^{25}Mg solid-state NMR in an ultra-high magnetic field: Structures of bacteriochlorophyll *c* complex, chlorosome

Mg atoms play an important role in biological materials, but ^{25}Mg NMR measurements are difficult since ^{25}Mg is low-γ nucleus and exhibits quadrupolar broadening in solids. An ultra-high magnetic field may, however, dramatically enhance sensitivity.

This Note introduces a study on stacking structures of bacteriochlorophyll *c* in chlorosome clarified using ^{25}Mg solid-state NMR at 21.8 T.

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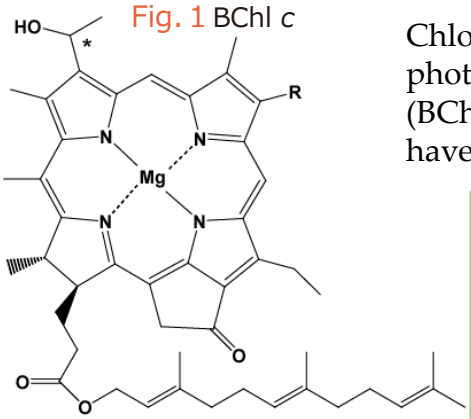
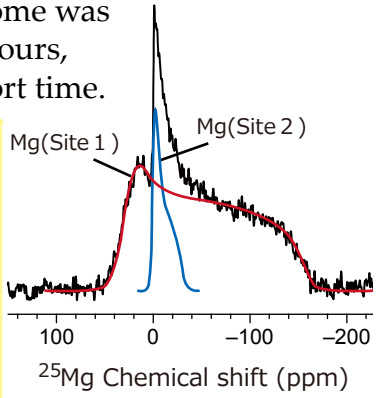
Fig. 1 BChl *c*



Chlorosome is a light-harvesting organ of green photosynthesis bacteria, and bacteriochlorophyll *c* (BChl *c*) aggregate in it. Stacking structures of BChl *c* have attracted interest for a long time.

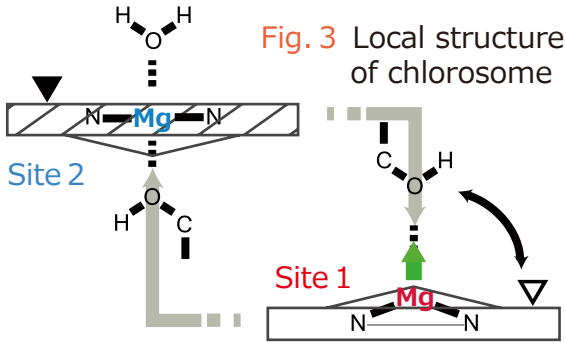
Using a 21.8 T ultra-high field, ^{25}Mg MAS NMR spectrum of chlorosome was obtained within 80 hours, unprecedentedly short time.

Fig. 2 ^{25}Mg spectrum at 21.8 T



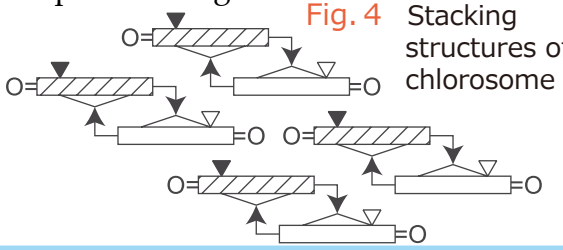
^{25}Mg spectrum of chlorosome suggests two Mg sites: Large quadrupolar or low symmetry Mg (Site 1) and small quadrupolar or high symmetry Mg (Site 2). Fig. 3 shows a plausible model: Mg-coordinated OH deviates Mg atom of Site 1 from the ring plane, whereas Mg atom of Site 2 stays within the plane because of a ligand water molecule.

Fig. 3 Local structure of chlorosome



Thus, BChl *c* molecules in chlorosome prove to have stacking structures depicted in Fig. 4.

Fig. 4 Stacking structures of chlorosome



This study demonstrates that ultra-high field NMR system is useful for low-γ nuclei in real samples, such as biological materials.

Reference: Y. Kakitani, Y. Koyama, Y. Shimoikeda, T. Nakai, H. Utsumi, T. Shimizu, and H. Nagae, *Biochemistry* **2009**, *48*, 74-86.