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Non-isothermal decomposition kinetics of pyridinium nitrate under nitrogen atmosphere

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Graphical Abstract

$$\mathbf{I} - [\mathrm{H-Pyr}]^{+}[\mathrm{NO_3}]^{-} \leftrightarrow \mathrm{HNO_3} + \mathrm{Pyr}$$

$$\mathbf{II} - [\mathrm{H-Pyr}]^{+}[\mathrm{NO_3}]^{-} + \mathrm{HNO_3} \leftrightarrow 2\mathrm{HNO_3} + \mathrm{Pyr}$$

$$\mathbf{III} - 2\mathrm{HNO_3} \leftrightarrow 2\mathrm{NO_2} + \mathrm{H_2O} + {}^{1}/_{2}\,\mathrm{O_2}$$

$$\mathbf{IV} - \mathrm{Pyr} \xleftrightarrow{\mathrm{HNO_3/NO_2}} \mathrm{HCN} + \mathrm{HCOH} + \mathrm{CO} + \mathrm{CO_2}$$

Highlights

- TG/DTG analyses showed endothermic thermal decomposition in the temperature region between 390K and 540K.
- Kinetic parameters were obtained from the Friedman and Kissinger-Akahira-Sunose methods.
- The activation energy increased with conversion degree, ranging from 76 to 112 kJ/mol.
- The variable activation energy dependence indicated a multi-step decomposition process.
- A decomposition mechanism for $[\mathrm{H–Pyr}]^{+}[\mathrm{NO_3}]^{-}$ under inert atmosphere was proposed.

Abstract

The thermal stability and decomposition kinetics of the ionic liquid pyridinium nitrate was investigated by non-isothermal thermogravimetric analysis in an inert atmosphere (nitrogen). For the kinetic experiments, the thermal behavior of the sample was studied in the temperature interval from 360 up to 600K at different heating rates (5, 10, 15 and 20 K/min).

The kinetic parameters of decomposition including activation energy and pre-exponential factor under nitrogen atmosphere were evaluated by menace of two model-free methods – Friedman and Kissinger-Akahira-Sunose. Depending on the used calculation model, the obtained activation energy and pre-exponential factor values with respect to the degree of sample conversion during the kinetic experiment for method ranged in the intervals of 76.36–112.56