Effect of compression in molecular spin-crossover chains

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The thermodynamic properties of a one-dimensional spin-crossover molecular chain under constant external pressure are investigated. The effective compressible degenerate Ising model is used as a theoretical basis. Analytical results for the crossover from low to high spin are obtained using the transfer matrix formalism. Exact expressions are obtained for the fraction of molecules in the high-spin state, the correlation function, and the heat capacity. The analysis of the range of parameters in which the spin-crossover occurs is carried out, and it is shown how the pressure changes the position of the crossover.

Keywords: spin-crossover, molecular chain, Ising model, magnetization, phonons.