Electronically Supporting Information

in the manuscript

SrFe₂(PO₄)₂: *Ab Initio* structure determination with X-ray powder diffraction data and unusual magnetic properties

Alexei A. Belik,^{*a} Masaki Azuma,^{a,b} Mikio Takano^a and Bogdan I. Lazoryak^c

^a *Institute for Chemical Research, Kyoto University, Uji, Kyoto-fu 611-0011, Japan.*

E-mail: belik@msk.kuicr.kyoto-u.ac.jp

^b *PRESTO, Japan Science and Technology Agency (JST), Kawaguchi, Saitama 332-0012, Japan*

^c *Department of Chemistry, Moscow State University, Leninsky Gory, Moscow 119992, Russia*

Fig. S1. The χT vs T curves in the field cooled mode at 0.1, 5, 15, 30, 50, and 90 kOe in the temperature range of 2–27 K

Fig. S2a. M vs H curves at $T = 5$ K between 0 to 50 kOe. Note the small hysteresis between ~ 10 and ~ 50 kOe (the second hysteresis). Inset gives the curves between -50 to 50 kOe.

Fig. S2b. M vs H curves at $T = 6$ K between 0 to 50 kOe. Note the small hysteresis between ~ 10 and ~ 40 kOe (the second hysteresis). Inset gives the curves between -50 to 50 kOe.

Fig. S2c. M vs H curves at $T = 8 \text{ K}$ between 0 to 30 kOe. Note the small hysteresis between ~ 5 and ~ 20 kOe (the second hysteresis). Inset gives the curves between -50 to 50 kOe.

Fig. S2d. First isothermal magnetization plots, M vs H , at $T = 2, 5, 6,$ and 8 K measured from 0 to 10 kOe.

Fig. S3. Magnetization curves, (a) M vs H and (b) dM/dH vs H , at $T = 9$, 10, 11, and 13 K measured from 50 to 0 kOe.

Fig. S4. The real ($\chi' = M'/H_{ac}$) and imaginary ($\chi'' = M''/H_{ac}$) parts of the *ac* susceptibility as a function of temperature (at 2–30 K) at different frequencies ($f = 100, 1000, 5000$, and 10000 Hz). Measurements were performed at $H_{dc} = 0$ Oe using an *ac* field with the amplitude $H_{ac} = 1$ Oe. The $\chi''(T)$ curve at $f = 100$ Hz was too noisy and not shown. Note that there is no anomaly at $T_2 = 11.3$ K.
(Frequency dependent *ac* susceptibility measurements at zero field were performed with a PPMS in the temperature range of 2–30 K (on cooling) at frequencies (f) of 10^2 , 10^3 , 5×10^3 , and 10^4 Hz at applied oscillating magnetic field (H_{ac}) of 1 Oe.)