

Crystallographic and Mössbauer studies of FeRh_2Se_4

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Single-phase FeRh_2Se_4 has been synthesized for the first time and studied by x-ray, Mössbauer, and magnetic measurements. The crystal structure is found to be monoclinic with the lattice parameters: $a = 6.310 \text{ \AA}$, $b = 3.643 \text{ \AA}$, $c = 11.14 \text{ \AA}$, and $\beta = 92.42^\circ$. The structure is characterized by ordered vacancies in alternate metal layers. The iron ions are found to be ferrous in charge state and occupy the metal layers that are without vacancies, which is "inverse" to the site distributions reported for similar structures. From quadrupole-splitting–isomer-shift correlation and magnetic susceptibility, it is inferred that Fe–Se bonds are highly covalent. The quadrupole splitting is observed to be 1.06 mm/s at 81 K and to decrease linearly with increasing temperature.