Electronic Supplementary Material (ESI) for Chemical Communications

Surface-assisted cis-trans isomerization of an alkene molecule on Cu(110)

Supporting Information

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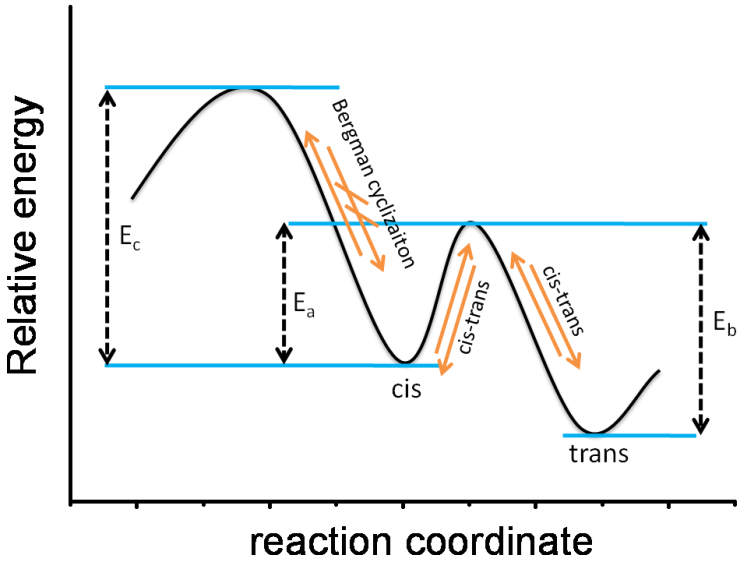

Scheme S1. Schematic reaction paths involving the cis-trans isomerization and Bergman cyclization of the DNHD molecule. The sequence of the three energy barriers should be: $E_a<E_b<E_c$.

After deposition of the cis-form molecule on the substrate held at low temperature (~170K), there is not enough thermal energy for cis to trans isomerization or Bergman cyclization. After slightly heating the sample to ~255K, the thermal energy is high enough to overcome the barrier (i.e. E_a) for cis to trans isomerization, while still not enough to trigger the Bergman cyclization. And then, at higher temperatures below ~400K, the thermal energy is high enough to overcome the barriers for both the cis to trans (i.e. E_a) and trans to cis (i.e. E_b) isomerization, and cis and trans forms should fluctuate at surface. Finally, after a further annealing to ~400K, the thermal energy is high enough to overcome the barrier for Bergman cyclization, and the cis forms are thermally triggered to Bergman cyclization. It should be noted that the isomerization behavior is reversible and the Bergman cyclization is irreversible. So the scenario is that at high enough temperature (~400K) once the trans-form molecules have the chance to change back to the cis-form, the Bergman cyclization is immediately triggered from the cis-form molecules, and finally all the trans forms are changed to cis forms followed by Bergman cyclization.