EXPERIMENTAL DETERMINATION OF GAS PHASE THERMODYNAMIC PROPERTIES OF BIMOLECULAR COMPLEXES

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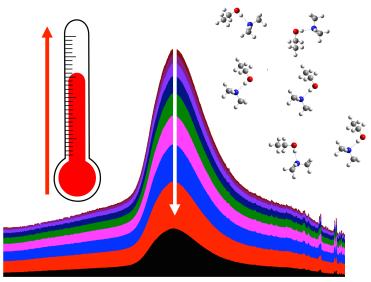

Accurate determination of the atmospheric abundance of hydrogen bound bimolecular complexes is necessary, as hydrogen bonds are partly responsible for the formation and growth of aerosol particles. The abundance of a complex is related to the Gibbs free energy of complex formation (ΔG), which is often obtained from quantum chemical calculations that rely on calculated values of the enthalpy (ΔH) and entropy (ΔS) of complex formation. However, calculations of ΔH and in particular ΔS are associated with large uncertainties, and accurate experimental values are therefore crucial for theoretical benchmarking studies. Infrared measurements of gas phase hydrogen bound complexes were performed in the 300 to 373 K range, and lead to a purely experimental determination of ΔH using the van't Hoff equation. Equilibrium constants were determined by combining an experimental and calculated OH-stretching intensity, from which values of ΔG and hence ΔS could be determined. Thus we can determine ΔG, ΔH and ΔS for a bimolecular complex. We find that in the 300 to 373 K temperature range the determined ΔH and ΔS values are independent of temperature.