A review is given of the state of the art methods commonly used for characterization of the inorganic matter and mineral matter in coal. The application of various separation procedures, macroscopic observations, reflected and transmitted optical microscopy, scanning and transmission electron microscopy, x-ray diffraction, differential thermal and thermogravimetric analyses, Mossbauer spectroscopy, IR spectroscopy, x-ray fluorescence, and chemical analyses are briefly discussed. Limitations of individual analysis methods and the interrelationships of types of methods, as well as chemical analyses (e.g. at. absorption spectroscopy, inductively coupled plasma at. emission spectroscopy, inductively coupled plasma mass spectroscopy, neutron activation analysis, low-temperature ashing, and high-temperature ashing) as well as mineral analyses.

04/00009 Molecular model of Estonian kukersite kerogen evaluated by 13C MAS NMR spectra

Lille, Ü. *et al. Fuel*, 2003, 82, (7), 799–804.

The chemical structure of Estonian kukersite kerogen is evaluated using a simulation of ^{13}C MAS NMR spectrum. A reasonable fit to the experimental NMR spectrum is obtained by assuming a model of the geomacromolecule with empirical formula $C_{421}H_{638}O_{44}S_4NCl$ and a set of structural elements comprising mainly alkylated phenolic structures particularly alkyl-1,3-benzenediols and condensed alicyclic rings. From the presented model new views are coming up on the carbon skeleton of kerogen and constraints on the phenol formation pathways in the retorting process, i.e. up to 80% of methylene groups in kerogen are located in aliphatic chains and the complicated mixture of phenols in the retort oil seems to result mainly from the thermal conversion of alkyl-1,3-benzenediol units originally present in kerogen.

04/00010 Novel phenolic biomarker triterpenoids of fossil laticifers in Eocene brown coal from Geiseltal, Germany

Simoneit, B. R. T. *et al. Organic Geochemistry*, 2003, 34, (1), 121–129.

Novel phenolic triterpenoids were tentatively identified with known mono$^-$, tri$^-$ and tetraaromatic oleanane, ursane, and lupane hydrocarbons and natural product precursors (α-amyrone, α-amyrin) in the extract of Eocene fossil laticifers called 'Affenhaar' from the Geiseltal lignites, Germany. The novel phenolic terpenoids are mono- and triaromatic hydroxytriterpenoids (OH at position 1, 2 or 3) of the oleanane, ursane, and lupane classes: hydroxy-23,25-dinoroleana-1,3,5(10),12-tetraene, hydrox-24,25-dinorlupa-1,3,5(10)-triene, hydroxy-24,25-dinorlupa-1,3,5(10),19-(22)-tetraene, hydroxy-24,25,26,27-tetranorursa-1,3,5,7,9,11,13-heptaene, hydroxy-24,25,26,27-tetranoroleana-1,3,5,7,9,11,13-heptaene, hydroxy-24,25,26,27-tetranoroleana-1,3,5,7,9,11,13-heptaene, and hydroxy-24,25,26,27-tetranorlupa-1,3,5,7,9,11,13-heptaene. The structures of the novel compounds were proposed based on the interpretation of the gas chromatography-mass spectrometry data of the underivatized and silylated total extract.

04/00011 On the molecular-level interactions between pyridine and Pittsburgh No. 8 Coal

Wertz, D. L. and Smith, E. R. *Energy & Fuels*, 2003, 17, (2), 482–488.

The polycyclic aromatic (PCA) units of Pittsburgh No. 8 coal, on the average, lie in short-range structural domains of about three layers. The species $C_{14}H_9$ is consistent with the average PCA unit in the coal, with a radius of 2.9 Å. The average distance between the PCA layers in the short-range domains of the coal is 3.9 Å. The addition of pyridine molecules did not alter structuring within the PCA units to an extent, measured by wide-angle X-ray scattering experiments, and it appeared that the interlayer structuring within the short-range structural domains in the coal is also not altered to a measurable extent. Instead, a quasi-stable adduct was formed between the three-layer domains of the coal and the pyridine molecules.

04/00012 On the relationship between coal plasticity and thermogravimetric analysis

Barriocanal, C. *et al. Journal of Analytical and Applied Pyrolysis*, 2003, 67, (1), 23–40.

Two series of bituminous coals of different rank, geographic origin and plastic properties were subjected to thermal treatment up to 1000°C in a nitrogen atmosphere at two heating rates (3 and 10°C min^{-1}), using two thermobalances of different design. Maximum fluidity of coal determined by the standardized Gieseler plastometry test was found to correlate well with the amount of volatile matter evolved up to 500°C and with that evolved in the plastic or fluid stage (between 375 and 500°C and 400 and 500°C). In addition, a good linear relationship was found between the temperature of maximum evolution of volatile matter derived from the DTG curve and the characteristic temperatures indicating the beginning, end and maximum value of the fluid stage of coal. Although the experimental values of the parameters derived from thermogravimetric analysis are affected by the heating rate applied and the design of the apparatus, the correlations based on the results are little affected by the above variables.

04/00013 Origin, alteration and geochemical correlation of Late Permian airfall tuffs in coal measures, Sydney Basin, Australia

Grevenitz, P. *et al. International Journal of Coal Geology*, 2003, 55, (1), 27–46.

The Late Permian Illawarra Coal Measures of the southern Sydney Basin contain tuffs derived from altered pyroclastic airfall material. These units represent ideal stratigraphic time planes because, as the products of airfall volcanic ashes, they are distributed over wide areas in short periods of geological time. Geochemical correlation of the tuffs of the Illawarra Coal Measures with similar units in the stratigraphically equivalent Newcastle Coal Measures offers a unique opportunity to understand the temporal and spatial relations during deposition of coal-bearing units in the Sydney Basin. Thirty-five core samples comprising 12 samples from each of the Burragorang and Farmborough Claystone Members and 11 samples from the Huntley Claystone Member were analysed for major and trace elements by X-ray fluorescence and instrumental neutron activation, and the results were subjected to stepwise discriminant analysis. The elements that served as the best discriminators between tuffs were, in order of atomic number, Ti, V, Sn, Hf and Th. Samples for basin-wide correlation were taken from thick interseam tuffs of the Newcastle Coal Measures and treated as unknowns in the discriminant model. The Burragorang Claystone Member shows a strong geochemical correlation with the Awaba Tuff, and the Farmborough Claystone Member correlates with the Warners Bay Tuff. The Huntley Claystone Member, however, has proved difficult to correlate with the Nobby's Tuff, the proposed stratigraphic equivalent in the Newcastle Coal Measures. Petrographic data for tuffs of the Illawarra Coal Measures indicate that they were deposited by airfall mechanisms and consist mainly of kaolinite and mixed-layer illite/smectite clays, quartz and plagioclase crystal fragments, lithic fragments and secondary calcite and siderite. Zr/TiO_2 and Nb/Y ratios, tectonic discrimination diagrams and chondrite normalized REE patterns (La/Yb = 3.3–11.9) are identical to those for tuffs of the Newcastle Coal Measures and are interpreted as being derived from magma that was calc-alkaline, rhyodacitic to rhyolitic in composition and derived from a continental volcanic-arc tectonic setting. The source of the tuffs is interpreted to be an active volcanic arc to the east of the present coastline (Currarong Orogen), but a lack of evidence from below the continental shelf makes it difficult to make concrete conclusions on its likely extent and composition.

04/00014 Palaeoecology of selected South African export coals from the Vryheid Formation, with emphasis on the role of heterosporous lycopods and wildfire derived inertinite

Glasspool, I. *Fuel*, 2003, 82, (8), 959–970.

The study of six bulk coal samples from the Early Permian Vryheid Formation of the Karoo Basin, South Africa has revealed the importance of wildfire in this coal-forming environment. Inertinite is a major constituent of these coals and was predominantly produced by wildfire. The accumulation of the peat in this setting was both autochthonous and hypautochthonous/allochthonous, conditions varying between the occurrence of standing water and desiccation. Woody gymnosperms and also lycopods were important components of the coal swamp vegetation, of which the diversity and abundance of the lycopods may be tentatively assessed by the distribution of megaspores in the coals. Consistent with lycopod reproductive strategy, these megaspores are more abundant and diverse where the vitrinite content is greater.

04/00015 Palynology, petrography and geochemistry of the Sewickley coal bed (Monongahela Group, Late Pennsylvanian), Northern Appalachian Basin, USA

Eble, C. F. *et al. International Journal of Coal Geology*, 2003, 55, (2–4), 187–204.

Forty-two bench samples of the Sewickley coal bed were collected from seven localities in the northern Appalachian Basin and analysed palynologically, petrographically, and geo-chemically. The Sewickley coal bed occurs in the middle of the Pittsburgh Formation (Monongahela Group) and is of Late Pennsylvanian age. Palynologically, it is dominated by spores of tree ferns. Tree fern spore taxa in the Sewickley include *Punctatisporites minutus, Punctatosporites minutus, Laevigatosporites minimus, Spinosporites exiguus, Apiculatasporites saetiger*, and *Thymospora* spp. In fact, *Punctatisporites minutus* was so abundant that it had to be removed from the standard counts and recorded separately (average 73.2%). Even when *Punctatisporites minutus* is removed from the counts, tree fern spores still dominate a majority of the assemblages, averaging 64.4%. Among the tree fern spores identified in the Sewickley coal, *Thymospora* exhibits temporal and spatial abundance variation. *Thymospora* usually increases in abundance from the base to the top of the bed. *Thymospora* is also more abundant in columns that are thick (> 100 cm) and low in ash yield (< 12.0%, dry basis). Calamite spores (e.g. *Calamospora* spp., *Laevigatosporites minor*, and *L. vulgaris*) are the next most abundant plant group represented in the Sewickley coal, averaging 20%. Contributions from