ESRF	**Experiment title:** X Ray diffraction study of self-organized tert-butyl-calix[4]arenes film deposited on Au(110)(1x2)	**Experiment number**: 32-03-674
Beamline: BM32	**Date of experiment**: from: 24 June 2008 to: 1st July 2008	**Date of report**: 14/10/2008
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Report:

We have deposited the tert-butyl-calix[4]arenes on Au(110). The molecule is 12 Å long and the initial substrate surface is a (1x2) missing rows reconstruction. The deposition temperature has been optimized following the disappearance of the 0 ½ fractional rods of the substrate and the optimum temperature has been found at in the range of ~ 200-250ºC. STM images obtained on a monolayer allow seeing a regular distribution of the molecules. They form long chains along the [1-10] direction (fig. 1). Each molecule appears as 4 circular lobes which can be assigned to the phenol groups, which mean that in this configuration, the tert-butyl groups cannot be imaged by STM. The detailed analysis of the STM images is quite difficult and a full interpretation can only be achieved thanks to the X-ray diffraction results. GIXRD data allow us to identify correctly the unit cell. The STM visible chains are formed by two different molecular conformers. In the unit cell, the molecules are rectangular and their dimensions are similar to those in gas phase, while in the centre of the unit cell, they adopt a more elongated geometry. The LEED pattern is also very complicated and due to the distortions of the low working energy, its analysis requires additional information provided by the X ray diffraction results. The experiment carried out at BM32 permits to resolve the structure: the tert-butyl-calix[4]arenes are arranged into a rectangular cell with 4 molecules per cell. Similarly to the « simple » calixarenes case, the substrate suffers a drastic reconstruction change and its surface became a (1x3) missing rows upon molecular absorption. The coincidence cell is a (21x14). In the [100] direction, the x14 corresponds in fact to a 4* (1x3) +1* (1x2), which is confirmed by the STM images (fig. 2) which show large bands assigned to the 1x3 together with some narrower bands corresponding to the (1x2), but without real space regularity.

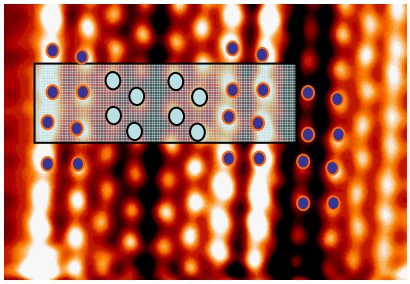

Fig 1: *High resolution STM image showing the molecular internal structure (10 nm x12 nm).*

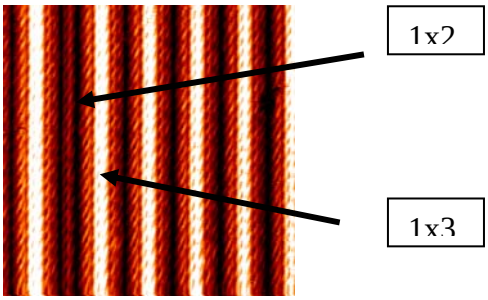

Fig. 2: *STM Image showing the (30 nm x30 nm) bands width alternating.*

In fig. 3, two scans aquired respectively in the H and K directions show the periodicity of the molecular overlayer. Due to the large surface periodicity and surface disordering, only some of the fractional rods are visible. The strongest reflexions arise from the averaged cells.

In conclusion, the gold substrate suffers a partial reconstruction and adapts itself to the molecules by adopting a (1x3) missing rows reconstruction probably due to a charge transfer. The coincidence cell is found to be a (21x14) corresponding in the K direction to the alternating large/narrow bands seen by ST;. In this work, the complementarity of the experimental techniques (STM, LEED and GIXRD) is of fundamental importance to resolve the structure.

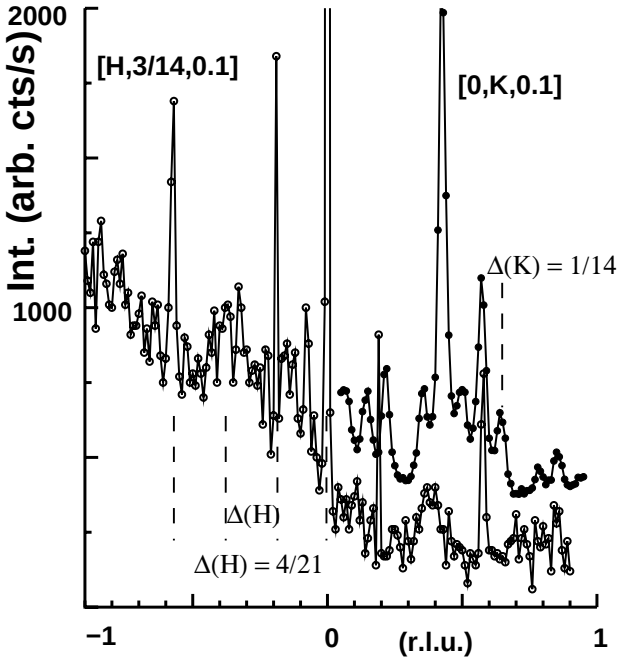

Fig 3: *H and K-directional scans (open and solid circles, respectively)indicating the periodicities of the (21x14)supercell. Due to the large surface periodiciy, and surface ordering, not all the reflections are observed, but mainly those coming from averaged supercells.*