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Neutron diffraction study of water intercalation in superconducting sodium cobaltate CINZIA METALLO, University of Tennessee, TAKESHI EGAMI, University of Tennessee/ORNL, THOMAS PROFFEN, LANL, DAVID MANDRUS, BRIAN SALES, ORNL — Neutron powder diffraction has been used to investigate the role of heavy water in deuterated sodium cobaltate $Na_{0.35}CoO_2 1.4D_2O$. In spite of the fact that superconductivity appears exclusively when water is intercalated in the (non superconducting) Na-deficient Na_xCoO_2, a clear understanding of the role of water has not been achieved. Neutron diffraction data at two different temperatures (T=15K, 100K) were analyzed using the Pair Density Function (PDF) technique, which gives information about local ordering in real space. The measured and calculated PDFs of $Na_{0.7}CoO_2$, $Na_{0.35}CoO_2 1.4D_2O$ and D_2O were compared. At both temperatures the D-D distance and the D-O-D angle in $Na_{0.35}CoO_2 1.4D_2O$ are significantly different from those of ordinary water. Two wide coexisting distributions of possible D-O-D bond angles are observed. We speculate that the altered geometry of the intercalated water molecules is due to a modification of the dynamics of the hydrogen bond. The possible implications are discussed in terms of electron conduction and superconductivity.

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