X-ray Absorption study of the solvation structure of Cu^{2+} in methanol and dimethyl sulfoxide

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Supporting information

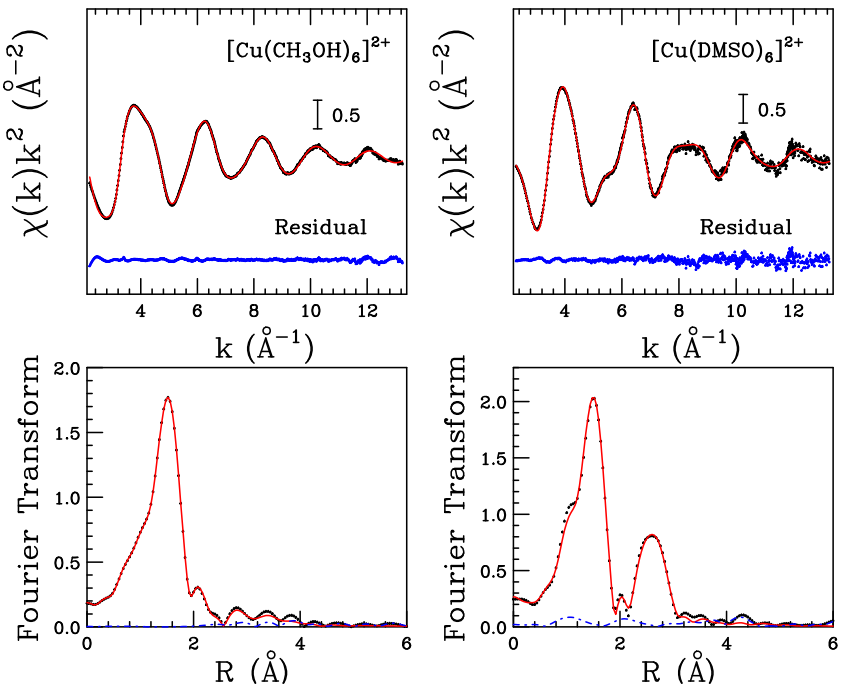

Figure S1. Comparison of the experimental Cu K-edge EXAFS spectra of Cu^{2+} in MeOH and DMSO solutions (red, solid line) and the theoretical signals calculated for a sixfold JT distorted octahedral geometry (black, dotted line). In the lower panels, the comparison of the modulus of the Fourier transform of the experimental k^2 EXAFS spectra (red, solid line) and the fitting results (black, dotted line) is shown.

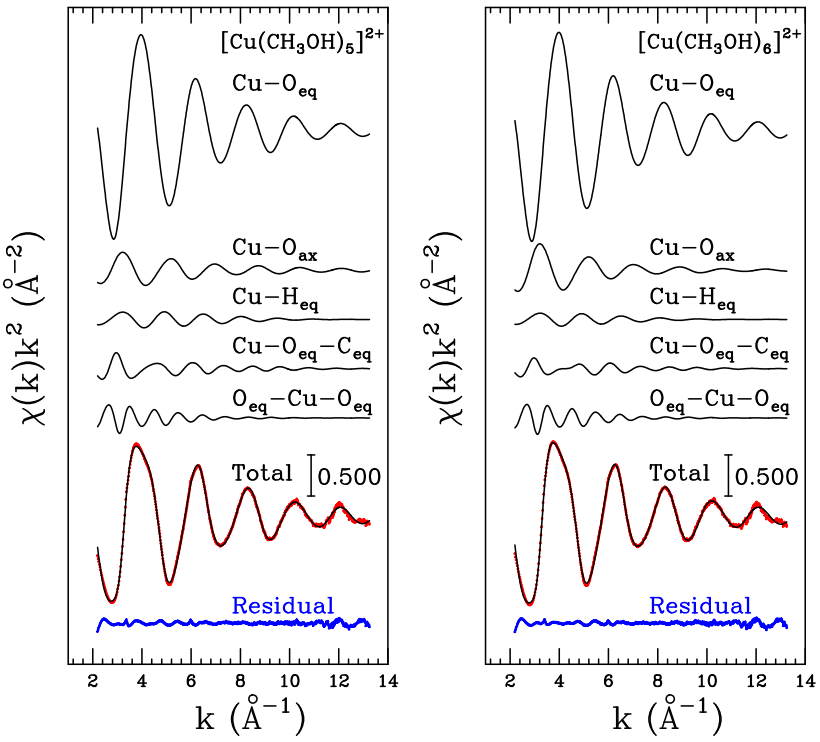

Figure S2. Comparison between the experimental and theoretical Cu K-edge EXAFS spectra of Cu^{2+} in MeOH calculated for a fivefold (left panel) and sixfold JT distorted octahedral (right panel) geometry. From the top to the bottom of each panel the following curves are reported: Cu-O_{eq}, Cu-O_{ax}, Cu-S_{eq}, Cu-S_{ax} and Cu-C_{eq} two-body signals, Cu-O_{eq}-S_{eq} and O_{eq}-Cu-O_{eq} three-body signals, total theoretical contribution (black line) compared to the experimental spectrum (red dotted line) and resulting residual (blue line)

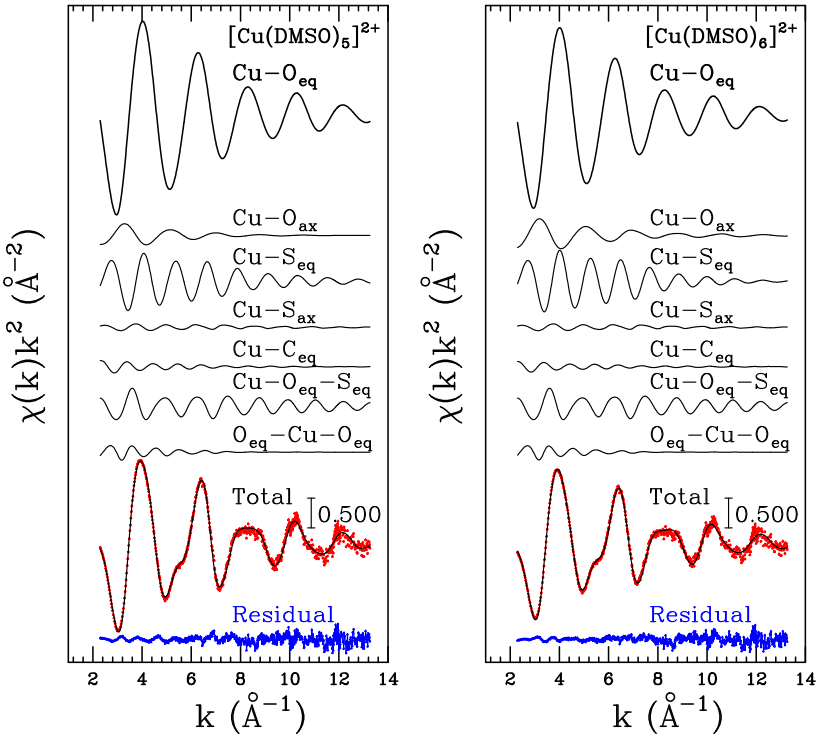

Figure S3. Comparison between the experimental and theoretical Cu K-edge EXAFS spectra of Cu^{2+} in DMSO calculated for a fivefold (left panel) and sixfold JT distorted octahedral (right panel) geometry. From the top to the bottom of each panel the following curves are reported: Cu-O_{eq}, Cu-O_{ax}, and Cu-H_{eq} two-body signals, Cu-O_{eq}-C_{eq} and O_{eq}-Cu-O_{eq} three-body signals, total theoretical contribution (black line) compared to the experimental spectrum (red dotted line) and resulting residual (blue line).

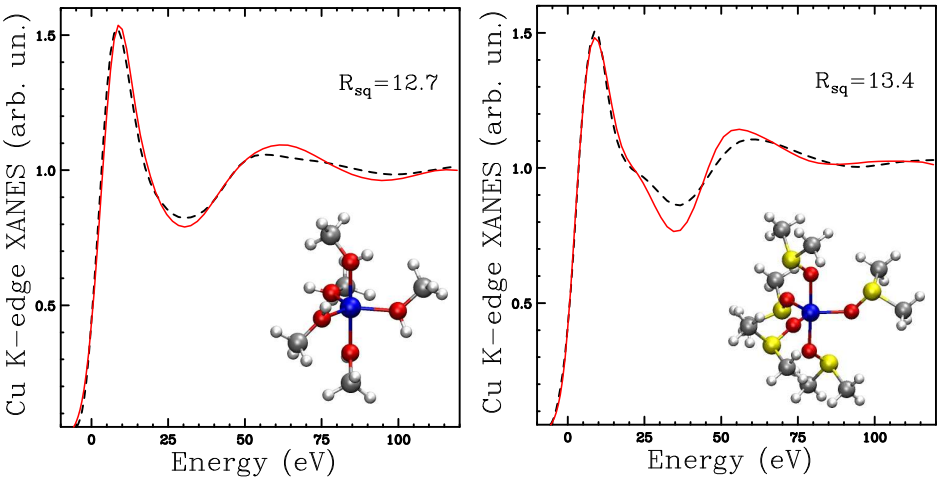

Figure S4. Comparison of the Cu K-edge XANES experimental spectra (black, dashed line) of Cu^{2+} in MeOH (left panel) and DMSO (right panel) solutions and the theoretical spectra (red, full line) calculated with a trigonal bipyramidal model.