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NATIONAL STANDARD OF THE PEOPLE'S REPUBLIC OF CHINA

GB/T 29858-2013

Standard guidelines for molecular spectroscopy multivariate calibration quantitative analysis

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Foreword

This standard was drafted in accordance with GB/T 1.1-2009 given rules.

The standard reference method using redrafted American Society for Testing Materials Standards ASTME1655-05 "infrared quantitative analysis through multivariate

The "establishment, and the degree of consistency ASTME1655-05 not equivalent.

This standard was proposed by the Ministry of Science and Technology of the People's Republic of China.

This standard by National Instrument Analysis and Testing Standardization Technical Committee (SAC/TC481) centralized.

This standard is drafted by. Beijing University of Chemical Technology.

Participated in the drafting of this standard. Research Institute of Petroleum, China Institute of Food and Drug test, the PLA General Logistics Department

Oil Institute, Beijing Academy of Agriculture and Forestry, Academy of State Grain Administration, China Agricultural University, Zhejiang University, China Petroleum Chemical

Research Institute, Chinese Academy of Agricultural Sciences, China Institute of Metrology, Hongyun Honghe Tobacco (Group) Co., Ltd.

1 Scope

This standard specifies the use of molecular spectroscopy with multivariate calibration as a quantitative measurement sample (Group) Guidelines content concentration (content) or the nature of the sample.

This standard applies to the mid-infrared spectrum (about 4000cm-1 ~ 400cm-1) and near-infrared spectrum (about 780nm ~ 2500nm) range

Of molecular spectroscopy.

2 Normative references

The following documents for the application of this document is essential. For dated references, only the dated version suitable for use herein

Member. For undated references, the latest edition (including any amendments) applies to this document.

GB/T 3358.1 Statistics Vocabulary and symbols - Part 1. General statistical terms and terms used in probability

GB/T 6379.2 measurement methods and results of Accuracy (trueness and precision) - Part 2. Determine the standard measurement method to repeat

Of the basic methods of reproduction

GB/T 8322 molecular absorption spectrometry term

GB/T 27407 laboratory quality control use performance statistics for quality assurance and control chart technical evaluation and analysis of the measurement system

3 Terms and Definitions

GB/T 3358.1, GB/T 8322 defined by the following terms and definitions apply to this document.

3.1

Correction calibration

The content of a set of samples or the nature of their spectra associated modeling process.

3.2

Correction Model calibrationmodel

Between the expression of a set of samples of the spectral content of their nature or the mathematical expression of the relationship.

3.3

Calibration Sample calibrationsamples

Calibration samples used to build the model, its concentration or nature of the data is known.

3.4

Prediction estimate

Calculate sample concentration or nature of the spectral calibration model and sample process.

3.5

Predictive value estimatevalues

And sample spectra using a calibration model to calculate the resulting sample concentration or nature of the data.

3.6

Validation samples validationsamples

Samples used to verify the performance of the model, its concentration or nature of the data is known.