

CHEMICAL ACTIVATION OF *tert*-BUTYL HYDROPEROXIDE BY Et₄NBr. NOTE ON INTRAMOLECULAR DYNAMICS

N.A. Turovskij¹, Yu.V. Berestneva² and E.V. Raksha³

¹ Federal State Budget Educational Institution of Higher Education “Donetsk State University” Donetsk, Russia

² Federal State budgetary Institution “V.K. Gusak Institute of Emergency and Reconstructive Surgery” of the Ministry of Health of the Russian Federation, Donetsk, Russia

³ International Intergovernmental Organization “The Joint Institute for Nuclear Research,” Dubna, Russia

E-mail: berestnevayuv@mail.ru

Organic hydroperoxides (RO-OH) are key intermediates in radical-chain oxidation processes occurring in the biosphere. Establishing the mechanism of chemically activated radical-pair decomposition of hydroperoxide compounds is an important priority task in the study of the complex metabolic processes of living cells both in health and in disease. The molecular recognition stage of the supramolecular catalytic decomposition reaction of RO-OH in the presence of tetraalkylammonium bromides was studied by complementary methods of chemical kinetics, NMR spectroscopy and molecular modeling [1-2].

The chemical activation features of *tert*-butyl hydroperoxide by tetraethylammonium bromide (Et₄NBr), including the structural models features of complex intermediates RO-OH – Et₄NBr are discussed (Fig. 1). Models that assume the combined action of the cation (Et₄N⁺) and the anion (Br[−]) of the salt in the process of hydroperoxide chemical activation are proposed. The specific solvation of the anion is taken into account by the supermolecule approximation. Structural reorganization of the hydroperoxide molecule along with changes in its molecular dynamics are discussed.

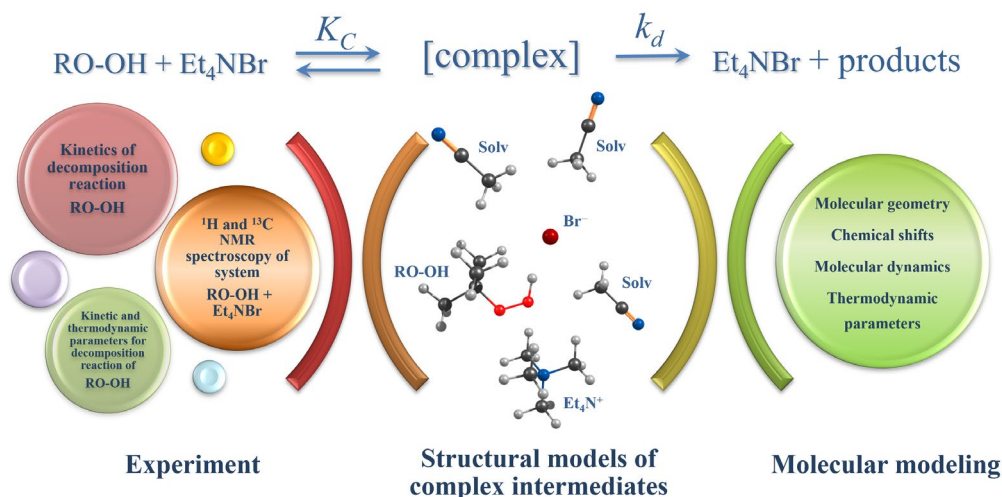


Fig. 1. Complementary methods in the study of chemical activation of *tert*-butyl hydroperoxide by Et₄NBr.

- [1] N.A. Turovskij, Yu.V. Berestneva, E.V. Raksha, M.Yu. Zubritskij, S.A. Grebenyuk (2014). NMR study of the complex formation between *tert*-butyl hydroperoxide and tetraalkylammonium bromides. *Monatsh. Chem.* 145, 1443-1448.
- [2] N.A. Turovskij, E.V. Raksha, Y.V. Berestneva (2020). Chemically activated decomposition of arylalkyl hydroperoxides in the presence of tetraalkylammonium bromides (Chapter). In: *Hydroperoxide Properties, Uses and Reactions*, Ed. Voleta Aubin, New York: Nova Science Publishers Inc. 4, 89-122.