Dissociative electron attachment to 3-bromopyruvic acid

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Synopsis: Fragmentation of gas phase 3-bromopyruvic acid ($BrCH_2COCO_2H$) caused by capture of low energy electrons (0-12 eV) was studied. Ion yields of negative ions formed via dissociative electron attachment were recorded.

Many cancer cells have aberrant energy metabolism therefore they consume more glucose than normal cells and rapidly convert it to lactate. Hexokinase type II (HK II) is the key enzyme for maintaining increased glycolysis in cancer cells where it is overexpressed. 3-bromopyruvate (3-BrPA), has an ability to inhibit HK II, hence it can cause cell death in cancer tissues.

Mitochondria are important in the control of both cell survival and cell death. Mitochondrial dysregulations, such as loss of trans-membrane potential, accumulation of reactive oxygen species (ROS), membrane permeability transition and release of pro-apoptotic factors lead to apoptosis [1]. 3-BrPA is a strong alkylating agent. It inhibits both HK II and mitochondrial oxidative phosphorylation, leading to a decrease of ATP formation which will lead to cell death [2]. Although 3-BrPA has been described as a good anti-cancer agent [3], the underlying molecular mechanism of cell death induced is still not clear.

In the present study we describe dissociative electron attachment (DEA) mechanisms leading anionic fragmentation of 3-BrPA. The peak resonances listed in the Table 1 were extracted from the recorded ion yields.

Table 1. DEA resonances

Anion	Peak resonance
3-BrPA-H	0 eV; 1 eV
3-BrPA-Br	0 eV; 2 eV
$BrCH(OH)_2$	0 eV
Br	0 eV; 2 eV; 5 eV
COOH	2.2 eV; 4.5 eV
COO	2.2 eV; 4.5 eV
OH	5 eV
O	5.5 eV

Dissociative electron attachment to 3-BrPA induces rich anionic fragmentation, prevailing 0 eV channels. The measurements have been carried out at the Siedlce University by means of crossed molecular beam apparatus coupled with trochoidal monochromator together with quadrupole mass spectrometer.

References

[1] Y. Higuchi Y 2004 *J Cell Mol Med* **8**, 455–464

[2] Y. H. Ko *et al.* 2004 *Biochem Biophys Res Commun* **324**, 269–275

[3] Y. H. Ko *et al.* 2001 *Cancer Lett* **173**, 83–91

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