



HAL
open science

Quasicrystal of fullerene C60?

René Ceolin, Viatcheslav Agafonov, Claude Fabre, André Rassat, Ary Dworkin, Daniel Andre, Henri Szwarc, A. Schierbeek, Patrick Bernier, Ahmed Zahab

► **To cite this version:**

René Ceolin, Viatcheslav Agafonov, Claude Fabre, André Rassat, Ary Dworkin, et al.. Quasicrystal of fullerene C60?. *Journal de Physique I*, 1992, 2 (1), pp.1-5. 10.1051/jp1:1992118 . jpa-00246454

HAL Id: jpa-00246454

<https://hal.science/jpa-00246454>

Submitted on 4 Feb 2008

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

Classification

Physics Abstracts

61.50J

Short Communication

Quasicrystal of fullerene C₆₀?

René Ceolin⁽¹⁾, Viatcheslav Agafonov⁽¹⁾, Claude Fabre⁽²⁾, André Rassat⁽²⁾,
Ary Dworkin⁽³⁾, Daniel Andre⁽³⁾, Henri Szwarc⁽³⁾, A.J. Schierbeek⁽⁴⁾,
Patrick Bernier⁽⁵⁾ and Ahmed Zahab⁽⁵⁾

⁽¹⁾ Laboratoire de Chimie Physique, Faculté de Pharmacie, 2 bis boulevard Tonnellé, 37042
Tours Cedex, France

⁽²⁾ Laboratoire d'Activation Moléculaire(*), Ecole Normale Supérieure, 24 rue Lhomond, 75231
Paris Cedex, France

⁽³⁾ Laboratoire de Chimie Physique des Matériaux Amorphes(**), Bâtiment 490, Université
Paris-Sud, 91405 Orsay, France

⁽⁴⁾ Delft Instruments X-Ray Diffraction, P.O. Box 811, 2600 AV Delft, The Netherlands

⁽⁵⁾ Groupe de Dynamique des Phases Condensées(***), Université de Montpellier 2, Place
Eugène Bataillon, 34060 Montpellier Cedex, France

(Received 30 October 1991, accepted in final form 13 November 1991)

Abstract. — X-ray measurements reveal a tenfold symmetry in a single crystal of fullerene C₆₀ grown from a n-hexane solution. Among various hypotheses, that of a quasicrystal is considered.

It is generally admitted that the crystalline structure of fullerene C₆₀ is face-centered cubic at room temperature [1], but a hexagonal close-packed lattice has also been proposed [2]. The structure seems also to depend on the presence of some amount of C₇₀ [3] or on the solvent from which the solid samples have been crystallized [4]. For instance, Hawkins *et al.* [4] assigned a P6₃/m space group to C₆₀ single crystals grown from n-hexane solutions, that is a structure which is neither hexagonal nor cubic closest-packed.

On the other hand, Fleming *et al.* [5] have described a pseudotenfold symmetry for crystals of C₆₀ or C₇₀ cocrystallized with n-pentane. They explain their results in terms of twinning of monoclinic crystals. We initially aimed to investigate the influence of solvents on the structure of crystallized C₆₀ and the observations we made on crystals grown from n-hexane led us to analogous apparent tenfold morphologies but a different assignment seems necessary.

(*) URA 1110, CNRS.

(**) URA D 1104, CNRS.

(***) URA 233, CNRS.

Experimental.

Soot was prepared according to the method of Haufler *et al.* [6] and purified as described elsewhere [7]. The purity of C₆₀ was tested by HPLC, IR, UV and mass spectroscopy. No impurity could be observed.

About 1 mg of C₆₀ was dissolved in ~ 100 ml of n-hexane and the solution was allowed to slowly evaporate. After a couple of days, shiny black crystalline rods (~ 75 μm length and 25-40 μm diameter) had grown.

Figure 1 shows two photographs which were recorded through scanning electron microscopy (SEM) with a JEOL apparatus. It can be seen that the rods are decagonal ones and that the side faces are rectangular. They are closely similar to the crystalline rod recorded on the SEM photograph shown by Fleming *et al.* [5]. Goniometric measurements show that the angle between any two adjacent side faces is equal to 36° within experimental uncertainty. The angles between the side faces and the pyramidal end faces are 32°.

X-ray Weissenberg photographs ($\lambda_{\text{CuK}\alpha} = 1.5418 \text{ \AA}$) reveal a crystallographic axis with a parameter equal to 10.25 Å along the oscillation direction (Fig. 2) which is the axis of the C₆₀ rod.

On a zero-level Weissenberg film (Fig. 3), symmetrical reflexions with equal intensities are located on each side of reciprocal lines between which the angles are equal to $\pi/5$ and $\pi/10$. Therefore, the oscillation direction seems to be a tenfold rotation axis.

Fleming *et al.* [5] describe an analogous crystal morphology as resulting from a particular twinning of a monoclinic lattice with a twinning angle equal to 35.5°. In order to compare our crystals with those of Fleming *et al.*, data collection has been performed with the Enraf-Nonius FAST system combined with a FR 571 rotating anode ($\lambda_{\text{CuK}\alpha} = 1.5418 \text{ \AA}$). The FAST detector is standardly equipped with a CAD4 kappa goniostat to orient the crystal.

The crystal has been oriented with the use of the goniostat, resulting in mm-symmetry of the diffraction pattern, which corresponds to some plane containing the crystal rod axis. Then ω changes were performed. The mm-symmetry is retained through $(36 \pm 0.005)^\circ$ ω rotations, but it is entirely lost when $(35.5 \pm 0.005)^\circ$ rotations are made.

All these results show that the tenfold symmetry really exists in the crystals we grew from n-hexane solutions.

Discussion and conclusion.

It has to be noted that our crystals are different from those obtained by Hawkins *et al.* [4] for crystals grown from n-hexane solutions because the symmetries are not compatible. Obviously, the morphologies of the two kinds of crystals are very different, as they describe crystalline platelets, while we have got decagonal rods.

We have tried to understand the structure of our crystals in terms of the lattice proposed by Fleming *et al.*. The morphologies of both systems are very close, but our results disclose definite differences. First, our value for the parameter along the crystal axis, 10.25 Å, is higher than the 10.1 Å value found by Fleming *et al.*. Then, their crystal overall symmetry corresponds to 35.5° rotations around the rod axis whereas such rotations do not match the symmetry of our samples. Instead, 36° rotations do. Thus, the crystals they have grown from n-pentane solutions are different from those we have obtained from n-hexane solutions.

Further studies are necessary to determine whether the tenfold symmetry of our crystals corresponds to twinning [8], to a microcrystalline structure [9] or to a quasicrystal [10].

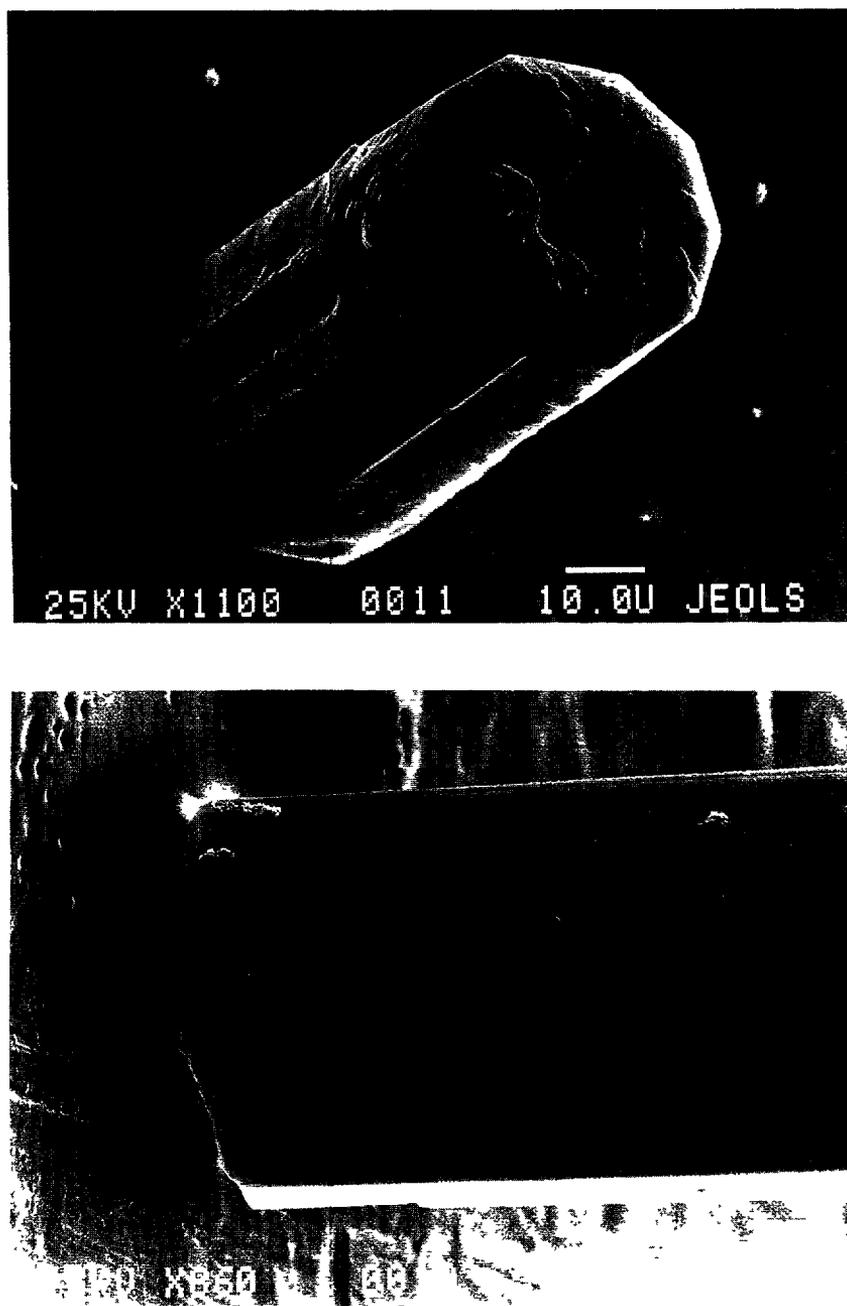


Fig. 1. — Scanning electron microscope photographs of single crystals of quasicrystalline fullerene C₆₀.

If this latter explanation happened to be true, it would be the first example of an organic, molecular, bi-dimensional quasi-crystal. Moreover the stacking unit, the C₆₀ molecule, is a unique entity.

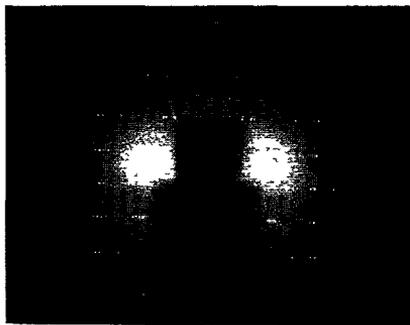


Fig. 2. — X-ray oscillation Weissenberg photograph of a single crystal of quasicrystalline fullerene C_{60} at room temperature. The oscillation direction corresponds to a crystalline axis.



Fig. 3. — Zero-level Weissenberg photograph of a single crystal of quasicrystalline fullerene C_{60} at room temperature.

It can be wondered whether the fivefold symmetry of the molecule is the origin of the crystallization process of this polymorph of C_{60} , as near fivefold symmetry is the origin of the dynamics-driven incommensurability of some crystalline phases of thiophene [11].

Acknowledgements.

We wish to thank Drs. P.Y. Sizaret, A.M. Carriot and B. Arbeille (Unité de Microscopie Electronique, UFR Médecine, Tours) for their invaluable assistance with the scanning electron microscope and the photographers M. Leroux and P. Milza who did a magnificent and rapid job with the Weissenberg pictures. We are also grateful to Dr. G. Fauvet, Enraf-Nonius France, for having organized the access to radiocrystallography apparatuses.

References

- [1] FLEMING R.M., SIEGRIST T., MARSH P., HESSEN B., KORTAN A.R., MURPHY D.W., HADDON R.C., TYCKO R., DABBAGH G., MUJSCE A.M., KAPLAN M.L. and ZAHURAK S.M., *Clusters and Cluster-Assembled Materials*, R.S. Averback, D.L. Nelson and J. Berhholc Eds., MRS Symposia Proc No. 206 (Materials Research Society, Pittsburgh, 1991).
- [2] KRÄTSCHMER W., LAMB L.D., FOSTIROPOULOS K. and HUFFMAN D.R., *Nature* **347** (1990) 354.
- [3] VAN TENDERLOO G., OP DE BEECK M., AMELINCKX S., BOHR J. and KRÄTSCHMER W., *Europhys. Lett.* **15** (1991) 295.
- [4] HAWKINS J.M., LEWIS T.A., LOREN S.D., MEYER A., HEATH J.R., SAYKALLY R.J. and HOLLANDER F.J., *J. Chem. Soc., Chem. Commun.* (1991) 775.
- [5] FLEMING R.M., KORTAN A.R., HESSEN B., SIEGRIST T., THIEL F.A., MARSH P., HADDON R.C., TYCKO R., DABBAGH G., KAPLAN M.L. and MUJSCE A.M., *Phys. Rev. B* **44** (1991) 888.
- [6] HAUFLE R.E., CONCEICAO J., CHIBANTE L.P.F., CHAI Y., BYRNE N.E., FLANAGAN S., HALEY M.M., O'BRIEN S.C., PAN C., XIAO Z., BILLUPS W.E., CIUFOLINI M.A., HAUGE R.H., MARGRAVE J.L., WILSON L.J., CURL R.F. and SMALLEY R.E., *J. Phys. Chem.* **94** (1990) 8634.
- [7] ALLEMAND P.M., KOCH A., WUDEL F., RUBIN Y., DIEDERICH F., ALVAREZ M.M., ANZ S.J. and WHETTEN R.L., *J. Am. Chem. Soc.* **113** (1991) 1050.
- [8] FUNG K., ZOU X.D. and YANG C.Y., *Philos. Mag. Lett.* **55** (1987) 27.
- [9] LAUNOIS P., AUDIER M., DENOYER F., DONG C., DUBOIS J.M. and LAMBERT M., *Europhys. Lett.* **13** (1990) 629.
- [10] STEURER W. and KUO K.H., *Acta Cryst.* **B46** (1990) 703.
- [11] ANDRE D. and SZWARC H., *Phase Transitions* **31** (1991) 59.