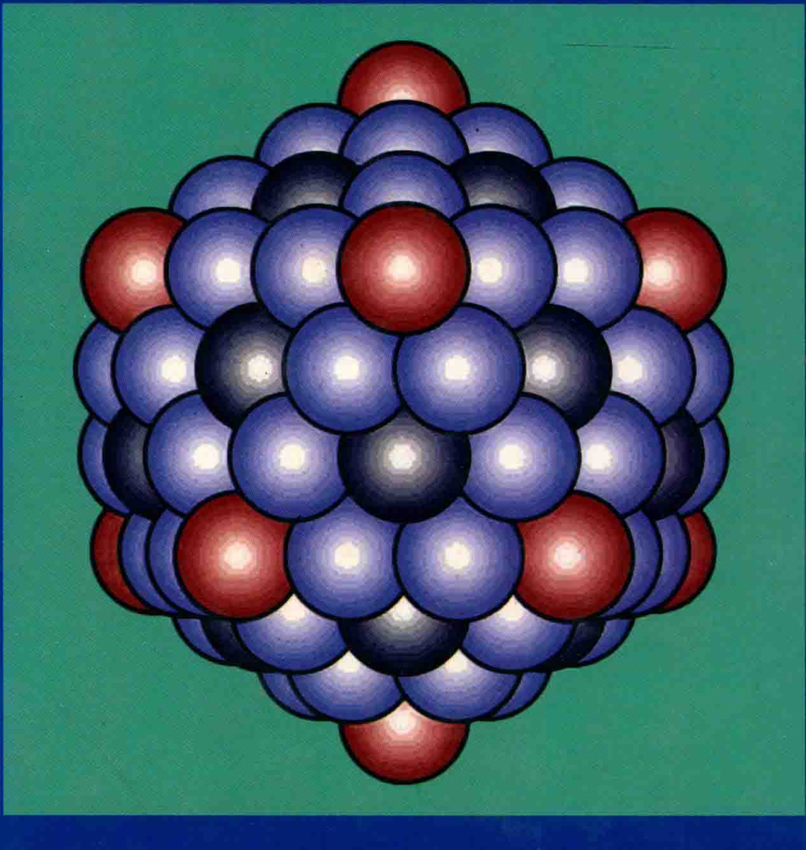
Proceedings of Nobel Symposium 117

The Physics and Chemistry of Clusters



Editors

Eleanor E.B. Campbell & Mats Larsson

World Scientific

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The Physics and Chemistry of Clusters

Visby, Sweden 27 June – 2 July 2000

Editors

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World Scientific

Singapore • New Jersey • London • Hong Kong

Published by

World Scientific Publishing Co. Pte. Ltd.
P O Box 128, Farrer Road, Singapore 912805
USA office: Suite 1B, 1060 Main Street, River Edge, NJ 07661
UK office: 57 Shelton Street, Covent Garden, London WC2H 9HE

British Library Cataloguing-in-Publication Data
A catalogue record for this book is available from the British Library.

The picture on the cover is a calculation of the icosahedral Ar147 cluster from M. Moseler.

THE PHYSICS AND CHEMISTRY OF CLUSTERS
Proceedings of Nobel Symposium 117

ISBN 981-02-4529-7

Printed in Singapore by World Scientific Printers

The Physics and Chemistry of Clusters

Foreword

Nobel Symposium nr. 117 was organized around the subject of the physics and chemistry of clusters, and was held in Visby on the island of Gotland, Sweden, from June 27 to July 2, 2000. The Symposium brought together leading investigators in the field of cluster science from all over the world.

Nobel Symposia were initiated in 1965 by the Nobel Foundation. A fund was created in 1982 jointly by money from the Nobel Foundation, the Knut and Alice Wallenberg Foundation, and the Bank of Sweden Tercentenary Foundation. It is stated in the regulations for the Symposia that they should be organized in scientific areas for which a Nobel Prize can be awarded. It is further stated that they should have a strong international participation, with at least 2/3 of the participants coming from non-Nordic countries. The number of participants should be limited to 30–40. In addition, students and young researchers can be invited as so-called observers. In Nobel Symposium nr. 117 about 30 young researchers participated in addition to the 35 established scientists.

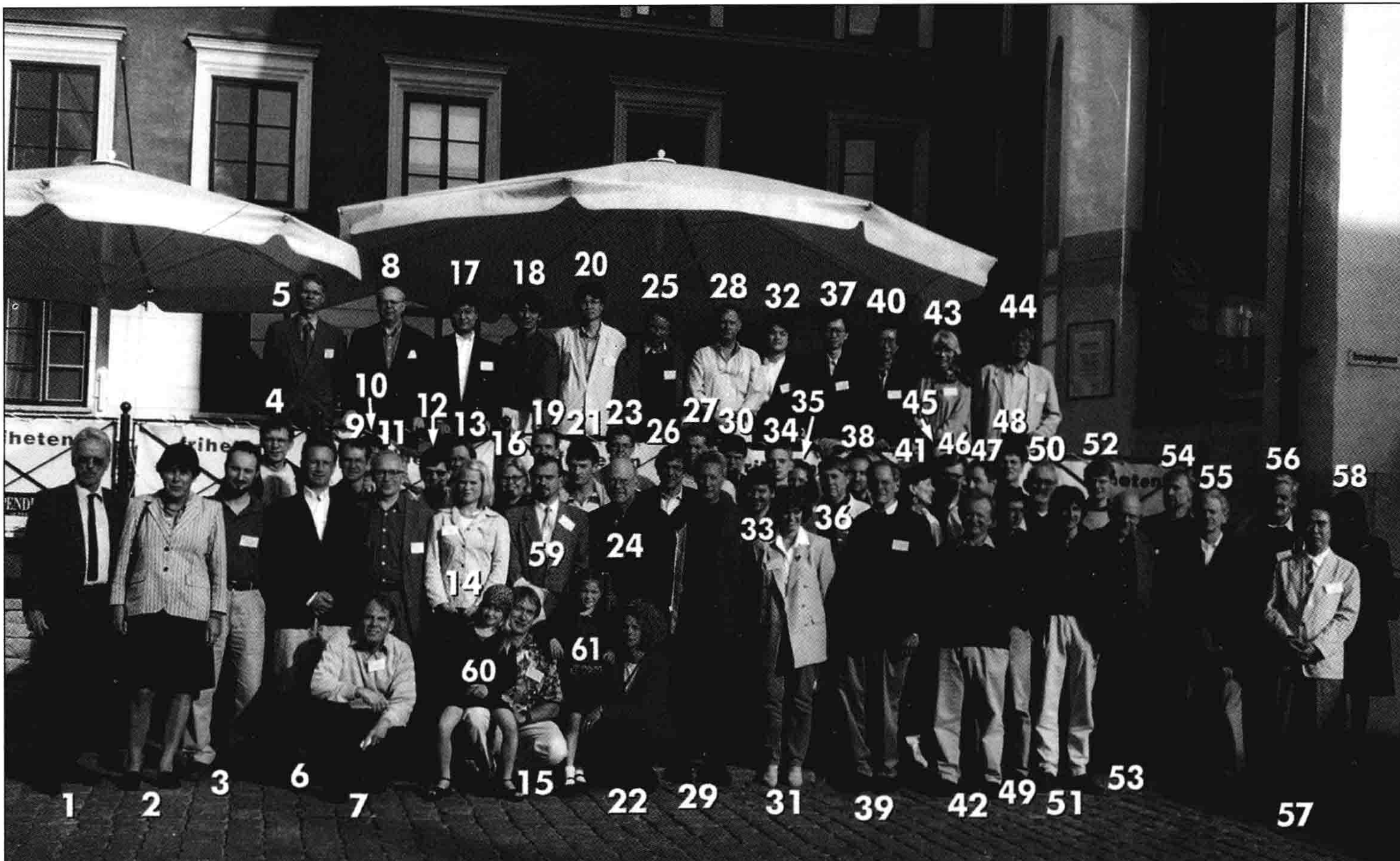
The main motivation for Sweden to organize Nobel Symposia is of course that it provides an excellent possibility for Swedish scientists to have close contacts with the internationally leading scientists in many fields, in particular those which are awarded a Nobel Prize.

The present book is the proceedings from the Nobel Symposium 117 on the physics and chemistry of clusters. It provides a very good insight to the remarkable diversity of the field, such as ultrahigh-resolution spectroscopy and ultrafast spectroscopy of clusters, size-dependent effects, catalysis, chemical reactivity, clusters at interfaces, fission of clusters, and the applications of spectroscopy of clusters to astrophysics.

We would finally like to express our gratitude to the Nobel Foundation for its generous financial support of Nobel Symposium 117.

Eleanor E.B. Campbell

Mats Larsson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List of Participants

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53. Uzi Landman
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56. Arne Rosén
57. Tamotsu Kondow
58. Renee Andersson
59. Vladimir Popok
60. Ms Saykally
61. Ms Saykally

The Physics and Chemistry of Clusters

Contents

VIRUS-LIKE CLUSTERS OF ATOMS

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The capsid shells of most viruses have icosahedral symmetry. The arrangement of protein capsomers within the shell is identical to that of the atoms in highly stable clusters. The classification scheme used to characterize viral structures can be applied, without change, to clusters of atoms and molecules.

1 The Structure of Viruses

Figure 1 shows a representation[1] of SV40, one of the most intensively studied spherical viruses. The reason for this intense interest is that it was found to be a contaminant in polio vaccine, after the vaccine had been given to millions of people. Also shown in Fig. 1, using the same size scale, is a cluster of atoms. It is difficult to see because of their different sizes, but the structure of these two objects is identical. The structural similarity is not limited to this particular cluster-virus pair (a simian virus and metal-covered fullerene cluster). A large variety of viruses find their structural analog in clusters that

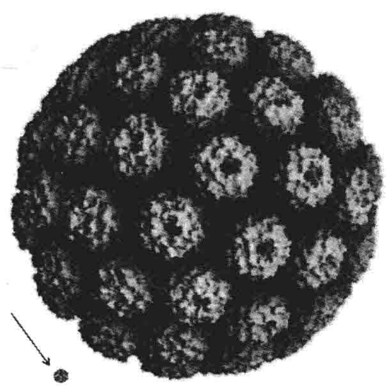

Figure 1. A simian virus 40 (Ref. 1) compared with a metal-covered fullerene cluster (arrow). The structure of both is T = 7.

demonstrate unusually high stability. Many viruses, unlike most clusters, are large enough to allow their structure to be observed directly by means of transmission electron microscopy and x-ray diffraction. We begin with a brief review of those aspects of viral structure that have direct application to clusters.

Ninety-five percent of all viruses that infect humans have icosahedral symmetry. The icosahedron is characterized by 20 identical equilateral faces arranged with a symmetry that includes 12 five-fold rotational axes. Actually, the icosahedral symmetry is restricted to the shell of pure protein that protects the genome. Our entire discussion will be restricted to the structure of this shell, called a capsid.

Viruses are small, as small as 20 nm. Therefore the capsid shell can contain only a very limited amount of genetic material (either DNA or RNA, depending on the virus type), only enough to code for the production of one or a few proteins. For this reason it was suggested very early that the capsid shell must consist of a repeating structural element.

Before the proteins self-assemble in an infected cell to form the icosahedral shell, they first polymerize. These capsomers, as they are called, are often, but not always, hexamers and pentamers. It is these capsomers that are the

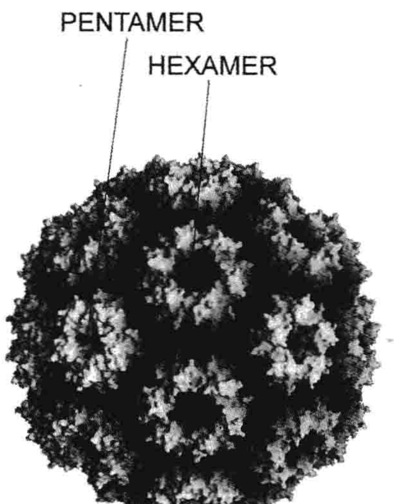

Figure 2. The capsid shell of the cowpea chlorotic mottle virus (Ref. 2) is composed of 12 protein pentamers and 20 hexamers. The structure is T = 3.

building blocks of the icosahedral capsid. Figure 2 shows a representation[2] of a plant virus composed of 32 capsomers that look circular. Closer inspection show that some have five-fold symmetry and some have six-fold symmetry. In fact, this cowpea chlorotic mottle virus (CCMV) capsid is made up of 12 pentamers and 20 hexamers.

Since viral capsomers are more or less close-packed, it is useful to consider the problem of how to pack circles onto an icosahedron. The solution to the problem of finding the densest packing of equal circles on a planar surface is trivial. However, the same problem when applied to a closed surface has no general solution. Consider first the simple case of the infinite plane. A plane surface can be tiled (completely covered) with equilateral triangles. This is sometimes referred to as triangulating, or tessellating a surface. If circles having a diameter equal to one side of the triangles are placed at each of the intersections of the tiles, the result is the densest possible packing of circles on the plane. Each circle is surrounded by six other circles. Suppose we now apply the same procedure to the closed surface of an icosahedron. Tiling this closed surface reduces to the problem of tiling each of the 20 triangular faces. Figure 3 shows a projection of an icosahedron onto a plane looking down one five-fold axis. Also shown in this figure are several ways of tiling the triangular faces. The number of tiles that can be fitted into a face is called the triangulation number. This number is the most common way of characterizing the structure of spherical viruses. For example, the cow-pea virus shown in Fig. 2 is referred to as having the T3 structure.

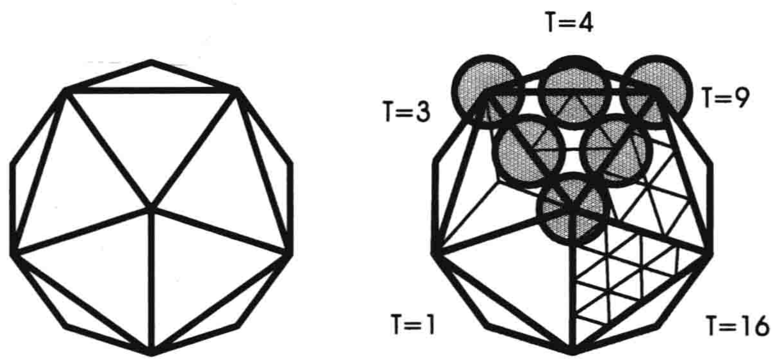

Figure 3. Projection of an icosahedron, looking down a five-fold rotational axis. Each triangular face can be covered with T equivalent triangular tiles. Viral structures are obtained by placing capsomers at each vertex of the tiles as shown for the case of T = 4.

Icosahedra can be triangulated in only a limited number of ways[3]. The first members of two series are shown in Fig. 4. The top row of configurations, corresponding to triangulation numbers 1, 4, 9, and 16, have the full symmetry of the icosahedral point group. The second series of configurations, shown in the bottom row, have a slightly lower symmetry. Inversion and reflection symmetry has been removed because the circles within the triangular face have been rotated as a group relative to the symmetry axes of the triangle. The reason for this rotation can be seen in Fig. 5. Without the rotation, a hole is left in the packing scheme where two triangles butt against one another. This packing void is filled by rotating the circles within a face. Such a rotation confers a chirality to the structure, which can be seen in Fig. 5 The simian virus is an example of a T7 structure for which the symmetry has been lowered and chirality has gained.

2 Calcium Clusters

Calcium clusters also have icosahedral symmetry,[4,5] a symmetry known to exist in large inert gas clusters[6,7,8,9,10,11,12] and suspected to exist in large sodium and magnesium clusters[13].

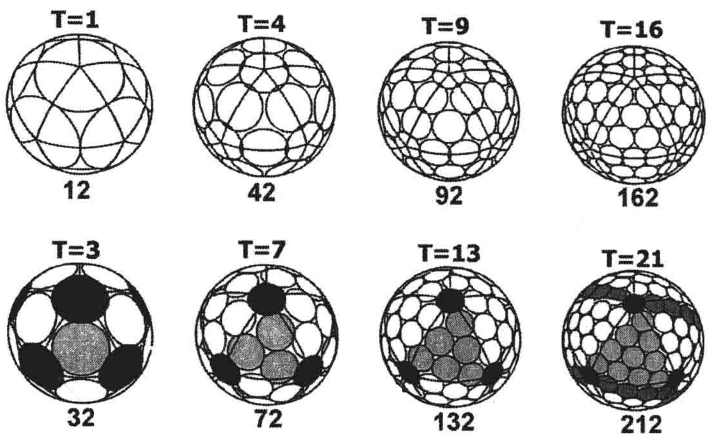

Figure 4. Only a limit number of structures are allowed using T equivalent tiles. The structures in the top row have I_h symmetry. The symmetry in the bottom row is reduced to I.

The technique used to reveal the structure of calcium clusters is photofragmentation. Light is used to heat the clusters to a temperature at which they begin to evaporate atoms on a time scale of interest. The evaporation process slows down each time a very stable cluster size is reached. Therefore, the concentration of such clusters tends to be the higher in the evaporative ensemble. This technique places restrictions on the materials and light sources. The clusters should be solid at the temperatures necessary for evaporation, since we are interested in studying the structure of a cluster with well-defined geometry. The cluster should also have a large photo-absorption cross-section at the wavelength of the warming laser. These conditions have been met in the following way.

Our cluster source is a low pressure, inert gas, condensation cell. Calcium vapor produced at 700C was quenched in cold He gas having a pressure of 1 mbar. Clusters condensed out of the quenched vapor were transported by the gas stream through a nozzle and through two chambers of intermediate pressure into a high vacuum chamber. Here the clusters were simultaneously warmed and ionized with a 10μJ, 2x2 mm, 10 ns, 380 nm light pulse. The laser power was chosen to cause an appreciable loss of cluster mass through single atom evaporation during the laser pulse duration. The wavelength was chosen to correspond to a plasmon resonance in calcium spheres expected at

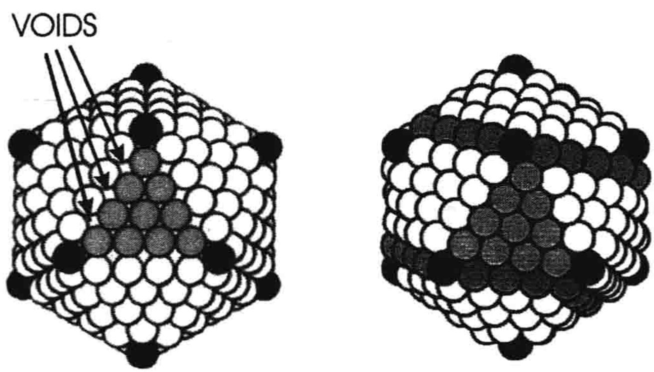

Figure 5. A T = 21 structure with full I_h symmetry has packing voids at the intersection of icosahedral faces. These voids can be filled by rotating the circular units inside a face by 19° either clockwise or counterclockwise, reducing the symmetry group to I and introducing chirality.