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Determination of a Weak Exchange Interaction in Magnetically Coupled Cluster System by EPR Singlet-Triplet Transition Lines

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Abstract

Exchange-coupled clusters of transition-metal ions are relevant to many different scientific areas, ranging from chemistry to solid-state physics, biology, material science and has been the subject of much research in recent years(1,2). Single crystal EPR spectroscopy works as a very effective tool for the measurement of J values for small exchange interactions. This makes EPR technique very suitable for detection of weak exchange coupling transmitted over long distances via extended atomic and melecular bridges. Large polyoxometallates (3) may provide ideal structural environments for the study of interactions between paramagnetic ions. The detailed nature of magnetic interaction (positive sign and magnitude of J~ 0.006 cm^{-1}) was clearly determined for di-copper(II) system by single crystal EPR spectroscopy (4). The single-triplet (S-T) transitions are forbidden by different symmetries of the wave functions. However, when the singlet ground state is mixed into triplet states, the S-T transitions can be allowed and observed as weak lines. These weak S-T lines are positioned symmetrically with respect to the main transitions in the distance equals to 2J from the center of the spectrum. This lines allow one to determine the J-value with very high accuracy when $|J| < h\nu \approx$ 0.32 cm^{-1}. Unfortunately, the S-T transitions in the single crystal were detected by EPR method only in a few complexes until now. We have measured single-triplet transition lines for several magnetically coupled cluster systems and determined their J values accurately. The temperature dependency of J was studied by monitoring the changes in S-T.

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