

## Long-Range Coupling of Paramagnetic Guest Molecules via Ion-Doped Water Framework

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The superexchange-like long-range coupling between molecular oxygen guests encaged in an ion-doped water framework was calculated by molecular calculations and demonstrated by the measurement of magnetization of guest molecules. In this work, abnormal proton positioning of an ion-doped water framework in the presence of paramagnetic oxygen molecules and the distortions of the water-water connection caused by orbital mixing between a paramagnetic guest and an ion-doped cage were demonstrated by a synchrotron high-resolution powder diffraction pattern refinement. The identified crystal structures of ionic oxygen clathrate hydrate well explain the superexchange-like long-range interactions occurring in ionic clathrate hydrates with paramagnetic guests.