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Erratum: Cubic-Rhombohedral Structural Phase Transition in Na_{1.32}Mn[Fe(CN)₆]_{0.83}·3.6H₂O [J. Phys. Soc. Jpn. 80 (2011) 074608]

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We reported crystal structure of the trigonal Na_{1.32}Mn[Fe(CN)₆]_{0.83}·3.6H₂O at 200 K with the hexagonal setting ($R\bar{3}m$, Space group No. 166 and Setting No. 1).¹⁾ 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.²⁾ Na⁺ 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_{1.32}Mn[Fe(CN)₆]_{0.83}·3.6H₂O 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 ²)
Fe ²⁺	$3a$	0.83	0	0	0	0.3(2)
Mn ²⁺	$3b$	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 ⁺	$6c$	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

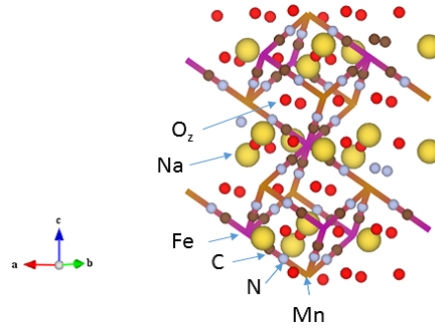


Fig. 1. (Color online) Crystal structure of trigonal $\text{Na}_{1.32}\text{Mn}[\text{Fe}(\text{CN})_6]_{0.83}\cdot 3.6\text{H}_2\text{O}$. Fe, Mn, and O_l are omitted for simplicity. Thick lines represent the nanocubes. z -coordinate of Na is exaggerated.

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,¹⁾ 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: 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.

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