COVER SHEET
FOR TRIP REPORTS SUBMITTED TO THE OFFICE OF ENERGY RESEARCH

ORNL/FTR--3669

DE90 014309

Destination(s) and Dates for Which Trip Report Being Submitted:

Frankfurt, Germany	6/18-20/90
Darmstadt, Germany	6/19/90
Freiburg, Germany	6/21-23/90
Rome, Italy	6/24-27/90
Paris, France	6/28-7/2/90

Name of Traveler: C. Bottcher

Joint Trip Report: _____Yes
_X_ No

If so, Name of Other Traveler(s): _____

OAK RIDGE NATIONAL LABORATORY

OPERATED BY MARTIN MARIETTA ENERGY SYSTEMS, INC.
POST OFFICE BOX 2008, OAK RIDGE, TENNESSEE 37831-6285

ORNL

FOREIGN TRIP REPORT

ORNL/FTR-3669

DATE: July 11, 1990

SUBJECT: Report of Foreign Travel by C. Bottcher, Research Staff Member, Physics Division

TO: Alvin W. Trivelpiece

FROM: C. Bottcher

PURPOSE

To attend a meeting of the General Committee of the International Conference on the Physics of Electronic and Atomic Collisions, held at Castelgandolfo, near Rome. The traveler also presented seminars and held discussions at some leading European centers of research in atomic physics: Frankfurt, G.S.I. (Darmstadt), Freiburg, and Paris.

SITES VISITED

6/18-20/90	University of Frankfurt	Frankfurt, Germany	W. Greiner
6/19/90	G.S.I.	Darmstadt, Germany	W. Greiner
6/21-23/90	University of Freiburg	Freiburg, Germany	J. S. Briggs
6/24-27/90	Castelgandolfo	Rome, Italy	F. Gianturco
6/28-7/2/90	University of Paris	Paris, France	R. McCarroll

UCN-2383A
(3 6-88)

ABSTRACT

The traveler participated in the committee meeting which set up the program for the next International Conference on the Physics of Electronic and Atomic Collisions, to be held in Brisbane, Australia. Seminars were presented at Frankfurt, Freiburg, and Paris. Discussions took place covering the following subjects of direct relevance to ORNL programs: pair production in relativistic heavy-ion collisions, angular correlations and post-collision interactions in the Coulomb three-body problem, and interactions of slow, highly charged ions with crystal surfaces.

The primary purpose of this trip was to participate in a meeting of the General Committee of the International Conference on the Physics of Electronic and Atomic Collisions, held at Castelgandolfo, near Rome. The subsidiary purpose was to maintain contacts with some of the leading European centers of research in atomic physics, namely Frankfurt (including GSI, Darmstadt), Freiburg, and Paris. Each has historically interacted with programs at ORNL, and members of groups and laboratories from those places are fairly regular visitors to the Physics Division of ORNL. Each is strong in both theory and experiment.

Frankfurt: June 18–20

The traveler spent two days in discussions with Prof. Walter Greiner and his colleagues at the Institute for Theoretical Physics of the J. W. Goethe University of Frankfurt. The main thrust of the group at present is the description of intermediate-energy (a few hundred MeV/nucleon) nuclear collisions by means of quantum molecular dynamics (QMD). In this phenomenology, classical dynamics is used to describe the motions of wavepackets of nucleons. Predictions are in remarkable agreement with almost all available data. Extensions to relativistic collisions using strings are under way and appear equally promising. Both approaches suffer from the shortcoming, frankly admitted, that some *ad hoc* assumptions are needed which are difficult to justify. The group expressed a strong and supportive interest in the project on colliding strings being pursued at ORNL by Dean, Strayer, and Wu.

Prof. J. Maruhn, in collaboration with Prof. P.–G. Reinhard of Erlangen, is applying basis-spline techniques to relativistic mean-field theories of nuclear structure. Use is made of the spline codes originally developed at ORNL. The method is superior to other techniques (finite difference, Fourier transforms) for calculations using Cartesian coordinates in three dimensions, i.e., without any assumptions regarding spherical or cylindrical symmetry.

During one afternoon's visit to GSI at Darmstadt, the traveler had discussions with Dr. Gerhardt Soff on the atomic theory program at GSI. Calculations are being pursued on electronic capture and excitation in ion-atom collisions around a GeV/nucleon using close coupling techniques. However, Soff regards this approach as unreliable for the higher energies, which are of most interest to accelerator designers. As he is also keenly interested in the electromagnetic production of W–pairs and Higgs bosons in heavy-ion collisions, we discussed recent ORNL preprints in some detail.

While at GSI, it was also possible to discuss new searches for positron peaks with Dr. W. König and other experimentalists. It appears that the most recent measurements confirm two peaks in the form of back-to-back electron-positron coincidences with sharp total energy, but a less well–defined energy difference. The new ESR ion storage ring is being tested, and it appears that cooling has been demonstrated by measuring the reduction in the Schottky noise, though no results have yet been publicly announced.

The traveler gave a seminar at Frankfurt on "Heavy-Ion Collisions at Ultra-relativistic Energies."

Freiburg: June 21–23

The Albert Ludwig University of Freiburg has a number of Physics Institutes and groups working in atomic and chemical physics. The traveler

had detailed discussions with the theory group of Prof. J. Briggs, and the experimental groups of Profs. W. Sandner and W. Mehlhorn.

The activity of Briggs's group is based on the unifying theme of the Coulomb three-body problem. With Dr. H. Klar and others, he has been calculating triply differential cross sections for electron-impact ionization of atomic hydrogen and helium in a distorted-wave formulation with correct three-body boundary conditions. This is the first reliable theory for intermediate energies, and it is in remarkable agreement with experiments. With Dr. J. Broad, they have produced an ingenious exact solution for electron–hydrogen scattering in a laser field by showing that the system is equivalent to a stationary two-center Coulomb arrangement. Incidentally, Dr. Broad is about to become Director of the Atomic Data Center at Boulder. Thus, we talked about the organization of the atomic data centers in the U.S., including that at ORNL, with which a continuing fruitful collaboration is expected. A postdoctoral fellow, Dr. Gernot Albers, is carrying out extremely interesting calculations in quantum optics using time-dependent wavepacket approaches very similar to those used on other problems over many years at ORNL. We initiated discussions on the possibility of closer interactions, including a visit to ORNL this fall.

The group of Prof. W. Sandner is very famous for their studies on the structure of two-electron atoms. They have been able to produce states in which both electrons are prepared in precisely defined hydrogenic orbits, and observe their subsequent evolution. As many as six tunable lasers are needed! Such experiments can explore many unsolved problems in classical and quantal dynamics touching on chaos and periodic solutions.

For many years, the group of Prof. W. Mehlhorn has pursued very accurate studies of the dynamics of photoionization and Auger emission, usually of fairly complex atoms in the first or second row of the periodic table. They have recently been studying Auger emission from inner shells following electron impact ejection of an inner electron. The final state thus involves one fast and two slow electrons. The interesting physics lies in the interaction of the slow electrons, which is largest when they have the same asymptotic velocity. Thus, the experiments look at the angular correlation of such electrons. Significant effects are found which can be described by semiclassical analyses of the type used to interpret the post-collision interaction experiments of Havener *et al*. at ORNL.

The traveler gave a seminar on "Numerical Studies of the Coulomb Three-Body Problem."

Castelgandolfo: June 24–27

The International Conference on the Physics of Electronic and Atomic Collisions (ICPEAC) is the largest and most successful in this field with 500-700 participants at each conference. The next meeting in the series (the XVII-th) is to take place in July 1991 in Brisbane, Australia. Over the years, ICPEAC has acquired a rather elaborate apparatus of governance, which is jealously protected by the regular participants. The gathering at Castelgandolfo (30 km from Rome) was technically of the Executive Committee (about six people), but it has become customary to extend invitations to all members of the General Committee (about 60 people) to assist with the main task, which was to make recommendations to the local (in this case, Australian) committee regarding the program. A complete program of about 60 invited speakers was constructed, and it is expected that most recommendations will be accepted. The organization and time allotted to contributed papers were also discussed, as were more general topics, such as the escalating cost of participation.

Of about 20 participants, only four were from the U.S.A., three being from national laboratories (two from ORNL). This may be related to the conference being unable to pay travel to committee meetings (though local expenses were generously subsidized by the University of Rome). Some degree of under-representation was reflected in the demographics of the suggested invited speakers. Out of 60 speakers, 16 were from the U.S.A. (10 from universities, 6 from national laboratories). In fairness, other factors entered, such as an effort to compensate for U.S. over-representation at the last two conferences and an increased number of nominations of Australians, Japanese, and East Europeans. The largest bloc is from Western Europe (about 20), reflecting the high level of activity and support for basic science in the European economic community.

The balance of interest in different subfields has shifted in some respects. The number of talks on collisions of highly charged ions with electrons or atoms is down, while the number on electron collisions with neutral atoms and molecules has increased. Regrettably, chemical reactive scattering is probably disappearing from the conference, but the representation of surface and cluster phenomena is growing.

Paris: June 28–July 2

On this final leg of his journey, the traveler visited three laboratories housed in the same building of the Université Pierre et Marie Curie, located in the heart of Paris. These were the theoretical group of Prof. R. McCarroll, and the experimental groups of J.–P. Briand and J. Mazeau.

Prof. McCarroll and his associates are currently chiefly interested in processes in interstellar clouds, such as ion–molecule reactions. Such reactions at low temperatures are controlled by long-range interactions. For polar molecules in particular, the theory is analytically tractable. For asymmetric top molecules of astrophysical significance, such as H_2O or NH_3, the analysis is complicated and group theory must be invoked. The group continues to be interested in electron capture by multiply charged ions at low or intermediate energies, including processes studied experimentally at ORNL. The approach here is heavily computational, using multistate close coupling expansions. Attention is currently focused on resolving discrepancies between theory and experiment, and the theories of different groups.

The group of J.-P. Briand is involved in an astonishing range of experiments on the spectroscopy and collisions of highly charged ions at many centers, including Saclay, Grenoble, GSI, and LBL. Experiments are conducted at both low and high energies. The group's success relies on their ability to engineer spectrometers (of milliradian precision) which can be carried to any facility and set up in a matter of hours. They provide a case study in the effectiveness of "suitcase physics" if properly managed.

Most of the scientific discussions on heavy-ion physics concerned recent experiments at Grenoble, ORNL, and LLNL of the interaction between a slow, highly charged ion and a crystal surface. These discussions were joined by Prof. S. Bliman (Grenoble) and Dr. J. N. Bardsley (LLNL). All observe that the subsequent radiation from the ion is anomalous compared with capture from atoms in the sense that low-lying states are preferentially populated. At least three theories have been proposed to explain this:

1) The *hollow atom* theory of Andra and others, that all electrons are initially captured in high-Rydberg states, which Auger decay to fill the lower states. Simple estimates give Auger rates too slow to account for the experiments.

2) The *boiling off* theory of Bardsley, based on classical plasma simulations, that the hollow atoms are formed with net positive energies and decay rapidly into the continuum. Low-lying states are populated by direct capture in close approaches to the surface.

3) The *transfer ionization* theory favored by the traveler, based on calculations on multiple capture done about six years ago, suggesting that in multiple capture events, some electrons would be propelled directly into low-lying states by electron correlation.

Each theory makes predictions which can be tested by future experiments. The entire controversy may be the most important current topic in low-energy heavy-ion physics. As one outcome of our discussions, Dr. Bardsley and the traveler plan to organize a workshop on the subject at Santa Barbara in the fall of 1991.

Prof. J. Mazeau and his collaborator, Dr. A. Huetz, have been studying the angular correlations of electrons ejected from atoms by electron impact and photoionization near threshold. Technically this requires the design of charged-particle spectrometers of high resolution and the ability to control experiments at very low count rates. The latter problem will be removed in the next version of the experiment using multichannel plates. Once again, the object is to probe the famous unsolved Coulomb three-body problem. This group has now carried out experiments to sufficient precision to uncover disagreements with the widely accepted theory of threshold ionization due to Wannier. In particular, the angular correlation is not universal, but depends on the initial state. (Experiments have been made on several of the rare gases.) Discussions centered on recent Russian work, and calculations are in progress by the traveler which might explain these phenomena. It was agreed to maintain close contact on theoretical and experimental advances.

The traveler gave a seminar on "Coulomb Three-Body Scattering Near Threshold."

APPENDICES

A. ITINERARY

1990

June 17	Travel en route from Oak Ridge to Frankfurt, Germany
June 18-20	J. W. Goethe University, Frankfurt, Germany
June 20	Travel en route from Frankfurt to Freiburg, Germany
June 21-23	Albert Ludwig University, Freiburg, Germany
June 23	Travel en route from Freiburg to Rome, Italy
June 24-27	Castelgandolfo, Italy
June 27-28	Travel en route from Rome to Paris, France
June 28-July 2	Université Pierre et Marie Curie, Paris, France
July 3	Travel en route from Paris to Oak Ridge

B. PERSONS CONTACTED

W. Greiner	J. W. Goethe University, Frankfurt, Germany
J. A. Maruhn	J. W. Goethe University, Frankfurt, Germany
G. Soff	J. W. Goethe University, Frankfurt, Germany
W. König	GSI, Darmstadt, Germany
J. S. Briggs	Albert Ludwig University, Freiburg, Germany
W. Mehlhorn	Albert Ludwig University, Freiburg, Germany
W. Sandner	Albert Ludwig University, Freiburg, Germany
J. T. Broad	Albert Ludwig University, Freiburg, Germany
H. Klar	Albert Ludwig University, Freiburg, Germany
F. Gianturco	University of Rome (Chairman, International Conference on the Physics of Electronic and Atomic Collisions)
J. N. Bardsley	Lawrence Livermore National Laboratory (Secretary, International Conference on the Physics of Electronic and Atomic Collisions)
R. McCarroll	Université Pierre et Marie Curie and/or CNRS, Paris, France
J. Mazeau	Université Pierre et Marie Curie and/or CNRS, Paris, France
J.-P. Briand	Université Pierre et Marie Curie and/or CNRS, Paris, France
A. Huetz	Université Pierre et Marie Curie and/or CNRS, Paris, France
S. Bliman	Université Pierre et Marie Curie and/or CNRS, Paris, France

C. LITERATURE ACQUIRED

Post Collision Interaction at High Impact Energies, W. Sandner, J. Phys. B19, L863 (1986).

Absolute Measurement of Auger Line Shifts After High-Energy Electron Impact Ionization, M. Völkel, M. Schnetz, and W. Sandner, J. Phys. B21, 4249 (1988).

Positional Correlation in Laser-Excited Three-Body Coulomb Systems, U. Eichmann, V. Lange, and W. Sandner, Phys. Rev. Letts. 64, 274 (1990).

Propensity Rules for Radiative and Nonradiative Decay of Doubly-Excited States, J. M. Rost and J. S. Briggs, submitted to Journal of Physics B.

Auger Line Shapes of Free Atoms, W. Sandner and M. Völkel, Phys. Rev. Letts. 62, 885 (1989).

Saddle-Point Resonances in Few-Body Systems, J. M. Rost and J. S. Briggs, submitted to Physical Review Letters.

$KL_{2,3}$ Ionization in Neon by Electron Impact in the Range 1.5-50 keV: Cross Sections and Alignment, A. Albiez, M. Thoma, W. Weber, and W. Mehlhorn, to be published in Z. Phys. D, 1990.

K/π Ratios in Relativistic Nuclear Collisions: A Signature for the Quark-Gluon Plasma?, R. Mattiello, H. Sorge, H. Stöcker, and W. Greiner, Phys. Rev. Letts. 63, 1459 (1989).

String Dynamics in Hadronic Matter, H. Sorge, A. von Keitz, R. Mattiello, H. Stöcker, and W. Greiner, UFTP preprint 245/1990.

Nuclear Stopping, Baryon Densities, Flow and Equilibration at AGS Energies, H. Sorge, A. von Keitz, R. Mattiello, H. Stöcker, and W. Greiner, UFTP preprint 243/1990.

Near Threshold (e,2e) Measurements for Neon, Argon and Krypton, P. Selles, J. Mazeau and A. Huetz, to be published in J. Phys. B, 1990.

Proceedings of European Conference on (e,2e) Collisions and Related Problems, invited papers and progress reports, Kaiserslautern, FRG, November 23-24, 1989.