On the combustion of terpenes biofuels

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Limonene and α-pinene were oxidized in a jet-stirred reactor at atmospheric pressure, in the cool flame regime, under fuel-lean conditions. Samples of the reacting mixtures were collected, dissolved in acetonitrile, and analyzed by high-resolution mass spectrometry. Direct flow injection or chromatographic separation by ultra-high-performance liquid chromatography and +/– heated electrospray ionization and +/– atmospheric pressure chemical ionization were used to characterize the oxidation products. H/D exchange using D_2O were performed for probing the presence of hydroxy and hydroperoxyl groups in the products. Reaction with 2,4-dinitrophenylhydrazine was used to assess the presence of carbonyl functions in the products. A large set of oxidation products, including highly oxygenated organic products with five and more oxygen atoms, was observed. Aromatic and/or polyunsaturated products were detected. Van Krevelen plots, computed oxidation state of carbon and degree of unsaturation in products were used to rationalize the results.