

CHARACTERIZATION OF C₅₇H₃₃N₃ ON Au(111) AND TRIAZAFULLERENES FORMATION BY CYCLODEHYDROGENATION.

*G. Otero*¹, *C. Sánchez-Sánchez*¹, *C. Rogero*¹, *M.F. Lopez*¹, *E. Román*¹, *F. Borgatti*²,
*M. Pedio*², *R. Felicci*², *S. Nannarone*², *B. Gómez-Lor*¹, *A.M. Echavarren*³, *J. Méndez*¹,
*J.A. Martín-Gago*¹

¹ *Instituto de Ciencia de Materiales de Madrid – CSIC, 28049-Madrid*

² *TASC – INFN, Area Science Park, Basovizza, Trieste*

³ *Instituto Catalán de Investigaciones Químicas – Tarragona*

oterog@icmm.csic.es

The understanding of the physical and chemical properties of new materials, especially the combination between organic molecules and metallic surfaces, is of a great relevance both from the point of view of new applications and basic science. Among the great quantity of organic molecules that can be studied, hydrogenated fullerenes, C_nH_x are very interesting because of its capacity to store hydrogen and their possible applications in optoelectronics [1]. In our case we have studied the C₅₇H₃₃N₃ [2] molecule deposited on a metal surface. It presents a structure similar to a flat cloverleaf of three leaves (Fig.1) in which the nitrogen atoms, lodged in central positions, favour the anchoring to the surface. An interesting property of this type of molecules is their capacity to lose hydrogen upon temperature, rendering possible the formation of closed fullerenes of the type C₆₀ (see Fig. 1). *Ab initio* calculations [1] predict that these molecules could loss the hydrogen when annealed at ~800K (cyclodehydrogenations).

In our work we studied in ultra high vacuum conditions with different spectroscopy and microscopy techniques (LEED, AUGER, XPS, UPS, NEXAFS and STM) the adsorption and the interaction between C₅₇H₃₃N₃ and Au(111) from coverages ranging from 0.1 ML to 5 ML. For room temperature deposition we observed that the molecules diffuse on the surface doing 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, being anchored to the surface (Fig. 2b). This process starts from the step edges, and it forms a complete molecular layer. In this situation the binding energy of both N1s and C1s core-level XPS peaks indicates a charge transfer process to the substrate. This core level analysis shows that the carbon atoms near the nitrogen are responsible for this charge transfer process. For annealing at higher temperatures (Fig. 2c) we observed with STM the occasional formation of triazafullerenes C₅₇H₂N₃ with similar structure to a deposited C₆₀ molecule.

References:

- [1] C. Koper, Tesis Doctoral, Non-Alternant Polycyclic Aromatic Hydrocarbons versus Closed Carbon Surfaces, Verbonden aan het Debye Instituut de Universiteit Utrecht, The Netherlands (2003).
- [2] B. Gómez-Lor, A.M. Echavarren, Organic Letters, **6** (2004) 2993.

Figures:

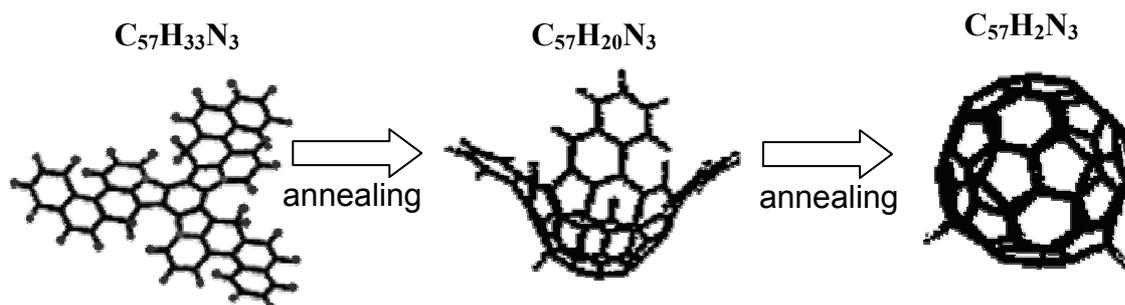


Fig. 1. Cyclodehydrogenation of $C_{57}H_{33}N_3$. For temperatures greater than 800K it is possible to lose hydrogen rendering possible the formation of closed fullerenes.

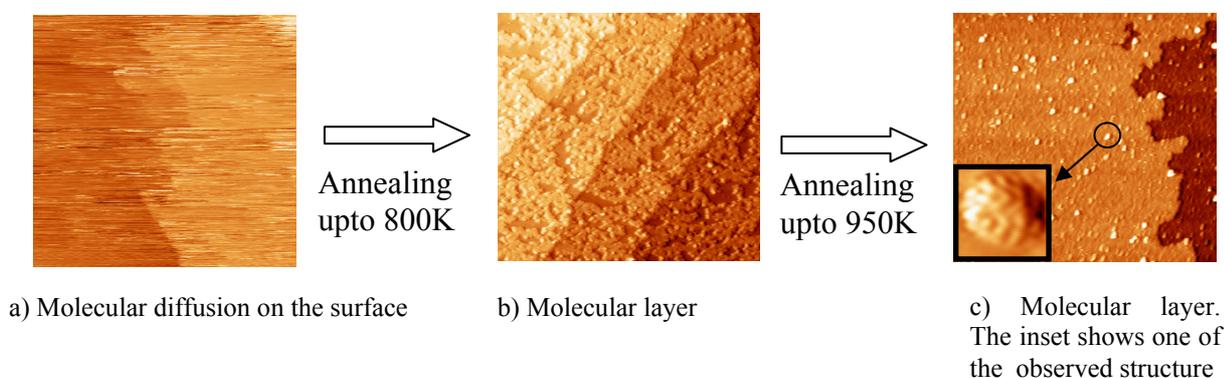


Fig. 2. Evolution with temperature of the morphology of 1 ML thick film of $C_{57}H_{33}N_3$ deposited at room temperature on Au(111).