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13. ABSTRACT *(Maximum 200 words)*

This is a report on the International Conference on Organic Superconductors which was held on May 20-24, 1990, at Fallen Leaf Lake, South Lake Tahoe, California. Sixty participants attended the conference from Japan, Europe, Canada, and the United States, and over forty papers were presented on recent developments in the field and reviews were given on the optical, thermo-electric and the fermiology-properties of organic conductors. A distinguished panel of experts discussed the prospects and the means for synthesizing new classes of conducting and superconducting organics. Papers presented at the conference will be published by Plenum Press under the title, "Organic Superconductivity", edited by V. Kresin and W. A. Little, late in 1990.

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Final Report

An International Conference on Organic Superconductors

May 20 - 24, 1990

Grant No. N00014-90-J-1384

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Stanford University,
Stanford,
CA 94305

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William A. Little
Principal Investigator

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Final Report
An International Conference on Organic Superconductors
May 20 - 24th, 1990
ONR Contract # N00014-90-J-1384

This is the final report on the International Conference on Organic Superconductors which was held on May 20 - 24th, 1990 at Fallen Leaf Lake, South Lake Tahoe, California with support from the Department of Energy and the Office of Naval Research under Contract #N00014-90-J-1384.

A total of sixty participants attended the conference, with Japan, Europe, Canada and the United States represented but not the Soviet Union, although the USSR does have a considerable effort in the area. Apparently, funding difficulties in the Soviet Union resulted in the nine expected participants from the Soviet Union having to cancel their attendance at the last moment. In line with our objective of introducing new blood to the field, we were glad to welcome among the sixty attendees, a total of twelve student participants who represented most of the key laboratories in the field. The conference was based on the Gordon Conference schedule, with a full morning program, early afternoons free for discussion, hiking, etc., reconvening of the meeting in mid-afternoon, and discussion and poster sessions in the evening. Each session was a mixed session, with topics on the physics, chemistry and material aspects of the subject in each. This worked very well resulting in almost 100% participation of the attendees at all the sessions.

It got off to an excellent start with the announcement on the first day, by the Jack William's group from Argonne National Laboratory, of a new high for the superconducting transition temperature of an organic compound, in a newly synthesized structure of the ET series, having a transition temperature in excess of 11.6K.

The similarities and differences between the organic and the high transition temperature superconducting cuprates were noted in a number of papers, and the physical properties of each were compared by several authors. A paper by Ron Elsenbaumer reported on recent advances in the preparation of highly conducting, processable polymeric materials. One can expect considerable progress in this area in the next few years. The panel discussion on new compounds brought forth a plethora of new ideas of interesting materials, which in many cases were compounds that were related to those that have received some attention to date, but which yet remain to be studied. The notes on the distinguished contributions to this session, which have been edited by Professor Dwain Cowan of Johns Hopkins University who chaired the session, will appear in the proceedings later this year, and will bring these ideas to a wider audience. Undoubtedly, these will receive close scrutiny by workers and potential workers in the field.

Among the interesting physical properties reported on were the optical properties of several of the prototypical organic salts, their behavior under pressure, their thermoelectric properties and their behavior in large magnetic fields. Several of the speakers did an excellent job for the students present by providing an up-to-date review of their fields before plunging into the details of their own contributions. In particular, reviews of optical properties, fermiology and thermoelectric effects were presented and these, which will appear in the proceedings, may well be expected to become a valuable reference for future workers in this, and other fields, in condensed matter physics and chemistry.

The proceedings of the conference which will be published as a book, and will include all but two of the papers given at the meeting. This will be published by Plenum Press under the title, "Organic Superconductivity" and will be edited by Vladimir Kresin and William A. Little. It is expected that the book, which will be of 385 pages, will be released in early December, 1990.

It would be appropriate to mention two items which were brought up by the participants and which might be of interest to funding agencies. The first was a perceived need to develop a better understanding of the process of electro-crystallization. This is a technique which plays a key role in the preparation of almost all the materials developed in the field, but is one which most of the participant felt was poorly understood and for which equipment was not readily available nor standardized. A scholarly study of this technique could have a significant impact on both the work on charge transfer salts and on the conductive polymers.

The second, was the remark by Professor J.P. Collman that the field of organic conductors, organic magnets and organic superconductors, which appears to many to have the potential of contributing an enormous amount to the development of new materials of commercial value in the coming years, is presently funded at a level, which is only of the order of one thousandth of that devoted to research in natural products chemistry! One cannot help but conclude that a better return on the funding dollar could be had by increasing by a modest amount the level of support to the organics, particularly to the synthesis of the organics.

Support from the Department of Energy and from the Office of Naval Research is gratefully acknowledged for the meeting.

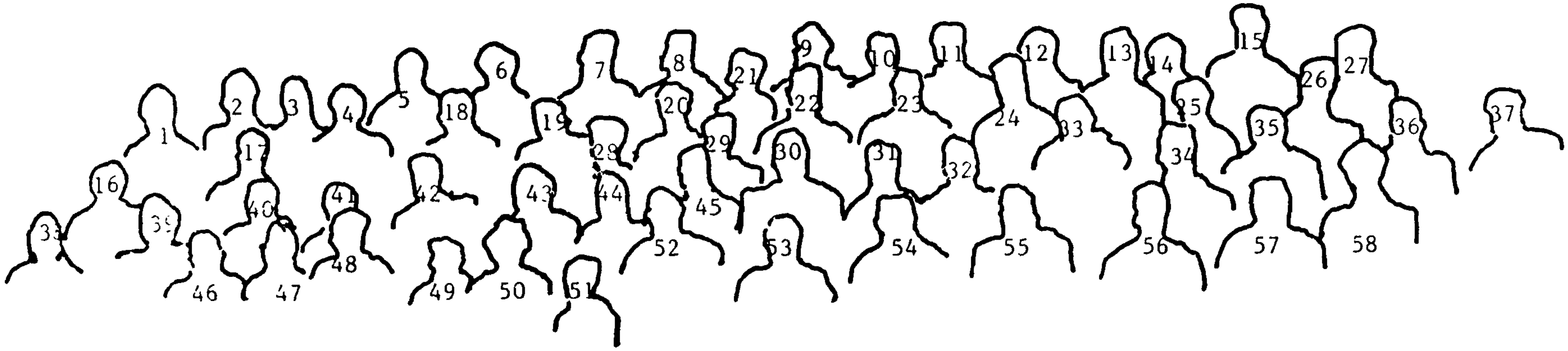
Respectfully submitted,

William A. Little
Principal Investigator

Attendees: International Conference on Organic Superconductivity

May 20 - 24th, 1990

Fallen Leaf Lake, South Lake Tahoe, California, USA



1. Liaping Le 2. S. Yoon 3. S. D'Arcangelis 4. W. A. Little 5. D. Cowan 6. L. Montgomery 7. P. Erk
8. M.Holcomb 9. J. Brill 10. J. Schirber 11. R. L. Greene 12. J. Medrano 13. J. Novoa 14 .M. Weger
15 .B. Bush

16. W. Kang 17. O. Klein 18. G. Gruner 19. J. Ladik 20. T. Ishiguro 21. S. Brown 22. M. Zisk 23. F. Wudl
24. H.Morawitz 25. F. Higuchi 26. V. Kresin 27. A. Blumstein

28. G. Friedman 29. R. Kelley 30. M. Beno 31. M. Dreiling 32. E. Pope 33. J. Lagowski. 34. A. H. Alberts
35. T. Timusk 36. R. Elsenbaumer 37. S Wolf

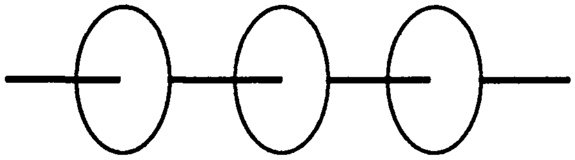
38. C. Caley 39. Y. Uemura 40. G. Saito 41. H. Wang 42. W. Smith 43. P. Chaikin 44. W. Fuller
45. S. Hannahs 46. R. Fainchtein 47. A. Hermann 48. J. Collman 49. H. Arnold 50. C. Agosta
51. A. Swanson 52. J. Williams 53. M. Whangbo 54. M. Tokumoto 55. G. Papavassiliou
56. K. Kornelson 57. J. Eldridge 58. H.Q. Lin

Absent: R. V. Kasowski

International Conference on Organic Superconductors

May 20 - 24, 1990,
Stanford Sierra Lodge, Fallen Leaf Lake,
South Lake Tahoe,
California, USA

Scientific Program
Abstracts
&
List of Participants



PROGRAM OUTLINE

SUNDAY	MONDAY	TUESDAY	WEDNESDAY	THURSDAY
	9:00 W. A. Little: Welcome & Introduction 9:30 R. L. Greene 10:15 Group Photograph	9:00 T. Timusk 9:45 T. Ishiguro 10:05 S. Hannahs 10:25 V. Kresin	9:00 J. Ladik 9:45 A. H. Hermann 10:05 J. E. Eldridge 10:25 E. E. Laukhina	9:00 P. Batail 9:45 J. P. Collman 10:05 W. Kang 10:25 C. C. Agosta
	10:45 COFFEE	COFFEE	COFFEE	COFFEE
	11:00 G. Saito 11:45 G. Gruner 12:10 J. Williams	11:00 Synthesis Panel D. Cowan, J. Collman, R.L. Elsenbaumer, B. Hoffman, F. Wudl	11:00 M. Takumoto 11:45 J. Schirber 12:05 H. H. Wang	11:00 E. B. Yasgubskii 11:45 R. V. Kasowski 12:05 A. I. Kotov 12:25 W. A. Little (Close)
	1:00 p.m. LUNCH	LUNCH	LUNCH	LUNCH
3:00 p.m. CHECK-IN	FREE	FREE	FREE	Adjourn Meeting
	4:00 pm R. L. Elsenbaumer 4:45 T. Uemura 5:15 S. Wolf 5:30 M. Whangbo	4:00 P. Chaikin 4:45 P. Erk 5:10 S. Pan 5:30 H. Q. Lin	4:00 M. Weger 4:45 G. C. Papavassiliou 5:10 D. Cowan 5:30 J. J. Lagowski	
7:00 p.m. DINNER	7:00 p.m. DINNER	7:00 p.m. DINNER	7:00 p.m. BANQUET	
8:00 p.m. RECEPTION	RESERVED	POSTER SESSION		

WELCOME

The members of the organizing committee wish to welcome you to the International Conference on Organic Superconductors at the Stanford Sierra Conference Center at South Lake Tahoe. This conference commemorates the twenty-first anniversary of the first such Conference which was held in the Fall of 1969, in Honolulu. The intent of that meeting was to bring together theoretical and experimental physicists, and theoretical, organic and inorganic chemists, and introduce them to the challenge of designing and synthesizing polymeric, organic compounds which would superconduct at high temperatures. That conference served to catalyze work in this area and within the next decade the first superconductors intercalated with organic compounds were prepared; in 1975, the first polymeric superconductor was synthesized; and, in 1980, the first organic superconductor was discovered. Much progress has been made in the past decade, with more than thirty organic superconductors now known, and some with transition temperatures above 11K. On the other hand, the search for high temperature superconductivity appeared more elusive, with little progress made until the discoveries of the high T_c cuprates in 1986. Today, however, the possibility remains as strong as ever, that the organics may yet yield materials with transition temperatures comparable to, or higher, than those of the cuprates.

In view of these recent developments, it seemed appropriate on this anniversary occasion, to bring together once more, a similar group of physicists and chemists to review the progress that has been made in recent years, and to consider new approaches to the synthesis of other classes of conducting or possibly superconducting compounds. This received the enthusiastic support of the United States Department of Energy and the Office of Naval Research. These agencies also have endorsed our proposal to include a substantial number of students in the meeting, recognising in so doing, the long term nature of the field, and the need for involving both the present and the next generation of scientists in it.

The program has been organized to include both review talks of each of several key areas which will serve as an introduction to those new to the field, and presentations of original, recent contributions by those most active in them. These two, in some sense, are expected to lay the ground work for the main focus of the meeting, which is to stimulate the participants to consider new and different materials to synthesize. This it is hoped, will lead to the discovery of new classes of superconductors, or materials with other novel properties. The program also has been organized in such a way as to keep the physicists and chemists together, interleaving recent theoretical and experimental work, with work on the synthesis or strategic design of chemical synthesis; rather than separating the sessions into those that are predominantly of interest to physicists, and others predominantly of interest to chemists. We have tried to leave ample time for discussion and interaction among the participants, both in and out of the formal sessions. We hope you will have an interesting and stimulating meeting, and the opportunity to enjoy the high Sierras.

W. A. Little

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International Conference on Organic Superconductors
(May 20-24, 1990, South Lake Tahoe, California, USA)

SUNDAY, MAY 20th

3:00 p.m. - 6:00 p.m.	CHECK-IN AND REGISTRATION
6:30 p.m.	DINNER
8:00 p.m. -10:30 p.m.	RECEPTION, Meeting Room 2A/B

MONDAY, MAY 21st

Chair: V. Kresin **SESSION I.**

9:00 a.m. W. A. Little, Stanford University, Stanford, CA
WELCOME AND INTRODUCTION

9:30 a.m. R. L. Greene, University of Maryland,College Park, MD
ORGANIC AND OXIDE SUPERCONDUCTORS:
AN EXPERIMENTAL COMPARISON.

10:15 a.m. Group Photograph

10:30 a.m. COFFEE

Chair: A. Hermann **SESSION II.**

11:00 a.m. G. Saito, Kyoto University, Kyoto, Japan
PRESENT STATUS OF ORGANIC SUPERCONDUCTOR
κ-(BEDT-TTF)$_2$ [Cu(NCS)$_2$]

11:45 a.m. G. Gruner, University of California, Los Angeles, CA
THE ELECTRODYNAMICS OF ORGANIC SUPERCONDUCTORS.

12:10 p.m.. J. M. Williams, Argonne National Laboratory, Argonne, IL
DESIGN STRATEGY FOR THE SYNTHESIS OF SUPERCONDUCTORS BASED ON BEDT-TTF AND RELATED ELECTRON-DONOR MOLECULES

1:00 p.m LUNCH

2:00 p.m. - 5:00 p.m. FREE

MONDAY, MAY 21st (Continued)

Chair G. Saito **SESSION III**

5:00 p.m. R. L. Elsenbaumer, Allied-Signal, Inc., Morristown, NJ
EMERGING STRUCTURE PROPERTY RELATIONSHIPS IN ELECTRICALLY CONDUCTIVE POLYMERS: POLY(THIENYLENE VINYLENES) AND POLY(PHENYLENE VINYLENES)

5:45 p.m. Y. J. Uemura, Columbia University, New York, NY
μSR MEASUREMENTS OF MAGNETIC PENETRATION DEPTH IN (BEDT-TTF)$_2$ Cu(NCS)$_2$: COMPARISONS WITH HIGH-T_c SUPERCONDUCTORS

6:10 p.m. S. A. Wolf, Naval Research Laboratory, Washington, D.C.
ORGANIC SUPERCONDUCTORS vs CUPRATES

6: 30 p.m. M. -H. Whangbo, North Carolina State University, Raleigh, NC
EFFECTS OF CH...ANION AND CH...DONOR CONTACT INTERACTIONS ON LATTICE SOFTNESS AND CRYSTAL PACKING PATTERN

7:00 p.m. DINNER

8:30 p.m.- 10:30 p.m. RESERVED

TUESDAY, MAY 22nd

Chair: J. M. Williams **SESSION IV**

9:00 a.m. T. Timusk, McMaster University, Hamilton, Ont. Canada
THE INFRARED RESPONSE OF THE EXOTIC SUPERCONDUCTORS

9:45 a.m. T. Ishiguro, Kyoto University, Kyoto, Japan
UNIAXIAL STRESS EFFECTS ON ORGANIC SUPERCONDUCTORS

10:05 a.m. S. T. Hannahs, Francis Bitter National Magnet Lab., Cambridge, MA
PRESSURE DEPENDENCE OF THE HALL EFFECT AND GIANT OSCILLATIONS IN (TMTSF)$_2$PF$_6$

10:25 a.m. V. Z. Kresin, Lawrence Berkeley Laboratory, Berkeley, CA
PAIR CORRELATIONS IN π-ELECTRON SYSTEMS

10:45 a.m. COFFEE

TUESDAY, MAY 22nd (Continued)

Chair: W. A. Little **SESSION V**

11:00 a.m. PROSPECTS FOR NEW DISCOVERIES IN THE ORGANICS

SYNTHESIS PANEL
D. O. Cowan, R. L. Elsenbaumer, J. Collman, B. Hoffman, F. Wudl

1:00 p.m. LUNCH

2:00 p.m. - 5:00 p.m. FREE

Chair: M. Weger **SESSION VI**

5:00 p.m. P. Chaikin, Princeton University, Princeton, NJ
THERMOELECTRIC AND OTHER ELECTRONIC EFFECTS IN ORGANIC CONDUCTORS.

5:45 p.m. P. Erk*, Universität Würzburg, Würzburg, Bundesrepublik Deutschland
STRUCTURAL AND ELECTRONIC PROPERTIES OF HIGHLY CONDUCTING DICYANOQUINONEDIIMINE (DCNQI) RADICAL ANION SALTS.

6:10 p.m. S. Pan*, University of Texas at Austin, Austin, TX
SCANNING TUNNELING MICROSCOPY OF QUASI ONE-DIMENSIONAL ORGANIC CONDUCTORS

6:35 p.m. H. Q. Lin*, Los Alamos National Lab., Los Alamos, NM
PHASE DIAGRAM OF ANISOTROPIC TWO-DIMENSIONAL QUARTER-FILLED BAND OF INTERACTING ELECTRONS

7:00 p.m. DINNER

8:30 p.m. **POSTER SESSION**

Meeting Room 2A/B
Open Bar

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* For Co-authors, see Abstracts

WEDNESDAY, MAY 23rd

Chair: M. -H. Whangbo **SESSION VII**

9:00 a.m. J. Ladik, Friedrich-Alexander-University, Erlangen-Nürnberg, Erlangen, FRG
WHAT WE CAN LEARN FROM THE HIGH-T_C SUPERCONDUCTORS FOR THE DESIGN OF ORGANIC SUPERCONDUCTORS ?

9:45 a.m. A. M. Hermann, University of Colorado, Boulder, CO
THALLIUM-BASED COPPER OXIDE SUPERCONDUCTORS

10:05 a.m.. J. Eldridge*, University of British Columbia, Vancouver, B. C., Canada
INFRARED OPTICAL PROPERTIES OF THE DEUTERATED FORM OF THE 10K ORGANIC SUPERCONDUCTOR (BEDT-TTF)$_2$ [Cu(NCS)$_2$]

10:25 a.m. E. E. Laukhina*, Chemogolovka, Moscow Region, USSR
CONVERSION OF THE POLYIODIDES OF ET INTO SUPERCONDUCTOR β-(ET)$_2$I$_3$ WITH $T_C = 7.5$K

10:45 a.m. COFFEE

Chair: R. L. Greene **SESSION VIII**

11:00 a.m. M. Tokumoto*, Electrotechnical Laboratory, Tsukuba, Ibaraki, Japan
FERMI SURFACE STUDY OF TWO-DIMENSIONAL ORGANIC METALS (BEDT-TTF)$_2$ X

11:45 a.m. J. Schirber*, Sandia National Laboratories, Los Alamos, NM
THE ROLE OF PRESSURE IN THE STUDY OF ORGANIC SUPERCONDUCTORS

12:05 P.m. H. H. Wang*, Argonne National Laboratory, Argonne, IL
TWO NEW AMBIENT PRESSURE ORGANIC SUPERCONDUCTORS: α– (BEDT-TTF)$_2$(NH$_4$)Hg(SCN$_3$) AND β_m-(BEDO-TTF)$_3$Cu$_2$(NCS)$_3$

1:00 p.m. LUNCH

2:00 p.m. - 5:00 p.m. FREE

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* For Co-authors, see Abstracts

WEDNESDAY, MAY 23rd (Continued)

Chair: P. Chaikin **SESSION IX**

5:00 p.m. M. Weger*, Hebrew University, Jerusalem, Israel
AN ELECTRONIC BAND STRUCTURE CALCULATION OF
$(\text{BEDT-TTF})_2\,\text{I}_3$

5:45 p.m. G. C. Papavassiliou*, National Hellenic Research Foundation, Athens, Greece
CONDUCTING AND SUPERCONDUCTING SOLIDS BASED ON SOME NEW DONOR MOLECULES

6:10 p.m. D. Cowan*, The Johns Hopkins University, Baltimore, MD
STUDY OF TTeF-TCNQ AND RELATED COMPOUNDS

6:35 p.m. J. J. Lagowski*, The University of Texas at Austin, Austin, TX
THE SYNTHESIS AND CHARACTERIZATION OF ORGANO-METALLIC MULTIDECKER SANDWICH POLYMERS

7:30 p.m. BANQUET

THURSDAY, MAY 24th

Chair: T. Ishiguro **SESSION X**

9:00 a.m. P. Batail, Universite Paris-Sud, Orsay, France
DESIGN, H-BONDING AND ELECTRONIC PROPERTIES OF ORGANIC - INORGANIC HYBRID SALTS

9:45 a.m. J. P. Collman, Stanford University, Stanford, CA
SHISH-KEBAB POLYMERS

10:05 a.m. W. Kang*, Princeton University, Princeton, NJ
ABSENCE OF SPIN-DENSITY WAVE TRANSITIONS IN $(\text{TMTSF})_2\,\text{NO}_3$

10:25 a.m. C. C. Agosta*, Francis Bitter Nastional Lab., Boston, MA
MAGNETO-RESISTANCE AND HALL EFFECTS OF $(\text{TMTSF})_2\,\text{ClO}_4$
IN A PULSED MAGNETIC FIELD

10:45 a.m. COFFEE

THURSDAY, MAY 24th (Continued)

Chair: W. A. Little

SESSION XI

11:00 a.m.	E. B. Yagubskii*, Institute of Chemical Physics, Chernogolovka, USSR NEW CLASS OF THE DITHIOLENE ELECTROCONDUCTING COMPOUNDS: CATION COMPLEXES OF METALS WITH DDDT
11:45 a.m.	R. V. Kasowski, E. I. Du Pont de Nemours & Co., Wilmington, DE MOLECULAR IDENTITIES IN FIRST PRINCIPLES SELF-CONSISTENT BAND STRUCTURE CALCULATIONS FOR ORGANIC SUPERCONDUCTING SALTS.
12:10 p.m.	A. I. Kotov*, Institute of Chemical Physics, Chernogolovka, USSR HIGHLY CONDUCTING COMPLEXES BASED ON AU(III)-BIS(1,3-DITHIO-2-THION-4,5-DITHIOLATO)
12:35 p.m.	W. A. Little, Stanford University, Stanford, CA CLOSING REMARKS
1:00 p.m.	LUNCH

Attendees Depart

MONDAY, MAY 21st

ABSTRACTS

SESSION I

Speakers

9:00 a.m.: W. A. Little
9:45 a.m.: R. L. Greene

SESSION II

11:00 a.m.: G. Saito
11:45 a. m.: G. Gruner
12:10 a.m.: J. M. Williams

SESSION III

5:00 p.m.: R. L. Elsenbaumer
5:45 p.m.: Y. J. Uemura
6:10 p.m.: S. A. Wolf
6:30 p.m.: M. -H. Whangbo

ORGANIC AND OXIDE SUPERCONDUCTORS: AN EXPERIMENTAL COMPARISON

R. L. Greene

Center for Superconductivity Research
Department of Physics
University of Maryland
College Park, MD 20742, USA

ABSTRACT

Both Organic superconductors and Oxide superconductors have unusual normal state and superconducting properties. It is likely that the mechanism for superconductivity in these materials is "unconventional". In this talk I will review the most reproducable currently available experimental data in order to identify the pairing state in these two classes of superconductors. Properties such as resistivity (ac and dc), specific heat, NMR, infrared reflectivity tunneling and electromagnetic penetration depth will be discussed and compared.

PRESENT STATUS OF ORGANIC SUPERCONDUCTOR κ-(BEDT-TTF)$_2$[Cu(NCS)$_2$]

Gunzi Saito, Hatsumi Mori* and Kokichi Oshima**

Dep. of Chemistry, Fac. of Science, Kyoto University,
Kyoto 606; *International Superconductivity Technology
Center, Nagoya 456, ** Dep. of Physics, Fac. of Science,
Okayama University, Okayama 700, Japan

ABSTRACT

Structural and physical properties of an organic superconductor κ-(BEDT-TTF)$_2$[Cu(NCS)$_2$] and its related new member (BEDT-TTF)$_2$[NH$_4$Hg(SCN)$_4$] (Tc=0.8K) will be presented. The Cu(NCS)$_2$ salt showed an inverse isotope effect, namely Tc of ^{13}C-salt is between those of the H-salt (10.4K) and D-salt(11.1K). Hc$_2$ values of this salt were obtained from the resistance recovery with the magnetic field. The resistive transition width showed characteristic broadening, which suggests the flux-flow resistance. The parallel Hc$_2$ values exceed Pauli limited value. The transport critical current density was estimated as Jc=100 A/cm^2 (5.1K, 0 T). The tunneling spectra and magnetic field penetration depth measurements suggest that the Cu(NCS)$_2$ salt has anisotropic gaps. Shubnikov-de Haas oscillations were observed in both salts.

THE ELECTRODYNAMICS OF ORGANIC SUPERCONDUCTORS

K. Holczer*, D. Quinlivan*, G. Gruner*, and F. Wudl**

Department of Physics and Solid State Science Center*,
University of California, Los Angeles,CA
Department of Physics**, University of California, Santa Barbara, CA

ABSTRACT

We have measured the superconducting penetration depth and surface impedance in κ-{BEDT-TTF}$_2$Cu{NCS}$_2$ using microwave techniques. $\lambda(T)$ is strongly suggestive of singlet pairing, with a magnitude in agreement with that evaluated from parameters which determine the optical properties in the normal state. Both the normal and superconducting state is characterized by extreme anisotropy, which determines the low frequency electrodynamics of the normal and superconducting state.

DESIGN STRATEGY FOR THE SYNTHESIS OF SUPERCONDUCTORS BASED ON BEDT-TTF AND RELATED ELECTRON-DONOR MOLECULES

J. M. Williams, H. H. Wang, K. D. Carlson, A. M. Kini,
M. A. Beno, U. Geiser and M.-H. Whangbo†

Chemistry and Materials Science Divisions,
Argonne National Laboratory, Argonne, IL 60439, USA
†Department of Chemistry, North Carolina State University,
Raleigh, NC, 27695, USA

ABSTRACT

The largest number of known organic superconductors have been derived from the electron-donor molecule BEDT-TTF in combination with simple [viz., I_3^-, IBr_2^-, AuI_2^- etc.] and complex [$Cu(NCS)_2^-$, $Hg_{3-x}Cl_8^{n-}$ etc.] anions. The BEDT-TTF/anion structure types are quite varied [β-, κ-, θ etc.] and structure-property relationships, which are invaluable in the design of new superconductors, exist only for the well-known β-phase materials. The design strategy for the synthesis of β-phase, and entirely new BEDT-TTF and related superconductors, will be presented.

Work at Argonne National Laboratory and at North Carolina State University was supported by the Office of Basic Energy Sciences (DOE), Division of Materials Sciences, U. S. Department of Energy, under Contract W-31-109-ENG-38 and Grant DE-FG05-86ER45259, respectively.

EMERGING STRUCTURE PROPERTY RELATIONSHIPS IN ELECTRICALLY CONDUCTIVE POLYMERS: POLY(THIENYLENE VINYLENES) AND POLY(PHENYLENE VINYLENES)

R.L. Elsenbaumer, H. Eckhardt, L.W. Shacklette, and K.Y. Jen

Polymer Sciences Laboratory
Allied-Signal, Inc.
P.O. Box 1021R
Morristown, NJ 07960 USA

ABSTRACT

The electronic and electrochemical properties of poly(p-phenylene vinylene), poly(thienylene vinylene), and derivatives containing electron donating substituents such as methyl, methoxy, ethoxy, and butoxy groups were studied using electrochemical and optical techniques. It was found that electrochemically derived band gaps agree well with band gap values obtained from optical measurements. Substitution with electron donating groups substantially lowers both oxidation potentials and band gaps. A similar effect is attributed to the introduction of a vinylene linkage between aromatic rings along the polymer backbones. Our findings imply that through the proper choice of base polymer and substituents one can adjust the electrochemical potentials for the onset of oxidation and reduction as well as substantially red shift the absorption edge of conjugated electrically conductive polymers. The ability to tailor these important properties provides unique application possibilities.

μSR measurements of magnetic penetration depth in $(BEDT-TTF)_2Cu(NCS)_2$

Comparisons with high-T_c superconductors

Y.J. Uemura

Department of Physics, Columbia University, New York, NY 10027

We have performed muon spin relaxation (μSR) measurements [1] in single crystals of $(BEDT-TTF)_2Cu(NCS)_2$, by applying an external magnetic field of 3.1 kG perpendicular to the conducting b-c plane. The muon spin relaxation rate σ increased with decreasing temperature below T_c towards $\sigma(T \rightarrow 0) \sim 0.12 \mu sec^{-1}$, which corresponds to a penetration depth $\lambda_{inplane} = 8000$ Å. The relaxation rate σ is proportional to $1/\lambda^2$ and consequently to n_s/m^* (carrier density / effective mass) in the clean limit. When we plot $\sigma(T \rightarrow 0)$ versus T_c, the point from the organic system lies close to the universal relation which we found in cuprate high-T_c superconductors [2]. This might suggest a common condensation mechanism of the organic and high-T_c superconductors, which share various features, such as, 2-dimensional electronic structure, strong correlation among charge carriers, low carrier density, large Ginzburg-Landau parameter κ, etc.

This work has been performed in collaboration with G. Saito, H. Yamochi, G.M. Luke, J.H. Brewer, and many other scientists.

[1] Y.J. Uemura *et al.*, Proceedings of the NATO Advanced Research Workshop on *Dynamics of Magnetic Fluctuations in High-T_c superconductors*, Crete, Oct. 1989, Plenum (1990), in press; Y.J. Uemura *et al.*, Proceedings of Int. Conf. Muon Spin Rotation, Oxford, April 1990, Hyperfine Interactions, in press.

[2] Y.J. Uemura *et al.*, Phys. Rev. Lett. 62, 2320 (1989).

ORGANIC SUPERCONDUCTORS VS. CUPRATES

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**Lawrence Berkeley Laboratory,
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ABSTRACT

Based on the recent evaluation of the major normal and superconducting parameters of high T_c oxides [1], a detailed comparison of the organic superconductors and the cuprates will be carried out. The criterion $\xi_0 << l$ (ξ_0 is the coherence length, l is the mean free path) appears to be satisfied for organic superconductors as well as for the new high T_c oxides. This leads to the possibility of observing a multigap structure. As a result, the experimental data can be interpreted in terms of usual s-wave pairing.

1. V. Kresin and S. Wolf, Phys. Rev. **B41**, 4278 (1990); preprint.

EFFECTS OF C-H···ANION AND C-H···DONOR CONTACT INTERACTIONS ON LATTICE SOFTNESS AND CRYSTAL PACKING PATTERN

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ABSTRACT

Crystal packing patterns and lattice softness of superconducting organic charge-transfer salts are examined by analyzing the nature of various C-H···anion and C-H···donor interactions present in the salts. Interaction energies calculated for these intermolecular contacts by ab initio correlated electronic structure calculations are discussed.

Acknowledgments

Work at North Carolina State University and at Argonne National Laboratory is supported by the Office of Basic Energy Sciences, Division of Materials Sciences, U. S. Department of Energy, under Grant DE-FG05-86ER45259 and Contract W-31-109-ENG-38, respectively.

TUESDAY, MAY 22nd

ABSTRACTS

SESSION IV

9:00 a.m.: T. Timusk
9:45 a.m.: T. Ishiguro
10:05 a.m.: S. T. Hannahs
11:25 a.m.: V. Z. Kresin

SESSION V

11:00 a.m.: SYNTHESIS PANEL

D. O. Cowan
J. P. Collman
R. L. Elsenbaumer
B. Hoffman
F. Wudl

SESSION VI

5:00 p.m.: P. Chaikin
5:45 p.m.: P. Erk
6:10 p.m.: S. Pan
6:35 p.m.: H. Q. Lin

POSTER SESSION

8:00 p.m.

THE INFRARED RESPONSE OF THE EXOTIC SUPERCONDUCTORS.

T. Timusk

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The three new families of superconductors, the organic conductors, the heavy Fermion metals and the high T_c oxides share an unusal response to infrared. All have a temperature dependent Drude-like mode and a temperature independent mid-infrared band. The fraction of oscillator strenth of the Drude portion is lowest in the organics highest in the oxides. Coupling of the midinfrared band to phonons is seen in all the systems through antiresonant phonon lineshapes. Together, these properties point to unconventional transport in the normal state.

UNIAXIAL STRESS EFFECTS ON ORGANIC SUPERCONDUCTORS

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ABSTRACT

The electronic structure of the organic superconductor is affected by the overlap between constituent molecules which is sensitive to the intermolecular spacing. Although the interaction is anisotropic, integrated effects on different directions have been investigated through either hydrostatic pressure application or chemical substitution. To elucidate the interactions more specifically, uniaxial stress is suitable. By suppressing thermal contraction in one direction $(ET)_2Cu(NCS)_2$ is uniaxially elongated, and shift in T_c and enhancement of resistance maximum are observed. This result is argued mainly in the light of intermolecular interactions. Also, application of the method to the other organic superconductors and a method to control the stress will be presented.

PRESSURE DEPENDENCE OF THE HALL EFFECT AND GIANT OSCILLATIONS IN $(TMTSF)_2PF_6$

S. T. Hannahs,[a] W. W. Kang,[b] J. S. Brooks,[c]
P. M. Chaikin,[b,d] and L. Y. Chiang[d]

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[b] Princeton University, Princeton New Jersey 08544
[c] Boston Univeristy, Boston Massachusetts 02215
[d] Exxon Research and Engineering, Annandale, New Jersey 08801

ABSTRACT

The compound $(TMTSF)_2PF_6$ exhibits a complicated pressure dependent Hall effect. We have measured this pressure dependence at low temperatures and high magnetic fields. Near the critical pressure where the ambient pressure Spin Density Wave (SDW) state is supressed leading to superconductivity, the Hall effect shows a complicated structure. At higher pressures and low temperatures the Quantum Hall Effect is observed along with a series of Field Induced SDW states. At higher temperatures we observe giant oscillations in the magneto-transport. We will discuss the pressure dependence of both the onset and frequencies of the FISDW and the giant oscillations.

PAIR CORRELATION IN π -ELECTRON SYSTEMS

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ABSTRACT

Pair correlations of the superconducting type in large aromatic molecules is discussed. The analysis is based on the theory of finite Fermi systems. Pair correlation of the π-electrons has many similarities with correlations in nuclei as well as with usual macroscopic superconductivity. The origin of the correlation is due to large electron-vibrational coupling and is virtual σ-π transitions. If the molecule contains several spatially separated groups of π-electrons, the Little mechanism can also contribute to pairing. The behavior of a large π-electron system in external electric and magnetic fields is affected by the pair correlation. Charge transfer in large systems also will be discussed.

THERMOELECTRIC AND OTHER ELECTRONIC EFFECTS IN ORGANIC CONDUCTORS

P. M. Chaikin

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Structural and Electronic Properties of Higly Conducting Dicyanoquinonediimine (DCNQI) Radical Anion Salts

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J. U. von Schütz, H.-P. Werner and H. C. Wolf
3. Physikalisches Institut, Universität Stuttgart, Pfaffenwaldring 57
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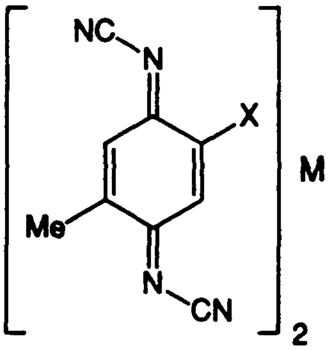
Abstract: The facile one-step synthesis of dicyanoquinonediimines (DCNQIs) from the corresponding substituted quinones provides an easy access to a large variety of powerful new electron acceptors. This new class of quinoid compounds has allowed for the preparation of numerous organic conductors with conductivities as high as $\sigma = 500,000$ Scm^{-1}.

Synthesis and structural results of the highly conducting salts $[2\text{-X-5-Me-DCNQI}]_2M$ (X = Cl, Br, I, Me, MeO; M = Cu, Ag, Li) will be presented with respect to the influence of substituents and counterions.



The DCNQI salts of non-copper cations behave als one-dimensional conductors and can be classified as metal-like semiconductors due to the temperature dependance of their conductivity. The one-dimensional behavior is implicated by the occurrance of $4k_f$ and $2k_f$ phase transitions.

A non-activated metallic conductivity is found in copper salts of the DCNQIs at higher temperatures. Chloro- and bromo-substituted salts undergo phase transitions into a semiconducting state similar to the corresponding non-copper salts. All the other copper salts retain their metallic conductivity down to the lowest temperatures with extremely high values of $\sigma = 500,000$ Scm^{-1}. The behaviour of the copper salts is discussed in terms of their structural and electronic properties, especially with respect to the electronic and ligating abilities of the DCNQI-acceptors, which provide the goal to a new building-concept for organic conductors.

SCANNING TUNNELING MICROSCOPY OF QUASI ONE-DIMENSIONAL ORGANIC CONDUCTORS

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R. Fainchtein

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ABSTRACT

We have studied samples of TTF-TCNQ, $(TMTSF)_2ClO_4$, and $(BEDT\text{-}TTF)_2Cu(NCS)_2$ with three different scanning tunneling microscopes covering a temperature range from 300K down to 0.043K. The images taken under ambient conditions clearly show linear chains with the expected spacing and small features due to the stacking of flat molecules. On TTF-TCNQ single crystal samples, both room temperature and low temperature topographic images taken in ultra-high vacuum clearly show one dimensional molecular chains forming lattice structures with period of about 1.2nm. At temperatures below approximately 80K a modulation with period of about 2.4nm has also been observed. This modulation is commensurate with the underlying lattice. We attribute this to the direct observation of charge density waves on this type of material. Low temperature spectroscopy data shows a 50mV energy gap, which confirms the CDW phase transition. These results confirm on a microscopic scale, for the first time, the known properties of these materials determined by macroscopic techniques like X-ray diffraction, neutron-scattering and dc conductivity.

PHASE DIAGRAM OF ANISOTROPIC TWO–DIMENSIONAL QUARTER–FILLED BAND OF INTERACTING ELECTRONS

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and

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ABSTRACT

Using the anisotropic two-dimensional extended Hubbard Hamiltonian, we propose a phase diagram to explain simultaneously (1) the pressure-induced BOW (spin-Peierls) to SDW transition in TMTTF salts; (2) the magnetic-field-induced SDW in TMTSF salts; and (3) the absence of SDW in BEDT-TTF materials. The phase diagram consists of three parts: the spin density wave(SDW), bond-order wave(BOW), and possibly "frustrated" phases. The spin-spin, bond-bond, and charge-charge correlation functions are calculated numerically. We examine in detail the separate roles of Coulomb interactions, band-filling, and degree of anisotropy. Our results provide a unified picture of the "normal", i.e., non-superconducting, phases.

WEDNESDAY, MAY 23rd

ABSTRACTS

SESSION VII

9:00 a.m.: J. Ladik
9:45 a.m.: A. M. Hermann
10:05 a.m.: J. Eldridge
10:25 a.m. E. E. Laukhina

SESSION VIII

11:00 a.m.: M. Tokumoto
11:45 a.m.: J. Schirber
12:10 a.m.: H. H. Wang

SESSION IX

5:00 a.m.: M. Weger
5:45 a.m.: G. C. Papavassiliou
6:10 a.m.: D. O. Cowan
6:35 p.m.: J. J. Lagowski

WHAT CAN WE LEARN FROM HIGH T_C CERAMIC SUPERCONDUCTORS FOR THE DESIGN OF ORGANIC SUPERCONDUCTORS?

Janos J. Ladik

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ABSTRACT

From the breakthrough in the field of inorganic superconductors (ceramic materials) we can see that the system has to be 1) two-dimensional, 2) it should have a broader partially filled band 3) some filled narrow bands. The latter two conditions fulfill the requirements of a generalized polarization model which includes as special case the excitonic model of superconductivity. At the end of the lecture some examples to design possible new organic superconductors will be presented.

THALLIUM-BASED COPPER OXIDE SUPERCONDUCTORS

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ABSTRACT

Stable bulk superconductors in the Tl-Ca-Ba-Cu-O system with zero resistance above 120K are discussed. Structural, magnetic, and electronic transport properties are presented. A variety of procedures for preparing bulk, wire, thick-film, and thin-film samples are discussed. Special emphasis is given to safe preparation procedures, wherein Tl is added through a vapor-phase reaction to Ca-Ba-Cu-O precursors. Transport data showing zero resistance temperatures of 120K for thick films and 113K for thin films formed by this process are presented. In some cases, highly oriented 2122 thin films with T_c about 100K were deposited. Deposition procedures, x-ray diffraction analysis, and transport measurements for these oriented films are presented.

INFRARED OPTICAL PROPERTIES OF THE DEUTERATED FORM OF THE 10K ORGANIC SUPERCONDUCTOR $(BEDT\text{-}TTF)_2[Cu(NCS)_2]$*

K. Kornelsen and J. Eldridge,

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and
Hau H. Wang and Jack M. Williams

Chemistry and Materials Science Divisions, Argonne
National Laboratory, Argonne, Illinois 60439 U.S.A.

ABSTRACT

Polarized reflectivity measurements at 295K, 100K, 50K and 25K are reported for (deuterated $BEDT\text{-}TTF)_2[Cu(NCS)_2]$ from 200 cm^{-1} to 6000 cm^{-1}. The optical conductivities obtained from Kramers-Kronig analyses show a dramatic increase in the far-infrared below 50K, and a mid-infrared band which is a maximum at 100K, which correlates with the minimum in the d.c. conductivity. The vibrational features have been assigned to a predominant mixture of normally-inactive a_g modes and normally-active b_{2u} modes of the ET molecule. A few of both types couple strongly to the charge carriers, and in particular appear to couple to those that oscillate between dimers oriented perpendicular to each other.

CONVERSION OF THE POLYIODIDES OF ET INTO SUPERCONDUCTOR β-$(ET)_2I_3$ WITH T_c=7.5K

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ABSTRACT

Five polyiodides of ET: α, β-$(ET)_2I_3$, ε-$(ET)_2I_7$, η-$(ET)I_3$, ζ-$(ET)_2I_{10}$ have been obtained by iodine oxidation of ET. The thermolysis of these compounds has produced crystals of the superconducting β^*–$(ET)_2I_3$ phase. On varying thermolysis conditions of ε- and ζ -modifications, there were obtained β^*-$(ET)_2I_3$ crystals with the superconducting transition that is fully completed by 6K (T_c=7.5K).

FERMI SURFACE STUDY OF TWO-DIMENSIONAL ORGANIC METALS (BEDT-TTF)$_2$X

M. Tokumoto, A. G. Swanson,[a] J. S. Brooks,[a]
S. T. Hannahs,[b] C. C. Agosta,[b] M. Tamura,[c]
H. Tajima,[c] H. Kuroda,[c] A. Ugawa,[d] K. Yakushi,[d]
N. Kinoshita, H. Anzai and J. R. Anderson[e]

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Observation of Shubnikov-de Haas (SdH) and de Haas-van Alphen (dHvA) oscillations in some two-dimensional organic metals (BEDT-TTF)$_2$X, including X=KHg(SCN)$_4$, θ-I$_3$ and β"-AuBr$_2$ salts, are reported.

In KHg(SCN)$_4$ salt, in addition to the SdH oscillations with frequency of 670 T corresponding to about 16 % of the first Brillouin zone(BZ), we observed splitting of each SdH peak which we ascribed to the "spin-splitting".

In θ-I$_3$ we have succeeded in an observation of quantum oscillations for the first time. We observed a "saw-tooth" dHvA oscillation indicating a highly two-dimensional and extraordinary clean electronic system. In addition to the fundamental frequency at 4170 T corresponding to 50.4 % of the first BZ and its higher harmonics, we observed an oscillation with lower frequency at 730 T corresponding to about 8.8 % of the first BZ.

THE ROLE OF PRESSURE IN THE STUDY OF ORGANIC SUPERCONDUCTORS

J. E. Schirber#, H. H. Wang* and J. W. Williams*

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Argonne National Laboroatory*, Argonne, IL 60439

ABSTRACT

A brief review of the key role played by pressure in the study of organic superconductivity will be given. Studies of the pressure dependence of the superconducting transition temperatures of the $(ET)_nX_m$ family using solid He pressure techniques will be discussed in detail, as well as our most recent results on the new BO materials.

Supported by US DOE under contract #DE-AC04-76DP00789.
* Supported by US DOE under contract #W-31-104-ENG-38.

TWO NEW AMBIENT PRESSURE ORGANIC SUPERCONDUCTORS: α-(BEDT-TTF)$_2$(NH$_4$)Hg(SCN)$_4$ AND β_m-(BEDO-TTF)$_3$Cu$_2$(NCS)$_3$

H. H. Wang, M. A. Beno, K. D. Carlson, U. Geiser,
A. M. Kini, and J. M. Williams

Chemistry and Materials Science Divisions
Argonne National Laboratory
Argonne, IL, 60439, USA

ABSTRACT

Two new ambient pressure organic superconductors have recently been characterized. The sulfur based material α-(BEDT-TTF)$_2$(NH$_4$)Hg(SCN)$_4$ becomes a superconductor at 1.15 K. The synthesis and related physical properties will be presented. Our efforts to replace the ammonium cation with other monopositive cations will be discussed. The first oxygen containing donor molecule salt, β_m-(BEDO-TTF)$_3$Cu$_2$(NCS)$_3$, superconducts at 1.06 K. Its synthesis and ESR properties will be compared with other BEDO-TTF based salts.

Work at Argonne National Laboratory is sponsored by the US Department of Energy (DOE), Office of Basic Energy Sciences, Division of Materials Sciences, under Contract W-31-109-ENG-38.

AN ELECTRONIC BAND STRUCTURE CALCULATION FOR β-(BEDT-TTF)$_2$I$_3$

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** Technical University, Darmstadt
@ Department of Physics, University of Stutgart
# Laboratoire de Physique des Solides,Orsay

ABSTRACT

The electronic band structure of β-(BEDT-TTF)$_2$I$_3$ was calculated, using the ASW method. The space between the 55 atoms per unit cell was characterized by 32 empty spheres. The calculation shows that the separation between the various bands is of order 0.2 eV, which is considerably less than the width of the bands (of order 0.5eV); thus the various bands intersect and the Huckel approximation is no longer valid. The band structure turns out to be two-dimensional, in accord with a previous calculation of Mori based on the Huckel approximation, and with experiment. A particular result of the calculation is that the empty spheres play an important role, and the charge in them depends critically upon the details of the calculation. Some computer runs suggest the presence of a gap somewhat above E_F. We performed a vacuum tunneling experiment to search for such a gap, but failed to observe it. At present, we cannot say whether the accuracy of the ASW method is sufficient to provide an accurate band structure.

CONDUCTING AND SUPERCONDUCTING SOLIDS BASED ON SOME NEW DONOR MOLECULES

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A. Hountas*, B. Hilti **, C. Mayer** and J. Zambounis**

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ABSTRACT

In this paper the preparation, crystal structure and properties of conducting and superconducting solids based on methylene-dithiotetrathiafulvalene, ethylene-dioxoethylene-dithiotetrathiafulvalene, ethylene-dioxomethylenediselenotetrathiafulvalene, ethylene-dioxovinylene-dithiotetrathiafulvalene and similar new π-donor molecules are described.

STUDY OF TTeF-TCNQ AND RELATED COMPOUNDS*.

D.O. Cowan (a), M.D. Mays (a), R.D. McCullough (a); T.J. Kistenmacher (b), T.O. Poehler (b); M.A. Beno (c), A.M. Kini (c), J.M. Williams (c), Y.K. Kwok (c), K.D. Carlson (c); L. Xioa (d), J.J. Novoa (d), M.H. Whangbo (d); J.P. Pouget (e).

(a) Department of Chemistry, The Johns Hopkins University, Baltimore, MD 21218 (b) Applied Physics Laboratory, The Johns Hopkins University, Laurel, MD 20707 (c) Chemistry and Materials Science Division, Argonne National Laboratory, Argonne, IL 60439 (d) Department of Chemistry, North Carolina State University, Raleigh, NC 27695-8024 (e) Universite Paris-Sud Laboratoire de Physique des Solides, Batiment 510, Centre Universitaire, 91405 ORSAY, Cedex, France

An improved synthesis of TTeF gives a 30% yield of the tellurium π-donor in a high purity state. Several inorganic and organic charge transfer salts have been prepared, from TTeF, e.g. salts of $TCNQ^-$, $TCNQF_4^-$, $DMTCNQ^-$, ClO_4^-, and ReO_4^-. X-ray diffraction, static magnetic susceptibility, electrical conductivity and thermoelectric power studies on TTeF-TCNQ as a function of temperature are interpreted in terms of a tight-binding electronic band structure calculation. The increase in electrical conductivity on going from S to Se to Te in TXF-TCNQ (where X = S, Se, Te) is shown to be consistent with the square of the donor bandwidths ($\sigma \propto W_D^2$). Preliminary measurements of other TTeF salts are described.

*This work was supported in part by the National Science Foundation, Solid State Chemistry Program, Grant DMR-8615305.

THE SYNTHESIS AND CHARACTERIZATION OF ORGANOMETALLIC MULTIDECKER SANDWICH POLYMERS

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The University of Texas at Austin
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ABSTRACT

The ligand exchange reaction of bis(η^6-naphthalene)chromium, to form poly[(μ-η^6,η^6-naphthalene)chromium] (poly[(μ-Np)Cr], Np=$C_{10}H_8$) and oligomers represents a generic synthetic pathway to organometallic polymers incorporating η-bonded bridging (μ) polycyclic arene ligands. The proposed mechanism of formation and the characterization of oligomers of poly[(μ-Np)Cr] is discussed to illustrate the assigned characterization of poly[(μ-Np)Cr], along with the electrochemistry of these kinds of species.

Direct metal atom synthesis is used to synthesize Np_2Cr; this route also can be used to produce multidecker sandwich polymers incorporating μ-arene moieties directly. Thus, the direct metal atom reaction of iron with dicyclopentadienylnickel (nickelocene), nickel with ferrocene, and chromium with $(C_6H_6)_2Mo$, results in the formation of ferrocene from nickelocene, nickelocene from ferrocene, and $(C_6H_6)_2Cr$ from $(C_6H_6)_2Mo$; multidecker sandwich polymers are also formed. For example CpNiCpFeCp (Cp=cyclopentadiene), CpFeCpNiCpFeCp, and BzMoBzCrBz (Bz=C_6H_6) were observed by mass spectrometry which undoubtedly represents fragments of higher polymers.

Complexing agents can act as dopants through mixing of density of states, and likewise can be utilized to effect distinct macromolecular architectures.

THURSDAY, MAY 24th

ABSTRACTS

SESSION X

9:00 a.m.: P. Batail
9:45 a.m.: J. P. Collman
10:05 a.m.: W. Kang
10:25 a.m. C. C. Agosta

SESSION XI

11:00 a.m.: E. B. Yagubskii
11:45 a.m.: R. V. Kasowski
12:10 p.m.: A. J. Kotov
12:35 p.m.: W. A. Little

ABSENCE OF FIELD INDUCED SPIN DENSITY WAVE TRANSITIONS IN $(TMTSF)_2NO_3$.

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ABSTRACT

An experimental selection rule for the coexistence of the superconductivity and the field-induced spin density wave (SDW) within a temperature-magnetic field phase diagram is observed in the Bechgaard salts. Yakovenko has recently proposed a theory that relates the superconductivity, the field-induced SDW, and the reentrant phase diagram within a single theoretical framework. In order to test this theory we have performed magnetotransport measurements in an organic conductor $(TMTSF)_2NO_3$ in pressure to 8 kbar, temperature down to 0.5 K, and field up to 10 tesla. The metallic state is stabilized above 8 kbar, but no superconductivity is observed down to 0.5 K. In the range of magnetic fields below 10 tesla the magnetoresistance looks reminiscent of the normal state magnetoresistance in $(TMTSF)_2ClO_4$ and $(TMTSF)_2PF_6$, but no field-induced transition is observed.

MAGNETO-RESISTANCE AND HALL EFFECT OF $(TMTSF_6)ClO_4$ IN A PULSED MAGNETIC FIELD

C. C. Agosta[a,b], S. Foner[a], J. S. Brooks[a,c],
W. G. Clark[d] and P. Chakin[e].

a) Francis Bitter National Magnet
Lab, b) IBM Postdoctoral Fellow, c)
Boston University*, d) University
of California at Los Angeles,
e)Princeton University

The organic superconductor $(TMTSF_6)ClO_4$ has a rich phase diagram which includes superconductivity, metalic behavior and spin density waves (SDW). In the region below 6K and above 28-30 tesla it is believed to be reentrant, losing its SDW properties and going back to a metalic phase. We have studied this region with a pulsed magnetic field apparatus to fields greater than 40 tesla. Our data includes both magneto-resistance and hall measurements taken with the field perpendicular to the a-b plane of the $(TMTSF_6)ClO_4$ sample. *Supported by NSF contract DMR-88-18510.

NEW CLASS OF THE DITHIOLENE ELECTROCONDUCTING COMPOUNDS: CATION COMPLEXES OF METALS WITH DDDT

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A.A. Ignatiev, L.I. Buravov, A.G. Khomenko,
V.E. Shklover*, S.S. Nahapetyan*, Y.T. Struchkov*

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Highly conducting compounds have been synthesized based on cation $M(dddt)_2$ (M = Ni, Pt, Au,; dddt = 5,6-dihydro--1,4-dithiin-2,3-dithiolato) complexes. The $[M(dddt)_2]^+$ cation chelates represent a new class of dithiolene compounds and their salts are metal complex analogs for the organic superconductors of BEDT-TTF cation radical salts family. Till now only anion and neutral metal complexes of dddt have been known, which are insulators. Crystals structures, conducting and optical properties of $[M(dddt)_2]^+$ salts have been studied.

MOLECULAR IDENTITIES IN FIRST PRINCIPLES SELF CONSISTENT BAND STRUCTURE CALCULATIONS FOR ORGANIC SUPERCONDUCTING SALTS

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ABSTRACT

The ab initio pseudofunction method with a full potential has been used to compute the electronic structure of β-$(BEDT\text{-}TTF)_2X$ ($X=I_3$, AuI_2, IBr_2) and κ-$(BEDT\text{-}TTF)_2Cu(NCS)_2$. The electronic structure is approximately molecular. The Fermi surface is similar to that obtained with the extended Huckel method. Comparison to Fermi surface and optical conductivity measurements will be shown. We will also show the electronic structure of TTF-TCNQ which is metallic but not superconducting.

HIGHLY CONDUCTING COMPLEXES BASED ON AU(III) - BIS(1,3-DITHIO-2-THION-4,5-DITHIOLATO)

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ABSTRACT

The anion [Au(dmit)]$_2$(dmit = 1,3-dithia-2-thione-4,5-di-thiolato) salts with various cations (Me_4N^+, Et_4N^+, n-Pr_4N^+, n-Bu_4N^+, $Et_2Bu_2N^+$, Et_3BuN^+, $EtBu_3N^+$, Me_3S^+, Bu_3S^+, pyridinium) was obtained in the partially oxidized state. Their conducting properties have been studied. A great number of these salts have a rather high room conductivity (σ = 1–500 Ohm^{-1}cm^{-1}), some of them retain metallic conductivity down to 1.5 K, others undergo the metal-semiconductor transition. The Au (dmit)$_2$ salt with the Et_4N^+ cation of the 1: 2 composition was obtained in two modifications (the α- and β-phases with metallic and semiconducting properties, respectively). The β-phase crystal structure was solved.

TUESDAY EVENING, MAY 22nd

ABSTRACTS

POSTER SESSION

SUPERCONDUCTIVITY, ELECTRICAL PROPERTIES, AND CRYSTAL AND BAND ELECTRONIC STRUCTURE OF CHARGE-TRANSFER SALTS DERIVED FROM THE NEW ELECTRON-DONOR MOLECULE BEDO-TTF.

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ABSTRACT.

Charge transfer salts of bis(ethylenedioxy)tetrathiafulvalene, BEDO-TTF, namely (BEDO-TTF)$_3$Cu$_2$(NCS)$_3$, (BEDO-TTF)$_2$AuBr$_2$, and (BEDO-TTF)$_m$X$_n$ where X$^-$ is I$_3^-$, AuI$_2^-$, Au(CN)$_2^-$, ClO$_4^-$, BrO$_4^-$, BF$_4^-$, PF$_6^-$, AsF$_6^-$, NO$_3^-$, C(CN)$_3^-$, and HgBr$_3^-$ have been synthesized. RF penetration depth measurements on crystals derived from (BEDO-TTF)$_3$-Cu$_2$(NCS)$_3$ exhibit superconductivity at 1.06±0.02 K. While the PF$_6^-$ salt is semiconducting and the AuBr$_2^-$, Au(CN)$_2^-$, and ClO$_4^-$ salts are metallic only near room temperature, (BEDO-TTF)$_2$AuI$_2$ shows metallic conductivity to low temperatures. Crystallographic investigations of BEDO-TTF salts show that the donor stacking in these new synmetals is remarkedly constant and does not appear to depend on stoichiometry. Band electronic structure calculations indicate that while (BEDO-TTF)$_2$AuBr$_2$ is a one-dimensional metal the Cu$_2$(NCS)$_3^-$ salt has a two-dimensional Fermi surface in accord with the observed electrical properties.

Work at Argonne National Laboratory and North Carolina State University is sponsored by the US Department of Energy (DOE), Office of Basic Energy Sciences, Division of Materials Sciences, under contract W-31-109-ENG-38 and Grant DE-FG05-86ER45259, respectively.

CONJUGATED IONIC POLYACETYLENES: SYNTHESIS OF A MODEL FOR A POLYMERIC HIGH T_c SUPERCONDUCTOR

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ABSTRACT

A synthetic process is described leading to a novel family of ionic polymers containing long sequences of conjugated double bonds. The charge density and charge distribution in these polymers depends both on the number and on the nature of side groups attached to the main chain. These polymers are soluble in common solvents and can, therefore, be processed easily. The synthetic method is quite general and may be utilized to generate a great variety of polymer structures. These structures bear structural similarity to the model proposed for an organic high temperature superconductor. They may also have potential application in the areas of energy storage and permselective membranes.

THE INFRARED OPTICAL PROPERTIES OF $(TMTSF)_2ReO_4$ AND $(TMTSF)_2BF_4$, COMPARED WITH SEVERAL MODEL CALCULATIONS

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ABSTRACT

We report high-resolution reflectivity measurements of the protonated and deuterated forms of $(TMTSF)_2ReO_4$ and $(TMTSF)_2BF_4$ at 300K and 25K, and for polarizations $\vec{E}||\vec{a}$ and $\vec{E}||\vec{b}'$, from 20 cm^{-1} to 8000 cm^{-1}. The vibrational features in the conductivity are assigned to multiply-split a_g modes and combinations. The predominantly-doublet splitting is discussed. The low-temperature energy gap is seen in both polarizations. The $\vec{E}||\vec{a}$ spectra were fitted to the "dimer", the "tetramer", the "phase-phonon", and a "one-dimensional CDW" model. The latter gave the best agreement with experiment, with gaps of 1120 cm^{-1} and 1700 cm^{-1} for the BF_4 and ReO_4 compounds respectively. The results show the validity of the one-dimensional band approach.

SEARCH FOR THE SUPERCONDUCTING ENERGY GAP IN THE 10K SUPERCONDUCTOR (BEDT-TTF)$_2$[Cu(NCS)$_2$]

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ABSTRACT

A composite-bolometer technique has been used to measure the far-infrared absorptance, of (ET)$_2$[Cu(NCS)$_2$] for polarizations $\vec{E} \| \vec{b}$ and $\vec{E} \| \vec{c}$, at temperatures above and below T_c. At 5.3K we observe no step-like structure in the absorptance, 1–R, which is non-zero down to below 10 cm^{-1}. R remains constant ($\approx$90%) between 10 cm^{-1} and 100 cm^{-1}. Likewise no structure is observed in the ratio of spectra taken at 11K and 7K. It is hoped to repeat the experiment by direct measurements of reflectivity from a large crystal.

NEW CATION-RADICAL SALTS OF BEDT-TTF WITH TETRAHEDRAL AND OCTAHEDRAL METAL COMPLEX ANIONS: SYNTHESIS, STRUCTURE AND PROPERTIES.

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ABSTRACT

New cation-radical salts of BEDT-TTF with the tetrahedral metal complex dianions $(MCl_4)^{2-}$ (M = Zn, Cd, Co, Mn, Cu), have been prepared. The salt $(BEDT\text{-}TTF)_3 CuCl_4 \cdot H_2O$ retains metallic properties down to 0.5 K. The crystal structure of this salt has been determined. The series of isostructural. cation-radical salts of bis-(ethilene) dithiotetrathiafulvalene (BEDT-TTF) with octahedral metal complex dianions $PtCl_6^{2-}$, $PtBr_6^{2-}$, $TeCl_6^{2-}$, $SnCl_6^{2-}$ have been obtained. The crystal structure of the $(BEDT\text{-}TTF)_4PtCl_6 \cdot C_6H_5CN$ salt has been determined. Though it should be attributed to the κ-type of BEDT-TTF metallic salts due to the packing motif of the BEDT-TTF molecules, it undergoes the first order transition into the insulating state below 250K. Applying the pressure higher than 6 kbar results in a new conducting state. The complexes of (BEDT-TTF) with anions $PtBr_6^{2-}$, $TeCl_6^{2-}$ and $SnCl_6^{2-}$ exhibit semiconducting properties.

QUASI-PARTICLES IN POLYMERIC CONDUCTORS

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In the fascinating field of conducting and superconducting polymers, many features of the fundamental mechanisms still remain to be fully understood. In particular, the role of quasi-particles such as solitons, polarons and bipolarons in the conduction process or superconductivity phenomenon is only beginning to be revealed [1]. For example, two opposing contentions have recently been made in the literature, regarding the relative stability of single charged soliton-antisoliton pairs as compared to similarly charged polarons. Bredas et al. [2] using essentially Huckel theory with σ-bond compressibility and Kivelson and Heeger [3] by arguing on the basis of the Su, Schrieffer and Heeger model [4], have shown that with consideration of electron-electron interactions, polaron formation is favored. Specifically, they studied the polyacetylene case, and estimated a binding energy of about 0.65 eV for the polaron, relative to the soliton-antisoliton system at infinite separation (cf. ref. 2). On the other hand, Fukutome has recently used a PPP-UHF type hamiltonian to show that, within that approach, the charged soliton lattice is always the ground state of the single doped chain of polyacetylene [5].

Both studies used comparatively crude approximations. In this paper we present studies based on the semi-empirical quantum calculations, at the AM1 level of approximation [6], and implemented for the calculation of infinite systems at the cluster approximation level [7] and full crystal orbital theory [8]. We use this technique to study the interaction between charged soliton and antisoliton systems and polaron formation in polyacetylene and polysulfurnitride, which is being studied for the first time in this connection.

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AB INITIO COMPUTATIONAL STUDY OF THE NATURE OF CHALCOGEN···CHALCOGEN CONTACT INTERACTIONS

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The nature of the short S···S, Se···Se and Te···Te contact interactions found in organic charge-transfer salts was investigated by performing ab initio SCF-MO/MP2 calculations on model systems. Our calculations show that, in the vicinity of the van der Waals X···X distance, the X···X interaction is substantially repulsive for X=O but essentially nonbonding in nature for X=S, Se and Te. The O···O interaction is repulsive at all O···O distances, while the X···X interaction (X=S, Se, Te) is slightly attractive in the region of the X···X distance greater than the van der Waals X···X distance by 0.6 ~ 0.8 Å.

Acknowledgements

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POLYHETEROTETRAHETERAFULVALENES, PRECURSORS OF CONDUCTING SOLIDS

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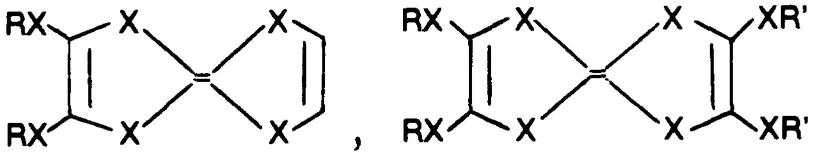
Methods for synthesis and properties of



and similar compounds (where : X= O,S,Se, etc; R, R=alkyl-group, ...) are described. Also, results on the crystal structure, and physical properties of a number of conducting solids based on these compounds are briefly discussed.

INTRAMOLECULAR VIBRATIONS IN POINT-CONTACT SPECTRA OF β-(BEDT-TTF)$_2$ I$_3$.

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The point-contacts between quasi 2-D organic conductor β-(BEDT-TTF)$_2$ I$_3$ and noble metals (Cu, Ag) were investigated at 4.2 K. The d^2U/dI^2 curves (derived from I-U characteristics) except two intensive maxima connected with e-p coupling in corresponding metal contain broad maximum in the region of 50 mev. It can be attributed to the interaction between electrons and intramolecular vibrations (presumably, C-S stretching in TTF-fragment of BEDT-TTF). It was shown recently that this mode has one of the highest coupling constants with conductive electrons. The increase of the force, pressing the two electrodes (and consequently local pressure in the contact area) causes the change of N-c-N contuct type to that of N-S-c-N type at 4.2 K. It is connected with the well known pressure induced phase transition $\beta_{1.5} \rightarrow \beta_8$ in β-(BEDT-TTF)$_2$ I$_3$. From the d^2U/dI^2 curves for the last type of contacts the value of superconducting gap was evaluated as $\Delta \approx 1.5$ mev and consequently $2\Delta/kT_c \approx 4.1$ just slightly above the BCS value.

STABILIZATION OF METALIC STATE IN MT_2I_3 SYSTEM.

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We have prepared the new 2:I salt with linear anion based on close related to ET molecule MT. MT_2I_3 crystals, obtained by electrocrystalization, demonstrate the metalic type conductivity, the magnitude of which is egual to $\sim$IOO $Om^{-I}sm^{-I}$ at RT and increases with T decrease down to $\sim$IOOK. According to thermopower, Hall coefficient and conductivity measurements data on further cooling title salt undergoes the metal-semiconductor transition accompanied by the inversion of dominated type of carriers (from holes to electrons). As a result the dielectric gap $\Delta E \gtrsim 0{,}03$ eV becomes open. Stabilization of metallic state is achieved by application of pressure $P \gtrsim 9$kbar. The disorder effect on transport properties and phase diagram in T-P plane are discussed.

IONIC AND ELECTRONIC TRANSPORT IN ORGANIC CRYSTAL ETAg$_x$Iy: DIRECT OBSERVATION.

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Ionic and electronic transport in ETAg$_x$Iy ($x \approx$ I.8, $y \approx$ 2.9) system was studied by the thermopower and conductivity measurements. This salt undergoes a lot of phase transitions with temperature decrease – from the gybrid state of hole type semiconductor and ionic conductor at $T \gtrsim$ I80K throw the quasimetalic state at I80K>T>80K to the electron type semiconductor at T<80K. The existance of definite ionic contribution (about IO^{-3} Om^{-I}sm^{-I}) to the conductivity in temperature range $T \gtrsim$ I80K was confirmed by the observation of characteristic polarisation effects. We have obtained the direct evidence of ionic transport by the detection of silver density changes (as we got to know about 30%) in the sample parts in the vicinities of the electrodes. The high pressure effect (up to I2kbar) on phase transitions in ETAg$_x$Iy is discussed too.

Transport and Magnetization Studies of $\beta''(\mathrm{BEDT\text{-}TTF})_2\mathrm{AuBr}_2$ in High Magnetic Fields

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ABSTRACT

Transport measurements reveal that $\beta''(\mathrm{BEDT\text{-}TTF})_2\mathrm{AuBr}_2$ is metallic down to 60 mK with no evidence for a superconducting transition. Tight binding calculations yield a Fermi surface containing both open and closed portions. The measurements of de Haas van Alphen and Shubnikov de Haas frequencies differ from the calculated frequencies and from the previous SdH measurements[1]. In this paper, we will discuss the discreprancies in these frequencies, our recent Hall measurements and the angular dependence of the transport measurements.

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