

Use of spectrometry in near-infrared region and chemometrics for organic material quality control

E.V. Vostroknutova, M.A. Yaburov, V.M. Golik, A.V. Saprygin

Joint Stock Company Ural Electrochemical Integrated Plant, Analytical Centre, Novouralsk, Russia

Incoming quality control of organic material used in manufacture of gas centrifuges for uranium isotope separation is carried out by standard laboratory methods, which are generally associated with high labor cost. At present, there is a possibility to develop express methods based on spectrometry in near-infrared region (NIR), which enables to determine certain parameters of material quality on the basis of spectral-response characteristics by means of parameter value and reference material spectrum comparison. In this case, experimental data are processed using chemometrics.

Near-infrared spectra of test objects, such as epoxy resins (ED-16, ED-20, DEG-1) and amine hardeners (triethanolamine, polyethylenepolyamine) were obtained by using Thermo Fischer Scientific Antaris II near-infrared spectrometer.

The quality parameters of selected material were determined: mass fraction of epoxy groups for epoxy resins, mass fraction of water for hardeners. Calibration models were developed by mathematical treatment of spectra produced by a training set of reference materials using projection of latent structure (PLS). Estimate of quality parameters for the developed model (root-mean-square errors of calibration (RMSEC) and prediction (RMSEP), correlation factor and basic component quantity proved their acceptability for practical use.

Thus, calibration models were developed for determination of epoxy groups' mass fraction in ED-16, ED-20, DEG-1 epoxy resins, and water mass fraction in triethanolamine and polyethylenepolyamine. It is the authors' opinion that the results obtained could be used to develop the express methods of incoming quality control for epoxy resins and amine hardeners.