

Assessment of Theoretical Methods for the Study of Hydrogen Abstraction Kinetics of Global Warming Gas Species During Their Degradation and Byproduct Formation (IUPAC Technical Report)

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Global climate change is a major concern as it leads to an increase in the average temperature of the earth's atmosphere. The existence and persistence of some gaseous species in the atmosphere contribute to global warming. Experimental techniques are used to study the kinetics and degradation of global warming gases. However, quantum mechanical methods are also useful for the kinetic and radiative forcing study of global warming species and can precede experimental investigations. Research has also been targeted to develop more adapted procedures using ab initio and density functional theory (DFT) methods.

This report provides a global perspective, in a simplified manner, of the theoretical studies of the degradation of gas species in the atmosphere, with an emphasis on the hydrogen abstraction kinetics of global warming gas species during their degradation and byproduct formation. En route, the results obtained from these studies are analyzed and compared with experimental data where available. Our analyses indicate that the theoretical predictions are in agreement with experimental findings, but the predicted parameters are dependent on the method being used. Theoretical methods are used to predict the thermodynamic parameters of reactions, and, with relevance to this report, the global warming potential (GWP) index can also be calculated. This report can be useful for future investigations involving global warming gaseous species while providing suggestions on how computations can fill in data gaps when experimental data are unavailable.

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Determination of the Photoluminescence Quantum Yield of Dilute Dye Solutions (IUPAC Technical Report)

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Procedures for the determination of photoluminescence quantum yields with optical methods are addressed, and challenges associated with these measurements are discussed. Special emphasis is dedicated to relative measurements of fluorescent (i.e., short excited-state lifetime), transparent, and dilute dye solutions in conventional cuvettes in a 0°/90° measurement geometry. Recommendations on the selection of suitable quantum yield standards are presented, and requirements for the documentation of photoluminescence quantum yields are derived.

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Provisional Recommendations

Provisional Recommendations are drafts of IUPAC recommendations on terminology, nomenclature, and symbols made widely available to allow interested parties to comment before the recommendations are finally revised and published in Pure and Applied Chemistry. Full text is available online.

Nomenclature of Flavonoids

Flavonoid structures, found in nature or obtained by synthesis, have become more and more complex, and a guide for aglycone names is provided here to permit the construction of the names for their polyglycosylated species with clarity and conciseness.

A joint working party of IUPAC/IUBMB members has prepared these recommendations, which establish rules for the general nomenclature of flavonoids, providing examples of acceptable trivial names, and names derived from trivial names, together with semi-systematic and fully systematic names that follow the published IUPAC recommendations.

Comments by 28 February 2014

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 <http://www.iupac.org/project/2009-018-2-800>