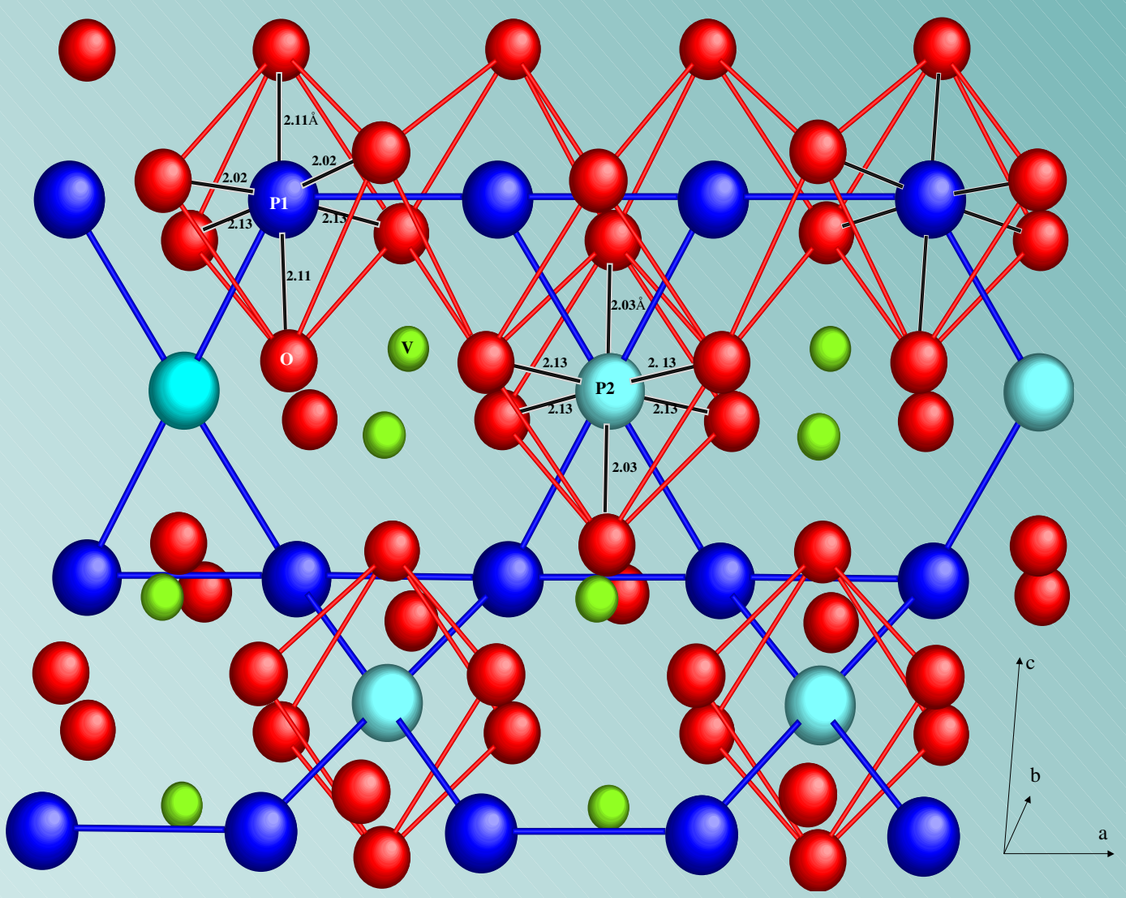
EPR in kagomé staircase compound $Mg_{2.997}Co_{0.003}V_2O_8$

P.Aleshkevych, J. Fink-Finowicki, H. Szymczak

Institute of Physics, Polish Academy of Sciences, Al. Lotnikow 32/46, PL-02-668 Warsaw, Poland

Purpose: investigation of local symmetry of Co ions in buckled kagomé staircase $Mg_{2.997}Co_{0.003}V_2O_8$ single crystals by EPR technique.



The crystal structure of the $Mg_{2.997}Co_{0.003}V_2O_8$.

$Mg_{2.997}Co_{0.003}V_2O_8$ single crystals:
- grown from polycrystalline feed rods by floating zone technique
- X-Ray: single-phase, orthorombic (Cmca) structure
- the samples were the roentgenographically oriented disks of 3 mm diameter and thickness of 0.5 mm

Main results:

The EPR spectra were observed at temperature below 40 K.

The spectrum consists of two groups of eight hyperfine structure components due to ^{59}Co nuclear spin I=7/2. The two nonequivalent positions produce the two group of the observed lines which is interpreted as being the consequence of the transitions between the lowest Kramers doublet (M_S=±1/2) levels.

The position of experimental resonance lines can be described by a spin-Hamiltonian of rhombic symmetry with an effective spin S=1/2 and nuclear spin I=7/2,

$$\hat{H} = \mu_B(\vec{B}g\hat{S}) + (\hat{S}A\hat{I})$$

where $\hat{S}$ - the spin operator, A -tensor of the hyperfine interactions and $\hat{I}$ - the nuclear spin operator. The components of the g-tensor can be written as follows:

$$g_x = (10/3 - 8/3\alpha) + k(1 - 2\alpha)$$

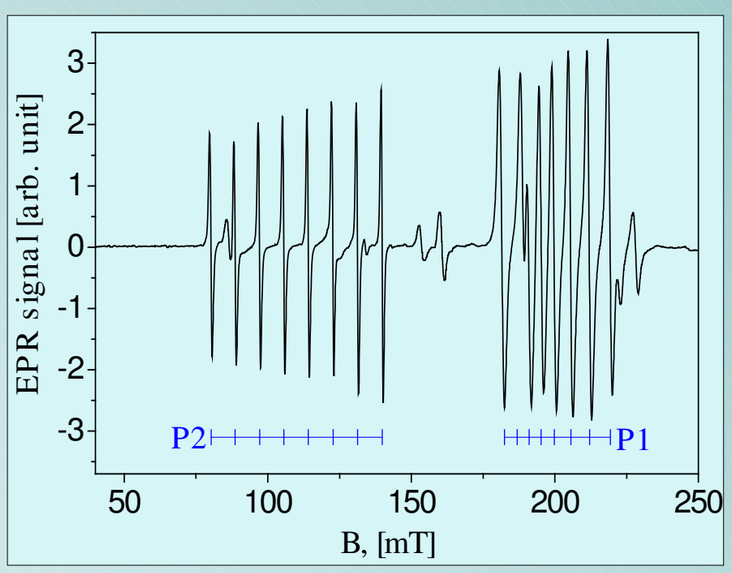
$$g_y = (10/3 + 4/3\alpha + 4/3r) + k(1 + \alpha + r)$$

$$g_z = (10/3 + 4/3\alpha - 4/3r) + k(1 + \alpha - r)$$

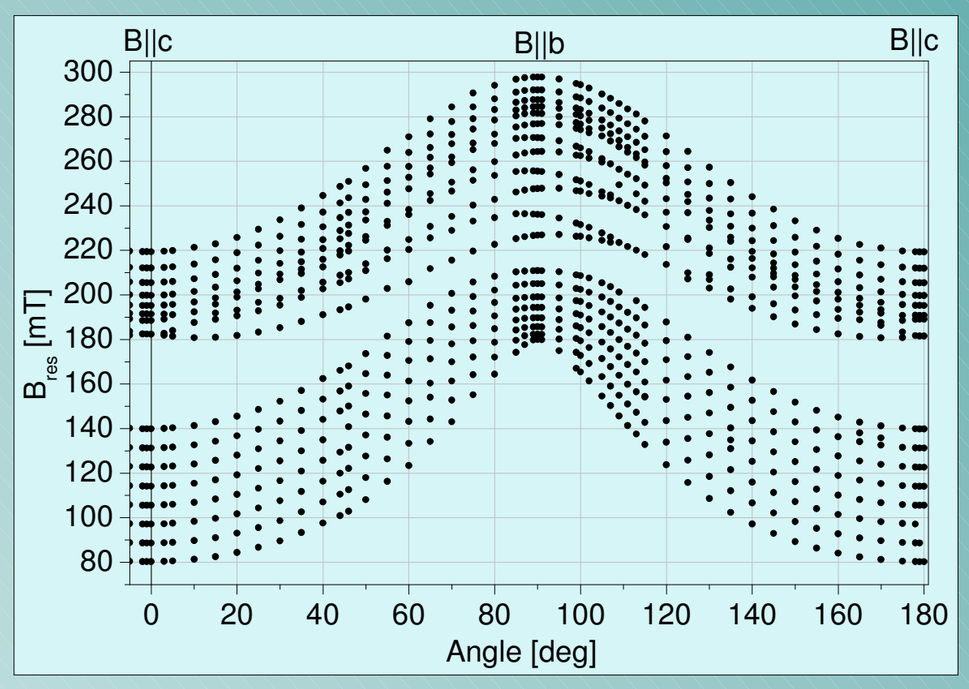
where α denotes the axial distortion, r is the rhombic distortions, k is the orbital reduction factor corresponding to the reduction of the orbital angular momentum by charge transfer from the paramagnetic ion to the surrounding oxygen ions.

The main values of the g, A tensors and distortion parameters for both positions

Position	g_a	g_b	g_c	A_a (x10^{-4} cm^{-1})	A_b (x10^{-4} cm^{-1})	A_c (x10^{-4} cm^{-1})	axial distortion	rhombic distortion	**Orbital reduction factor**
P1	7.038(1)	2.42(1)	3.36(1)	373.6(3)	72.7(7)	79.2(4)	-0,608	-0,208	0,941
P2	3.247(4)	3.47(1)	6.095(2)	34.8(2)	72.2(4)	242.6(1)	-0,402	-0,048	0,936



The EPR spectrum of $Mg_{2.997}Co_{0.003}V_2O_8$ for the magnetic field applied parallel to the c axis at T=4.2K.



The angular dependence of the EPR spectrum in the plane bc at T=4.2K.

Conclusions
- The orbital contribution to the magnetic momentum of Co ions is reduced.
- The local symmetry of oxygen octahedron surrounding Co ions in “cross-tie” and “spine” positions was found to be rhombic.
- The main values of the g-factors and hyperfine structure were determined for both cobalt positions.

The work was partly supported by Polish Committee for Scientific Research (KBN) under the project 1 P03B 038 27.