$LiBi_3S_5$—A Lithium Bismuth Sulfide with Strong Cation Disorder

Supporting Information

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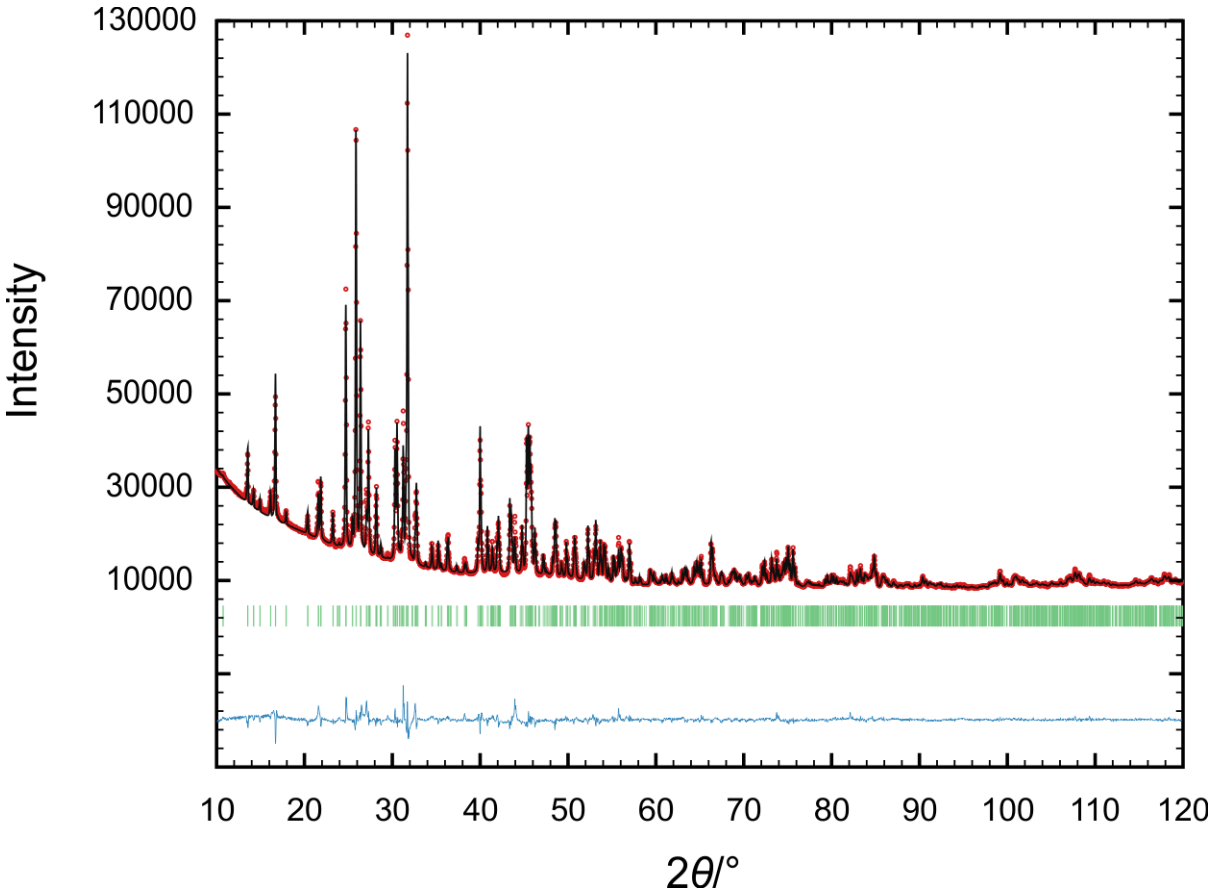

Fig. S1. X-ray powder diffractogram of $LiBi_3S_5$ with the results of the Rietveld refinement (black: measured, red: calculated intensities, green: Bragg positions, blue: intensity difference).

Table S1. Details of X-ray powder diffraction at $LiBi_3S_5$.

Sum formula	$LiBi_3S_5$
T/K	298
Crystal system	monoclinic
Space group	$C2/m$
λ_1/pm	154.056
λ_2/pm	154.439
Z	4
M/g mol^{-1}	794.2
a/pm	1310.23(6)
b/pm	400.054(18)
c/pm	1650.92(7)
β/°	94.0840(10)
V/10^6 pm^3	863.15(7)
ρ_{calc}/g cm^3	6.112
μ/mm^{-1}	128.51
R_p	0.0188
R_{wp}	0.0286
R_{exp}	0.0084
R_B	0.0658
R_F	0.0426
S	3.36

Table S2. Atomic coordinates, displacement parameters, and site occupation factors (s.o.f.) for $LiBi_3S_5$ at ambient temperature as derived from X-ray powder diffraction.

Atom	Wyckoff site	*x*	*y*	*z*	$U_{iso}/10^4$ pm^2	s.o.f.
Bi1	4*i*	0.2378(2)	½	0.11120(14)	0.0223(13)	0.875(4)
Li1	4*i*	0.2378(2)	½	0.11120(14)	0.0223(13)	0.125(4)
Bi2	4*i*	0.4725(2)	0	0.21770(13)	0.0198(12)	0.862(3)
Li2	4*i*	0.4725(2)	0	0.21770(13)	0.0198(12)	0.138(3)
Bi3	4*i*	0.21592(16)	0	0.39037(13)	0.0180(11)	0.943(5)
Li3	4*i*	0.21592(16)	0	0.39037(13)	0.0180(11)	0.057(5)
Bi4	2*a*	0	0	0	0.019	0.467(4)
Li4	2*a*	0	0	0	0.019	0.533(4)
Bi5	2*d*	0	½	½	0.019	0.172(4)
Li5	2*d*	0	½	½	0.019	0.828(4)
S1	4*i*	0.3776(10)	0	0.0548(7)	0.010(4)	1
S2	4*i*	0.1107(10)	0	0.1494(7)	0.013(4)	1
S3	4*i*	0.3408(10)	½	0.2562(7)	0.019(4)	1
S4	4*i*	0.0650(8)	½	0.3725(7)	0.007(4)	1
S5	4*i*	0.3611(9)	½	0.4618(7)	0.017(4)	1

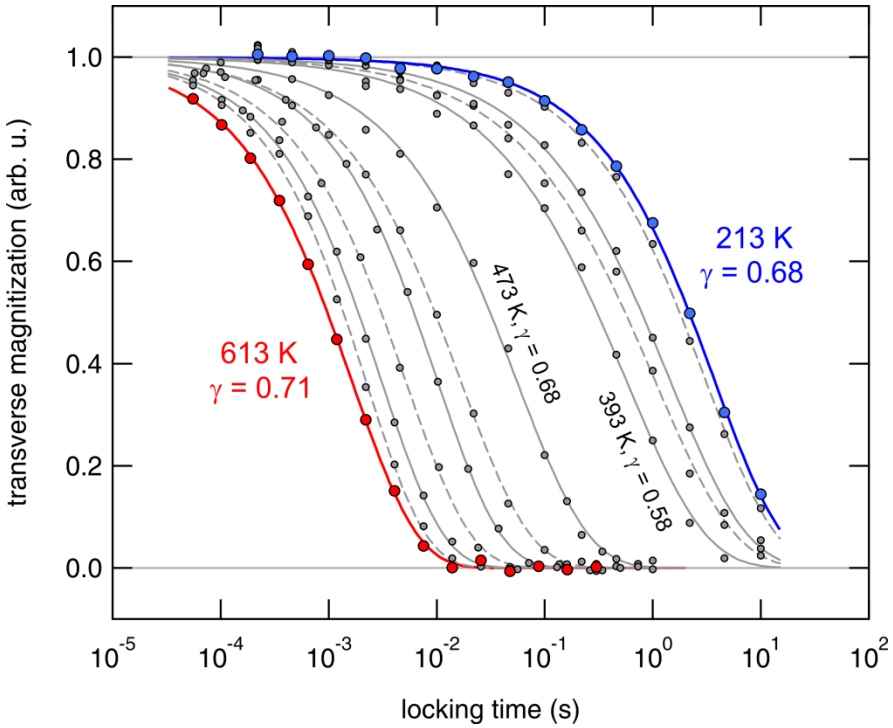

Fig. S2. ^{7}Li-NMR $R_{1\rho}$ magnetization transients recorded in the rotating frame of reference using a spin-lock frequency of 30 kHz; temperatures ranged from 213 to 613 K. The solid and dashed lines represent fits according to stretched exponentials yielding the parameters $R_{1\rho}$ and γ. Note that the x axis is scaled logarithmically.