Electronic Supplementary Material (ESI) for Dalton Transactions.

Charge density studies of single and transient (single to double) Boron-Oxygen bonds in $(NH_4)_2B_4O_5(OH)_4 \cdot 2H_2O$

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Supporting information

The ICSD deposition numbers 2181471-2181472 contain the supplementary crystallographic data for investigated system. This data can be obtained freely via

http://www.ccdc.cam.ac.uk/data_request/cif,

by e-mailing

data_request@ccdc.cam.ac.uk

or by contacting directly the Cambridge Crystallographic Data Centre (12 Union Road, Cambridge CB2 1EZ, UK. Fax: +44 1223 336033).

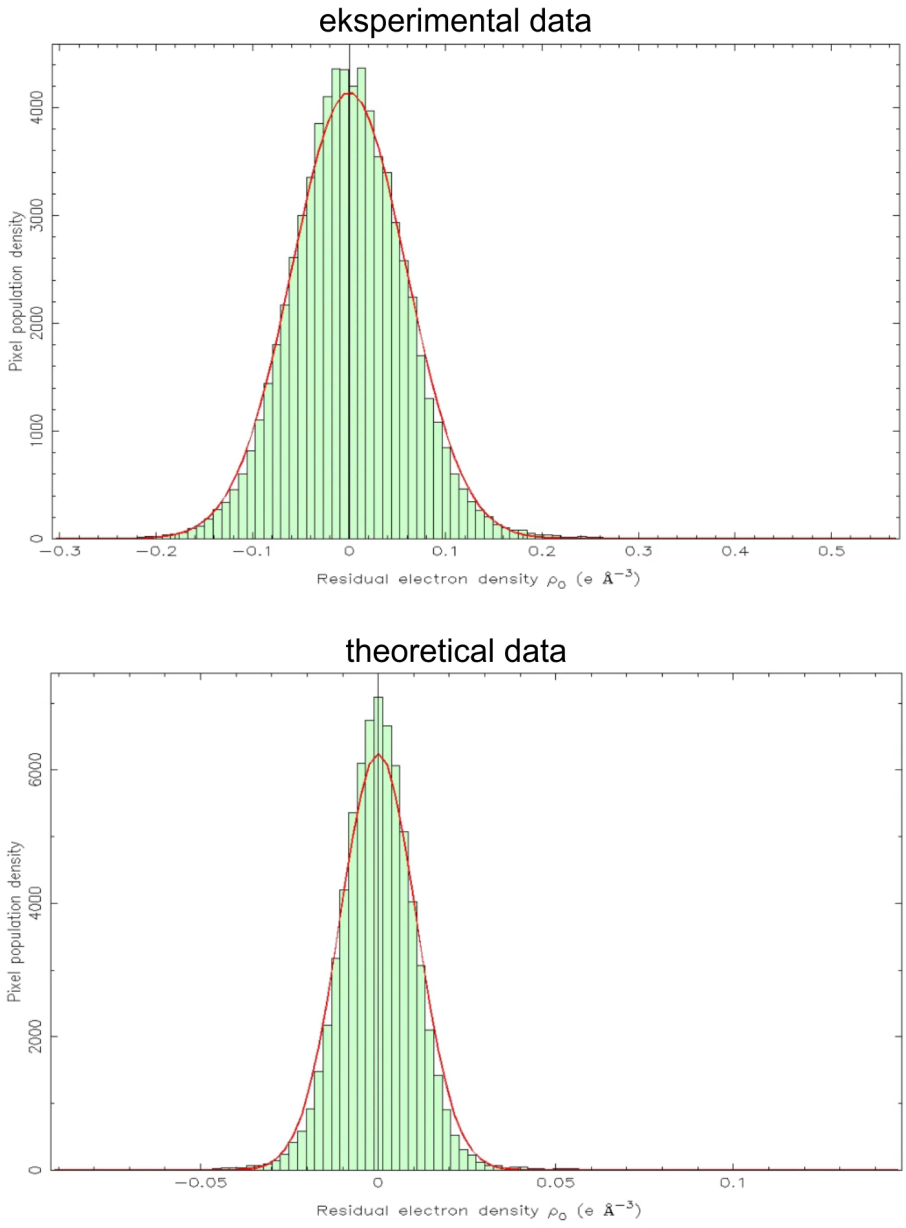


Figure 1: Normal distribution of residual electron density.

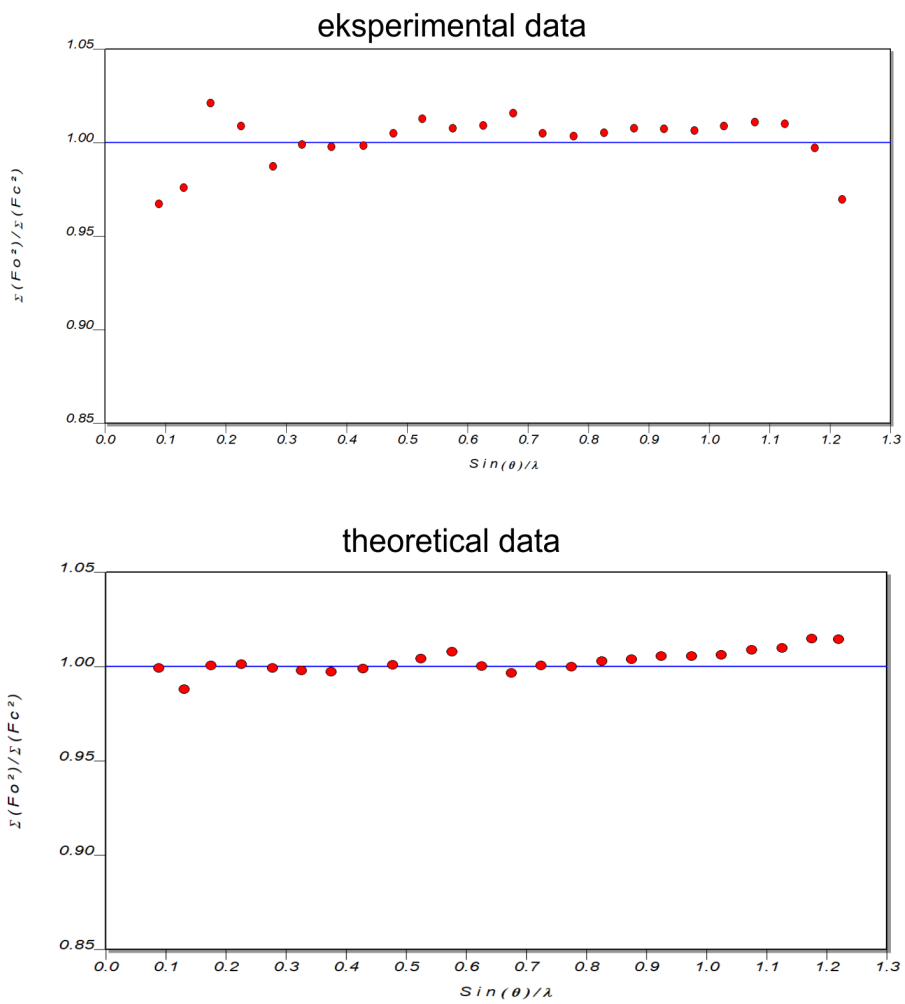


Figure 2: Ratios of the sums of observed and calculated structure-factor amplitudes as a function of sin θ/λ.

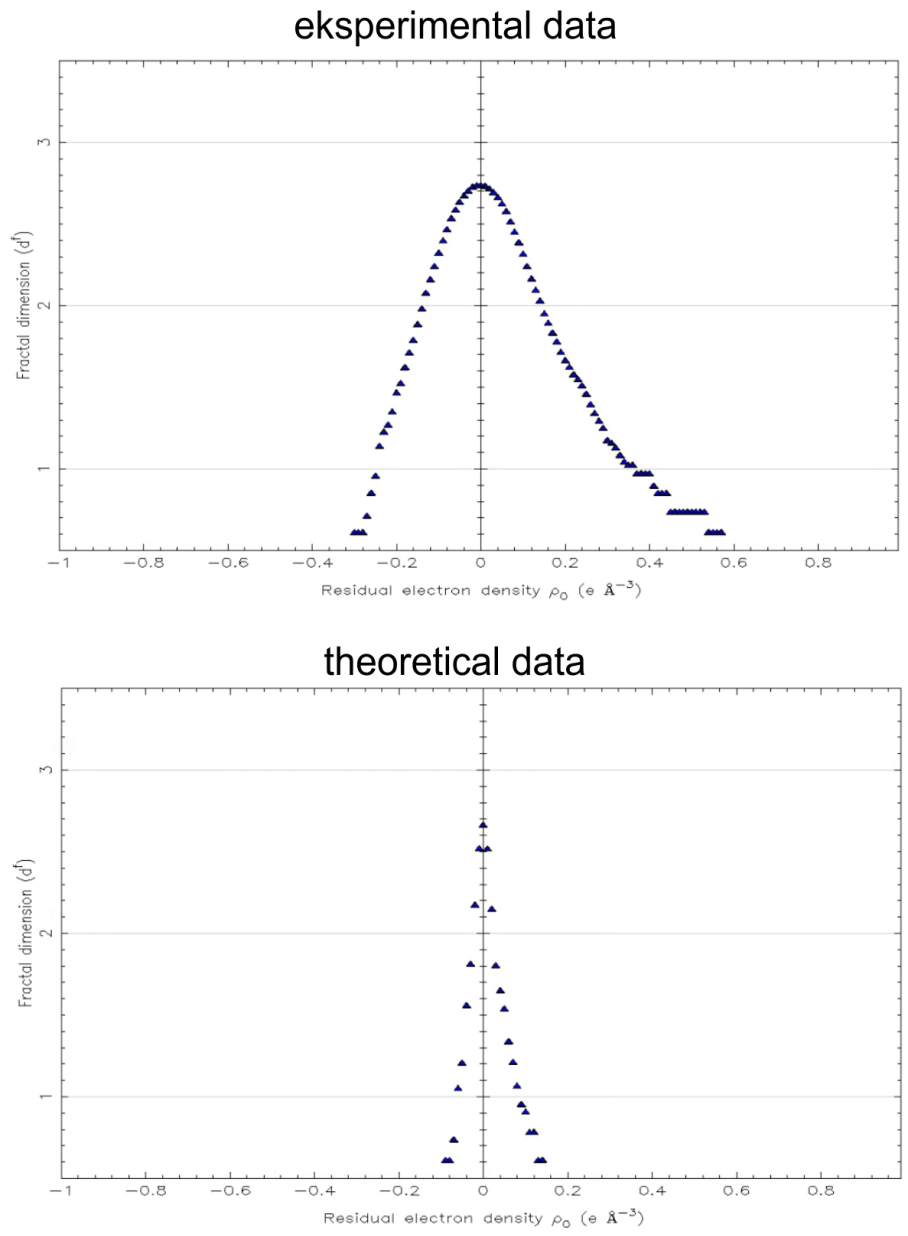
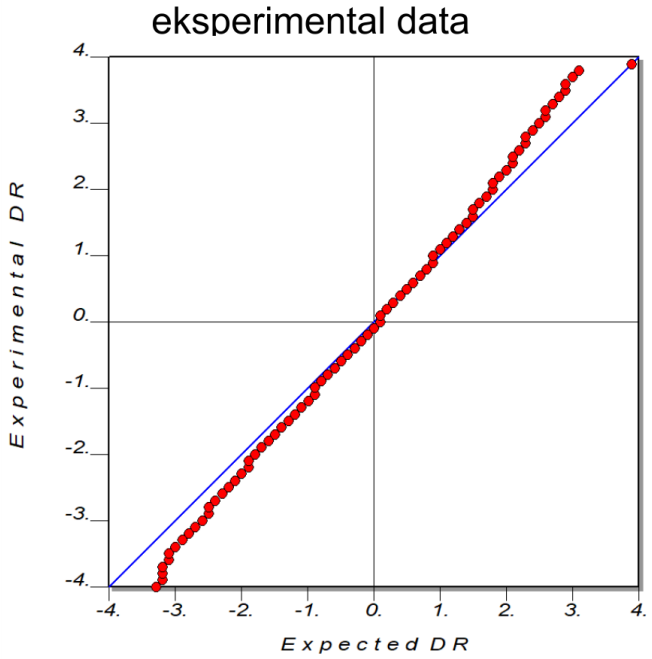


Figure 3: Fractal dimension versus residual density.



theoretical data

In the case of our theoretical calculations, the theoretical dynamic structure factors were generated by CRYSTAL17 without any uncertainties. To build a proper input file (hkl file) suitable to XD, for each structure factor we used an arbitrary uncertainty equal to 0.001. That is why there is no sense to present corresponding normal probability plot for theoretical data.

Figure 4: Normal probability plot.