IUPAC Physical Chemistry Division

Report to the Council (August 1999)

Organizational work

The IUPAC Division I on Physical Chemistry consists of 7 Commissions with a total of 7 × 6 = 42 Titular (TM), 46 Associate Members (AM) 44 National Representatives (NR) and 40 additional members within subcommittees. The work is coordinated by the Division Committee consisting of 7 TM and 4 AM. There is an additional Subcommittee on Plasma Chemistry attached directly to the Division Committee with its Chairman as an AM. The seven Commissions cover different fields of Physical Chemistry. This working force is engaged in 51 projects some of which are ongoing while most of them are time-limited between 2 and 12 years.

In view of the recently proposed changes in the structure of IUPAC the Division Committee decided at its meeting in February 1992 to reshape the divisional structure. The Commission structure is expected to be abandoned, which gave rise to some concerns expressed at the 1998 Bureau meeting. The Division Committe proposes to continue with two Commissions in the future Division of Physical Chemistry. One would have to do with the terminology, symbols and units in Physical Chemistry — it would essentially be a Commission I.1 (possibly enlarged) covering all aspects of Physical Chemistry with respect to terminology and symbols. It would take care of the continued work on revisions of the Green Book, provide a permanent link to other related international bodies such as IUPAP and ISO TC-12, but also initiate projects in certain more specialized fields of Physical Chemistry. As opposed to the present Commission I.1 the new commission would have to rely much more on internal knowledge since the fruitful interactions with other commissions at General Assemblies will be lacking in the future and much more will have to be done through correspondence or internet communication. The second Commission would evolve from present Commissions I.2 and I.4 and would cover the work on compilation and critical evaluation of data. The two aspects of IUPAC work: (i) nomenclature, terminology and symbolism and (ii) compilation and evaluation of data were felt to be so important that a need for a long-term structural organization was thought to be essential in ensuring smooth continuation of the work.

It is not easy to assess the impact of IUPAC work, but some indication is given by citations in the literature. The Green Book is cited in instructions for authors of several leading journals in Physical Chemistry, it is cited in many textbooks on Physical Chemistry or more special fields. Large sections are reproduced in the CRC Handbook of Chemistry and Physics and it has been cited some 200 times in the primary literature covered by ISI. The data compilations on atmospheric reactions or on thermodynamic properties of important substances are also reproduced in the CRC Handbook with specific mentioning of primary IUPAC sources. So we in the Physical Chemistry Division think that such work has contributed to the reputation of IUPAC and should continue as long as needed with as little perturbation as possible. A complete list of publications produced by the Division is given as an appendix in order to provide a record of what has been achieved within the present structure.

Changes were envisaged in the structure of the future Division Committee which will have to take up many more responsibilities. We shall need a broadly based committee with experts from

different fields of physical chemistry to ensure competent initiation and evaluation of projects. Thus, for the transition period 2000-2001 we proposed a committee with four officers, as we have at present, plus all the seven present-Commission chairmen. In addition we wanted a broadly oriented physical chemist such as a journal editor from outside and keep the titular members elected in 1997 for their 4-year period. The new Division Committee would keep track of all the projects within the Division and would alocate the National Representatives to work in different projects according to their interest.

Scientific work

Commission I.1 on symbols, terminology and units is exceptional in that it deals with Physical Chemistry as a whole and covers the aspects of terminology, symbols and units of physical quantities. Its work strongly depends on the recommendations produced in other Commissions including some from other Divisions of IUPAC (especially II.1, III.2, III.3, and some commissions from Division V). Its sole project the *Revision of the Green Book: Quantities, Units and Symbols in Physical Chemistry* consists of preparation of the third edition planned for 2000. The typing of the whole text into a standard computer-readable format (Revtex) is taking time. It is being carried out under the supervision of M. Quack and a meeting of I.1 was held in March 1999 in order to finalize most of the text. Some sections however are still open and will have to be reconsidered at the General Assembly in Berlin. The main changes with respect to the second edition, except for producing the book on a computer, involve extensions in the field of surface chemistry and the treatment of uncertainties of measurement.

Commission I.2, the largest and most productive in the Division, covers the field of thermodynamics. In the period since the General Assembly in Geneva it has produced numerous publications covering different types of work: evaluated data compilations, terminology recommendations, guidelines and monographs. It continued work on organizing conferences (15^{th} ICCT took place in Porto, July 1998, the 16^{th} is due in Halifax, August 2000) and workshops (on safe refrigerants in Pisa, September 1999).

Commission I.2 agreed to enter a Joint IUPAC/CODATA project on *Standardisation of Physico-Chemical Properties: Electronic Data Files* with Professor Kehiaian as the CODATA project officer. From Commission I.2, the active participants will be Professor Grolier, Drs Stolen, Deiters and Vogel.

Commission I.3 on Electrochemistry completed two projects: (i) Spectroelectrochemistry: a survey of in situ spectroscopic techniques published in *Pure Appl. Chem.* **70** (7) (1998) 1395-1414 and (ii) Nanostructures in electrochemistry: *in situ* local probe techniques in electrochemistry which resulted in the publication of a book with the same title by Verlag Chemie in March 1998.

A new project on Electrochemistry for the environment (Ch. Brett) has been reviewed under the new system and has been accepted.

Commission I.4 on Chemical Kinetics has a very active subcommitte on Gas Kinetic Data Evaluation for Atmospheric Chemistry. They have an ongoing project and produced two evaluations under IUPAC sponsorship in the reporting period:

> R. Atkinson, D. L. Baulch, R. A. Cox, R. F. Hampson, Jr., J. A. Kerr (Chairman), M. J. Rossi, J. Troe, Evaluated Kinetic and Photochemical Data for Atmospheric Chemistry.

Supplement V. IUPAC Subcommittee on Gas Kinetic Data Evaluation for Atmospheric Chemistry, *J. Phys. Chem. Ref. Data* **26** (1997) 509-1011;
{disk version of Summary Table published in *Atmos. Environ*. **30** (1996) 3903}.

R. Atkinson, D. L. Baulch, R. A. Cox, R. F. Hampson, Jr., J. A. Kerr (Chairman), M. J. Rossi and J. Troe, Evaluated Kinetic and Photochemical Data for Atmospheric Chemistry. Supplement VI. IUPAC Subcommittee on Gas Kinetic Data Evaluation for Atmospheric Chemistry, *J. Phys. Chem. Ref. Data* **26** (1997) 1329-1499.

These IUPAC data compilations are the main sources of kinetic data for the ever increasing modelling activities on atmospheric chemistry. They have been extensively reproduced in the CRC Handbook of Chemistry and Physics. The subcommitte meets regularly at least once a year and continues work on further supplements including photochemical data and heterogeneous chemistry. The publication of evaluated data on a special web site are also being considered.

Commission I.5 on Molecular Structure and Spectroscopy is working on 11 projects most of which have been completed or are nearing completion. The GA in Berlin will be used for the final revisions of several documents.

150/18/93 Practical Standards for NMR, (R. K. Harris)

This project is reaching its final stages. Much time has been spent recently in clarifying and annotating the important accompanying tables listing data for each NMR-active nucleus. This is now essentially complete, and final modifications are being made to the main text, principally by Dr Becker and Professor Harris. Subject to approval by the remaining members of the Working Party, it is hoped to present the completed document at the Berlin meeting and subsequently to send it to 15 chosen experts for comment, as required for IUPAC documents.

150/19/93 Guidelines for the Presentation of Instrumental Parameters in Optical and Nuclear Magnetic Resonance Fourier Transform Spectroscopies, (J. E. Bertie)

This project was split into two parts I 1995. The part for NMR was transferred to project 150/22/95, described below, and has been published in Pure and Applied Chemistry

The final report of the remaining part of this project, for optical spectroscopy, has been published in *Pure Appl. Chem*. **70** (1998) 2039 - 2045. It is in the final stages of appearing on our web site. To fulfil part of its purpose, the paper has been sent to many journal editors to ask if they would reprint it or send it to their referees and authors. Several journals have indicated their interest. Specifically *Applied Spectroscopy* and the *Australian Journal of Chemistry* have stated their intent to reprint the article. The *Journal of Molecular Spectroscopy* has indicated its interest in including on its web site a statement of the existence of the document with a hyperlink to the IUPAC web site. This is probably the preferred way to distribute the work of the Commission in the future.

150/20/93 Nonlinear Spectroscopy for Molecular Structure Determination (S. Tsuchiya)

The project is completed. The final report of this project is the 268-page book entitled *Nonlinear Spectroscopy for Molecular Structure Determination* edited by R.W. Field, E. Hirota, J.P. Maier and S. Tsuchiya, published by Blackwell Science in January 1998.

150/2/95 The Computation of Experimental Structure and Properties of Small Molecules by *Ab Initio* Calculation, (R. Janoschek)

A 79-page report was reviewed by the Commission in Geneva. Many changes and additions have been made to incorporate the Commissioners' views. The final report has been completed and will be reviewed by the Commission in Berlin.

150/22/95 Parameters and Symbols for use in Nuclear Magnetic Resonance R. K. Harris

The final report has been published in *PAC* **69** (1997) 2489 - 2495. It is published on the Commission's web site and has been reprinted in *Magnetic Resonance in Chemistry* **36** (1998) 145-149 and in *Solid State NMR* **10** (1998) 111 - 116.

150/23/95 Spectroscopic Intensities; Related Quantities, Nomenclature, and Symbols (J. E. Bertie)

This project has led to the author redrafting the page on "Spectroscopic Nomenclature" published annually in *Applied Spectroscopy*, and to contributions to project 154/5/97 of the Subcommittee on Notations and Conventions for Molecular Spectroscopy. These contributions have fairly well complemented the Green Book's content on this subject, and the project will be terminated in Berlin

150/24/95 Spectroscopy under Extreme Conditions of Temperature and Pressure (A. M. Heyns)

Much progress has been made on this project. A 6-page summary has been received and will be presented to the Commission in Geneva. The full report currently occupies 150 pages and needs rigorous editing which will start in Berlin.

150/25/98 Quantities, Terminology and Symbols in Photothermal and Related Spectroscopies (N. Hirota and M. Terazima)

The first draft of the report of this project is completed and copies were sent out recently to prospective collaborators for review and suggestions. The 29-page draft contains 5 sections including the origins of photothermal effects, a glossary of terms and symbols for physical parameters in photothermal effects. The draft will be reviewed by the Commission in Berlin.

Subcommittee on Notations and Conventions for Molecular Spectroscopy

Two projects are under way, both coordinated by R. S. McDowell and J. K. G. Watson:
154/5/97 Notations and Conventions in Molecular Spectroscopy Part 4. Vibrational-Rotational Spectroscopy and Part 5. Electronic-Vibrational-Rotational Spectroscopy

The Subcommittee has exchanged several drafts of this document and met at the Columbus Conference. The document now comprises about 45 pages in final IUPAC format, and is nearing completion. Final revisions are planned for Berlin and the document is expected to be sent for IUPAC approval and publication by the end of 1999.

Part 5 is a large and complex project involving all degrees of freedom. It will be taken up more effectively after the completion of Part 4, and is likely to continue beyond 2001.

Subcommittee on Theoretical Chemistry

The project 155/1/95 on Guidelines for the Presentation of Methodological Choices in the Publication of Computational Results (J. E. Boggs) has evolved to include three parts.

Part A is for *ab initio* electronic structure calculations. The final report has been published in PAC 70, 1015-1018 (1998), and has been put onto the IUPAC web site. The reprints have been distributed to journal editors to help them to guide authors and referees on the appropriate presentation. They have been well received by editors and authors alike.

Part B is for Semi Empirical calculations. A draft report was reviewed by the Commission in Geneva. After a lengthy hiatus, the author is seeking input for the final revision.

Part C is for molecular dynamics, molecular mechanics and empirical force-field calculations. It is being pursued in collaboration with Commission I.7 which initiated a similar project in Geneva. Dr. Terry Stouch leads the I.7 project and has been made a member of the Subcommittee to avoid duplication of effort.

Commission I.6 works on different tasks which can be grouped under the headings: General, Environmental Protection and Advanced Materials.

General

The project on Pillared clays and pillared layers (R. Schoonheydt) is focused on nomenclature and characterization and is forwarded for final refereeing.

Measurement and Interpretation of Electrokinetic Phenomena (Gonzalez-Caballero; L. K. Koopal)
A Feasibility Study Document has been produced by the group which was sent out for external review by the Division. The reviews were positive

Environmental Protection

Environmental Protection: Surface, Colloid and Catalytic Aspects (J. Ralston)
This project comprised the involvement in 3 meetings: (1) "Colloids in the Aquatic Environment" (Gregory, London 1992, proceedings: *Colloids Surfaces A*, **73** (1993); (2) "Soil Pollution" (Iyer, Madras 1994); (3) "Environmental Catalysis" (Misono, Tokyo 1995, proceedings: *Catalysis Today*, **35**, 1-2, (1997). The project is completed.

Colloid Chemical and Catalytic Processes for the control and Protection of Environmental Pollution (L. K. Koopal, M. Misono, I. Dékány)
This project has been centered on the IUPAC sponsored International Conference "Interfaces Against Pollution" (Koopal, Wageningen 1997). The Proceedings have been published in *Colloids and Surfaces* A, **151** (1999) 1-2.

Advanced Materials

Nomenclature of structural and compositional characteristics of ordered microporous materials (K. K. Unger, Liebau, Delmon, R. Schoonheydt)
The title of this project has changed somewhat in the course of the project. The recommendation document regarding this project will be sent out for refereeing to the Division.

IUPAC Strategic Initiative in Materials: An important part of the projects of Commission I.6 are connected with the preparation or characterization of new advanced materials. This domain is not exclusively that of commission I.6 and certainly in this field collaboration with other Commissions and Divisions through the Inter Divisional (limited-lifetime) working party co-chaired by Professor John Corish (Inorganic Division) and Professor Robert Gilbert (Macromolecular Division) is important. All initiatives regarding new materials have been reported to this working party.

Further collaboration: Other fields of collaboration emerge with the Commissions on Electrochemistry (e.g., electrochemistry at interfaces, nanostructures, poisons for catalysts),

Fundamental Environmental Chemistry (see Subcom. E) and Biophysical Chemistry (e.g., microcalorimetric techniques, the role of adsorption at interfaces, terminology of liquid vesicles and membranes).

The relatively new **Commission I.7** on Biophysical Chemistry works on 6 projects.

Recommendations for the presentation of NMR structures of proteins and nucleic acids (K Wüthrich)

The final document was published in *Pure Appl. Chem* **70** (1998) 117-142. It will also appear shortly in leading structural journals *Biochemistry, J. Mol. Biol.* and *J. Biomol. NMR*. This document will be useful and valuable in the standardization of reporting of NMR structures of proteins, nucleic acids and macromolecules in general.

Recommendations for reporting the results of computations in biophysical chemistry (T. Stouch)

The working party has met twice at conferences and plans to meet again (6 members) with J E Boggs (SC 155) in New Jersey in autumn 1998 in order to produce (i) an educational paper and (ii) a draft of recommendations.

Terminology in the field of lipid vesicles (liposomes) (H. Hauser)

A 3-day meeting of the six-membered working party was organized in April 1998. General consensus has been achieved among the members on most points and a document containing recommendations on nomenclature and symbols in the field of liposome science is being drafted.

Three more projects are all expected to be finished at the General Assembly in 1999: Electrochemical biosensors (D. Thévenot), Recommendations for the measurement and for the presentation of results obtained on biological substances with scanning calorimetry (F Schwarz, H-J Hinz) and Nomenclature for lipid mesophases (M. Caffrey).

Tom Cvitas
President Physical Chemistry Division

19 July 1999

I U P A C

Publications of the Physical Chemistry Division

Commission I.1 Symbols, terminology and units

1. McGlashan, M. L.: Manual of Symbols and Terminology for Physicochemical Quantities and Units, *Pure Appl. Chem.* **21** (1970) 1-38. [superseded 1975]

2. Paul, M. A.: Manual of Symbols and Terminology for Physicochemical Quantities and Units, 2nd ed., Butterworths, London 1975. [superseded 1979]

3. Whiffen, D. H.: Manual of Symbols and Terminology for Physicochemical Quantities and Units, 3rd ed., *Pure Appl. Chem.* **51** (1979) 1-41. [superseded 1987]

4. Homann, K.: Abbreviated list of quantities, units and symbols in physical chemistry, Blackwell Scientific Publications, Oxford 1987. [superseded 1993]

5. Mills, I., T. Cvitaš, K. Homann, N. Kallay, K. Kuchitsu: Quantities, units and symbols in physical chemistry, Blackwell Scientific Publications, Oxford 1988, x + 134. [superseded 1993]

6. Russian translation of 5: Nomenklaturniye pravila IUPAC po Khimii, Vol. 6, Fizicheskaya Khimiya, Nacionalnii Komitet Sovetskih Khimikov, Moscow 1988.

7. Hungarian translation of 5: Riedel, M.: *A fizikai-kémiai definiciók és jelölések*, Tankönyvkiadó, Budapest 1990.

8. Japanese translation of 5: Kuchitsu, K.: *Quantities, Units and Symbols in Physical Chemistry*, Kodansha, Tokyo 1991.

9. Portuguese translation of 4:

10. Roumanian translation of 4: *Revista de Chimie*, 40 (1989) 661-664.

11. Homann, K.: Abbreviated list of quantities, units and symbols in physical chemistry, Blackwell Scientific Publications, Oxford 1993.

12. Swedish translation of 11: Holmström, B.

13. Mills, I., T. Cvitaš, K. Homann, N. Kallay, K. Kuchitsu: Quantities, units and symbols in physical chemistry, 2nd ed., Blackwell Scientific Publications, Oxford 1993, x + 166.

14. German translation of 10: Hausmann, M.: Größen, Einheiten und Symbole in der Physikalischen Chemie, Verlag Chemie, Weinheim 1996.

Commission I.2 Thermodynamics

1. Recommendations: [N - nomenclature], [R - recommendations and guidelines]

1.01 Rossini, F.D., K. Schaefer, D.M. Newitt: Resolution on publication of calorimetric and thermodynamic data, *Pure Appl. Chem.* **2** (1960) 339-342 [R]

1.02 Rossini, F.D.: Values of the fundamental constants for chemistry, *Pure Appl. Chem.* **9** (1964) 453-459 [Data - superseeded 1993]

1.03 Rossini, F.D.: A report on the international practical temperature scale of 1968, *Pure Appl. Chem.* **22** (1970) 555-570 [R]

1.04 Cox, J.D.: A guide to procedures for the publication of thermodynamic data, *Pure Appl. Chem.* **51** (1979) 393-403 [R]

1.05 Olofsson, G.: Manual of symbols and terminology for physicochemical quantities - Appendix IV, *Pure Appl. Chem.* **53** (1981) 1805-1825 [N]

1.06 Cox, J.D.: Assignment and presentation of uncertainties of the numerical results of thermodynamic measurements, *Pure Appl. Chem.* **54** (1982) 1239-1250 [R]

1.07 Goldberg, R.N., R.D. Weir: Conversion of temperatures and thermodynamic properties to the basis of the international temperature scale of 1990, *Pure Appl. Chem.* **64** (1992) 1545-1562 [R]

1.08 Ewing, M.B., T.H. Lilley, G.M. Olofsson, M.T. Rätzsch, G. Somsen: Standard quantities in chemical thermodynamics, *Pure Appl. Chem.* **66** (1994) 533-552 [N, R]

1.09 Guidelines for publication of equations of state - I. Pure Fluids, *Pure Appl Chem* **69** (1997) 1237-1249.[N,R]

1.10 Boly, A., U. K. Deiters, C. J. Peters, T. W. de Loos: Nomenclature for phase diagrams with particular reference to vapour-liquid and liquid-liquid equilibria, , *Pure Appl Chem* **70** (1998) 2233-2257.[N]

2. Educational: Experimental Techniques and Theory

2.01 Experimental Thermodynamics - III, Measurement of transport properties of fluids - Chemical Data Series, No. 37, Blackwell Scientific Publications, Oxford 1991, xx + 459.

2.02 Experimental Thermodynamics IV. Solution Calorimetry, Blackwell Scientific Publications, Oxford 1994, xviii + 331.

2.03 Transport Properties of Fluids; their correlation, prediction and estimation, Cambridge University Press (1996), xiv + 483.

3. Compilations of Critically Evaluated Data and Standard Reference Values:

a) Books

3a.01 Electrolyte Data Collection - 1a: Conductivities, transference numbers, limiting ionic conductivities (methanol)- Chemistry Data Series XII, DECHEMA.

3a.02 Electrolyte Data Collection - 1a: Conductivities, transference numbers, limiting ionic conductivities of ethanol solutions- Chemistry Data Series XII, DECHEMA, 1993, xviii + 248.

3a.03 Electrolyte Data Collection - 2: Dielectric properties of water and aqueous electrolyte solutions - Chemistry Data Series XII, DECHEMA, 1992.

3a.04 Electrolyte Data Collection - 2a: Dielectric properties of non-aqueous solutions - Chemistry Data Series XII, DECHEMA, 1992.

3a.05 Electrolyte Data Collection - 3 Viscosities of non-aqueous solutions (aprotic and protic non-alcohol solutions), Part a (C1-C3) and Part b (C4-C8), Chemistry Data Series XII, DECHEMA, 1996.

3a.06 Enthalpies of vaporization of organic compounds - A critical review and data compilation, Chemical Data Series, No. 32, Blackwell Scientific Publications, Oxford 1985, 1-300.

3a.07 Heat Capacity of Liquids: Volume I - Critical Review and Recommended Values, *J. Phys. Chem. Ref. Data*, Monograph No. 6, Amer. Chem. Soc., 1-813 (1996).

3a.08 Heat Capacity of Liquids: Volume II - Critical Review and Recommended Values, *J. Phys. Chem. Ref. Data*, Monograph No. 6, Amer. Chem. Soc., 814-1596 (1996).

3a.09 International Thermodynamic Tables of the Fluid State - 8: Chlorine, Chemical Data Series, No. 31, Pergamon Press, Oxford 1985, xviii + 162.

3a.10 International Thermodynamic Tables of the Fluid State - 9: Oxygen, Chemical Data Series, No. 33, Blackwell Scientific Publications, Oxford 1987, xviii + 231.

3a.11 International Thermodynamic Tables of the Fluid State - 10: Ethylene (ethene), Chemical Data Series, No. 34, Blackwell Scientific Publications, Oxford 1988, xxviii + 299.

3a.12 International Thermodynamic Tables of the Fluid State - 11: Fluorine, Chemical Data Series, No. 36, Blackwell Scientific Publications, Oxford 1990, xviii + 193.

3a.13 International Thermodynamic Tables of the Fluid State - 12: Methanol, Chemical Data Series, No. 38, Blackwell Scientific Publications, Oxford 1992, xxii + 295.

3a.14 International Thermodynamic Tables of the Fluid State - 13: Methane, Blackwell Science, Oxford 1996, xxii + 219.

b) Scientific Publications:

Transport Properties of Gases and Liquids:

3b.1.01 Equilibrium and transport properties of the noble gases and their mixtures at low density, *J. Phys. Chem. Ref. Data* 13 (1984) 229-303.

3b.1.02 Viscosity of nitrogen, oxygen and their binary mixtures in the limit of zero density, *J. Phys. Chem. Ref. Data* 14 (1985) 209-226.

3b.1.03 Thermal conductivity of fluid air, *J. Phys. Chem. Ref. Data* 14 (1985) 227-234.

3b.1.04 Viscosity and thermal conductivity of dry air in the gaseous phase in a wide range of temperature and pressure, *J. Phys. Chem. Ref. Data* 14 (1985) 947-970.

3b.1.05 Standard reference data for thermal conductivity of liquids, *J. Phys. Chem. Ref. Data* 15 (1986) 1073-1088.

3b.1.06 Viscosity and thermal conductivity coefficients of gaseous and liquid argon, *J. Phys. Chem. Ref. Data* 15 (1986) 1323-1337.

3b.1.07 Improved tables for calculation of nonspherical contributions to second virial coefficients, *Int. J. Thermophys.* **7** (1986) 1115-1133.

3b.1.08 Viscosity and thermal conductivity of normal hydrogen in the limit of zero density, *J. Phys. Chem. Ref. Data* **15** (1986) 1315-1322

3b.1.09 Viscosity of carbon dioxide, methane and sulfur hexafluoride in the limit of zero density, *J. Phys. Chem. Ref. Data* **16** (1987) 175-187

3b.1.10 Viscosity of normal deuterium in limit of zero density, *J. Phys. Chem. Ref. Data* **16** (1987) 189-192

3b.1.11 Equilibrium and transport properties of eleven polyatomic gases a t low density, *J. Phys. Chem. Ref. Data* **16** (1987) 445-467 .

3b.1.12 Viscosity and thermal conductivity of nitrogen for a wide range of fluid states, *J. Phys. Chem. Ref. Data* **16** (1987) 993-1023.

3b.1.13 Viscosity of liquid toluene in temperature range 25-75oC, *Int. J. Thermophys.* **8** (1987) 641-647.

3b.1.14 Transport properties of isobutane, *J. Chem. Eng. Data* **32** (1987) 1-8.

3b.1.15 Thermal conductivity of liquid n-alkanes, *Int. J. Thermophys.* **9** (1988) 351-363.

3b.1.16 Thermal conductivity of nitrogen and carbon monoxide in the limit of zero density, *J. Phys. Chem. Ref. Data* **18** (1989) 565-581.

3b.1.17 Thermal conductivity of ethane in the critical region, *Int. J. Thermophys.* **10** (1989) 409-415.

3b.1.18 Viscosity of refrigerants R12, R113, and R114 and mixtures of R12 + R114, at high pressure, *Int. J. Thermophys.* **10** (1989) 701-712.

3b.1.19 Absolute measurements of thermal conductivity of mixtures of alcohols with water, *Int. J. Thermophys.* **10** (1989) 793-803.

3b.1.20 Theoretically based data assessment for correlation of thermal conductivity of dilute gases, *Int. J. Thermophys.* **10** (1989) 805-818.

3b.1.21 Correlation and prediction of thermal conductivity and other properties of gases at zero density, *Int. J. Thermophys.* **10** (1989) 983-993.

3b.1.22 On the validity of the simplified expression for thermal conductivity of Thijse et al., *Physica A* **148** (1988) 153-164 .

3b.1.23 On the theory of oscillating cup viscometers, *Physica A* **149** (1988) 107-122

3b.1.24 Viscosity of methane at 25 _C up to 10 kbar, *Physica A* **151** (1988) 153-166 .

3b.1.25 On the temperature function of the viscosity of nitrogen in the limit of zero density, *Z. phys. Chem*. **270** (1989) 1145-1152.

3b.1.26 Thermal conductivity of carbon dioxide, High Temp. High Press. **21** (1989) 225-231.

3b.1.27 Prediction of viscosity of fluid mixtures over wide ranges of temperature and pressure, *Chem. Eng. Sci*. **44** (1989) 2181-2189.

3b.1.28 Working equations of a vibrating wire viscometer, *Physica A* **156** (1989) 909-920.

3b.1.29 Benzene - A further liquid thermal conductivity reference material, *J. Phys. Chem. Ref. Data* **19** (1990) 113-117.

3b.1.30 Thermophysical properties of alkali metal vapours - I: Theoretical calculation of the properties of monoatomic systems, *Ber. Bunsenges. Phys. Chem*. **90** (1990) 53-59.

3b.1.31 Transport properties of carbon dioxide, *J. Phys. Chem. Ref. Data* **19** (1990) 763-808.

3b.1.32 Thermal conductivity of a moderately dense gas, *Chem Phys*. **145** (1990) 19-26.

3b.1.33 Thermal conductivity of ethane in the critical region, *J. Chem. Phys*. **92** (1990) 5454-5462.

3b.1.34 Guarded parallel-plate instrument for measuring thermal conductivity of fluids in the critical region, *Rev. Sci. Instrum*. **60** (1990) 3466-3474.

3b.1.35 Measurements of thermal conductivity of nitrogen with a parallel-plate instrument, *Int. J. Thermophys.* **11** (1990) 597-601.

3b.1.36 Absolute vibrating-wire viscometer for liquids at high pressures, *Int. J. Thermophys.* **12** (1991) 231-244.

3b.1.37 Measurement of viscosity of benzene, toluene, and m-xylene at pressures up to 80 MPa, *Int. J. Thermophys.* **12** (1991) 449-457.

3b.1.38 Measurement of viscosity of n-heptane, n-nonane and n-undecane at pressures up to 80 MPa, *Int. J. Thermophys.* **12** (1991) 801-810.

3b.1.39 Viscosity of three binary hydrocarbon mixtures, *J. Chem. Eng. Data* **36** (1991) 85-88.

3b.1.40 The viscosity of carbon dioxide up to 450 MPa. *High Temperature - High Pressure* **23** (1991) 87-95.

3b.1.41 Viscosity of liquid toluene at temperatures from 25 to 150 _C and at pressures up to 30 MPa. *J. Chem. Eng. Data* **37** (1992) 349-355.

3b.1.42 Transport properties of ethane - I: Viscosity, *Int. J. Thermophys.* **15** (1994) 1-31.

3b.1.43 Transport properties of ethane - II: Thermal conductivity, *Int. J. Thermophys.* **15** (1994) 33-66.

3b.1.44 Vapour-liquid equilibria in alkan-1-ol + *n*-alkane mixtures, *Pure Appl. Chem*. **66** (1994) 553-564.

3b.1.45 Viscosity of selected liquid n-alkanes, *J. Phys. Chem. Ref. Data* **23** (1994) 41-53.

3b.1.46 Status of the round robin on the transport properties of R134a, *Int. J. Thermophys.* **16** (1995) 63-78.

3b.1.47 A round robin project on the transport properties of R134a, *Int. J. Refrig*. **18** (1995) 355-357.

3b.1.48 Reference correlation of the viscosity of propane, *J. Phys. Chem. Ref. Data* **27** (1998) 947-970.

3b.1.49 The thermal conductivity of methane in the critical region., *J. Chem. Phys*. **105** (1996) 10535-10555.

3b.1.50 Transport properties of 1,1-difluoroethane (R152a). *Int. J. Thermophys.* **17** (1996) 397-404.

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