Structural analysis of trace degradation compounds in OLED materials heated under various atmospheres by using LC/HRMS^n

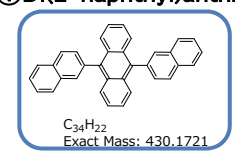
It is essential to analyze trace impurity compounds because OLED materials require high-purity quality for longer lifetime, high reliability. LC(Liquid chromatography) separation and acquisition of high-resolution mass spectra enable high accuracy of chemical formula estimation and detailed structural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

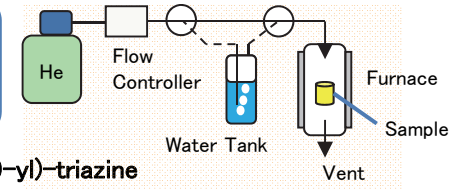
Objective

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^n

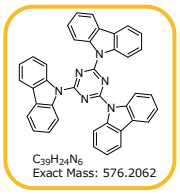
Experimental

①Di(2-naphthyl)anthracene





②Tri(9H-carbazol-9-yl)-triazine



a. He atmosphere
b. He atmosphere including H_2O
【Heating condition】
RT→20℃/min→500℃

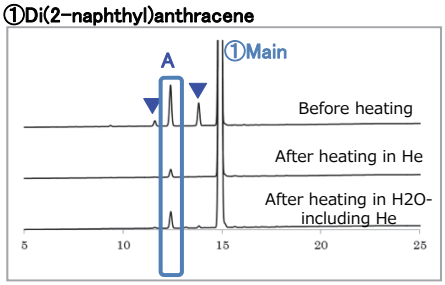
Preparation of THF solution of residue after sample heating

LC/UV
LC/HRMS^n

LC/UV results

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

①Di(2-naphthyl)anthracene

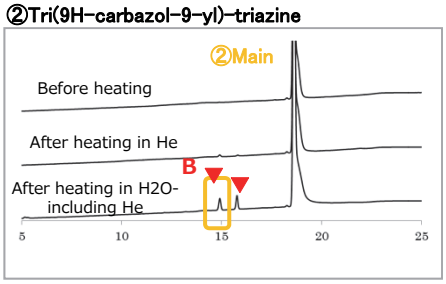


Peak area ratio (%)

	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



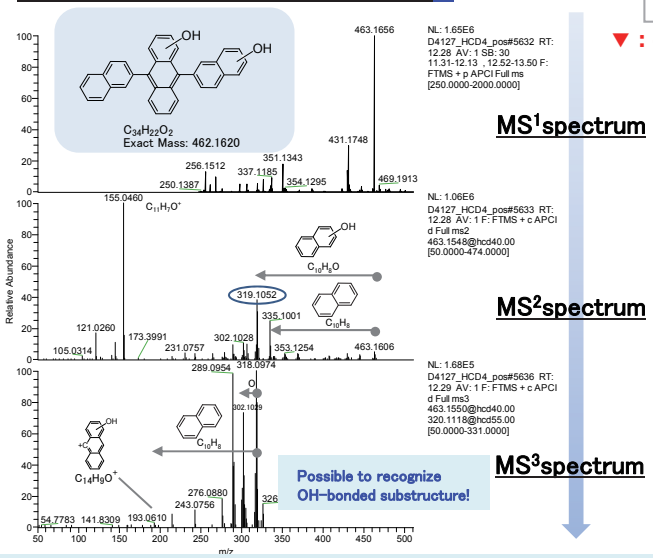
Peak area ratio (%)

	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

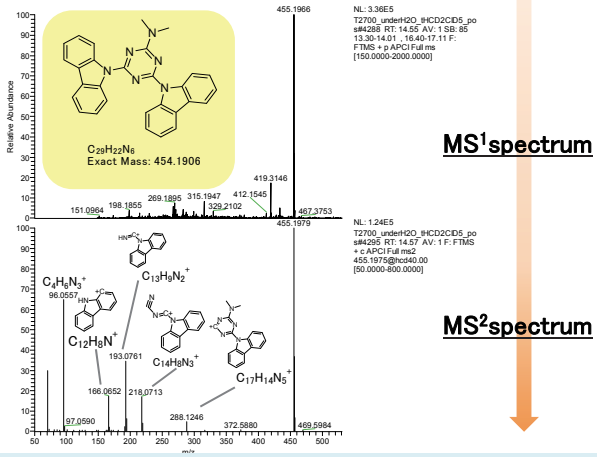
▼ : degraded compounds due to heating under water-including He

LC/HRMS^n results

✓ **Mass spectra of impurity peak A**



✓ **Mass spectra of impurity peak B**



MS^n 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.

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