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Thermal conductivity in terbium-based compound : KTb3F10

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KTb3F10 is a terbium-based compound with a cubic structure (Fm-3m space group), in which the magnetic Tb ions form an unusual network of corner sharing octahedra [1-4]. Tb ions sit on the 24e Wyckoff site (C4n point group) and are surrounded by 8 fluorine atoms, forming a slightly distorted dodecahedra cage. Interestingly, because of the cubic three-fold symmetry, there are three possible orientations of this fluorine cage in the structure : the 4-fold axis of each cage can be parallel to either of the three cubic axes. This compound exhibits a very low thermal conductivity at room temperature, about 2 W/m/K which is expected in amorphous materials such as glass. More interestingly, the thermal conductivity curve at low temperatures is not proportional to T3 as expected for a system where only phonons conduct heat but instead comprises a local extremum. Since this unexpected feature has been observed in other Tb based compounds, which all have low energy CEF levels, magnetic excitations are likely to play a role in this macroscopic property. Indeed, measurements have shown that the magnetic field was able to drastically affect the thermal conductivity in those terbium-based compounds, while phonons should not be affected in the approximation of an absence of CEF-Phonon coupling. In that context, neutron diffraction and inelastic neutron scattering experiments as well as calculations were carried out to characterize the magnetic properties of KTb3F10 and emphasize the microscopic signature of such coupling.

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Primary author: DEMORTIER, OLIVIER (Laboratoire Léon Brillouin, CEA Saclay)

Co-authors: IVANOV, Alexandre (ILL); FAUQUÉ, Benoît (Collège de France); ROESSLI, Bertrand (Paul Scherrer Institut); RESSOUCHE, Eric (Université Grenoble Alpes, CEA, IRIG, MEM, MDN, 38042 Grenoble, France); DAMAY, Francoise (LLB); LE BERRE, Françoise (Institut des Molécules et Matériaux du Mans); Dr BOURDAROT, Frederic (CEA-Grenoble); LHOSTE, Jérôme (Institut des Molécules et Matériaux du Mans); SIBILLE, Romain (Paul Scherrer Institut); PETIT, Sylvain (LLB CEA-CNRS-Université Paris-Saclay); FENNELL, Tom (Paul Scherrer Institut); COLIN, claire (Institut Néel, CNRS & Université Grenoble Alpes)

Presenters: IVANOV, Alexandre (ILL); FAUQUÉ, Benoît (Collège de France); ROESSLI, Bertrand (Paul Scherrer Institut); RESSOUCHE, Eric (Université Grenoble Alpes, CEA, IRIG, MEM, MDN, 38042 Grenoble, France); DAMAY, Francoise (LLB); LE BERRE, Françoise (Institut des Molécules et Matériaux du Mans); Dr BOURDAROT, Frederic (CEA-Grenoble); LHOSTE, Jérôme (Institut des Molécules et Matériaux du Mans); DEMORTIER, OLIVIER (Laboratoire Léon Brillouin, CEA Saclay); SIBILLE, Romain (Paul Scherrer Institut); PETIT, Sylvain (LLB CEA-CNRS-Université Paris-Saclay); FENNELL, Tom (Paul Scherrer Institut); COLIN, claire (Institut Néel, CNRS & Université Grenoble Alpes)

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