

Powder diffraction crystal structure analysis using derivative difference minimization. The example of 1-(tetrazol-5-yl)-2-nitroguanidine potassium salt

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Supplementary material

Fractional atomic coordinates and thermal parameters (\AA^2) obtained by DDM for samples A and B.

	<i>x</i>	<i>y</i>	<i>z</i>	<i>B</i> _{iso}
Sample A				
K	0.2858(2)	0.8859(1)	0.0744(3)	^a
O1	0.1246(6)	0.1149(3)	0.241(1)	2.7(1)
O2	0.3244(6)	0.0257(3)	0.637(1)	2.8(1)
C1	0.247(1)	0.3220(5)	0.489(2)	1.9(2)
C2	0.286(1)	0.5329(5)	0.584(2)	1.6(1)
N1	0.2493(8)	0.1185(5)	0.494(1)	2.9(1)
N2	0.3131(7)	0.2163(3)	0.635(1)	2.2(1)
N3	0.129(1)	0.3400(3)	0.227(2)	1.7(1)
N4	0.3249(7)	0.4152(4)	0.664(1)	1.2(1)
N5	0.1633(7)	0.5753(4)	0.325(1)	2.3(1)
N6	0.1801(8)	0.6936(4)	0.357(1)	2.4(1)
N7	0.3125(8)	0.7142(4)	0.624(1)	2.4(1)
N8	0.3807(8)	0.6147(3)	0.770(1)	1.9(1)
H1	0.105(8)	0.290(4)	0.09(1)	6.0
H2	0.113(8)	0.417(4)	0.14(1)	6.0
H3	0.39(1)	0.387(3)	0.87(1)	6.0
^a Anisotropic thermal parameters of K are: U ₁₁ , 0.050(2); U ₂₂ , 0.028(1); U ₃₃ , 0.030(2); U ₁₂ , -0.006(1); U ₁₃ , 0.002(2); U ₂₃ , 0.001(1).				
Sample B				
K	0.2853(3)	0.8863(2)	0.0737(4)	2.45(8)
O1	0.1234(8)	0.1166(5)	0.245(1)	2.4(2)
O2	0.3252(7)	0.0262(5)	0.632(1)	2.3(2)
C1	0.248(1)	0.3262(7)	0.486(2)	0.7(2)
C2	0.291(1)	0.5323(7)	0.587(2)	0.6(2)
N1	0.247(1)	0.1213(7)	0.499(2)	2.1(2)
N2	0.3151(9)	0.2193(6)	0.633(1)	1.2(2)
N3	0.1317(8)	0.3398(5)	0.227(2)	1.8(2)
N4	0.323(1)	0.4120(7)	0.666(1)	2.0(2)
N5	0.165(1)	0.5712(6)	0.324(1)	1.4(2)
N6	0.180(1)	0.6904(7)	0.354(1)	1.4(2)
N7	0.307(1)	0.7157(6)	0.623(2)	2.4(2)
N8	0.376(1)	0.6187(6)	0.769(2)	1.6(2)

Fractional atomic coordinates and thermal parameters (\AA^2) obtained by Rietveld refinement for samples A and B.

	<i>x</i>	<i>y</i>	<i>z</i>	<i>B</i> _{iso}
Sample A				
K	0.2870(3)	0.8860(1)	0.0773(4)	^a
O1	0.1222(8)	0.1153(3)	0.244(1)	2.0(2)
O2	0.3202(7)	0.0247(3)	0.631(1)	2.0(1)
C1	0.240(2)	0.3231(6)	0.480(2)	1.8(3)
C2	0.292(1)	0.5307(6)	0.595(2)	1.7(2)
N1	0.248(1)	0.1225(6)	0.505(2)	3.8(2)
N2	0.3150(9)	0.2191(4)	0.640(1)	2.1(2)
N3	0.1296(8)	0.3412(4)	0.222(1)	2.3(2)
N4	0.3259(9)	0.4137(4)	0.659(1)	2.3(2)
N5	0.163(1)	0.5745(5)	0.326(2)	2.0(2)
N6	0.180(1)	0.6954(6)	0.362(1)	1.9(2)
N7	0.315(1)	0.7173(5)	0.620(2)	3.1(2)
N8	0.3809(9)	0.6187(4)	0.773(2)	1.9(2)
^a Anisotropic thermal parameters of K are: U_{11} , 0.045(2); U_{22} , 0.030(2); U_{33} , 0.025(2); U_{12} , -0.003(2); U_{13} , -0.001(2); U_{23} , 0.007(2).				
Sample B				
K	0.2848(6)	0.8854(3)	0.0752(7)	1.8(1)
O1	0.127(1)	0.1149(6)	0.247(2)	-0.7(3)
O2	0.324(1)	0.0255(8)	0.625(2)	2.1(2)
C1	0.252(3)	0.327(1)	0.468(4)	1.9(5)
C2	0.284(2)	0.531(1)	0.587(4)	-1.7(4)
N1	0.255(2)	0.126(1)	0.525(2)	0.8(4)
N2	0.306(2)	0.224(1)	0.634(3)	1.7(4)
N3	0.130(1)	0.3407(8)	0.222(2)	1.4(3)
N4	0.325(1)	0.410(1)	0.666(2)	0.7(4)
N5	0.164(2)	0.576(1)	0.321(2)	0.3(2)
N6	0.175(2)	0.694(1)	0.362(2)	1.8(4)
N7	0.315(2)	0.712(1)	0.612(3)	1.8(2)
N8	0.374(1)	0.618(1)	0.772(2)	-0.3(3)
N8	0.374(1)	0.618(1)	0.772(2)	-0.3(3)

Variable parameters after DDM and Rietveld refinements for samples A and B

Sample A, DDM refinement

FWHM parameters V, W: 0.046926, 0.002041;
Anisotropic strain broadening parameters $S_1 \dots S_6$: 2.25392, 0.00000, 3.56990, -0.07778, -0.76963, -0.03919;
Pearson VII peak shape parameter: 1.7089;
Asymmetry coefficient: 0.15337;
Preferred orientation coefficients $P_1 \dots P_6$: 15.65830, 0.00000, 42.10891, 0.38834, 5.88969, 0.51854.

Sample A, Rietveld refinement

FWHM parameters V, W: 0.066676, -0.002243;
Anisotropic strain broadening parameters $S_1 \dots S_6$: 1.83701, 0.00000, 2.81627, 0.10795, -0.69548, -0.16963;
Pearson VII peak shape parameter: 1.3192;
Asymmetry coefficient: 0.11184;
Preferred orientation coefficients $P_1 \dots P_6$: 17.61159, 0.00000, 53.34301, -0.19715, 7.47189, 0.41286;
Polynomial background coefficients $B_0 \dots B_5$: 332.53, 11.009, 81.469, -461.38, 393.51, -95.556.

Sample B, DDM refinement

FWHM parameters V, W: 0.033288, 0.008366;
Anisotropic strain broadening parameters $S_1 \dots S_6$: 1.85734, 0.01000, 2.96342, 0.08009, -1.87592, 0.21289;
Pearson VII peak shape parameter: 1.6648;
Asymmetry coefficient: 0.10502;

Sample B, Rietveld refinement

FWHM parameters V, W: 0.044844, 0.003921;
Anisotropic strain broadening parameters $S_1 \dots S_6$: 2.09548, 0.01000, 4.87556, 0.14211, -1.40771, 0.10087;
Pearson VII peak shape parameter: 1.3227;
Asymmetry coefficient: 0.10068;
Polynomial background coefficients $B_0 \dots B_5$: 264.70, -218.65, 53.566, -135.67, 700.33, -447.19.