# PCP7-1

## Accurate Determination of Composite Crystal Structure of $Sr_{14-x}Ca_xCu_{24}O_{41}$ Using the Akaike Information Criterion

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The composite crystal structures of the spin-ladder compound, $Sr_{14-x}Ca_xCu_{24}O_{41}$ have been accurately determined using the Akaike Information Criterion (*AIC*) to solve the possible overfitting of atomic parameters. For $Sr_{14}Cu_{24}O_{41}$ as parent material of $Sr_{14-x}Ca_xCu_{24}O_{41}$, the minimizing *AIC* method removes an anomalous behavior of the Cu-O bonds along the 1-D Cu-O chain in the two-legged $Cu_2O_3$ ladder. Our study reveals the importance of the Cu-O-Cu rung with a strong Cu-O bond in $Sr_{14-x}Ca_xCu_{24}O_{41}$.

In the modulated structure of $Sr_{14}Cu_{24}O_{41}$, non-symmetric hole transfers from the O atom in the $CuO_2$ chain to the Cu-O-Cu rung in the ladder have been elucidated. The Bond-valence sum analysis of the modulated $CuO_2$ substructure of $Sr_{14}Cu_{24}O_{41}$ shows the role of large displacive modulation of O atom in the $CuO_2$ chain and the valence fluctuation of Cu atom with a periodicity almost 200 times that of the average $CuO_2$ lattice. There exist the $<Cu^{2+}>$-$<Cu^{3+}>$-$<Cu^{2+}>$ arrangements without the discommesuration in the $CuO_2$ chain. The mutual incommensurability between the average substructures is precisely characterized and the chemical formula of $Sr_{14}Cu_{24}O_{41}$ should be exactly expressed as $(Sr_2Cu_2O_3)_{0.6995}CuO_2$.

The minimizing *AIC* method has enabled us to successfully select the correct superspace group of $Sr_{14-x}Ca_xCu_{24}O_{41}$.

[1] Y. Gotoh *et al.*, Phys. Rev. B **68**, 224108 (2003).
[2] Y. Gotoh, J. Phys. Soc. Jpn., **87**, 124601 (2018).

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