

TRANSFORMING MOLECULES: FROM POLYCYCLIC AROMATIC HYDROCARBONS TO TRIAZAFULLERENES.

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Polycyclic Aromatic hydrocarbons are very interesting molecules because their potential use as precursors in a controlled synthesis of fullerenes alternative to those based on graphite vaporization [1]. The main idea of this work is that this type of molecules could undergo a surface catalyzed reaction and consequently, losing hydrogen and forming fullerenes. Indeed, *ab initio* calculations [2] have predicted that aromatic hydrocarbons could experience hydrogen removal when annealed at ~800K (cyclodehydrogenations). In this work, we focus our interest on the adsorption and the interaction of C₅₇H₃₃N₃ [3] on Au(111) surface, from coverages ranging from 0.1 ML to 5 ML, and the possibility of closed fullerenes formation on this surface (Fig. 1).

We studied in ultra high vacuum conditions the adsorption and interaction between the ‘flat’ molecule C₅₇H₃₃N₃ (Fig. 1) and the Au(111) surface from coverages ranging from ~0.1 ML to ~5 ML by means of a combination of different experimental techniques (LEED, AUGER, XPS, UPS, NEXAFS and STM). For room temperature deposition we observed that the molecules diffuse on the surface making difficult the observation by STM (Fig. 2a). We observed with NEXAFS, for coverages of ~1 ML, that the molecules are adsorbed parallel to the surface, while for coverages of ~5 ML the molecules are randomly distributed. After annealing the sample at temperatures near ~800K, the molecules react with the surface, resulting anchored to it (Fig. 2b). This process starts from the step edges, and it leads to the formation of a complete molecular layer. In this situation the binding energy of C1s core-level XPS peak indicates a charge transfer process from the molecule to the substrate. This core level analysis shows that the carbon atoms surrounding the nitrogen ones are involved in this charge transfer mechanism. For higher annealing temperatures (Fig. 2c) we observed with STM the occasional formation of triazafullerenes C₅₇H₂N₃, with similar electronic molecular features to a deposited C₆₀ molecule.

References:

- [1] Y. Tobe, N. Nakagawa, K. Naemura, T. Wakabayashi, T. Shida and Y. Achiba, *J. Am. Chem. Soc.*, **120** (1998) 4544.
- [2] C. Koper, Tesis Doctoral, Non-Alternant Polycyclic Aromatic Hydrocarbons versus Closed Carbon Surfaces, Verbonden aan het Debye Instituut de Universiteit Utrecht, The Netherlands (2003).
- [3] B. Gómez-Lor, A.M. Echavarren, *Organic Letters*, **6** (2004) 2993.

Figures:

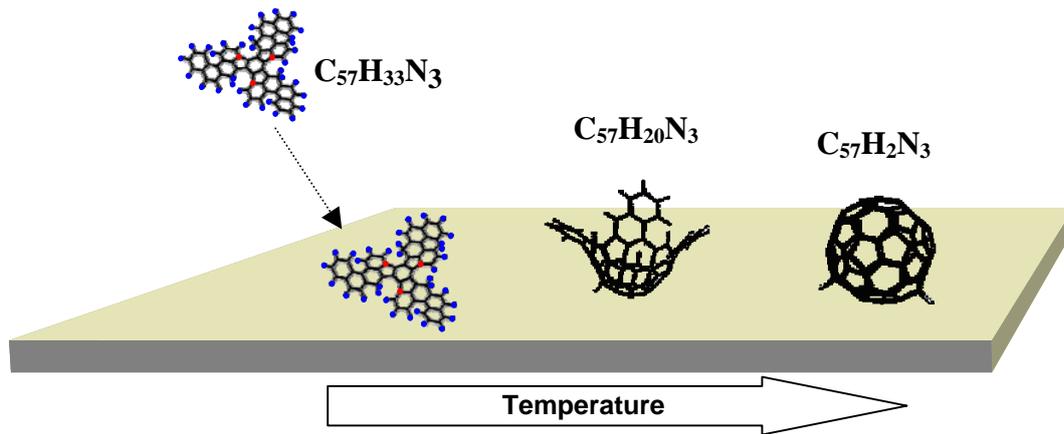


Fig. 1. Cyclodehydrogenation of $C_{57}H_{33}N_3$. For temperatures greater than 800K it is possible to lose hydrogen rendering possible the formation of closed fullerenes.

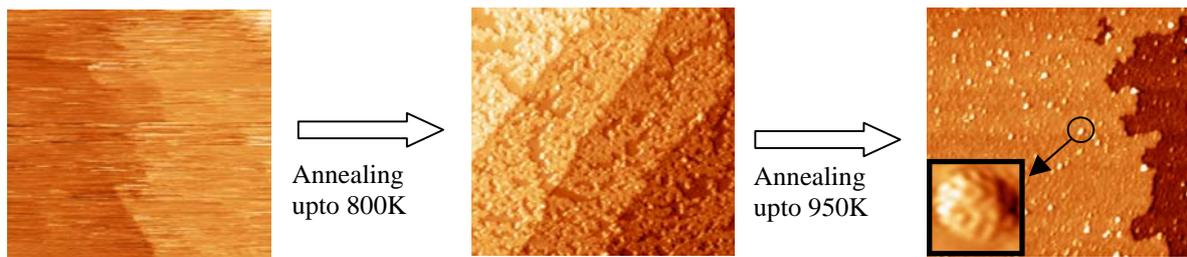


Fig. 2. Evolution with temperature of the morphology of 1 ML thick film of $C_{57}H_{33}N_3$ deposited at room temperature on Au(111).