

## **Reverse Monte Carlo refinement of single crystal diffuse neutron scattering and correlated magnetic disorder with program rmc-discord**

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A new software program for the analysis of single crystal diffuse scattering from disordered materials has recently been released. The rmc-discord Python package can extract short-range correlations from disordered crystals including the spin-spin correlations from magnetic diffuse neutron scattering data. An introduction to the program will be given including an overview of graphical user interface use for setting up a refinement. Using the program, it is shown with the mineral bixbyite, a geometrically frustrated magnetic, that reverse Monte Carlo can resolve subtle features of reciprocal space and differences between antiferromagnetic spin-pair correlation strength of nearest neighbor iron and manganese sites. Extensions to other systems generated by forward Monte Carlo method will also be discussed including future development for magnetic systems. This research used resources at the Spallation Neutron Source, a DOE Office of Science User Facility operated by the Oak Ridge National Laboratory.