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PROGRAM AND ABSTRACTS

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250 COULOMETRIC CO_2 TITRATION FOR THE DETERMINATION OF H_2O+ IN ROCKS. S. W. Tweedy, T. L. Pinkston, D. W. Koppenaal, Bureau of Economic Geology, The University of Texas at Austin, University Station, Box X, Austin, Texas 78713

A coulometric titration method has been adapted for the determination of H_2O+ (bound water) in rocks. The method involves pyrolysis of the dried sample and quantitative conversion of the liberated water to carbon dioxide by reaction with 1,1'-carbonyldiimidazole. The carbon dioxide is then absorbed in solution and titrated coulometrically. The method appears to be superior in precision and accuracy when compared with an established Karl Fischer titration procedure for H_2O+ determination and has the following advantages over other methods used in similar analyses: (1) high temperature pyrolysis insures total liberation of water, (2) standardization of the titrant is precluded, (3) large (~200 mg) samples can be accommodated, (4) condensation problems existent in the Penfield method are avoided. Accuracy of $\pm 4\%$ with precision of 3% is achieved at H_2O+ concentration levels of one weight percent. Description of the system used, along with comparative data for performance on standard reference rock samples will be presented.

251 SOME COMMON THERMOANALYTICAL CHARACTERISTICS OF DURABLE PRESS RESINS BASED ON CYCLIC UREA, Brenda J. Trask and B. A. Kottes Andrews, Southern Regional Research Center, 1100 Robert E. Lee Blvd., P. O. Box 19687, New Orleans, LA 70179

Thermal analyses, including Differential Scanning Calorimetry (DSC), Thermogravimetry (TG), and Differential Thermogravimetry (DTG), were performed on a series of derivatives of cyclic urea. Such compounds are used extensively for durable press finishing of cotton textiles. Two common features were discovered after more than 12 resins were analyzed under nitrogen. These features related to the presence of an oxygen-containing substituent on the ring carbons or the ring nitrogens. The former substitution was expressed as an exothermic response between 200°-300°C and the latter as an endotherm between 300°-400°C. Specific substituent modifications that changed these responses are described.

252 DIGITAL SIMULATION AND PEAK RESOLUTION IN DIFFERENTIAL SCANNING CALORIMETRY. Guang-Way Jang and Krishnan Rajeshwar, Department of Chemistry, The University of Texas at Arlington, Arlington, Texas 76019-0065

An equivalent-circuit model is presented for a commercial heat-flux differential scanning calorimetry (DSC) cell. This model is developed in a form which permits direct comparison with experimental data. The various thermal resistance factors in the cell are computed via this model. In particular, the influence of variables such as the heating rate and the thermal characteristics of sample and the purge gas atmosphere, is critically examined. A digital simulation method is finally used to test the influence of these variables on peak shape and resolution. The simulated and experimental thermograms demonstrate for the first time that better peak resolution and sensitivity can be achieved in DSC by using a high conductivity purge gas such as helium.

253 GoIGO (GOOD IN GARBAGE OUT)
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Access to powerful computing ability in the laboratory has contributed to an increasing use of sophisticated computational techniques by chemists. Generally, the results of a computation are considered to be correct. However, even when the data is correct, the results of a computation can be grossly incorrect. This is because of the fact that most computing machines have limitations which basically arise from the finite representation of the numbers, leading to round-off and truncation errors. On the first glance the magnitude of these errors appears to be small but their effect can be amplified because of accumulation, ill-conditioning of algorithm, cancellation, and instability. In this paper we will discuss such computational errors, as well as strategies to minimize them.