

## **Magnetic field effects on the initiation of chain oxidation**

**Anton K. Kuzaev, Aleksey M. Grobov, Evgenii M. Pliss and Anatoly L. Buchachenko**

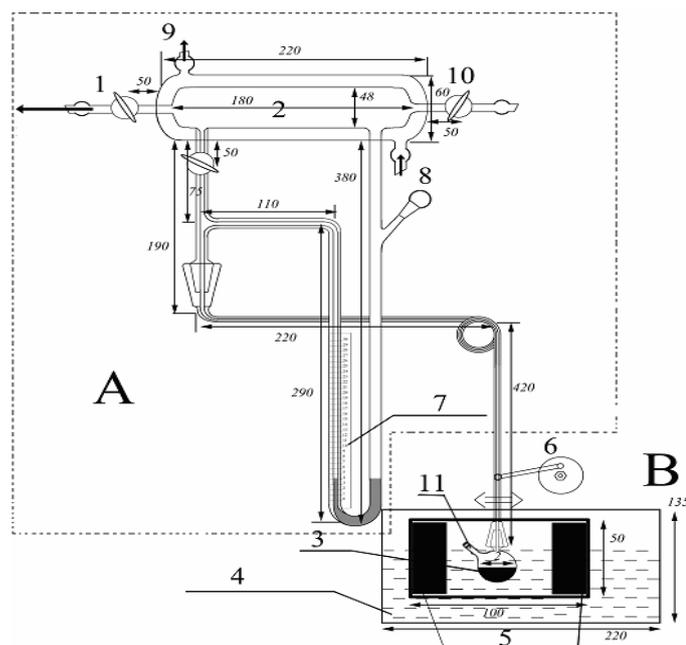
### **1. Experimental details**

All substrates and solvents (chlorobenzene, acetonitrile) were purchased from Aldrich (St. Louis, Missouri, U.S.). Their purity was monitored by HPLC (HPLC Flexar, PerkinElmer, USA) and chromatography-mass spectrometry (GC/MS Clarus 680T MS, PerkinElmer, USA). Initiators (Polyscience Inc.) –  $\alpha,\alpha'$ -azobisisobutyronitrile (AIBN), 2,2-azobis(2,4-dimethylvaleronitrile) (AMVN) and dibenzoyl peroxide (BP) – were recrystallized three times from ethanol.

The initiation rate ( $W_i$ ) was determined by two methods: 1) by the Kinetic Chain Initiated Reaction (KIR) method through the initiated oxidation rate by equation (2) using known values of  $k_2 \cdot k_5^{-0.5}$ ; 2) using inhibitors or the Acceptors of Free Radicals (AFR) method with equation (3):  $W_i = f[\text{InH}]_0/\tau_{\text{ind}}$  (3), where  $f$  is the stoichiometric coefficient of inhibition,  $\tau_{\text{ind}}$  – the duration of the induction period, InH – phenolic inhibitor Trolox (from Aldrich) or the stable nitroxyl radical 2,2,6,6-tetramethylpiperidin-1-oxyl (TEMPO). To determine the TEMPO concentration in the medium of Ar, the EPR spectroscopy method (Adani CMV spectrometer) was used. The kinetics of oxygen absorption was monitored using a highly sensitive capillary microvolumometer with a cell allowing injecting and taking samples during the experiment. Microvolumometer was equipped with the magnetic unit. The installation design is shown in Figure S1.

The magnitudes of the magnetic effect during initiation ( $\text{MFE}_i$ ) were calculated from the ratio:  $\text{MFE}_i = (W_i)_H/(W_i)_O$ , where  $(W_i)_H$  and  $(W_i)_O$  are initiation rates in a given magnetic field and in the Earth's natural field, respectively. The oxygen concentration constant was 7.8 mM. Experimental data were obtained at 343 K, when even substrates (ethylbenzene and methyl oleate) with low  $k_2$  values were oxidized with a chain length  $\nu \geq 10$ . In order to avoid the influence of viscosity on the passage of radicals to the volume, all experiments were carried out in solutions of chlorobenzene and/or acetonitrile. The experimental data were processed using the optimization program "Kinetica-2012".

## 2. Microvolumometer equipped with the magnetic unit.



**Figure S1** The scheme of the experimental setup. A. Micro volume-meter; B. Magnet. 1. Valve leading to vacuum lines and a tank with the gas mixture; 2. Thermostated tank for the gas mixture; 3. Reactor; 4. Reactor's temperature control bath; 5. Neodymium magnets; 6. Stirrer; 7. Measuring unit; 8. Thermostatic flow; 9. Thermostatic flow; 10. Maintenance valve. 11. Glass tap for insertion or sampling. Dimensions are given in mm (the figures in picture).