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Computational Chemistry Study of Amine Complexation

Stefan Andersson^a and Eirik Falck da Silva^{a*}

^a SINTEF Industry, P.O. Box 4760 Torgarden, N-7465 Trondheim, Norway

Abstract

Solvent management and the understanding of solvent degradation is important to the improvement of CO₂ absorption technology. It has long been suspected that metal ions can contribute to catalyzing solvent degradation. It has also been suspected that amine solvents and degradation products can complexate metal ions. Together this suggests a complex interplay between solvent components and metal ions. This also has the potential to influence the level of corrosion seen in a capture plant.

Obtaining direct insight into such phenomena experimentally is difficult. We have therefore undertaken a computational chemistry study to explore amine complexation to iron metal ions, Fe²⁺ and Fe³⁺. In this study we look at the correlation between complexation energies calculated with computational chemistry tools and concentrations of metal ions measured in amine thermal degradation experiments.

The data on metal solubility in amine solutions are from the PhD thesis of Ingvild Eide-Haugmo.¹ The thermal degradation experiment has been reported on in journal publications. The metal solubility data were obtained by ICP-MS analysis of the solvent at the end of the 5 week experiments. The solvents had a 0.5 loading and were kept at 135C for 5 weeks.

The computational chemistry calculations were carried out with DFT methods and a continuum solvation model. The B3LYP/ 6-31G** method was used together with the SMD solvation model. A broad range of different complex structures were explored. In Figure 1 is shown a stable complex for ethylenediamine (EDA).

In Figure 2 we show results for complexation with Fe²⁺ while Figure 3 shows corresponding results for Fe³⁺. The results show a fairly strong correlation. In this work we have so far only looked at the complexation of the solvent amine itself. We have not studied the complexation of carbamate species yet. In a thermal degradation experiment, degradation products are known to form. It may be that for some solvents degradation products contribute significantly to the metal solubility. This is something one may be able to resolve with further work. One should not read too much into the absolute values calculated from the current computational chemistry work, further work would be needed to draw conclusions on absolute values. The results do however suggest strong complexation between metal ions and amines.

In this work we have only focused on complexation of potential solvent amines. We do however intend to expand this work to also cover reactive amine species and solvent degradation products.

* Corresponding author. Tel.: +47 948 45 691
E-mail address: eirik.silva@sintef.no

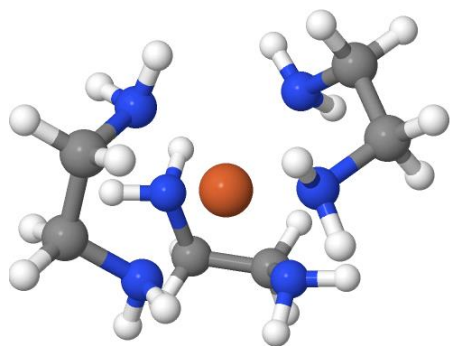


Figure 1. Complexation of 3 ethylenediamine (EDA) molecules with Fe^{2+}

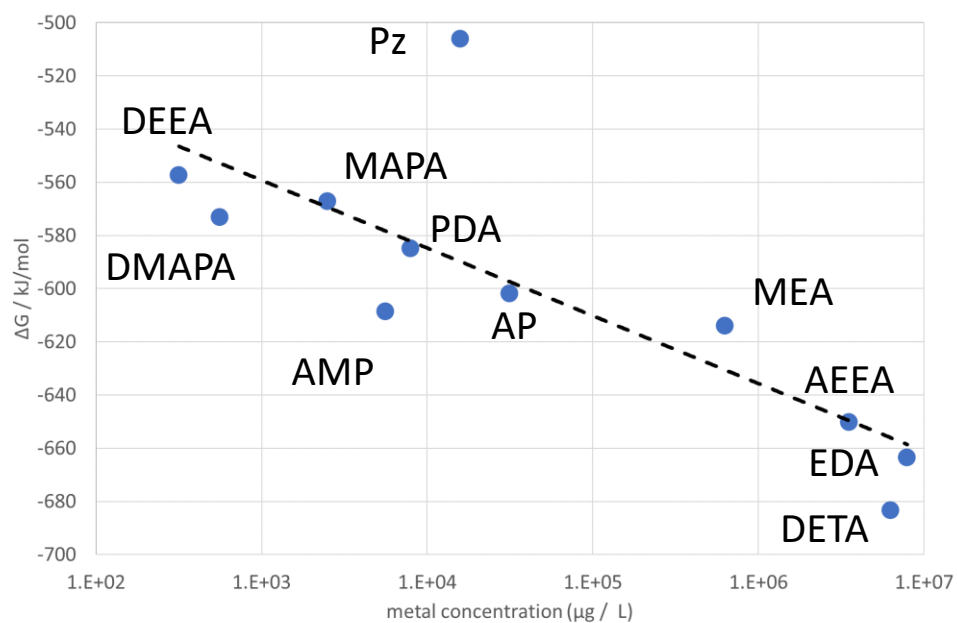


Figure 2. Complexation energy for different amines with Fe^{2+} plotted against iron concentration in thermal degradation experiments. DEEA: Diethylethanamine; DMAPA: Dimethylaminopropylamine; MAPA: 3-amino-1- methylaminopropane; AMP: 2-amino-2-methylpropanol; AP: 3-aminopropanol; Pz: Piperazine; PDA: propylenediamine; MEA: 2-ethanolamine; AEEA: N-(2-hydroxyethyl)- ethylenediamine; EDA: Ethylenediamine; DETA: Diethylenetriamine.

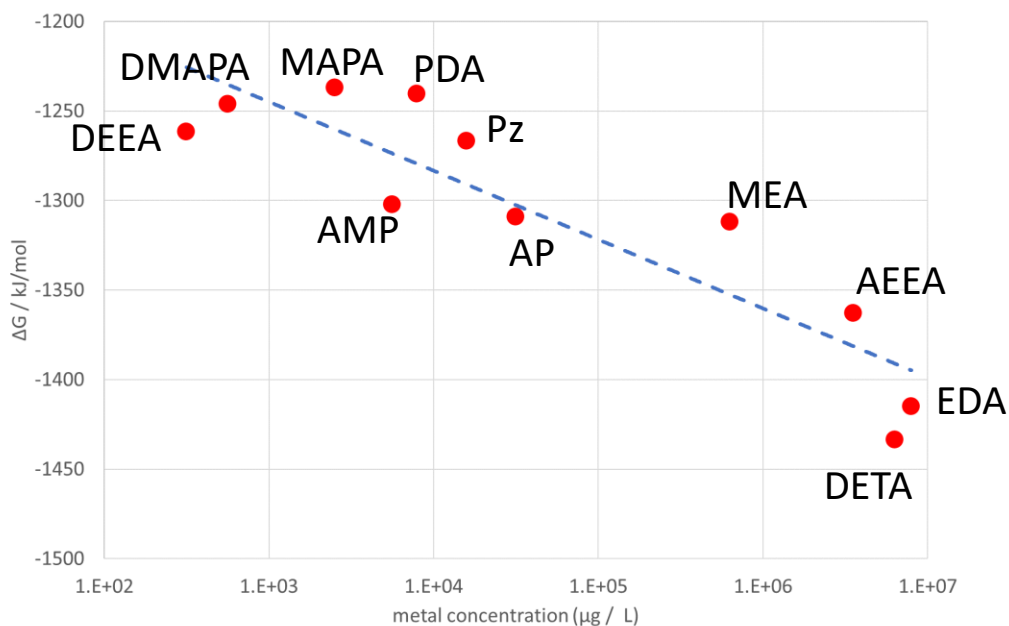


Figure 3. Complexation energy for different amines with Fe^{3+} plotted against iron concentration in thermal degradation experiments.

References:

- 1) Eide-Haugmo, I., (2011), Environmental impacts and aspects of absorbents used for CO₂ capture, doctoral thesis, NTNU.
- 2) Eide-Haugmo, I., Lepaumier, H., Einbu, A., Vernstad, K., Da Silva, E. F., & Svendsen, H. F. (2011). Chemical stability and biodegradability of new solvents for CO₂ capture. *Energy Procedia*, 4, 1631-1636.

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