Supplementary Materials

Pattern analysis and interpretation of scattering from short-range order stacking in layered composite crystal $Na_xCoO_2 \cdot yD_2O$ (x~0.35, y~1.3)

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Table I. Probability table for 2H-$Na_xCoO_2 \cdot yD_2O$ (x ~ 0.35, y ~ 1.3).

Table II. Fractional coordinates; occupancies, *g*; and isotropic atomic displacement parameters, *B*; for 2H-$Na_xCoO_2 \cdot yD_2O$ (x ~ 0.35, y ~ 1.3).

Table I Probability table for 2H-$Na_xCoO_2 \cdot yD_2O$ (x ~ 0.35, y ~ 1.3).

	G_1	G_2	G_3	G_1	G_2	G_3	H_1	H_1	H_1	$H_{1'}$	$H_{1'}$	$H_{1'}$
${}^tG_1$	O	O	O	O	O	O	O	O	O	E	O	O
${}^tG_2$	O	O	O	O	O	O	O	O	O	O	E	O
${}^tG_3$	O	O	O	O	O	O	O	O	O	O	O	E
${}^tG_1$	O	O	O	O	O	O	E	O	O	O	O	O
${}^tG_2$	O	O	O	O	O	O	O	E	O	O	O	O
${}^tG_3$	O	O	O	O	O	O	O	O	E	O	O	O
${}^tH_1$	A_{11}	A_{12}	A_{13}	O	O	O	O	O	O	O	O	O
${}^tH_1$	A_{21}	A_{22}	A_{23}	O	O	O	O	O	O	O	O	O
${}^tH_1$	A_{31}	A_{32}	A_{33}	O	O	O	O	O	O	O	O	O
${}^tH_{1'}$	O	O	O	A_{44}	A_{45}	A_{46}	O	O	O	O	O	O
${}^tH_{1'}$	O	O	O	A_{54}	A_{55}	A_{56}	O	O	O	O	O	O
${}^tH_{1'}$	O	O	O	A_{64}	A_{65}	A_{66}	O	O	O	O	O	O

Note 1: Arrays, $\boldsymbol{E}$, $\boldsymbol{O}$, $\boldsymbol{A}_{st}$, $\boldsymbol{G}_q$, ${}^t\boldsymbol{G}_q$, $\boldsymbol{H}_r$, and ${}^t\boldsymbol{H}_r$, are defined as follows,

$$\boldsymbol{E} \equiv \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \quad \boldsymbol{O} \equiv \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad \boldsymbol{A}_{st} \equiv \begin{pmatrix} 0 & \alpha_{st} & \alpha_{st} & \alpha_{st} \\ \alpha_{st} & 0 & \alpha_{st} & \alpha_{st} \\ \alpha_{st} & \alpha_{st} & 0 & \alpha_{st} \\ \alpha_{st} & \alpha_{st} & \alpha_{st} & 0 \end{pmatrix}, \quad \boldsymbol{G}_q \equiv$$

$$\begin{pmatrix} G_{1q} & G_{2q} & G_{3q} & G_{4q} \end{pmatrix}, {}^t\boldsymbol{G}_q \equiv \begin{pmatrix} G_{1q} \\ G_{2q} \\ G_{3q} \\ G_{4q} \end{pmatrix}, \boldsymbol{H}_r \equiv \begin{pmatrix} H_r & H_r & H_r & H_r \end{pmatrix}, \text{ and } {}^t\boldsymbol{H}_r \equiv \begin{pmatrix} H_r \\ H_r \\ H_r \\ H_r \end{pmatrix}.$$

Note 2: When the structure is analyzed on the assumption that all $\boldsymbol{A}_{st}$ are equal to each other, or all α_{st}'s are equal to 1/9, the commensurate model does not significantly improve the fitting results. When $\boldsymbol{A}_{s3} = \boldsymbol{A}_{s5} = \boldsymbol{O}$, i.e. $\alpha_{s3} = \alpha_{s5} = 0$, the R factors are lowered to $R_p = 4.0\%$ and $R_{wp} = 5.8\%$ with the values from $\alpha_{s1} = \alpha_{s4} = 0.220$, $\alpha_{s2} = \alpha_{s6} = 0.113$ to $\alpha_{s1} = \alpha_{s4} = 0.141$, $\alpha_{s2} = \alpha_{s6} = 0.192$. As dependency of the R factors on the values of α_{s1}, α_{s2}, α_{s4}, α_{s6} is weak and it is difficult to know the optimum values for α_{st}, $\alpha_{s1} = \alpha_{s2} = \alpha_{s4} = \alpha_{s6} = 1/6$ and $\alpha_{s3} = \alpha_{s5} = 0$ have been selected as a typical value set of α_{st} to obtain a satisfactory convergence.

Table II Fractional coordinates; occupancies, *g*; and isotropic atomic displacement parameters, *B*; for 2H-$Na_xCoO_2 \cdot yD_2O$ (x ~ 0.35, y ~ 1.3).

Host part	*x*	*y*	*z*	*g*	*B* (Å^2)
Co1	0	0	0	1	0.735(4)
Co2	1/2	0	0	1	= *B*(Co1)
O1	2/3	1/3	-0.2328(5)	1	= *B*(Co1)
O2	0.1672(7)	-0.1672	-0.1942(2)	1	= *B*(Co1)
Guest part	*x*	*y*	*z*	*g*	*B* (Å^2)
Na1	0	0	0	1[a]	= *B*(Co1)
Na2	1/3	2/3	0.1596(12)	0.192[a]	= *B*(Co1)
O3	0.6840(6)	0.6662(8)	0.2808(6)	0.857(1)	= *B*(Co1)
D1	0.7352(6)	0.6876(11)	0.4747(5)	= *g*(O3)	5.73(3)
D2	0.4934(5)	0.5496(6)	0.2712(7)	= *g*(O3)	= *B*(D1)
O4	2/3	1/3	0.3798(10)	0.146(3)	= *B*(Co1)
D3	0.41(3)	0.299(2)	= *z*(O4)	= *g*(O4)	= *B*(D1)

a = 5.6418(2) Å, *c* = 4.9029(3) Å, and γ = 120°. Local symmetry: *x*, *y*, *z*; −*y*, *x*−*y*, *z*; *y*−*x*, −*x*, *z*; −*x*, −*y*, −*z*; *y*, *y*−*x*, −*z*; *x*−*y*, *x*, −*z*. [a] Na content was fixed to the analytical value.

Reference

Takada K., Onoda M., Argyriou D.N., Choi Y.-N., Izumi F., Sakurai H., Takayama-Muromachi E. and Sasaki T. (2009). *Chem. Mater.* **21**, 3693-3700.