



Implications of VOC Oxidation in Atmospheric Chemistry: Development of a Comprehensive AI Model for Predicting Reaction Rate Constants

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Abstract. Volatile Organic Compounds (VOCs) significantly influence global atmospheric chemistry through oxidative reactions with oxidants. These reactions produce key precursors to the formation of atmospheric fine particulate matter (PM_{2.5}) and ozone (O₃), which in turn play a crucial role in regulating O₃ pollution and reducing PM_{2.5} concentrations. With the increasing diversity of VOCs, the need for advanced modeling techniques to accurately estimate the atmospheric oxidation reaction rate constants (k_i , where $i \in \{•OH, •Cl, NO_3, \text{ or } O_3\}$) has become more urgent. Here we introduce Vreact, a Siamese message passing neural networks (MPNN) architecture that jointly models VOC–oxidant reactivity. The model simultaneously predicts $\log_{10}k_i$ values and achieves a mean squared error (MSE) of 0.299 and a coefficient of determination (R²) of 0.941 on the internal test set. This framework overcomes the single-oxidant constraint of traditional models, enabling unified and scalable prediction of VOC oxidation kinetics across multiple oxidants. An interactive web tool (<http://vreact.cn/wind.site:8001>) is provided to facilitate non-expert access to reactivity screening. Vreact offers valuable insights into the formation and evolution of atmospheric pollutants, and serves as a critical resource for developing effective control and emission strategies, ultimately supporting global efforts to mitigate air pollution and improve public health.

1 Introduction

The rapid advancement in data-driven methodologies has revolutionized various fields, such as protein structure prediction (Abramson et al., 2024), molecular generation (Zhang et al., 2023), organic reaction prediction (Burés and Larrosa, 2023), and bioinformatics (Theodoris et al., 2023). Environmental challenges, particularly those associated with atmospheric chemistry and climate change, have also benefited from these innovations. As pollutants evolve under both anthropogenic and natural influences, the understanding of their chemical and physical properties has become increasingly vital for addressing global air quality and climate issues. Volatile Organic Compounds (VOCs) are organic chemicals that readily

Atmospheric Oxidation Rate Program

David Baud



Atmospheric Oxidation Rate Program:

Atmospheric Oxidation Rate Program Philip H. Howard, William M. Meylan, 1992-06-26 Use the same powerful software package that has been the standard at the U S and German Environmental Protection Agencies for estimating atmospheric degradation rates Atmospheric Oxidation Rate Program quickly and accurately estimates the gas phase reaction rate between organic chemicals and hydroxyl radicals using estimation methods developed by Dr Roger Atkinson Ozone reaction rates can also be estimated for olefinic and acetylenic compounds The program calculates hydroxyl radical and ozone rate constants and you can enter chemical structures using SMILES notation The atmospheric half life is estimated using an average hydroxyl radical concentration and an average ozone concentration The program will run on any IBM or IBM compatible computer with 350K RAM Atmospheric Oxidation Rate Program will be an indispensable tool for environmental chemists engineers toxicologists atmospheric scientists and regulators **Office of Air Programs Publication** ,1971

Environmental Health Perspectives ,1993 **Handbook of Property Estimation Methods for Chemicals** Donald Mackay, Robert S. Boethling, 2000-03-29 A complete restructuring and updating of the classic 1982 Handbook of Chemical Property Estimation Methods commonly known as Lyman s Handbook the Handbook of Property Estimation Methods for Chemicals Environmental and Health Sciences reviews and recommends practical methods for estimating environmentally important properties of organic chemic Chemical Engineering Progress ,1991 **Toxicological Profile for Formaldehyde** ,1999 **Toxicological Profile for Hexamethylene Diisocyanate** ,1998 **Acid Precipitation** ,1984 **EM** ,1997 **Energy Research Abstracts** ,1980 **The Department of Energy's Atmospheric Chemistry Program** National Research Council (U.S.). Committee on Atmospheric Chemistry, Charles E. Kolb, 1991 **Transactions of Society for Mining, Metallurgy, and Exploration, Inc** ,1990 **American Industrial Hygiene Association Journal** ,1963 **Books in Print** ,1994 **CEP Software Directory** ,1999 Toxicological Profile for Chlorpyrifos ,1997 *Unclassified Research and Development Programs Executed for the Division of Reactor Development and Technology and the Division of Research, May, 1965 / .* ,1965 **Journal of the Air Pollution Control Association** ,1979 **Power** ,1923 **Environmental Toxicology and Chemistry** ,2003

Whispering the Techniques of Language: An Mental Journey through **Atmospheric Oxidation Rate Program**

In a digitally-driven world wherever displays reign supreme and immediate interaction drowns out the subtleties of language, the profound secrets and emotional subtleties hidden within phrases often move unheard. Yet, set within the pages of **Atmospheric Oxidation Rate Program** a interesting fictional treasure pulsating with raw thoughts, lies an exceptional quest waiting to be undertaken. Written by an experienced wordsmith, this enchanting opus attracts readers on an introspective trip, gently unraveling the veiled truths and profound impact resonating within the material of each word. Within the mental depths of the touching evaluation, we can embark upon a heartfelt exploration of the book is key subjects, dissect their fascinating writing type, and yield to the strong resonance it evokes strong within the recesses of readers hearts.

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