



Investigating the Vapour Pressures of Nitroaromatic Compounds Using Knudsen Effusion Mass Spectrometry

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Atmospheric aerosols directly and indirectly affect the Earth's climate. Further understanding of aerosol formation and evolution is required to improve aerosol representation in models. The saturation vapour pressure of a secondary organic aerosol (SOA) can be used to predict partitioning between the gaseous and particulate state. The extent of this partitioning affects how the SOA behaves in the atmosphere.

Due to the sheer number of SOAs present in the atmosphere (estimated at over 100000)[1] it is not possible to measure the saturation vapour pressure of each individually. Instead group contribution methods (GCMs) are commonly used to predict vapour pressure. The reliability of a GCM depends on how well represented the functionality present in the compound of interest is in the reference data set. There is a lack of atmospherically relevant data for nitroaromatic compounds in the most commonly used GCMs (Myrdal and Yalkowsky method[2] contains 3, Nannoolal method[3] contains 13, Moller method[4] contains 19, SIMPOL method[5] contains 25 however many of these are taken from single data points, and EVAPORATION method[6] contains 0). This leads to experimentally determined values differing from GCM predictions by orders of magnitude. With further experimentally determined vapour pressure data these reference data sets can be expanded and the methods will have the appropriate tools to more accurately predict the vapour pressures of nitroaromatic compounds.

In this study we present results from recent experiments using Knudsen effusion mass spectrometry (KEMS) and comparison with GCMs. Specifically Mono-substituted nitrophenols, mono-substituted nitrobenzoic acids, and nitrobenzaldehydes were selected for study. All compounds selected were purchased at a purity of 99% or higher to minimise errors introduced by impurity.

References

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