameters. The isotropic atomic displacement parameters of K atoms are constrained to be those of Ba atoms (B_{Ba}).

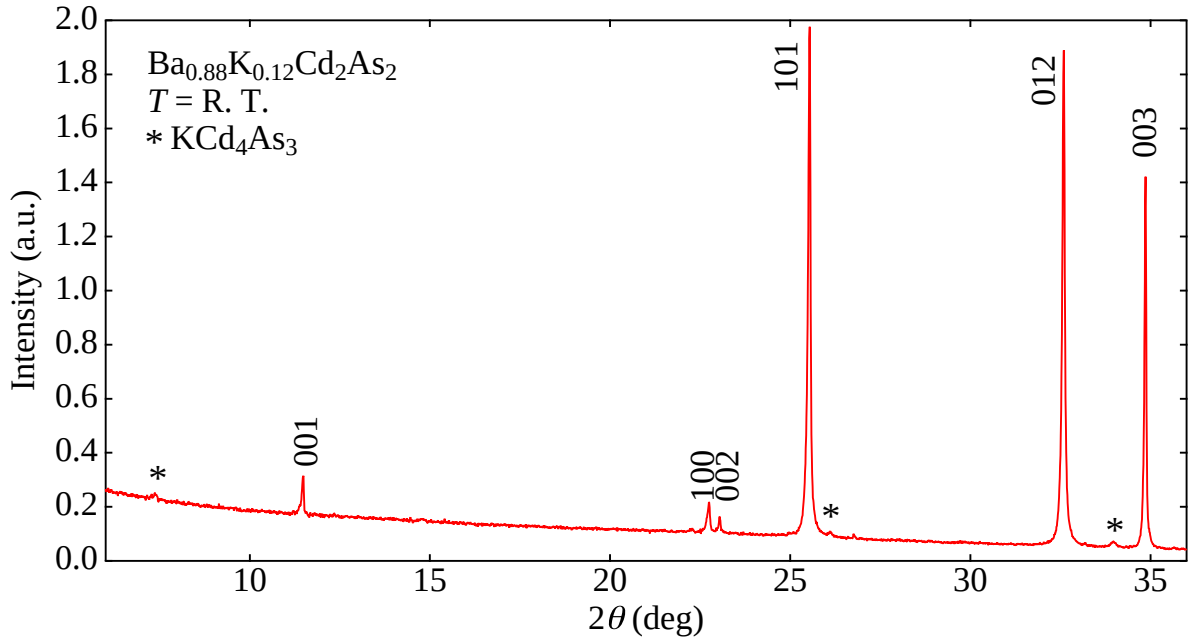

FIG. S3. X-ray diffraction pattern for $Ba_{0.88}K_{0.12}Cd_2As_2$ at room temperature. KCd_4As_3 appears as an impurity phase.

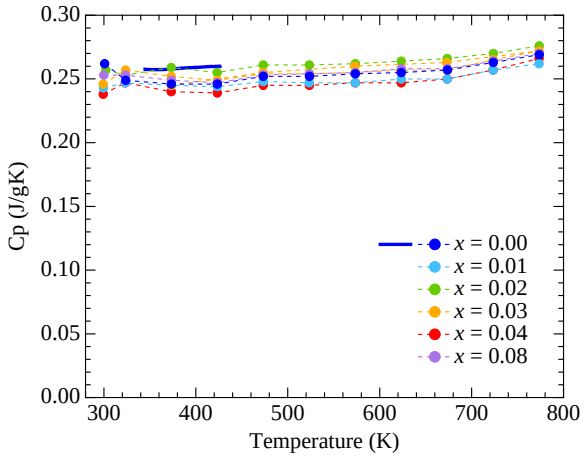

FIG. S4. Temperature dependence of the specific heat for $Ba_{1-x}K_xCd_2As_2$ measured by the laser-flash method (circles) and the differential scanning calorimetry (solid line).