The possibility of existence the magnetic field induced structural phase transition in $KEr(MoO_4)_2$

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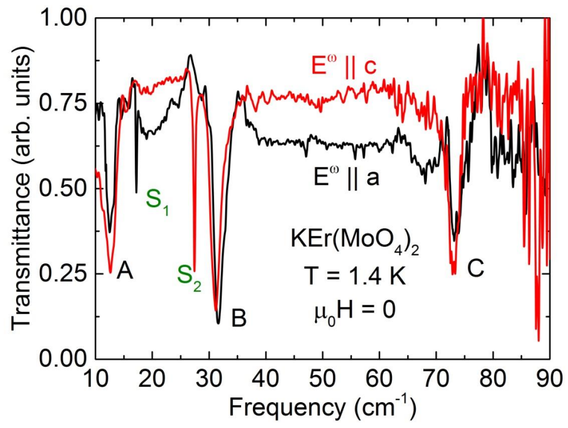
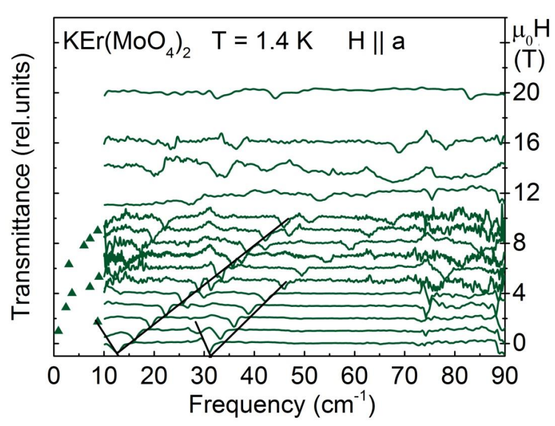
I. Introduction

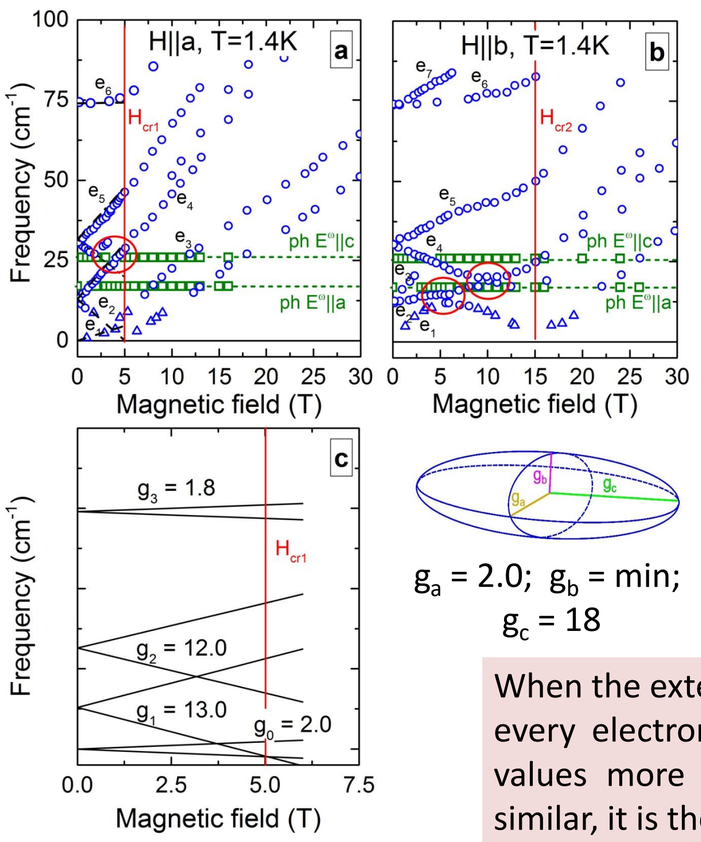
The crystals of double rare-earth (*RE*) molybdates $MRE(MoO_4)_2$ (like a $KEr(MoO_4)_2$ studied in this work) are the isostructural Jahn-Teller type compounds in which the rhombic unit cell contains several *RE* ions (namely, 4) in the initial - orthorhombic at 300K - phase [1]. The anisotropy of elastic properties of these crystals is determined by its layered structure [2]. The study of the phase transitions induced by external magnetic field, and the phase diagrams as a functions of temperature and magnetic field at different directions, was discovered the uniqueness of such crystallographic systems [3]. The aim of this work is as to study the changes in FIR spectra $KEr(MoO_4)_2$ in the vicinity of phase transition observed before at HII*a* [3], so as to obtain the magnetic field dependencies of the energies of electronic (polaron) excitations when magnetic field is applied along the different crystallographic axes.

II. FIR spectra in magnetic field





Mode	Energy	Origin
A	13 cm^{-1}	(gs→1st exc.)
B	31.5cm^{-1}	(gs→2nd exc.)
C	74 cm^{-1}	(gs→3rd exc.)
S_1	17 cm^{-1} (E^ω||a)	phonon
S_2	26 cm^{-1} (E^ω||c)	phonon



$g_a = 2.0$; g_b = min; $g_c = 18$

(**Top Left**) The FIR transmittance spectra **in zero magnetic field** at two polarizations $E^\omega||a$ (black curve) and $E^\omega||c$ (red curve) (T = 1.4 K).

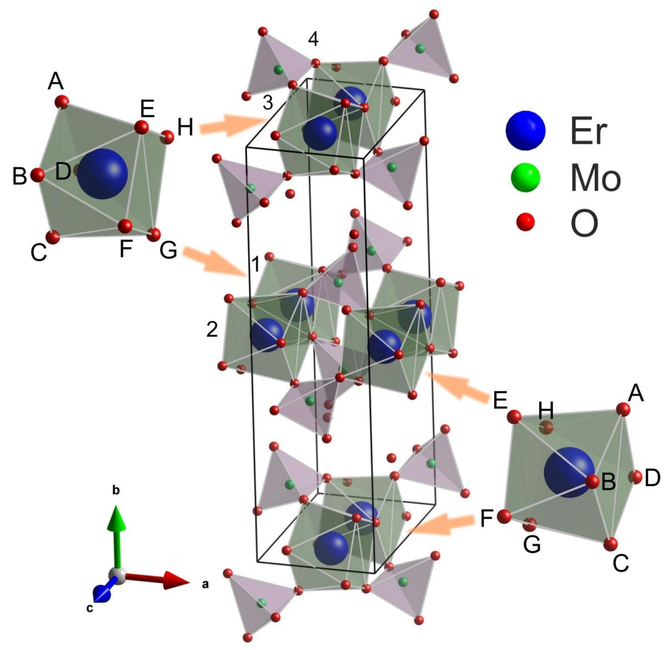
(**Top Center**) FIR transmittance spectra of electronic excitations in $KEr(MoO_4)_2$ **in magnetic field H||*a*** at T=1.4K. ▲ correspond to the electronic excitation energies, were obtained by means ESR spectroscopy method.

(**a, b**) The frequency – magnetic field dependences of the low energy excitations in $KEr(MoO_4)_2$. ○, Δ – electronic-type excitations and □ – phonon-type excitations. With the dashed lines showed calculated branches.

(**c**) The calculated energy levels diagram in a low magnetic field.

When the external magnetic field is switched on along HII*a* or HII*b*, the splitting of every electronic excitation on two components is observed. At magnetic field values more than H_{cr1} ~5T and H_{cr2} ~15T, correspondingly, their behavior is similar, it is the same for the both components, in contrast to the low-field region.

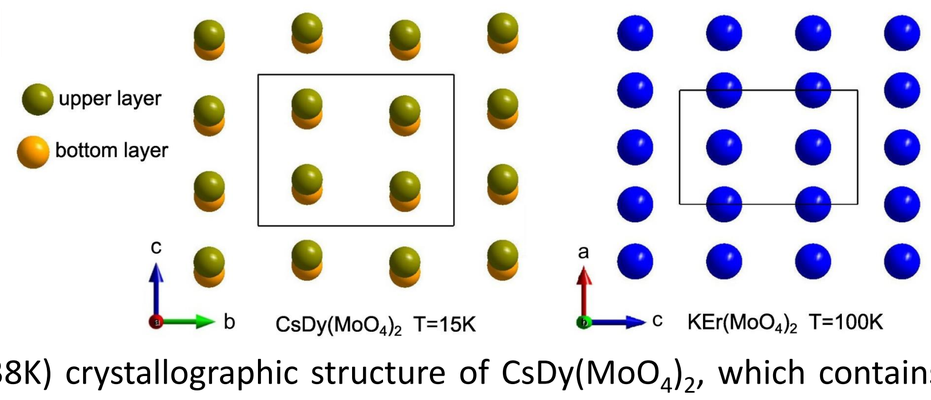
III. Crystal structure



- Non-magnetic potassium layers (is omitted for clarity) are located between erbium layers and have common tetrahedral anions.
- The centers 1 and 2 belong to one of the layers, they are energy equivalent to 3 and 4, the latter are in the nearest layers.
- The tetrahedrons $[MoO_4]$ have shared oxygen ions with polyhedrons $[REO_8]$ and potassium layers. The switching on the external magnetic field may lead to the different local distortions in *ac* plane for the nearest *RE* ions.

IV. The possibility of existence the phase transition

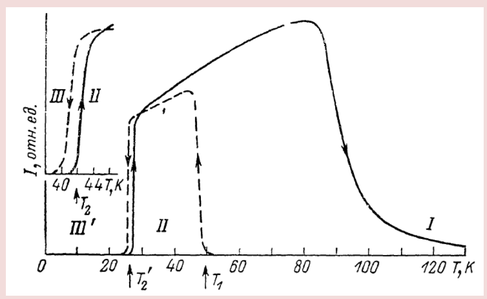
Compound	a, Å	b, Å	c, Å	group	H_{cr}, T
$KEr(MoO_4)_2$	5.060	18.19	7.892	*Pbcn* (100K)	4÷5 (1.8K)
$KTm(MoO_4)_2$	5.047	18.28	7.892	*Pbcn* (300K)	~4 (1.7K)
$KDy(MoO_4)_2$	5.078	18.12	7.943	*Pbcn* (100K)	~4 (2.0K)



As an example, we use the low-temperature (T < 38K) crystallographic structure of $CsDy(MoO_4)_2$, which contains two layers of *RE* ions in unit cell and that does not have a spatial inversion center [4].

The crystallographic properties of structural phases for spontaneous phase transitions in $CsDy(MoO_4)_2$ [4].

Pccm	300 K	1 leyer	2 centers	
Pcca	50 K	2 layers	4 centers	8.2 cm^{-1}
P2 1/c	15 K	2 layers	4 centers	Noncentro-symmetric group



Experimental temperature dependence of mode with ω = 8.2 cm^{-1} in Raman spectra of $CsDy_{0.93}Gd_{0.07}(MoO_4)_2$ [5]. Insert: for $CsDy(MoO_4)_2$. Dashed line – cool, solid line – heat.

V. Conclusions

The external magnetic field directed along *a* and *b* crystallographic axis makes the small rotation of tetrahedrons around Er^{3+} ions that in results the local distortions take place (different for two types polyhedrons for nearest Er^{3+} ions in *ac* plane). These local distortions lead to decreasing of elastic energy due to changes in the parameters of the spin-orbit interaction. The low frequency phonon, responsible for the shear displacements of the *RE* layers (with energy less than 8 cm^{-1} like in $CsDy(MoO_4)_2$), makes cooperative effect and as a result a phase transition takes place. We suppose that the *RE* layers become inequivalent and also the operation of spatial inversion between the nearest polyhedrons in the layers may be lost. The role of low-energy phonons (S_1 and S_2) in the occurrence of phase transition remains unclear yet.

[1] S. Chong, S. Perry, et al., *Acta Crystallogr.*, Sec. **E 76,** 1871 (2020). https://doi.org/10.1107/S205698902001542X
[2] A. A. Loginov, , *Fiz. Nizk. Temp*. **28**, 1056 (2002). [Low Temp. Phys. **28**, 755 (2002)]. http://doi.org/10.1063/1.1521295
[3] V. I. Kut'ko, *Fiz. Nizk. Temp*. **31**, 3 (2005). [Low Temp. Phys. **31**, 1 (2005)]. https://doi.org/10.1063/1.1820349
[4] E. N. Khatsko, et al., *Fiz. Nizk. Temp*. **30**, 184 (2004). [Low Temp. Phys. **30**, 133 (2004)]. https://doi.org/10.1063/1.1645155
[5] V.I. Fomin, V.P. Gnezdilov, V. V. Eremenko, N. M. Nesterenko, *Solid State Physics*, **31**, N 5, 266 (1989).

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