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Physical Chemistry: Neither Fish nor Fowl?

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1. Introduction

The birth of a new discipline, called 'physical chemistry', is sometimes related to the names OSTWALD, ARRHENIUS and VAN'T HOFF and dated back to the year 1887, when OSTWALD founded the *Zeitschrift für physikalische Chemie*.[1] But as many historians have pointed out, the phrase 'physical chemistry' was widely used before that and the topics under investigation partially go back to Robert BOYLE's attempts to connect chemistry with concepts of mechanical philosophy.[2] The idea of a sudden birth of physical chemistry in 1887 seems to be a founder myth.[3] But there is no doubt that in the late nineteenth-century there was a rapid growth of research in fields now understood as physical chemistry: chemical thermodynamics, electrochemistry, photochemistry, spectroscopy, chemical kinetics etc.[4]

Historians (and sociologists) of science have proposed several categories to describe the genesis and to fix the identity of scientific 'disciplines', 'fields', 'traditions', 'paradigms', 'research schools' etc.[5] In what follows, I will not consider sociological categories but concentrate on knowledge based philosophical or methodological aspects to describe characteristics of physical chemistry as a research field. Certainly, physical chemistry is in a sense related to physics as well as to chemistry establishing some relation between the two fields. But what kind of relation does it establish? Is it a kind of reductive relation *reducing* or integrating chemistry to some unifying physical science, as NERNST and even OSTWALD thought?[6] Or should we treat physical chemistry as a *link* between physical methods and concepts and chemical topics? Or does it just *fill a gap* between chemistry and physics, which

1 E.g. EYRING 1976.

2 There was actually a journal called *Annalen der Physik und der Physikalischen Chemie* (1819-23) as the predecessor of POGGENDORFF's later *Annalen der Physik und Chemie*; Herrmann KOPP holds an independent chair of "Physikalische Chemie" at Heidelberg since 1863; and BOYLEs famous "Sceptical Chymist" was subtitled "Physico-Chymical Doubts and Paradoxes ..." Among eighteenth- and early nineteenth-century chemists celebrated as the forefathers of physical chemistry were MACQUER, LAVOISIER, DUMAS, BERTHOLLET, DAVY, FARADAY, BUNSEN, LANDOLT, ROSE, GULDBERG, WAAGE (SERVOS 1990).

3 Cf. DOLBY 1976, ROOT-BERNSTEIN 1980, BARKAN 1990, NYE 1993.

4 Important studies in the history of physical chemistry are: BARKAN 1990, BITTRICH 1986, BRUSH 1976, DOLBY 1976, DUBPERNELL/WESTBROOK 1978, EYRING 1976, GIRNUS 1982, 1986, GUÉRON, MAGAT 1971, KING 1981, LAIDLER 1985, 1993, NYE 1993, ROOT-BERNSTEIN 1980, PARTINGTON 1964, SERVOS 1990, WINTERMEYER 1975.

5 A short survey with special reference to the historiography of chemistry is given by NYE (1993, chapt. 1).

6 Cf. NYE 1993: 108f.

would otherwise be neglected? Or is it even a *new type of research field* once emerged from a fruitful combination of chemistry and physics but now in some sense wedging them?

My *overall thesis* is that we can make sense of all these interpretations, if we restrict them to certain aspects. If the perspectives are mixed unreasonably, we get into trouble with the meaning of ‘physical chemistry’.[7] In what follows I will try to clarify the aspects and give an outline of characteristics of physical chemistry.

2. Filling the gap between chemistry and physics

My first point is that *physical chemistry has always filled a knowledge gap in material science,* as long as we take physics and chemistry in a narrow sense. Let me give an outline of the topics of material science by giving a typology of material investigations (Fig. 1).

“simple” properties		**contextual factors**		**“composed” properties**
				mechano-electrical 1)
mechanical 1)	←	mechanical (directional) forces		*thermo-electrical* 1)
thermodynamical 1)	←	heat and (hydrostatic) pressure		*electro-optical* 1)
electrical 1)	←	electric fields		...
magnetical 1)	←	magnetic fields	→	*photo-chemical* 3)
optical 1)	←	light		*electro-chemical* 3)
chemical 2)	←	chemical reagents		*thermo-el.-chem.* 3)
				...

1) physical (material) properties, 2) chemical properties, 3) physico-chemical properties

Figure 1: Typology of material properties according to relevant contextual factors of experimental investigations. Selection of only one factor yields ‘simple’ properties (left side); selection of two or more factors yields ‘composed’ properties (right side).

Material science is concerned with the behaviour of material objects under certain contextual conditions: mechanical (directional) forces, heat and (hydrostatic) pressure, electric and magnetic fields, light and chemical reagents.[8] According to the list of contextual factors we can define simple material properties (like mechanical, thermodynamical, electrical, magnetical, optical and chemical properties). Certainly, every context can be described in terms of each factor. But if we introduce neutral or standard conditions for each of them (e.g. standard pressure and temperature, zero magnetic and electric field, inert container material etc.), then we can concentrate on a single factor as the relevant one for the object’s behaviour. In that way, *chemical properties* are kept distinct from the rest which may be called *physical material properties*. In the same way, we can introduce ‘composed’ material properties, if two or more contextual factors are considered to be relevant (like thermo-electrical, electro-optical, photo-chemical, electro-chemical, thermo-electro-chemical properties and so on). Whenever the chemical factor (i.e. a chemical reagent) is considered to be one of the relevant factors we can speak of a *physico-chemical property*. In sum, we can carefully distinguish

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7 LAIDLER (1993: 7), for instance, after trying to clarify the meaning of 'physical chemistry' concludes in resignation: "Although I cannot precisely define what physical chemistry is I can recognize it when I see it, and I am sure most of us can. Perhaps I can do no better than say that anything covered in this book, and much else besides, is physical chemistry!"

8 For more details see SCHUMMER 1994, 1997a.

between *chemical, physico-chemical and physical material properties*. Now, let us see, which of these fields are left for physical chemists.

Chemists are first and foremost interested in chemical properties accompanied by a chemical reaction, i.e. a change of chemical identity on the level of pure substances.[9] Hence, they give place to the investigation of mixing materials without chemical reaction. This field is covered by *solution theory* and *theory of phase equilibria*, both are central topics of physical chemistry. Next in our list, physico-chemical properties (electro-, thermo- and photochemical) seem to found the most prominent fields of physical chemistry: *electrochemistry, chemical thermodynamics and photochemistry*.

3. Applying physical methods and concepts to chemical topics

Do investigations of *physical material properties* belong to the domaine of physics or physical chemistry? There certainly are controversial claims due to different definitions of the discipline's identity. If there is a distinct border between research fields at all, we might draw the line according to different historical 'interests'. The 'chemical interest', on the one hand, aims at the *diversity of chemical substances* – as a heritage of natural history. Chemists' laboratory practice has enlarged the number of chemical substances to more than 15 mio now, and their concern is specially with the variety of material properties. One the other hand, the 'physical interest' aims at 'universal' properties and laws abstracting from any peculiarities of a certain material object – as a heritage of natural philosophy. The difference may be illustrated by electric properties.

Take, for instance, OHM's law (U: voltage, I: electric currency, R: const. resistance):

$$dU = R \cdot dI \qquad \text{(I)}$$

There is no reference to certain materials, because the law was intended to express an *universal electric property* of matter. Meanwhile, OHM's law does not claim to be universal any longer, because there are many materials which do not obey the law. But for those materials which do at least approximately, the law is extremely useful to introduce *specific electric properties*: Define a geometric standard form of material objects, g, and express R in terms of specific electric conductivity of material i (c_i)

$$R = g/c_i \qquad \text{(II)}$$

Then mathematical transformation of OHM's law yields

$$c_i = g \cdot dI/dU \qquad \text{(III).}$$

Hence, we can characterize each material in terms of its *specific* electric conductivity by simply measuring dI/dU of a standard sample.

Following our distinction between 'scientific interests' we have turned from physics (electricity) to physical chemistry (electrochemistry). One can easily find the same switch with all the other physical material properties. For instance, general thermodynamics provides specific heat capacities, isothermal compressibilities and so on, LAMBERT-BEER's law provides optic absorption coefficients, POISSEUILLE's law provides specific viscosity, and so on. All these cases demonstrate that physical chemistry more than just fills a gap between chemistry and physics. It fruitfully applies physical concepts amd methods (here: the

9 The concept of chemical reaction is introduced in detail in SCHUMMER 1994, pp. 41 f.; 1996, sect. 5.2.2.

mathematical frame and quantitative approach, instruments and techniques of measurement) to the chemical problem of characterizing materials in a subtly differentiated way.

4. What about eliminative discipline reduction?

There is another historical fact, which may further clarify the twisted line between (physical) chemistry and physics.

Zweiter Theil.

Spezielle Chemie oder Lehre von der Affinität der einzelnen Stoffe.

ERSTER ABSCHNITT.

Figure 2: Extract from the table of content of GMELIN's *Handbuch der anorganischen Chemie* (GMELIN 1852, p. XXV). After giving a short outline of the physical nature, the chemistry of each imponderable substance is discussed in terms of relations to other substances (imponderable and ponderable).

During the first half of the nineteenth century physical material properties were still part of the domaine of *inorganic chemistry* (fig. 2). For light, heat, electricity (and magneticsm) had been taken as *imponderable chemical substances* since LAVOISIER. While physicists were concerned with the *nature* of light, heat, electricity, magneticsm and matter in general and each of their own, chemists were investigating their effects on different materials. Roughly speaking, physics was a science of the *nature of substances of their own* (a heritage of natural philosophy's substantialism) and chemistry was a science of *relations of different substances*. As long as, for instance, heat could be considered as a substance (possibly) different from materials, phenomena like boiling or melting were part of (inorganic or physical) chemistry. The borderline could easily be drawn by empirically distinguishing the objects of investigations.

But things changed, when physicists succeeded in settling the natures of substances in an unified frame. As the most prominent step, heat was identified with motion of corpuscles.[10] In corpuscularian terms, boiling a piece of material was just setting particles in motion. Since this should be describable in terms of classical mechanics, as the leading theory of physics, the

10 Notice that corpuscularians in the Newtonian tradition still hypothesized heat corpuscles so that boiling a piece of matter means mixing different kinds of corpuscles. For details of the development of the kinetic theory cf. BRUSH 1976.

whole field of thermodynamics was claimed to belong to the domain of physics. In succession, the claim of physics went along with unifying the nature of the former simple substances electricity and light. Unification seems to be accomplished at the latest in quantum electrodynamics.

As a consequence, we have now two controversial claims to physical material properties. Should we take, for instance, specific heat capacities (and the whole of thermodynamics) or optical absorption coefficients (and the whole of spectroscopy) as parts of physics or as parts of physical chemistry?

Philosophical analysis may help to settle the difference. In fact, it depends on what we consider as criterion for the identity of a research field. If we subscribe to the *epistemological or methodological criterion*, then the field is fixed by the type and purpose of investigation. In this case, there is no need to expel properties like specific heat capacities from physical chemistry because of a change of theory. One the other hand, if we subscribe to the *ontological criterion*, the field is fixed by ontological commitments of the underlying theory. Then we adopt *eliminative discipline reduction* and should consequently treat thermodynamics as a branch of physics, if the reductive program has success.

There are good reasons to prefer the first approach, leaving the research field of physical chemistry free of theoretical changes.[11] For the identity of research fields should generally be kept free from ontological commitments of its theories, because otherwise the consequences are counter-intuitive. Historical disciplines like physics mostly cover areas of investigation which are treated by different theories. In nineteenth-century physics, for instance, there was no ontological link between mechanics and electrodynamics on a theoretical level. Hence, we would have to treat them as strictly separate fields. The case is even worse in seventeenth-century optics, where the same optical phenomena were treated by rival theories (corpuscularian and wave theory). According to the ontological criterion there would be no competition of rival theories within one field, but rather a dubious competition of different fields. And any change of the dominant theory would simply be a turn to another research field losing all continuity. Finally, we should not forget research fields, which use clusters of theories in a more pragmatic or even instrumentalist way; they would not have any identity at all according to the ontological criterion. We will see later that a pragmatic pluralism of models is actually a trait of physical chemistry.

Since these consequences do not fit at all our historical and philosophical understandig of scientific research fields, it seems more reasonable to drop the ontological criterion and take *specific physical material properties as belonging to the domain of physical chemistry*.

5. Characteristics of theoretical approaches in Physical Chemistry

If this is right, then another trait of physical chemistry becomes understandable. Physical chemists do not only investigate material properties empirically, they also like to explain them on theoretical level. In fact, they like to refer to models often taken from physics. In this regard, physical chemistry seems to include a *reductive approach* relating chemistry to physics. That was the idea of NERNST, for instance, arguing “that physics forms the theoretical basis of all sciences, including chemistry.“ (NYE, 1993: 109) But we should carefully point out in which sense there is a reductive approach.

Since we have rejected the idea of *eliminative* reduction of research fields, there is no reductive relation between fields in this sense. As long as physical chemists do their research, it is reasonable to speak of physical chemistry as an individual research field. Instead, physical chemists try to relate empirical facts about material behaviour to theoretical models. It is their

[11] Cf. CRANE/MELLOR 1990 for the flaw of physicalism.

aim *to reduce the diversity of material behaviour to the simplicity of comprehensive models, as far as possible*. It should be emphasized that this task is quite different from that of the physicist. The latter tries to reduce general laws about matter, for instance, the named laws of OHM, POISSEUILLE, general thermodynamics, and so on to fundamental theories. It appears to be ironic that from the chemical point of view, the physicist provides only *qualitative explanations* for material behaviour in general. In fact, he leaves the task to physical chemists, to explain the different behaviour of the 15 mio and more chemical substances in *quantitative terms*. I will give an outline of what I think are main *characteristics of the theoretical approach of physical chemistry*.

(1) As just mentioned, physical chemists try to explain the *specific* behaviour of chemical substances and mixtures in *quantitative* terms. Models are jugded by their discriminative force with respect to the diversity of materials and contextual conditions.[12]

(2) Perhaps the next most obvious point is that physical chemists use a *variety of models* in nearly every field. It is sometimes said that the pluralistic account is due to the complexity of the object of investigation, but it is rather due to the diversity of materials, contexts and purposes.

In thermodynamics and electrochemistry, for instance, the law of perfect gas, RAOULT's and HENRY's law, DEBYE-HÜCKEL theory, the solid state aproaches of DEBYE and of EINSTEIN and so on work quite well in certain cases, but are useless in others, which should be treated by different aproaches. It is also up to practioneers, to decide whether they should take the isoterms of LANGMUIR, BRUNAUER-EMMETT-TELLER, FREUNDLICH or another equation to describe their absorption process. In chemical kinetics the (mechanically based) collision theory is in competition with the (thermodynamically based) theory of activated complexes. In coordination chemistry we still find in use crystal field theory, valence-bond theory and molecular orbital theory. In fact, quantum chemistry seems to be the art of deliberatly constructing appropriate models for different kinds of materials and problems.[13]

I think we can generalize what HUHEEY (1983: 286) has pointed out regarding the variety of acid-base concepts: "the differences between the various acid-base concepts are not concerned with which is 'right' but which is *most convenient to use in a particular situation*." The theoretical approach of physical chemistry is neither dogmatic nor intended to be universal. Instead we find a *pragmatic pluralism of models* appropriate to certain materials, contexts and problems. Unlike the universalistic accounts of natural philosophy the value of each model increases as far as the scope of reasonable use has been precisely restricted.[14]

(3) In an important paper on theories of chemistry CALDIN (1960: 218) has rightly pointed out: "models [of chemistry] are subjected less to testing than to adaptation,

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12 Perhaps the most intriguing case here is the methodological difference between solid state physics and solid state (physical) chemistry: two disciplines that jointly developed during the last 60 years. In a case study of models of transition metal oxides HOFMANN (1990) has carefully analysed "a clear divergence between two evaluative criteria for models of solid state phenomena" (p. 416), which he assigns to the way of reasoning of physicists and chemists respectively. With regard to CARTWRIGHT's (1983) concepts of phenomenological and fundamental laws he points out that the model should be, on the one hand, an application of some theoretical formalism (physicist's preference) and, on the other hand, it should "depict the causal relationships essential to phenomena" (p. 411) (chemist's preference). Because solid state physicists and chemists lay different stress on these evaluative criteria, they prefer different types of models. HOFMANN illustrates the difference by the constrast between MOTT and SLATER.

13 Cf. LOWDIN 1967.

14 For a more general discussion of this point cf. CHRISTIE 1994.

elaboration, and exact specification. This is characteristic of physical chemistry". CALDIN rejects generalized accounts of methodology, especially that of POPPER, who takes theories just as candidates for empirical tests: "Popper's account [...] should apply best to those parts of science where theories are general in scope, precisely formulated, clear-cut in application [...] Such fields may be sought in mathematical physics. In chemistry, however, many of our theoretical hypotheses are by contrast restricted in scope, contain undetermined parameters, require additional hypotheses in application, and do not give numerically exact predictions. [...] The refutation or support of these hypotheses is not however the main purpose or result of experimental investigations in physical chemistry; [...] the rôle of experiment is usually to give them more exact specification. The improvement of theories is a characteristic result of such work." (p. 221) Physical chemists are concerned with *refinement and adaptation of models* to certain cases instead of testing general hypotheses.

(4) Physical chemists commonly use *semi-empirical approaches*. Most of their models contain parameters open for experimental specification. Here, on theoretical level, we meet again what has been said about the relation of general laws of physics (like OHM's law) and specific material properties (sect. 3): general equations must be adjusted to each material by introducing specific parameters drawn from experiments.

Examples are: specific parameters for various types of thermodynamic equations of state, activity coefficients, activation energies and so on. If models of different fields are interrelated, then empirical data of one field may even be useful for the others: e.g. spectroscopic measurement of molecular energy levels for statistical treatment of thermodynamics or adjustment of quantum chemical computation; measurement of specific transport coefficients (viscosity, diffusion, thermal conduction) for kinetic theory, collision theory or thermodynamic equations of state in terms of VAN DER WAALS.

Specific parameters and properties are collected in handbooks of considerable size.[15] Due to the semi-empirical approaches, these handbooks are actually part of the theoretical machinery of physical chemistry.

(5) In physical chemistry the sources of model building are not restricted to physical theories, as NERNST thought. In contrast, we have also considerable *import of chemical concepts and theories*. The most prominent example is, of course, *physical organic chemistry* in the line of LEWIS:[16] For instance, valence theory and theories of reaction mechanism basically rest upon chemical concepts of affinity and classical structure theory. Similar remarks can be made about *quantum chemistry*. For quantum chemical models and approximations cannot be deduced from first principle quantum mechanics but are mostly guided by chemical concepts and purposes.

For example: Quantum chemists do not consider bulk materials but use the isolated molecule or pars-pro-toto approach of classical chemistry: properties of the bulk are represented by a single molecule. They further use Born-Oppenheimer approximation which provides classical structures of the nuclei analogue to chemists' structural formulas (WOOLLEY 1978, WEININGER 1984). They neglect electronic correlation in order to select certain electrons which may be useful for remodelling concepts of classical chemistry (HÜCKEL theory for the concept of aromaticity, valence bond theory and localized orbitals for the classical concepts of directed bonds etc.) (PRIMAS 1985). They separate molecular systems in order to describe interactions of the resultant subsystems in classical terms (ligand field

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15 Notice, that perhaps the most famous handbook was a result of the collaboration of the chemist H.H. LANDOLT and the physicist R. BÖRNSTEIN, their *Physikalisch-chemische Tabellen* (1st edn. 1883), later expanded and entitled *Zahlenwerke und Funktionen aus Naturwissenschaft und Technik*.

16 Cf. NYE 1993, chap. 6.

theory, tight binding model etc.) (HARTMANN 1965). They ‘explain’ the periodic system of chemistry by separating electronic ‘sub-shells’ according to different angular momemtum (s, p, d etc.), although quantum mechanics does not allow definite values for the angular momentum of single electrons in stationary many-electron systems (HARTMANN 1965, SCERRI 1991). And they even use ad-hoc hypotheses, like PAULI’s exclusion principle (HALL 1986) or the exclusion of superpositions of enantiomers (PRIMAS 1981: 12), to exclude chemically absurd predictions.[17]

Physical chemists fruitfully combine different sources of chemistry and physics to build new types of models apart from any reductive account. In this regard, physical chemistry is actually an *emergent discipline*.

Conclusions

It is the aim of this paper to clarify the role of physical chemistry establishing relations between physics and chemistry. Let me summarize the results:

(1) According to the systematics of material investigation, *physical chemistry has a research field of its own* that lies between physics and chemistry, both taken in a narrow sense. The field includes physico-chemical properties, chemical properties without chemical reaction and specific physical material properties.

(2) In so far as chemistry in a broader sense is concerned with material differences, *physical chemists treat chemical problems by applying physical concepts, methods and instruments*. This point was illustrated by turning from OHM’s law to specific electric conductivities.

(3) In spite of some reductive success of physical theories, eliminative discipline reduction can be rejected for several reasons. Instead, there are some *non-eliminative reductive approaches within physical chemistry*, which are quite different from that of physics.

(4) A closer look on theoretical reasoning has revealed some further *methodological characteristics of physical chemistry supporting the idea of an emerging discipline*: (a) Physical chemists try to explain *material diversity* in quantitative terms. They use (b) a *pragmatic pluralism of models*, which are (c) rather subject to *refinement and adaptation* than to crucial tests. We further found (d) an extensive use of *semi-empirical approaches* and (e) the emergence of new types of models from *combining physical and chemical concepts and theories*.

What about the crucial question: Is physical chemistry a branch of chemistry, a branch of physics or is it a discipline of its own? In the light of the various aspects discussed, a general and simple answer appears to be a matter of taste. I would prefer to follow the traditional line and take it as a branch of chemistry in a broader sense, keeping in mind that physical chemistry has actually developed many distinct characteristics.

References

BARKAN 1990: D. K. Barkan: *Walther Nernst and the Transition to Modern Physical Chemistry*. Ph.D. Dissertation, Harvard University.

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[17] For further literature reflecting quantum chemical modelling cf. HABERDITZL/LAITKO 1967, GEY/PARTHEY 1984, TRINDLE 1984, LIEGENER/DEL RE 1986, TOMASI 1988, HOFMANN 1990, SCHUMMER 1997b.

BITTRICH 1986: H.-J. Bittrich: “Entstehung und Evolution der Physikalischen Chemie”, in: Akademie der Wissenschaften der DDR (ed.): *Philosophische, historische und wissenschaftstheoretische Probleme in Chemie und Technik*, Berlin, pp. 201-213.

BRUSH 1976: S.G. Brush: *The Kind of Motion we call Heat*, Amsterdam.

CALDIN 1960: E.F. Caldin: “Theories and the Development of Chemistry”, *The British Journal for the Philosophy of Science*, **10**, 209-222.

CARTWRIGHT 1983: N. Cartwright: *How the Laws of Physics Lie*, New York.

CHRISTIE 1994: M. Christie: “Philosophers versus Chemists Concerning ‘Laws of Nature’”, *Studies in History and Philosophy of Science*, **25**, 613-629.

CRANE/MELLOR 1990: T. Crane, D.H. Mellor: “There is No Question of Physicalism”, *Mind*, **99**, 185-206.

DOLBY 1976: R.G.A. Dolby: “The Case of Physical Chemistry”, in: G. Lemaine et al. (eds.): *Perspectives on the Emergence of Scientific Disciplines*, The Hague, pp. 63-73.

DUBPERNELL, WESTBROOK 1978: G. Dubpernell, T.H. Westbrook (ed.): *Selected Topics in the History of Electrochemistry*, Princeton.

EYRING 1976: H. Eyring: “Physical Chemistry: The Past 100 Years”, *CENews*, **54**, 88-104.

GEY/PARTHEY 1984: E. Gey, H. Parthey: “Quantenchemie – eine interdisziplinäre Entwicklung”, *Wissenschaft und Fortschritt*, **34**, 282-285.

GIRNUS 1982: W. Girnus: *Grundzüge der Herausbildung der physikalischen Chemie als Wissenschaftsdisziplin: Eine wissenschaftshistorische Fallstudie zur Disziplinengenese in der Wissenschaft. Dissertation,* Akademie der Wissenschaften der DDR.

GIRNUS 1986: W. Girnus: “Bemerkungen zur Entwicklung der Elektrochemie im 19. Jahrhundert”, in: Akademie der Wissenschaften der DDR (ed.): *Philosophische, historische und wissenschaftstheoretische Probleme in Chemie und Technik*, Berlin, pp. 97-112.

GMELIN 1852: L. Gmelin: *Handbuch der Anorganischen Chemie* (5th edn), vol. 1, Heidelberg.

GUÉRON, MAGAT 1971: J. Guéron, M. Magat: “A History of Physical Chemistry in France”, *Annual Review of Physical Chemistry*, **22**, 1-25.

HABERDITZL/LAITKO 1967: W. Haberditzl, H. Laitko: “Reduziert sich die theoretische Chemie auf angewandte Quantenmechanik und Quantenphysik?”, *Wissenschaftliche Zeitschrift der Humboldt-Universität zu Berlin, M-N Reihe*, **16**, 961-2.

HALL 1986: P.J. Hall: “The Pauli Exclusion Principle and the Foundation of Chemistry”, *Synthese*, **69**, 267-272.

HARTMANN 1965: H. Hartmann: “Die Bedeutung quantenmechanischer Modelle für die Chemie”, *Sitzungsberichte der Wissenschaftlichen Gesellschaft der Johann Wolfgang Goethe Universität*, 151-168.

HOFMANN 1990: J. R. Hofmann: “How the Models of Chemistry Vie”, *PSA*, vol. 1, 405-419.

HUHEEY 1983: J.E. Huheey: *Inorganic Chemistry. Principles of Structure and Reactivity* (3rd edn), Cambridge et al.: Harper International.

KING 1981: C. King: “Experiments with Time: Programs in the Development of Chemical Kinetics”, *Ambix*, **28**, 70-82.

LAIDLER 1985: K. J. Laidler: “Chemical Kinetics and the Origins of Physical Chemistry”, *Archive for the History of Exact Sciences*, **32**, 43-75.

LAIDLER 1993: K. J. Laidler: *The World of Physical Chemistry*, Oxford.

LIEGENER, DEL RE 1987: C. Liegener, G. Del Re: “The Relation of Chemistry to other Fields of Science: Atomism, Reductionism, and Inversion of Reduction”, *Epistemologia*, **10**, 269-284.

LOWDIN 1967: P.O. Lowdin: “Nature of Quantum Chemistry”, *International Journal of Quantum Chemistry*, **1**, 7-12.

NYE 1993: M. J. Nye: *From Chemical Philosophy to Theoretical Chemistry. Dynamics of Matter and Dynamics of Disciplines 1800-1950*, Berkeley-Los Angeles-London.

PARTINGTON 1964: J.R. Partington: “The History of Physical Chemistry” in: *A History of Chemistry*, vol. 4, London: Macmillan, pp. 567-746.

PRIMAS 1981: H. Primas: *Chemistry, Quantum Mechanics and Reductionism*, Berlin-Heidelberg-New York.

PRIMAS 1985: H. Primas: “Kann Chemie auf Physik reduziert werden?”, *Chemie in unserer Zeit*, **19**, 109-119, 160-166.

ROOT-BERNSTEIN 1980: R.S. Root-Bernstein: *The Ionists: Founding Physical Chemistry, 1872-1890.* Ph.D. Dissertation, Princeton University.

SCERRI 1991: E. Scerri: “The Electronic Configuration Model, Quantum Mechanics and Reduction”, *The British Journal for the Philosophy of Science*, **42**, 309-325.

SCHUMMER 1994: J. Schummer: “Die Rolle des Experiments in der Chemie”, in: P. Janich (ed.): *Philosophische Perspektiven der Chemie*, Mannheim, pp. 27-51.

SCHUMMER 1996: J. Schummer: *Realismus und Chemie. Philosophische Untersuchungen der Wissenschaft von den Stoffen*, Würzburg.

SCHUMMER 1997a: J. Schummer: “Towards a Philosophy of Chemistry”, *Journal for General Philosophy of Science* (forthcoming).

SCHUMMER 1997b: J. Schummer: “Problems with Physicalistic Reduction: The Chemical Core of Chemistry” (submitted for publication).

SERVOS 1990: J. W. Servos: *Physical Chemistry from Ostwald to Pauling: The Making of a Science in America*, Princeton.

TOMASI 1988: J. Tomasi: “Models and Modelling in Theoretical Chemistry”, *Journal of Molecular Structure (Theochem)*, **179**, 273-292.

TRINDLE 1984: C. Trindle: “The Hierarchy of Models in Chemistry”, *Croatica Chemica Acta*, **57**, 1231-1245.

WEININGER 1984: S.J. Weininger: The Molecular Structure Conundrum: Can Classical Chemistry be Reduced to Quantum Chemistry”, *Journal of Chemical Education*, **61**, 939-944.

WINTERMEYER 1975: U. Wintermeyer: *Zur Geschichte der Entwicklung der physikalischen Chemie*, Dissertation, Universität Frankfurt/M.

WOOLLEY 1978: R.G. Woolley: “Must a Molecule Have a Shape?”, *Journal of the American Chemical Society*, **100**, 1073-1078.