CHEMICAL SCIENCE

Observation of reactions involving the variation of states and phases induced by external forces, and clarification of the nature of chemical bonds are the eternal subjects of chemistry. What we human beings have found, analyzed, uncovered and understood is only the tip of the iceberg of vast chemical knowledge. The variety of facilities installed in SPring-8 and the variety of scientists gathering there are now unveiling the mysteries of chemistry. The present section compiles eight highlighted outcomes of the excellent experiments carried out during the period of 2003B and 2004A.

The 1st article features the *femtosecond* nuclear motion that occurs when a core-excited CF_4 molecule happens to dissociate entirely to form an F⁺ ion and an electron. This ultrafast process has been observed by measurement of electron-ion momentum correlation. The 2nd article introduces the application of two-dimensional ultra-small-angle X-ray scattering (2D-USXAS) to the in situ study of the aggregated structure of stretched rubber using X-ray scattering by silica particle fillers containing in an elastomer. The phenomenon of structural variation on a size scale of 100 nm-10 µmol is observed for the first time here, though its existence has been speculated on the basis of viscoelastic experiments. The following three articles are the outcomes of X-ray powder diffraction experiments carried out with the large Debye-Scherrer camera installed at BL02B2 combined with analyses by the maximum entropy method (MEM) and the Rietveld method. The porous coordination polymers are thought to be promising as an alternative material of zeolites, and the synthetic method and its properties are being extensively studied. The skeletal framework has been thought to be rigid but careful analysis of X-ray diffraction (XRD) patterns in the 3rd article reveals that the framework shrinks when guest molecules are incorporated into the pores of the coordination polymers. The porous coordination polymer adsorbs hydrogen molecules effectively and the authors of the 4th article are the first to succeed in determining the position of hydrogen molecules by the XRD technique. The 5th paper is the first to report that a charge ordering pattern in an organic conductor can be observed before and after the metal-insulator (M-I) transition known as the 'Peierls transition' by the same XRD technique. The 6th article deals with a new technique, nuclear resonant inelastic scattering (NRIS). The change in the spin state donated by the electronic configuration in the t_{2g} and eg orbitals of octahedrally coordinated iron complexes including ⁵⁷Fe was fully analyzed by NRIS. The nature of the chemical bonds are discussed in the 7th and 8th articles. The former article reports that shape resonance energy is dependent on intramolecule distance in core-level molecular photoionization as well as on the ionization cross section observed by high-resolution photoelectron spectroscopy. The latter clarifies the electronic structure of the hydrogen bond in various phases of H_2O at low temperatures by oxygen K-edge absorption fine structure technique and the spectra may suggest the presence of an unknown phase of ice at the temperatures of 4-50 K.

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