Electron attachment studies with 2,3-dimethoxy-5-methyl-1,4-benzoquinone F. Ferreira da Silva^{* 1}, J. Ameixa^{* 2}, J. Khreis^{† 3}, and S. Denifl^{† 4}

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Synopsis We demonstrate that low-energy electron (< 3 eV) interaction with 2,3-dimethoxy-5-methyl-1,4benzoquinone (DMB) in the gas phase leads to a wide assortment of anionic fragments. DMB is the functional head-group of ubiquinone electron carrier involved in the electron transport chain in mithochondrial membrane. This study is a key contribution to a more comprehensive understanding of the electron transport in the mithochondrial membrane by ubiquinone.

The electron transport chain is the final stage of aerobic respiration and plays the final role in reducing ADP to ATP by oxidative phosphorylation in mithocondria membrane. In this process, ubiquinone acts as an electron carrier [1]. Remarkably, no other molecule can perform this function. Briefly, ubiquinone is composed by a quinone derivative head-group which works as an electron carrier as well as an hydrophobic-tail formed by isopropenoid subunits [2]. In order to understand the fundamental processes of electron transport by ubiquinone, we have performed studies on electron attachment to 2,3-dimethoxy-5-methyl-1,4benzoquinone (DMB $-C_9H_{10}O_4$) in the gas phase. This compound represents the functional unit of ubiquinone. The measurements were carried out utilizing a high resolution double focusing mass spectrometer in reversed Nier-Johnson geometry. The incident electron current was set to 10 μA and the energy resolution at 0 eV is \sim 1 eV and the mass resolution is about $m/\Delta m = 1000$. At electron energies < 3 eV we observe the formation of the parent anion, $C_9H_{10}O_4^-$ as well as the following fragments: $C_9H_9O_4^-$, $C_8H_6O_4^-$, $C_7H_4O_4^-$. The highest anionic yield corresponds to the fragment $C_8H_6O_4^-$ formed by the loss of a hydrogen atom and a methyl group. The most relevant recorded ion yields are presented in Figure 1. Additionally, we report more six anionic fragments formed by DEA at higher energies. The corresponding peak resonance energies are listed in Table 1. Therefore, gas-phase DMB

exhibits a highly reactive behavior upon interaction with electrons close to 0 eV.



Figure 1. Ion yield of $C_9H_{10}O_4^-$, $C_8H_6O_4^-$, $C_7H_4O_4^-$ for electron attachment to DMB as a function of electron energy. Also shown is molecular structure of DMB (mass 182 u).

Table 1. Resonance energies of anions formed upon electron attachment to DMB.

		Resonance Energies (eV)			
Mass (Da)	Anion	I^{st}	2^{nd}	3^{rd}	4^{th}
182	$(DMB)^{-}$	0	-	-	-
166	$(DMB-H-CH_3)^{-1}$	1.9	-	-	-
152	$(DMB - 2CH_3)^{-1}$	2.8	4.9	10.7	14.5
137	$(C_6 H_7 O_4)^{-1}$	3.2	7.3	-	-
125	$(C_5HO_4)^{-1}$	2.9	5.9	-	-
124	$(C_5 O_4)^{-1}$	3.1	7.1	8.8	-
123	$(C_6H_3O_3)^2/(C_7H_7O_2)^2$	7.0	9.1	8.8	-
110	$(C_6 H_6 O_2)^{-1}$	7.0	9.9	-	-
97	$(C_4 H O_3)^{-1}$	6.4	-	-	-

References

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