Supporting Information:

Functionalization of the C(100)-2×1 Surface by 1,3-Dipolar Cycloadditions: A Theoretical Prediction

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Optimized geometries for the reactants, transition states and products of the CH_3N_3 and CH_2N_2 reactions with the C_9H_{12} surface model are presented in Figure 2 and Figure 3 (see in the following page), respectively.

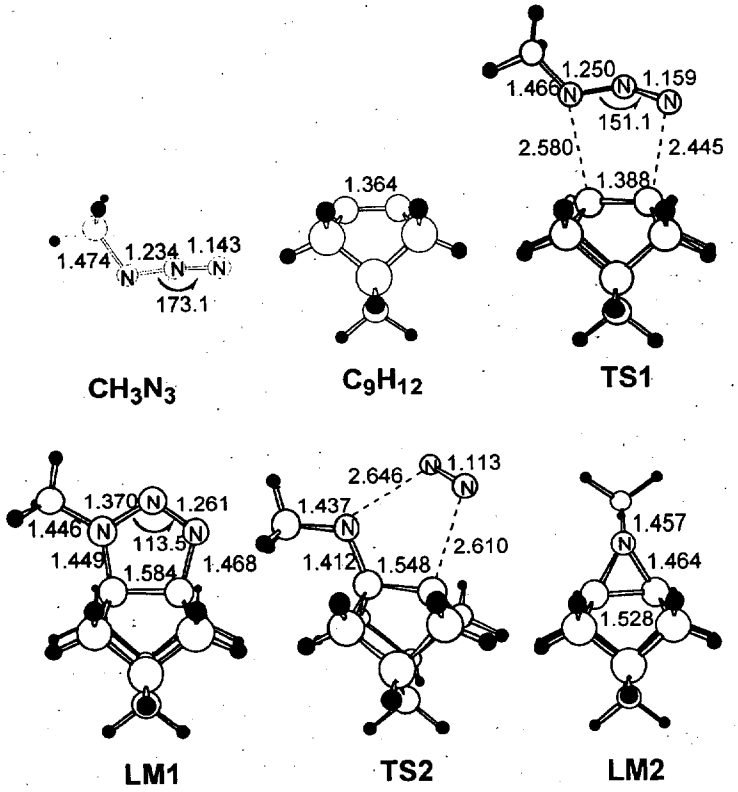

Figure 2 $CH_3N_3 + C_9H_{12}$

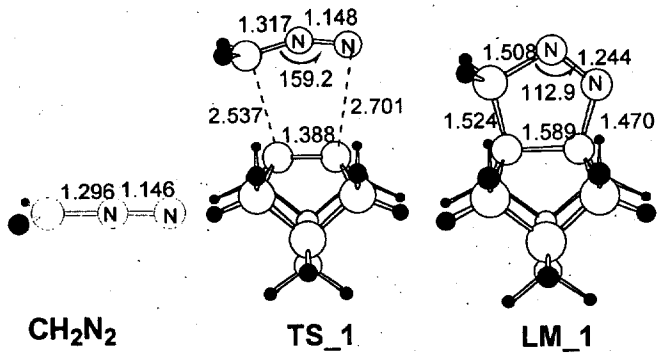

Figure 3 $CH_2N_2 + C_9H_{12}$