

河北大学 2005 年博士研究生入学考试试题 A

| 学科、专业 | 研究方向 | 考试科目及科目代码 | 考试时间 |
|-------|------|-----------|------|
| 分析化学 | | 专业英语 | |

一、汉译英 (10 分)

原子吸收光谱法；原子荧光光谱法；原子发射光谱；
紫外分光光度法；气相色谱法；高效液相色谱法；
毛细管电泳；环境分析；生物分析；药物分析；材料分析。

二、译成中文 (20 分)

What is chemometrics?

Chemometrics (化学计量学) is a new cross chemical branch which uses the theory and methods developed in statistics, mathematics and computer science and other related disciplines to optimize the procedure of chemical measurement, and to extract useful information from chemical measurements as much as possible.

Chemometrics starts from chemical measurement which differs from the computational chemistry which is purely based on quantum chemistry. Thus, chemometrics is essentially the theory and methodology of chemical measurement.

Chemometrics provides theory and methodology for the chemical measurements, and analyzes the various spectral data from chemical measurements in order to solve the difficult problems in

chemistry and chemical engineering. Its researches cover the whole process of chemical measuring, including: sampling theory and methods, experimental design and optimization for chemistry and chemical engineering processes, chemical signal processing, multivariate calibration and resolution, chemical pattern recognition, simulation of chemistry and chemical engineering processes, quantitative structure and activity relationship (QSAR), chemical database and artificial intelligence and chemical expert systems.

It is a new chemical branch of extensive contents, which provides lots of new idea, new way and new methods for solving the problems in many chemical branches, such as analytical chemistry, environmental chemistry, pharmaceutical chemistry, organic chemistry and chemical engineering and etc.

Chemometrics has been becoming a new branch in chemistry and analytical chemistry, it was the two factors that promoted this development.

Firstly, the appearance of lots of chemical instruments made the fact possible that chemists and analytical chemists could acquire chemical measurement data much easily than ever before. It was surprising for chemists to find at the first time that the most difficult problem was not the acquirement of chemical data, instead, how to

extract the useful information from the huge amount of data was a really difficult problem faced by chemists. Thus, building in the chemometric methods into the analytical instruments in order to construct the new generation of the intelligent instruments is an attractive research direction in analytical chemometrics.

On the other hand, the recent quick developments of computer and information sciences gave some new opportunities to chemometrics. The new methods for signal processing, especially the methods of wavelet analysis, brought along the new ideas of data-compressing, de-noising and removing-background from instruments for chemometrics.

From now on, chemometrics has its 30 years' history. From the relationship between analytical chemistry and chemometrics, one can see that chemometrics may provide the fundamental basis of analytical chemistry, since analytical chemistry is essentially a chemical measurement science. Furthermore, the development of chemometrics will also provide new theory and methods for analysts to construct the new generation of the intelligent analytical instruments. It may be the point of break-through in analytical chemistry in next century. In addition, with the development of internet techniques and micro-computer, the techniques related to

chemical databases will be also developed quickly. Using the technique of data mining, combining the numeric methods (the main part of chemometrics) and logic induction methods will result in lots of new opportunities for chemometricians to solve the difficult problems in chemistry. The future of chemometrics in analytical chemistry is promising.

However, the relationships of chemometrics with other chemical branches, such as environmental chemistry, pharmaceutical chemistry, agricultural chemistry, food chemistry and chemical engineering and etc., will also become more closed, the application of chemometrics in these chemical branches will be more extensive.