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# Modeling of lattice constant and their relations with ionic radii and electronegativity of constituting ions of A2XY6 cubic crystals using Artificial neural network method

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## Abstract

In the present study a new empirical model is proposed to describe and predict the lattice constants for a series of cubic crystals, all of which have the A2XY6 composition (A = K, Cs, Rb, Tl; X = tetravalent cation, Y = F, Cl, Br, I). The model is based on a thorough analysis of structural properties of 85 representative crystals from this group using Particle Swarm Optimization (PSO) algorithm integrated with an Artificial Neural Network (ANN). It was shown that the lattice constant is a linear function of theionic radii and electronegativity of the constituting ions. As a result of the performed analysis. It gives very good agreement between the experimental andmodeled values of the lattice parameters, with a mean squared error of 0.0256. The developed approach can be efficiently used for a simple, fast and reliable prediction of lattice constants and interionic distances in isostructural materials having a similar composition.

**Keywords:** Peroveskite,Lattice constant,ANN,PSO,Prediction

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