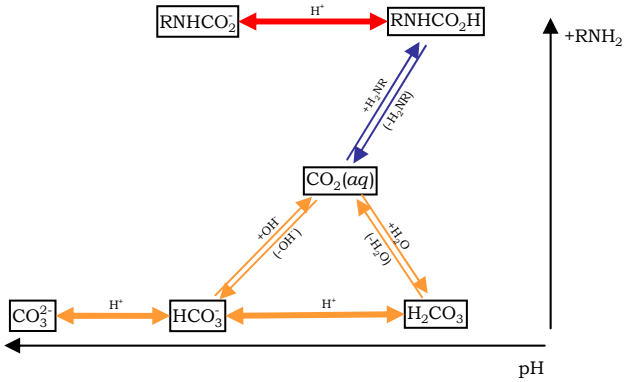
CHEMOMETRICS

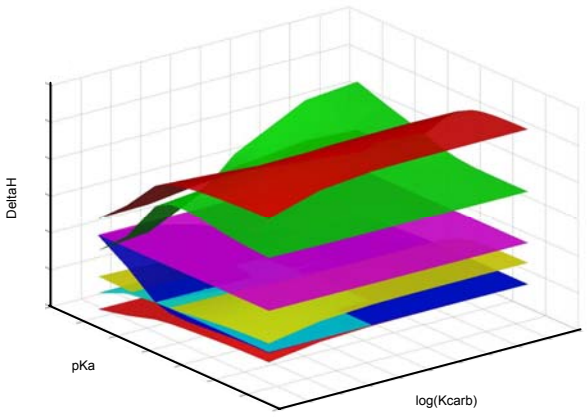
RESEARCH LABORATORY

THE UNIVERSITY OF NEWCASTLE AUSTRALIA

Research Focus

Amongst several other, non-energy related projects, the Chemometrics laboratory is currently investigating the fundamental understanding of the interaction of CO_2 with organic amines and other bases in aqueous solution. This research is relevant for post-combustion capture (PCC) of CO_2 in coal fired power stations and several other applications. There is a strong collaboration with CSIRO Energy Technology in Newcastle and the Swiss Federal Institute of Technology (ETH).





Current Projects

The immediate goal of our research is to determine all relevant rates and equilibrium constants for all reactions between CO_2 and organic amines. A complete reaction scheme for monobasic amines is given in the scheme to the right. The results will include the temperature dependences of all constants as well as the heat capacities of all reactions. The second goal is to model the performance of single amine and amine mixture solutions in pilot plant situations. The modelling results will continuously be compared with laboratory and pilot plant absorbers at CSIRO. Plant modelling is based on molecular mechanisms and not on empirical reactions which are traditionally used in the engineering contexts. It is our belief that this more scientific approach will advance the understanding of CO_2 amine interactions in significant ways; e.g. it allows the detailed analysis of all components of the overall interaction of CO_2 with amines as a function of amine parameters such as pK_a-values, reaction enthalpies, carbamate formation, etc. The graph displays the resolution of the overall cyclic reaction enthalpy into the different components as a function of amine protonation and carbamate formation constant. PCC is done in concentrated solutions, thus the incorporation of activity coefficients is crucial. In a related project we are investigating different activity coefficient approximations for their applicability in situations relevant for PCC. Software for all the above computations is developed in Matlab.

Equipment

The chemometrics laboratory has a complete range of instrumentation for the investigation of chemical processes in solution; this includes in particular kinetic and equilibrium studies. Spectroscopic instrumentation includes NMR facilities, UV-Vis and IR spectrometers as well as access to MS equipment; analytical instrumentation: HPLC, GC, AA and ICP; general lab facilities with fume cupboards for synthetic work. In addition to this, the laboratory has several fully computerised titration set-ups that include potentiometric and spectrophotometric instruments for equilibrium studies and a stopped-flow instrument with diode-array detection for fast kinetic studies. Currently, the laboratory, in collaboration with Dr Graeme Puxty of CSIRO, is in the process of building a research calorimeter designed by Professor Hungerbühler at the ETH. Most relevant is a complete range of software for the modelling and analysis of chemical processes in solution.

Contact Us

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