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Bismuth-Rich Intermetallic Rods with Strong Spin-Orbit Coupling

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During the search for novel topologically non-trivial materials, materials containing heavy elements, with large spin-orbit coupling were investigated. A particular focus lay on materials containing the heaviest non-radioactive element bismuth, as its large spin-orbit coupling has proven highly advantageous in finding compounds that exhibit the desired properties. In the course of these investigations, the novel bismuth-rich mixed halide $Bi_{21}Rh_4Cl_6I_7$ was found.[1] The black needle-shaped crystals of this material showcase an orthorhombic structure that consists of infinite intermetallic rods $^1_\infty[Bi_9Rh_2]^{3+}$ and discrete anionic groups $[Bi^{II}_2Cl_5I_2]^3$ and $[Bi^{III}Cl_4I_2]^3$. The rods consist of Rh-centered $[RhBi_8]$ polyhedra that alternately share triangular and rectangular faces. Using traditional electron counting rules, the intermetallic rod can be interpreted as a covalent polymer with Rh_2 dumbbells bonded to molecular Bi_2 and Bi_5 units, while a quantum-chemical bonding analysis shows that the bonds involving Rh atoms are largely diffuse, while two-center bonds dominate in the bismuth units. Resistivity measurements indicate two temperature regimes, of which one showcases a temperature-independent resistance and this, along with the strong spin-orbit coupling inherent to this bismuth-rich compound, makes it a candidate for a topological insulator.

[1] M. A. Herz, K. Finzel, W. Schnelle, M. Ruck, *Z. Anorg. Allg. Chem.* **2023**, e202300124.