**Mechanistic Kinetic Analysis of Fast Pyrolysis of Vanillin to Primary Phenols**

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**Vanillin\_kinetics\_DFT** folder has three subfolders: Intermediates, Products, and Transition States (TS). In the Intermediates folder, there are 11 free radicals; the products folder contains 12 files, which correspond to all products in Figures 1 and 2 in the manuscript. The notations correspond to that used in the manuscript. The transition state geometries of the propagation reactions are given in the transition state folder under Reaction #.

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| --- | --- | --- |
| **Intermediates** | **Products** | **Transition States (TS)** |
| **IM1**  **IM2**  **IM3**  **IM4**  **IM5**  **IM6**  **IM7**  **Methyl**  **Methoxyl**  **Ethyl**  **Hradical** | **P1**  **P2**  **P3**  **P4**  **P5**  **P6**  **Methane**  **Ethane**  **Formaldehyde**  **CO**  **Aldehyde**  **R** | **TS1**  **TS2**  **TS3**  **TS4**  **TS5**  **TS6**  **TS7**  **TS8**  **TS9**  **TS10**  **TS11**  **TS12**  **TS13**  **TS14**  **TS15**  **TS16**  **TS17**  **TS18** |

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