PHOTON FACTORY, IMSS, KEK

Merry Christmas and Happy New Year! It is our great pleasure to send our second facility report of the year in this glorious season. This time, we would like to introduce two recent scientific outcomes that have been accomplished by the use of our synchrotrons.



The first outcome is concerned with κ -D₃(Cat-EDT-TTF)₂, a very interesting material of which the macroscopic properties are controlled via hydrogen bonds. The hydrogen bonds, which are considered to play significant roles not only in solid-state physics but also in biological systems, have been intensively studied so far. In the figure, we show how the two phases of this material are switched by changes in temperature. The most striking

feature observed for the low-temperature phase at BL-8A is the displacement of the deuterium (D) from the midpoint to a position closer to (farther from) the oxygen. Interestingly, such displacement is accompanied by charge disproportionation at the Cat-EDT-TTF molecules, which is also confirmed by our X-ray diffraction experiments. We expect that this outcome will lead to further understanding of the interplay between the two fundamental degrees of freedom, namely, those of the hydrogen and the electron, in near future. (For the details, see "A. Ueda et al., J. Am. Chem. Soc. **136**, 12184 (2014).")



Next, we introduce new findings related to photosynthesis. Without doubt, the photosynthesis is one of the most important chemical reactions, being indispensable to energy and oxygen generations. Recently, a high-accuracy structural

determination of the so-called light-harvesting complex 1 (LH1) has succeeded at BL-1A. According to that study, first, the LH1 is not a complete circle but an oval, and two particular units (No. 1 and No. 8 in the middle panel of the figure above) are considered to be most tightly connected to the reaction center. Next, it has special holes in the ring of the LH1, which are thought to be pathways through which reduced ubiquinones escape to the outside. Lastly, the role of Ca was also identified; Ca atoms reside between each pair of the units and work to stabilize the whole structure. The BL-1A has contributed substantially to this determination of the Ca position, since the BL-1A supplies a high-brilliance X-ray at 3.0 Å wavelength that fits the Ca absorption edge. (For the details, see "S. Niwa et al., Nature **508**, 7495 (2014).")

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