ABSTRACT

Khat pyrolysis, Penolic compounds, Khat smoke, Geometry optimization, Molecular geometries Herein, we report phenolic reaction products from the thermolysis of khat that is important in understanding the smoking of khat under conditions that are representative of cigarette smoking. Phenolic compounds occur naturally and are precursors for grave environmental health problems such as cancer and cell injury. This study investigates the phenolic compounds generated from the thermal degradation of Catha edulis, computes the global energies and entropies of selected phenolic compounds and their derivatives, and performs their geometry optimization using Gaussian '09 computational code. In addition, we report on the elemental speciation of thermal char from khat pyrolysis. The thermal degradation of khat was conducted in an inert nitrogen environment at 1 atmosphere at a contact time of 2s using a quartz tubular reactor. The pyrolysis effluent was characterized using a Gas-chromatograph coupled to a mass spectrometer. The GC-MS results indicated that khat pyrolysis yielded a significant number of phenolic compounds such as phenol, p-cresol, catechol, hydroquinone and substituted methoxy phenols. The maximum release of these compounds occured between 400 and 550 °C. Hydroquinone gave the highest yield of 21.32% in the entire pyrolysis temperature while p-cresol gave a yield of 2.54% in the same temperature range. Phenolic compounds exhibited endothermicity with increase in temperature. Because of the potent nature of khat cigarette, it is necessary for government authorities, policy makers and medical practioners to mount campaigns against khat smoking.