

## Structural Characterisation of *p*-semiquinone Radical in a Crystal: X-ray Structure and EPR Evidence

Krešimir Molčanov<sup>a</sup>, Biserka kojić-Prodić<sup>a</sup>, Mario Roboz<sup>b</sup>, Božidar S. Grabarić<sup>b</sup>, <sup>a</sup>*Rudjer Bošković Institute, Zagreb, Croatia.* <sup>b</sup>*Faculty of Food Technology and Biotechnology, University of Zagreb, Croatia.*  
E-mail: [kojic@irb.hr](mailto:kojic@irb.hr)

In membrane-located proteins, quinone system plays a significant role in electron-transfer reactions. The described work illustrates that semiquinone radical is stabilized in the solid state.

Thin dark-red plate-like crystals of *p*-semiquinone radical were grown by evaporation of mildly alkaline, saturated water solution of hydroquinone. Although stable in air, larger single crystals decay after *ca.* 20 h exposure to X-rays or UV radiation producing amorphous yellow substance identified as a mixture of quinone and quinhydrone.

Solid-state electronic paramagnetic resonance spectra of crystalline *p*-semiquinone detected its paramagnetic properties revealing four symmetrically equivalent protons.

Crystal structure was determined at 100 and 150 K (monoclinic, space group P 21/c,  $a = 3.78 \text{ \AA}$ ,  $b = 5.98 \text{ \AA}$ ,  $c = 10.79 \text{ \AA}$ ,  $\beta = 90.66^\circ$ ). In both of them, *p*-semiquinone molecule is centrosymmetric (four protons are, therefore, equivalent), with C-O bond length of  $1.295 \text{ \AA}$ , corresponding to bond order of 1.5. Molecules are hydrogen bonded into infinite chains (O-H $\cdots$ O distance of  $2.70 \text{ \AA}$  with the proton disordered between two oxygen atoms. This packing is very similar to that of quinhydrone; the unit cell can be transformed into a half of the unit cell of quinhydrone.

**Keywords:** radical, *p*-semiquinone, EPR