Calorimetric Study of Diluted Spin Ice Materials TAO-RAN LIN, University of Waterloo, XIANGLIN KE, Pennsylvania State University, MISCHA THESBERG, McMaster University, PETER SCHIFFER, Pennsylvania State University, ROGER MELKO, MICHEL GINGRAS, University of Waterloo — Spin ice materials Dy$_2$Ti$_2$O$_7$ and Ho$_2$Ti$_2$O$_7$ have been the subject of ongoing interest for over ten years. The cooperative magnetic ground state can be mapped onto the proton disordered ground state in water ice, and its residual entropy follows the same Pauling’s estimate. Interestingly it was found in a previous study that, upon dilution of the magnetic rare earth ions Dy$^{3+}$ and Ho$^{3+}$ by non-magnetic substitutes Y$^{3+}$, the residual entropy depends non-monotonically on the dilution level. In this work we investigate through Monte Carlo simulations microscopic models to account quantitatively for the calorimetric experimental measurements, and thus also the residual entropies as a function of dilution. Features of the dilution physics in the specific heat are captured quantitatively by the microscopic models and the interplay between dilution and frustration is understood on the basis of a Bethe lattice calculation. The effect of the dipolar interactions between magnetic spins are exposed numerically for various dilution concentrations. Our work explains the previous discrepancy of the residual entropy between different species of rare earth ions and the generalized Pauling’s estimate.

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