

# Structural analysis of trace degradation compounds in OLED materials heated under various atmospheres by using LC/HRMS<sup>n</sup>

It is essential to analyze trace impurity compounds because OLED materials require high-purity quality for longer lifetime, high reliability. LC(Liquid chromatography) separation and acquisition of high-resolution mass spectra enable high accuracy of chemical formula estimation and detailed structural analysis.

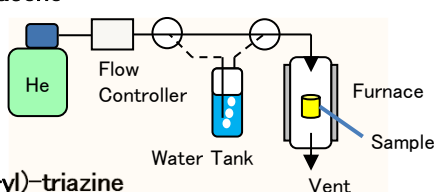
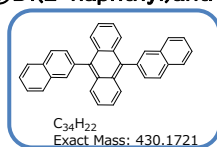
## Objective

Final goal : Application to quality evaluation during vacuum thermal evaporation of OLED materials.

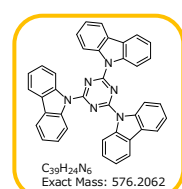
Characterization of decomposition compounds for each OLED material after heating under various atmospheres by using LC / HRMS<sup>n</sup>

## Experimental

### ①Di(2-naphthyl)anthracene



### ②Tri(9H-carbazol-9-yl)-triazine



a. He atmosphere  
b. He atmosphere including H<sub>2</sub>O  
【Heating condition】  
RT→20°C/min→500°C

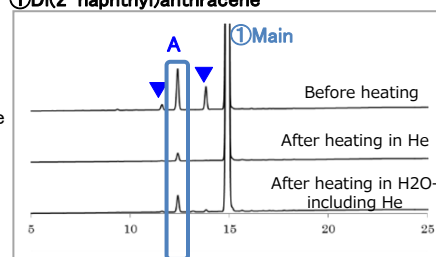
Preparation of THF solution of residue after sample heating

LC/UV  
LC/HRMS<sup>n</sup>

## LC/UV results

### ✓ Comparison of LC/UV chromatograms (254nm)

#### ①Di(2-naphthyl)anthracene

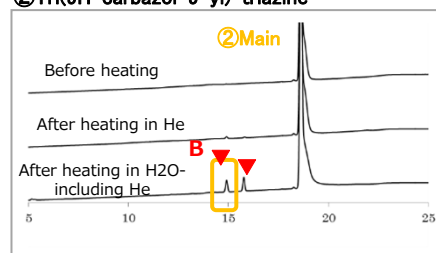


Peak area ratio (%)

	Main	A
Before heating	92.69	4.39
After heating in He	99.02	0.92
After heating in H2O-including He	97.90	1.77

▼ : degraded/sublimed compounds due to heating under He

#### ②Tri(9H-carbazol-9-yl)-triazine



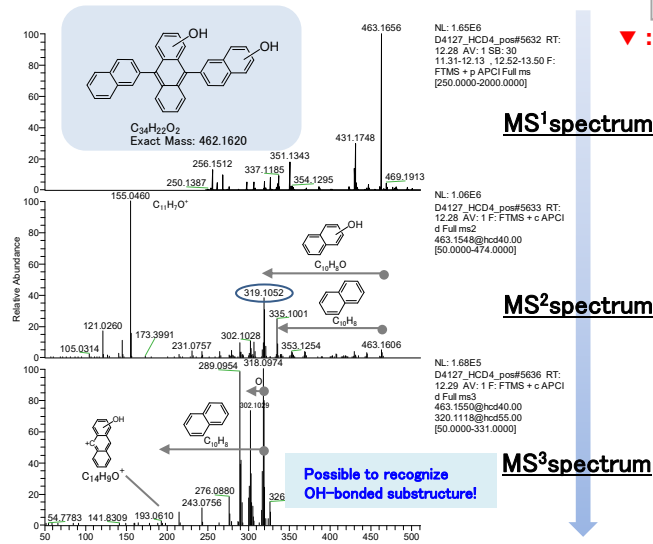
Peak area ratio (%)

	Main	B
Before heating	99.69	0.00
After heating in He	98.81	0.55
After heating in H2O-including He	95.24	2.12

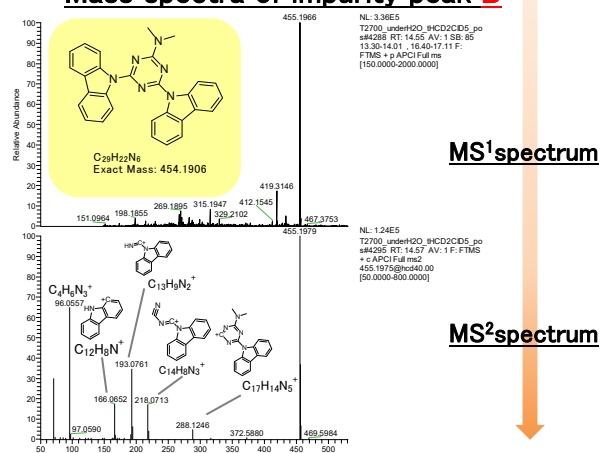
▼ : degraded compounds due to heating under water-including He

## LC/HRMS<sup>n</sup> results

### ✓ Mass spectra of impurity peak A



### ✓ Mass spectra of impurity peak B



MS<sup>n</sup> analysis is effective for detailed structural analysis.

(e.g. estimation of bonded substructure, analysis of compounds which is difficult to cleave)

**Hydrocarbon materials** : Amounts of impurities decreased after heating under He

**Heteroelement materials** : Impurities with carbazole- decomposition were generated due to heating under water-including He.