Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

On the Formation of Pyridine in the Interstellar Medium

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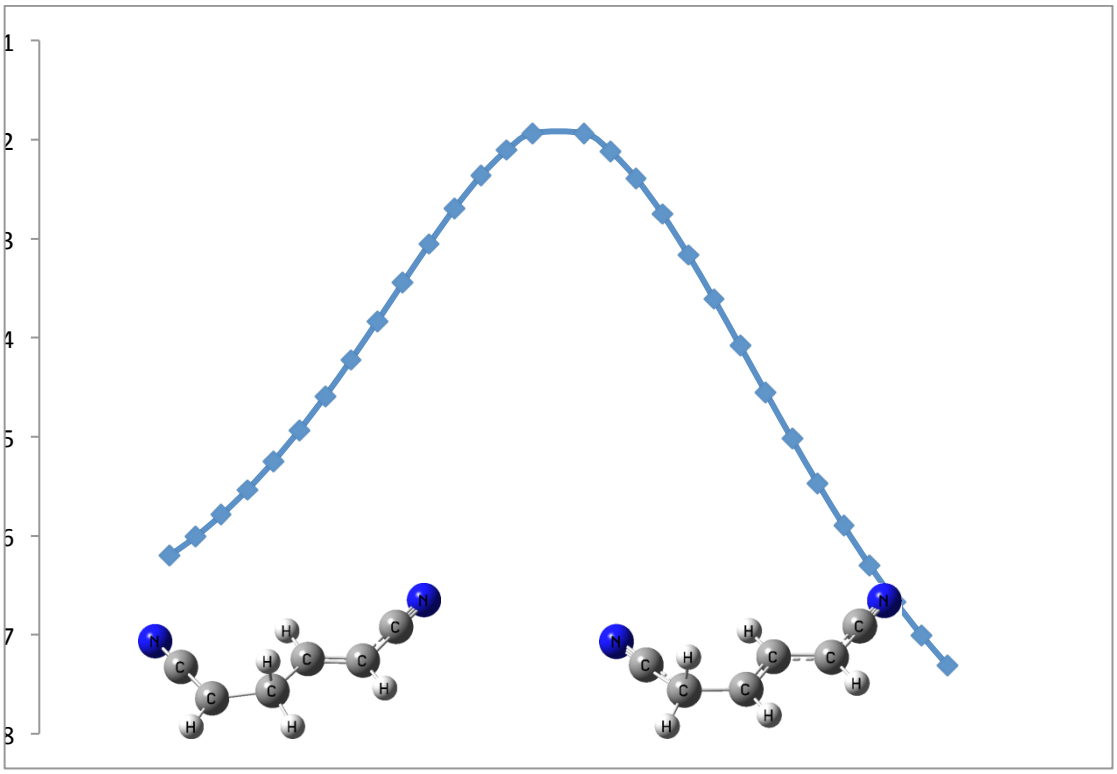
Figure S1. IRC calculations for bottom path of Figure 4.

tsi6i7



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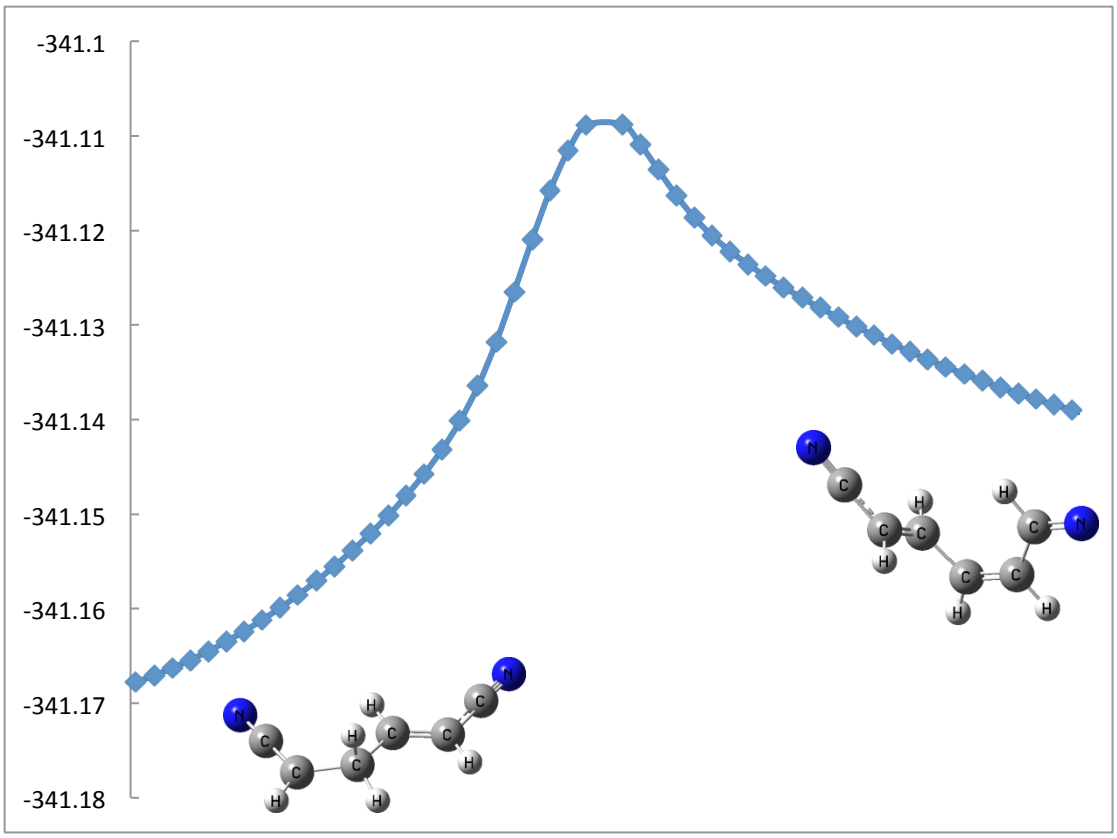
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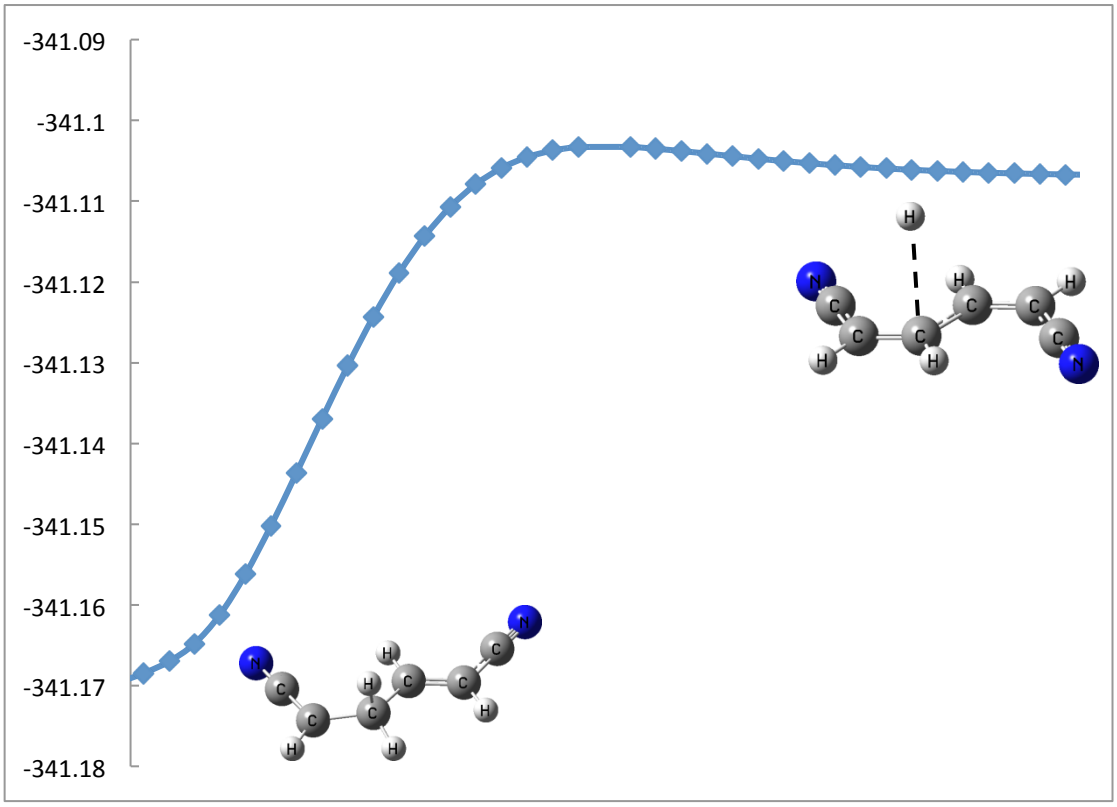
tsi6p3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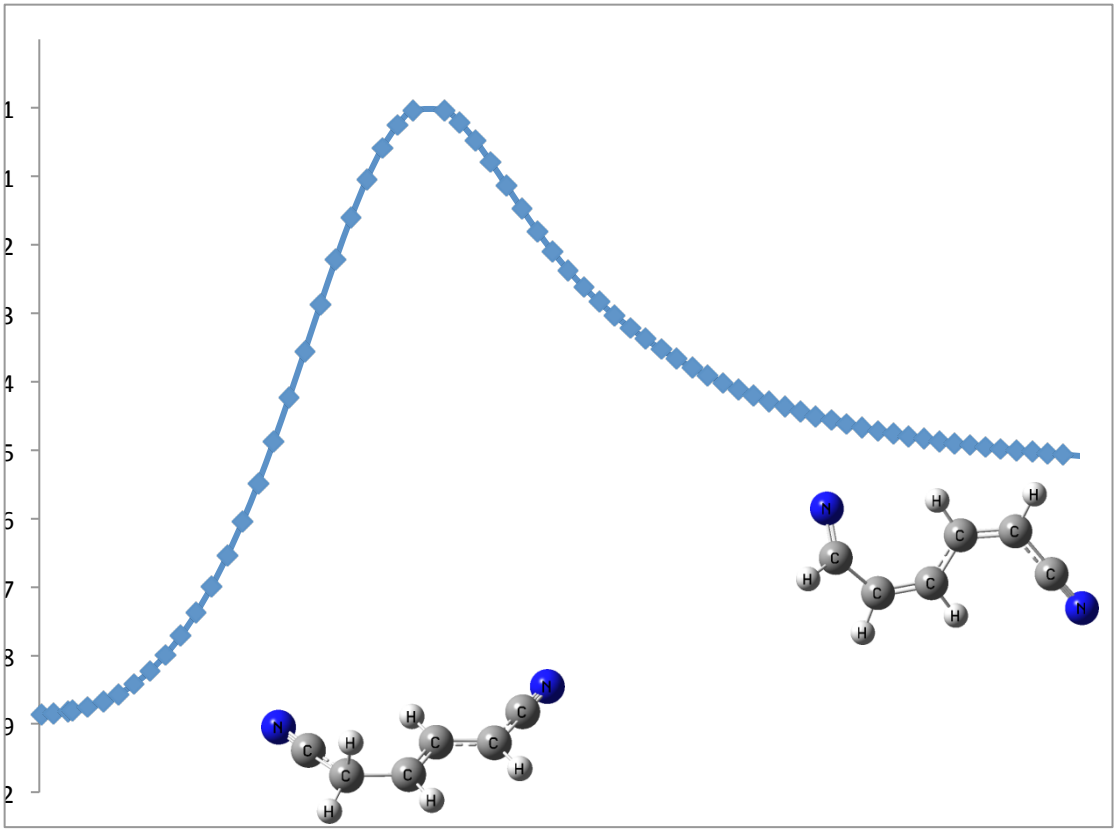

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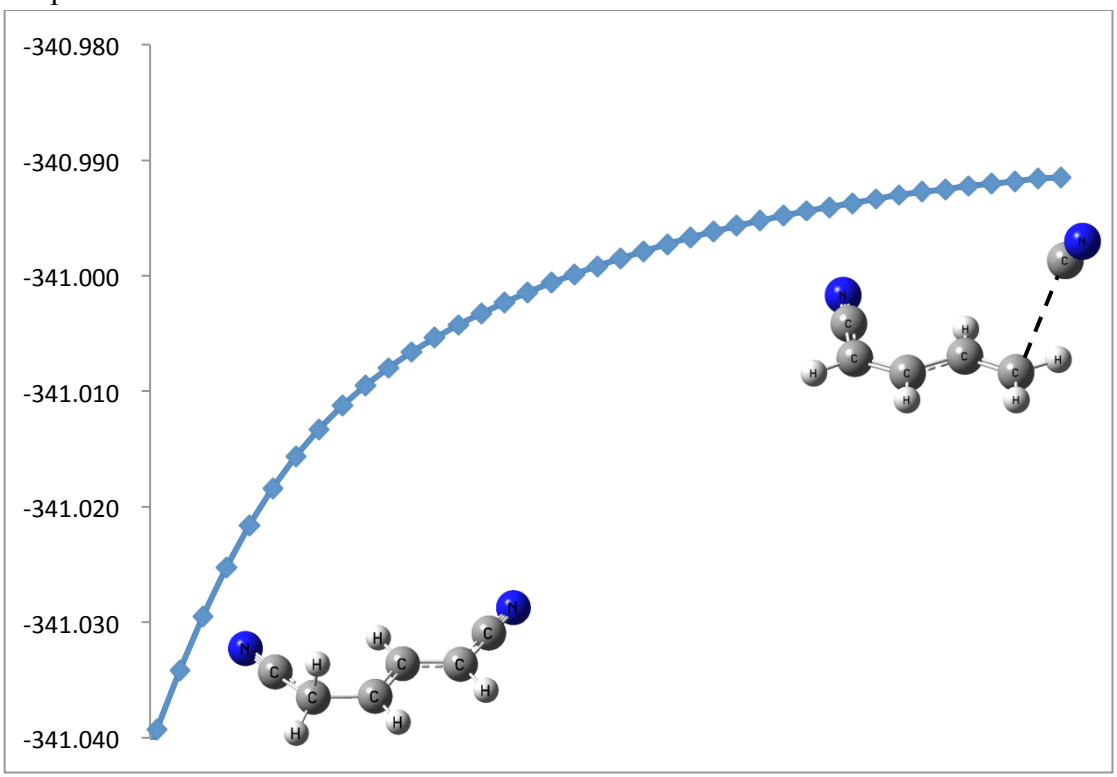

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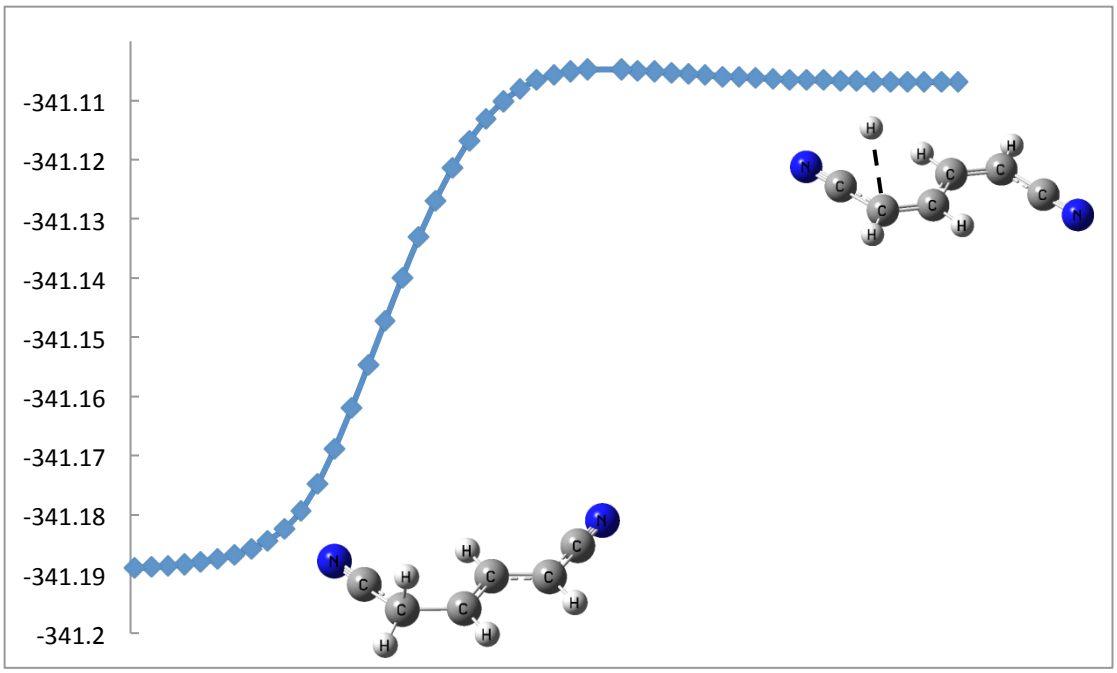

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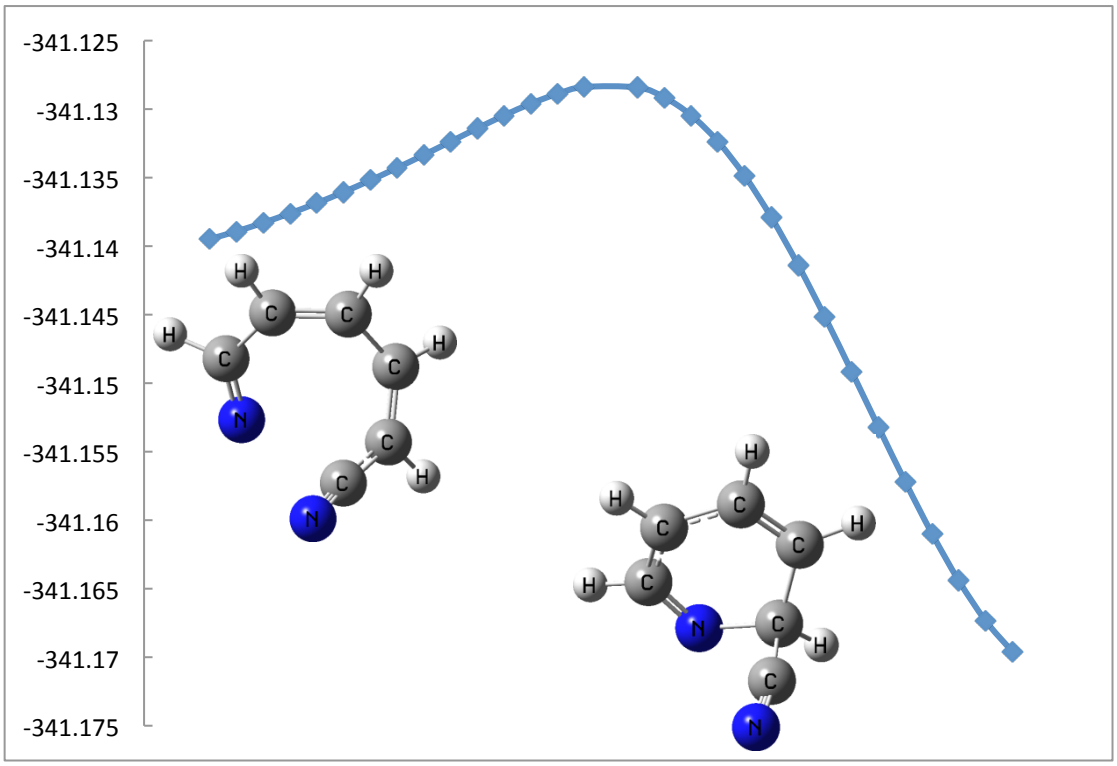

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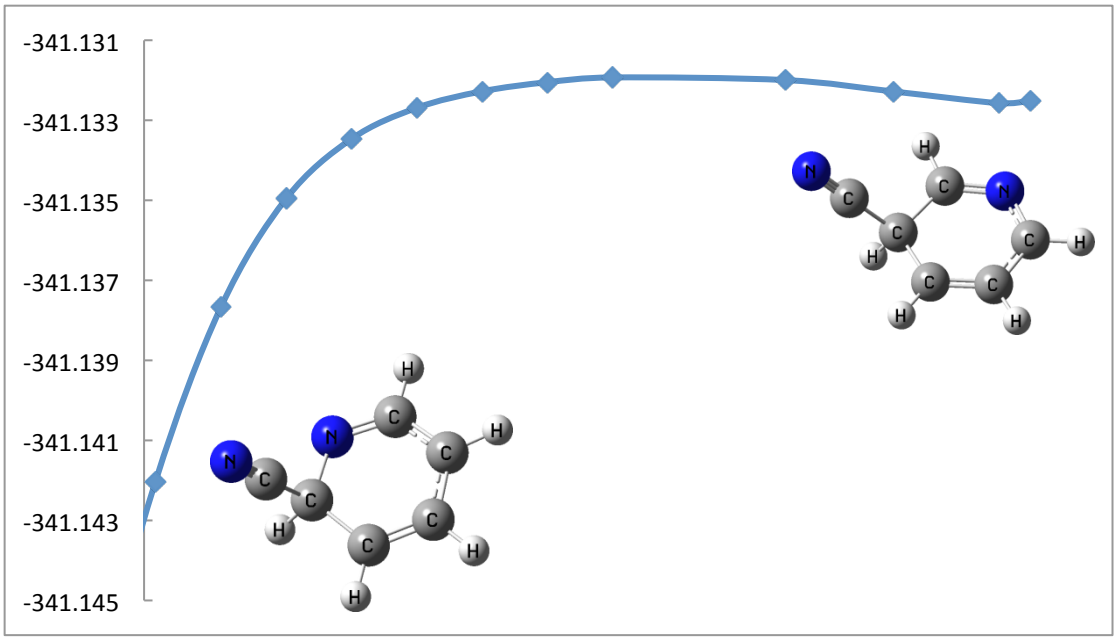

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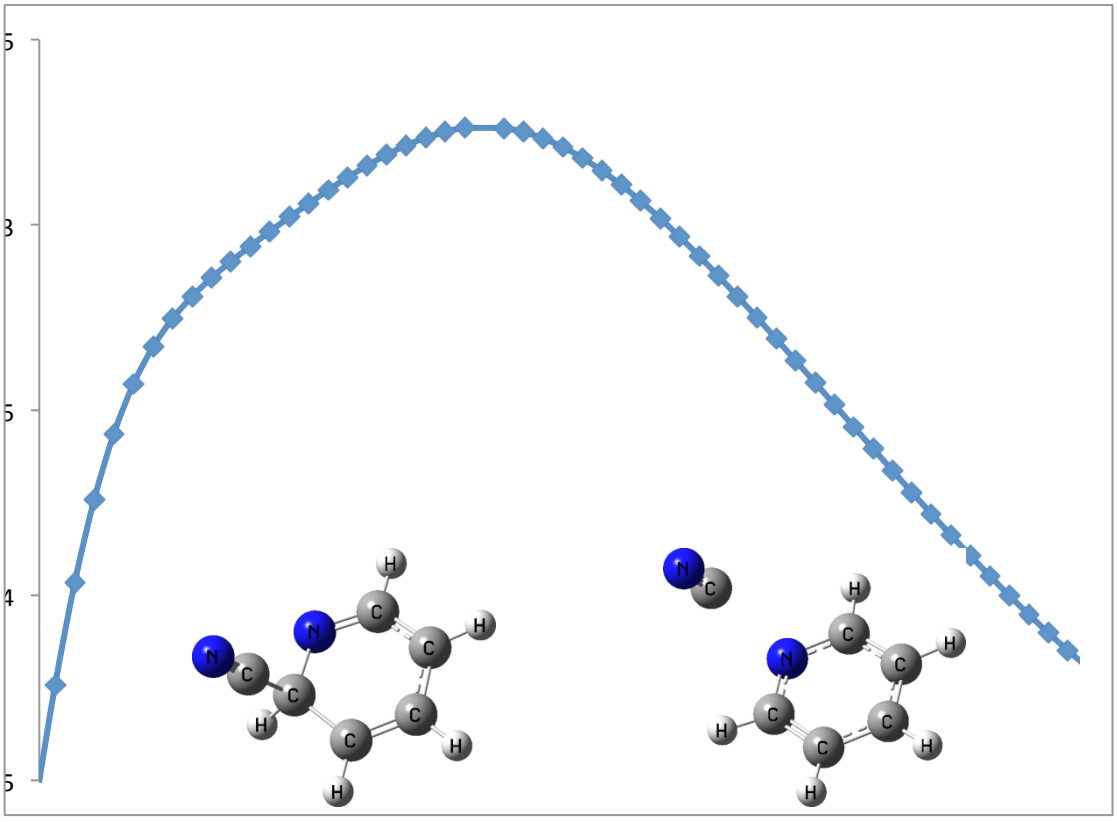

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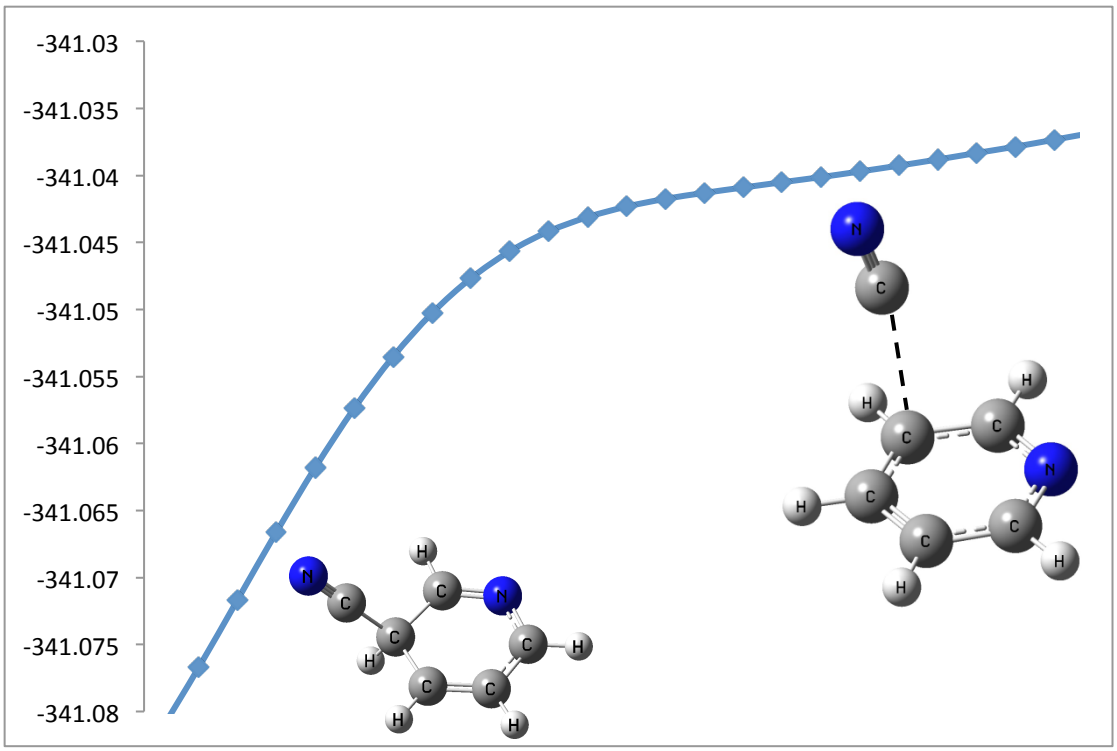

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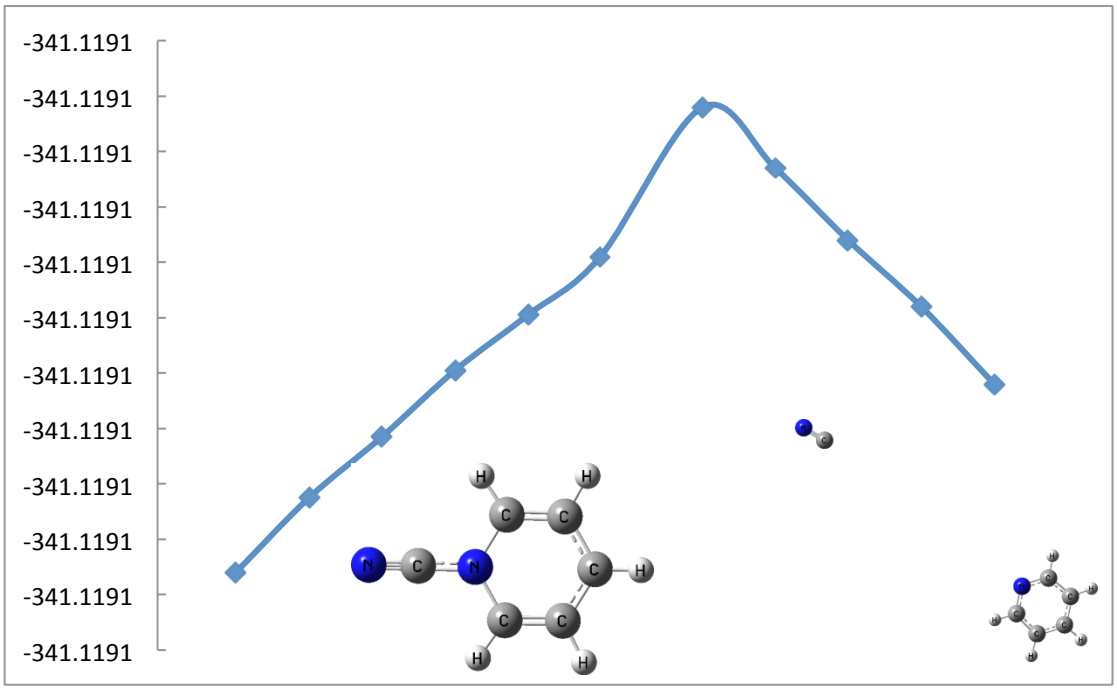

Table S1. The product branching ratios of path1 and path2, which are obtained by employing RRKM rate constants computed with B3LYP/ cc-pVTZ zero-point energy corrected CCSD(T)/cc-pVTZ energies, and B3LYP/cc-pVTZ harmonic frequencies at collision energies of 0, 0.1, 0.6, 8.4, 12.5, 41.8, 83.7, 92.0, 104.6, and 125.5 kJ mol^{-1}. The collision energies correspond to average kinetic energy of an ideal gas molecule at 0, 10, 50, 671, 1000, 1678, 3356, 6712, 7383, 8390, and 10068 K, respectively.

Branching Ratio (path 1)

kJ /mol Product	**0.0 (0 K**	**0.1 10 K**	**0.6 50 K**	**8.4 671 K**	**12.5 1000 K**	**41.8 3356 K**	**83.7 6712 K**	**92.0 7383 K**	**104.6 8390 K**	**125.5 10068 K)**
P1	1	1	1	1	1	0.911	0.996	0.995	0.994	0.993
P2	0	0	0	0	0	0.001	0.004	0.005	0.006	0.007

Branching Ratio (path 2)

kJ/mol Product	**0.0 (0 K**	**0.1 10 K**	**0.6 50 K**	**8.4 671 K**	**12.5 1000 K**	**41.8 3356 K**	**83.7 6712 K**	**92.0 7383 K**	**104.6 8390 K**	**125.5 10068 K)**
p1	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.001	0.002
p2	0.277	0.275	0.268	0.190	0.163	0.094	0.068	0.065	0.061	0.056
P3	0.723	0.725	0.732	0.810	0.827	0.906	0.932	0.935	0.938	0.942