Supporting Information

Development of an automatic, high-throughput structural refinement method using Rietveld analysis

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Table S1. The parameters for $CaMnTi_2O_6$ refined during Rietveld analysis. Initial values for the parameters marked with * are randomly generated by software developed in this study.

Symbol	Note	Symbol	Note
t_0	Peak shift parameter 1	η_{L0}*	Mixing parameter 1
t_1	Peak shift parameter 2	η_{L1}*	Mixing parameter 2
t_2	Peak shift parameter 3	η_{H0}*	Mixing parameter 3
t_3	Peak shift parameter 4	η_{H1}*	Mixing parameter 4
b_0*	Background parameter 1	*a*	Lattice parameter, *a*
b_1*	Background parameter 2	*c*	Lattice parameter, *c*
b_2*	Background parameter 3	Mn1-*z*	Fractional coordinate, *z* for Mn on tetrahedral site
b_3*	Background parameter 4	Mn2-*z*	Fractional coordinate, *z* for Mn on square planar site
b_4*	Background parameter 5	Ca2-*z*	Fractional coordinate, *z* for Ca on 2*c* site
b_5*	Background parameter 6	Ti-*x*	Fractional coordinate, *x* for Ti
b_6*	Background parameter 7	Ti-*y*	Fractional coordinate, *y* for Ti
b_7*	Background parameter 8	Ti-*z*	Fractional coordinate, *z* for Ti
b_8*	Background parameter 9	O1-*x*	Fractional coordinate, *x* for O1 on 4*e* site
b_9*	Background parameter 10	O1-*z*	Fractional coordinate, *z* for O1 on 4*e* site
b_{10}*	Background parameter 11	O2-*x*	Fractional coordinate, *x* for O2 on 4*d* site
b_{11}*	Background parameter 12	O2-*z*	Fractional coordinate, *z* for O2 on 4*d* site
*s**	Scale factor	O3-*x*	Fractional coordinate, *x* for O3 on 4*d* site
*U**	FWHM parameter 1	O3-*z*	Fractional coordinate, *z* for O3 on 4*d* site
*V**	FWHM parameter 2	O4-*x*	Fractional coordinate, *x* for O4 on 4*e* site
*W**	FWHM parameter 3	O4-*z*	Fractional coordinate, *z* for O4 on 4*e* site
a_0*	Asymmetric parameter 1	O5-*x*	Fractional coordinate, *x* for O5 on 8*f* site
a_1*	Asymmetric parameter 2	O5-*y*	Fractional coordinate, *y* for O5 on 8*f* site
a_2*	Asymmetric parameter 3	O5-*z*	Fractional coordinate, *z* for O5 on 8*f* site

Table S2. Reliability factors of Rietveld analysis for various compounds and measurement technique.

Compound	Space group	Incident X-ray	Method	R_{wp} (%)	R_B (%)	R_F (%)	Time / s
Fapatite $Ca_{10}(PO_4)_6F_2$	$P6_3/m$ (Hexagonal)	CuKα	Manual*	8.215*	3.782*	1.924*	-
			Auto	8.119	3.718	2.202	172
Cimetidine $C_{10}H_{16}N_6S$	$P2_1/c$ (Monoclinic)	Synchrotron λ = 0.152904 nm	Manual*	6.805*	3.542*	3.304*	-
			Auto	5.970	2.407	3.036	1636
$MnTiO_3$	$R3c$ (Trigonal)	CuKα	Manual	7.699	1.695	1.572	539
			Auto	7.626	1.762	1.549	146
$MnTiO_3$	$R3c$ (Trigonal)	Synchrotron λ = 0.052035 nm	Manual	3.515	0.995	0.565	~4500
			Auto	3.267	0.961	0.553	1049

*The manual analysis results for $Ca_{10}(PO_4)_6F_2$ and $C_{10}H_{16}N_6S$ are referred from examples supplied with RIETAN-FP version 2.83 software package.