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Monte Carlo Simulation of Spin-Crossover Compounds CHARLES J. PYE, CARSTEN TIMM, Department of Physics and Astronomy, University of Kansas, Lawrence, Kansas 66045 — A Monte Carlo simulation employing cluster updates is used to study a classical model of three-dimensional spin-crossover compounds. These compounds are characterized by magnetic ions that can be in a high-spin or low-spin state. We here consider the case of diamagnetic (S = 0) low-spin state appropriate for Fe(II) compounds. The values of the magnetization average, Binder cumulant, and high-spin/low-spin (HS/LS) fraction are studied over a wide range of values for the system size, temperature, magnetic field, HS/LS energy difference, nearest neighbor HS/LS coupling, and exchange interaction. We also address the phase diagram of the spin-crossover model.

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