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ORNL**FOREIGN TRIP REPORT**

ORNL/FTR 3764

DATE: October 8, 1990

SUBJECT: Report of Foreign Travel of C. E. Klots, Senior Research Staff Member,
Chemical Physics Section, Health and Safety Research Division

TO: Alvin W. Trivelpiece

ORNL/FTR--3764

FROM: C. E. Klots

DE91 000776

PURPOSE: To present an invited paper at the Gordon Conference on Molecular Clusters, Volterra, Italy (September 3-7); to present an invited paper at the International Symposium of Small Particles, Konstanz, Germany (September 9-14); to visit the University of Freiburg; and give a lecture at the University of Paris.

SITES

VISITED:	9/2-7/90	Gordon Conference Molecular Clusters	Volterra, Italy	W. Castleman
	9/9-14/90	International Symposium of Small Particles	Konstanz, Germany	E. Recknagel
	9/17/90	Universität	Freiburg, Germany	O. Hertel
	9/18-19/90	Université	Paris, France	S. Leach

ABSTRACT: Accounts are given of the two major international conferences on the physics and chemistry of small particles, commonly referred to as van der Waals particles. Details of special interest to Oak Ridge National Laboratory personnel are cited. Information exchanges at Freiburg and Paris are described.

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INTRODUCTION

Interest in the properties of small particles has grown so rapidly that there are now two major international conferences in the field. The International Symposium on Small Particles has been in existence for several years, with its size doubling every second year. It is primarily for physicists. By contrast, the Gordon Conference on Molecular Clusters, designed primarily for chemists, is brand new. Most of what follows will describe these conferences.

GORDON CONFERENCE ON MOLECULAR CLUSTERS

The first of what promises to be a continuing series of Gordon conferences on clusters, and also the first Gordon conference on any subject held outside the United States, took place in the hill town of Volterra, Italy. The familiar format of four invited speakers per day permitted a thorough examination of a small number of topics. Thus Levy (Chicago) and Schlag (Munich) described in great detail their high resolution studies of spectroscopic shifts of electronic transitions upon gradual solvation in van der Waals molecules. The structure of these aggregates are obtained either from rotational constants or from the electronic shifts plus exciton theory. Kit Bowen (John Hopkins) argued persuasively that his photoelectron spectra studies of negatively charged water clusters reveal no indication of surface states for the extra electron. This result made a number of people unhappy. Bob Stanley (Penn State) described elegant ion-dip spectroscopy experiments in which a species in an excited state may be photoionized by a second color or dumped back to the ground state by stimulated emission.

The traveler had been invited to speak on the theory of metastable evaporation and how it can be used to study the energetics of cluster formation. It was shown that recent measurements of metastable decay of carbon clusters do not implicate magic numbers but rather magic layers. It was also shown that this heretical result follows independently from recent measurements of kinetic energy release during evaporation. The discussion which ensued was heated.

A large number of poster papers were also presented at the meeting. This and the attendance of many graduate students, mostly from Europe, suggests a healthy future for this particular conference.

INTERNATIONAL SYMPOSIUM ON SMALL PARTICLES

By contrast, this symposium is an established institution. The number of attendees (now about 350) continues to double with each second conference. The number of invited presentations was more than twice that of the Gordon Conference. Over three hundred poster papers were given at Konstanz.

Nevertheless, certain themes tended to dominate the discussion. Absorption spectra of alkali metal clusters have been measured by Brechignac (Paris), Broyer (Lyon), and Knight (Berkeley) and can be understood in terms of surface plasmon theory plus splittings due to

deformations from spherical geometry. Mottelson (Copenhagen) discussed the origin "even-odd" magic numbers and their gradual disappearance with increasing cluster size. Another kind of electronic magic was discussed by Whetten (UCLA) who has been studying electron solvation in alkali-halide crystals where an excess electron may occupy a lattice defect.

Carbon clusters kept cropping up. Bethune (San Jose) and Krätschmer (Heidelberg) presented evidence that the C_{60} molecule can now be made in macroscopic amounts. Its properties seem to be those expected for a fullerene. Thus the traveler's invited talk, in part also on the energetics of evaporation from carbon clusters, again provoked much discussion.

This talk also showed how evaporative kinetics can be used to test Mottelson's ideas on even/odd magic. Further cooperation between Oak Ridge National Laboratory (ORNL) and Copenhagen on this subject is planned.

UNIVERSITY OF FREIBURG

Immediately after the conference, the traveler visited Professor I. Hertel's group in Freiburg, where metastable evaporation from carbon is being studied. Hertel is the editor of *Z. Physik D.* and asked the traveler to submit a feature article on the subject to his journal.

UNIVERSITY OF PARIS

The traveler spent two days at the University of Paris at Orsay. A seminar, "Generalized Arrhenius Plots," was presented in which it was shown how one should analyze experimental data which Sidney Leach, Odille Dutuit, and Paul-Marie Guyon take on rate constants as a function of energy. Several examples were shown which demonstrate how one can extract numbers in a simple and model-free fashion, compared with the tedious and model-free methods they now use.

Leach is abreast of almost all European science. For example he knew already about Krätschmer's synthesis of C_{60} . Collaborations with him, such as that of John Miller, will inevitably be fruitful for ORNL. As an example, he noted that his work is supported because of its astrophysical implications. Because C_{60} is believed to be formed in carbon-rich stars (the universe's first molecule), the traveler's work on the stability of this species thus has broad ramifications.

SUMMARY

With the incredible flood of written literature which inundates our libraries, personal contacts and attendance at meetings become increasingly important, on the one hand for learning what is new and important and, on the other, for making more visible work done for the Department of Energy at ORNL. While this insight is not new, its validity is underscored by the several events described above. Likewise, chance conversations such as those between the traveler and Mottelson and Leach reveal new directions to be taken.

APPENDIX

ITINERARY

August 27-31, 1990	Vacation in United States
September 1-2, 1990	Travel from Boston to Volterra, Italy
September 3-7, 1990	Attend Gordon Conference on Molecular Clusters
September 8-9, 1990	Weekend Travel to Konstanz, Germany
September 10-14, 1990	Attend Symposium on Small Particles
September 15-16, 1990	Weekend Travel to Freiburg, Germany
September 17, 1990	University of Freiburg
September 18-19, 1990	University of Paris
September 20-21, 1990	Travel from Paris, France, to Oak Ridge, Tennessee

PERSONS CONTACTED

Volterra, Italy

I. Hertel, Freiburg
 O. Echt, Konstanz
 W. Castleman, Penn State
 E. Schlag, Munich
 J. Jortner, Tel Aviv
 M. Johnson, New Haven
 K. Bowen, Baltimore
 A. Stace, Brighton
 M. Henchman, Gottingen
 M. Bowers, Santa Barbara
 J. Lissy, Illinois
 T. Mark, Salzburg
 C. Lifschitz, Jerusalem

Konstanz, Germany

E. Recknagel, Konstanz
 C. Brechignac, Paris
 B. Mottelson, Copenhagen
 R. Whetter, UCLA
 W. Knight, Berkeley

A. Ding, Berlin
L. Bartell, Michigan
J. Gspann, Karlsruhe
D. Bethune, San Jose
T. Kondow, Japan
K. Meiwes-Broer, Bielefeld
T. Martin, Heidelberg
R. Smalley, Houston
G. Torchet, Paris

Freiburg

I. Hertel
H. Haberland

Paris

S. Leach
J. Belloni
J. Faure
O. Dutuit
P. M. Guyon

- END -

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