

Editorial

Bayesian Statistics in Data Separation of Indicators for Neutralization Titration

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We have systematically investigated thermally-accessible structural changes of (chiral) Cu (II) complexes by means of XRD or spectroscopic methods. We also observed solid-state CD spectra and Non-Linear Optics (NLO) for some bimetallic assemblies involving chiral copper (II) complexes exhibiting thermally-accessible structural changes associated with Jahn-Teller distortion [1]. In addition, we have developed “separated” structural analysis of each component from powder XRD (PXRD) patterns for composite materials of metal oxides (LiMnO₂ or TiO₂) and (chiral) metal complexes of various ratios, which indicated IR spectral shifts by the ratios [2]. Recently, we could observe NLO of composite materials of LiMnO₂ and chiral Cu (II) complexes showing no NLO as sole components due to slight structural changes as composites confirmed by separated PXRD analysis for the first time [3]. This optical property may potentially apply for metal complex dyes and semiconductor metal oxides of dye-sensitized solar cells. Even in Chromatography and Separation Techniques, separated detection and treatment of data may be important factor among experimental works. We have also discussed statistical treatment of data using basic student’s chemical experiments as well as our own study on separated observation of multi-components hybrid materials by means of polarized spectroscopy. Herein, we show our (Atsuo Yamazaki, Yosuke Mori, Maiko Ito, Takashiro Akitsu) approach of Bayesian statistics and its application to neutralization titration (oxalic acid by Naoh), a typical experiments of analytical chemistry.

$$p(T,E)=p(T)p(E | T)=p(E)p(T|E)$$

$$p(T|E)\alpha p(T)p(E | T)$$

T (theory) and E (experimental), and when the two events that combined probability p (T, E) is posterior probability p the other one events around the probability p(T) [or p(E)] and (E | T) [or p (T | E)] of the expressed product. Given a theory T is T,

if the posterior probability p (T | E) probability after test results found the T prior probability p (T) in the odds before you can see test results and test results posterior probability p (E | T) of can be interpreted as proportional to the area. As an expression of the best estimate of the average, median, and often are fit often within the range of standard deviation from the average. Therefore, these three values are being best estimates. Depending on the indicators (PP and MO), color pH optimum to be confirmed statistically.

Oxalic acid 2-hydrate crystals (molecular: 126.07) of 1.6 g were measured. And the concentration was diluted in 0.05 mol/L. 0.1 mol/L Naoh atitration of oxalic acid (10.00 cm³) was carried out three times by using indicators phenolphthalein (PP; pH 8.3[colorless]-10.0[red]) (Table 1) or methyl orange (MO; pH 3.1[red]-4.4[yellow]) (Table2). In contrast to constant results of PP indicator, test of the year at the neutralization titration data of the Naoh solution (MO indicator) data showed considerable variation, for example as shown in (Figure 1).

year	2010	2009	2008	2007
no. of data	32	32	36	31
average	0.097986	0.095661	0.090581	0.105785
std	0.004488	0.003082	0.011625	0.011775
median	0.097623	0.096323	0.097483	0.098318
frequency	0.1	0.1	0.1	0.1

Table1: Naoh Titration of Oxalic Acid (indicator PP).

year	2010	2009	2008	2007
no. of data	30	23	29	26
average	0.121013	0.132278	0.150757	0.127802
std	0.02319	0.040205	0.041579	0.020248
median	0.117305	0.104174	0.168673	0.127575
frequency	0.12	0.11	0.13	0.19

Table2: Naoh Titration of Oxalic Acid (indicator MO).

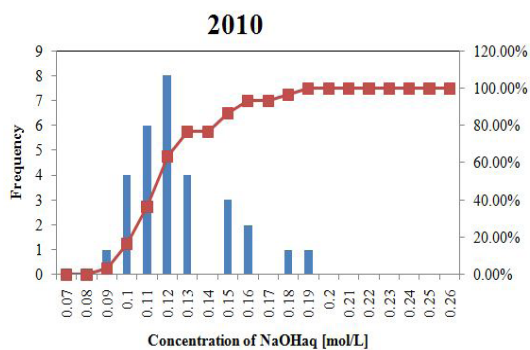


Figure1: Naoh Titration of Oxalic Acid (indicator MO) in 2010.

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