Low-T Mechanisms of Ammonia Synthesis on Co_3Mo_3N

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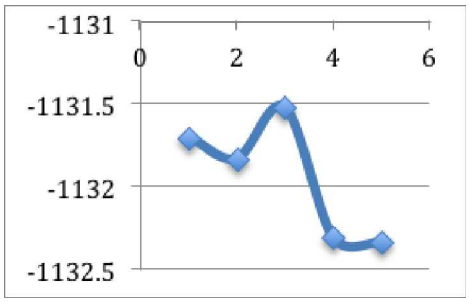
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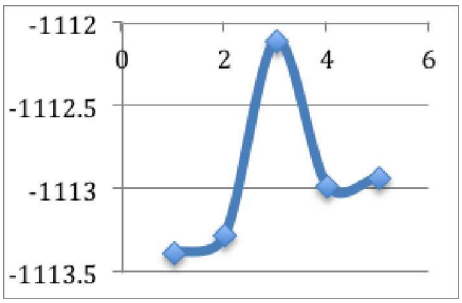
[3] *School of Chemistry, Cardiff University, Cardiff CF10 1AD, UK*

Figure S1 Detailed barrier potential energy surface from NEB calculations

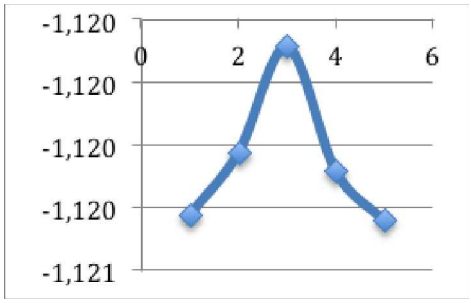
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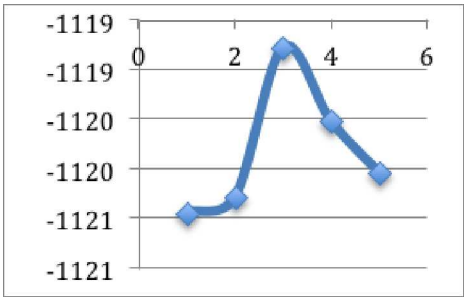
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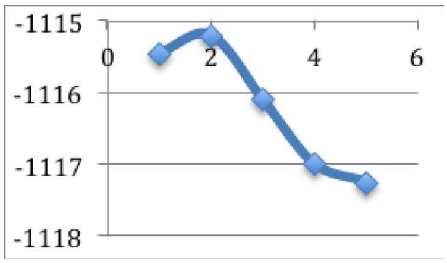
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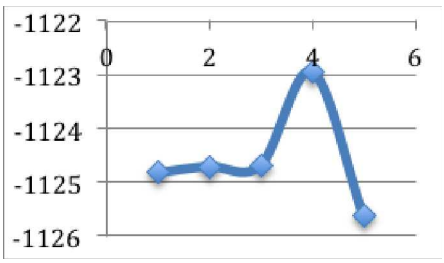
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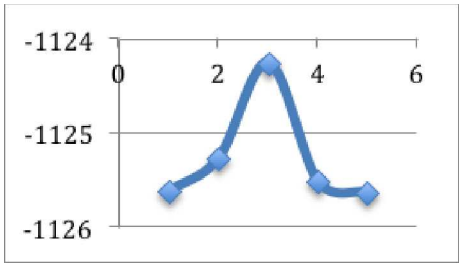
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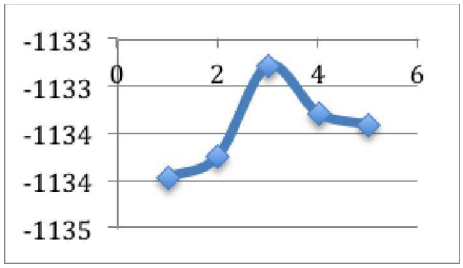
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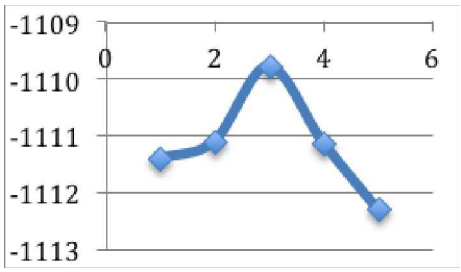
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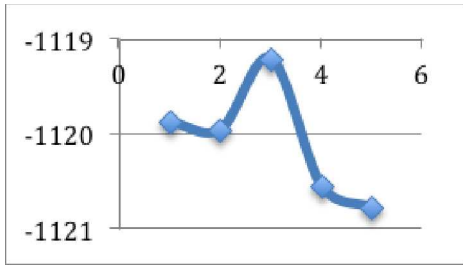
LH_FG



LH_HI



LH_JK



LH_KL

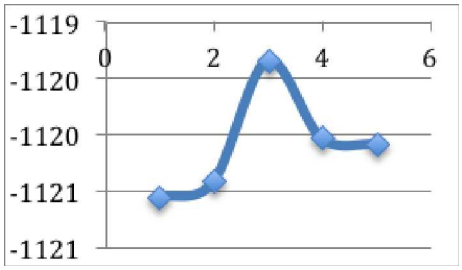


Figure S2 The coordinates of the structure of the various intermediates and transition states

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