Detailed structural analysis of compounds containing heteroatoms -Analysis of OLED materials-

2D NMR measurements using hydrogen and carbon nucler are often used for detailed structural analysis of organic compounds, but when the structure contains heteroatoms, structural information may not be sufficiently obtained. Here, we introduce an example in which 2D NMR measurements using multinuclear are effective for detailed structural analysis of OLED materials.

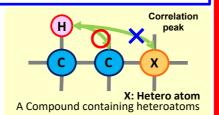
Background

HMBC: HMBC is one of 2D NMR methods that can provides information on the positional relationships between atoms separated by 2-3 bonds.

TH-13C HMBC measurement Correlation peak C C C C

A compound composed of hydrogen and carbon

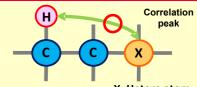
Correlation peaks of hydrogen and carbon distant from 2-3 bonds are detected. **Structural information** can be obtained.



Some correlation peaks are not detected. Enough structural information is not available.

Detailed structural analysis is difficult!

Multinuclear HMBC measurement

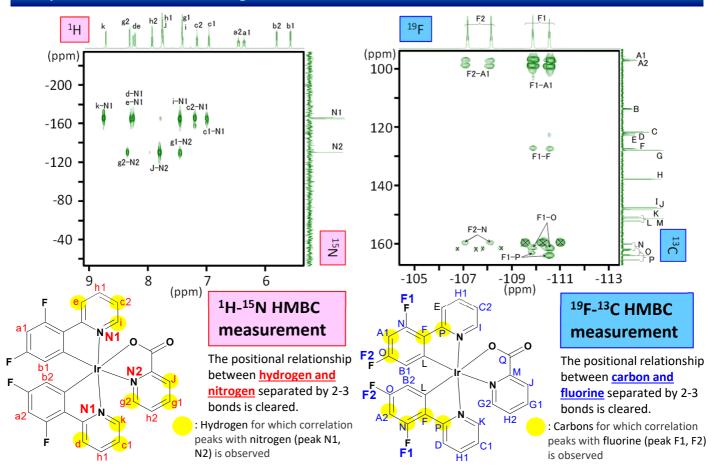


X: Hetero atom Compounds containing heteroatoms

Structural information around heteroatom can be obtained.

It is an effective tool for detailed structural analysis by combining the results of ¹H-¹³C HMBC measurement!

Analysis of OLED materials using multinuclear 2D NMR measurement



The structural information around nitrogen and fluorine was obtained, which enabled more detailed structural analysis!