

# Vibrational properties and magnetic specific heat of the covalent chain antiferromagnet RbFeSe<sub>2</sub>

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## Abstract

© 2018 American Physical Society. The magnetic specific heat of RbFeSe<sub>2</sub> and the spin state of Fe<sup>3+</sup> ions in the compound have been studied. Phonon dispersion and phonon density of states (PDOS), element specific and total, were evaluated from first-principles calculations. It is shown that iron atoms in quasi-one-dimensional chains have dramatically different vibrational properties against Rb and Se atoms: the Fe PDOS is mostly concentrated within two Einstein-like optical phonon peaks at high frequencies. Analysis of our Mössbauer data for RbFeSe<sub>2</sub>, utilizing the calculated Fe PDOS as well as our optical absorption measurements, have shown full agreement with the location of the high-frequency optical-type lattice vibrations within the FeSe<sub>4</sub> tetrahedra. The calculated PDOS was utilized to evaluate the lattice contribution to the specific heat. The phonon heat capacity has been used to evaluate the magnetic specific heat of the quasi-one-dimensional antiferromagnetically correlated Fe<sup>3+</sup> ion chains in RbFeSe<sub>2</sub>. An intermediate spin state  $S=3/2$  has been found most closely relevant to our magnetic entropy analysis for Fe<sup>3+</sup> ions in RbFeSe<sub>2</sub>.

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