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Supporting information for article:

X-ray diffraction study of the atomic interactions, anharmonic displacements and inner-crystal field in orthorhombic KNbO3

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Some statistical indicators clarifying the significance of the different structural models of $KNbO_3$ are given below.

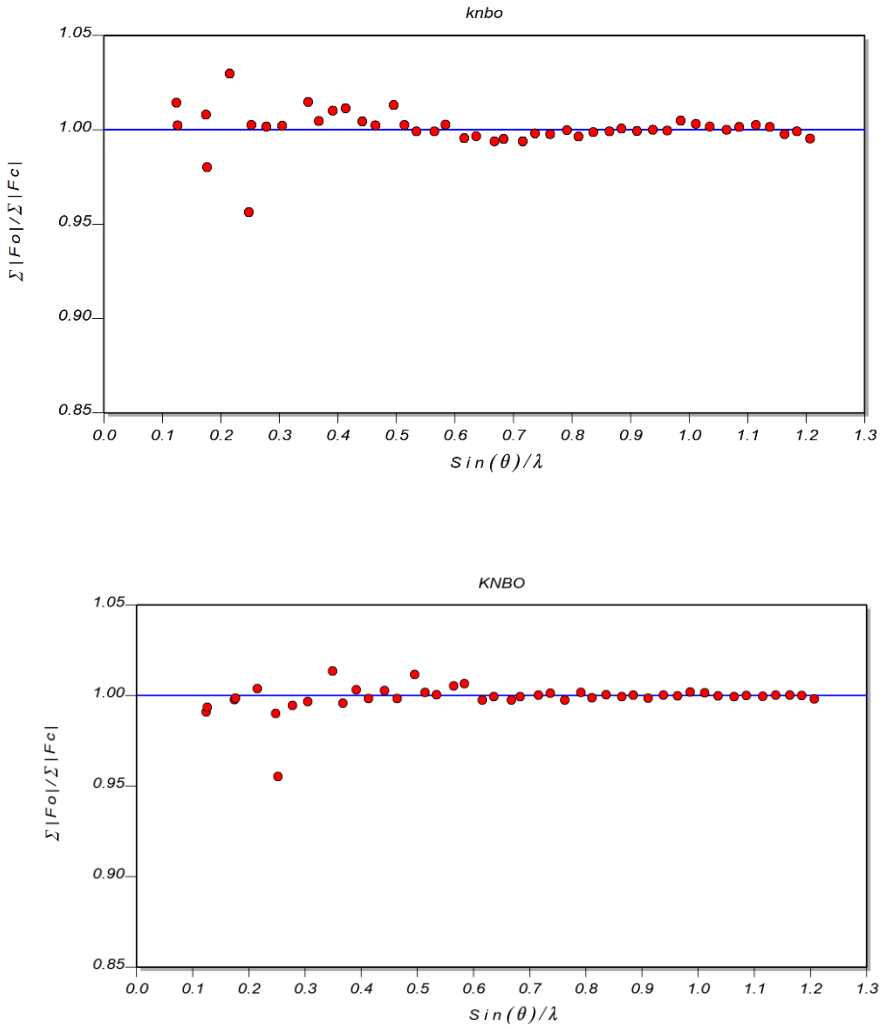

Figure S1 Distribution of the quantity $\sum F_o / \sum F_c$ over the resolution: upper graph is linked with spherical atom harmonic model, the bottom graph reflects the multipole anharmonic model. (A. Stash. XDRKplot, 2007-2010, Moscow, Russia)

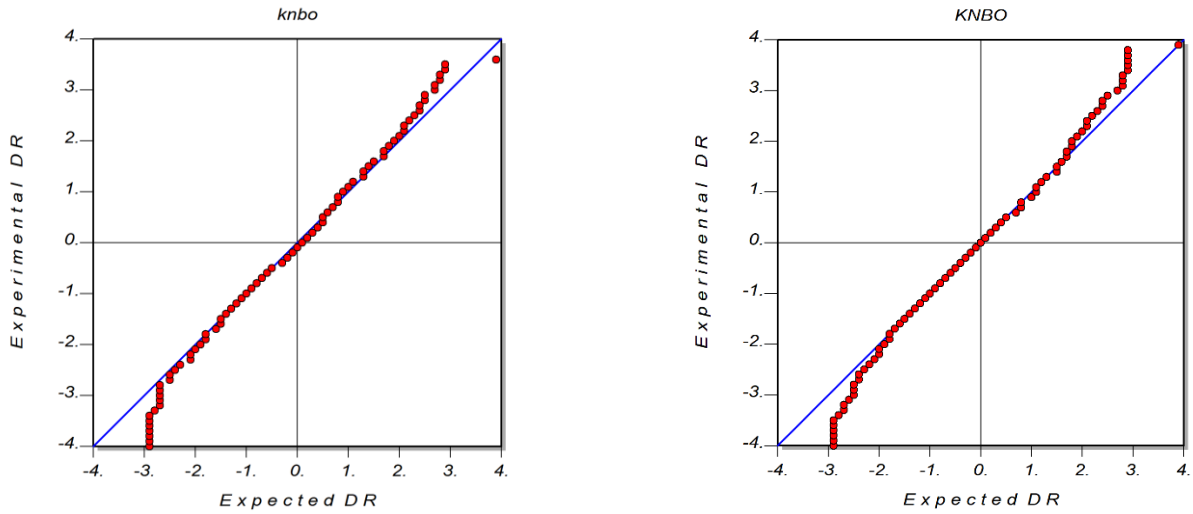

Figure S2. Normal probability plots, $\delta R_i=(F_o - F_c)_i/\sigma_i$ (F_o), for $KNbO_3$ (S.C. Abrahams & E.T. Keve. *Acta Cryst*. 1971 **A27**, 157). Left: the spherical atom harmonic model, F_c; right: the multipole anharmonic model, F_c. (A. Stash. XDRKplot, 2007-2010, Moscow, Russia)

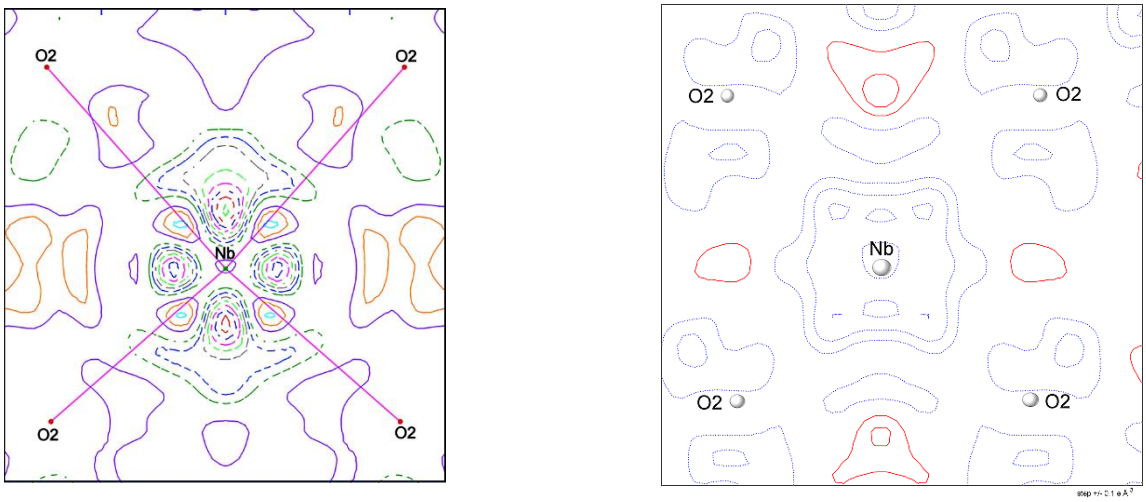

Figure 3S. Residual electron density maps showing the density, which is not covered by the chosen structural model. Left: spherical atom harmonic model; right: the multipole anharmonic model. Positive values are shown by solid lines, negative values are depicted by dashed lines. The line step is 0.1 e·Å^{-3}.

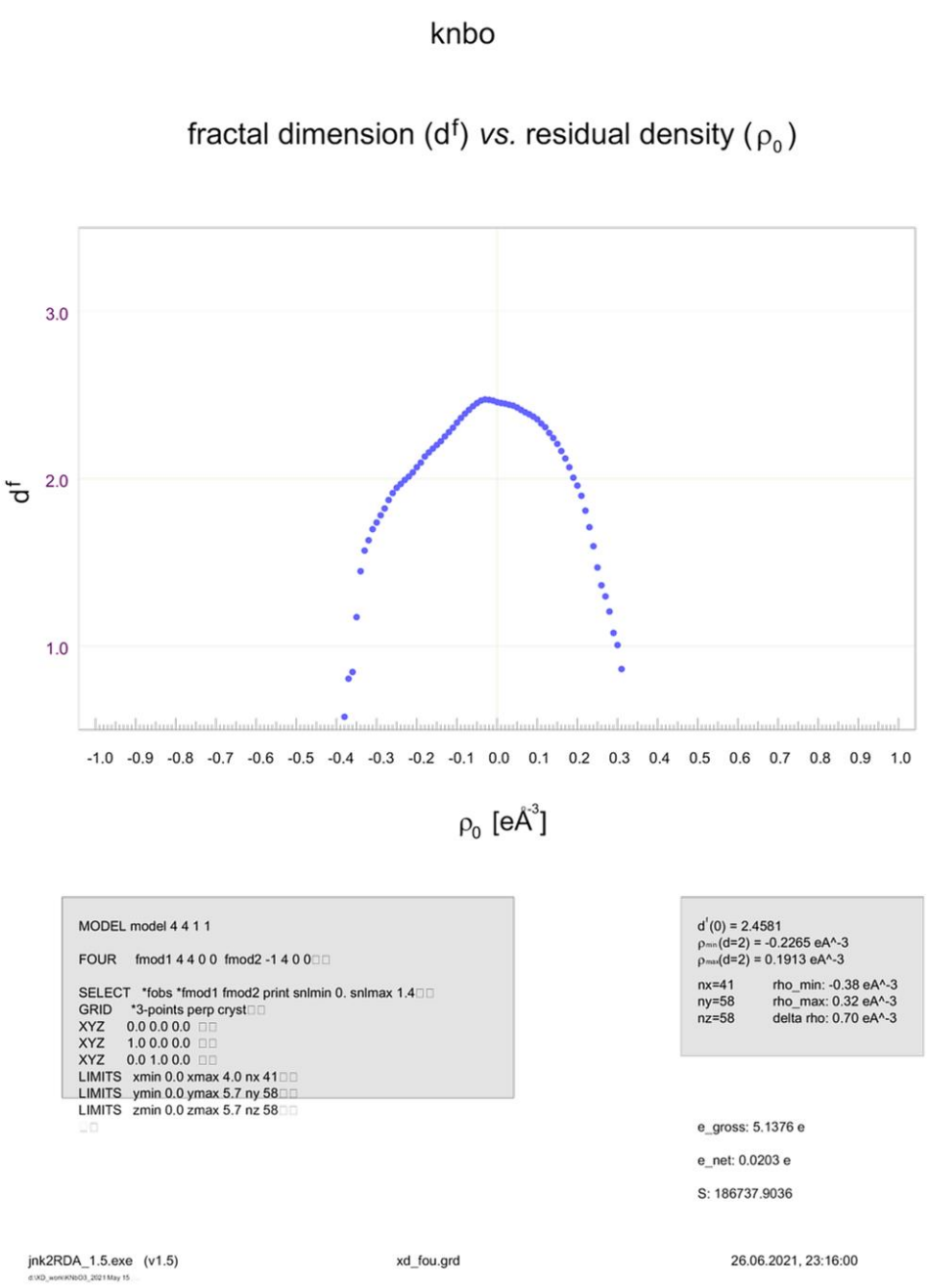

Figure 4S. Fractal dimension distribution d^f of the residual electron density in the unit cell : multipole + anharmonicity model. See Meindl, K.& Henn, J. *Acta Cryst*. 2008, ***A64***, 404-418. The distribution is close to hyperbola (the ideal case).