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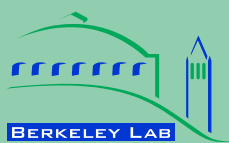
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Unit price scaling trends for chemical products

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Abstract

To facilitate early-stage life-cycle techno-economic modeling of emerging technologies, here we identify scaling relations between unit price and sales quantity for a variety of chemical products of three categories - metal salts, organic compounds, and solvents. We collect price quotations for lab-scale and bulk purchases of chemicals from both U.S. and Chinese suppliers. We apply a log-log linear regression model to estimate the price discount effect. Using the median discount factor of each category, one can infer bulk prices of products for which only lab-scale prices are available. We conduct out-of-sample tests showing that most of the price proxies deviate from their actual reference prices by a factor less than ten. We also apply the bootstrap method to determine if a sample median discount factor should be accepted for price approximation. We find that appropriate discount factors for metal salts and for solvents are both -0.56, while that for organic compounds is -0.67 and is less representative due to greater extent of product heterogeneity within this category.

1. Introduction

Prospective life-cycle techno-economic modeling of emerging technologies is a growing research field, combining scenario analysis with consequential life-cycle assessment (LCA) to assess the potential impacts of technologies and infrastructure systems that are not yet operating at commercial scale. This modeling method can produce insights that may help guide fundamental research and stimulate effective innovation in the most critical areas. Recent examples of techno-economic analysis include Van Dael et al. (2015) for ultrasonic production of biofuels and Kuppens et al. (2015) for fast pyrolysis for the valorization of short rotation coppice. This type of early-stage modeling, when applied to technologies that involve chemical synthesis processes, may require knowledge of the sales price structure for a wide variety of chemical reagents and solvents in various quantities. Lab-scale prices of chemicals are usually standardized and easily accessible (e.g., supplier Sigma Aldrich). However, discovering their bulk prices is more difficult, typically requiring extensive inquiries and sometimes bilateral negotiations. In this work, we propose a price scaling method that can facilitate the prospective techno-economic modeling process, by quickly deriving proxies of bulk prices of chemicals at quantities of interest, in place of ad hoc solicitation of price quotations from actual suppliers.

It is widely understood that suppliers offer price discounts for purchases in larger quantities. Munson and Rosenblatt (1998) surveyed the literature on quantity discounting and distinguished between buyer's perspective, seller's perspective, and joint buyer-seller models of price discounts. They supplemented this literature review with interviews of numerous industrial buyers and sellers to determine how quantity discounting theory corresponds with actual practice. However, they offered no quantitative guidelines of actual price discount factors in industry. Anderson (2009) identified detailed cost components and demonstrated a bottom-up cost estimation approach. He also noticed the price discount effect without quantified characterization. Hart and Sommerfeld (1997) collected price data on 24 chemical products at lab-scale and medium scale (approximately 25 kg) quantities, and used a log-log linear regression model to derive quantity discount factors. They found that a discount factor of -0.75 most accurately described the observed price reductions. However, they did not consider larger bulk quantities, and they did not distinguish between different types of chemical products. Here,

we build on this knowledge of quantity discounting of chemical products by applying a log-log price discount model to different categories of chemicals including metal salts, organic compounds and solvents, in larger quantities up to metric tons. We also provide a validation framework to provide additional insights on the uncertainties and limitations of the methodology.

Our method consists of two parts. In the modeling part, we use a log-log linear regression model to relate the unit sales price of a chemical product (e.g. in units of dollars per kg) to the amount of the purchased product (e.g. in units of kg). We consider the slope coefficient obtained from the ordinary linear regression as the price discount factor for each chemical product in the given data set. The mean and median of those discount factors within each product category (metal salts, organic compounds and solvents) become representatives of the discount factor for that category. Consequently, rapid and informed estimation of prices of specific chemicals can be obtained as inputs to prospective techno-economic modeling of emerging technologies, based on current sales prices for laboratory scale quantities.

In the validation part, we first test the price approximation errors using out-of-sample mean and median discount factors. Then we propose a bootstrap method to systematically test whether the sample median of each category is sufficiently robust as a representative value. This information is revealed by examining the “fatness” of the distribution of bootstrapped medians for each product category. We show from our price data set that the sample medians of the metal salts and the solvents can be accepted as representative discount factors, while that of the organic compounds cannot, if we set 1.5 as the acceptance/rejection threshold width of the 90% confidence interval of the bootstrapped median distribution.

The remainder of this report is organized as follows: Section 2 describes the modelling process of identifying individual price discount factors and inferring prices of materials of the same category. Section 3 validates the proposed approach by first testing the price approximation accuracy and then applying the bootstrap method. Section 4 concludes this report.

2. Modelling the price discount effect

2.1 Log-log linear regression model

We obtained price quotations for a variety of chemical reagents and solvents (25 metal salts, 11 organic compounds and 16 solvents) at different transaction scales (from grams to tons). The quotes were obtained from several chemical suppliers through their company websites and through personal communication with sales representatives. Specifically, the lab-scale quotes were queried from the U.S. supplier Sigma-Aldrich, and the bulk-scale quotes were from U.S. supplier BOCSCI and from Chinese suppliers registered at the Alibaba.com online platform. The bulk-scale quotes are “free on board” (FOB), meaning that the transportation costs to the shipping port is paid by the supplier. Data were collected during the time window from 2011 to 2014. BOCSCI quotes for 20 metal salts and four organic compounds were obtained in 2011 and the rest of the data were collected during the year of 2014.

Our objective is to quantitatively determine the price discount factors. For each material, we fit

the collected price data into models that characterize the relation between the price and the order quantity. Consequently, we identify the model described by Equation (1) to be the most accurate in terms of R^2 goodness of fit:

$$p(q) = b \times q^\gamma \quad (1)$$

where

p is the unit price (e.g., \$/kg) as a function of the order quantity q (e.g., kg)
 b is a scale parameter
 γ is the quantity discount factor.

In theory, $\gamma < 0$ because of quantity discount and $\gamma > -1$ to guarantee $p(q)$ is still increasing in q . However, these inequalities may not necessarily hold empirically, given that the effect of supplier non-homogeneity is not fully controlled.

The two parameters γ and b are the parameters to be estimated. Their best estimates (in the sense of least squared error) can be readily solved for by standard linear regression, since the model has its linear equivalent described by Equation (2):

$$\log_{10}(p) = \gamma \times \log_{10}(q) + \log_{10}(b) \quad (2)$$

Given the limited number of price points for each chemical in the data set, the model must be very parsimonious to avoid over-fitting. In equation (2), γ has clear interpretation – it is the rate of change of the order of magnitude of the price with respect to the order of magnitude of the quantity.

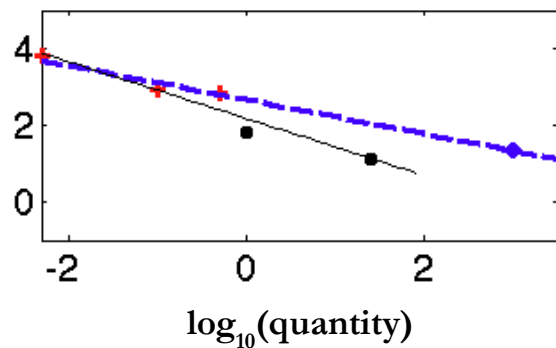
2.2 Individual price discount effects

For each material, we estimate γ first using the bulk prices exclusively from BOCSCI, the U.S. domestic vendor, and then using the bulk prices exclusively from Alibaba.com suppliers. For both sets of bulk price data, we use the same set of lab-scale prices from Sigma-Aldrich.

The price discount profiles of all the considered materials are available in Figures A1-A3 in the Appendix A. Figure 1 shows the price discount of a representative chemical product, cobalt(II) chloride. The horizontal and the vertical axes represent the quantity (in kilogram) and the per unit price, respectively, both on the \log_{10} scale. The red crosses represent lab-scale data points. The blue diamond shapes represent U.S. domestic bulk prices from BOCSCI and the black circles represent those from Alibaba suppliers. The blue dashed lines fit with BOCSCI prices as well as the lab-scale prices, while the black solid lines fit with Alibaba prices as well as the lab-scale prices. The slope of each line is the price discount factor γ . The price unit is 2014 U.S. \$.

Figure 1. Price discount of cobalt(II) chloride.

$\log_{10}(\text{price})$



The fitting overall is accurate with high R-squared values and significant t-values. This is partly due to a careful choice of model and partly due to limited data points. Figures A1-A3 show that bulk prices offered by Alibaba suppliers are in general lower than by the U.S. domestic supplier. While it is reasonable to infer that the Chinese suppliers tend to offer lower prices, this price difference may also be partly due to how the data are collected. Specifically, most of the sales quantities provided by the Chinese suppliers are labeled as “minimum” sales quantities that support their associated price, while the BOCSOI prices were all offered at the sales quantities that we specified in our inquiry. It can thus be expected that those Alibaba.com prices may be biased. On the other hand, both BOCSOI and Alibaba.com prices that we collected could be systematically higher than the actual transaction prices, since bulk prices, in general, can decrease as bilateral negotiations proceed.

Hereafter we only consider data from Alibaba suppliers as bulk price data for brevity of discussion, since we have more of those data available than those from BOCSOI. Figure 2 shows histograms of the distributions of the values of the resulting discount factors.

Figure 2. Distributions of cost discount factors.

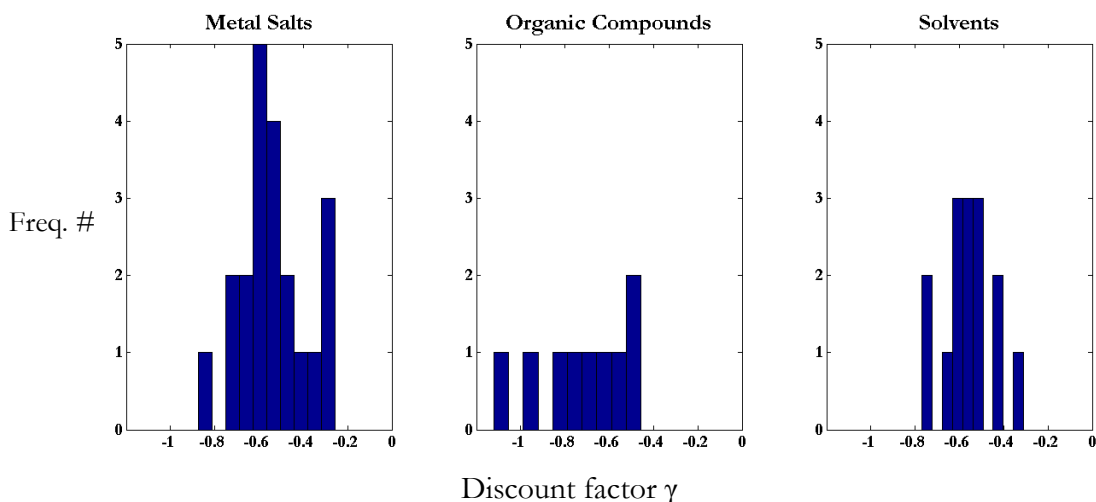


Figure 2 shows that the discount factors of metal salts and of the solvents are more narrowly distributed than those of the organic compounds. Given insufficient samples, it is still early to draw general conclusion on the price discount behavior of the category of organic compounds. One reason for the wider distribution may be that organic compounds have more sophisticated and varied molecular structures, requiring specialized production processes for different compounds at different costs. Furthermore, we do not fully control the purity of the materials by the bulk suppliers, as we accept the quotes as long as the supplier indicates that the purity is at least 95%. Another factor may contribute to the dispersion of discount factors with overseas sourcing, as we do not fully control the heterogeneity of those suppliers but accepted an Alibaba supplier as long as it provided quotes of the product.

2.3 Inferring prices of a new product

Our goal of this work is to be able to predict the bulk price of a chemical product when only its lab-scale prices are available. To this end, we propose to use the median of the sampled discount factors of its product category as the representative value of price discount for the material of interest. Two natural candidates of such representative values are the median and the mean of the sample price discount factors. We opt for the sample median, denoted as γ_m , since the sample mean is more sensitive to outliers when data points are few and is thus less statistically robust, as justified by the numerical tests in the next section. The values of γ_m for metal salts, organic compounds and solvents are -0.56, -0.67, and -0.56, respectively.

Consequently, at any bulk order quantity q , the price proxy \tilde{p} can be given by:

$$\tilde{p}(q) = p_i(q) \left(\frac{q}{q_i}\right)^{\gamma_m} \quad (3)$$

where p_i and q_i are the price and the quantity of a given lab-scale data point, respectively.

3. Validating the price inference

3.1 Out-of-sample test errors

To test the effectiveness of the method described above, we first evaluate the out-of-sample prediction accuracy. Specifically, for a category with N chemical products for which the prices are available and the individual discount factors are learned, we split the materials such that $N-1$ materials are in the training group and the remaining one is used for testing. The median price discount factor of the training group serves as the representative discount value γ_m . As for the testing material, q_i and p_i are chosen to be the largest lab-scale quantity where a price quote is available and the associated price, respectively. Similarly, q and p are the largest available bulk quantity and the associated price, respectively. We compute the price proxy $\tilde{p}(q)$ according to Equation (3), and then compare it against the actual value p . We repeat this procedure N times, each time with a different material being used for testing.

The test errors in terms of the magnitude that \tilde{p} differs from p are summarized in Table 1. The results with the mean discount factors of training groups as the representative values are also included for comparison purposes. Notice that p should not be treated as the exact value, since it is provided by a single supplier, involving internal volatility and bias. For this reason we do not present the relative errors of \tilde{p} with respect to p .

Table 1. Percentage of tests that result in the specified magnitude of difference between price proxy \tilde{p} and its true value p .

| Product group | Choice of γ_m | Magnitude of difference | | |
|-------------------|----------------------|--------------------------|-------------------------|-------------------------|
| | | $0.1p < \tilde{p} < 10p$ | $0.2p < \tilde{p} < 5p$ | $0.5p < \tilde{p} < 2p$ |
| Metal salts | Median | 81.0 | 76.2 | 52.4 |
| | Mean | 81.0 | 76.2 | 47.6 |
| Organic compounds | Median | 66.7 | 33.3 | 11.1 |
| | Mean | 55.6 | 44.4 | 22.2 |
| Solvents | Median | 86.7 | 66.7 | 26.7 |
| | Mean | 88.7 | 66.7 | 26.7 |

Table 1 shows that most of the price proxies (81.0% of metal salts, 66.7% of organic compounds and 86.7% of solvents) deviate from their actual reference prices by a factor less than ten. However, the approximation is not fully accurate, since only a small portion (52.4% of metal salts, 11.1% and 26.7%) of the proxies deviate from the reference values by a factor smaller than two. Therefore, given the data that we experiment with, the proposed method is likely to correctly estimate the order of magnitude of the product price, but is unreliable for finer estimation. Table 1 also shows that using the mean discount factor of the training groups is less robust, with more occurrences of estimation off by a certain factor.

We expect an enhancement of estimation accuracy if the data set is enriched with additional quotations. However, the enhancement may be limited by the inherent discrepancies between different chemical materials as well as the uncertainties in suppliers, purities, etc. The results shown in Table 1 are conservative, since we choose the maximum available bulk quantity and the associated price for testing. In general, smaller bulk quantities incur less price volatility.

3.2 Bootstrapping-based validation approach

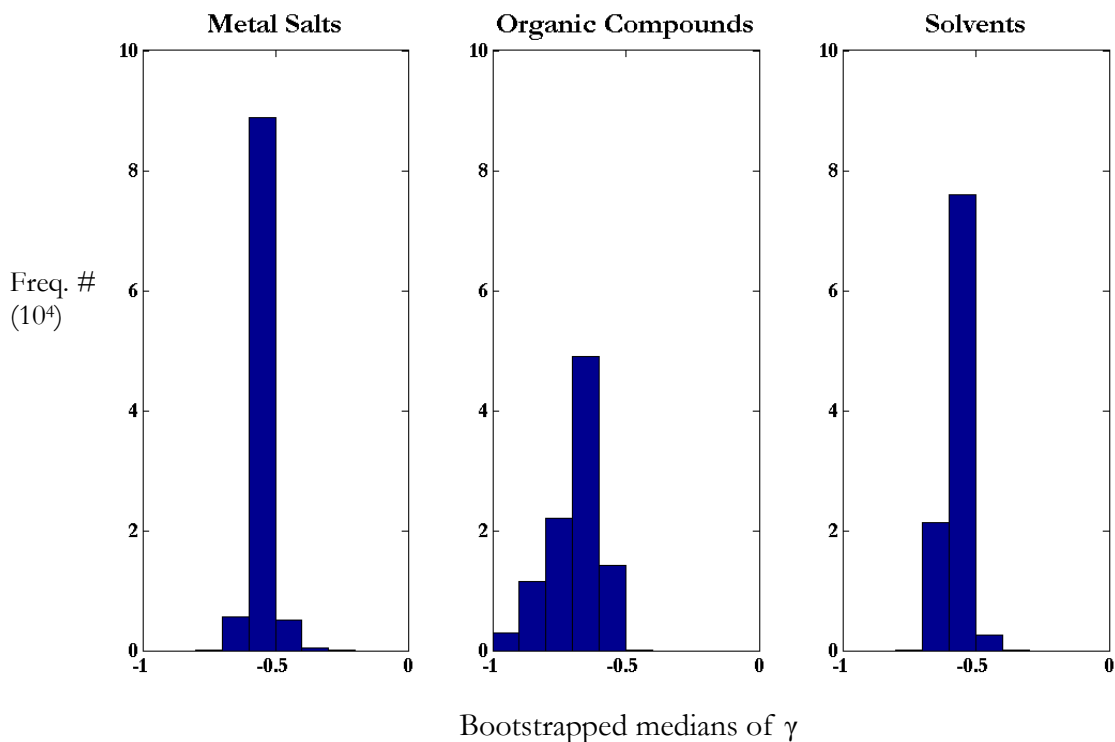
Our recommended discount factor of each product category for future analyses are the median of the sampled discount factors, as explained in Subsection 2.3. Ideally, the best representative discount factor of each product category is the median of the discount factors of all its products. However, such population-level statistic is unachievable with finite samples. Subsequently, a natural question arises as to how robustly the sample median approximates the population median. The level of this robustness is a strong indicator of the effectiveness of our bulk price approximation, since one can expect gross price misestimates if the sample median value of the discount factors changes dramatically by replacing only a few sample materials with some others.

In this subsection, we apply the bootstrap method to quantify the robustness level of γ_m , the median of the sample discount factors. The bootstrap method is primarily used to infer probabilistic information (e.g., distribution, confidence interval, etc.) of sample statistics of interest, such as moments, quantiles, etc. It is particularly appropriate when the underlying population distribution is unknown or intractable and/or the sample size is not large enough. The reader may refer to reference Davison and Hinkley (1997) for a general introduction as well as extensive applications of the bootstrap method.

We adopt the basic bootstrap method in our context. We assume that the sample of M price discount factors obtained from Section 2.2 for each product category are randomly drawn from the population of discount factors of all the chemicals of that category. Starting from this original sample, we consecutively construct $B = 100,000$ “bootstrap” samples of the discount factors. Each bootstrap sample is of size M and is constructed by randomly replacing one discount factor in its preceding sample with another discount factor that is randomly sampled from the original sample. Since each bootstrap sample, by our assumption, is a representation of the unknown population, the median discount factor of each sample is also a representation of the population median. The dispersion of those bootstrapped medians reflects our uncertainty about the true population median. In fact, bootstrapped (common) statistics asymptotically converge to their true values under mild regularity conditions as the sample size goes to infinity (Bickel & Freedman (1981)).

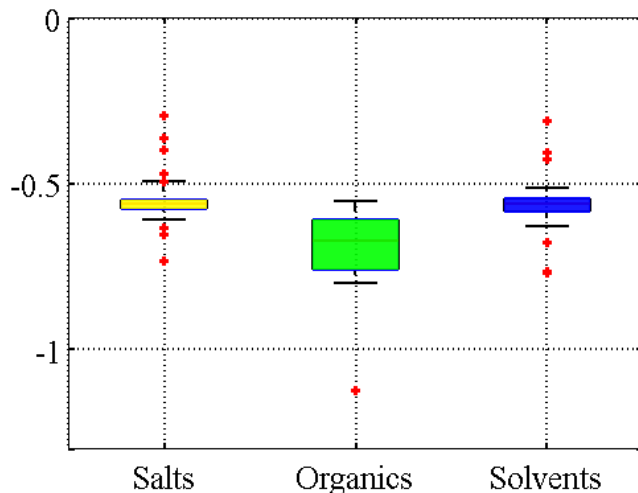
We implement the above bootstrapping procedure to our samples and obtain the distributions of the bootstrapped medians of price discount factors for the three product categories, as shown in Figure 5. Apparently, the bootstrapped medians are more narrowly distributed in the cases of metal salts and solvents, compared with those in the case of organic compound. We thus expect that the representative discount factors that we choose for the metal salts and solvents are likely to generate more accurate price estimates than in the case of organic compound, which is consistent with the results in Table 1.

Figure 3. Distribution of bootstrapped medians of cost discount factors.



We next demonstrate a simple quantified method for interested researchers to determine if γ_m should be accepted for price approximation based on the distribution of the bootstrapped medians. Specifically, one can specify a certain degree of dispersion of the bootstrapped medians as the threshold rule of acceptance/rejection. Such rule can be made on an ad hoc basis: it reflects the error tolerance of the interested life-cycle techno-economic modeling, contingent on the modeling purposes and/or stages. To illustrate, suppose we set the rule to be “accept the sample median of discount factors for price approximation only if the 90% confidence interval length of its bootstrap distribution is no larger than 0.15”. Then, we accept the sample median discount factors of the metal salts and the solvent, but reject that of the organic compounds, since their 90% confidence interval lengths 0.12, 0.12 and 0.25, respectively. Figure 6 is a boxplot illustration, where the horizontal edges of each box are the 25th and the 75th percentiles of the bootstrap distribution, the whiskers delimit the 90% confidence interval and the red dots represent the bootstrapped medians outside of the 90% confidence interval.

Figure 4. Boxplot illustration of the bootstrapped median distribution.



4. Discussion and conclusions

In this work, we develop a framework of analyzing price discount effect of chemical products. We consider a model that is able to characterize the price discount by linear regression of log-log relations. Using lab-scale and bulk-scale quotations from U.S. and Chinese suppliers, we identify discount factors for 25 metal salts, 11 organic compounds and 16 solvents. Using the median discount factor of each category, a price proxy of a material at any bulk purchase scale can be readily computed. The out-of-sample tests show that most of the price proxies deviate from their actual reference prices by a factor less than ten. We also apply the bootstrap method to determine if a sample median discount factor should be accepted for price approximation. Through this work, we find that the degrees of price discount of the sample metal salts and solvents have smaller variation within their respective categories, compared with those of the sample organic compounds. We also find that sourcing from overseas brings down the order cost, but with greater cost uncertainty.

Our work focuses on price discounts that are primarily driven by quantities of individual purchases. It should be noted that other scaling mechanisms may also affect the price of chemical products. For example, Lieberman (1984) noted a learning curve effect in the chemical industry, where price reductions occurred due to increasing cumulative production quantities of a product. This may be particularly relevant for emerging technologies that require specialty chemicals that are currently produced and used at small scale, but may be used in much larger quantities if the technology scales up considerably. In addition to estimating the cost of a single chemical product, various methodologies for project-level cost-estimation were discussed in Dysert (2003).

The price discount factors identified in this work can enable more robust prospective techno-economic modeling of emerging technologies. On the other hand, their accuracy can be further enhanced with an augmented data set, finer categorization of the materials and more control of the factors such as supplier attributes and product purities.

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Appendix A: Price Discount of Materials

Figures A1-A3 show the price discount profiles of 25 metal salts, 11 organic compounds and 16 solvents, respectively. The horizontal and the vertical axes represent the quantity (in kilogram) and the per unit price, respectively, both on the log₁₀ scale. The red crosses represent lab-scale data points. The blue diamond shapes represent U.S. bulk prices from BOCSCI and the black circles represent those from Alibaba suppliers. The blue dashed lines fit with BOCSCI prices as well as the lab-scale prices, while the black solid lines fit with Alibaba prices as well as the lab-scale prices. The slope of each line is the price discount factor γ . The price unit is 2014 U.S. \$. The quantity unit is kilogram for solids and liter for liquids. Data of bulk prices either in the U.S. or from Alibaba suppliers are not available for some materials.

Figure A1. Price discounts of 25 metal salts.

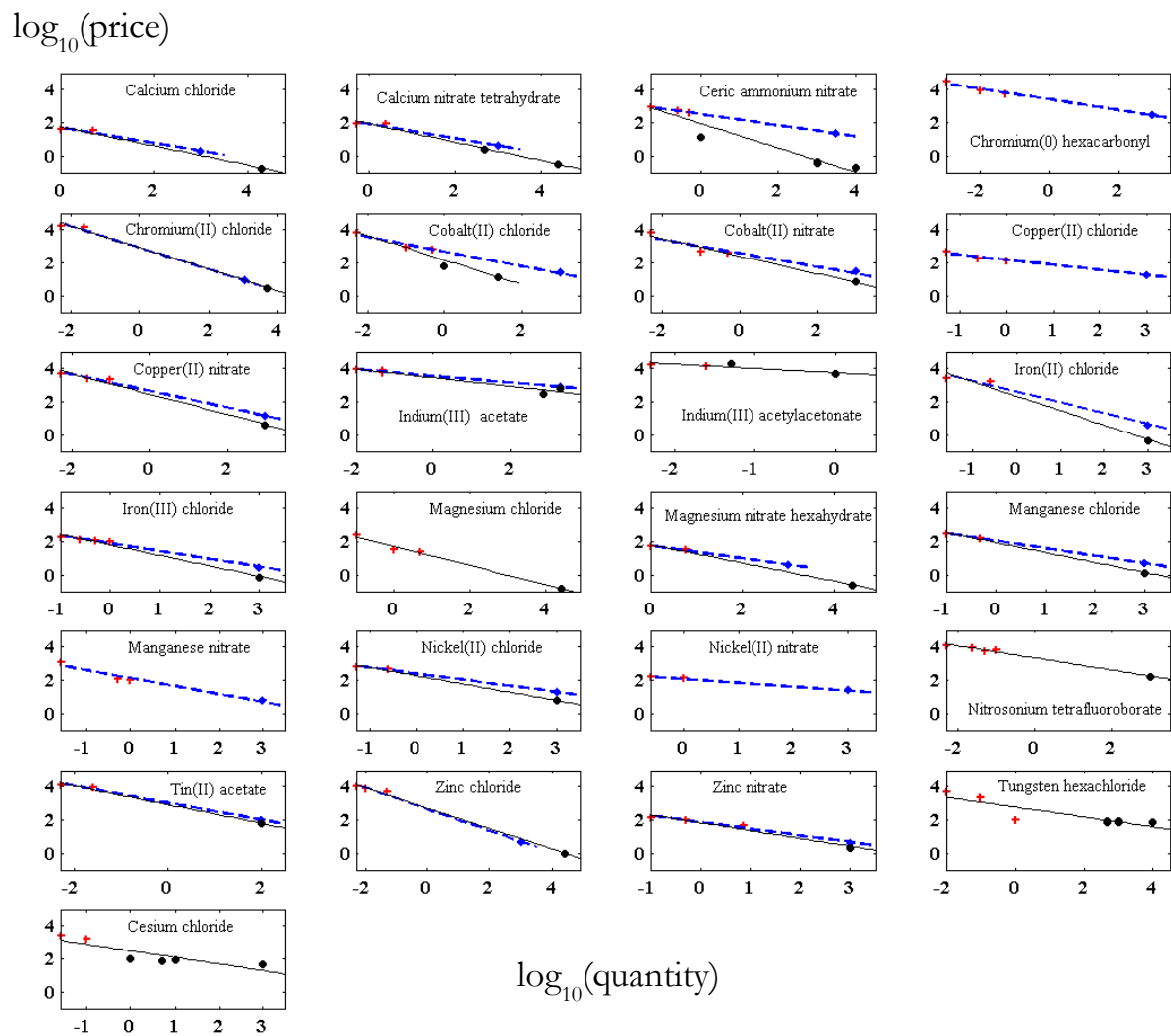


Figure A2. Price discounts of 11 organic compounds.

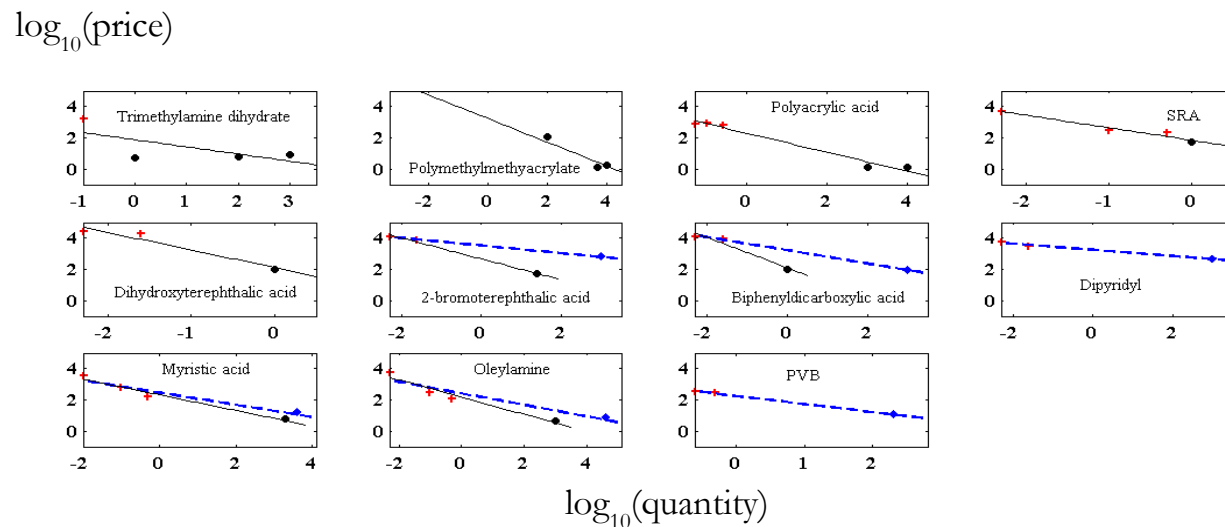


Figure A3. Price discounts of 16 solvents.

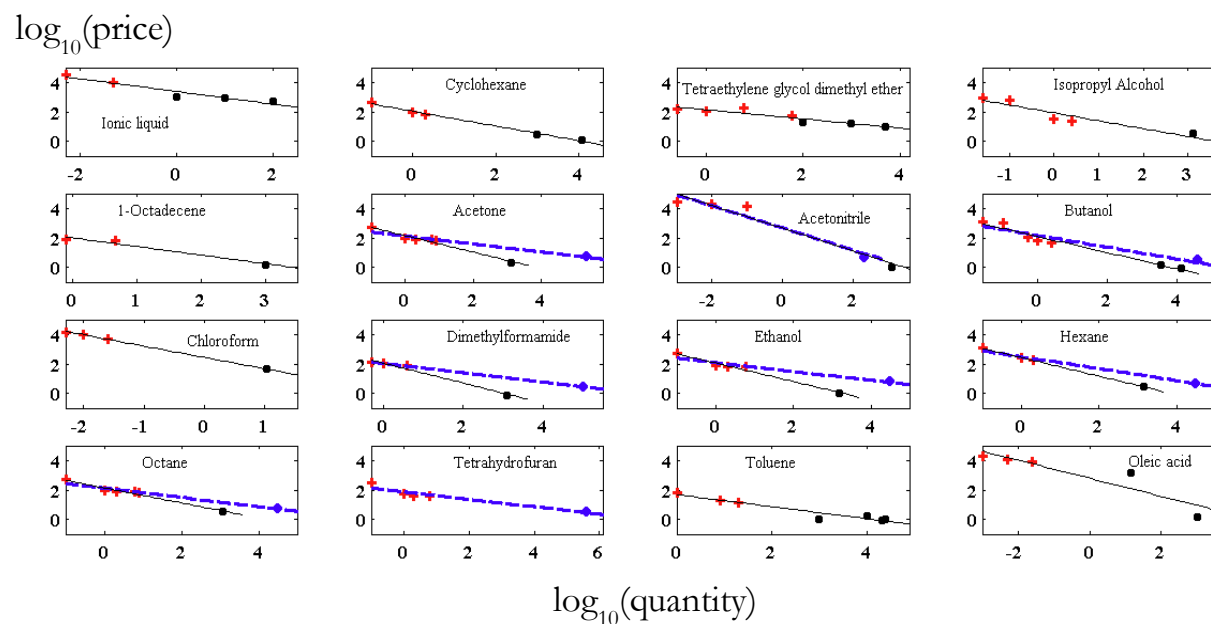


Table A1. Price quotes collected from Sigma Aldrich, BOSCI and Alibaba

| Chemical Name | Category | Quantity Unit | Sigma Aldrich | | | | BOSCI | Alibaba | | | | | | |
|---|------------|---------------|---------------|-------|--------|-------|-------|---------|----------|-------|-------|------|--|--|
| | | | | | | | | | | | | | | |
| | | kg | 1 | 5 | | | 1000 | 20000 | | | | | | |
| Calcium chloride | metal salt | | 40.7 | 32.4 | | | 1.9 | 0.18 | | | | | | |
| | | kg | 0.5 | 2.5 | | | 1000 | 500 | 25000 | | | | | |
| Calcium nitrate tetrahydrate | metal salt | | 90 | 79.4 | | | 3.9 | 2.4 | 0.325 | | | | | |
| | | kg | 0.05 | 0.25 | 0.5 | | 3000 | 1 | 1000 | 1000 | 10000 | | | |
| Ceric ammonium nitrate | metal salt | | 860 | 514 | 395 | | 22 | 12.5 | 0.38 | 0.415 | 0.2 | | | |
| | | kg | 0.001 | 0.01 | 0.05 | | 1000 | | | | | | | |
| Chromium(0) hexacarbonyl | metal salt | | 31100 | 8630 | 5950 | | 290 | | | | | | | |
| | | kg | 0.005 | 0.025 | | | 1000 | 5000 | | | | | | |
| Chromium(II) chloride | metal salt | | 17760 | 13920 | | | 7.9 | 3 | | | | | | |
| | | kg | 0.005 | 0.1 | 0.5 | | 1000 | 1 | 25 | | | | | |
| Cobalt(II) chloride | metal salt | | 6340 | 875 | 659 | | 23 | 65 | 13 | | | | | |
| | | kg | 0.005 | 0.1 | 0.5 | | 1000 | 1000 | | | | | | |
| Cobalt(II) nitrate | metal salt | | 6420 | 480 | 380 | | 28 | 7.2 | | | | | | |
| | | kg | 0.05 | 0.25 | 1 | | 1000 | | | | | | | |
| Copper(II) chloride | metal salt | | 466 | 184.4 | 136.5 | | 19 | | | | | | | |
| | | kg | 0.005 | 0.025 | 0.1 | | 1000 | 1000 | | | | | | |
| Copper(II) nitrate | metal salt | | 5020 | 2568 | 2130 | | 13 | 3.75 | | | | | | |
| | | kg | 0.01 | 0.05 | 0.05 | | 2000 | 700 | 2000 | | | | | |
| Indium(III) acetate | metal salt | | 9210 | 7570 | 5397.8 | | 798 | 318 | 630 | | | | | |
| | | kg | 0.005 | 0.025 | | | | 0.05 | 1 | | | | | |
| Indium(III) acetylacetonate | metal salt | | 17000 | 15200 | | | | 19120 | 4635 | | | | | |
| | | kg | 0.025 | 0.25 | | | 1000 | 1000 | | | | | | |
| Iron(II) chloride | metal salt | | 2796 | 1678 | | | 3.9 | 0.425 | | | | | | |
| | | kg | 0.1 | 0.25 | 0.5 | 1 | 1000 | 1000 | | | | | | |
| Iron(III) chloride | metal salt | | 188 | 143.2 | 117.2 | 99 | 2.9 | 0.705 | | | | | | |
| | | kg | 0.1 | 1 | 5 | | | 25000 | | | | | | |
| Magnesium chloride | metal salt | | 235 | 36.4 | 24.2 | | | 0.155 | | | | | | |
| | | kg | 1 | 6 | | | 1000 | 25000 | | | | | | |
| Magnesium nitrate hexahydrate | metal salt | | 50.8 | 33.58 | | | 4 | 0.24 | | | | | | |
| | | kg | 0.1 | 0.5 | | | 1000 | 1000 | | | | | | |
| Manganese chloride | metal salt | | 293 | 166.6 | | | 4.9 | 1.35 | | | | | | |
| | | kg | 0.025 | 0.5 | 1 | | 1000 | | | | | | | |
| Manganese nitrate | metal salt | | 1220 | 114.4 | 106 | | 5.9 | | | | | | | |
| | | kg | 0.05 | 0.25 | | | 1000 | 1000 | | | | | | |
| Nickel(II) chloride | metal salt | | 634 | 488 | | | 19 | 5.8 | | | | | | |
| | | kg | 0.25 | 1 | | | 1000 | | | | | | | |
| Nickel(II) nitrate | metal salt | | 150.4 | 126.5 | | | 23 | | | | | | | |
| | | kg | 0.005 | 0.025 | 0.05 | 0.1 | | 1000 | | | | | | |
| Nitrosonium tetrafluoroborate | metal salt | | 12340 | 9140 | 5900 | 6895 | | 165 | | | | | | |
| | | kg | 0.005 | 0.03 | | | 100 | 100 | | | | | | |
| Tin(II) acetate | metal salt | | 12920 | 8640 | | | 98 | 60 | | | | | | |
| | | kg | 0.005 | 0.01 | 0.05 | | 1000 | 25000 | | | | | | |
| Zinc chloride | metal salt | | 11120 | 7390 | 4770 | | 4.7 | 1 | | | | | | |
| | | kg | 0.1 | 0.5 | 7 | | 1000 | 1000 | | | | | | |
| Zinc nitrate | metal salt | | 147 | 96 | 48.76 | | 3.9 | 2 | | | | | | |
| | | kg | 0.01 | 0.1 | 1 | | | 500 | 1000 | 10000 | 500 | 1000 | | |
| Tungsten hexachloride | metal salt | | 4830 | 2325 | 96.5 | | 78.8 | 77.5 | 76.8 | 86.5 | 79.50 | | | |
| | | kg | 0.025 | 0.1 | | | 1 | 5 | 10 | 1000 | | | | |
| Cesium chloride | metal salt | | 2464 | 1690 | | | 100 | 72.58 | 85 | 47.5 | | | | |
| | | kg | 0.1 | | | | 1 | 100 | 1000 | | | | | |
| Trimethylamine N-oxide dihydr | OC | | 1760 | | | | 5 | 6.5 | 8 | | | | | |
| | | kg | 0.0005 | | | | 100 | 5000 | 10000 | | | | | |
| Elvacite 2041 (polymethylmeth | OC | | 439000 | | | | 125 | 1.3 | 1.65 | | | | | |
| | | kg | 0.05 | 0.1 | 0.25 | | 1000 | 10000 | | | | | | |
| Polyacrylic acid | OC | | 810 | 922 | 678 | | 1.33 | 1.23 | | | | | | |
| | | kg | 0.005 | 0.1 | 0.5 | | 1 | | | | | | | |
| SRA | OC | | 5180 | 312 | 220 | | 50 | | | | | | | |
| | | kg | 0.005 | 0.025 | | | 1 | | | | | | | |
| 2,5-dihydroxyterephthalic acid | OC | | 27300 | 18840 | | | 100 | | | | | | | |
| | | kg | 0.005 | 0.025 | | | 1000 | 25 | | | | | | |
| 2-bromoterephthalic acid | OC | | 12080 | 8040 | | | 600 | 50 | | | | | | |
| | | kg | 0.005 | 0.025 | | | 1000 | 1 | | | | | | |
| 4,4'-biphenyldicarboxylic acid | OC | | 13260 | 9140 | | | 86 | 100 | | | | | | |
| | | kg | 0.005 | 0.025 | | | 1000 | 10 | | | | | | |
| 4,4'-dipyridyl | OC | | 5660 | 3112 | | | 450 | 5000 | | | | | | |
| | | kg | 0.01 | 0.1 | 0.5 | | 4000 | 2000 | | | | | | |
| Myristic acid | OC | | 3420 | 622 | 152.8 | | 14.9 | 5.75 | | | | | | |
| | | kg | 0.005 | 0.1 | 0.5 | | 40000 | 1000 | | | | | | |
| Oleylamine | OC | | 5840 | 316 | 124.92 | | 7.5 | 4.65 | | | | | | |
| | | kg | 0.25 | 0.5 | | | 200 | | | | | | | |
| PVB | OC | | 324 | 275 | | | 11 | | | | | | | |
| | | kg | 0.005 | 0.05 | | | | 1 | 10 | 100 | | | | |
| Ionic liquid (IL) | solvent | | 32300 | 9980 | | | | 975 | 800 | 560 | | | | |
| | | L | 0.1 | 1 | 2 | | | 1283.70 | 15404.36 | | | | | |
| Cyclohexane | solvent | | 465 | 90.9 | 63.25 | | | 2.73 | 1.29 | | | | | |
| | | kg | 0.25 | 1 | 6 | 60 | | 100 | 1000 | 5000 | | | | |
| Tetraethylene glycol dimethyl e solvent | | | 159.6 | 110 | 191.67 | 52.42 | | 18 | 15 | 10 | | | | |

Table A1 (continued). Price quotes collected from Sigma Aldrich, BOSCI and Alibaba

| Chemical Name | Category | Quantity Unit | Sigma Aldrich | | | | | BOSCI | Alibaba | | | |
|-------------------|----------|------------------|---------------|-------|----------|-------|-------|--------|---------|----------|-------|-------|
| | | | | | | | | | | | | |
| Isopropyl Alcohol | solvent | kg | 1 | 8 | 20 | | | | 1000 | 10000 | 25000 | 21000 |
| | | | 62 | 20.75 | 14.35 | | | | 1 | 1.75 | 1 | 0.85 |
| 1-Octadecene | solvent | L | 0.025 | 0.1 | 1 | 2.5 | | | 1267.43 | | | |
| | | kg | 908 | 630 | 31.8 | 23.44 | | | 3.23 | | | |
| Acetone | solvent | kg | 1 | 6 | | | | | 1000 | | | |
| | | L | 79.4 | 66.17 | | | | | 1.57 | | | |
| Acetonitrile | solvent | | 0.1 | 1 | 2 | 6 | 8 | 200000 | 1272.26 | | | |
| | | | 520 | 98.8 | 76.5 | 82.33 | 63.75 | | 5.9 | 2.11 | | |
| Butanol | solvent | L | 0.001 | 0.01 | 0.1 | | | 200 | 1234.57 | | | |
| | | | 25600 | 18200 | 13630.25 | | | | 4.5 | 1.05 | | |
| Chloroform | solvent | L | 0.025 | 0.1 | 0.5 | 1 | 2.5 | 40000 | 3378.38 | 13513.51 | | |
| | | | 1244 | 1025 | 108.2 | 65.3 | 42.6 | | 3.5 | 1.55 | 0.90 | |
| Dimethylformamide | solvent | L | 0.005 | 0.01 | 0.025 | | | | 11.15 | | | |
| | | | 13200 | 10550 | 5280 | | | | 42.61 | | | |
| Ethanol | solvent | L | 0.5 | 1 | 4 | | | 100000 | 1267.43 | | | |
| | | | 129.4 | 108.5 | 74.25 | | | | 2.8 | 0.79 | | |
| Hexane | solvent | L | 0.1 | 1 | 2 | 6 | | 30000 | 1515.15 | | | |
| | | | 478 | 83.1 | 63.75 | 69.25 | | | 6.6 | 0.99 | | |
| Octane | solvent | L | 0.1 | 1 | 2 | | | 30000 | 1422.48 | | | |
| | | | 1205 | 239.5 | 170.75 | | | | 5.3 | 2.81 | | |
| Tetrahydrofuran | solvent | L | 0.1 | 1 | 2 | 6 | 8 | 30000 | 1124.86 | | | |
| | | | 500 | 94.9 | 72.75 | 81.33 | 60.56 | | 6.1 | 3.38 | | |
| Toluene | solvent | L | 0.1 | 1 | 2 | 6 | | 400000 | | | | |
| | | kg | 304 | 52.2 | 37.25 | 42.17 | | | 3.4 | | | |
| Oleic acid | solvent | kg | 0.001 | 0.005 | 0.025 | | | | 1000 | 14.4 | | |
| | | | 19800 | 12360 | 7900 | | | | 1.5 | 1450 | | |