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Quantum-Chemical investigation and isoconversional approach for non-isothermal decomposition of Gemcitabine

Refaat Mohamed Mahfouz, Ereen A Rezkallah, Abeer Ibrahim and **AbdeRahman A Dahy**
Assiut University, Egypt

Geometry optimization of gemcitabine molecule was carried out by DFT with B3LYP/6-311++G (d, p) level in gas phase. Reactivity parameters were calculated and discussed. Non-isothermal decomposition of gemcitabine anticancer drug was carried out in static air. The kinetic data were analyzed by isoconversional method. The decomposition proceeds in two decomposition steps occurred in the temperature range of (260-380°C) and (360-690°C) attributed to the degradation of furan and pyridine rings, respectively. The results of the application of linear (Tang) and non-linear (Vyazovkin) isoconversional methods on the present kinetic data globally showed dependence of the activation energy on the extent of conversion. Analysis of the non-isothermal data by Master-plots indicated that the decomposition process is controlled by phase boundary (R2) model. Using the model free isoconversional method, the isothermal conversion as a function of time was predicated isothermal data were computed. Analysis of the predicated isothermal data by reduced time plots (RTPs) method gave the same reaction model as derived from non-isothermal data. The kinetic and thermodynamics parameters calculated by both non-isothermal and predicated isothermal data were evaluated and discussed.

rmhfouz@science.au.edu.eg

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