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Mechanism Development and Structure-Activity Relationships for Gas-Phase Atmospheric Chemistry

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Message from the Guest Editors

Atmospheric gas-phase chemistry plays a critical role in determining the concentrations of air pollutants. Each compound may form many other unique compounds and intermediates when it oxidizes in the atmosphere. Therefore, a complete gas-phase atmospheric chemical mechanism consists of on-the-order-of several million reactions and compounds. Now, there are important efforts to build highly detailed gas-phase mechanisms that attempt to be as complete as possible. However, many of the required reactions for highly detailed mechanisms must be constructed from structure activity relationships. On the other hand, more simplified gas-phase atmospheric chemical mechanisms are used in meteorological air quality models for making public policy. Both types of chemical mechanisms and their development procedures are of interest for this Special Issue. Methods of condensation, including machine learning and other approaches, used to link the development of simplified mechanisms to the highly detailed gas-phase mechanisms are of deep interest for this Special Issue.

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Message from the Editor-in-Chief

Continued developments in instrumentation and modeling have driven atmospheric science to become increasingly more complex with a deeper understanding of concepts, mechanisms, and interactions. This is the field that innovation built and it has led to a better appreciation for the complexity with atmosphere. Human life is intertwined in this complexity as we strive to better understand our atmosphere. Climate change is constantly stretching the limits of our thinking and forcing new ideas and concepts to be played out. Welcome to the Anthropocene!

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