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Applications of Bayesian Corrections for Systematic Errors in Rietveld Refinements

Anton Gagin and Igor Levin

Supplementary Information:

Applications of Bayesian Correction for Systematic Errors in Rietveld Refinements

Anton Gagin and Igor Levin

Materials Measurement Science Division

National Institute of Standards and Technology

Gaithersburg MD 20899

Correspondence e-mail: igor.levin@nist.com

Table S1: Atomic coordinates and displacement parameters in AgNbO₃ obtained from the standard and GL Rietveld refinements using the LXRD and SXRD data. The numbers in parenthesis represent estimated standard deviations (1 esd). For the GL refinements, two models were used. In the first model (“complete”), all three correction types were included, whereas the second model (“mult + add”) considered the multiplicative and additive corrections only. The discrepancies larger than 2 esd are highlighted in yellow. The U_{iso} values for all the oxygen sites were constrained to be equal.

	Standard	GL (complete)		GL (mult+add)	
		LXRD	SXRD	LXRD	SXRD
a , Å	5.55281(3)	5.55335(4)	5.5541(1)	5.5545(2)	5.55370(2)
b , Å	5.60888(2)	5.60963(4)	5.6108(1)	5.6109(2)	5.60965(2)
c , Å	15.65166(7)	15.6548(1)	15.6520(2)	15.6540(4)	15.65439(6)
<i>x</i>	0.7574(5)	0.7582(6)	0.7585(7)	0.757(1)	0.7586(4)
<i>y</i>	0.2313(4)	0.2332(6)	0.2329(6)	0.2334(9)	0.2320(3)
<i>Ag1</i>	<i>U</i> ₁₁ , Å ²	0.0009(9)	-0.003(1)	0.007(5)	0.001(3)
	<i>U</i> ₂₂ , Å ²	0.034(1)	0.013(2)	0.018(3)	0.020(3)
	<i>U</i> ₃₃ , Å ²	0.0083(9)	0.004(2)	0.007(4)	0.000(2)
	<i>U</i> ₁₂ , Å ²	0.011(3)	0.004(5)	-0.004(5)	0.001(8)
<i>Ag2</i>	<i>x</i>	0.7568(5)	0.7559(7)	0.7558(7)	0.756(1)
	<i>U</i> _{iso} , Å ²	0.0215(7)	0.012(1)	0.012(3)	0.010(2)
<i>Nb</i>	<i>x</i>	0.7459(4)	0.7462(6)	0.7455(6)	0.745(1)
	<i>y</i>	0.7278(2)	0.7272(4)	0.7273(4)	0.7284(6)
	<i>z</i>	0.6248(2)	0.6246(4)	0.6249(4)	0.6246(5)
	<i>U</i> _{iso} , Å ²	0.0080(3)	0.0063(5)	0.006(3)	0.0032(8)
<i>O</i>	<i>U</i> _{iso} , Å ²	0.0009(8)	0.002(2)	0.005(4)	-0.005(3)
<i>O1</i>	<i>x</i>	0.706(3)	0.687(5)	0.700(5)	0.681(7)
	<i>y</i>	0.753(2)	0.766(4)	0.752(4)	0.755(5)
<i>O2</i>	<i>x</i>	0.797(3)	0.805(5)	0.803(5)	0.803(7)
<i>O3</i>	<i>x</i>	0.459(1)	0.458(3)	0.456(3)	0.464(4)
	<i>y</i>	0.517(2)	0.523(3)	0.520(3)	0.527(4)
	<i>z</i>	0.6142(9)	0.612(2)	0.613(2)	0.614(2)
<i>O4</i>	<i>x</i>	0.977(2)	0.977(3)	0.982(3)	0.983(5)
	<i>y</i>	0.472(2)	0.460(3)	0.465(3)	0.467(4)
	<i>z</i>	0.6397(9)	0.642(1)	0.638(2)	0.637(2)
				0.979(2)	0.982(3)
				0.471(2)	0.462(3)
				0.6401(9)	0.640(2)

Table S2: Atomic coordinates and displacement parameters in AgNbO₃ obtained from the standard and GL Rietveld refinements using the NPDF and GEM data fitted separately and jointly with the LXRD and SXRD data. The numbers in parenthesis represent estimated standard deviations (1 esd). The discrepancies larger than 2 esd are highlighted in yellow.

	Standard				GL			
	NPDF	GEM	NPDF+LXRD	GEM+LXRD	NPDF	GEM	NPDF+LXRD	GEM+LXRD
<i>a</i>, Å	5.54864(4)	5.55486(9)	5.55277(3)	5.55318(4)	5.5486(2)	5.5550(5)	5.5539(1)	5.5525(2)
<i>b</i>, Å	5.60486(4)	5.61120(9)	5.60854(3)	5.60925(4)	5.6049(1)	5.6109(4)	5.6103(1)	5.6072(1)
<i>c</i>, Å	15.64265(9)	15.6593(2)	15.65213(8)	15.6535(1)	15.6437(5)	15.662(2)	15.6526(2)	15.6520(8)
<i>x</i>	0.7573(6)	0.759(2)	0.7578(4)	0.7600(9)	0.755(1)	0.757(3)	0.7578(4)	0.758(2)
<i>y</i>	0.2294(4)	0.2297(8)	0.2329(2)	0.2314(6)	0.2323(6)	0.230(2)	0.2329(2)	0.234(1)
<i>Ag1</i>	<i>U</i>₁₁, Å²	0.0073(8)	0.008(4)	0.008(1)	0.010(3)	0.010(1)	0.014(7)	0.008(1)
	<i>U</i>₂₂, Å²	0.0096(7)	0.007(2)	0.0092(9)	0.008(2)	0.010(1)	0.011(4)	0.0092(9)
	<i>U</i>₃₃, Å²	0.012(1)	0.010(3)	0.010(1)	0.008(2)	0.010(2)	0.008(6)	0.010(1)
	<i>U</i>₁₂, Å²	-0.004(1)	-0.002(3)	-0.003(1)	0.002(2)	-0.005(2)	-0.009(7)	-0.003(1)
<i>Ag2</i>	<i>x</i>	0.7585(7)	0.757(2)	0.7571(4)	0.7565(9)	0.758(1)	0.755(4)	0.7571(4)
	<i>U</i>₁₁	0.014(1)	0.011(4)	0.007(1)	0.010(3)	0.015(2)	0.008(5)	0.007(1)
	<i>U</i>₂₂	0.025(1)	0.012(2)	0.033(1)	0.017(2)	0.027(2)	0.012(5)	0.033(1)
	<i>U</i>₃₃	0.0085(9)	0.013(3)	0.012(2)	0.011(2)	0.010(2)	0.010(6)	0.012(2)
	<i>U</i>₂₃	-0.004(1)	-0.013(2)	0.007(2)	-0.014(2)	-0.006(2)	-0.012(4)	0.007(2)
<i>Nb</i>	<i>x</i>	0.7446(4)	0.745(2)	0.7453(3)	0.7448(8)	0.7445(5)	0.746(2)	0.7453(3)
	<i>y</i>	0.7267(1)	0.7266(4)	0.7268(2)	0.7261(3)	0.7261(2)	0.7249(7)	0.7268(2)
	<i>z</i>	0.6241(2)	0.6243(5)	0.6248(2)	0.6245(4)	0.6239(2)	0.6247(8)	0.6248(2)
	<i>U</i>₁₁, Å²	0.0060(2)	0.0046(9)	0.0051(3)	0.0046(6)	0.0052(4)	0.004(1)	0.0051(3)
	<i>U</i>₂₂, Å²	0.0074(2)	0.0047(7)	0.0080(4)	0.0054(6)	0.0076(4)	0.005(1)	0.0080(4)
	<i>U</i>₃₃, Å²	0.0068(2)	0.0088(6)	0.0082(3)	0.0083(5)	0.0075(3)	0.007(1)	0.0082(3)
	<i>U</i>₁₂, Å²	-0.0035(8)	0.009(3)	-0.001(1)	0.009(2)	-0.0072(9)	-0.006(4)	-0.001(1)
	<i>U</i>₁₃, Å²	-0.000(5)	0.001(2)	-0.0014(8)	0.000(1)	-0.0019(9)	-0.005(3)	-0.0014(8)
	<i>U</i>₂₃, Å²	-0.0004(9)	0.005(3)	0.005(1)	0.009(3)	-0.003(1)	0.003(5)	0.005(1)
<i>O1</i>	<i>x</i>	0.6933(6)	0.695(1)	0.6918(9)	0.695(1)	0.6940(9)	0.698(3)	0.6918(9)
	<i>y</i>	0.7665(4)	0.7688(8)	0.7668(6)	0.7683(7)	0.7641(6)	0.765(2)	0.7668(6)
	<i>U</i>₁₁, Å²	0.0125(10)	0.011(2)	0.015(2)	0.010(2)	0.013(1)	0.013(5)	0.015(2)
	<i>U</i>₂₂, Å²	0.0089(9)	0.010(2)	0.010(1)	0.009(2)	0.004(1)	0.010(5)	0.010(1)
	<i>U</i>₃₃, Å²	0.0070(9)	0.005(3)	0.002(1)	0.008(2)	0.007(1)	0.001(7)	0.002(1)
	<i>U</i>₁₂, Å²	0.003(1)	0.001(3)	-0.001(2)	0.001(2)	0.001(1)	-0.009(5)	-0.001(2)
<i>O2</i>	<i>x</i>	0.8024(6)	0.806(1)	0.8009(9)	0.806(1)	0.8033(9)	0.806(3)	0.8009(9)
	<i>U</i>₁₁, Å²	0.0060(2)	0.013(3)	0.009(1)	0.016(2)	0.009(1)	0.011(6)	0.009(1)
	<i>U</i>₂₂, Å²	0.0074(2)	0.010(3)	0.013(2)	0.014(3)	0.028(2)	0.012(6)	0.013(2)
	<i>U</i>₃₃, Å²	0.0068(2)	0.002(2)	0.006(1)	0.000(2)	0.001(1)	0.000(8)	0.006(1)
	<i>U</i>₁₂, Å²	-0.0035(8)	-0.006(3)	0.003(2)	-0.004(3)	0.000(2)	0.004(6)	0.003(2)
<i>O3</i>	<i>x</i>	-0.000(5)	0.4699(4)	0.4667(4)	0.4701(3)	0.4671(4)	0.466(1)	0.4667(4)
	<i>y</i>	-0.0004(9)	0.5347(5)	0.5356(4)	0.5342(4)	0.5353(4)	0.535(1)	0.5356(4)
	<i>z</i>	0.6108(1)	0.6104(2)	0.6106(2)	0.6103(2)	0.6111(2)	0.6109(5)	0.6106(2)
	<i>U</i>₁₁, Å²	0.0101(4)	0.014(1)	0.0092(7)	0.014(1)	0.0098(6)	0.009(2)	0.0092(7)
	<i>U</i>₂₂, Å²	0.0101(4)	0.005(1)	0.0067(6)	0.0049(9)	0.0095(6)	0.007(2)	0.0067(6)
	<i>U</i>₃₃, Å²	0.0137(8)	0.013(2)	0.013(1)	0.015(2)	0.014(1)	0.012(4)	0.013(1)
	<i>U</i>₁₂, Å²	-0.0065(7)	-0.005(2)	-0.003(1)	-0.006(2)	-0.011(1)	-0.010(4)	-0.003(1)
	<i>U</i>₁₃, Å²	-0.0029(9)	-0.003(2)	0.000(2)	-0.005(2)	-0.002(1)	-0.009(4)	0.000(2)
	<i>U</i>₂₃, Å²	0.0067(9)	0.008(3)	0.011(2)	0.007(2)	0.003(1)	0.006(4)	0.011(2)
<i>O4</i>	<i>x</i>	0.9665(2)	0.9669(4)	0.9665(4)	0.9676(4)	0.9667(4)	0.966(1)	0.9665(4)
								0.9657(9)

<i>y</i>	0.4739(3)	0.4730(5)	0.4729(4)	0.4730(5)	0.4727(5)	0.471(1)	0.4729(4)	0.471(1)
<i>z</i>	0.6379(1)	0.6380(2)	0.6377(2)	0.6380(2)	0.6382(2)	0.6393(5)	0.6377(2)	0.6392(4)
<i>U</i> ₁₁ , Å ²	0.0084(5)	0.006(2)	0.0071(7)	0.006(1)	0.0102(9)	0.005(3)	0.0071(7)	0.005(2)
<i>U</i> ₂₂ , Å ²	0.0100(5)	0.007(1)	0.0092(7)	0.009(1)	0.0093(8)	0.006(2)	0.0092(7)	0.007(2)
<i>U</i> ₃₃ , Å ²	0.0103(7)	0.012(2)	0.011(1)	0.011(2)	0.011(1)	0.012(4)	0.011(1)	0.012(4)
<i>U</i> ₁₂ , Å ²	0.0123(10)	0.017(3)	0.007(1)	0.018(2)	0.010(2)	0.011(5)	0.007(1)	0.008(4)
<i>U</i> ₁₃ , Å ²	0.0007(9)	0.002(2)	-0.002(1)	0.005(2)	0.000(1)	0.003(5)	-0.002(1)	0.000(4)
<i>U</i> ₂₃ , Å ²	-0.0014(9)	-0.003(2)	0.000(1)	-0.005(2)	0.002(1)	-0.001(4)	0.000(1)	-0.003(4)

Table S3: Atomic coordinates and displacement parameters of Ag and Nb in AgNbO₃ obtained from the standard and GL Rietveld refinements using the same 25-parameter model while fitting separately the NPDF, GEM, LXRD, and SXRD data. The numbers in parenthesis represent estimated standard deviations (1 esd).

Standard				GL					
	NPDF	GEM	LXRD	SXRD	NPDF	GEM	LXRD	SXRD	
a, Å	5.54955(4)	5.55504(9)	5.55281(3)	5.55336(4)	5.5488(2)	5.5532(3)	5.5542(1)	5.5545(2)	
b, Å	5.60570(4)	5.61141(9)	5.60887(2)	5.60963(4)	5.6054(1)	5.6098(3)	5.6107(1)	5.6108(2)	
c, Å	15.6451(1)	15.6597(2)	15.65164(7)	15.6548(1)	15.6446(5)	15.655(1)	16.6519(2)	15.6540(4)	
x	0.7578(5)	0.758(1)	0.7584(4)	0.7582(6)	0.757(1)	0.758(2)	0.7575(6)	0.758(1)	
y	0.2291(5)	0.2310(7)	0.2335(3)	0.2340(6)	0.2346(7)	0.233(2)	0.2349(4)	0.2343(8)	
Ag1	U₁₁, Å²	0.0017(7)	0.004(2)	0.013(1)	0.001(3)	0.001(1)	0.006(4)	0.010(4)	0.005(5)
	U₂₂, Å²	0.0100(8)	0.005(2)	0.013(1)	0.004(2)	0.006(1)	0.010(5)	0.008(2)	0.005(3)
	U₃₃, Å²	0.016(1)	0.013(2)	0.018(2)	0.015(3)	0.010(3)	0.008(6)	0.016(3)	0.011(4)
	U₁₂, Å²	-0.003(1)	-0.004(2)	0.006(3)	0.003(4)	-0.004(2)	-0.008(5)	-0.001(4)	-0.002(7)
x	0.7602(7)	0.757(1)	0.7562(4)	0.7559(6)	0.762(2)	0.758(3)	0.7559(6)	0.757(10)	
U₁₁	0.018(1)	0.015(2)	0.003(1)	0.006(3)	0.021(3)	0.021(7)	0.009(4)	0.006(5)	
Ag2	U₂₂	0.024(1)	0.012(2)	0.046(2)	0.027(3)	0.041(3)	0.018(7)	0.036(3)	0.031(4)
	U₃₃	0.008(1)	0.013(2)	0.011(2)	0.000(2)	0.011(3)	0.017(8)	0.004(3)	-0.001(3)
	U₂₃	-0.006(1)	-0.017(2)	0.011(2)	0.005(3)	-0.005(3)	-0.014(5)	0.008(3)	0.006(4)
x	0.7446(4)	0.7444(9)	0.7466(3)	0.7462(6)	0.7455(8)	0.746(2)	0.7457(5)	0.7457(9)	
Nb	y	0.7282(2)	0.7274(3)	0.7274(2)	0.7273(4)	0.7272(3)	0.7252(7)	0.7282(3)	0.7287(7)
	z	0.6243(2)	0.6237(2)	0.6252(2)	0.6253(4)	0.6252(3)	0.6250(6)	0.6252(3)	0.6256(5)
	U_{iso}, Å²	0.0070(1)	0.0051(2)	0.0107(3)	0.0061(4)	0.0072(3)	0.006(1)	0.007(1)	0.004(1)