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New Structure-Activity Relationships (SAR) for H atom abstraction branching ratio for OH reaction with alkenes and dienes

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Large amounts of unsaturated hydrocarbons are continuously being emitted into the Earth's atmosphere, originating from both biogenic and anthropogenic sources. The degradation of unsaturated VOCs in the troposphere is mainly initiated by reactions with OH radicals. For these OH reactions the addition channel is always the dominant one. However there are some contributions from hydrogen abstraction reactions, which can contribute up to 40% of the total rate coefficient. Because of the large variety of VOCs emitted in the atmosphere, it is impossible to pretend to study the reactions for each compound separately in laboratory experiments or by theoretical work. A solution is to develop Structure-Activity Relationships (SAR) for the various reaction pathways, which allows for the prediction of total rate constants and detailed primary product distributions. In our work we have measured the branching ratios between the abstraction and addition channels for various OH + alkenes (and dienes) reactions. We propose, from our experimental H atom abstraction branching ratio, a new Structure-Activity Relationships (SAR) based on Atkinson SAR concept but including new data on H atom abstraction channels.