pH behaviour of the water chemical shift in ^{1}H NMR of red cells with low transmembrane magnetic susceptibility difference

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The ^{1}H magic angle spinning (MAS) NMR spectrum of water in erythrocyte suspensions shows peaks from each of the intracellular and extracellular water pools. The splitting is a true chemical shift and is brought about by the elimination of water exchange under MAS conditions due to physical separation of the two water populations. The size of the chemical shift difference is determined by the concentration of intracellular protein affecting the average extent of hydrogen bonding of water (Larkin *et al.*, 2007). We present here a model of the chemical shift behaviour for water in erythrocytes under normal high resolution NMR conditions based on results from MAS experiments on these cells exposed to different pH and osmotic conditions. The model accurately predicts the chemical shift of water for a static sample, and the results demonstrate that in high resolution NMR experiments the chemical shift of water will appear to be invariant if differences in magnetic susceptibility across the cell membrane are minimal (< 10% of the magnetic susceptibility of water). Thus changes in the shape and chemical shift of the water resonance are not due to pH changes in the physiological range (6-8). The findings are fundamental to an interpretation of the mechanism of chemical shift effects on the water resonance that may occur in functional magnetic resonance imaging.

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