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An unique model for joint refinement of (polarised) neutron and X-ray data

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A new charge and spin density model and the corresponding refinement software were recently developed to combine X-ray and polarised neutron diffraction experiments [1,2]. This joint refinement procedure allows for an access to both the charge and spin densities but also to spin up ( ) and spin down ( ) electron distributions. These two quantities (and) were thus separately modelled and for the first time it was possible to compare them with theoretical results. The first part of the presentation will introduce the refinement procedure and describe its application to the case of an end-to-end azido double bridged copper(II) complex[3]. The results of this joint refinement of X-ray and polarized neutron diffraction data will be compared to theoretical calculations. The second part will be devoted to recent applications to other materials including a purely organic radical.

[1] *Deutsch, M., Claiser, N., Pillet, S., et al., M., Acta Cryst. A 68, 675-686 (2012).,* ***[2]*** *Lecomte C., Deutsch M., Souhassou M., et al., ACA Transactions (2011).,* ***[3]*** *Deutsch, M., Gillon, B., Claiser, et al., M., submitted to IUCrJ*

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