



Date: October 2014

To: Chemistry in Refining Overhead Stakeholders

From: Pat McKenzie, Business Development Director for OLI
Andre Anderko, Managing Director and CTO, OLI

Re: OLI assessment of dibutylamine hydrochloride / OLI quotation for thermophysical modeling

Reference: 14-OLI-N0064-3

SUMMARY

One of the Chemistry in Refining Overhead stakeholders has interest in the behavior of the dibutylamine hydrochloride salt point as part of their simulation studies. This component is not currently in the OLI MSE databank. This client requested any feedback that OLI might have regarding the behavior of this amine and its chloride salt. Citing the low vapor pressure relative to other amines, our client considers this an important amine for simulation. Thus, this proposal gives an estimate for adding this amine and also addresses the question: "... [from OLI's] knowledge of diethylamine (DEA) and dimethylamine (DMA) chloride salt formation which currently exist in OLI, where would [OLI] expect dibutylamine chloride salt formation temperature to form be relative to the DMA and DEA."

Part 1: BEHAVIOR OF DIBUTYLAMINE CHLORIDE (DBA·HCL)

Andre Anderko, OLI's Managing Director and CTO, in consultation with OLI's thermophysical modeling team, has prepared these comments regarding DBA·HCL behavior:

- There are experimental data for the vapor pressure over dibutylamine chloride at low temperatures (for aerosol applications) and at high temperatures (where it is liquid).
- At low temperatures, the vapor pressure decreases in the series DMA·HCl > DEA·HCl > DBA·HCl. So, the salt point temperature would be highest for DBA·HCl.
- However, as the temperature increases, the vapor pressures become closer and are similar in the range 230 – 300 C (where the hydrochlorides are liquid).



- In the intermediate temperature range, which is of interest for our applications, the series DMA·HCl > DEA·HCl > DBA·HCl would still probably hold but the differences will be small.

Further, the team believes that the biggest difference lies then not in the salt point but in the vapor pressure of the dibutylamine itself (as opposed to dibutylamine chloride). Because of the low vapor pressure, dibutylamine will much more readily partition into the liquid (mostly hydrocarbon) phase than the lighter amines. Under some conditions, this may reduce its availability to form the hydrochloride. **This should be the key effect.** So, a more detailed analysis would require modeling.

Part 2: ESTIMATE

To add this component to the OLI MSE databank, OLI would require parameters for the two binary systems of dibutylamine – H₂O and dibutylamine hydrochloride – H₂O (items 001 and 002 in the table below). For maximum accuracy, OLI also recommends parameters for dibutylamine – hydrocarbons. Finally, OLI has two data sources for dibutylamine hydrochloride; nonetheless, OLI recommends a literature search for additional data to completely model this system.

ITEM	Component	Time, USD	Amount, USD
001	Dibutylamine – H ₂ O	10 days	\$12,000
002	Dibutylamine hydrochloride – H ₂ O	5 days	\$6,000
003	Dibutylamine hydrocarbons	15 days	\$18,000
004	Literature search (included in the overall project)	4 days	\$4,800
TOTAL with extra hydrocarbon work			\$36,000

The prices shown in the table above represent a 50% cost-share with OLI on the work for priority treatment of this chemistry. **Cost could be divided among interested stakeholders.** The resulting parameters would then be treated in the same manner as the prior OLI’s Chemistry in Refining Overhead parameter development: proprietary to the funding stakeholders for a minimum of 2 years following the completion of the project.

OLI can also undertake this work on a totally proprietary basis to a single stakeholder, provided the stakeholder can supply proprietary data for this information. In that case, the prices shown in the table should be increased by a factor of 2.