

Supporting Information

Electronic Structure and Transport in the Potential Luttinger Liquids $\text{CsNb}_3\text{Br}_7\text{S}$ and $\text{RbNb}_3\text{Br}_7\text{S}$

Fabian Grahlow^a, Fabian Strauß^b, Marcus Scheele^b, Markus Ströbele^a, Alberto Carta^c, Sophie F. Weber^c, Scott Kroeker^d, Carl P. Romao^{*c} and H.-Jürgen Meyer^{*a}

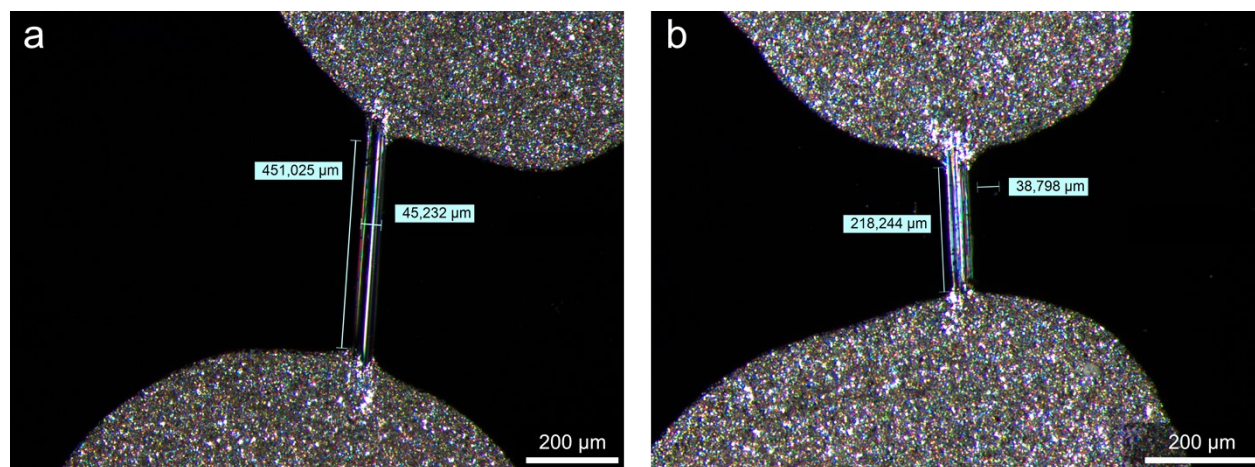


Figure S1: Optical micrographs of a (a) contacted $\text{CsNb}_3\text{Br}_7\text{S}$ crystal and a (b) contacted $\text{RbNb}_3\text{Br}_7\text{S}$ crystal.

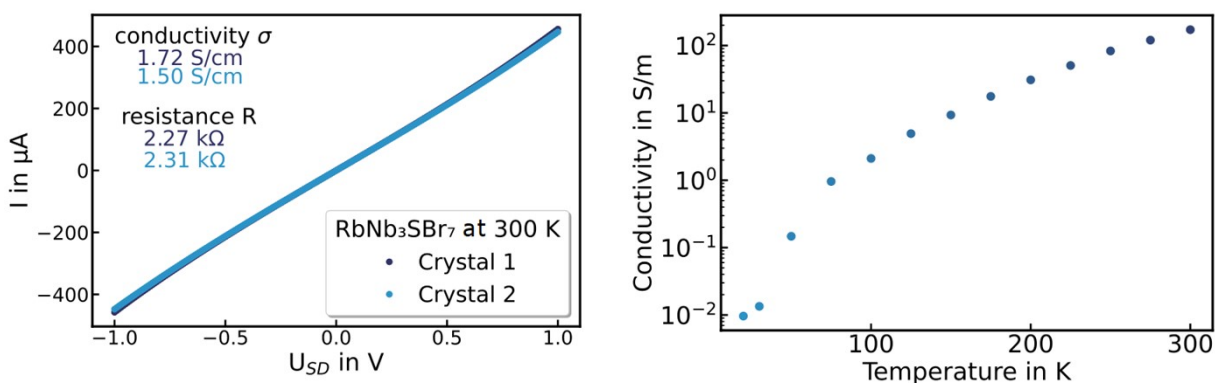


Figure S2: (left) Dark currents of $\text{RbNb}_3\text{Br}_7\text{S}$ Crystals on silicon with 770 nm dioxide layer at 300 K. (Right) Electrical conductivity of $\text{RbNb}_3\text{Br}_7\text{S}$ versus set temperature in a range of 20 K to 300 K.

^a Section for Solid State and Theoretical Inorganic Chemistry

Institute of Inorganic Chemistry

Eberhard-Karls-Universität Tübingen

Auf der Morgenstelle 18, 72076 Tübingen, Germany

^{*a} E-mail: juergen.meyer@uni-tuebingen.de

^b Institute for Physical and Theoretical Chemistry

Eberhard-Karls-Universität Tübingen

Auf der Morgenstelle 18, 72076 Tübingen, Germany

^c Department of Materials, ETH Zurich,

Wolfgang-Pauli-Str. 27, 8093 Zürich, Switzerland

^{*c} E-mail: carl.romao@mat.ethz.ch

^d Department of Chemistry, University of Manitoba, Winnipeg, Manitoba R3T 2N2, Canada

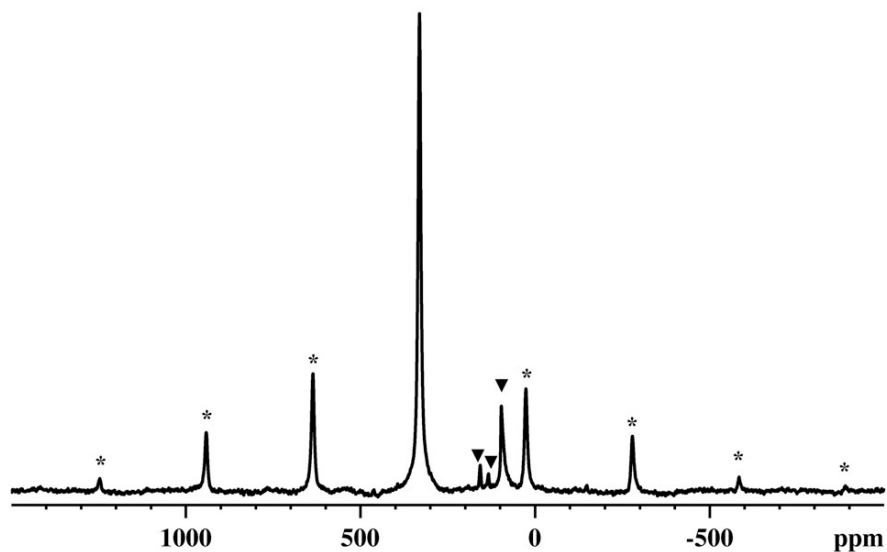


Figure S3: ^{133}Cs MAS NMR spectrum of $\text{CsNb}_3\text{Br}_7\text{S}$ acquired at 65.5 MHz with a spinning rate of 20.000(3) kHz. Spinning sidebands are marked with asterisks; peaks from minor impurities or decomposition products are indicated by arrows.

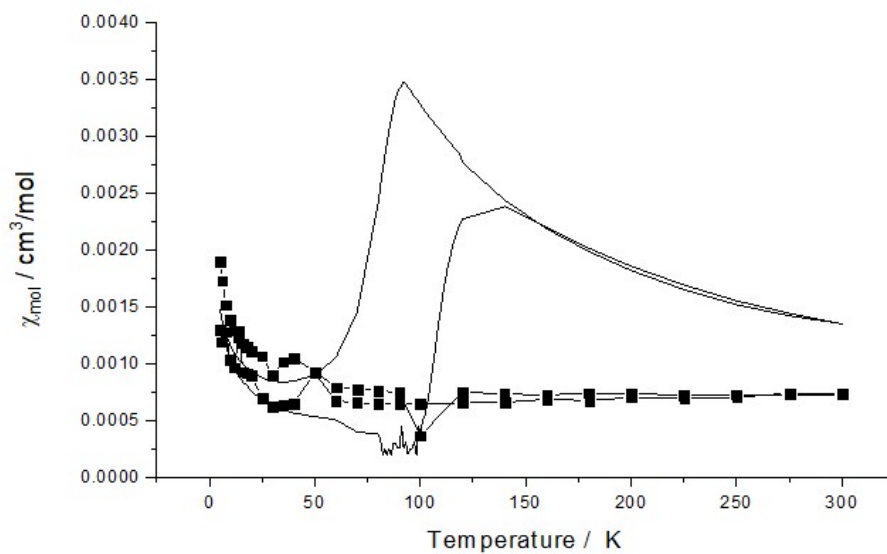


Figure S4: Measured magnetic susceptibility during one heating/cooling cycle at 100 Oe for Nb_3Cl_8 (line) and $\text{CsNb}_3\text{Br}_7\text{S}$ (line with squares).

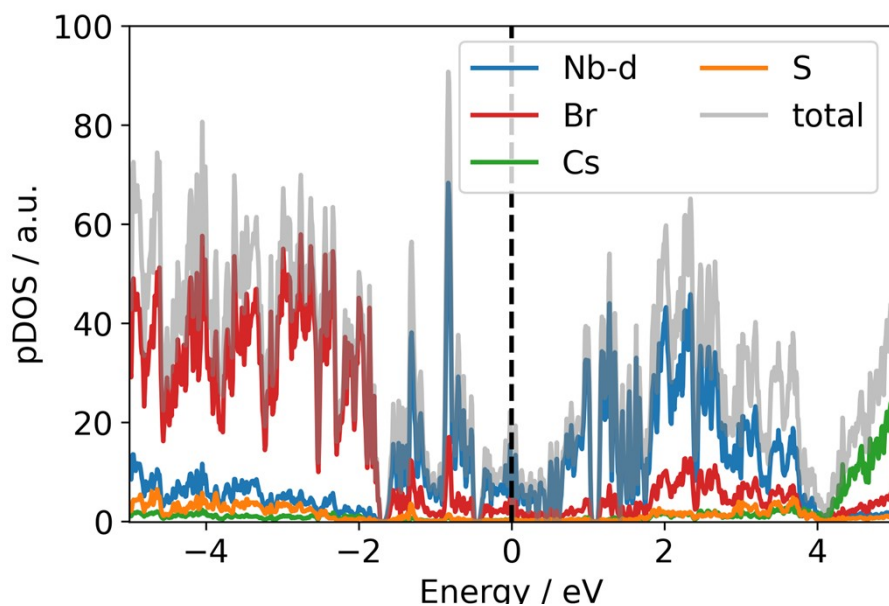


Figure S5: Calculated projected density of electronic states in CsNb₃Br₇S. The Fermi energy is shown as a black line.

Table S1: Parameters of the tight-binding model corresponding to the bond-centred Wannier functions of CsNb₃Br₇S.

R (unit cell translation)	t (hopping integral) / eV	Note
[0 0 0]	7.05	On-site bond energy
[0 0 0]	-0.20	Nearest neighbor intra-chain hopping
[0 0 1]	0.02	Next-nearest intra-chain hopping
[0 0 0]	-0.01	Nearest inter-chain hopping

Table S2: Calculated phonon frequencies at Γ of CsNb₃Br₇S.

Phonon frequency / cm ⁻¹				
0.00	0.00	0.00	13.82	19.00
22.51	30.40	36.64	38.67	43.39
44.75	45.29	46.37	46.77	48.39
48.87	49.56	52.99	53.70	60.98
61.65	63.65	64.04	64.20	64.22
64.54	71.97	74.61	75.42	76.19
79.48	79.70	81.84	83.49	83.53
83.97	85.83	87.15	87.45	91.20
92.28	92.43	93.26	94.01	96.09
96.48	96.84	99.12	99.95	100.35
103.28	103.46	104.84	105.28	106.97
107.81	108.53	110.47	114.45	115.29
115.87	116.33	120.49	120.61	122.27
122.29	127.94	128.16	129.81	131.58
131.70	131.83	132.11	133.17	134.87
135.14	137.85	138.71	139.79	140.27
144.25	145.04	145.26	146.83	148.07
148.69	150.41	150.49	151.01	152.26
154.77	155.07	167.36	167.92	169.24
170.62	174.51	174.71	191.26	191.41
195.37	195.41	198.30	204.25	210.01
210.04	210.17	212.79	212.86	215.80
216.07	217.71	217.79	219.59	222.61
228.86	229.39	229.53	231.31	232.42
238.55	239.04	243.34	243.73	246.34
250.03	251.19	253.81	255.17	255.42
264.96	266.98	311.65	311.80	329.66
330.67	332.12	332.23	342.05	342.21
389.45	390.98	394.79	395.03	