

外部評価：Assessment from Outside

外部評価・提言委員会

The Appraisal Panel

【センター長による注】ミクロ熱研究センターは、平成10年度末に10年の時限を迎えることになっている。それに先立ち、これまでの研究・教育・社会活動に対する外部評価を受け、時限到来後の将来構想に対する有効な提言を受けるために、国の内外の学識経験者による外部評価・提言委員会が組織された。本年1月に、佐野博敏先生を委員長とする外部評価・提言委員会の報告書が完成したので、その中から「評価の概要」と「評価と提言のまとめ」を抜粋し、ここに再録した。なお、本レポートが外国にも数多く配布されていることを考慮して、2名の「外国人委員による英文の評価レポート」も再録した。時限到来後の新センター構想に関しては、外部評価を受けた時点と、新規概算要求を行った時点とで、表現の違いが幾分存在するが、これは文部省との交渉の過程で設立目的をより鮮明にするために取られた措置であり、内容に大きな相違が有るわけではない。

委員会の構成（平成9年8月現在の役職）

- 委員長 佐野 博敏（東京都立大学(前)総長, 大妻学院理事,
大妻女子大学教授)
- 委員 岩村 秀（有機化学基礎研究センター長,
九州大学教授有機化学基礎研究センター）
- 委員 郷 信広（京都大学教授大学院理学研究科）
- 委員 長島 昭（慶應義塾常任理事, 慶應義塾大学教授）
- 委員 村上 幸夫（日本熱測定学会会長, 大阪市立大学理学部客員教授）
- 委員 森田善一郎（住友金属工業(株)顧問, 大阪大学名誉教授）
- 委員 山田 安定（山田科学振興財団理事長, 早稲田大学教授）
- 委員 Professor David N. Hendrickson
Department of Chemistry, University of California
at San Diego, USA
- 委員 Professor William A. Wakeham
Chairman of IUPAC I.2 Commission on Thermo-
dynamics
Imperial College of Science, Technology and
Medicine, UK

The Microcalorimetry Research Center will face to the time limit of ten years at the end of March in 1999. The School of Science decided to set up an appraisal panel consisting of persons of learning and experience to check and review this Center and to give suggestion to a new conception after the time limit. The Appraisal Panel completed the final report in January 1998 and submitted it to the Dean of the School of Science. The summary of the assessments written in Japanese are reproduced in this Annual Report. Two reviews by the appraisers from foreign countries written in English are also reproduced for the convenience of non-native readers. The member of the Appraisal Panel is as follows.

Committee of the Appraisal Panel

<i>Chairman</i>	Hirotooshi SANO The former President, Tokyo Metropolitan University; Trustee and Professor, Otsuma Women's College
<i>Appraiser</i>	Nobuhiro GO Professor, Graduate School of Science, Kyoto University
<i>Appraiser</i>	David N. HENDRICKSON Professor, University of California at San Diego, USA
<i>Appraiser</i>	Hiizu IWAMURA Director, Institute for Fundamental Research in Organic Chemistry; Professor, Kyushu University
<i>Appraiser</i>	Zenichiro MORITA Adviser, Sumitomo Metal Industries, Ltd; Emeritus Professor, Osaka University
<i>Appraiser</i>	Sachio MURAKAMI President, The Japan Society of Calorimetry and Thermal Analysis; Emeritus Professor, Osaka City University
<i>Appraiser</i>	Akira NAGASHIMA Trustee of Keio; Professor, Keio University
<i>Appraiser</i>	William A. WAKEHAM Chairman of IUPAC I.2 Commission on Thermodynamics; Professor, Imperial College of Science, Technology and Medicine, UK
<i>Appraiser</i>	Yasusada YAMADA Director, Yamada Science Foundation; Professor, Waseda University

評価の概要

【1】マイクロ熱研究センターの設置目的の達成への評価

マイクロ熱研究センターの設置目的に対する研究活動については、当センター設置以前からの学問研究の理念と伝統をよく維持し発展している。

- 1) 研究対象温度ならびに測定試料量など、マイクロ熱測定の限界を拡大すべく自然科学の多様な分野について追求されている。すなわち、種々のマイクロ熱量計の開発に成功し、これらを応用して興味ある先進的な自然科学現象の研究に役立つことが実証されている。そのための研究テーマもよく精選され、従来不可能であった微量試料による極低温での温度や極微の熱量の測定を可能とすることによって、それぞれの分野やテーマにおいて熱科学の基礎研究が大きく拡大進展され成功をおさめている。これらのことは、国外の委員を含めて全委員の高く評価するところである。また、この成果を確固とした土台として従来試みることが困難であった新しい分野への挑戦が可能となったのである。
- 2) 上記の高い達成目標を立てるとともに、多大の困難が予見されながらも、生命科学の基礎的理解に寄与すべく生体関連物質の精密熱測定をも当センターが目標としたことについては、その識見と意欲が高く評価される。上記の成果を土台として第2の目標とした生体関連物質の学問的研究成果としては、水素結合系や動的電子系など生命現象の基礎的理解に貢献する成果が数多く達成されている。しかし狭義の生体関連物質に限定した場合には、内外の委員が評価するように、含水蛋白質のガラス転移の画期的業績が挙げられているにしても、上記の他分野の業績の量には及ばないという指摘もあった。しかしこの指摘は、生体関連物質への熱測定研究の高いハードルを示したものであり、そのゆえにこの分野に挑戦してきた当センターの意欲をむしろ評価し激励するのが本意であって、困難な実状を理解し一層の支援が望まれるという補足説明があった。
- 3) 国際協力の実を挙げる目的は、上記の広い自然科学の各分野において多彩な共同研究の成果が挙げられていて、その点では当センターがフランス（マルセイユ）および米国（ジョンズ・ホプキンス）とともに世界の3大中心の一つと評価されている。共同研究の計画、協力体制の企画などが綿密に検討され、それらが着実に実践されたということが出来る。実際に、1996年に当センターが運営したIUPAC化学熱力学国際会議でも大成功をおさめている。このよう

な成果が現状の限られた人員と組織で挙げられていることは、当センターならびに大阪大学理学部・同大学院理学研究科の関係者の献身的な努力に基づくものであると評価される。

【2】教育面，社会的要請，ならびにセンターの運営についての評価

学界活動はいうまでもなく活発に行われていて、さらに一般的な学内外に対する多面的な活動が積極的に行われていると評価される。別項にも述べるように、熱科学データの汎用性のゆえに、将来はデータベースのサービスなど学界・産業界への貢献への期待も指摘された。なお当センターの小規模な実状に対して、むしろもっと配慮すべきであるという同情も少なくなかった。

【3】現代科学における熱力学的研究の位置と重要性

現代の自然科学や科学技術がそれぞれの専門に分化していく状況において、その流れを認めざるを得ないがゆえに、一切の見落としのない情報提供をしてくれる熱力学的研究は各専門分野を結びつけ、別の側面から自然現象の認識を提供するが、その重要性は今後ともますます非常に大きくなるであろう。これはすべての委員が異口同音に指摘しているところである。大阪大学理学部の発足以来、維持発展させてきた物質の「構造」と「エネルギー」の両視点からの研究の伝統は、当センターにおいて正しく把握されていて、わが国はもちろん世界的にも大きい信頼を得ているが、このことも熱力学の重要性が広く認められている反映である。

【4】時限到来後の将来計画

当センターから披露された将来計画では、複雑系熱力学と物性熱力学の2部門が示されたが、複雑系の選択は、これが生命科学を含めて来世紀の新しい科学の重要な命題であることは間違いなく、克服すべき困難は少なくないと考えられるが、その先見性と意欲に委員会委員全員の激励するところである。一方の物性熱力学は、着実にその基礎を築いてすべての分野の発展に貢献するものであり、これが不可欠の部門であることにも全員が賛意を示すところである。また、将来のセンターが大学院理学研究科附属とする案についても、自然認識のための高等教育における大学院教育の重要性、大阪大学の重点化構想、センターの発展性など、いずれの点から考察しても、それが望ましい案であるとして支持するものである。

ただし、当センターの挙げてきた輝かしい研究成果についての外部評価・提言委員会全員の評価は、すでに述べた通り大変に高く、したがって将来計画に対する期

待も非常に大きいものがあることも否めない。そこで、当センターから紹介された将来計画はかなり激しく自己規制されたものであると思われるが、特色を有する世界の3大研究拠点の一つとして評価されている実状に相応しい規模、多くの研究部門、人員、設備を備えた研究機関としての将来構想をもつべきであるという一致した希望が出されたのも当然であろう。たとえば、少なくともさらに理論・計算分野の部門や人員の充実、熱力学データベース、モデリングサービス部門等の設置による学界、産業界との連携も効果的と考えられる。組織・体制についても、学内共同利用研究機関、さらに全国共同利用研究機関とすれば、広い分野に基礎的関連をもつ熱科学の特性をいっそう発揮できると考えられる。

外部評価・提言委員会としては、世界ならびにわが国の熱科学の研究拠点の存続と発展の為に、当センターの実績に相応しい将来構想には大きい目標を描きつつ、当センターが測定限界を飛躍的に拡大したように、計画の実現においても着実に歩を進められるよう期待する。

特に本質的な問題ではないが、新センターに用いられている「分子熱力学研究センター」という名称は、研究目的からすると、その役割を十分に表しているとはいえないので、端的に「熱科学研究センター」とするのがふさわしいのではないかと提言が一部の委員から出された。これら以外にも幾通りかの名称が考えられるが、最終的にどれを採択するかは、当事者である大阪大学理学部が決めることである。

評価と提言のまとめ

上記の評価の概要から、当外部評価・提言委員会は以下のように総括して講評し必要かつ重要な諸点を提言するものである。

- ◆ 「マイクロ熱研究センター」の設置目的に対する研究活動は、全体として非常に高く評価する。今後ともこの研究活動を維持発展していくことを強く期待する。
- ◆ 現在および将来の自然科学ならびに科学技術の趨勢から考えて、熱科学研究の重要性はますます増大することは疑いない。そこで、当センターの活動の持続と発展は、学界、産業界を通じ社会に大きく貢献すると考え、その推進への理解と支援を要請する。
- ◆ 当センターは世界の熱科学の3大研究拠点の一つとしての評価を確立していて、それにふさわしい組織・体制の実現に向けての諸整備への支援を望みたい。
- ◆ 当面の計画として、複雑系熱力学研究部門および物性熱力学研究部門の両部門は相補的かつ相乗的效果をもたらすために不可欠な必要最小限の2部門であって来世紀の学問研究への適正な見通しに基づいているので、少なくとも発展の第一歩としてその実現が肝要である。
- ◆ さらに状況が許せば、理論・計算部門やデータベース部門などを追加することにより、いっそう学界、産業界、国の内外に貢献し、これがフィードバックされて将来の当センター発展を助けるという良い循環を生むと考えられる。このような長期将来構想による理解と支援が重要である。
- ◆ 当面は、大阪大学大学院理学研究科附属の組織が望ましいが、熱科学が広く自然科学、科学技術の各分野と不可欠の関連があり、相互に不可欠の関係があるので、その特色を生かした学内あるいは学外共同研究の組織や体制を将来構想の視点として考えておくことも大切である。



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September 12, 1997

From: Professor David N. Hendrickson
University of California, San Diego

A handwritten signature in dark ink that reads 'David N. Hendrickson'.

Subject: Appraisal of Microcalorimetry Research Center, Faculty of Science,
Osaka University

During the period of September 1-7, 1997, I visited Japan. On September 2, I traveled from Osaka to Tokyo to consult with Professor H. Sano, who is the Chairman of the Appraisal Committee. On Thursday, September 4, I met in the morning for 1-1/2 hours with members of the Steering Committee of the Microcalorimetry Research Center. In the afternoon of the same day, I met for one hour with Professor Kushida, Dean of the Faculty of Science. I have also studied the report "Materials for the Appraisal Panel of Microcalorimetry Research Center, Faculty of Science, Osaka University" prepared by Professor Michio Sorai, Director of the Microcalorimetry Research Center. The matter before the Appraisal Panel is an evaluation of the Microcalorimetry Research Center. There are basically two components to this evaluation. One is an appraisal of the success of the Microcalorimetry Research Center since its inception in May, 1989. The other element that needs to be evaluated is the proposal for the new institute called the "Research Center for Molecular Thermodynamics".

Past Progress

The three goals set for the Microcalorimetry Research Center in 1989 were:

1. To develop very accurate and precise microcalorimeters and thereby to expand the research area in which thermodynamic investigations play important roles;
2. To contribute to fundamental understandings of life science by precise calorimetry for bio-related materials; and
3. To develop international collaborations and to mutually confer benefits.

It is the considered opinion of this appraiser that all three goals have been achieved. It is quite clear from the list of international collaborators and the publication list of the Microcalorimetry Research Center that goal number 3 has been achieved. Collaborations

have been established with well known scientists from several countries. There have been many joint publications. In several cases, the information learned from the thermodynamics studies has proven to be very complimentary to data obtained in other laboratories by means of various non-thermodynamic techniques. For example, many chemical systems have been studied by a variety of spectroscopic techniques. In such spectroscopic examinations, generally local molecular events are examined, such as whether an electron transfer is occurring or a molecule is static or dynamic. A detailed thermodynamic characterization of the same chemical system has given additional significant insight into what cooperative interactions exist between molecular units. Thermodynamic characterizations, together with other physical data such as from spectroscopic techniques, have given considerably more insight into phenomena than either approach alone can give. Thus, collaborations, both internationally and domestically, enhance dramatically the effectiveness and impact of the Microcalorimetry Research Center.

It is also clear that the other two goals of the Center have also been achieved since 1989. Very accurate and precise microcalorimeters have been developed. This has allowed an expansion of the research areas of the Microcalorimetry Research Center. The thermal denaturations of several proteins have been studied. DSC studies have been carried out on the thermal unfolding of various proteins such as the acid proteinase from *Aspergillus niger*, the proteinase inhibitor SSI, subtilisin, and lysozyme. Calorimetric studies have been completed on several proteins to characterize the nature and importance of water molecules. In crystals of proteins such as cytochrome c there are different types of water molecules. Certain waters molecules are found in the "pores" of the proteins; some of these H₂O molecules are, in fact, highly conserved. Other H₂O molecules are just solvate molecules in the crystals. Thermodynamic studies have given insight into the importance of these different H₂O molecules.

There is no question that the research efforts carried out at the Microcalorimetry Research Center are of very high quality. The reputation of this Center is strong throughout the world. The importance of having such a center of excellence in a broad base of calorimetry is widely recognized. There are some who would say that the study of thermodynamics is an old science and that no problems remain to be solved by thermodynamics. Nothing could be further from the truth! Surely, many young scientists look to find new physical techniques with which to pursue science. There is a drive to set new trends. However, it is quite clear that thermodynamic studies are imperative to thoroughly characterize many chemical systems. There are just no other techniques that can give the same information. Furthermore, thermodynamics is still playing a crucial role in discovering new phenomena.

Future Plans

The proposal is to establish a "Research Center for Molecular Thermodynamics" for the next ten-year period. The basic founding idea is to develop the complementary roles between microscopic molecular sciences and macroscopic thermodynamics. The new Research Center is planned to have two research divisions: (1) Thermodynamics for Complex Systems, and (2) Thermodynamics for Materials Science. The timeliness of these plans is excellent. The studies of molecules have evolved to the point where scientists are employing molecular building blocks to fabricate new materials and systems. In the last few years, new areas of chemistry have appeared, such as the areas of supramolecular chemistry and molecule-based magnets.

Supramolecular chemistry is a highly interdisciplinary field of science covering the chemical, physical, and biological features of chemical species of greater complexity than molecules themselves. Supramolecular chemical systems consist of molecular units held together and organized by means of intermolecular (non-covalent) binding interactions. It is clear that thermodynamics will play a crucial role in the study of supramolecular chemistry.

In the second example mentioned, chemists are employing molecules as building blocks to make new magnetic materials. There have been several new interesting magnetic materials prepared by this relatively new approach. Already, thermodynamics data have proved considerably useful in characterizing these new magnetic materials. The above are only two of several examples of complex molecular systems that are amenable to thermodynamics studies.

The other major thrust of the new Research Center centers on thermodynamics for materials science. There is no question that materials science has become one of the hot areas of study in the physical sciences. It is the intent of the new Research Center to build calorimeters workable under extremely high pressure, strong magnetic fields, and alternating electric currents. This is to be applauded. There clearly is a strong need to have such facilities available to study new materials as they are discovered. This new Research Center could make an internationally recognized impact in this area.

Concluding Remarks

There is no question that the Research Center for Molecular Thermodynamics should be funded. This appraiser feels that the past impact of this center has been so strong that it warrants additional support, over and above what it has had in the present ten-year tenure. In particular, it would be most appropriate to provide the funds for additional staff.

REPORT TO APPRAISAL PANEL

MICROCALORIMETRY RESEARCH CENTER **Faculty of Science, Osaka University**

prepared by

Professor W.A. Wakeham

INTRODUCTION

The assessment of the Microcalorimetry Research Center is based upon several independent sources of information. First, a knowledge of similar centers throughout the world through Chairmanship of Commission I.2 on Thermodynamics of the International Union of Pure and Applied Chemistry; secondly, upon the material prepared by the laboratory for the appraisal panel and, finally, upon a visit to the Center in September 1997, during which a tour was made of the laboratories and discussions held with the Steering Committee.

APPRAISAL OF PAST PERFORMANCE AGAINST OBJECTIVES

At the beginning of its existence the Center established three objectives. The published results of the Center in this period demonstrate that it has both developed new microcalorimeters and extended their application to new areas. These new instruments are respected throughout the world as unsurpassed for their resolution, accuracy and precision. An inspection of the Center has revealed the quality of the conception of the instruments and the workmanship and skill that has gone into the design and construction of these instruments. The Center now has a unique set of instruments that encompass a wider range of temperatures and materials. The attention to detail evident in the instrument design and the building design is impressive and reinforces the view gained from reading the scientific output.

It is evident, too, that the range of applications of the instruments and microcalorimetry has been increased during the period of the Center's activity. Its work covers studies on liquid crystals, magnetic systems, clathrate compounds, fullerenes, clays in water and two-dimensional solids and others. Some of the

studies conducted on these systems have revealed entirely new phenomena while others have elucidated structures or processes postulated by others. In any event, the studies have been carefully focused within the overall objective and brought to fruition by careful experimentation.

I have no doubts that the first objective of the Center has been fulfilled.

The second objective of the Center was to contribute to fundamental understanding of life science by precise calorimetry of bio-materials. While this has not been a dominant theme of the Center, very considerable progress has been made in meeting the objective set. A new instrument has been commissioned in the period especially for measurements on bio-materials. With this instrument there has been a concentration of effort upon studies of thermal denaturation of proteins and the thermal unfolding of macromolecules to elucidate their function has been carried out. Although this work has extended the range of materials with which the Center is comfortable, excellent work, comparable with the best in the world, has been carried out in the review period and there is evidence that the group has now developed the expertise and maturity in the field of bio-materials that it sought initially.

I regard the second objective as having been met in large measure.

There can be no doubt whatsoever that the Center has met its third objective since the number of collaborations that have taken place is extremely large. Moreover, discussion revealed that the nature of these collaborations is very varied, some involving simply the preparation of materials elsewhere, others involving the short-term exchange of people for mutual benefit, and others have been a joint project involving the examination of a material with two or more complementary techniques in a number of locations. In this way, the cause of the scientific investigation has been enhanced, and all partners in the exchange have benefited greatly. The organisation of the 14th ICCT in Osaka represented a very significant step for the Center since it brought all the thermodynamic and calorimetric community to its door at one time.

ASSESSMENT BY REPUTATION

Necessarily, the judgement of the quality of the research work in the Center by means of international opinion is a little subjective. Quality can be noted in experimental work from the internal consistency and accuracy of results and by this criterion the Center attains the highest quality. One can also judge from the quantity of papers published in the journals with the highest standards of reviewing. Here again the Center obviously achieves the highest standards. The students produced by the Center are also a measure of quality if they attain high positions in academe or industry. The evidence placed before me suggests that students graduating from the Center are much in demand and, from my personal knowledge, are judged to have a high level of competence.

Thus, all objective measures suggest that the Center attains a very high standard internationally. I have consulted widely my colleagues on the Commission for Thermodynamics of IUPAC to discover their opinion of the Center from an international perspective. Without exception, those colleagues have used the phrase a 'Center of Excellence' to describe the Research Center for Microcalorimetry. Indeed, to show the high esteem in which the Center is held, the Commission recently elected Professor Sorai to Associate Membership in succession to Professor Matsuo. The Commission wished to honour the Center in this way as a mark of respect for its quality. The Center certainly ranks with equivalent centers in France and the US in the top three in the world for quality. There would be no universal agreement of the best among equals.

THERMODYNAMICS IN MODERN SCIENCE

There is a natural question when considering the future of such a Center about whether there is a need for such relatively traditional studies at a time when synthetic chemistry and other more modern forms of chemistry seem to offer greater insight. I believe that there is an urgent need for the type of work carried out by the Center but only if the high quality and accuracy of the work is maintained. There is surely no place for a series of inferior institutions pursuing lesser goals, but there will be a place for one Center of Excellence providing fundamental experimental

information against which modern theories must be tested. An understanding of molecular influences upon macroscopic and mesoscopic behaviour can only be claimed when the excellent data that are acquired in this laboratory, and a few others like it, are satisfactorily represented by theory. The field is therefore fundamental to the development of statistical thermodynamic theories, the study of the origins of forces between molecules in pairs and in groups. It will remain so for the future as novel materials and more complex molecules become more important in other areas of fundamental science and applications.

RESEARCH CENTER FOR MOLECULAR THERMODYNAMICS

This new Center is conceived to extend the work of the previous Center into the realm of more complex systems. They are more complex either by virtue of their molecular size, or by the existence of fields or boundaries within them. This endeavour seems totally appropriate for the evolution of the activity since it is consistent with the direction in which both the science and technology is moving generally as we approach the 21st century. Such systems pose challenges sufficiently great for the experimentalist that one needs a team of the calibre now assembled at Osaka to tackle them.

A second area proposed for the Center is that of extreme conditions, represented by pressure, temperature or magnetic field. Again, such conditions for simple or complex materials provide new challenges for experiment and theory and can be expected to reveal a host of new phenomena upon investigation. Much is already being considered about materials at extreme conditions in other branches of science; as always, the fundamental thermodynamic data will be vital to the complete elucidation of the observed behaviour.

Thus the proposed activities seem to me to fit with developments in other related sciences; the expertise existing in the Center will surely be of distinct advantage in this endeavour.

I therefore strongly support the establishment of the proposed Center.

COMMENTARY ON THE PROPOSED CENTER

I would like to add a few comments on the proposed Center. First, and most obviously, I believe it should be associated with the Graduate School of Science. My understanding of arrangements suggests that this would have a beneficial effect upon research performance without a detrimental effect upon teaching.

Secondly, I believe the Center should be encouraged to co-operate not only with other experimental groups but also with some involved in theoretical calculations. There is already some collaboration but I can see benefits for both sides from an increase. I would also support the stay of a guest professor on the same grounds that it would deepen collaboration to mutual benefit.

Thirdly, the systems to be studied and the conditions to be encompassed suggest that further calorimeters will need to be developed to satisfy the requirements of the new perspective. To this end, it will be necessary to provide additional capital expenditure to realise the plan proposed.

CONCLUSION

Overall, I have no doubts that the Mircocalorimetry Research Center has fulfilled its objectives and established itself as a leading laboratory in the field in the world. It is to be commended upon these achievements.

