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THE CRYSTAL STRUCTURES OF $RbMnP_2O_7$

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The crystal and magnetic structures of $RbMnP_2O_7$ have been determined. The crystal structure (a=7.3672(2), b=9.6782(2), c=8.6467(2)Å, β=105.488(1)° space group $P2_1/c$, was determined from X-ray and neutron powder diffraction, and was found to be isostructural with $RbFeP_2O_7$. Magnetic susceptibility measurements showed that $RbMnP_2O_7$ behaves as a Curie-Weiss paramagnet at high temperatures and orders antiferromagnetically bellow a Neel temperature of 20K. From low temperature neutron diffraction, the magnetic structure was found to be commensurate with the nuclear cell, with a magnetic symmetry group $P2_1^-/c$.

Introduction. Diphosphates of the trivalent transition metals of the stoichiometery $A^IM^{III}P_2O_7$ (A=alkali metal, M= V,Fe,Mo) exhibit several structure types [1–3]. The frameworks of these phases are built up fromcorner-sharing MO_6 octaedra and P_2O_7 groups. The size of the alkali metal cation plays an important role in the crystal structures of $A^IM^{III}P_2O_7$. The diphosphate group is very adaptive to the bonding

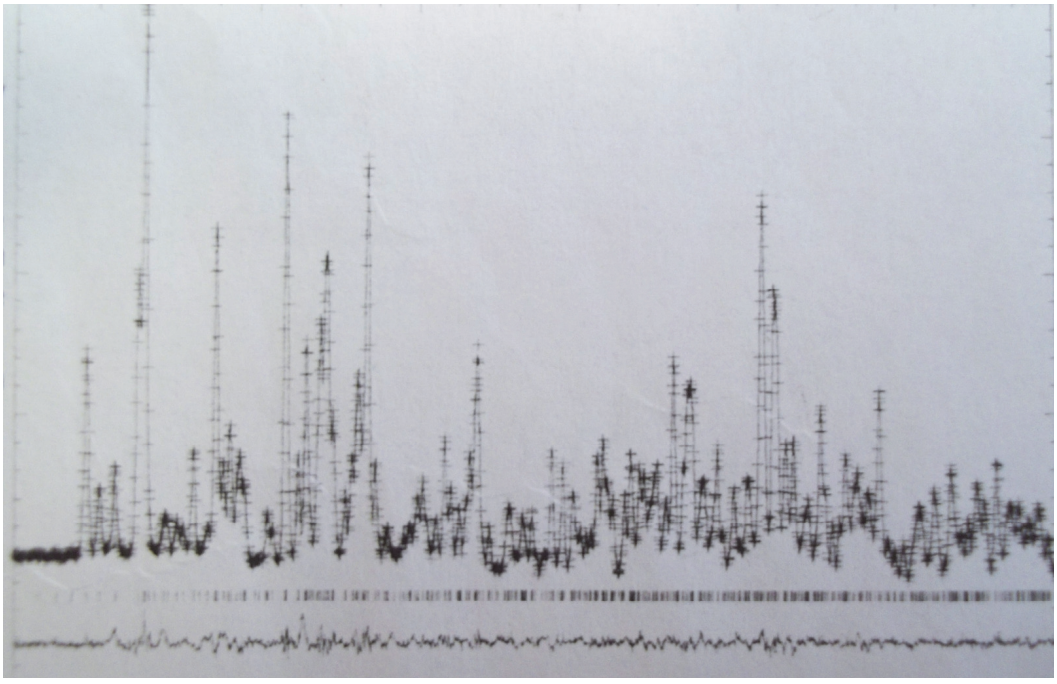

Figure 1. 2(˚) diagram

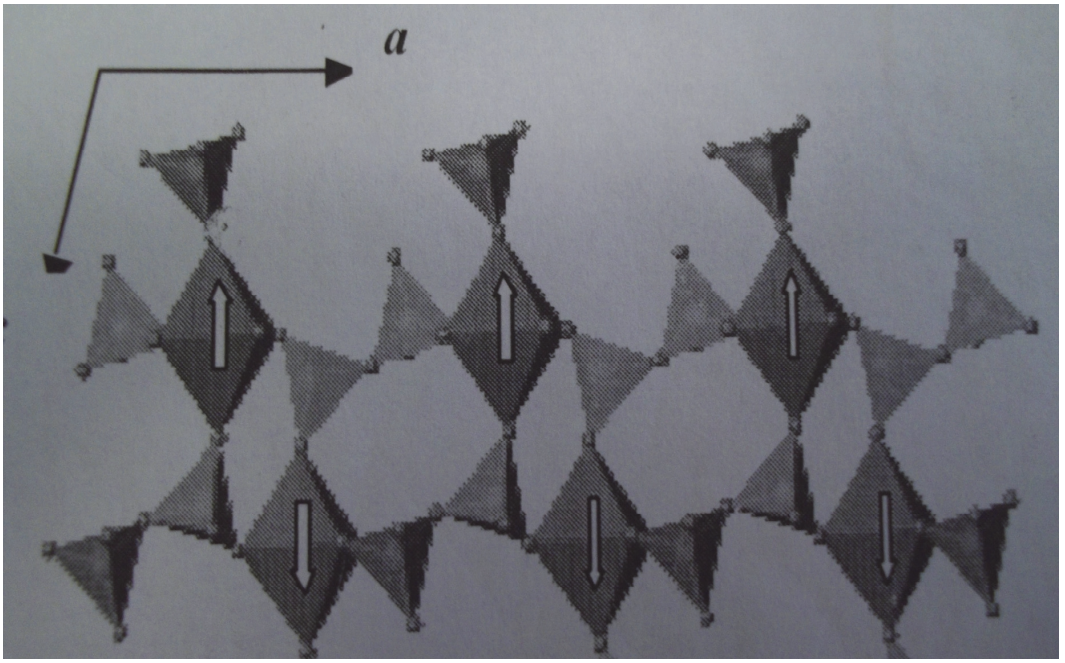

Figure 2. Orientated closely Mn–O bonds

requirements of other groups in the structure by adjusting the P–O–P bond angle and configuration of two phoshates tetraedra. In our continuing study of magnetic exchange interactions in these systems, we have investigated the nuclear and magnetic structure of $RbMnP_2O_7$ using neutron powder diffraction data recorded on HRPT at a wavelength of 1.886 Å at 2K and 100K. Analysis was performed using the GSAS suite of programs and the Rietveld plot from the 2K data is displayed in figure1.

Results and discussion. The resulting nuclear structure was found to consist of a framework of corner-sharing $Mn0_6$ octaedral and P_2O_7 groups, creating intersecting tunnels, with the Rb+ cation located at the intersection of these tunnels. The $Mn0_6$ octaedral were found to display an untypical (2+2+2) distorted arrangement (2 long, 2 medium and 2 short bonds) instead of the traditional (4+2) Jahn-Teller distortion expected for Mn^{+3}. The diphosphate group contained two distorted PO_4 tetraedra, with long P-O bonds to the bringing O atom and shorter bonds to terminal O atoms.

After the nuclear contribution was fitted for the 2K neutron diffraction pattern, extra peaks and intensity were evident and were assigned as magnetic diffraction. Subsequently, the nuclear and magnetic cells were found to be commensurate and consistent with the magnetic space group $P2_{1}./c$, with the magnetic moments lying in the ac plane resulting in a moment of 3.65 μ_b. The relative direction of the four Mn spins in the unit cell were found to be (0.23, 0.90, 0.26)+, (0.23, 0.60, 0.76)-, (0.77, 0.40, 0.25)+ (0.77, 0.10, 0.75)-, orientated closely to the two long axial Mn–O bonds (fig. 2).

Conclusion

Interestingly, this magnetic structure was found to consist of both antiferromagnetic and ferromagnetic exchange interactions mediated through Mn–O–Mn–O pathways.

Referenses

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АНОТАЦІЯ

Лаврик Р.В. *Кристалічна структура $RbMnP_2O_7$ // Біоресурси і природокористування. – 2015. – 7, №1–2. – С. 37–39.*

Досліджено кристалічну і магнітну структуру $RbMnP_2O_7$. Параметри кристалічної решітки (a=7.3672(2), b=9.6782(2), c=8.6467(2)Å, β=105.488(1)° просторової групи $P2_1/c$, було визначено рентгеновською та нейтронною силовою дифракцією, яка підтвердила ізоструктурність отриманого фосфату з $RbFeP_2O_7$.

АННОТАЦИЯ

Лаврик Р.В. *Кристаллическая структура $RbMnP_2O_7$ // Биоресурсы и природопользование. – 2015. – 7, №1–2. – С. 37–39.*

Исследована кристаллическая и магнитная структура $RbMnP_2O_7$. Параметры кристаллической решетки (a=7.3672(2), b=9.6782(2), c=8.6467(2)Å, β=105.488(1)° пространственной группы $P2_1/c$, были определены рентгеновской и нейтронной силовой дифракцией, которая подтвердила изоструктурность полученого фосфата с $RbFeP_2O_7$.