

La₃Cl₃BC – Structure, Bonding and Electrical Conductivity

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A new rare earth carbide boride halide, La₃Cl₃BC, has been prepared by heating a mixture of stoichiometric quantities of LaCl₃, La, B and C at 1050 °C for 10 days. La₃Cl₃BC (La₃Br₃BC type) crystallizes in the monoclinic system with space group *P*2₁/*m* (No. 11), *a* = 8.2040(16), *b* = 3.8824(8), *c* = 11.328(2) Å, β = 100.82(3)°. In the structure, monocapped trigonal prisms containing B–C units are condensed into chains along the *b* direction, and the chains are further linked by Cl atoms in the *a* and *c* directions. The condensation results in a polymeric anion $_{\infty}^1[\text{BC}]$ with a spine of B atoms in a trigonal prismatic coordination by La, and the C atoms attached in a square pyramidal coordination. The B–B and B–C distances are 2.16 and 1.63 Å, respectively. La₃Cl₃BC is metallic. The EH calculation shows that the distribution of valence electrons can be formulated as (La³⁺)₃(Cl[−])₃(BC)^{5−} · e[−].

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