# PHYSICAL CHEMISTRY 2014

12th International Conference
on Fundamental and Applied Aspects of
Physical Chemistry

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25. Anniversary of the Society of Physical Chemists of Serbia

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# ANALYSIS OF 4,4′-BIS(2,2′DIPHENYL VINYL)-1,1′-BIPHENYL USING THE ATMOSPHERIC-PRESSURE SOLIDS ANALYSIS PROBE FOR IONIZATION

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## ABSTRACT
An Atmospheric pressure Solids Analysis Probe (ASAP) mass spectrometer are used for investigation the ionization mechanism and fragmentation pathways of 4,4′-bis(2,2′diphenyl vinyl)-1,1′-biphenyl (DPVBi). DPVBi is material used in OLEDs (organic light-emitting diode). Results obtained indicate that by controlling ion source conditions it is possible to optimize forming of desired precursor ion, primarily radical cation and in less content protonated ion of DPVBi. The results presented illustrate the usefulness of ASAP MS in the characterization of DPVBi compounds.

## INTRODUCTION
ASAP mass spectrometry is a direct analysis ionization technique derived from atmospheric-pressure chemical ionization (APCI) that was introduced in 2005 [1]. In the ASAP the samples are first vaporized using heated desolvation gas (nitrogen) followed by ionization by electrical discharge at a corona needle [2]. This ionization method belongs to the group of the ambient desorption methods, like as Desorption Electrospray Ionisation (DESI) and Direct Analysis in Real Time (DART) [3 – 5]. The ASAP ionization source is integral part of a commercial electrospray (ESI) or atmospheric pressure chemical ionization mass spectrometer, and this method can be used for rapid qualitative analysis of various materials using only slightly modified commercial ESI-MS. The ASAP method is applied primarily to analysis of volatile and semivolatile solid materials, both polar and non-polar. Due to the significant differences in the mechanism of ionization this method offered the scope for analyzing some compound that do not ionize effectively by the ESI. It should be mentioned that the advantage of ASAP is important for the analysis of non -polar compounds where the ions of interest could not be easily ionized by ESI-MS.

To date, ASAP has facilitated the analysis of steroids, drugs, nucleosides, polymers, and chemicals in food [5 - 7].
In this work, the applicability of the ASAP for characterization 4,4′-bis(2,2′diphenyl vinyl)-1,1′-biphenyl (DPVBi) has been investigated.
DPVBi is material used in OLEDs and it is the particular important to find conditions for its detection [8, 9]. A structure of DPVBi is shown at Figure 1. It should be noted that this compound did not ionized effectively by ESI.

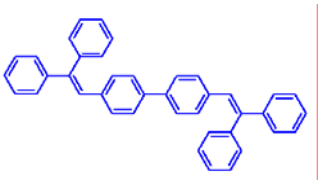

**Figure 1.** Structure of 4,4′-bis(2,2′diphenyl vinyl)-1,1′-biphenyl (DPVBi).

**EXPERIMENTAL**
The ASAP (mass analysis was performed by Acquity Tandem Quadrupole Detector (Waters, USA) – "Vinča" Institute of Nuclear Sciencies) consists of a glass capillary with sealed end onto which solid or liquid sample is deposited.

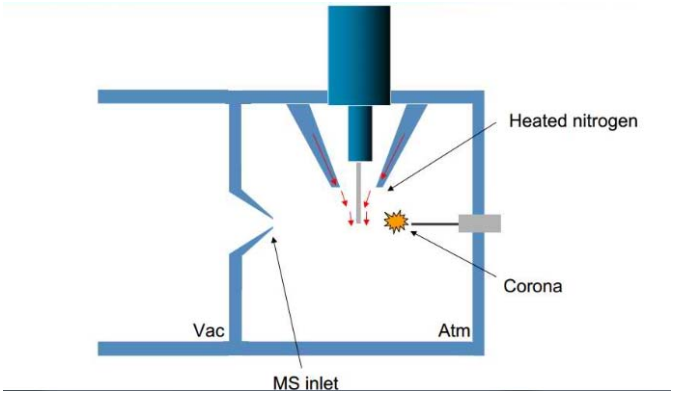


**Figure 2**. A schematic of the ASAP ion source (Waters corporation)

As can be seen in Figure 2, streams of nitrogen gas introduces into the ASAP source housing e.g. desolvation gas) enabling analyte vaporization. Namely, desorption occurs upon interaction with a hot desolvation nitrogen stream, whereby the solid evaporates from the glass's surface and then ionized at atmospheric pressure by the corona discharge. Typically, the temperature of desolvation gas was set in the range from 200 to 400°C, with the flow rate ranging from 500-800 L/h. Before use, probes should be conditioned (baked) to remove any residual contamination. This is usually achieved by heating the probe at 500 ˚C for at least 30 s. The ASAP source was operated in positive ion mode with a corona voltage in the range from 2kV to 4.0kV and a cone voltage over the range 10 – 50 V.

## RESULTS AND DISCUSSION

In the Figures 3 and 4 are shown positive-ion ASAP mass spectrum of DPVBi obtained at the corona voltage of 4.35kV and under cone voltage in the range from 20 to 40V, respectively.

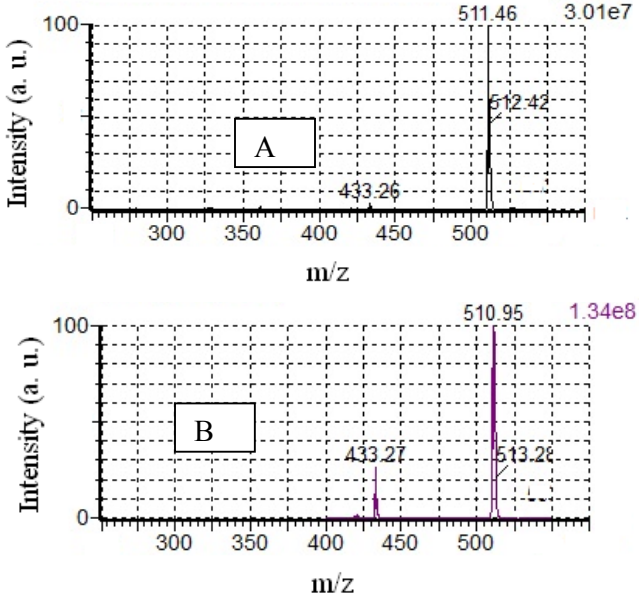


**Figure 3.** Positive-ion ASAP mass spectrum of DPVBi obtained at the corona voltage of 4.35kV, under cone voltage of 20 V (A), and 30 V (B)

As shown in Figure 3(A) at the cone voltage of 20V the predominant ion was protonated ion of DPVBi. Otherwise, applying of higher cone voltage above 30V causes formation of predominant, radical cation of DPVBi (m/z 510.95, Fig. 3B). With the enhancement of temperature from 250 to 400 ˚C, the signal intensity of this radical cation slightly increased. It should be noted that at the corona voltage below 3.0 kV either the radical cation or protonated ion of DPVBi could not be detected. Beside these main molecular ions shown in Fig. 3, it was detected appearance of two other peaks, one observed at m/z 433.27 and another at m/z 356.26 which eventually could be considered as fragments of DPVBi molecule (Fig.4).

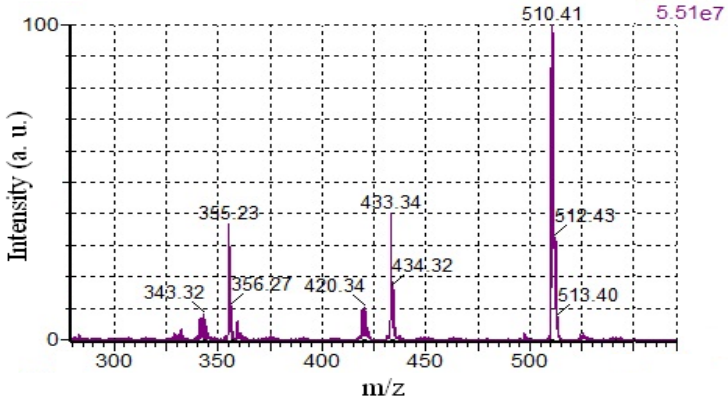


**Figure 4.** Positive-ion ASAP mass pectrum of DPVBi obtained at the corona voltage of 4.35kV, under cone voltage of 40 V.

Thus, masses with m/z 433.27 and 356.26 could be attributed to fragments of DPVBi molecule after one or two phenyl group loss, respectively. Whether these masses represent DPVBi fragments or they are ions of some other origin has to be additionally established.

## CONCLUSION

Work herein demonstrates that ASAP can be used successfully for the characterization of 4,4′-bis(2,2′diphenyl vinyl)-1,1′-biphenyl. Reliable method for monitoring of this compound and its photo-degradation products could be of importance for further improvements in OLEDs technology.

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