Determination of position-specific carbon isotope ratios of propane from natural gas

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On-line gas chromatography–pyrolysis coupled to gas chromatography–isotope ratio mass spectrometry was used here for the position-specific isotope analysis (PSIA) of propane. First, based on the conversion rate of propane and its products, 800–840 °C was considered optimal for propane pyrolysis. The major pyrolytic fragments of propane included CH_4, C_2H_4, C_3H_6, and C_2H_6. Subsequent isotope labeling experiments showed that CH_4 and C_2H_6 were derived entirely from the terminal carbons, whereas C_2H_4 and C_3H_6 were derived from both terminal and central positions of propane. Therefore, the ^{13}C enrichment factor associated with the major reactions during the pyrolysis process and position-specific $\delta^{13}C$ values of propane can be estimated from the amount and $\delta^{13}C$ values of the pyrolytic fragments using isotope mass balance. The obtained enrichment factors depended on the pyrolysis temperature, which can be used to calculate position-specific $\delta^{13}C$ values for propane measured with this system. The results suggest that a relatively accurate site-preference value for propane can be obtained by this method. Therefore, the combination of compound-specific isotope analysis and PSIA of propane will be a powerful tool to discriminate the different origins of gases.