X-ray photoelectron spectroscopy study of coals with different rank

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Nowadays the increasing amounts of NO_x and N_2O converted from coal nitrogen, led to the investigation of the combustion processes and coal properties that contribute to maximise the nitrogen production and influence the variation in the emissions. Therefore it is important to determine the molecular structure of nitrogen in coal.

X-ray Photoelectron Spectroscopy (XPS) analyses were performed in vitrinite-rich coals of increasing rank to determine the nitrogen functionalities (pyridine at 398.8 eV, pyrrol around 400.2 eV, quaternary nitrogen around 401-402 eV and nitrogen-oxide around 403 eV). Nitrogen in the studied coals was found to be predominantly pyrrol. However, the coals storage procedure determined the degree of nitrogen oxidation and the other nitrogen functionalities (Fig. 1 and 2). Due to this fact, the ratios of pyridinic to pyrrolic nitrogen and pyridinic to quaternary nitrogen vary with increasing rank and also with the oxidation of the coals. The analyses of a set of non-oxidised coals with rank lower than 1.41% vitrinite reflectance permitted the observation of the decreasing of pyrrolic and quaternary nitrogen and an increase of the pyridine with increasing coal rank.

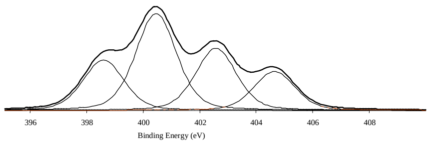

Figure 1: Representative XPS spectra of nitrogen (1s) obained on oxidised coal.

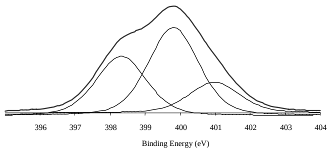

Figure 2: Representative XPS spectra of nitrogen (1s) obained on non-oxidised coal.

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Synthetic isotope mixtures for the calibration of ion current ratio measurements in carbon and oxygen in carbon dioxide

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Different sets of synthetic isotope mixtures for the calibration of carbon and oxygen ion current ratio measurements obtained by mass spectrometry have been prepared by mixing carbon dioxide isotopically enriched in ^{18}O ($^{nat}C^{18}O_2$) and natural carbon dioxide ($^{nat}C^{nat}O_2$), and by mixing different natural CO_2 gases with slightly different carbon and oxygen isotopic compositions [1].

These mixtures act as Primary Standards to the SI-scale for carbon and oxygen isotope amount ratio measurements in CO_2. They will help to anchor existing carbon Isotope Reference Samples (i.e. NBS19, IAEA-CO-9) and therefore offer the basis for comparability of carbon (and oxygen) isotope measurement results, without any assumptive correction for the oxygen isotopes.

Via such 'absolute' isotope amount ratio measurements of carbon and oxygen on CO_2 produced from the Primary Standard to the VPDB-scale NBS19, calibrated by means of synthetic isotope mixtures, 'absolute' isotope amount carbon and oxygen ratios corresponding with the zero point of the VPDB conventional scale were calculated to be $R_{13/12}$= (11 137 6 ± 16)$\cdot 10^{-7}$ and $R_{18/16}$ = (208 824 ± 48)$\cdot 10^{-8}$ respectively.

References

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