Electronic Supplementary Materials

A theoretical investigation on the thermal decomposition of pyridine and the effect of H_2O on the formation of NO_x precursors

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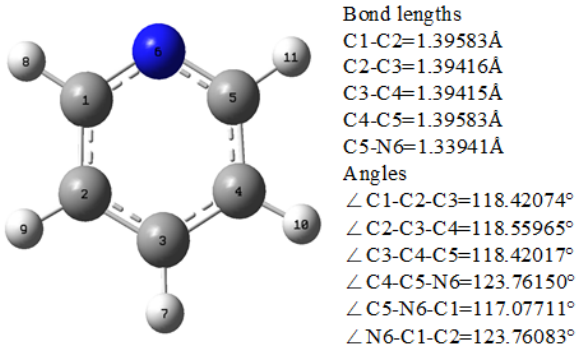

Figure S1. The optimized geometry and key parameters of pyridine (the gray, blue and white spheres represent carbon, nitrogen and hydrogen atoms, respectively)

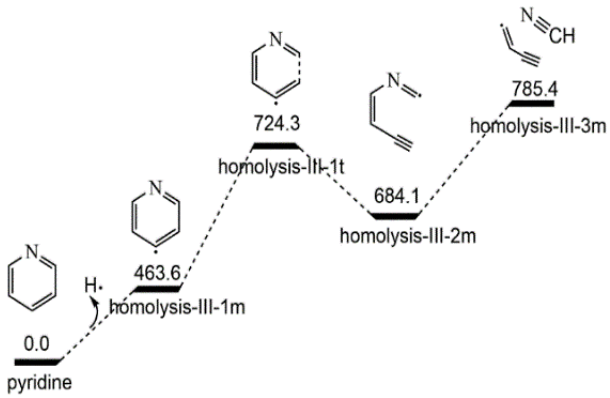

Figure S2. The energy profile of the optimal pathway proposed by Yoshihiko et al.[26]calculated at B3LYP/6-31G(d,p) level

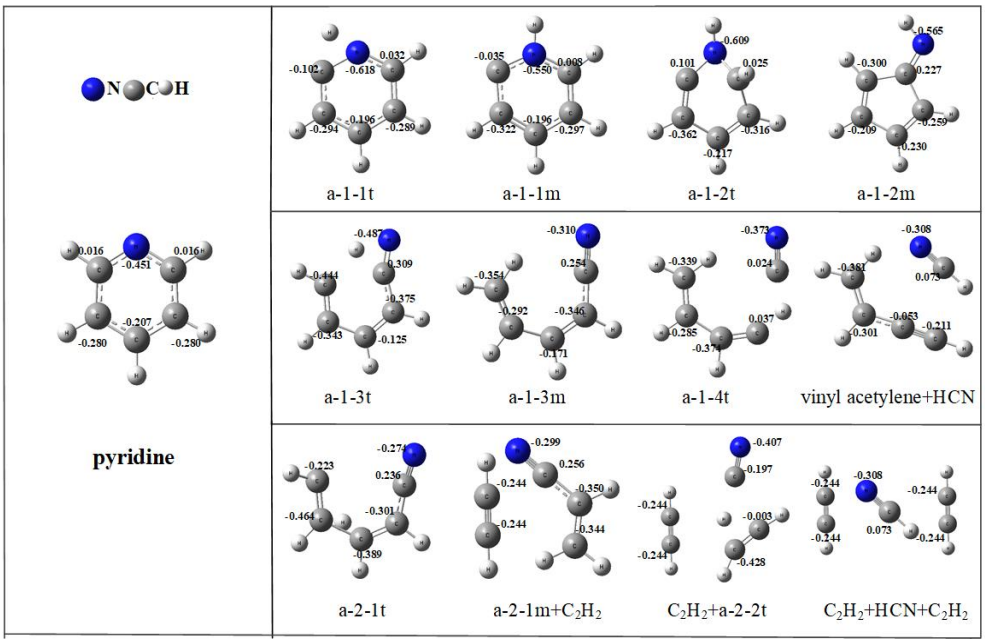

Figure S3. Optimized geometries and NPA charge distributions of intermediates and transition states in pyridine pyrolysis following Reaction-a (numerical values are NPA changes in a.u.).

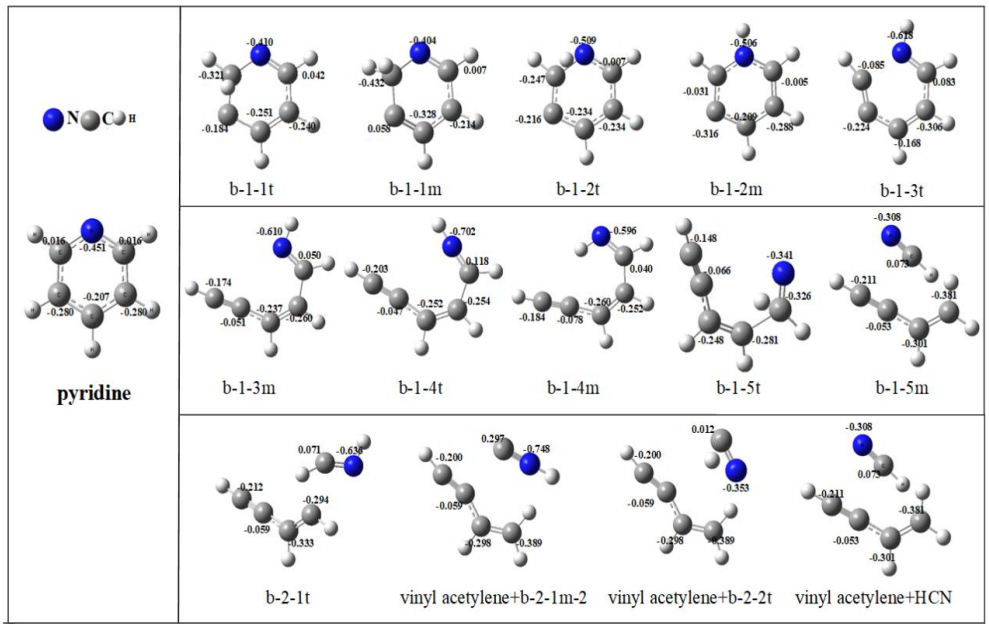

Figure S4. Optimized geometries and NPA charge distributions of intermediates and transition states in pyridine pyrolysis following Reaction-b (numerical values are NPA changes in a.u.)

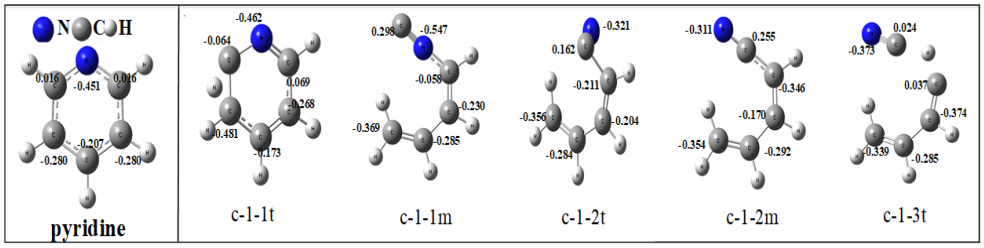

Figure S5. Optimized geometries and NPA charge distributions of intermediates and transition states in pyridine pyrolysis following Reaction-c (numerical values are NPA changes in a.u.)

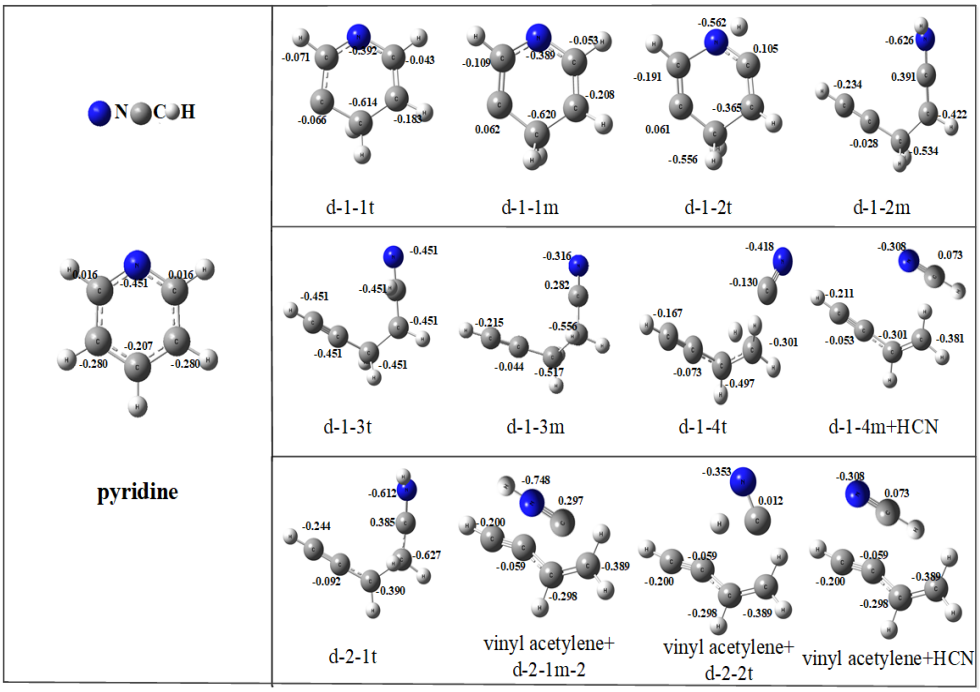

Figure S6. Optimized geometries and NPA charge distributions of intermediates and transition states in pyridine pyrolysis following Reaction-d (numerical values are NPA changes in a.u.)

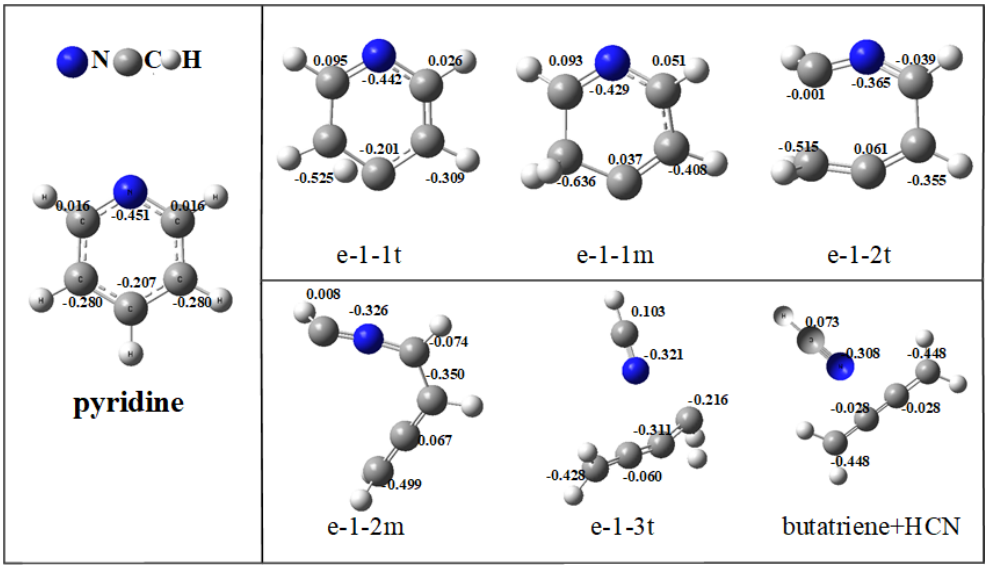

Figure S7. Optimized geometries and NPA charge distributions of intermediates and transition states in pyridine pyrolysis following Reaction-e (numerical values are NPA changes in a.u.)