Structure and magnetic interactions in $Ba_{3-x}Sr_xCr_2O_8$

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We have recently reported on a non-linear tuning of the magnetic interaction constant J_0 in the spin dimer system $Ba_{3-x}Sr_xCr_2O_8$ by varying the Sr content x[1]. In the present work we show that this peculiar behavior of J_0 can be explained by changes in the crystal structure, probed with neutron powder diffraction. Performing theoretical calculations based on those structural details, we could well reproduce the change of J_0 by taking into account a structural transition due to the Jahn-Teller active Cr^{5+}-ions. This transition, lifting the magnetic frustration in the system, is heavily influenced by disorder arising from partially exchanging Ba with Sr.

References:

[1] H. Grundmann, A. Schilling, C.A. Marjerrison, H.A. Dabkowska, B.D. Gaulin, Mat. Res. Bull. 48, 3108-3111 (2013)