

~ Application Note for DART ~

Analysis of low polar compound by DART

~ analysis of organic electroluminescence materials ~

Introduction

In MS Tips No. D031 we introduced the example of high polar compound analysis with DART. This application note introduces the example of the analysis of low polar compounds

For the mass spectrometric analysis of organic electroluminescence (EL) materials, which have been one of the typical luminescent materials in LC/MS (APCI, APPI), GC/MS (refer to MS Tips 78 and 87), MALDI-TOFMS, and TOFSIMS have been used.

This time, we have analyzed organic EL materials using DART as follows.

Methods

The samples were adhered to the tip of a glass rod and presented directly to the DART™ ion source.

Sample	4,4'-Bis(carbozoi-9-yl)biphenyl (CBP) 4,4'-Bis(2,2-diphenyl-ethen-1-yl)biphenyl (DPVBi) (made by Luminescence Technology Corp., Taiwan)
Mass spectrometer	JMS-T100TD time-of-flight mass spectrometer
Ionization	DART (+)
Helium gas temperature	250 °C

Results and discussion

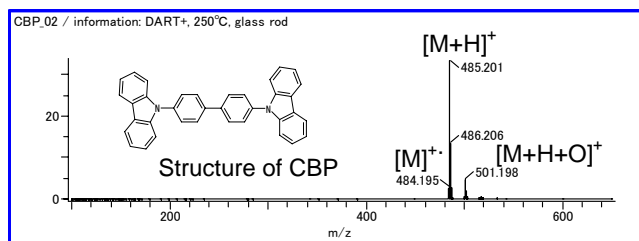


Fig. 1 DART(+) mass spectrum of CBP

Table 1 Estimated composition of CBP

Observed	Calculated	Error (10 ⁻³ u)	Estimated composition	Unsat.
485.20113	485.20177	-0.64	C ₃₆ H ₂₅ N ₂	25.5
501.19760	501.19669	0.92	C ₃₆ H ₂₅ N ₂ O	25.5

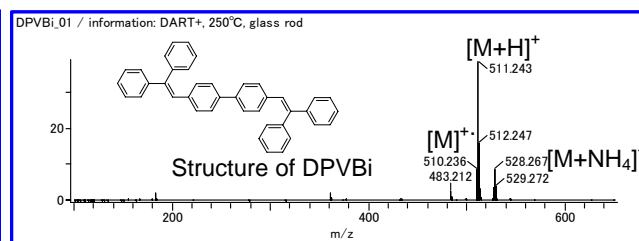


Fig. 2 DART(+) mass spectrum of DPVBi

Table 2 Estimated composition of DPVBi

Observed	Calculated	Error (10 ⁻³ u)	Estimated composition	Unsat.
511.24287	511.24258	0.29	C ₄₀ H ₃₁	25.5
528.26722	528.26912	-1.90	C ₄₀ H ₃₄ N ₁	25.5

In both samples, [M+H]⁺ was detected as base peak. In addition, [M+NH₄]⁺ and [M]⁺ were also detected. With CBP, ion which can be deduced as [M+H+O]⁺ from the accurate mass has also been detected. DART has been proven effective in the analysis of low polar compounds such as organic EL.