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Structure-activity relationships to estimate the effective Henry's law coefficients of organics of atmospheric interest

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The oxidation of volatile organic compounds emitted in the atmosphere involves complex reaction mechanisms which leads to the formation of oxygenated organic intermediates, usually denoted as secondary organics. The fate of these secondary organics remains poorly quantified due to a lack of information about their speciation, distribution and evolution in the gas and condensed phases. A significant fraction of secondary organics may dissolve into the tropospheric aqueous phase owing to the presence of polar moieties generated during the oxidation processes. The partitioning of organics between the gas and the aqueous atmospheric phases is usually described in the basis of Henry's law. Atmospheric models require a knowledge of the Henry's law coefficient (H) for every water soluble organic species described in the chemical mechanism. Methods that can predict reliable H values for the vast number of organic compounds are therefore required. We have compiled a data set of experimental Henry's law constants for compounds bearing functional groups of atmospheric relevance. This data set was then used to develop GROMHE, a structure activity relationship to predict H values based on a group contribution approach. We assessed its performance with two other available estimation methods. The results show that for all these methods the reliability of the estimates decreases with increasing solubility. We discuss differences between methods and found that GROMHE had greater prediction ability.