Magnetic fields induced structural modification in magnetoelastic $KEr(MoO_4)_2$

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MOTIVATION: The $KEr(MoO_4)_2$ is a layered magnetoelastic 'virtual' Jahn-Teller crystal. We have shown that external magnetic field affects the electronic shell of erbium ion over quadrupolar moment and triggers remarkably strong magnetostrictive response H_{cr2} = 15,6 T [1]. In this work we study Zeeman effect in $KEr(MoO_4)_2$ at external magnetic field up to 30T by far infrared (FIR) spectroscopy. **The aim of this study is to clarify the relationship between the anomalous behavior of low-energy excitations and the microscopic mechanisms responsible for magnetic-field-induced lattice distortions.**

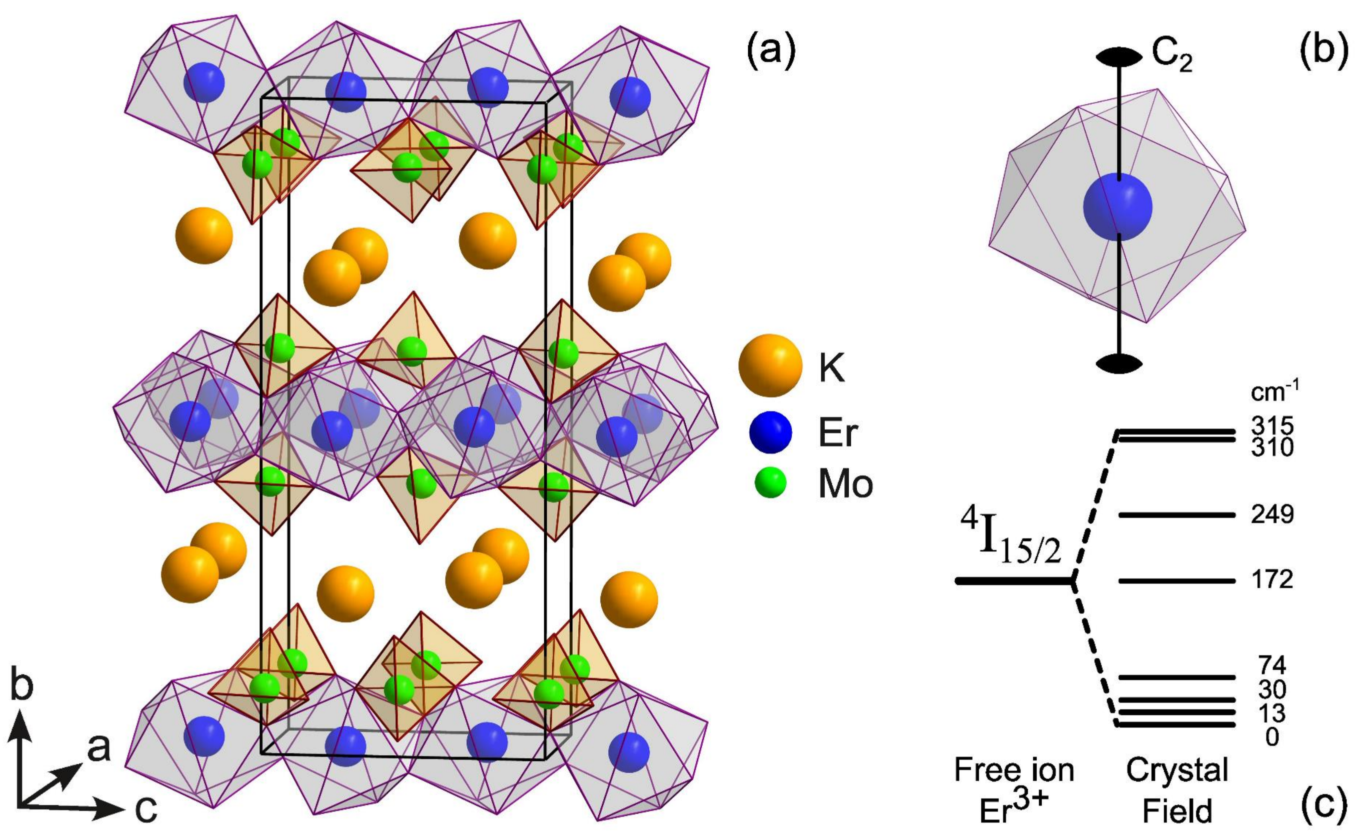

Fig. 1. a) Crystallographic structure of $KEr(MoO_4)_2$ [2]. b) Local environment of Er^{3+} ion. c) The splitting of the Er^{3+} multiplet $^4I_{15/2}$ into eight Kramers doublets by CEF.

The visualization of the total quadrupolar moments rotation in magnetic field and distortions of oxygen local environment of Er^{3+} ion [1].

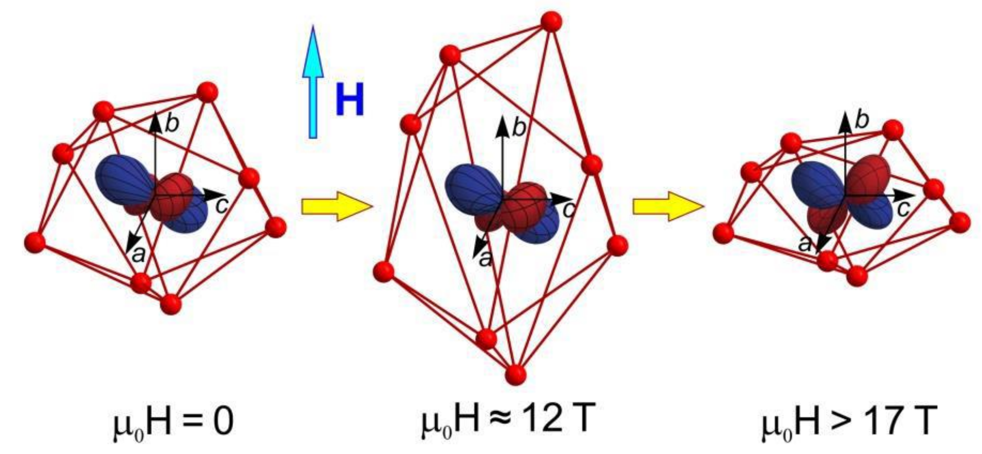

Fig. 2. The absolute-value isosurfaces of the calculated quadrupolar moment with a negative (positive) sign is indicated by a blue (red) color.

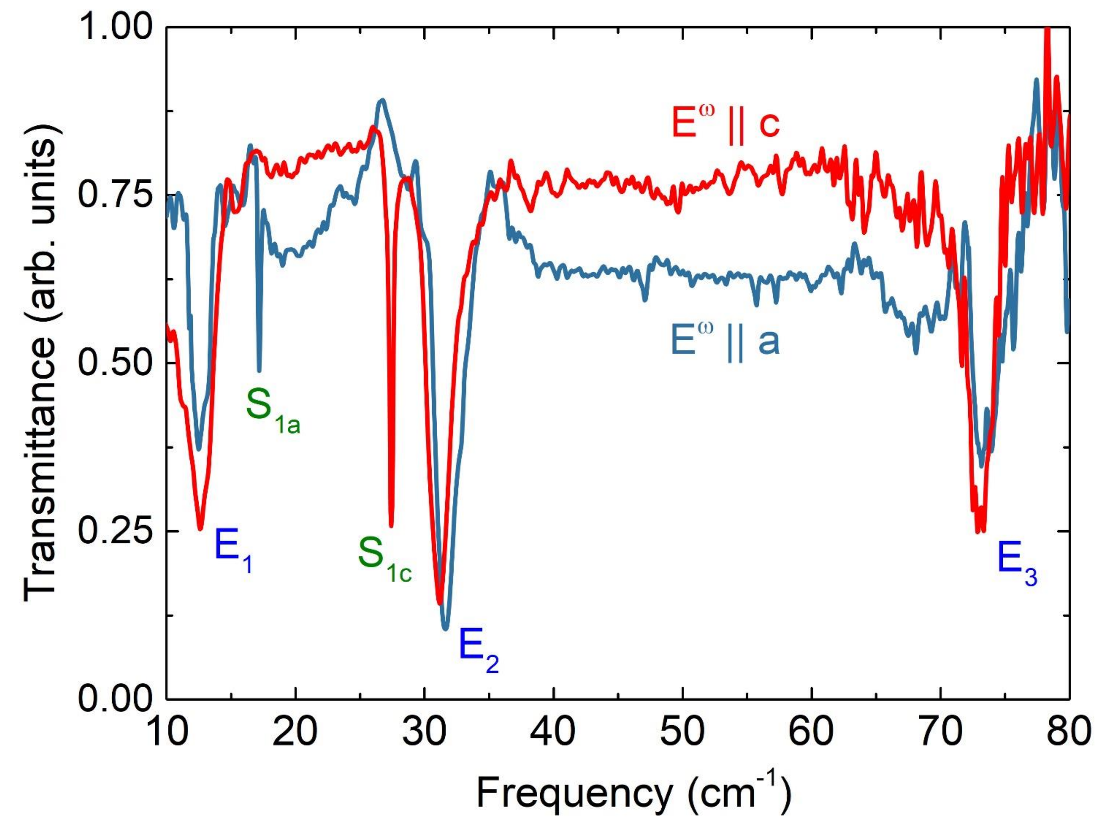

Fig. 3. Transmittance THz spectra of $KEr(MoO_4)_2$ at T = 1.4 K in zero magnetic field at polarizations E^ω || a (blue) and E^ω || c (red).

RESULTS:

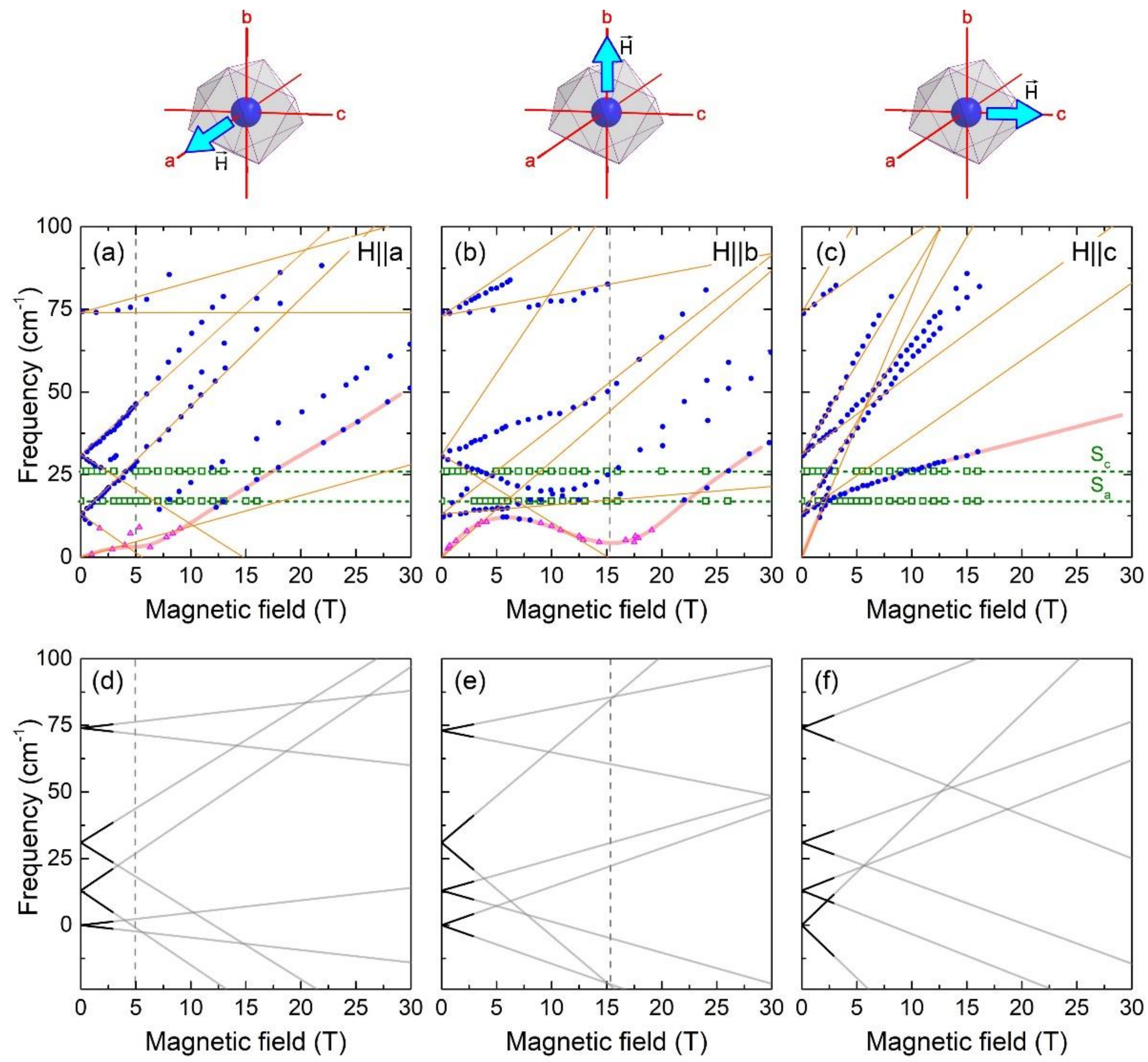

Fig.4. a), b), c) frequency-magnetic field dependencies of low frequencies excitations in $KEr(MoO_4)_2$ (T = 1.4 K). Closed blue and magenta symbols – experimental results of electronic excitations, phonon-type excitations denoted by open square symbol with green color. The solid orange lines – calculated electronic transitions between energy levels in the linear Zeeman approximation. The linear Zeeman approximation give the best fit to the experimental results in low field region up to 2 T (see bright fragments of the energy levels lines on plots d), e) and f)). The transitions between the ground state levels presented by solid red line.

Table 1. The m_j values obtained within the linear Zeeman approximation.

	m_{ja}	m_{jb}	m_{jc}
E_0 (ground state)	0.8	2.6	7
E_1 = 13 cm^{-1}	5	2.1	2.9
E_2 = 31.5 cm^{-1}	4.6	6.3	2.7
E_3 = 74 cm^{-1}	0.8	1.5	2.9

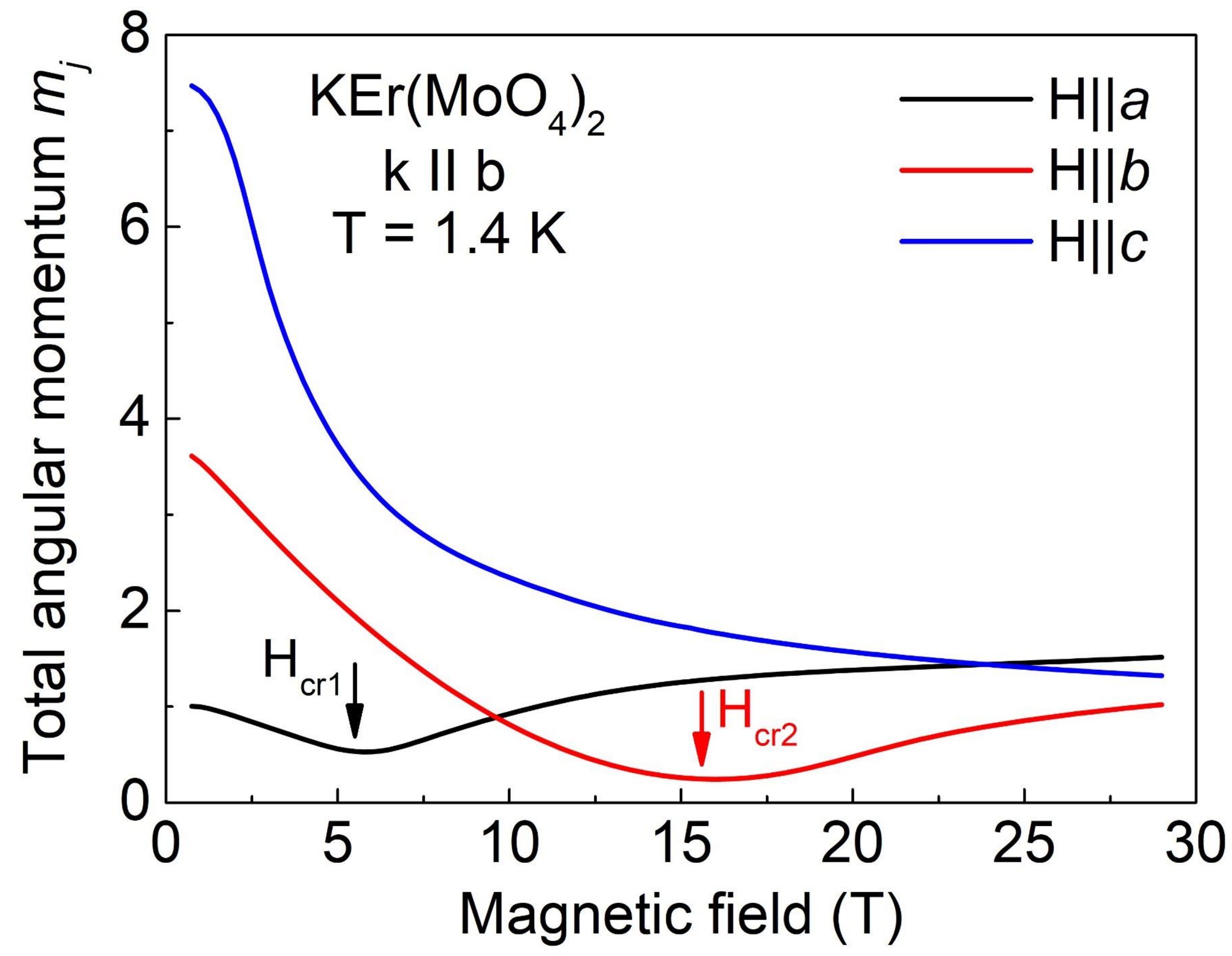

Fig.5. The magnetic field dependence of the projections of the total angular momentum m_j obtained with equation $m_j(H) = \Delta E_0/\mu_B H$.

In $KEr(MoO_4)_2$, for $H||b$, a pronounced strong magnetostrictive response is observed at H_{cr2} ≈ 15 T [1], accompanied by a sharp increase in the magnetization. A similar anomaly in the magnetization curve occurs for $H||a$ at a magnetic field of about H_{cr1} ≈ 5 T [3]. These peculiarities are associated with minima in the $m_j(H)$ curves (see Fig.5). The $m_j(H)$ behavior indicates a strong field dependence of the magnetic anisotropy, which may serve as an indicator the presence of magnetic-field-induced structural phase transitions in the studied compound.

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