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Supporting Information

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$K_7B_7Si_{39}$, a Borosilicide with the Clathrate-I Structure?

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S1: Scanning Electron Microscopy

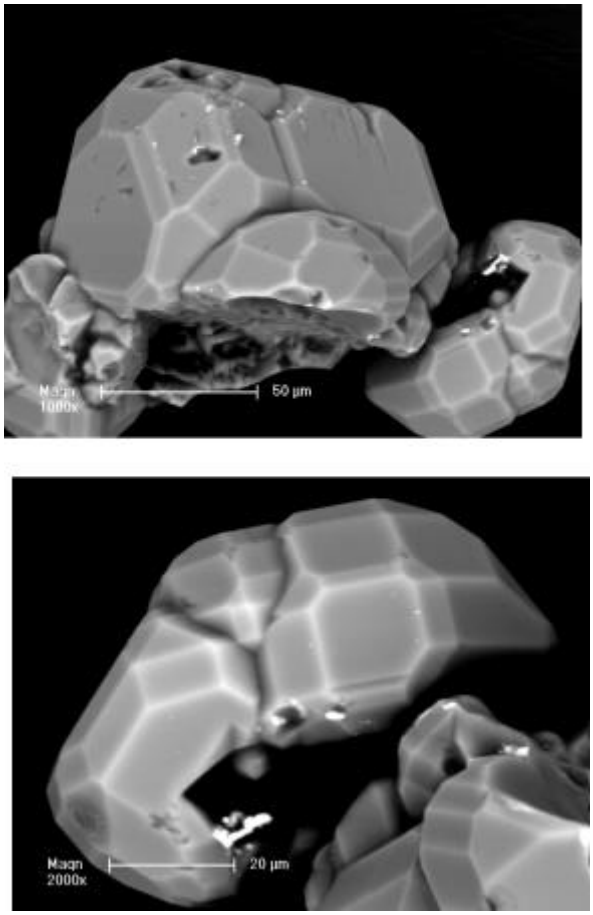

Fig. S1. SEM images of $K_7B_7Si_{39}$ cystals.

S2: EDXS

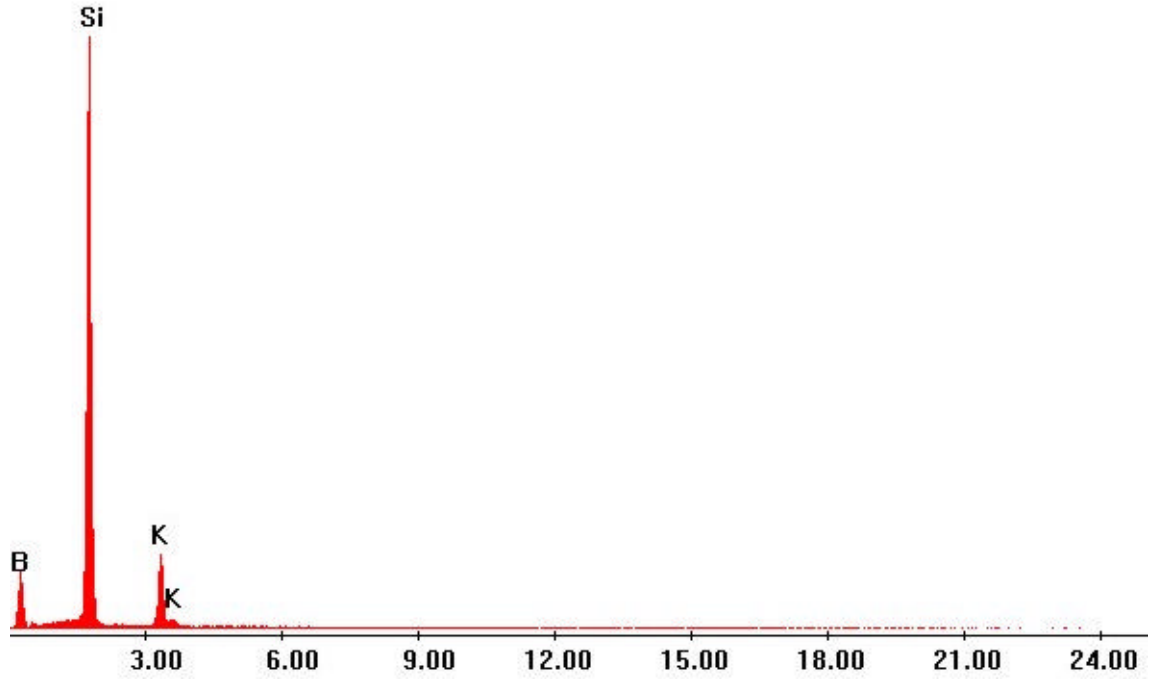

Fig. S2. EDX-spectrum of the $K_7B_7Si_{39}$ crystal, which was investigated by single crystal diffraction. The molar ration K:Si was determined to be ≈ 7:41. The quantitative determination of Boron was not possible by this method.

S3: Lattice parameters of silicides with clathrate-I structure

Composition	***a* / Å**	**XRPD Method**	**Literature**
$K_7B_7Si_{39}$	9.952(1)	Guinier, single profile fit	this work
$K_{7-x}B_{7-x}Si_{39+x}$ ($x\approx0.75$)*	9.971(1)	Guinier, single profile fit	this work
$Na_{6.2(1)}Si_{46}$	10.199(1)	Guinier, single profile fit	[7]
$K_{7.0(1)}Si_{46}$	10.278(1)	Guinier, single profile fit	[7]
$Na_2Ba_6Si_{46}$	10.275(1)	single crystal	[9]
$K_8Ga_8Si_{38}$	10.427(1)	single crystal	[4a]

*Composition was estimated from a linear extrapolation between K_7Si_{46} and $K_7B_7Si_{39}$.

S4: SAED

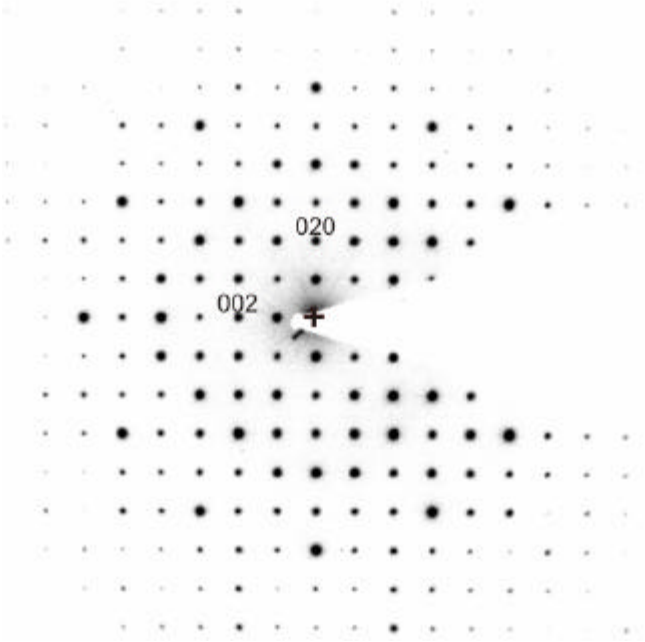

Fig. S4. Electron diffraction pattern, zone axis [100].

Simulated kinematical ED patterns are in rather good qualitative accordance with experimental SAED patterns for the prominent zone axes [100], [110], and [111]. Differences between the simulated and experimental intensities may be explained as effects of dynamical diffraction.

S5: Resistivity

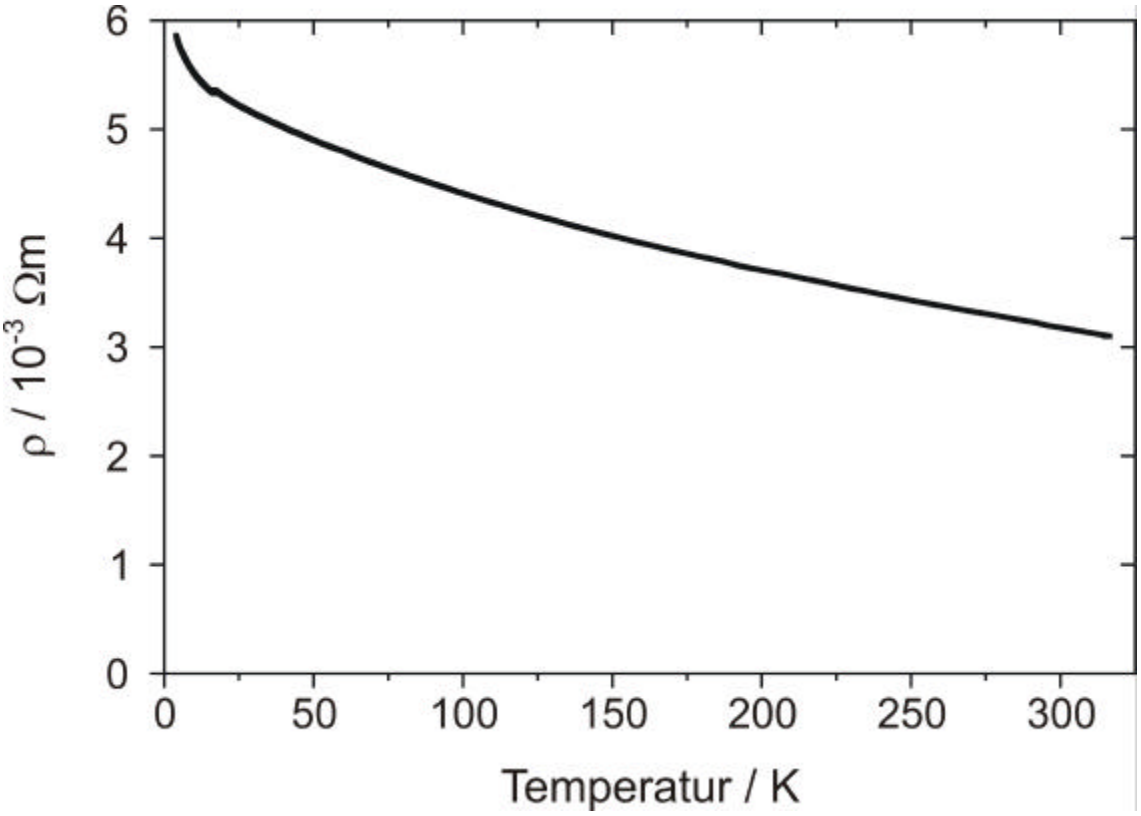

Fig. S5. Plot of the resistivity dependence on temperature.

S6: Data collection and handling

Composition	$K_{7.04(2)}B_{6.8(3)}Si_{39.2(3)}$
Space group	$Pm\bar{3}n$, $Z = 1$
a / Å	9.952(1)
Volume / Å³	985.7(3)
Diffractometer and software	RIGAKU Spider diffractometer with rotating anode and Varimax optics, AgKa_1 radiation, *?* = 0.56087 Å, structure refinement on F with WINCSD.
$2q_{max}$, $\sin(q/l)_{max}$	98°, 1.35
$N(hkl)_{measured}$, $N'(hkl)_{independent}$	21526, 1845
$N(hkl)$ with $F > 4s(F)$	1238
Refined parameters	29
$R(F)$, $R(F^2)$	0.116, 0.06

S7: Atomic coordinates and displacement parameters of $K_7B_7Si_{39}$

Atom	Site	Occ.	*x*	*y*	*z*	$B_{iso/eq}$ (Å²)
K1	2*a*	0.52(1)	0	0	0	0.49(2)
K2	6*d*	1	1/4	1/2	0	1.50(2)
Si1	6*c*	1	1/4	0	1/2	0.46(2)
(Si/B)21	16*i*	B21: 0.213(9) Si21: 0.287(9)	0.1828(2)	*x*	*x*	0.49(2)
(Si/B)22	16*i*	B21: 0.212(9) Si21: 0.288(9)	0.1974(2)	*x*	*x*	0.40(2)
Si31	24*k*	0.32(1)	0	0.1159(4)	0.3069(4)	0.49(5)
Si32	48*l*	0.347(3)	0.0145(2)	0.1252(2)	0.2924(2)	0.51(3)

$B_e = 1/3\ [B_{11}\ a^{*2}\ a^2 + ... + 2\ B_{23}\ b^*\ c^*\ b\ c \cos\alpha]$

Atom	B_{11}	B_{22}	B_{33}	B_{12}	B_{13}	B_{23}
K1	0.49(3)	B_{11}	B_{11}	0	0	0
K2	1.02(5)	1.73(4)	B_{22}	0	0	0
Si1	0.55(4)	0.42(2)	B_{22}	0	0	0
(Si/B)21	0.49(3)	B_{11}	B_{11}	-0.10(3)	B_{12}	B_{12}
(Si/B)22	0.40(3)	B_{11}	B_{11}	0.02(4)	B_{12}	B_{12}
Si31	0.56(8)	0.46(9)	0.45(7)	0	0	-0.20(7)
Si32	0.43(7)	0.51(4)	0.59(4)	-0.06(3)	0.01(4)	-0.09(4)

$T = \exp[-1/4\ (B_{11}\ a^{*2}\ h^2 + ...\ 2\ B_{23}\ b^*\ c^*\ k\ l)]$