

## 碳源甲基苯热裂解机理的密度泛函动力学研究

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**摘要** 在热力学研究的基础上,用UB3LYP/3-21G<sup>\*</sup>方法对甲苯热裂解机理进行了动力学研究。计算得到了甲苯的5种热裂解路径的活化能。用过渡态理论,计算得到了这些路径在298~1223K温度范围内的速率常数。动力学计算结果表明:甲苯在热解温度低于963K时的主反应路径为甲苯热裂解生成苄基自由基的反应,其速控步的活化能 $\Delta E^{\ddagger}=402.27\text{kJ/mol}$ ;当温度高于963K达1223K左右时,主反应路径转为苯环上脱甲基生成苯基和甲基自由基的路径,该路径的活化能 $\Delta E^{\ddagger}=456.91\text{kJ/mol}$ 。以上研究结果与实验结果相一致。

**关键词** [碳](#) [复合材料](#) [甲苯](#) [裂解](#) [过渡态理论](#) [反应动力学](#)

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## DFT kinetic study of the pyrolysis mechanism of toluene used for carbon matrix

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**Abstract** Based on the thermodynamic data, the pyrolysis mechanism of the carbon matrix toluene used for carbon material was studied by dynamic computation using the UB3LYP/3-21G<sup>\*</sup> method in the Gaussian 98 program package. The transition states were found by the QST2 method and were proved by IRC calculations. The activation energies of the five reaction paths were calculated, and the rate constants from 298—1223 K were obtained by the transition states theory. The dynamic calculation results show, when the pyrolysis temperature of toluene is lower than 963 K, the main reaction path is the breaking of the C—H bonds of the methyl on the benzene ring. The reaction is completed via the process: reactant→intermediate→product, with reactant→intermediate as rate-control step and activation energy  $\Delta E^{\ddagger}=402.27\text{kJ/mol}$ . When temperature is higher than 963 K, but below 1223 K, the main reaction paths is the one that produces benzene radical and methyl radical. The corresponding activation energy is  $\Delta E^{\ddagger}=456.91\text{kJ/mol}$ . This mechanism is in accord with the experimental result.

**Key words** [CARBON](#) [COMPOSITE WOOD](#) [METHYLBENZENE](#) [PYROLYSIS](#) [TRANSITION STATE THEORY](#) [REACTION KINETICS](#)

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