

Structural analysis of OLED materials

Using high resolution MS and high-sensitivity NMR, we performed the structural analysis of OLED materials. The elemental composition and partial structure were identified by MS and MS/MS measurement. 2D NMR provided the detailed chemical structure including the site of substitution. We were also able to discriminate and quantify the *anti* and *syn* isomers.

MS

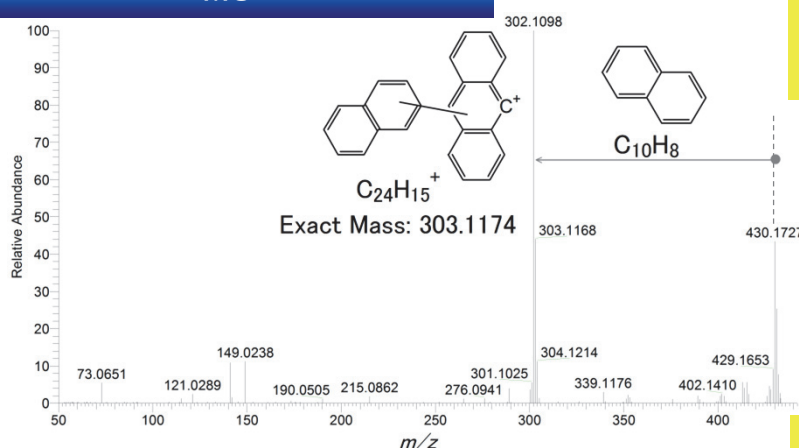
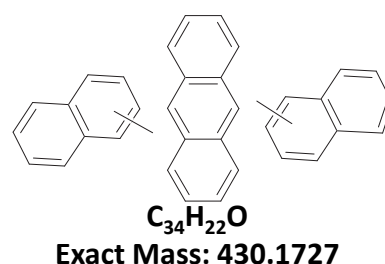


Fig. 1 MS/MS spectrum (Precursor ion : 430)

① Measured accurate mass

→ **Elemental composition**

② MS/MS fragment → **Partial structure**



2D NMR experiments gave correlations

between carbons and protons.

The site of substitution can be determined from 2D NMR results.

2D NMR

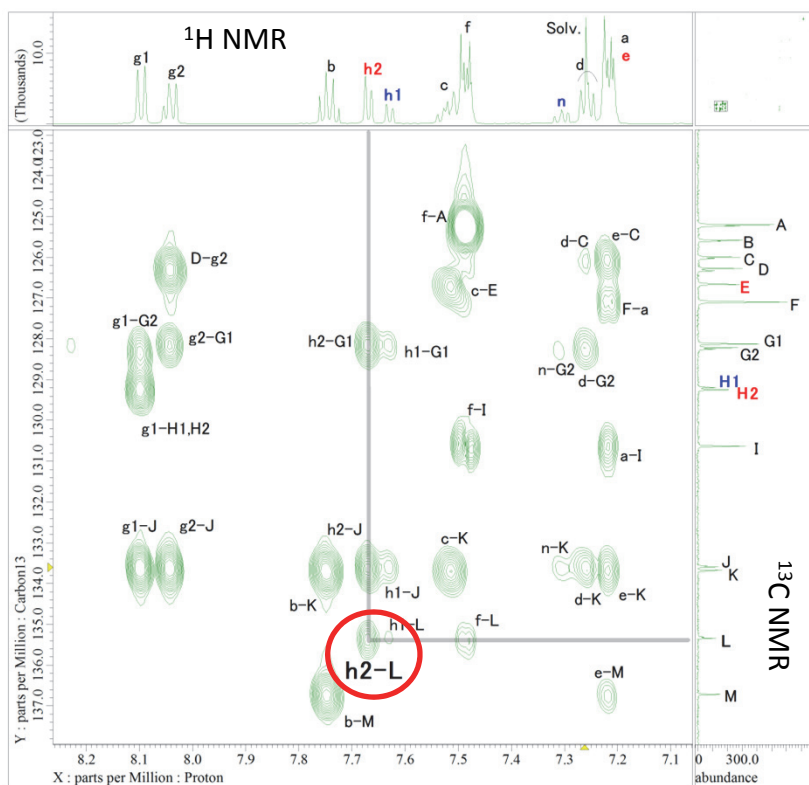
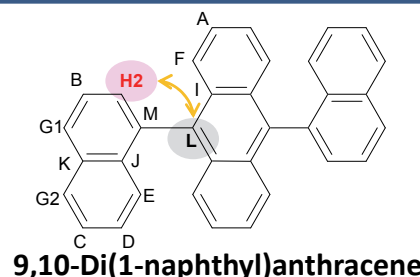
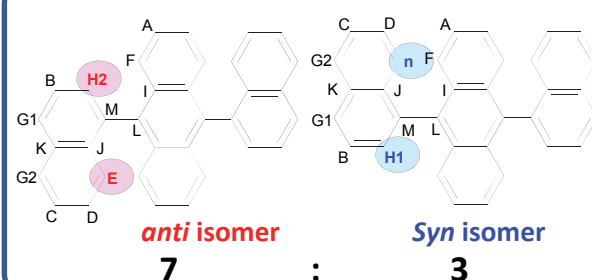


Fig. 2 HMBC (Heteronuclear Multiple Bond Coherence) spectrum



9,10-Di(1-naphthyl)anthracene

Appearance of peaks h2 and h1 indicated the existence of *anti* and *syn* isomers, and molar ratio was determined from integrated value of each peak.



Detailed structure of OLED materials including the site of substitution becomes clear.