

## Erratum: Cubic-Rhombohedral Structural Phase Transition in Na<sub>1.32</sub>Mn[Fe(CN)<sub>6</sub>]<sub>0.83</sub>·3.6H<sub>2</sub>O [J. Phys. Soc. Jpn. 80 (2011) 074608 ]

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(Received June 5, 2018)

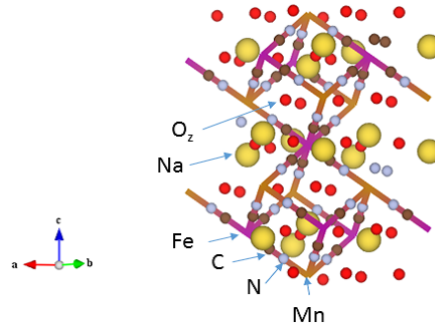
KEYWORDS: Trigonal phase, Prussian blue analogue

We reported crystal structure of the trigonal Na<sub>1.32</sub>Mn[Fe(CN)<sub>6</sub>]<sub>0.83</sub>·3.6H<sub>2</sub>O at 200 K with the hexagonal setting ( $R\bar{3}m$ , Space group No. 166 and Setting No. 1).<sup>1)</sup> In the analysis, however, we have chosen a wrong unit cell, *i.e.*,  $a_H = a_C\sqrt{2}$  and  $c_H = c_C\sqrt{3}$  (subscript H and C represent hexagonal setting and pseudo-cubic setting, respectively). The unit cell is four times larger in volume than the appropriate unit cell,  $a_H = a_C/\sqrt{2}$  and  $c_H = c_C\sqrt{3}$ .

We have re-analyzed the same X-ray power diffraction pattern with use of Rietan-FP program.<sup>2)</sup> Na<sup>+</sup> is put between the Fe and Mn along  $c$  axis ( $6c$ ). C, N, and the ligand oxygens ( $O_l$ ) are put on the edge ( $18h$ ) on the nanocube. The zeolite oxygen ( $O_z$ ) is put at the face centered position ( $9d$

**Table I.** Occupancy ( $g$ ), atomic positions ( $x, y, z$ ), and isotropic atomic displacement parameter ( $B$ ) of Na<sub>1.32</sub>Mn[Fe(CN)<sub>6</sub>]<sub>0.83</sub>·3.6H<sub>2</sub>O in the rhombohedral phase ( $R\bar{3}m$ : hexagonal setting) at 200 K.  $O_l$  and  $O_z$  are ligand oxygen and zeolite oxygen, respectively. For C, N, and  $O_l$ , linear constraints between the atomic coordinates, *i.e.*,  $z = \frac{x}{2}$ , are adopted.  $x$  and  $B$  of  $O_l$  are fixed as the same as those of C. The cell parameters are  $a_H = 7.5156(5)$  Å and  $c_H = 18.0323(13)$ .  $R_{wp}$ ,  $R_I$ , and  $S$  are 10.51%, 9.52%, and 2.39, respectively.

Atom	site	$g$	$x$	$y$	$z$	$B$ (Å <sup>2</sup> )
Fe <sup>2+</sup>	$3a$	0.83	0	0	0	0.3(2)
Mn <sup>2+</sup>	$3b$	1	0	0	1/2	2.5(2)
C	$18h$	0.83	0.213(1)	0.787	0.106	5.7(7)
N	$18h$	0.83	0.135(1)	0.865	0.068	1.5(4)
Na <sup>+</sup>	$6c$	0.66	0	0	0.242(2)	12.8(4)
$O_l^{2-}$	$18h$	0.057(9)	0.213	0.787	0.106	5.8
$O_z^{2-}$	$9d$	0.543	1/2	0	1/2	17.8(7)
$O_z^{2-}$	$9e$	0.543	1/2	0	0	17.7



**Fig. 1.** (Color online) Crystal structure of trigonal  $\text{Na}_{1.32}\text{Mn}[\text{Fe}(\text{CN})_6]_{0.83}\cdot 3.6\text{H}_2\text{O}$ . Fe, Mn, and  $\text{O}_l$  are omitted for simplicity. Thick lines represent the nanocubes.  $z$ -coordinate of Na is exaggerated.

and  $9e$ ) of the nanocube. The occupancies ( $g$ ) for Fe, Mn, Na, C and N are fixed as the chemical composition. For oxygens, a linear constraint between  $g_s$ , *i.e.*,  $g(9d) = g(9e) = 0.6 - g(18h)$ , is adopted, so that the oxygen content coincides the chemical composition. The obtained results are listed in Table I. Figure 1 shows crystal structure of the trigonal  $\text{Na}_{1.32}\text{Mn}[\text{Fe}(\text{CN})_6]_{0.83}\cdot 3.6\text{H}_2\text{O}$ .

Let us compare the magnitude and direction of the Na displacements from the central position of the nanocube. In the previous analysis,<sup>1)</sup> the Na displacement was  $1.69(4) \text{ \AA}$  and  $0.22(4) \text{ \AA}$  toward the Fe site for  $6c$  and  $18h$  sites, respectively. In the present analysis, the Na displacement [ $= 0.14(4) \text{ \AA}$ ] toward the same direction is confirmed. The different magnitude may be ascribed to the different structural model:  $\text{O}_z$  is put at the face centered position in the present model while their positions were adjusted in the previous model. Thus, the previous conclusion "cubic-trigonal phase transition is regarded as an order-disorder transition of the Na ions" is supported by the correct structural analysis.

## Acknowledgments

This work was supported by Grants-in-Aid (No. 21244052 and No. 22013003) for Scientific Research from the Ministry of Education, Culture, Sports, Science and Technology, Japan. The synchrotron-radiation X-ray powder diffraction experiments were performed at the SPring-8 BL02B2 beamline with the approval of the Japan Synchrotron Radiation Research Institute (JASRI)

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