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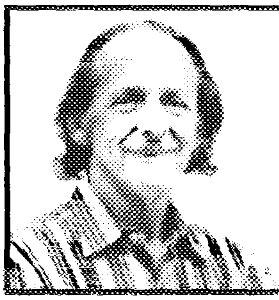

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# Journal Citation Studies. 46. Physical Chemistry and Chemical Physics Journals. Part 1. Historical Background and Global Maps

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This is the 46th in a series of journal citation analyses reported in *Current Contents®* (*CC®*) over the past two decades. It is my ambition to eventually round out these studies so that we can provide a successor to the monograph known to college and research librarians the world over as Brown's *Scientific Serials*.[1] Of course, the *Science Citation Index®* (*SCI®*) and its annual volumes of the *Journal Citation Reports®* (*JCR®*) are far more detailed tools for collection managers. But the very brevity of Brown's analysis has a special virtue that we hope to emulate by updating and expanding the brief reports we published earlier in *Science*[2] and *Nature*.[3]

In this three-part journal study, we focus on 31 periodicals from physical chemistry and chemical physics, two disciplines that today are inextricably linked. However, this was not always the case, as we shall see in the discussion that follows. In this essay we will cover the general history and development of the two fields as well as some of their current concerns. The latter were identified by examining ISI®'s 1983 research-front data. Keep in mind that the historical section in this essay must necessarily be limited to a broad overview of the two fields. Entire books have already been written on these subjects. But it is important that we review these developments here in order to provide an understanding of the present interrelationship between physical chemistry and chemical physics. Parts 2 and 3 of our study will then concentrate on the 31 physical chemistry/chemical physics journals listed in Table 1.

## History

Physical chemistry began as the study of the "physical" properties of chemical substances. Many of these properties were discovered in the nineteenth century. For example, in the early 1800s Humphry Davy (UK) and Jöns Jakob Berzelius (Sweden) demonstrated for the first time the electrical nature of chemical affinity, the relationship between substances that causes them to combine.[4] (p. 8-9) It was Hermann Kopp (Germany), however, who made the first real effort, in 1840, to measure the properties of chemical substances while correlating these qualities with chemical composition. For example, he tested substances at different temperatures and measured their resulting changes in volume; his studies on ice were so precise that they are still valid today.[5] (p. 392)

In the mid-nineteenth century, Jean Baptiste André Dumas (France) advanced the first theory of chemical types, a classification of "parent" compounds together with their substituted derivatives if both share the same fundamental chemical properties.[4] (p. 427) Shortly thereafter, in 1869, Dmitri Mendeleev (Russia), J. Lothar Meyer (Germany), and John Alexander Reina Newlands (UK) independently developed similar versions of the periodic law that

**Table 1:** Core physical chemistry/chemical physics journals indexed by the *SCI*® in 1983.

| |
|---|
| Annual Review of Physical Chemistry |
| Berichte der Bunsen-Gesellschaft fur Physikalische Chemie |
| Chemical Physics |
| Chemical Physics Letters |
| Faraday Discussions of the Chemical Society |
| International Journal of Chemical Kinetics |
| International Journal of Quantum Chemistry |
| Journal of Catalysis |
| Journal of Chemical and Engineering Data |
| Journal of Chemical Physics |
| Journal of Chemical Thermodynamics |
| Journal of Colloid and Interface Science |
| Journal of Computational Chemistry |
| Journal of Magnetic Resonance |
| Journal of Molecular Spectroscopy |
| Journal of Molecular Structure |
| Journal of Photochemistry |
| Journal of Physical Chemistry |
| Journal of Solution Chemistry |
| Journal of the Chemical Society—Faraday Transactions I |
| Journal of the Chemical Society—Faraday Transactions II |
| Journal of the Chemical Society—Perkin Transactions II |
| Kinetics and Catalysis—English Translation |
| Molecular Physics |
| Photochemistry and Photobiology |
| Radiation Physics and Chemistry |
| Surface Science |
| THEOCHEM—Journal of Molecular Structure |
| Theoretica Chimica Acta |
| Zeitschrift fur Physikalische Chemie—Leipzig |
| Zhurnal Fizicheskoi Khimii |

states that the properties of elements are functions of their atomic weights. From this law Mendeleev created the periodic table of elements of which an enlarged version is still used today.[4] (p. 317-8); [6]

In the 1870s Josiah Willard Gibbs, then at Yale University, used the term "phases" for the homogeneous strata of chemical substances. Phases (such as solids, liquids, and gases) are uniform in both composition and physical state. Gibbs then formulated the "rule of phases" according to their dependence on physical conditions such as pressure and temperature. This rule states that when a substance is in equilibrium, the sum of its phases and of possible variations of phases which can occur within it is always equal to three.[7] (p. 217-8); [8] (p. 319-20); [9] The rule "was published in the rather obscure *Transactions of the Connecticut Academy* and [was] overlooked for 20 years."[8] (p. 319) A classic case of delayed recognition, this 321-page paper, "On the equilibrium of heterogeneous substances,"[10] "was only slowly recognized for its significance. Because of its abstract mathematical treatment and austere style, American physicists and chemists were unable to master its import."[5] (p. 405) Once Gibbs was rediscovered he became an important figure. The two parts of his classic have been co-cited in hundreds of papers. Over 40 of these cites involve articles published in the last few years. Figure 1 is a graph of this paper's citation history from 1955 to 1984.

Wilhelm Ostwald (Germany), Jacobus H. van't Hoff (Holland), and Svante August Arrhenius (Sweden) organized the physical laws of chemical phenomena into one field and established *Zeitschrift fur Physikalische Chemie* in 1887.[5] (p. 391); [7] (p. 216); [11] The publication of this journal is considered the beginning of physical chemistry as a formal branch of chemistry.[11] The first volume of the new journal published Arrhenius's theory of ionization that in part stated that ions form when a salt dissolves in water.[5] (p. 413-5) Not surprisingly, the journal that these three researchers founded is part of the core group of journals in this three-part study. (See Table 1.) It will be discussed in more detail in Part 2.

Physical chemistry continued to mature in the early 1900s. *Transactions of the Faraday Society*, the precursor to the *Journal of the Chemical Society—Faraday Transactions I* and *II*, was founded in 1905 during this period in which physical chemistry and chemical physics were established as serious subjects.[12] *General Discussions of the Faraday Society* also began around this time (1907) as a part of the *Transactions*. Today it is known as *Faraday Discussions of the Chemical Society* (see Table 1), although for 25 years (1947-1972) it was

**Figure 1:** Chronologic distribution of 1955-1984 *SCI®* citations to J.W. Gibbs's two-part article, "On the equilibrium of heterogeneous substances."

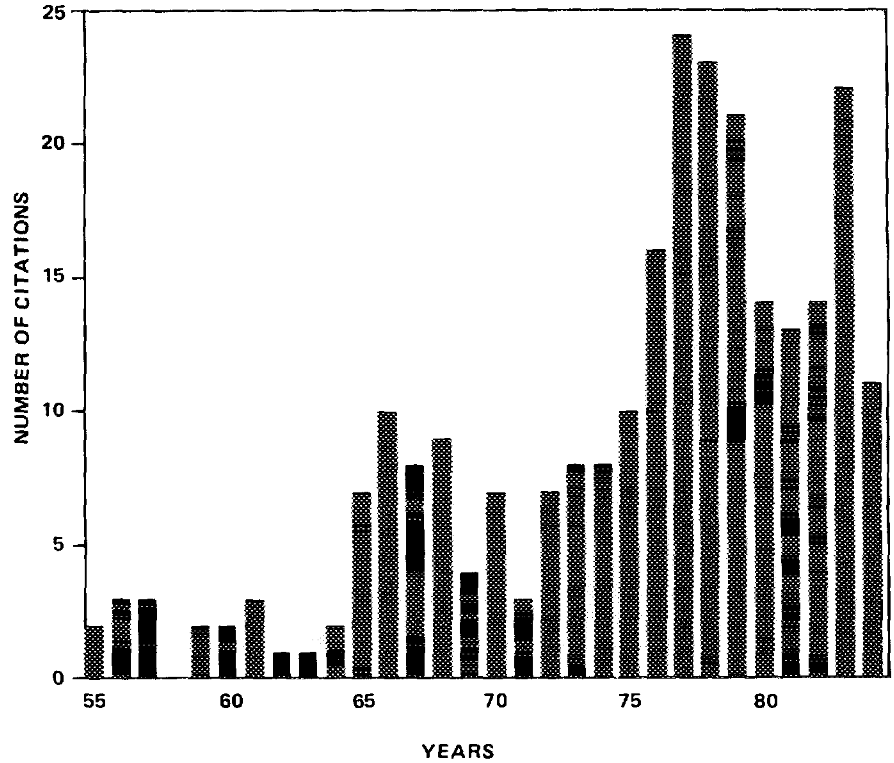
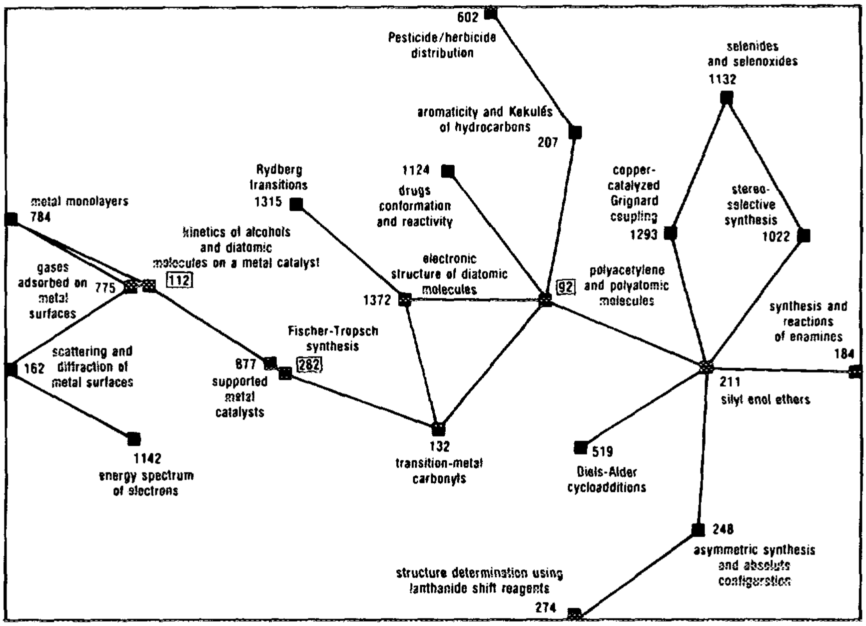



**Table 2:** The 1983 *SCI®* research-front specialties that include at least 100 citing documents published in core physical chemistry/chemical physics journals. A = research-front number. B = title. C = number of core physical chemistry/chemical physics journals that cite the research front. D = number of 1983 articles from these core journals that cite the research front.

| A | B | C | D |
|---|---|---|---|
| 83-0023 | Phase equilibria and thermodynamics of hard-sphere fluids and binary liquids | 13 | 256 |
| 83-0058 | Surface analysis of metal alloys, hydrides, and semiconductors by Auger electron spectroscopy and other techniques | 13 | 191 |
| 83-0075 | Processes of photoelectrochemical cells and applications to solar energy conversion | 23 | 541 |
| 83-0092 | *Ab initio* and other molecular-orbital calculations of force fields and electronic structure of polyacetylene and polyatomic molecules | 21 | 783 |
| 83-0112 | Kinetics of adsorption, desorption, and decomposition of alcohols and diatomic molecules on a metal catalyst | 7 | 150 |
| 83-0185 | Properties of chaotic and dynamic systems | 9 | 152 |
| 83-0190 | Theoretical studies of van der Waals interaction potentials | 10 | 147 |
| 83-0262 | Renormalization group approach in gauge theory of critical behavior and other properties of two-dimensional lattices | 10 | 130 |
| 83-0282 | Mechanism of the hydrogenation of carbon monoxide on supported metal catalysts; Fischer-Tropsch synthesis | 7 | 120 |
| 83-0291 | Calculations of electronic structure, magnetism, and other properties of alloys | 11 | 132 |
| 83-0297 | Vibrational relaxation and dephasing in picosecond laser Raman and infrared scattering | 9 | 133 |
| 83-0547 | Use of nuclear magnetic resonance in the analysis of protein and peptide structure | 16 | 269 |
| 83-0807 | Structure and physical properties of ice | 14 | 113 |

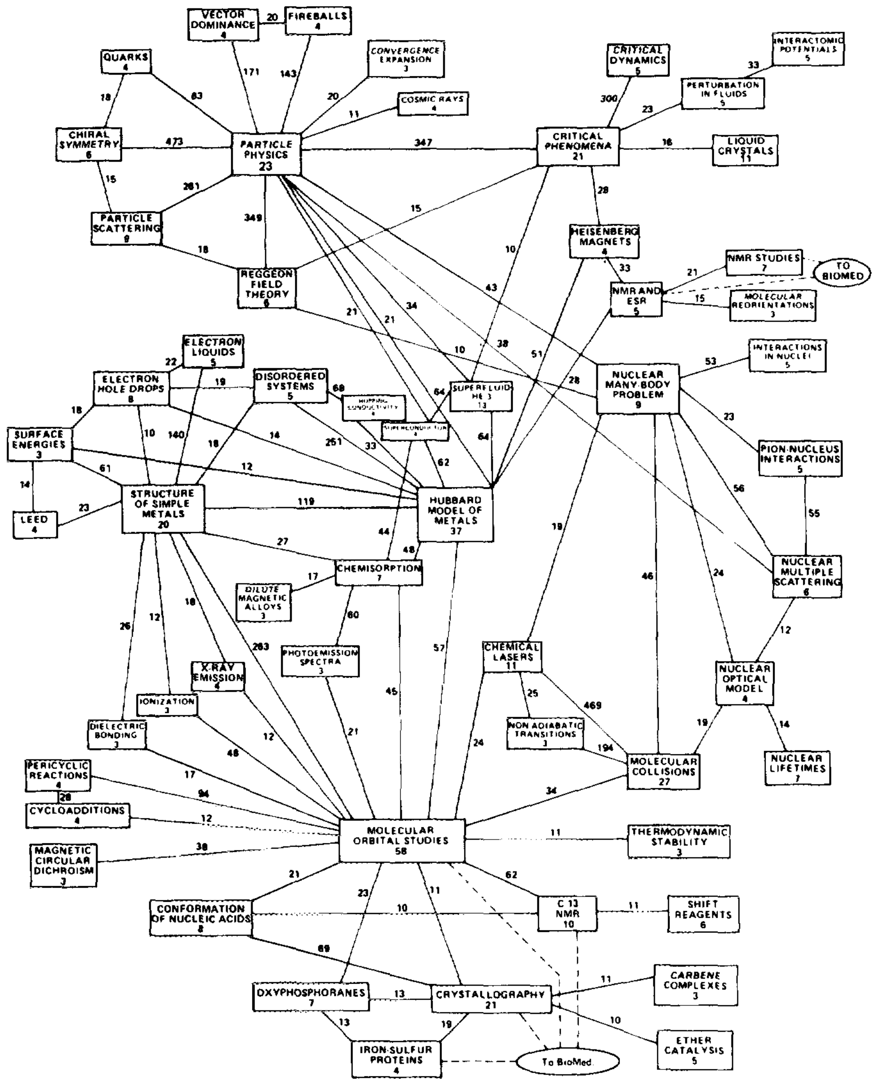
**Figure 2:** The 1983 map for "Molecular-orbital calculations of electronic structure applied to organic synthesis and adsorption studies on catalyst surfaces." This map includes three research fronts from Table 2 (#92, #112, and #282).




**Key**

83-0092 *Ab initio* and other molecular-orbital calculations of force fields and electronic structure of polyacetylene and polyatomic molecules
83-0112 Kinetics of adsorption, desorption, and decomposition of alcohols and diatomic molecules on a metal catalyst
83-0132 Synthesis, structure, and reactions of transition-metal carbonyls and other clusters
83-0162 Scattering and diffraction studies of metal surfaces by electron energy loss spectroscopy
83-0184 Synthesis and reactions of enamines
83-0207 Theory of aromaticity and Kekulé structures of conjugated hydrocarbons
83-0211 Preparation and use of silyl enol ethers in organic synthesis
83-0248 Use of chiral reagents for asymmetric synthesis and determination of absolute configuration
83-0274 Structure determination using lanthanide shift reagents
83-0282 Mechanism of the hydrogenation of carbon monoxide on supported metal catalysts; Fischer-Tropsch synthesis
83-0519 Synthesis, rearrangements and fragmentation studies of Diels-Alder cycloadditions
83-0602 Determination of organic compounds, pesticides, and herbicides and their distribution in the environment
83-0775 Infrared study of carbon monoxide and other gases adsorbed on metal surfaces
83-0784 Chemisorption properties of metal monolayers and gases on single-crystal metal surfaces
83-0877 Characterization and activity of supported metal catalysts
83-1022 Stereoselective synthesis of organic compounds and natural products
83-1124 Molecular-orbital studies of the conformation and reactivity of drugs
83-1132 Reactions of selenides and selenoxides
83-1142 Characterization of the energy spectrum of electrons at various surfaces
83-1293 Use of copper-catalyzed Grignard coupling reactions in organic synthesis
83-1315 Spectroscopic studies of electronic structure and Rydberg transitions of atoms, ions, and chemisorbed molecules
83-1372 *Ab initio* molecular-orbital calculations of ionization potentials and core energies; electronic structure of diatomic molecules by photoelectron spectroscopy

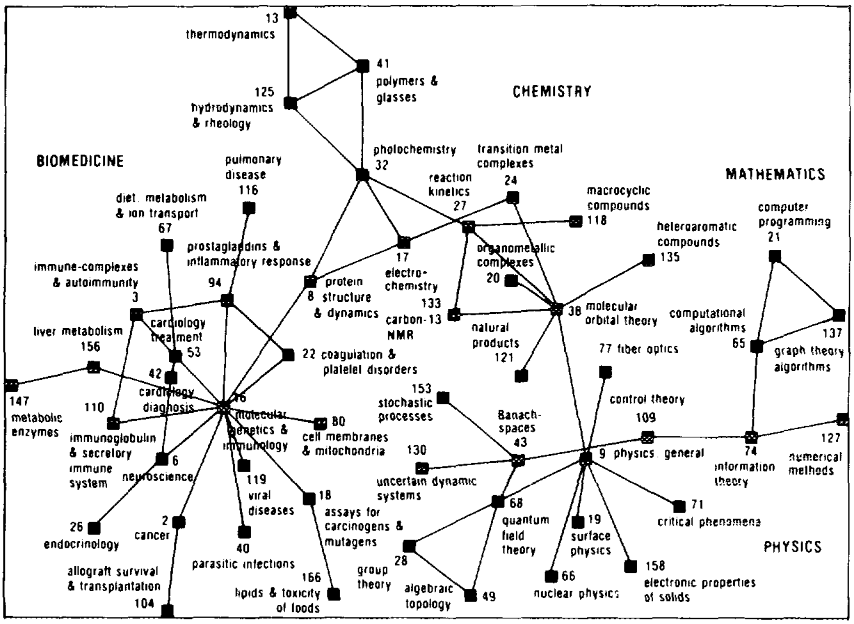
**Figure 3:** The 1974 map of chemistry and physics. Serial numbers are for identification only. Lines between nodes represent co-citation strength, an indicator of semantic distance.




known simply as the *Discussions of the Faraday Society*.

Chemists working in the early twentieth century found themselves confronted with complex problems that they could not solve using conventional chemical methods. They needed to understand the physical properties of elements and compounds at molecular and submolecular levels, the traditional domain of physicists. Thus the development of chemical physics began as a

**Figure 4:** Multidimensional scaling map of the natural sciences for 1983. Serial numbers are for identification only. Lines between nodes represent co-citation strength, an indicator of semantic distance.




common area of study between physical chemists and physicists. Max Planck, Albert Einstein, and Niels Bohr contributed to this new field with their work in quantum theory.[7] (p. 232) Bohr developed the quantum model of the hydrogen atom in 1913.[5] (p. 502-4); [8] (p. 74; 347)

Physical chemistry and chemical physics continued their parallel development throughout the twentieth century. Subdisciplines such as chemical kinetics, thermodynamics, quantum mechanics, and physical organic chemistry developed with the help of Arthur Amos Noyes, Edward Washburn, Francis Owen Rice, Morris Kharasch, Linus Pauling, John C. Slater,[5] (p. 531-58) and Louis P. Hammett. Slater was the first to write a textbook on chemical physics, in 1939,[13] that has since appeared in several editions, the most recent in 1970. This book was cited 624 times in the 1955-1985 *SCI*. Just one year later, in 1940, Hammett published *Physical Organic Chemistry*.[14] This classic has been explicitly cited over 3,200 times since 1955. Hammett, who is now 91, is a past recipient of numerous awards, including the American Chemical Society's William H. Nichols Medal (1957) and the Willard Gibbs and Priestley Medals (1961). He also won the James Flack Norris Award (1960, 1966), the Lewis Medal (1967), and the National Medal of Science (1968), to name a few.

Despite this parallel development, physical chemistry and chemical physics remained separate because each involved different methodological approaches to problem solving. According to Subbiah Arunachalam, editor, *Indian Journal of Technology*, chemists are content to live in a concrete world, with its myriad substances and compounds and their reactions. But physicists have learned to live with less concrete situations—they attempt to reach levels of understanding inaccessible through the conceptual tools of chemistry.[15]

## Research Fronts

Today, recent research in physical chemistry and chemical physics includes the analysis "of the flow of energy between atoms and molecules, [which] underlies the study of lasers, combustion and catalysis, photosynthesis, atmospheric and interstellar chemistry, and the fabrication of microelectronic circuitry"; high-resolution spectroscopy of polyatomic ions;[16] and the production of metals for industry.[17] These topics are illustrated in the 1983 *SCI* research fronts listed in Table 2. A research front consists of a group of current papers that cites one or more older well-cited papers identified as core for that topic. It also includes the core papers. From these research-front data we can then identify which research fronts are cited by specific journals.

In Table 2 we've listed only those fronts that include at least 100 citing papers published in 1983 in the 31 core journals given in Table 1. In column C of Table 2 we provide the number of core journals represented in each front; column D lists the number of 1983 articles from these journals that cited the research front. We did not calculate the total number of publications for each of the fronts. But, as an example, about 1,100 papers were published on "Phase equilibria and thermodynamics of hard-sphere fluids and binary liquids" (#83-0023), and they cited 95 core documents. It is significant that only about 260 of the papers were published in 13 of the core journals. Over 800 papers were published in non-core journals.

Three fronts (#83-0058, #83-0282, #83-0291) in Table 2 are related to the properties or analysis of metals or metal alloys. Over 400 papers were published on those topics. Equally active, with over 540 papers, is front #83-0075, which deals with processes of photoelectrochemical cells and applications to solar energy conversion. The wide range of topics in this table illustrates that today's physical chemists work in many diverse areas of science with impacts in mathematics, medicine, and botany as well as chemistry and physics.[18]

Without a "map" showing the semantic connections between these topics, it is harder to perceive how they interact. The map in Figure 2 on molecular-orbital theory includes three of the fronts from Table 2 ("*Ab initio* and other molecular-orbital calculations of force fields and electronic structure of polyacetylene and polyatomic molecules" [#83-0092], "Kinetics of adsorption, desorption, and decomposition of alcohols and diatomic molecules on a metal catalyst" [#83-0112], and "Mechanism of the hydrogenation of carbon monoxide on supported metal catalysts; Fischer-Tropsch synthesis" [#83-0282]).

**Table 3:** The national affiliations of papers citing *SCI*® research front #83-3402, "Generation of solitons and electrochemical properties of doped polyacetylene and other one-dimensional polymers; Peierls distortion reduced by electron correlation." A = number of items citing the research front. B = percent of all items citing the research front.

| | A | B |
|---|---|---|
| US | 261 | 41.2 |
| Japan | 117 | 18.5 |
| France | 54 | 8.5 |
| FRG | 43 | 6.8 |
| Italy | 26 | 4.1 |
| USSR | 23 | 3.6 |
| UK | 17 | 2.7 |
| Israel | 11 | 1.7 |
| Poland | 11 | 1.7 |
| Belgium | 10 | 1.6 |
| China | 8 | 1.3 |
| GDR | 6 | 1.0 |
| Sweden | 5 | 0.8 |
| Austria | 4 | 0.6 |
| Canada | 4 | 0.6 |
| India | 4 | 0.6 |
| Mexico | 4 | 0.6 |
| Finland | 3 | 0.5 |
| Spain | 3 | 0.5 |
| Switzerland | 3 | 0.5 |
| Hungary | 2 | 0.3 |
| The Netherlands | 2 | 0.3 |
| Australia | 1 | 0.2 |
| Brazil | 1 | 0.2 |
| Unassigned | 10 | 1.6 |
| **TOTAL** | 633 | 100% |

A more precise view of the world of chemistry is seen in Figure 3, which shows the 1974 map of chemistry and physics. This map makes it easier to view the complex borderland between chemistry and physics. An even more extensive map (for 1983) is shown in Figure 4. The relationship between chemistry and biomedicine and biochemistry is more apparent in this map. Incidentally, the map in Figure 2 is represented by point #38 in Figure 4.

Were there time and space to do so, we could create similar but more detailed maps from a subset of the *SCI* constituting the citation index drawn from the core journals listed in Table 1. However, we can get a comparable perspective by examining the list of research fronts that are most prominently cited in these journals. (See Table 2.)

If we want to get a country-by-country perspective on research areas in physical chemistry and chemical physics, we can also use our *SCI* data. Table 3 shows the percentage of citing papers by country that were published in a research front on electrochemical properties of doped polyacetylene and other one-dimensional polymers (#83-3402). For example, the number of papers from Japan in that front is much larger than its overall 1983 *SCI* share of 5 percent. This is, of course, only an example and may be quite different for other fronts. Some old-fashioned fields of physical chemistry are more popular in certain countries. This may be because they use alternative technologies or simply because they are unable to conduct more modern research.

## Conclusion

This concludes the first part of our study on physical chemistry/chemical physics and the journals that are most prominent in these fields. As we have seen in the research fronts and maps provided in this essay, physical chemistry and chemical physics have become closely intertwined despite their different approaches to the physical world. Their interdependence will become even more evident in our analyses in Parts 2 and 3 of this study.

* * * * *

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## REFERENCES

1. **Brown C H.** *Scientific serials.* Chicago: Association of College and Reference Libraries, 1956. 189 p.
2. **Garfield E.** Citation analysis as a tool in journal evaluation. *Science* 178:471-9, 1972.
3. --------------. Significant journals of science. *Nature* 264:609-15, 1976.
4. **Bynum W F, Browne E J & Porte R,** eds. *Dictionary of the history of science.* London: Macmillan Press, 1981. 494 p.
5. **Ihde A J.** *The development of modern chemistry.* New York: Harper & Row, 1964. 851 p.
6. Science: scientific inventions, discoveries, and theories. *Information Please Almanac 1983.* New York: A&W, 1982. p. 356.
7. **Lockemann G.** *The story of chemistry.* New York: Philosophical Library, 1959. 277 p.
8. **Barrow G M.** *Physical chemistry.* New York: McGraw-Hill, 1979. 832 p.
9. **Wheeler L P.** *Josiah Willard Gibbs.* New Haven, CT: Yale University Press, 1951. p. 79.
10. **Gibbs J W.** On the equilibrium of heterogeneous substances. *Trans. Connecticut Acad.* Vol. III. Oct. 1875-May 1876. p. 108-248; May 1877-July 1878. p. 343-524. (Reprinted in: *The collected works of J. Willard Gibbs.* New Haven, CT: Yale University Press, 1957. Vol. 1. p. 55-353.)
11. **Maron S H & Prutton C F.** Introduction. *Principles of physical chemistry.* New York: Macmillan, 1966. p. 1-3.
12. **Young D A.** Personal communication. 13 November 1985.
13. **Slater J C.** *Introduction to chemical physics.* New York: Dover, 1939. 521 p.
14. **Hammett L P.** *Physical organic chemistry.* New York: McGraw-Hill, 1940. 404 p.
15. **Arunachalam S.** Personal communication. 24 October 1985.
16. **Leone S R.** Molecular energy transfer of ions. *Phys. Today* 38(11):S.15-S.16, 1985.
17. **Sohn H Y.** Developments in physical chemistry and basic principles of extractive and process metallurgy in 1983. *J. Metals* 36(4):48-54, 1984.
18. **Castellan G W.** Preface to the first edition. *Physical chemistry.* Reading, MA: Addison-Wesley, 1971. p. vii-ix.