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ONLINE ISSN : 1349-273X

PRINT ISSN : 1346-8804

**Journal of the Japan Petroleum Institute**

Vol. 46 (2003) , No. 1 pp.1-14

[\[PDF \(250K\)\]](#) [\[References\]](#)

## The Autoxidation of Simple Esters: Towards an Understanding of the Chemistry of Degradation of Polyol Esters Used as Lubricants

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(Received: July 18, 2002)

The liquid phase oxidation of a series of neopentyl esters, chosen to model the more complex polyol esters used as lubricants, has been studied in two ways. In one, detailed product analyses, following reaction with oxygen in a closed reactor at elevated temperatures, allows for mechanisms to be proposed. In the second, the esters were reacted with two different alkoxy radicals, the results leading to valuable information about the relative rates of attack on the various C-H bonds. For example, it was found that attack could take place readily on both the alkyl and acyl groups in the ester and that the  $\beta$ -acyl C-H bonds are more susceptible to attack than  $\alpha$ -C-H bonds.

To support the proposals for the mechanisms, details are given of experiments in which reactions of specific peroxy radicals derived from esters were studied in detail and compared with similar experiments with alkylperoxy radicals. The reactions of peroxy radicals formed from esters are similar to those derived from alkanes and it is possible to use rate constants for reactions of alkylperoxy and related oxygenated radicals to model successfully the reactions of the esterperoxy radicals.

Overall the mechanisms for the autoxidation of the esters can be explained in terms of well-established mechanisms associated with the autoxidation of alkanes, as would be expected from the similarity of the peroxy radical chemistry of the two systems. However, care has to be taken in accounting for the influence of the functional group which has a profound effect on the point of attack in the case of the autoxidation of the esters.

**Keywords:** [Polyol ester](#), [Neopentyl ester](#), [Lubricant](#), [Autoxidation](#), [Hydroperoxyl radical](#), [Alkoxy radical](#)

To cite this article:

John R. LINDSAY SMITH, Eiji NAGATOMI and David J. WADDINGTON, *Journal of the Japan Petroleum Institute*, Vol. **46**, No. 1, p.1 (2003) .

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doi:10.1627/jpi.46.1

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