Solubility enhancement of aromatic amino acids and peptides in aqueous solution of divalent transition-metal cations - QENS study

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Generally, the solubility of aromatic amino acids decreases in solution containing multivalent transition-metal ions, such as Cu^{2+}, Pt^{2+}, $Pd^{2+}$and Co^{3+}, due to the formation of complex precipitates. Surprisingly, we have observed considerably enhanced solubility of tryptophan (Trp) in $CuCl_2$ aqueous solution with a high local concentration of Cu^{2+} at thesurface of Trp [Phys. Rev. Lett. 117, 238102 (2016)]. The solubility increases by 2-5 times that of Trp in pure water. Based on first principle calculations, this unexpected phenomenon is attributed to the strong interaction between $Cu^{2+}$and the aromatic ring in Trp, referred to as cation–? interaction which modifies the electron distribution of the aromatic ring in Trp and increases the water–aromatic ring interaction.

The self-diffusion behavior of Trp water solution with and without Cu^{2+} has been determined using quasielastic neutron scattering (QENS) on the PELICAN instrument at Australian Nuclear Science and Technology Organization. Two samples of Trp-D_2O (mol ratio of 1:100) and Trp-D_2O-$CuCl_2$(1:100:1) have been studied. The measured QENS spectra were fitted with a Lorentzian function. An estimate of self-diffusion coefficients are obtained by fitting the linear part of the half-width at half-maximum (HWHM) of the Lorentzian function versus Q^2 with the Fick's law. The values are $(2.6 \pm 0.1) \times 10^{-5}$ cm^2/s and $(1.9 \pm 0.1) \times 10^{-5} cm^2/s$ for Trp-D_2O and Trp-D_2O-$CuCl_2$, respectively. Though these values reflect the dynamics of the entire system, they are dominated by Trp. The significant difference indicate that Trp in D_2O containing Cu^{2+} moves much more slowly as compared with that without Cu^{2+}. This observation confirms the enhancement of water affinity of Trp in the presence of Cu^{2+}.