Retention of Xe in Copper-Ion-Exchanged MFI at 300 K as a Stable and New Compound, $XeCu^+$, Exhibiting Covalent Bonding Nature

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A stable and new type of Xe compound, $XeCu^+$, was found to be easily formed at room temperature into MFI-type zeolite by utilizing it as a reaction pot in sub-nm size. The presence of prominent interaction between the monovalent copper ion and Xe which has a covalent nature was distinctly evidenced from the experiments, such as in situ synchrotron X-ray absorption fine structure (XAFS), adsorption heats, Xe-NMR, and diffuse reflectance (DR) measurements. The structural data, Cu^+-Xe bond length of 0.244 nm, was, for the first time, obtained distinctly and directly by XAFS spectra including both extended X-ray absorption fine structure (EXAFS) and X-ray absorption near edge structure (XANES) methods, as well as the bonding energy of 60 kJ mol^{-1} through the direct adsorption energy measurements. The bonding nature between Cu^+ and Xe in MFI was discussed with the aid of density functional theory (DFT). An easy preparation of Xe bonded to the copper ion and the structural and electronic analysis of this species may represent a first step toward the possible preparation of the bonded species between Xe and various kinds of metal ion and their extended chemistry.