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ON THE NEGLECT OF THE PHILOSOPHY OF CHEMISTRY[1]

ABSTRACT. In this paper I present a historiography of the recent emergence of philosophy of chemistry. Special attention is given to the interest in this domain in Eastern Europe before the collapse of the USSR. It is shown that the initial neglect of the philosophy of chemistry is due to the unanimous view in philosophy and philosophy of science that only physics is a *proper* science (to put in Kant's words). More recently, due to the common though incorrect assumption that chemistry can in principle be reduced to physics, the neglect continued, even when interest in sciences such as biology and psychology entered more strongly in philosophy of science. It is concluded that chemistry is an autonomous science and is perhaps a more 'typical' science than physics.

> Kant said that there are in the world 'two things which never cease to call for the admiration and reverence of man: the moral law within ourselves, and the stellar sky above us.' But when we turn our thoughts towards the nature of the elements and the periodic law, we must add a third subject, namely, 'the nature of the elementary individuals which we discover everywhere around us.'
>
> Dmitri Mendeleev (1889)

> Physicists in general tend to restrict themselves to the small part of the physical world with which they deal, and to leave out of their studies all such features as the structure and properties of substances in relation to their chemical composition, and the reactions that change one substance into another.
>
> Linus Pauling (1950)

1. INTRODUCTION

Until about 1960, philosophy of science dominated by logical positivism, consisted mainly of philosophy of physics, although philosophy of mathematics, biology, psychology, history, and social science always held some residual interest; see for example Nagel

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(1961) and Hempel (1965). It is instructive to consult the content pages of *The Journal of Unified Science (Erkenntnis)*, the 'house journal' of the *Vienna Circle* – home of the logical positivists – or the titles of the contributions at the *International Congress for the Unity of Science* from 1931 to 1940. Nowhere is there any indication that chemistry might be part of science, despite numerous references to logic, mathematics, physics, probability, causality, biology, psychology, some references to sociology, semantics, language, measurement, induction, space and time, physicalism, astronomy, medical psychology, economics, history; and even – on occasion – to values and aesthetics. No word however on chemistry. Similarly, in the 18 parts of the *Foundations of the Unity of Science: Toward an International Encyclopedia of Unified Science*, published between 1938 and 1970, the only reference to chemistry is found in Kuhn's (1962) *The Structure of Scientific Revolutions*, together with a few pages on chemical bonding in Frank's (1946) contribution on the foundation of physics.

By 1990 mathematics, biology, and cognitive science occupy respectable areas within the philosophy of science and there is interest in the philosophy of economics and astronomy. The philosophy of medicine too is on the rise, though hardly interacts with mainstream philosophy of science. A vast literature on the philosophy of the social sciences and the humanities (philosophy of social science, of literature, of art, of history) has appeared. However most of it is not part of philosophy of science, as normally understood, partly due to the divide between analytic and continental philosophy. The philosophy of law and the philosophy of religion belong to separate parts of philosophy. Considerable interest in the philosophy of linguistics tends to be brought under the philosophy of language (or mind). Finally, there is some interest in the philosophy of technology (including engineering and agricultural sciences) and considerable interest in environmental philosophy, a subject usually considered part of applied ethics.

Finally, in 1994 philosophy of chemistry was born. That is not to say *nothing* happened before 1994 (see sections 3 and 4). But it was in March 1994 that the *First International Conference on Philosophy of Chemistry* took place in London, followed a month later in Karlsruhe by the *Tagung Philosophie der Chemie: Bestandsauf-*

nahme und Ausblick.[2] In October of that year the American *Philosophy of Science Association* organised for the first time in its history a colloquium on the philosophy of chemistry during its biannual congress.[3] In November the *Second Erlenmeyer Kolloquium* on the philosophy of chemistry took place at Marburg[4] and in December the meeting *Riflessioni Epistemologiche e Metodologische sulla Chimica* was held in Rome.[5] In 1995, there were seven contributions to the philosophy of chemistry at the 10th International Congress of Logic, Methodology and Philosophy of Science held at Florence.[6] In 1995 too the journal *Hyle: An international Journal for the Philosophy of Chemistry* published its first volume (in electronic form) and in 1997, its third, now full-fledged volume appeared in printed form. The *International Society for the Philosophy of Chemistry* was formally established at an international symposium on the philosophy of chemistry and biochemistry held at Ilkley (U.K.) in July 1997. Again in 1997 a special issue of *Synthese* on the philosophy of chemistry came out bringing it to a broader philosophical audience. In 1999 the first issue of the *Foundations of Chemistry* appeared.

The modest purpose of this paper is to investigate the degree to which it is true that philosophy of chemistry is a neglected area. Section 2 is concerned with early contacts between philosophy and chemistry; section 3, ‘philosophy of chemistry marginalised’, concerns literature in English up to about 1970; section 4 is on philosophy of chemistry and dialectical materialism, from 1962 to 1986; section 5 is on changes in post-1960 philosophy of science; and section 6 lists a number of research areas that might give an outline of the philosophy of chemistry. The emphasis in this paper is on ontological and epistemological aspects of chemistry, not on the historical, social, or ethical dimensions of how it has developed and will change the world.[7] This is an important limitation, but it conforms to the fact that the question of the neglect of the philosophy of chemistry is almost always raised within the context of ‘traditional’ philosophy of science. Here is a further list of issues I will *not* discuss (all of which, nevertheless, could be counted under the philosophy of the material sciences in a wide sense): the transition from alchemy to chemistry, chemical evolution as the evolution of inorganic and organic molecules preceding biological evolution; issues associated with biochemistry and molecular biology (e.g.

classical and molecular genetics, immunology); chemical (material) systems as the building blocks of more complex systems (including systems theory and synergetics); the 'contemplative' interests in crystal structures; and most issues concerning thermodynamics.[8]

While there has been more interest in the *history* of chemistry, this area too is neglected when compared with physics.[9] The history of chemistry is relevant to the philosophy of chemistry in a number of ways (see also section 5). For example, studies concerning when chemistry 'became' a science will have to use a philosophy of science to establish whether the practice of chemistry meets the criterion of being a science.[10] Similarly if it is stated that Lavoisier presented the first quantitative chemical law, this is simultaneously a statement in the philosophy of science. Finally, any historical episode and its later renderings that bear on the relation of, or distinction between physics and chemistry, is relevant; primarily because of the constant rewriting of the history of science that privileges physics.[11]

2. EARLY CONTACTS BETWEEN PHILOSOPHY AND CHEMISTRY

There is an extensive literature on the concepts of substance and matter in the history of western metaphysics, dominated by publications on Aristotle and Locke. But many other philosophers (and physicists and chemists) figure as well (Averroës, Boyle, Descartes, Faraday, Gassendi, Leibniz, Mach, Newton, Ostwald, Priestley, Spinoza, to name but a few). However it is rare for these discussions to be related directly to modern chemistry. Typically, Düring's (1944) *Aristotle's Chemical Treatise: Meteorologica, Book IV* is a curiosity in using the word 'chemical' in the title.[12] Perhaps one could distinguish two lines in these developments; one a more 'purely' philosophical, metaphysical line with the key words 'substance' and 'essence' running from Thales to Aristotle via Locke to Kripke (1972) and Putnam (1975), and 'side tracks' like Mach and Ostwald. Secondly, the more scientific line concerned with the ontology of kinds of matter, with key-words like 'element' and 'compound/mixture', followed by 'valence' and explanations of the properties of substances in terms of their composition, and later quantum chemistry. This line could also start with Thales and Aristotle and then move via Averroës, Gassendi and Boyle to Lavoisier, Dalton, Kekulé, Butlerov and London and Pauling.

A slightly different way of putting this is to suggest that there are two separate issues: firstly, the ontology of *matter, in general*, to be dealt with in relation to micro- and astrophysics; secondly, the ontology of *particular kinds of matter*, i.e. chemical kinds.[13] Discussions in both the history of philosophy and the philosophy of science have been mainly concerned with the first issue. Atomism[14] has been discussed in numerous publications,[15] though as Paneth (1962 [1931]) noted: "the physical aspect (divisibility, mutual attraction and repulsion, and so on) has been discussed much more than the chemical (qualitative characteristics, valency, etc.)." Presumably, the common identification of chemical and physical atomism is based on the assumption that the final ontology of everything (including chemistry) is whatever physics says it is.

A rather different interaction between philosophy and chemistry can be found with those philosophers who, in their general philosophy, were influenced by their knowledge of chemistry. This includes in particular the philosophy of nature of the German philosophers Kant, Hegel, and Schelling (and to a lesser extent Fichte and Schopenhauer),[16] as well as the French philosophers of science, Duhem, Bachelard and Meyerson.

Kant made detailed contributions to the chemistry of his time (Carrier, 1990). He considered Stahl (founder of the phlogiston theory), Galilei, and Toricelli paradigmatic practitioners of the scientific method.[17] Hence his often quoted view of chemistry as an *uneigentlichen Wissenschaft* ("not a proper science") should be read with care.[18] For Kant the difference between science that is and is not proper, is roughly the difference between 'pure' and empirical science, where 'purity' is guaranteed by metaphysics and mathematics. The distinction runs parallel to that between primary and secondary qualities and between hard and soft (or 'special') sciences. The application of mathematics introduces the pure part and at the highest level of abstraction there is the metaphysical *a priori*. For Kant, this *a priori* of the 'special metaphysics' of natural bodies is not the *a priori* of the (more general) *transcendental* metaphysics of nature. The latter investigates the possibility of experience *per se*, the former the possibility of particular natural things, for which in order to ‘construct’ them, one needs mathematics. Physics is proper because it has a pure and an empirical part. A natural science is proper to the extent that mathematics is applied in it. Sciences like chemistry and psychology are rational (because they use logical reasoning), though not *proper* science, because they miss the basis of the synthetic *a priori*.[19]

In the crucial passage[20] Kant not only says that chemistry and psychology do not count as proper sciences because they use no mathematics, but that this requirement would be difficult *ever* to fulfil (emphasis added). However there are some ambiguities if one compares this with older texts of Kant, in particular those referring to psychology. In the nineteenth century it led to extensive debates among interpreters; some scholars even went so far as to say that the often quoted passage is an oversight (Drews, 1894: p. 259), and is inconsistent with the rest of this writings.[21]

Though Kant had made brief comments about science in his *Kritik der reinen Vernunft* and in the *Prolegomena*, his most worked out views can be found in the preface of his *Metafysische Anfangsgründe der Naturwissenschaft*. The title already indicates that, notwithstanding Kant’s ‘Copernican Revolution’, science is only possible because of certain metaphysical foundations. Already in his own time this stance had little impact on the development of science; still Kant’s views on science have probably been more influential than one is aware of. For Kant a necessary requirement of ‘proper’ science is its tie to metaphysics and mathematics. Though the metaphysics has been dropped, the idea that ‘proper’ science is something that uses mathematics has been prevalent to the present day. To put it crudely, the logical positivists, following Hume, threw out metaphysics, replacing it by logic to line it up side by side with mathematics as the ‘metaphysical foundations’ of all ‘proper’ science.

One thing the nineteenth century German *Naturphilosophen* did was to pick up the notion of affinity or valency from chemistry and make it the basis of a very general notion of chemism. Chemism played an important role in Hegel’s philosophy of nature. For him chemism stands between mechanism and teleology. A ‘chemical object’ (not restricted to ‘ordinary’ chemical objects) is, intriguingly, an independent totality that is (nevertheless) defined in terms of its relation to other things.[22] Chemical objects in this sense share a family connection that separates them off from mechanical and teleological objects. Hegel's logic of chemism is not simply generalised from the empirical evidence of chemistry, but develops its own theoretical perspective, which can then be applied more generally to a number of spheres. Von Engelhardt (1984, 1993) has been stressing how important Hegel's philosophy of nature is. Its neglect is due to the incorrect ascription (to Hegel by Hegel scholars) of a contempt for both empirical work and modern research.[23] For Hegel the presence of separation and continuity at all levels makes the explanation of the natural order possible. The philosophy of chemistry might therefore be regarded as a crucial part of Hegel's philosophy of nature.[24]

The German tradition of philosophy of nature also had an effect on practising chemists with philosophical interest. Mittasch (1948), a well-known chemist in the history of catalysis, wrote widely on the philosophy of nature, on Schopenhauer and chemistry, on Nietzche and chemistry (including hundreds of pages of unpublished manuscripts on Nietzsche's philosophy of nature), on catalysis and determinism, and on the concept of causality of Robert Mayer. Without exception, this has had no impact on twentieth century philosophy of science, which was completely separated from 'metaphysical' philosophy of nature.[25]

In a tradition that can be associated more with that of Mach and Duhem, the German philosopher-chemist Ostwald (1902, 1907) had two aims. First, to distinguish between what is given in experience and what is postulated by the mind: nothing *compels* us to affirm that mercury oxide 'contains' mercury and oxygen. Second, to show that energy is the most general concept of the physical sciences. Such a view implies that thermodynamics is the most basic physical science. Like Ostwald, Duhem claimed that thermodynamics was the most basic science.[26] Needham (1996, 1996a) has shown that Duhem developed what he regarded as an essentially Aristotelian view of chemistry, as an alternative to the corpuscular view and based on his understanding of phenomenological thermodynamics, derived from the Aristotelian idea of "two contradictory opinions of the nature of a mixt" (Duhem, 1902: p. 15).[27] It is against this background that Duhem's attack on the indefiniteness of the atomic hypotheses has to be judged; in his view these hypotheses are otiose, appealing to *a priori* considerations. For example he did not accept that van 't Hoff's stereochemical representations should be understood as a fully fledged geometric picture of something real.[28]

Bachelard, initially a chemistry teacher at a provincial French college, later became a philosopher of science with a strong influence in France (notably on Foucault). However, in the few English publications on Bachelard's philosophy of science, chemistry is never mentioned,[29] and Bachelard's historical approach is not always appreciated. As one of the reviewers of a reprint of Bachelard's *Le pluralisme cohérent de la chimie moderne* (1932) said: It is nothing but a historical story translated in philosophical terminology.[30] Theobald (1982; see also Vinti, 1996), who published rather extensively on the philosophy of chemistry (see next section), summarised the little that Bachelard had *specifically* said on chemistry as follows:

- 'The thought of the chemist' oscillates between pluralism on the one hand and the reduction of this pluralism on the other.
- Each chemical substance refers to all the others – knowing about a chemical substance includes knowing how it is 'located' among other substances and how it behaves in all chemical reactions in which it can take part. That is to say chemistry has a pluralistic ontology (or an ontology of relations, more than of 'substances', let alone atoms), leading on to the importance of chemical synthesis.[31]
- Continuity is opposed: 'incompatible' sets of concepts and principles can be applied to phenomena.[32]

Further, one may find in Bachelard's work the suggestion that, compared with (mathematical) physics, the philosophical neglect of chemistry parallels modern philosophical preference for form at the expense of substance. Bachelard puts this in a way that won't win him many supporters in the prevailing tradition of the philosophy of science, as when he speaks of: "chemistry's unconscious dreamwork"[33] and "[w]ater is, in other words, a universal glue".[34]

Not all history reviewed above is equally important. One issue stands out as being relevant to a contemporary philosophy of chemistry (as well as contributing to its neglect):

- In general, since Aristotle, the concept of *hyle* or ‘stuff’ has been suppressed in philosophy (of science), in favour of Euclidean geometry and Newtonian mechanics as a universal model for scientific knowledge,[35] illustrated for example by Kant’s influential view that chemistry is not a proper science.
- More specifically, views like those of Ostwald and Duhem, who stressed the priority of thermodynamics and the operational definition of homogeneity, pure substance and such like (independent of atomic models or interpretations), were marginalised.

3. PHILOSOPHY OF CHEMISTRY MARGINALISED

I suggest the main reasons for the absence of interest in chemistry in traditional philosophy of science, as it developed between 1930 and 1960, were as follows (all four points can been seen as set on the stage by Kant’s pronouncements on the difference between physics and chemistry):[36]

1. Pre-1960 interest was almost exclusively in *theoretical* science. Thus experimental and applied physics (at least 90% of a physics department?) was as much neglected as was chemistry. That chemistry is not a theoretical science in the sense of theoretical physics tends to be supported by chemists themselves who, in the words of the chemist-philosopher Polanyi (1958: p. 156) have always been wary of theoretical ‘speculation’ unsupported by detailed experimental observations. Similar views, echoing Kant, have been expressed by many philosophers of science: “The truth is that chemistry indeed has no place in the strict scientific scheme. . . . The part played by chemistry in the growth of science has been a pragmatical, heuristic one” (Dingle, 1949).

2. Physics and chemistry were lumped together as *exact* natural sciences with emphasis on studying its *logical* structure. This meant that the interest was in laws in the sense of mathematical equations stating relations between magnitudes and theories that were axiomatisable, at least in principle. In that sense there are few laws and theories in chemistry and most of the numbers chemists manipulate are values of *physical* magnitudes. If anything, philosophers took this one step further; e.g. Hartmann (1948), again echoing Kant:

"all of chemistry that is lawlike is pure physics". Rare attempts to get chemistry to live up to the model of an exact formalistic science failed to have any impact on the philosophy of science.[37]

3. Chemists are more inclined to be instrumentalists or pragmatists than scientific realists looking for strictly universal laws. Although speculative, there is considerable circumstantial evidence for it. Consider Pauling (1950) who said: "A physical law is a succinct description of the results of a number of experiments. It is not an inflexible, unchanging dogma. It describes only the experiments that have been carried out up to the time the law is stated. . . . these basic laws of nature may, as a result of some new experiment, not be exactly right next year."[38]

4. In the natural sciences from 1500 to 1900, there were more physical than chemical 'big' theories. Moreover, since the end of the nineteenth century philosophical interest has primarily been in the idea of unified theories (and hence unified science, the most fundamental theories, and concomitant ideas about reduction).[39] There have been no theoretical developments in chemistry that could compete on these terms with physics. One might also compare the philosophy of biology here. The infiltration of an all-embracing neo-darwinism (evolutionary theory and molecular biology), dominating biology and spreading to other sciences and spheres of life, may soon have the effect of biology replacing physics as the dominant discipline scrutinised by philosophy of science.

Mainstream philosophy of science simply regarded chemistry as part of physics and an unimportant part at that, because of the emphasis on the structure of formalisable theories. Chemical examples were used, for example in discussing the status of dispositional properties. However, such examples had nothing to do with anything that might be considered *typically* chemical (as distinct from physical). There was only one 'early' subject that had some specific connection to chemistry (as well as to biology and psychology): the concern with the idea of emergence.[40] This is the view that (Broad, 1925: pp. 58–59) "there need not be any peculiar *component* which is present in all things that behave in a certain way" and that "the characteristic behaviour of the whole *could* not, even in theory, be deduced from the most complete knowledge of the behaviour of its components taken separately or in other combinations, and of their proportions and arrangement of this whole”.[41]

In the 1960s a few publications specifically on the philosophy of chemistry appeared. It was suggested that ‘theory’ means something different to a chemist than to a (theoretical) physicist; what comes under a chemical law or theory is not ‘the same’, but ‘similar’ or ‘analogous’ things. For example, Caldin (1959, 1961) notes that often experiments in chemistry are not meant to test a model or theory, but are attempts to make it more precise.[42] This applies in particular to the refinement of molecular structure. In a comment on Caldin (1959), MacDonald (1960) wrote: “it would appear that the chemist regards theories – or perhaps better *his* theories (!) – as far less sacrosanct [than the physicist], and perhaps in extreme cases is prepared to modify them *continually* as each bit of new experimental evidence comes in.” Though chemists may sometimes test theoretical models in critical cases, this is not characteristic of chemistry: “the thesis that theories are tested by attempts to falsify them is not supported”. If anything, chemistry supports Lakatos’ methodology of research programmes.

Further, Churchman and Buchanan (1969) as well as Theobald (1976) found that the Hempel-Oppenheim scheme of deductive-nomological explanation is not applicable to examples from chemistry. This however may be more to do with the highly abstract characteristics of the Hempel-Oppenheim scheme and the sort of criticisms that can be levelled at it from a more pragmatic stance (van Fraassen, 1980), than with any difference between physics and chemistry.

The question of differences between physics and chemistry with respect to subject matter and method has often been addressed, but it is typical of the neglect of the philosophy of chemistry that these tend to be isolated observations.[43] There was one substantial publication written from a phenomenological (Husserlian) perspective. Ströker (1967) argues that chemistry cannot restrict itself purely to mathematical-functional relationships, but is always concerned with phenomena ‘happening to’ substances and with phenomena ‘because of the substances’.[44]

Many of the isolated, marginalised publications on the philosophy of chemistry in this period seem to be by chemists who developed an interest in the philosophy of science. This applies most particularly to the more substantial publications. Even then, as Bunge (1985: pp. 219f) noted:[45] "Given the popularity and prestige of chemistry, it is strange that the corresponding philosophy hardly exists. The publications in this field are only a handful . . . Not even the distinguished philosophers of science Meyerson, Broad and Bachelard, who started out as chemists, made any significant contributions to the philosophy of chemistry: they preferred to write about other sciences." Even if there appeared an occasional paper on the philosophy of chemistry, it had no further impact. Typically, when the *British Journal for the Philosophy of Science* published in 1962 two installments of a paper of Paneth on the epistemological status of the chemical concept of element (Paneth, 1962 [German original, 1931]),[46] there were only two brief responses disputing historical details concerning Locke and Lavoisier.[47] Neither the republication of Paneth's article nor the earlier exchange between Caldin (1959) and MacDonald (1960) in the same journal had any further impact.[48]

4. PHILOSOPHY OF CHEMISTRY AND DIALECTICAL MATERIALISM

In the period 1949 to 1986 a number of publications on the philosophy of chemistry, primarily in German and Russian, appeared in Eastern Europe. This included a range of books devoted solely to the subject.[49] In the former DDR (German Democratic Republic) there were twenty-four people who wrote their dissertation (Ph.D. or higher degree) on the philosophy of chemistry (Schummer, 1996a). Although about a third were on historical, economic, or educational subjects, most concerned the philosophy of chemistry proper: issues such as laws, theories, models, causality, the structure of organic molecules, quantum chemistry, the theory of acids and bases. In the *Deutsche Zeitschrift für Philosophie*, between 1962 and 1983, thirteen articles appeared on the philosophy of chemistry and more in other journals.[50] The number appearing in the Russian journal *Voprosi Filosofii* [*Problems of Philosophy*] was about two times higher.[51] Of the three hundred articles on the philosophy of the natural and social sciences that appeared in volumes 1–25 (1953–1977) of the *Deutsche Zeitschrift für Philosophie*, only a small number were on the philosophy of chemistry.[52] Nonetheless this was larger than the number of articles appearing in the same period in *all* English language philosophy journals. The same is true when comparing Russian and English language publications. The number of English articles was perhaps comparable to those published in Rumanian journals.[53] Moreover, course books were written on 'philosophical problems of chemistry' and used in teacher training and technical colleges. Such books were also prescriptions for how to talk about chemistry from the perspective of dialectical materialism. But they were well written and included the latest developments of discussions in philosophical literature. A typical format for such a book would be to have chapters on: philosophy and natural science, materialism and dialectics in chemistry, epistemological problems in chemistry, chemistry and society, philosophical views of particular scientists (e.g. Ostwald and Mittasch were discussed against the background of a critique of positivism).[54]

One reason for this interest in chemistry goes back to Hegel (cf. section 2), who 'used' chemistry to illustrate the dialectic of quantity and quality.[55] This point had been taken up by Engels in his *Dialectics of Nature*.[56] For the purpose of this paper dialectical materialism can be taken as the view that [i] everything that exists consists of matter-energy, [ii] this matter-energy develops in accordance with universal laws, [iii] knowledge is the result of a complex interaction between human(s) and their 'external' world (but both humans and their external world are part of the same material world). It would not be particularly difficult to transcribe a contemporary view in analytic philosophy which combined non-reductive materialism with a 'dynamic' or 'interactive' cognition theory into dialectical materialism (and have it accepted for publication in a journal in Eastern Europe in the 1960s or 1970s).

In applying the conceptual scheme of dialectical materialism to the natural sciences, a number of issues directly relevant to the philosophy of chemistry emerged. For example, in Kedrov's (1962) influential account any *type* of change (or 'movement' in Engels' sense)[57] must correspond to a particular type of matter. He distinguished the following 'levels' of change and matter: [i] nuclear physical; [ii] electrical (as in atoms), [iii] chemical (within a molecule), [iv] molecular-physical (as in liquids), [v] geological (as in minerals). From level [iii] onwards there is also a line towards biological forms of change. The essence of each qualitatively new form of 'movement' is to be found in the interaction between elements at a lower level. In general, any form of strict reductionism is opposed; physics and chemistry are "both separate and together".[58] The irreducible macroscopic character of typical chemical phenomena was stressed; e.g. reaction velocity only makes macroscopic sense. That chemical laws had a higher "specificity, complexity, and individuality" was also used to argue against reductionism.

Kedrov's views were discussed in many German publications which often criticised his failure to go into chemical detail. In one typical example he incorrectly assumed all chemical change involves molecules. The general tone of this discussion is very similar to both old and new 'emergence' literature in English.[59] Further, much was written on the relation between physics and chemistry.[60] Derivatively, there was considerable interest in the subject matter of chemistry. In the terminology of Engels and Kedrov the question was: what is specific to the *chemical* form of movement? In brief the conclusion reached was that the subject of chemistry is a set of laws (Richter and Laitko, 1962; Laitko, 1967), governing 'chemical forms of movement' (Rosenthal, 1982) and the transformation of chemical matter.[61] Each chemical transformation corresponds to a chemical law. It was argued that 'transformation of matter' includes polymorphous transformations and radioactive decomposition, leading to an extensive discussion of the precise definition of chemistry. Engels' definition, "the science of qualitative changes in bodies, which take place in conformity with change in their quantitative composition" is better than many text book definitions, but it excludes isomeric transformations.[63] Hence it was proposed that "chemistry is the science of the qualitative changes of bodies that occur under the influence of changes in their quantitative composition and structure" (Zhdanov, 1965).

A general reason for the interest in the philosophy of chemistry was a strong concern not to separate science, education, and philosophy. For example, in the DDR, similar articles on the philosophy of chemistry could appear in *Chemie in der Schule* or in the *Deutsche Zeitschrift für Philosophie*. Although at times the writing is dominated by ideologically correct qualifiers, as when different views on the Brönsted theory of acids are formulated in terms of 'reactionary bourgeois theories', 'Maoist accounts' and the 'correct dialectic' approach (Simon, 1975), this is epiphenomenal to the substantial issues being discussed. In some cases the principles of dialectical materialism were a true stimulus to tackle philosophical issues, in other cases the obligatory jargon is simply tacked on.[63] For example, Poller (1966: p. 334) writes: "Both [redox] reactions must proceed simultaneously (Principle of the unity of the 'struggle' of contradictions!)" – scare quotes and exclamation mark in original.[64] But this sentence 'stands out' amidst a set of sophisticated arguments against the suggestion that quantum chemistry could, in principle, give an exact account of *what* is going on in a redox reaction. Similarly, Poller expresses the view that knowing *what* happens is not the same as knowing *how* it happens (with reference to Marx and Engels), an argument not much different from that of any contemporary critique of reductionism (such as Dupré, 1993).

It is possible that an extra stimulus for the interest that developed in the philosophy of chemistry was spawned by an article in 1949 in *Voprosi Filosofii* by Tatevskii and Shakhparanov. They argued that "the physical theory of resonance is erroneous and the philosophical setting of its authors and propagandists is Machistic"[65] and "hostile to the Marxist view".[66] This publication was itself triggered by a book by the chemist G. V. Chelintsev, a professor of chemical warfare at the Voroshilov Military Academy, who had attacked Pauling's resonance theory of aromatic[67] organic compounds and proposed an anti-resonance benzene theory.[68] The theory of resonance can be understood as a synthesis of classical structural ideas and quantum mechanical concepts.[69] This presents a possible problem for materialism in the following sense. How could something ('resonance') that has no material base in a particular molecular structure be the cause of anything?[70]

Apparently Chelintsev had Lysenkoistic aspirations.[71] The issue fell on fertile ground, not so much because of the principles of dialectical materialism, but also because there had been priority disputes since 1863 about the originators of the theory of chemical structure (Butlerov, Couper and Kekulé), in particular between

German and Russian historians. In Moscow two conferences were held in 1950 and 1951 at the Institute of Organic Chemistry of the USSR Academy of Sciences,[72] though conclusions were different from the 1948 meeting at the Academy of Agricultural Sciences where Lysenkoism was the outcome. The greatness of the "Russian scientific genius Aleksandr Mikhailovich Butlerov" was heralded; the term 'resonance' could not be used – its 'idealist' associations were to be shunned; chemists who had used the term 'resonance' in their writings were required to acknowledge their mistake. However at both conferences, Chelintsev's 'new structural theory', was decisively, and with little discussion, rejected as worthless.[73] At the level of chemical research the difference between 'bourgeois' resonance theory and the continuation of the 'great tradition of Butlerov' amounted to no more than substituting 'mutual influences' for 'resonance', which was probably better anyway, because even those who introduced resonance theory (Pauling, Wheland) had not said that the theory was about 'things' that 'resonate'.

When Stalin died in 1953 much rhetoric disappeared.[74] What remained was [i] the old priority dispute, which will probably remain unresolved forever,[75] and [ii] the philosophical problem of what sense it might make to say that something that does not exist (viz. the different resonance structures of benzene) can be used to explain all kinds of things.[76] That this example of the politicisation of science had more to do with nationalism than with dialectical materialism is confirmed by the fact that in the DDR, the general issue of the significance of the development of quantum chemistry was often discussed, though the Russian 'hype' about Butlerov had little impact – after all, Kekulé was German.[77] The issue was further complicated when Pauling, the main architect of modern resonance theory, started to publish on 'life and death in the atomic era' (Pauling, 1964). After the 1951 meeting and report from Moscow, the *Chemical and Engineering News* (September 10, 1951) carried the headline "Soviets Blast Pauling/Repudiate Resonance Theory" and as late as 1965 Russian chemistry text books had to avoid the term 'resonance'. But in November 1961 Pauling gave a lecture entitled "The theory of resonance in chemistry" at the Institute of Organic Chemistry of the USSR Academy of Science to an audience of about twelve hundred people. The lecture was translated and published in a Russian journal (Pauling, 1962), after which Pauling became the most admired Western chemist in the Soviet bloc.[78]

As Laitko (1996) notes, after 1956 there were no longer constraints on talk about 'resonance'. However, the philosophical discussion about the status of resonance theory continued and moved to the general theme of the relation of chemistry to quantum mechanics. Whereas chemistry moved on (to the molecular-orbital method and the further development of quantum chemistry), the philosophical problem of the intrusion of instrumentalism into bonding theory was there to stay. Vermeeren (1986) correctly points out that *because* of the language barrier and the political overtones of that exchange, the scientific and philosophical importance of the problem was underestimated (and still is): Whether it is called mesomerism, resonance, mutual influence, idealised valence bond structure, or whatever, for the first time 'non-existent' chemical structures were 'in the air', problematising the notion of chemical identity. A pragmatic chemist might be happy to say that a chemical bond is "a figment of the imagination" and in the same breath that "[f]ew would say that there is no such thing as a chemical bond" (Sutcliffe, 1996: p. 654), but this won't satisfy most philosophers of science.

Many publications appeared drawing negative conclusions concerning the reduction of chemistry to quantum mechanics (via quantum chemistry).[79] For example Laitko (1967) argues against the reductionism of Kitajgorodskij (1966) that chemistry can be 'brought back' (is *zurückbar*), but not reduced to quantum mechanics. He expresses agreement with Shakhparanov (1962: p. 32) who emphasises that the 'higher' notion of individualisation makes chemistry more specific and more concrete (whereas quantum mechanics is more general and more abstract). The connection between the valence-structure method and classical chemical formulae is discussed, as too is the underlying issue of 'model': do quantum chemists use (approximate) models of quantum physical systems or do they use chemical theories? And it is argued that the chemical and quantum mechanical structure of molecules should be distinguished. Because quantum mechanics in its standard Copenhagen interpretation was seen as undermining materialistic principles, chemistry became the 'first science' to deal with the material properties of the world. If quantum mechanics is to chemistry as statistics is to economics (Kedrov, 1962; Vihalemm, 1974),[80] the concept of molecular structure would vie for the priority of most fundamental concept of chemistry, though having no ground at all in quantum mechanics.

In this literature *both* the idea that chemistry was qualitatively different from physics in some absolute sense *and* the idea that chemistry could be reduced to physics via quantum chemistry, was regarded as a fetish. Although phrased in dialectical jargon, the view would not seem to be very different from that of supervenience in analytic philosophy.[81] Also the arguments are often similar to issues raised in later literature on the relation of chemistry to quantum mechanics. For example Laitko (1967) says: "The quantum chemical methods of approximation are of such a kind that when introducing the simplifications, chemical considerations play an essential role, considerations which are of course supported by experimentation and the traditional chemical ways of thinking".[82]

With the decline of dialectical materialism as a political force, discussions on the philosophy of chemistry in Eastern Europe disappeared, though some of the authors who were involved are still active in this area.[83] In conclusion three things may be noted about this rather extraordinary period of interest in the philosophy of chemistry.

- Only when political dogma's merge with the power hunger of mediocre scientists do extreme situations like the Lysenko affair arise. The more common situation is that either the political dogma's are tagged on to the scientific results without in any way influencing the work of the scientists or, in more foundational or philosophical issues, the dogma's stimulate the scientist-philosopher to explore new avenues without feeling bound by the canonical reading of those dogma's.
- The debates about the theory of resonance show that, if anything, nationalistic concerns were of much greater importance than the dogma's of dialectical materialism. The concerns of the debates and power machinations in Moscow promoting Butlerov had no followers whatsoever in the DDR.[84]
- Many of the ideas put forward by the best philosophers of chemistry in the USSR and the DDR, phrased in the termin-

ology of Engels, Marx, and Lenin, are surprisingly similar to those that arose as part of the naturalistic turn in Anglo-American philosophy after the end of the cold war.

5. CHEMISTRY AND POST-1970 MAIN STREAM PHILOSOPHY OF SCIENCE

Since the 1960s, though many different strands of philosophy of science have emerged that made room for chemistry, only rarely has it been for anything *specific* to chemistry:

1. Interest arose in historical case studies to provide arguments for and against the rationality of scientific practice, both within philosophy of science 'proper' and in the sociology (or anthropology) of science. Since Kuhn (1962) referred to the revolution brought about by Priestley and Lavoisier (who removed phlogiston from the language of chemistry), philosophical reflection has increased, roughly in proportion to the number of 'big' theories in chemistry and the number of 'major' developments that have taken place. For example in Kuhn (1962), Boyle, Dalton, Lavoisier, and Priestley figure prominently. In Latour's seminal *Science in Action* (1987) there are more references to Crick, Mendeleev, and Pasteur than to Einstein, Newton and Copernicus (and more references to engineers such as Diesel and Reynolds than to physicists). In a work, entitled *Method and Appraisal in the Physical Sciences* – note that *physical sciences* include chemistry –, there are five big case studies: atomism versus thermodynamics; Young versus Newton; oxygen versus phlogiston; Einstein versus Lorentz; rejection of Avogadro's hypothesis (Howson, 1976).[85] Phlogiston figures as an example in numerous publications as a 'prototypical example of a non-referring term in a successful theory', as does the 'chemical revolution' in the post-Kuhn debates about the rationality of science.[86]

2. An interest developed in the experimental side of natural science. This reacted against the bias within philosophy of science towards (formal) theory. Although initially this research concentrated on things like air pumps, Faraday's experiments, electron microscopes, pulsars, and atomic parity violation experiments, recently a reasonable balance has been struck and several detailed chemical case studies have been published.[87] Hacking's popu-

lar introduction to the philosophy of natural science (1983) no doubt privileges physics, partly because of the book's concern for the instrumental side of science. Consequently, there are detailed discussions of microscopes, 'making' quarks, etcetera. But there are *also* discussions of Boyle, Dalton, Davy, Lavoisier, as well as references to Paracelsus, Berzelius, Brønsted, Kekulé, Lewis, Pasteur, Prout, and von Liebig. Still, the more influential contributions to the 'experimental turn' are all about physics. Most of the chemical case studies, moreover, are not based on what might be specific for chemistry. They are case studies which 'test' positions in the philosophy of 'general' science. For example, the polywater episode is used by van Brakel (1993) to argue that it is spurious to appeal to distinctions like experimenting 'on' and 'with' if one takes the role of experimentation in science seriously and that any (alleged) reality of scientific entities depends on much more than experimenting 'on' or 'with'. Similarly, Ramsey (1990) used a case study in chemical kinetics to discuss general issues of realism and anti-realism and to argue against Latour's idea of blackboxing instruments. In (1992) he argues that the 'contingency' does not disappear if the instruments are available 'off the shelf'; they merely become epistemologically 'translucent' rather than 'black'. Publications such as these are written on the assumption of the unity of science: scientists use instruments – are they 'translucent' or 'black'? Even the answer 'sometimes one, sometimes the other' is not seriously considered. If one looks for conclusions that may tell us specifically about chemistry, the observations are often superficial.[88]

3. Interest in reduction, directed at providing a unified picture of science, continued and became even more important under the new label of supervenience, at the same time shifting in emphasis from physical microreduction to mind/brain supervenience. Here we can speak of a true neglect of chemistry, one not even warranted by prevailing fashion. There is lots of literature on the (alleged) reduction or supervenience of macro/micro-physics, macro/micro-genetics, mind/brain, social/individual, moral/physical, and even aesthetic/physical,[89] but very little on the relations of chemistry to micro- or macro-physics. The reason for this is that reduction of chemistry to physics is taken for granted because of a few influential statements by Dirac, Heisenberg, Reichenbach, and

Jordan.[90] However, all more detailed investigations show that chemistry cannot be reduced to physics, or at least that the example fails to fit 'standard' theories of reduction, particularly 'classical' notions of molecular structure or chemical bond are not easily reconciled with quantum mechanics.[91] However, the importance of this fact (of the irreducibility of chemistry to quantum mechanics) has not had any impact on mainstream philosophy. Of course much depends on how the term 'reduction' is meant. If 'reduction' is used in the sense of 'higher-level theory plus its interpretation can be deduced from the basic theory' then it is a brute *fact* that (Primas, 1991):

– chemistry has not been reduced to physics;
– chemical purity is not a molecular concept;
– the theory of heat has not been reduced to statistical mechanics;
– temperature is not a molecular concept;
– classical physics is not a limiting case of Einsteinian physics, nor a universal limiting case of quantum physics.

If reduction isn't simply taken for granted, many foundational issues ask for philosophical attention. Examples are: the relation of chemical bond and quantum mechanics, the understanding of the periodic table (Scerri, 1993a, 1997), and the Pauli exclusion principle (Hall, 1986; Scerri, 1995; Schröder, 1998).

4. On a smaller scale the old interest in the logical reconstruction of scientific theories remained. Here the amount of interest in chemical theories is noteworthy. See for example Hettema and Kuipers (1988) on the periodic table;[92] Kamlah (1984) on phlogiston; Balzer et al. (1987) and Lauth (1989) on stoichiometry; and Lauth (1993) on Avogadro's number. These are all studies in the paradigm of structuralist philosophy of science, a stage set by Sneed and Stegmüller. More recently considerable interest in chemistry arose from the approach known as *Protoscience*, in this case, *Protochemistry*, which aims at the reconstruction of the methods of chemistry and leads from the pre-scientific every day practices of mastering properties of substances to scientific theories of modern chemistry (see further section 6).

5. Finally and most recently, interest has developed in the cognitive science of science, which focuses on the context of discovery rather than of justification. Here too case studies from the history

of chemistry play a role in the discussion, in particular the chemical revolution of Lavoisier.[93]

In judging whether chemistry is a neglected science in philosophy, it should be realised that there are many publications on what might be called "general philosophy of science", which are not about any science in particular, although it is often presupposed that "science" means "natural science". This includes publications about induction, laws, causality, Bayesianism, determinism, explanation, verisimilitude, types of scientific realism, scientific rationality, models for scientific change, and so on. While the main subject may be a general issue, if an example from chemistry is chosen, this may be of interest in its own right; see for instance the exchange between Howson and Franklin (1991) and Maher (1993), in which Mendeleev's predictions figure as the major example of a Bayesian prediction model.[94]

Moreover, issues relevant to the philosophy of chemistry may arise via examples used in general philosophical discussions. Chemists may be surprised to hear how popular it is among philosophers to discuss the properties of water. It would be easy to give a list of 100 publications that have appeared since Putnam's seminal (1975), in which water (and its 'twin' on Twin Earth) figure prominently in the defence of a causal theory of reference (with ramifications throughout the philosophy of science, mind, and language). Although many of the arguments in this literature are based on thought experiments, which are chemically extremely implausible or impossible, nevertheless this vast literature includes publications that are also relevant to the philosophy of chemistry.[95] To give the flavour of these discussions let me give a few recent examples. In the prestigious journal *Mind* eight pages were recently devoted to a discussion of the relevance of Chomsky's (1995) observation that tea and Sprite are not called water although they contain roughly the same proportion of H_2O as tap water (Abbott, 1997). On a different track, LaPorte (1996) argues that others concerned with the subject greatly overestimate the role of microstructure in advocating theories of causal reference and he discusses the difference between H_2O and D_2O, that between ruby, topaz, and corundum; jade and nephrite; diamond and charcoal; and similar examples. Many of these debates touch on the general issue of the tension between the manifest and scientific image and the 'dilemma' concerning whether physics or chemistry should be claimed the final arbiter of substances.[96] If chemistry is *primarily* the science of macroscopic substances, whereas 'micro' or 'submicro' talk, though important, useful, insightful, and so on, does not change what matters, namely the properties of *macroscopic* substances then these substances and their properties cannot be *reduced* to talk of molecules or solutions of the Schrödinger equation (van Brakel, 1997, 1999a).

On a somewhat different track, discussions in the philosophy of mind often hide unresolved issues in the philosophy of chemistry. For example, Kim (1995) says there is no need to worry about mental causation because the reasoning that leads to worries about mental causation can be generalised to show that there cannot be causation in chemistry, biology, geology, or any other science other than basic microphysics.[97] The comment suggests that much of the discussion in the philosophy of mind on such issues as eliminativism, reductive materialism, and anomalous monism can be transposed to the philosophy of chemistry. For example: Does it make sense to say that chemistry is ontologically about the same (material?) world as physics, but conceptually autonomous? (See further last item section 6.)

Finally, philosophers borrowing ideas from chemistry have gone beyond nineteenth century interest in 'affinity'. For example, modern definitions of the chemical notion of valence figure, as analogies, in esoteric ongoing discussions about the possibility of reducing truth to non-semantic notions (Field, 1972; Putnam, 1978; Weatherall, 1993). There are also formal analogies in which chemical examples play a role. For example there is a mathematical similarity in the description of neural nets (or connectionism) on the one hand and immunology and autocatalytic networks on the other (Farmer, 1990). Or, there are possibly incorrect analogies, as when the discussion of Kant's argument that a hand can be embedded in space in two ways is connected to the question whether enantiomorphism (the 'chemistry of space') is a manifest or a dispositional property.[98] Finally, philosophers may 'borrow' some idea from chemistry, which may, in retrospect, bear on the philosophy of chemistry; an example is Frege's famous *Begriffsschrift* (a formal language for 'pure thought'), published in 1879, which is based partly on his knowledge of the language of chemistry and ‘borrows’ the chemical concepts ‘(un)saturated’ and ‘disintegration’ (Majer, 1996).

6. CONCLUDING REMARKS

Developments since 1960 have had some impact in restoring the balance between chemistry and physics in philosophical discourse. But although there is by now an extensive literature in the philosophy of science that appeals to detailed examples from chemistry, the number of studies that address issues that are specific to chemistry or its autonomy is still quite small. The only substantial exception to this is the discussion of reducibility (see references in note 91). The specific relevance of chemistry for discussions on reduction has received a further boost from the renewed interest in ‘emergence’ (Beckerman, 1992; Schröder, 1998).

Here is a list of other issues in the philosophy of chemistry that go further than merely taking examples from chemistry to illustrate some view or other in the philosophy of ‘unified’ science.

6.1. *The Science of Stuffs*

Schummer (1996) presents the foundations of an ordering of ‘stuffs’, i.e. chemical substances, that allow the pursuit of the synthesis of new stuffs.[99] He claims that chemistry is governed by an action-related conception of knowledge as distinct from the non-interactive approach that characterises the emphasis on formalisation and mathematication of physical science. There is therefore some similarity with the emphasis on the interactive aspects of the experimental side of science (mentioned under point 2 in the previous section). But the fact that chemistry is constantly enlarging the world it studies by making new stuffs, and the differences between the chemical space of stuffs[100] and the time-space of physics, make the interaction of cognitive and material praxis in chemistry very different from that in physics and biology.

This implies that the method of chemistry is neither to be characterised as empirical-inductive, nor as hypothetico-deductive. The experimental praxis of making new things (new ‘stuffs’) is different from that of making careful measurements or carrying out ‘crucial’ experiments. There is a side to chemistry that makes it more akin to technology than to physics (Schummer, 1997c). To study the world from the stuff perspective is vastly different from the mechanistic study of primary qualities. Relative to the stuff perspective, talk of atoms and molecules is subsidiary. Any transformation of 'stuff' is first and foremost a qualitative change. Proposing an underlying quantitative description cannot fully grasp the 'emergent' property. A simple example could be the difference between a liquid and a vapour. It is not difficult to blur this distinction under special experimental conditions (of pressure and temperature), but that does not undermine the qualitative difference between a liquid and a vapour or, speaking more scientifically, the sense of ascribing thermodynamic properties to the interface between a liquid and a vapour (van Brakel, 1997).

Schummer (1997) gives an extensive inventory of what further is 'peculiar' to chemistry, compared with the 'received' view of science. When compared with physics, the most striking is perhaps the abstraction from form, size and mass. As long as an object can be placed in an experimental context, chemists do not care about spatial co-ordinates or the number of its physical parts. In physics two objects are identical, if and only if they have the same space-time co-ordinates; in contrast, two objects are chemically identical if and only if they are found at the same place in chemical space (which means that they enter into the same chemical reactions). Further, knowledge about material properties cannot be completed, because there is no end to making new stuffs.[101] Not only do chemists have reference rules that use names or labels and rules that use identification conditions (*cf.* the discussion on reference from Russell to Kripke); they also have reference rules that provide laboratory rules for producing stuff.

6.2. *Protochemistry*

Protochemistry aims at a reconstruction of chemical scientific knowledge. It is the theory that is methodologically prior to chemistry. All experimental science has a technical or instrumental basis that should not be identified (as philosophers of science from logical empiricists to naturalised epistemologists of science tend to) with 'measuring experience', but with setting technical goals and their successful realisation. Against that background protoscience can be considered to be the study of the *normative* criteria for the use of experimental technology in science. It distinguishes itself from ‘received’ philosophy of science by focusing on the praxis in which new concepts and laws are not ‘discovered’, but ‘constructed’. That is to say the commitment is explicitly *against* scientific realism – the methodological constructivism of ‘protoscience’ is a blend of instrumentalism and pragmatic realism. The historically grown scientific language is investigated both at the object level (vocabulary concerning operations, tools, instruments and technical terms) and the meta-level (the discourse *about* the object level). The aim of science is seen *not* as the description of nature, but as the theoretical-instrumental support of ‘poietic practices’, i.e. practices that aim at the production of material goods.

Hence scientific objects are not simply found in nature, but ‘constructed’ in the sense that ‘scientific experiences/data’ are only obtained *after* the technical and conceptual construction of instruments. What is meant here by (re)construction has similarities to the operationalism of Bridgeman (1950) and Dingle (1949), the making-worlds view of Goodman (1987) and social construction in the sense of Latour (1987), but it is different from all of them in starting explicitly from the daily life world.[102] This is an approach that is to be applied to any knowledge domain, and most of the work on ‘protoscience’ has been directed at physics (including geometry). More recently a substantial number of publications have appeared (mainly in German) on protochemistry.[103] When applied to chemistry, the difference with other sciences shows at once, because of the characteristics of the proto-concepts involved in practices like cooking, brewing, dyemaking, metallurgy, making medicinal stuffs, and so forth: colours, tastes, hardness/viscosity, melting and boiling point, homogeneity, purity, toxicity, inflammability, and similar properties of materials. First reflection draws attention to the peculiarities of the notions ‘stuff’ or ‘substance’ (against the background of the practices just indicated). This involves simple observations like: “if two arbitrary cut parts of a thing display the same ‘essential’ material properties then it is ‘essentially’ uniform”. Then come the rules and laws that characterise chemical practice. And so on. Contrary to what one might expect the most *basic* laws are those that state the existence of particular pure stuffs and their properties, that is the reproducible identification and synthesis of substances and the reproducible measurement of their properties. All further theorising remains dependent on the validity of these basic laws, which are tied to what it is technically possible to make. Talk of atoms and molecules plays little role in *proto*chemistry (and similarly for the quarks or strings in protophysics).

6.3. *Chemical Synthesis*

Under this heading come discussions about concepts like reactivity, steric interaction, stability, equilibrium, (chemical) bond, bond strength, electron orbitals, solvation, valency, transition state, catalyst.[104] Although chemical *synthesis* is one of the most characteristic features that distinguishes chemistry from other sciences, philosophers have paid virtually no attention to it.[105]

There has been an almost stable exponential growth of the number of chemical substances over the past 200 years; 1820: 10^3, 1860: 10^4, 1900: 10^5, 1960: 10^6, 1985: 10^7 (Schummer, 1997a). Not only are more and more substances added by, as it were, more of the same, but substances are added with completely novel properties. For example 'starburst' dendrimers (also called cascade molecules, arborols, or micellanes) are heterocyclic molecules that consist of a central polyfunctional core to which successive branched layers (called 'generations') are added. Each subsequent generation brings about a doubling of the end groups and a change of conformation until the dendrimer adopts a spherical shape. The volume inside is shielded from relatively large molecules while still remaining accessible to small ones.[106]

Probably reactivity is the most important dispositional notion in chemistry. A chemical reaction can be defined as a change of number, kind or mass of pure materials, while number, kind and mass of elementary materials remain constant (Schummer, 1997). Chemical reactions play at least three different roles: [i] they provide an inventory of possible chemical changes; [ii] they yield information on the structure of molecules; [iii] they contribute to the 'emergence' of new compounds. Because chemistry is *essentially* about transformations, the concept of time is a necessary ingredient of any theory that is truly chemical. It 'enters' chemistry via [i] the second law of thermodynamics; [ii] the concept of molecular diffusion, and [iii] reaction kinetics proper (Benfey, 1963). Although the first two could be taken as ‘physical’, reaction kinetics is essential to chemistry. The second law of thermodynamics can predict from a present state but has nothing to say about the time required to attain a future one.

6.4. *Chemical Thermodynamics and Physical Chemistry*

For various reasons, physical chemistry might well be considered a separate science. On the one hand parts have names like quantum chemistry, chemical thermodynamics, interface chemistry, colloid chemistry, electrochemistry.[107] On the other hand most of it is not concerned with chemical reaction. I suggest that the best (pragmatic, not essentialistic) choice is to consider chemistry the science of the transformation of substances, including the transformation of substances that do not involve chemical reactions – after all the mathematics for describing chemical reactions isn’t very different from that used for describing the grinding of solid particles or radioactive disintegration. This implies, *inter alia*, that metallurgy, usually distinguished from chemistry and sometimes ‘generalised’ (together with polymer science) to material science would be part of it, as too would so called unit operations in chemical engineering, whether chemical, physical, or mechanical.[108] And nuclear physics aimed at the production of materials might better be called nuclear chemistry.

Thermodynamics that takes on gravity, interfaces or time is already ‘underdeveloped’ from a scientific point of view and raises many foundational issues, often of a paradoxical nature. Not only are there the vagueries about irreversible thermodynamics and the well-known Gibbs paradox,[109] but there are other antinomies as well.[110] Consider for example crystals. They can never be perfect, the ‘positions’ of atoms being average positions (they vibrate), whereas these average positions differ in different ‘cells’ (atoms are never in a homogeneous field of forces). Problems concerning the relation of thermodynamics and statistical mechanics have often been discussed (Sklar, 1993), but an almost completely neglected area is interface chemistry, raising poignantly the problem of the relation between different levels of description.

The phase rule[111] and the theory of chemical thermodynamics provided Gibbs with the theoretical background for the concept of phase (the state of aggregation of a substance such as solid, liquid, vapour) and, hence, made it possible to give precise definitions of 'solution', 'compound', 'pure substance', 'element', independent of any atomic hypothesis. A material is pure if it is perfectly homogeneous after being subjected to successive and maximally different modes of fractionating (i.e. when attempts at further purification produce no further change in properties).[112] This forms the basis for a purely macroscopic approach to chemistry (Ostwald, 1907; Timmermans, 1963 [1928]; Prélat, 1949; van Brakel, 1999a).

6.5. *Molecular Structure*

The notion of structure has different meanings at different levels of description. For example:[113]

– Structure as a rough 'summary' of reaction possibilities, i.e. structure given by the (macroscopic) network of relations between substances and the chemical reactions into which they enter.[114] This structure is a little potted theory in its own right and provides a model for the chemical behaviour (the reactivity in various environments) of macroscopic masses of the relevant compounds. When combined with different compounds different parts of the structure may be relevant.
– Geometric structure at the (micro)level of molecules: spatial arrangement of atoms, crystal structures, glasses.
– Valence structure, i.e. structure at the (micro)level of atoms and bonds between atoms: arrangement of electron configurations.[115]
– Mathematical structure of the quantum mechanical description for a particular system.

It is trivial that at every level of description there is structure. A reductionistic view will take for granted that all the higher level structures will, if they make sense, eventually be found back at the most fundamental level: all higher level structures are mirrored at the lower level. Defenders of this view seem to presuppose that as quantum mechanical structures have been used to make excellent predictions of higher level properties, that is sufficient to prove that complete reduction is possible in principle.

A pure substance is often considered a collection of molecules of the same type. But this definition doesn't work for enzymes, antibodies, viruses, or more generally isochemical compounds and homeomers (Pirie, 1952). Then there is the problem of definite and indefinite compounds – a distinction already recognised by Mendeleev. The concept of molecule too is inapplicable to metals, salts, electrolytes (including water) and dissociating liquids; and molecular interpretations break down in heterogeneous catalysis, autocatalytic and cyclic reactions (Manzelli, 1996).[116] And many more problems with the concept of molecule arise.[117] It sounds good to say something like "molecule is the smallest 'particle' of a definite compound which still has the same properties". But 'smallest particle' only makes sense for ideal gases and a few liquids, not for diamond/soot, salt crystals, proteins, cellulose or micelles. And even in cases like alcohol or helium it is unclear what could be meant by saying that the properties of the assembly of molecules are the same as those of the compound. Alcohol is transparent and may contain dimers; helium gas has a particular pressure. The concept of molecular structure seems to derive its meaning more from the way molecules are represented in models than from anything else.[118] At the microlevel the static architectonics of bonds are no more than a convenient selective idealisation of much more fluid relationships. Molecule is an indispensable, but through-and-through theoretical concept, part of theories that are impressively empirically adequate, but without a clear idea of what entities are thought to exist. Moreover, to the extent that it makes sense to say things like "a pure substance consists of identical molecules", any empirical evidence for this statement depends on a prior understanding of what a pure substance is (van Brakel, 1997).[119]

6.6. *Chemical Laws*

At the moment there is virtual consensus that [i] biology is a science and [ii] it has no laws in the sense of 'laws in physics'.[120] There is considerable disagreement in what sense biology is different from physics, but there is consensus that the difference is big. Typically in this discussion, chemistry (if mentioned) is lumped with physics,[121] though in the ‘old days’ it was lumped with biology and the rest of science (as sciences without ‘proper’ laws). It is not surprising then that opinions have differed on how many chemical laws there are.[122] Answers include: no laws, two laws, three, many.

The laws of definite proportions and of stoichiometry (of multiple proportions) are two of the important laws of chemistry associated with the development of the atomic theory in the early nineteenth century. Christie (1994) shows that they have characters which cannot be reconciled with philosophers’ accounts of laws of nature. They are non-universal, and one of them is imprecise. Unlike philosophers, chemists have recognised this diversity for at least a hundred years.[123] Mendeleev’s law of periodicity says that the properties of the elements are a periodic function of their atom numbers; there exists a periodicity in the properties of the elements governed by certain intervals within their sequence arranged according to their atomic numbers. But the possession of particular shell configurations is neither necessary nor sufficient for inclusion of an element in any particular group of the table. The law expresses an appropriate trend among the properties of the elements and their compounds. The regularity it captures cannot be expressed in nomological fashion using non-chemical concepts.

Hence, the suggestion (referred to above and echoing Kant) that there are no laws in chemistry because even the best examples (like the law of stoichiometry) have exceptions. On the other hand, according to Caldin (1959) there are empirical laws of two kinds in chemistry: [i] statements that there are definite kinds of material; [ii] statements concerning functional relations which express the properties of these substances. And according to Laitko (1967) the notion of ‘generality’ in connection with laws should not be understood in terms of ‘applicable to all objects’, but as ‘universal’ even if it applies to a limited number of objects. Hence chemistry has millions of laws: each reaction equation provides a law.[124]

If one applies ‘strict’ criteria, there are no chemical laws. That much is obvious. The standard assumption has been that there are strict laws in physics, but that assumption is possibly mistaken.[125] Perhaps chemistry may yet provide a more realistic illustration of an empirical science than physics has hitherto done.

6.7. *Independence of Chemistry*

Most writers on the latter-day successors of reductionism (including advocates of 'radical' emergentism) propose by implication, substance monism and explanatory pluralism: [i] the only *things* there are, are physical things – all true descriptions and explanations concern the states and behaviour of things composed only of physical entities, but [ii] not all true descriptions or explanations are in, or are translatable into, the language of physics. But nothing forces us to take this view. Consider instead a form of anomalous monism applied to chemistry.[126] On this view causation is a relation between events, not between events *as* one thing or another. Events cause one another independently of how they are described, even independently of how they are identified. For example, the same event can have a chemical and a neurophysiological description, or a moral and a physical description, or a macroscopic and a microscopic physical description, and so on. Of course, the only way to talk about causes is under some description or other, but there is no need or ground for favouring one privileged description as more fundamental.

Often monism is taken to imply an asymmetry of a reductionistic sort, as when one says materialism is a form of monism. But the anomalous monism here proposed should be seen as *anomalous* in a variety of ways and should not be taken as a variant of materialism. The God's-Eye-point-of-view-meta-description that gives the 'true' identification of events has to be abandoned. We can only ask about criteria of identification if something is in place – we can only quantify over something if there is already a domain of individuals. The request for individuation stops somewhere. In a physical discourse events can be identified as physical events; in a chemical discourse as chemical events. But because chemical and physical predicates are not 'made' for one another – after all, that is why the whole discussion about reduction arose – it is not possible to say whether an event identified under some physical description is exactly the same event (or not) as the one that is described under a chemical description (or a psychological, or a moral description, etc.). Of course rough hints are possible, but they don't give exact descriptions, not even of the space-time boundaries. Moreover, talking about one event and one other event is only by way of speaking, because there are no discourse independent identification criteria of one or the other event. Any parcelling out of events bounded in time and space only makes sense given a particular discourse in place.

It is not that first there are physical events and chemical events and then some physical events turn out to be identical with some chemical events. In ordinary language all events are EVENTS, no matter whether they are described in physical, social, chemical, or whatever terms. By assuming that each event that can be given a chemical description also has a physical description (although we cannot specify it or provide exact criteria of identification) some insight is gained in the *autonomy* of the chemical *and* the physical, while still keeping both in the same boat.

NOTES

1. Much shorter predecessors of this paper were presented at the *First International Conference on Philosophy of Chemistry*, London, March 26–27, 1994, at the *Tagung Philosophie der Chemie: Bestandsaufnahme und Ausblick*, Karlsruhe, April 16–17, 1994, and published in German in Psarros et al. (1996).
2. The contributions were published in Psarros et al. (1996). The *Arbeitskreis Philosophie und Chemie* was founded at a meeting in Coburg (Germany) in June 1993.
3. Three papers were presented: Rothbart (1994), Scerri (1994), Ramsey (1994). Papers presented at earlier meetings include Hofmann (1990) on solid state chemistry, Ramsey (1990) on numerical and causal accuracy in reaction kinetics, and Hofmann and Hofmann (1992) on Darcy's law. Though the journal *Philosophy of Science* started in 1933, there have been very few articles on the philosophy of chemistry. Malisoff (1941) is the text of a public lecture on "Chemistry: Emergence without mystification"; Kent (1958) is a paper on scientific naming in which Lavoisier and Faraday play a central role; Kultgen (1958) concerns the distinction between elements as separate homogeneous substances and as a material part of compounds. Early publications in *The British Journal for the Philosophy of Science* on the philosophy of chemistry are: Feibleman (1954), where chemistry is mentioned in the context of von Bertalanffy's theory of general systems theory; Pirie (1952), on the concept of pure substance; Bradley (1955), which attempts an operational interpretation (in the sense of Bridgeman and following the lead of Ostwald) of classical chemistry (Dalton, Gay-Lussac, Avogadro, Cannizzaro); and Ellis (1957), who uses Gay-Lussac's law of combining volumes as an example to compare process and non-process explanations.

4. The proceedings have been published in Janich and Psarros (1996). The first *Erlenmeyer-Kolloquium der Philosophie der Chemie* took place in November 1993 (proceedings: Janich, 1994a); also in 1993 there were meetings on the history and philosophy of chemistry in Bradford and Perugia.
5. Papers were published in Mosini (1996). Also the *Atti del V Convegno Nazionale di Storia e Fondamenti della Chimica* were published in 1994 (Marino, 1994), proceedings of a meeting in Perugia in October 1993. As the title indicates, this was the fifth meeting of its sort (the first one taking place in 1985). Probably the first journal in which papers on the philosophy of chemistry were published with some regularity was the Italian journal *Epistemologia* (Lévy, 1979; Del Re, 1987; Liegener and Del Re, 1987; Villani, 1993; Mosini, 1994; Psarros, 1995). Earlier interest in the philosophy of chemistry in various countries was usually tied to meetings with a predominantly historical orientation. In Italy the initial interest came from Chairs in theoretical chemistry, not philosophy (*cf.* Del Re, 1981; Paolini, 1981). In the Netherlands some interest began in 1981, stimulated by A. Rip, H. Vermeeren and P. van der Vet (*Chemisch Magazine*, October 1981, pp. 591–598) – *cf.* Vermeeren (1986), van der Vet (1979, 1987, 1989), Zandvoort (1985, 1988). There was however little follow up.
6. For names and titles of presentations see *Hyle – Bibliographie (post 1990 literature)* at the *Hyle* website (http://www.uni-karlsruhe.de/∼philosophie/hyle.html). At earlier meetings of the International Congress of Logic, Methodology and Philosophy of Science, there had been only rare, and isolated claims for the philosophy of chemistry, for example van Brakel and Vermeeren in 1979 at the *6th International Congress* in Hannover and Ruthenberg and Ramsey at the *9th International Congress* in Uppsala in 1991.
7. In Germany, in response to the negative image of the chemical industry, a programme ‘Chemistry and the Humanities’ was started, leading to Mittelstraß and Stock (1992).
8. In the final section I briefly refer to issues in physical chemistry. On the significance of the *essential* macroscopic character of thermodynamics in relation to chemistry see Baracca (1996), van Brakel (1997, 1999a). *Cf.* also the discussion of Duhem’s view in the next section and Heisenberg (1942: pp. 246–258) who subdivides chemistry into ‘heat’, ‘chemical laws’, ‘limits’ [of distinguishing mechanical and chemical descriptions at the ‘lowest’ level of the *material* world], and ‘chance’. For a comprehensive survey of the philosophical issues surrounding the relation of thermodynamics and statistical mechanics see Sklar (1993).
9. See Brush (1978) for a rather old, but still pertinent assessment of why there has been relatively little interest in the history of chemistry. Recently the history of chemistry in Europe got a small boost from a four year research programme (1993–1996), financed by the European Science Foundation. Important recent publications on the history of chemistry include Bensaude-Vincent and Abbri (1995), Duncan (1996) and Nye (1993).

10. This would include literature on the transition from alchemy to chemistry (e.g. Ströker, 1967), or more generally the 'Aristotelian side' of chemistry (Needham, 1996, 1996a; Schummer, 1996). See for some recent discussions on the 'emerging' *science* of chemistry the special issue of *Science in Context*, vol. 9, No. 3 (1996).
11. Although Boyle is known as 'the father of chemistry' (*cf.* the title of Pilkington, 1959), it is wrong to stress the connection between Boyle's chemistry and his corpuscular philosophy. At the end of the 19th century the atom definitively changed hands from the (German) chemists to the (English) physicists. Typically, neither in his address on molecules to the British Association for the Advancement of Science in 1873, nor in his article on Atoms in the *Encyclopaedia Britannica*, did Maxwell mention Dalton. See for a brief account of these examples van Brakel (1997, 1999a) and for more details Klein (1994, 1994a) on Boyle and Gavrogulu (1994) or Gavrogulu and Simoes (1994) on Maxwell.
12. For Aristotle's notions of element and substance from a philosophy of chemistry perspective see Böhme (1980), Schummer (1996: pp. 98–122 and *passim*), and also Lewis (1996), whose Ph.D. thesis on Aristotle's *Metereologics* is entitled *Body, Matter and Mixture: The Metaphysical Foundations of Ancient Chemistry*.
13. See van Brakel (1991, 1997). Peirce already made the distinction in 1861 (Tursman, 1989). *Cf.* the chemist Williamson who wrote in the *Chemical Gazette* of 1851 (quoted in Benfey, 1963): "We are all agreed that chemistry is concerned with the material process of the transformations and changes which matter undergoes, and that the study of the properties of matter in themselves, as long as they undergo no change, belongs to physics."
    Lavoisier's (1789) view was that chemistry is the quantitative science of the macroproperties of substances and their transformations. He supported an atomic view of matter, but he did not use atoms and molecules in the explanations of observed chemical phenomena (Abbri, 1996). Mendeleev aimed both at the unification of the many natural sciences and the autonomy of chemistry: atoms are the ultimate constituents of nature; chemistry studies their properties *qua* difference from each other; physics their properties *qua* similarity (Kultgen, 1958; Kedrov, 1969; Mendeleev, 1889).
14. Across centuries 'atomism' can mean: atoms are the four elements water, fire, earth, and air, or the three principles Mercury, Sulphur, and Salt, or Lavoisier's 33 simple substances, or atoms, or molecules, or quarks, or the referents of a hidden variable interpretation of quantum mechanics. The word 'molecule' was introduced as a neologism by Gassendi in 1637 (Bloch, 1971: p. 267). The idea of a molecule, as a new category distinct from 'atom', 'body', and 'substance' was perhaps first formulated by Beeckmans in 1620 (Kubbinga, 1984, 1988). For Beeckmans *homogenea physica* were substance-characteristic particles ('substantial individuals') consisting of a number of atoms of different form and size, organised in structure – a concept

already ‘predicting’ isomerism. Pre-Avogadro chemists tended to use the terms ‘atom’ and ‘molecule’ interchangeable.

15. A recent example is Pyle (1997).
16. For references to the older literature on this theme see von Engelhardt (1986). Also the philosophical interest of the German chemists Ostwald, von Liebig, and Mittasch can be placed in this tradition. At the height of publication on the history and philosophy of chemistry in the German Democratic Republic (see section 4), many theses and articles appeared on Ostwald and von Liebig (and also on Schelling and Goethe).
17. Vasconi (1996) has suggested that under the influence of the work of Lavoisier, Kant’s transcendental system undergoes revision. *Cf.* note 23.
18. For a recent discussion in English see Nayak and Sotnak (1995), though little is added to what had been discussed in the German literature of the past century.
19. *Cf.* Kant’s ‘a procedure which resembles chemistry’ (Körner, 1991), a procedure needed in the analysis of moral commonsense.
20. The crucial passage reads (Kant, *Schriften,* 4: p. 470): “So lange also noch für die chemischer Wirkungen der Materien auf einander kein Begriff ausgefunden wird, der sich construiren läßt, d.i. kein Gesetz der Annacherung oder Entfernung der Theile angeben läßt, nach welchem etwa in Proportion ihrer Dichtigkeiten u.d.g. ihre Bewegungen sammt ihren Folgen sich im Raume *a priori* anschaulich machen und darstellen lassen (eine Forderung, die schwerlich jemals erfüllt werden wird), so kann Chemie nichts mehr als systematische Kunst oder Experimentallehre, niemals aber eigentliche Wissenschaft werden, weil die Principien derselben blos empirisch und keine Darsellung *a priori* in der Anschauung erlauben, folglich die Grundsätze chemischer Erscheinungen ihrer Möglichkeit nach nicht im mindesten begeiflich machen, weil sie der Anwendung der Mathematik unfähig sind.”
21. It was suggested that psychology might score better as a ‘proper science’ than chemistry, because Kant works with the distinction of ‘body nature’ (*res extensa*) and ‘thinking nature’ (*res cogitans*). In his lectures on metaphysics Kant described psychology as “metaphysische Erfahrungswissenschaft vom Menschen” [in “Nachricht von der Einrichtung Vorlesungen Winterhalbenjahren von 1765–1766”, *Schriften*, 2: p. 316) and used the expression *mathesis intensorum*, suggesting that even if not now, psychology *could* become a proper science – though it should be noted that these are views from Kant’s ‘pre-critical’ period. In the preface of the *Metafysische Anfangsgründe der Naturwissenschaft* (1786) there is no word about *mathesis intensorum*. And there he says: “Noch weiter aber, als selbst Chemie muss empirische Seelenlehre jederzeit von dem Range einer eigentlich so zu nennenden Naturwissenschaft entfernt bleiben” (*Schriften*, 4: p. 471). Altogether there are very few references to chemistry in Kant’s writings on the philosophy of science. In a lecture in 1783 Kant says “Unstreitig sollte die Physik also auch die ersten Gründe von der Chemie zugleich enthalten” (*Schriften*, 29: p. 173) and there are the following brief utterances in the *Nachlass*: “Chemie ist bloß

physisch." "Die ganze Chemie gehort zur Physik – in der Topik aber ist vom Übergange zu ihr die Rede." "Die Chemie ist ein Theil der Physik aber nicht ein bloßer Übergang von der Metaph. zur Physik. – Dieser enthält blos die Bedingungen der Möglichkeit Erfahrungen anzustellen" *Schriften*, 14: p. 470, 31: p. 288, 31: p. 316).

22. See Burbidge (1996), Snelders (1993), von Engelhardt (1993) and references given there.
23. But see Burbidge (1993: pp. 615–616): "Hegel has had to rework his philosophy of nature in the light of the results of empirical chemistry. His first attempt to force it into a tri-partite scheme did not do justice to the significant differences between amalgamation, oxidation and acidification, and completely ignored the use of chemistry in refining. . . . it suggests that in 1817 Hegel revised the syllogistic structure of the logic of chemism in the light of empirical chemistry."
24. Schelling developed his philosophy of nature in response to Hegel. In Book II of *Ideas for a Philosophy of Nature*, Schelling gives a detailed account of the chemical properties of bodies and chemical processes on the basis of a dynamic account of matter. According to Schelling "attractive and repulsive forces constitute the *essence* of matter itself" (1988 [1797]: p. 165).
25. In a quite different tradition from that of German philosophy of nature, Peirce too believed that the notion of valency as developed by Frankland, Mendeleev and others was one of the most important ideas in the history of science. He used the concept in what he called phanerochemistry, which, in going beyond chemistry and being applicable whenever there is a 'connection-of-two' has some similarities to Hegel's chemism, though it is closely intertwined with the idiosyncracies of Peirce's three categories and his notion of semiotic (Tursman, 1989).
26. Prélat (1947) and Timmermans (1963 [1928]) are later examples of such a macroscopic approach to chemistry.
27. Needham (1996) has attempted to provide a systematic account of the Aristotelian theory of the generation of substances by the mixing of elements. Needham (1996a, 1996b) has pursued the interpretation of a macroscopic, thermodynamical perspective on chemical substances from an elementary viewpoint in the spirit of Duhem (1902), showing the general lines along which an explicit ontology – in Quine's sense – of macroscopic theory might be developed.
28. Nevertheless it would be incorrect to describe Duhem as an anti-realist or instrumentalist (Needham, 1998).
29. For example Gutting (1987), Tiles (1987), Tijiattas (1991). Typically, in Tiles' (1985) book on Bachelard's philosophy of science, the two publications with 'chemistry' in the title (Bachelard, 1932, 1971) aren't mentioned once.
30. "Cette philosophie de la chimie est en fait une stylisation de l'histoire, simple traduction de l'événement historique en style philosophique" (Bensaude-Vincent, 1974). For a critique of Bachelard's approach to the history of

chemistry, directed at Bachelard's comments about Bertholet see Stengers (1995). *Cf.* Duhem's comments on Bertholet (Needham, 1998: p. 57).

31. Schummer (1996: pp. 180, 182, 226) stresses Bachelard's observation that the purity of substances should not be taken as a 'natural-given', but as the result of human operations (*cf.* Bachelard, 1934: p. 79). Bellu (1979) used Bachelard's (1949) in support of the contradictory unity of conservation and transformation.
32. In Bachelard (1934: pp. 170–177) there is the intriguing comment that experiments on the stretching of colloidal gels allow "the physicist to act upon the *chemical nature* of substances" (emphasis in original).
33. Or from French chemists for that matter: Delhez (1974).
34. Or, a bit more specific: "The hypotheses of 'native chemistry' which stems from the work of *homo faber* are at least as important psychologically as the ideas of 'natural geometry' . . . both the remotest reverie and the harshest toil [should] be reintegrated into the psychology of *homo faber*." Quotations from Bachelard (1942: pp. 142–148), as translated by McAllester Jones (1991).
35. *Cf.* note 99.
36. For reasons more 'internal' to chemistry that might explain the 'neglect' of the philosophy of chemistry see Eisvogel (1996), Janich (1994), Ruthenberg (1996), Psarros (1996a), Scerri and McIntyre (1997) and brief observations in Bunge (1982), Janich (1992: p. 173, 1994a: p. 86f), Liegener and del Re (1987), Ströker (1967), Del Re (1996).
37. See Mulckhuyse (1961) for an early attempt to do philosophy of chemistry that meets the formalistic standards of traditional philosophy of science. He presents an axiomatisation in first order logic of the 'classical' (van 't Hoff type) theory of chemical structure. For a critique of the limited scope of his project see Schummer (1996: pp. 248f, 255).
38. See also quotation of Meyerson in note 45.
39. In Causey's book *Unity of Science* (1977), there are less than four pages on chemistry (pp. 51–54). *Cf.* first paragraph section 1.
40. See Hempel (1965: pp. 259–264); Nagel (1961: pp. 366–380).
41. Nevertheless Broad seemed to assume that emergent properties strongly supervene on microstructural properties (Beckermann, 1992). That is to say: the emergent properties cannot be defined in terms of (deduced from) microstructural properties. But given both kinds of properties, these are connected by necessary laws (a view scarcely differing from the original concept of a psychophysical law). Though Broad himself did not use specific chemical examples (*cf.* note 45), he may well have been influenced by examples like the colours of dyestuffs. For example, if hydrochloric acid is slowly added to crystal violet the colour changes from blue-violet to green to colourless. The colours, though non-reducible and 'emergent' properties are connected by law to microstructural properties (*in casu* the charge of the nitrogen atoms in the molecule).
42. *Cf.* Theobald (1976): "Theories are rarely highly controlled by observation in chemistry, since [they] are generally rationalising constructions covering

vast arrays of experimental data, rather than precise mathematical formulations vulnerable to a single quantitative misfortune." Caldin (1961) is a short introduction to the philosophy of science using chemistry as example; as to the philosophy of chemistry it doesn't add much to Caldin (1959).

43. At a text book level the difference has been ascribed to that between energy and matter, to that between all matter and individual kinds of matter, and to that between the study of microscopic and macroscopic phenomena.
44. "Doch handelt es sich bei ihnen um solche [phenomena], die, anders als die rein physikalisch betrachteten, den Charakter *stofflicher* Veränderung haben . . . [phenomena] *an* Stoffen und *um* der Stoffe willen . . . Die Chemie kann auf die Frage, *was* die Stoffe und ihre Qualitäten *sind* nicht verzichten" (Ströker, 1967).
45. The list of examples quoted is not completely convincing. Polanyi (1958) could be added to the list. On the other hand, Broad started his study in Cambridge with physics, chemistry, botany, and mineralogy, but after two years decided that his future lay in philosophy. There isn't one reference to chemistry in the Broad volume in the *Library of Living Philosophers*. Meyerson (1991), in his historical account of explanation in the sciences, discusses the resistance to Lavoisier's theory at some length (pp. 546–563), but in his long chapters on Hegel and Schelling there is no reference to chemistry. Still there are other occasional references to it, for example (Meyerson, 1930: p. 31): "The existence of the silver-element is only a hypothesis which is obtained after many deductions; and pure silver, like the mathematical lever, the ideal gas, or the perfect crystal are abstractions created by a theory."
46. In this paper Paneth (1962) argues that the concept of element has a double meaning: [i] indestructable substance present in compounds and simple substances; [ii] simple substance: isolated basic substance uncombined with any other. Only the latter appears to our sense. Ruthenberg (1997) has pointed out the Kantian echo in Paneth's view: the simple substances are the *Phenomena* and the basic substances are the *Noumena*. See van der Vet (1979) on the Paneth-Fajans debate and chemical identity.
47. *The British Journal for the Philosophy of Science*, 14 (1963) 39–40, 316–317.
48. *Cf.* note 3.
49. Including Budreiko (1970), Garkovenko (1970), Ionidi (1958), Kedrov (1969), Laitko and Sprung (1970), Shakhparonov (1957, 1962), Simon et al. (1982), Zhadanov (1960).
50. Publications on the history and philosophy of chemistry appeared in the *Wissenschaftliche Zeitschrift* of the following universities and colleges: Humboldt-Universität Berlin, Ernst-Moritz-Arndt-Universität Greifswald, Friedrich-Schiller-Universität Jena, Pädagogische Hochschule "Wolfgang Ratke" Köthen, and Technischen Hochschule für Chemie "Carl Schorlemmer" Leuna-Merseburg, as well as in *Chemie in der Schule, Wissenschaft und Fortschritt, Rostocker Philosophische Manuskripte*, and others. The major contributors were [number in square brackets is number of (co-authored) publications listed in Schummer, 1996a]: H.-J. Bittrich [6], K.

Buttker [6], W. Fleischer [7], G. Fuchs [14], H. Laitko [9] U. Niedersen [14], R. Simon [23], W.-D. Sprung [19], I. Strube [7], F. Welsch [12].

51. The most influential writers in the USSR who published on the philosophy of chemistry were the philosophers of science Kedrov and Kuznetsov and the chemist Zhdanov. Kedrov published numerous books and articles in the philosophy of natural science. One of his earliest publications was a thorough-going article on Dalton which was translated into English (Kedrov, 1949). He was among the high-ranking Russian philosophers and gave one of the plenary lectures at the *XV World Congress on Philosophy* (1973, Varna, Bulgaria) with the title “Sur la synthèse des sciences”. Zhdanov published widely, in philosophy and chemical journals, on esthetics and in the *Pravda*. Kuznetsov published less, but often about the philosophy of chemistry. See Kedrov (1956, 1962, 1969), Kuznetsov (1963, 1964), Kuznetsov and Pechenkin (1972), Kuznetsov and Shamin (1993), Zhdanov (1950, 1960, 1963, 1965).
52. See Laitko (1996) for an insider’s account of the socio-historical factors that stimulated interest in the philosophy of chemistry in the DDR. He stresses that, compared with the interest in physics and biology, it wasn’t much and this seems true if one notes that, except for a few references to the history of chemistry, there is no philosophy of chemistry in Woodward and Cohen (1991), a volume containing a large number of papers from a German-American Summer Institute on science studies in the German Democratic Republic held in 1988.
53. Most of the contributions from Rumania were by E. Bellu, some of which were published in English or French (Bellu, 1973, 1979).
54. See Simon, Niedersen and Kertscher (1982).
55. The translation of the authorised Russian version of the law reads: “The law of the transition of quantitative changes into qualitative is a law according to which small, at first insignificant, quantitative changes, having reached a certain point, break (*narusajut*) the measure of the object and (thereby) evoke fundamental (*korennye*) qualitative changes. As a consequence, objects change, the old quality disappears and a new quality comes to be” (Bochénski, 1963: p. 17). See for the application of the law to chemistry, Kedrov (1962) and Kuznetsov (1963, 1964).
56. Engels (1940). This book consists of unfinished notes. Kedrov made a chrestomathic reconstruction (Engels, 1979) of how the book might have looked if Engels had finished it. He used extensive texts from Engels’ *Nachlass* and added parts from his other publications and from the Marx-Engels correspondence. He added brief connecting texts so that the whole was unified. According to Kedrov, Engels was strongly influenced in his view on the natural sciences by Carl Schorlemmer’s book on the history of organic chemistry. Schorlemmer was the first Marxist natural scientist and friend of Marx and Engels. This explains the significant presence of chemistry in the *Dialectics of Nature*, even more so in the extended ‘Kedrov’-version (Engels, 1979), than in the ‘Haldane’-version (Engels, 1940). This ‘historical’ aspect

of the connection between dialectical materialism and chemistry was stressed by Kedrov in numerous publications.

57. "Motion in the most general sense, conceived as the mode of existence, the inherent attribute of matter, comprehends all changes and processes occurring in the universe, from mere change of place right to thinking" (Engels, 1940: p. 35).
58. This is the principle of subordination and objectivity. See on these issues: Niedersen (1983), Poller (1966), Richter and Laitko (1962), Simon (1975).
59. For a detailed modern discussion of 'emergence', using primarily chemical examples (solubility, spatial structure of molecules, Pauli's exclusion principle) see Schröder (1998).
60. For example Laitko (1965), Laitko and Sprung (1970), Rosenthal (1982). Richter and Laitko (1962) argued that chemistry and molecular physics should be considered as two branches of macrophysics.
61. The material carriers of chemical change are atoms, molecules, radicals and ions (both of atoms and atom groups).
62. Isomers are compounds composed of the same elements in the same proportions, but different in properties because of differences in structure. Tautomers are isomers that change into one another rapidly and are usually in equilibirum with one another. The structure of isomers and tautomers is real in a way that the 'resonance' (Pauling) or 'mesomer' (Ingold) 'structure' of benzene and other (pseudo-)aromatic compounds is not.
63. Literally so, in that such statements occur in the preface of a book, or in the introduction or conclusion of an article. For example, in the preface of a book on the history of spectral analysis, Kedrov (1956) writes: "Am Beispiel der Entwicklungsgeschichte der Spektroanalyse wird versucht, mit Hilfe der marxistisch-dialektischer Logik allgemeine Wege zur Erkenntnis der Wahrheit durch den Menschen zu verfolgen".
64. "Beide [redox] Reaktionen müssen gleichzeitig ablaufen (Prinzip von der Einheit und vom 'Kampf' der Gegensätze!)" (scare quotes around 'Kampf' and exclamation mark in original).
65. 'Machistic': referring to Lenin's crititicism of Mach in his chief philosophical work *Materialism and Empirio-Criticism* (1st Russian edition, 1909).
66. For extensive quotations in English and a critique of the mathematical physics of Tatevskii and Shakhparanov (1949) see Wheland (1955: pp. 613–615), who concludes: "these authors have been misled by the carelessly worded expositions of the theory, which give an erroneous impression of its physical meaning, and which are unfortunately all too common". But note that Wheland found the criticism serious enough to warrant rebuttal.
67. Aromatic character is defined as possessing the physical properties of delocalized electrons, typically associated with bezenoid aromatics. If aromaticity is held to be a purely electronic property (i.e. of cyclic electronic delocalisation) aromaticity may also occur in cyclic molecules containing nitrogen, boron, or even sulphur or phosphorus atoms.

68. See for a detailed, though rambling, description of the following events (Graham, 1966: ch. VII) and also Vermeeren (1986) and Stork (1963).
69. Structure theory in the sense of van ‘t Hoff studies the geometry of the fixed positions of atoms in a molecule without considering the nature of the binding forces. The idea of structure as a static architectonics of atoms, and of bonds between them as the defining structure, was slowly undermined during the development of the theory of resonance structures between 1872 (Kekulé) and 1931 (Pauling). In a benzene molecule it is not possible to specify exactly where there are single and double bonds. The ‘real’ microsituation is a kind of mixture of a number of (logically) possible fixed arrangements of nuclei (of atoms) and electrons. At different stages the structure of the benzene molecule was represented as ‘intermediate’ between two, three, and five structures. There is no end to the extent of this kind of hybridity: to explain the reactions of anthracene over four hundred different diagrams have been utilised.
70. Pauling introduced the term ‘resonance’ and his theory was extended and completed by Wheland who stressed that (1955: p. 612) “the individual structures which contribute to the state of a resonance hybrid are merely intellectual constructions, and hence . . . they do not correspond to any actual molecules.” Such quotations were reiterated over and over again in the discussion in Moscow.
71. The general thrust of my account on the resonance issue is quite different from Laitko (1996). Though it would go too far to discuss the disagreement in detail, let me just mention two points. Laitko was himself an important contributor to the discussions in the DDR (Laitko, 1965, 1967; Laitko and Sprung, 1970; and many more; *cf.* Schummer, 1996a) and seems oversensitive to what one might call the Lysenko fallacy. Secondly, and possibly related to the first point, he seems to be too sensitive to any suggestion that the nature of chemical bonds cannot be explained exclusively by quantum mechanics, a sensitivity that was common in the DDR when such statements appeared in Russian publications (*cf.* Heber, 1964; Laitko, 1965: 334n16). Laitko (1965: 334n14) writes “Leider wird von einigen marxistischen Autoren bis in die jüngste Zeit die Meinung vertreten, die Mesomerie- und Resonanzvorstellungen selbst (nicht nur bestimmte Arten ihrer philosophischen Interpretation) seien ihrer Grundlage nach idealistisch [referring to Shakhparonov, 1962: pp. 100–102] . . . Die marxistische Philosophie sollte die progressive Tendenz der Durchdringung der Chemie mit quantenmechanischen Anschauungen und Verfahren mit allen Mitteln fördern.” This is a statement sounding quite different from the views expressed in Laitko (1967) and discussed in the main text below.
72. The conferences took place February 2–7, 1950 and June 11–14, 1951. Kursanov et al. (1951) is the report of the first conference. This report stresses the importance of Butlerov and the incompatability of the ‘idealistic’ resonance theory with Butlerov’s concept of structure, but it rejected Chelintsev’s positive proposals for an alternative: “A number of Soviet chem-

ists have repeatedly called G.V. Chelintsev's attention to these and many other unavoidable contradictions between the basic facts of physics and chemistry on the one hand and his [Chelinstev's] postulates with their consequences on the other. It is significant that even the author himself does not apply his 'new structural theory' in his writings." The second conference confirmed the decisions of the first conference, rejected Chelintsev's views even more explicitly, argued that the theory of resonance leads to agnosticism and replaced it by a theory of mutual influences (which is more akin to what had become known as the 'molecular orbit' method). The final report criticised Soviet philosophers, chemists, and physicist, each for slightly different reasons, but basically for not noting this infiltration of idealistic tendencies. Of the second report only a stenographed version was published and I've drawn on Graham's (1971: pp. 307–312) summary of its major parts. Probably it still formed the basis of a 1954 report of the Academy of Science that was also published in German (AN SSSR, 1954).

73. Chelintsev made another attempt when an edited collection of Butlerov's works appeared in 1951 (Graham, 1971: p. 312), but this had no impact.
74. The last 'official' commitment to a 'purely Butlerovean' theory of structure for organic chemistry (incorporating new developments in quantum mechanics) appeared in a book published by a committee of the department of chemical science of the Academy of Sciences of the USSR (AN SSSR, 1954).
75. See Bykov (1962) and Rocke (1981). According to Rocke (1981: p. 51): "Remarkably, the principal developers of those ideas [including Butlerov] had reached a satisfactory settlement by 1868, corresponding to what I call a 'weak Kekulé' position; it has been historians who have since muddled this interpretation." For a non-biased view on the Butlerov-Kekulé controversy from the Russian and the German side respectively, see Kuznetsov and Shamin (1993) and Stork (1963).
76. This criticism of resonance theory was most fully presented in a book by Shakhparanov (1957) – co-author of the 1949 paper in *Voprosi Filosofii* that spawned the philosophical debate – and still present in Zhdanov (1960), but fizzled out (see for example Budreiko, 1970), partly because interests in the philosophy of chemistry became more determined by issues surrounding the influential work of Kedrov (1969). The translation of Shakhparanov's short book in German was not well received by philosophers of chemistry in the DDR, primarily because Shakhparanov's chemical expertise was unconvincing. Earlier criticisms were repeated: Shakhparanov confused the use of visual models with being committed to idealism. Resonance structures in fact illustrate the dialectical character of nature (a point already made in 1939 by Haldane, the translator of Engels' *Dialectics of Nature*). And it was stressed that even the 'ordinary' double and triple bonds as depicted in structural formulae of molecules are not always 'pointing to' identical material entities, illustrating Shakhparanov's lack of chemical expertise. In a review of Shakhparanov's book in *Voprosi Filosofii* the situation was well summed up by Abramova et al. (1963): "The resonance theory as a method for quantum

mechanical calculations of molecules has been surpassed by better methods and it is doubtful whether it is necessary to repeat again old and not very well supported criticisms of Machism and agnosticism at the defenders of resonance theory.... The relation of scientific abstraction to objective reality is not as simple as the critics of resonance theory have often tried to present it". See also Kuznetsov and Pechenkin (1972).

77. Stork (1963), in the DDR journal *Chemiker Zeitung/Chemische Apparatur* completely rejects the Russian accusation that the resonance theory developed by Pauling, Wheland, and Ingold fails both empirically and philosophically (because of 'subjective idealism, mechanism, and agnosticism' – in the sense of Lenin). He explicitly criticises 'the Russians' for not mentioning important western authors like Ingold and at the same time placing much weight on '(older) Russian chemists', giving the incorrect impression that the state of the art in structural chemistry is mainly due to Russian chemists, whereas western chemists have produced little else but a false resonance theory (Stork, 1963: p. 616).
78. For example, Laitko (1967) starts his overview of philosophical questions concerning chemistry with a reference to Pauling: "Important chemists like Linus Pauling have become conscious of their humanistic responsibility and raise their voice against the misuse of science for agressive, antihuman purposes. In the socialist world stability and military security contributes considerably to increasing welfare and better public health".
79. See, amongst others, Haberditzl and Laitko (1967), Kitajgorodskij (1966), Poller (1966), Niedersen (1983), Fuchs (1964, 1965).
80. *Cf.* Bernal (1954: p. 796): "Physics is a tool to the chemist just as chemistry is a field of intellectual exercise to the physicist".
81. Consider Poller (1966): "Dem Verhältnis von Quantenmechanik und Chemie wird man jedoch weder durch die These von der Absorption der Chemie durch die Quantenmechanik noch durch eine metaphysische Trennung und eklektische Nebeneinanderstellung beider gerecht [tun]. Vielmehr muß dieses Verhältnis im dialektische Sinne als eine Einheit beider Seiten, die ihren Gegensatz nicht ausschließt, erfaßt werden. Auch daraus folgt, daß Quantenmechanik und Chemie nicht identisch sein können, denn 'Bewegung ist nicht bloß Ortsveränderung', sondern 'sie ist auf den übermechanischen Gebieten auch Qualitätsänderung' [quotations from Marx/Engels, *Werke*, Bd. 20, p. 517]".
82. *Cf.* Primas (1983, 1991).
83. R. Vihalemm from Estonia, referred to above (Vihalemm, 1974) presented papers at the 10th International Congress of Logic, Methodology and Philosophy of Science held in Florence (1995) and at a symposium on the philosophy of chemistry in Ilkley, U.K. (1997); Laitko and Niedersen published extensively in the DDR period and also, amongst others Laitko (1996) and Niedersen (1994). See also references for Kuznetsov in note 51.
84. Similarly, in the DDR much work was done on German 'philosopher-chemists' such as Mittasch and Ostwald, which found no hearing elsewhere.

85. Other early examples of such studies include Gay (1976, 1978) on the theory of chemical radicals and the asymmetric carbon atom and Frické (1976) on Dalton versus Avogrado; Bantz (1980) uses theories of chemical bonding (Heitler-London, Lewis) as a case study for the structure of discovery. Recent examples of detailed case studies include Zandvoort (1985) on nuclear magnetic resonance, and Zandvoort (1988) on polymer chemistry as a testing ground for Lakatos' notion of research programmes. Diamond (1988) uses the polywater episode to test the thesis that younger scientists are the first to shift (result negative). Rothbart (1993) discusses intertheoretic analogies during the 19th century unification of organic and inorganic chemistries (*cf.* Brooke, 1971). Thagard (1990) uses the chemical revolution as model for his computational theory of conceptual change. McEvoy (1989) writes about it in the tradition of Foucault. Francoeur (1997) is a case study in the sociology of science concerning molecular modelling as a constitutive element of the practice of chemistry. Finally, in a series of short papers Akeroyd (1986, 1988, 1990a, 1993, 1996, 1997) has used a range of examples from the history of chemistry to 'test' various models of the growth of science, in particular those of Popper, Lakatos, and Laudan. Akeroyd (1990) uses a chemical example to propose, by analogy, a new model of scientific development.
86. See, amongst others, Toulmin (1957), Putnam (1975), Kitcher (1978), Laudan (1984: pp. 68–102), Nola (1980), Shapere (1984: pp. 325–333), Donovan (1988), Zucker (1988), Sankey (1991), McAllister (1993), Shelton (1995), Allchin (1997).
87. See Ramsey (1994) on the notion of 'ideal type' (in the sense of Weber) using ideal reaction types of metal alloys as an example and Rothbart (1994), Rothbart and Slayden (1994) and Rothbart and Scherer (1997) on spectrometers.
88. Few practicing chemists will be surprised to hear that "the epistemological instability of chemical kinetic data was due to a number of factors including the resolving power of the instruments, the recognized lack of clear theories about chemical processes, and the recognized lack of experimental data on many chemical reactions" (Ramsey, 1992).
89. See for examples, references and discussion van Brakel (1996).
90. Reichenbach (1978 [1929]: p. 129), Dirac (1929), Heisenberg (1959: p. 89), Jordan (1957 [1947]: p. 19). Many chemists defend this picture as well; see for example Bader et al. (1994) and for discussion van Brakel (1999a).
91. From a philosophy of science perspective see Lévy (1979), Liegener (1994), Liegener and Del Re (1987, 1987a), Needham (1999), Scerri (1991, 1991a, 1993, 1997, 1997a, 1998), Scerri and McIntyre (1997), van Brakel (1997, 1999a), and supported from within quantum chemistry: Amann (1990), Claverie and Diner (1980), Primas (1983, 1985, 1991), Paolini (1981), Woolley (1991).
92. See Scerri (1997) for a critique of Hettema and Kuipers' (1988) claim that they have successfully axiomatised the periodic table.
93. See Thagard (1989, 1990); various contributions in Giere (1992).

94. It has been argued that Mendeleev's 'dramatic' predictions of new elements may have contributed little to the acceptance of his periodic system. For example, the citation which accompanies his being awarded the Davy Medal by the Royal Society of London makes no mention of these predictions (Scerri, 1997). However, in his Faraday lecture in 1889, Mendeleev said "When, in 1871, I described to the Russian Chemical Society the properties, clearly defined by the periodic law, which such elements ought to possess, I never hoped that I should live to mention their discovery to the Chemical Society of Great Britain as a confirmation of the exactitude and the generality of the periodic law" and in a note he adds: "I foresee some more new elements, but not with the same certitude as before. I shall give one example, and yet I do not see it quite distinctly".
95. See on water as the prototypical example of a natural kind Mellor (1977), Putnam (1990), van Brakel (1986, 1990); the same applies to the related philosophical and linguistic discussion on the nature of mass terms: Needham (1993), Psarros (1996).
96. 'Manifest' versus 'scientific' imagery stems from Sellars (1963). The former is the daily practice or common-sense-life-form and refers to things like water, milk-lapping-cats, injustice-angry-people, as well as sophisticated interpretations of 'people-in-the-world'. The scientific image is concerned with things like neurons, DNA, quarks, and the Schrödinger equation, again including sophisticated reflection and a promise of more to come.
97. *Cf.* Johnston (1997) who uses water and diamond/soot to argue that what some call the hard part of the mind-body problem is perfectly general and has nothing to do with special features of mind and body. A somewhat different example is Searle (1983) who maintains that mental states are realized in and caused by the brain in much the same was as the liquid character of water is realized in and caused by the movement of individual ('non-wet') molecules.
98. See Le Poidevin (1994) and Nerlich (1995). The antimony is that one hand is a reflection of the other whereas no rigid motion in infinite Euclidean space can map the one embedding into the other. *Cf.* Van Cleve and Fredrick (1991).
99. Schummer (1996) argues that after Thales considered everything to be water, there was a subsequent *Entstoffichung* of philosophy (giving utter priority to form over substance or 'stuff'), of the world (mechanical world picture), of knowledge (substance reduced to secondary properties or to Kant's *Ding-an-sich*), of language (mass terms reduced to form terms as in Quine's reduction of material objects to quadruples of numbers) and of science.
100. Seen as a network, chemical space consists of the pure substances at the nodes; the relationships between the nodes are chemical reactions correlated to experimental practice. Chemical space (not to be confused with the 'chemistry of space', *cf.*, note 98) contains all possible substances. Its relational structure is described in terms of the operational definitions of 'element', the notion of chemical mass equivalent, and chemical reactivity (Schummer, 1996: pp. 182–223).

101. There is no *a priori* reason why the number of elements is smaller than the number of compounds – it cannot be excluded that infinitely many elements do not combine to compounds.
102. The *lebensweltliche Basis*, which may be connected to *Lebenswelt* in the sense of Husserl, *form of life* in the sense of Wittgenstein or even *Dasein* in the sense of Heidegger (van Brakel, 1998).
103. See Gutman and Hanekamp (1996), Janich (1992, 1994a), Psarros (1995, 1995a).
104. Talk of electron orbitals or shells may sound physical, but reference to them is not sanctioned by our present understanding of quantum mechanics; at that level they are ontologically redundant. To assume that appeal to electronic orbitals is a reason for basing the presentation of chemistry on quantum mechanics has been called the 'orbital fallacy' (Scerri, 1991; *cf.* his 1997a).
105. But see section 3 on chemism, section 4 on chemical movement and Schummer (1996: pp. 229–296, 1997b, 1997c).
106. Potential applications of dendrimers include: synthetic models for enzymes and globular proteins, catalysts and template reagents, biosensors, drug carriers and transporters, unimolecular micelles and reverse micelles, synthetic membranes, molecular electronic devices, and photographic imagery.
107. Schummer (1997c) refers to colloid and interface chemistry as solution theory and theory of phase equilibria. Note that chemical physics is not the same as physical chemistry. See for a case study on solid state physics and solid state (physical) chemistry Hofmann (1990).
108. Examples of chemical operations are synthesis, oxidation, polymerisation. Physical operations like distillation, extraction, crystallising, melting can be used to divide mixed and pure materials. Mechanical operations such as filtration, centrifugation, grinding can be used to separate heterogeneous and homogeneous substances. An industrial chemical process as well as a synthesis of chemical products on laboratory scale consists of a sequence of such 'unit operations'. Chemical operations are always followed by physical and/or mechanical operations to purify and concentrate the product ('downstream processing'). Also note that for a chemical reaction to take place there has to be energy transfer and a mechanical pathway.
109. Gibbs' paradox says that the entropy of mixing two substances (no matter how 'similar' they are) is $2R\ln 2$ (R is the gas constant), but collapses to 0 when the substances are identical. This finds its base in the fact that mixtures can be separated, which makes no sense for a pure substance. Denbigh and Redhead (1989) dissolve Gibbs' paradox by taking entropy to be observable (though dispositional). For a recent discussion of the debate see Mosini (1995).
110. Aristotle (*On Coming-to-be and Passing-away*, I. 10) already noted that mixing was a problem for any kind of atomism. In physical chemistry one talks about solutions, mixtures, suspensions, colloids, alloys, etc. which are all defined as something being *distributed uniformly* in a *continuous medium*,

but at the atomic level this is a *contradictio in terminis*. Duhem later used a similar argument when opposing atomistic interpretations of (chemical) substances. Cf. Needham (1996a).

111. According to Gibbs's phase rule a system of *c* components in *p* phases has $c - p + 2$ degrees of freedom. It is a law completely free from all hypothetical assumptions as to the molecular condition of the substances involved.

112. Categories that cause problems for this simple definition of chemical substance include (Timmermans, 1963): [i] racemates or enantiomers (species containing equal numbers of molecules of each of two optical optimers); [ii] azeotropic mixtures, dissociative compounds in equilibrium; [iii] certain types of mixed crystals (polymorphic compounds); [iv] systems that are not in 'pure' thermodynamic equilibrium (supercooled water, Brownian motion, systems in transformation); [v] isotopes.

113. Maccoll (1964), Schummer (1996: pp. 252–289).

114. The chemical sign system, developed since the 1860s, is not a pictorial or iconic sytem, i.e. about molecular formulae or drawings or other 'pictorial' models, but about material properties, in particular dynamic properties like reactivities and reaction mechanisms. Hence, there is a close connection between the network of chemical space and the sign system used to name the nodes. The complex system of naming used in chemistry is 'exact', but not mathematical. See for recent studies on the language of chemistry: Bensaude and Abbri (1995), Hoffmann and Laszlo (1991), Laszlo (1993), Schummer (1996c, 1997: section 7), contributions in Janich and Psarros (1996).

115. An example of the significance of valence as an 'archestructural' concept is the inequality of $[Cr(H_2O)_6]Cl_3$ and $[Cr(H_2O)_4Cl_2]Cl.2H_2O$. The idea of valency as a number is in accord with the conception of chemistry in which structure is taken to be fundamental. The idea of valency as the combining power of atoms is a mental construction (and as such perfectly valid). That is, either one puts structure first and makes atoms and bonds subsidiary concepts and valency only a number, or one derives structure from the 'combining power' of atoms with valency bonds. Mosini (1996a) argues that the concept of valence cannot be reduced to physics – though this would not challenge the unity of science (because it supervenes on physical properties).

116. Ostwald was the first to observe oscillating behaviour in the oxidation reaction of metals in acids. The phenomenon was first studied systematically by the Russian biochemist Belusov in 1951, but his paper was rejected by different chemical journals, because the accepted thermodynamic theory did not allow for systems oscillating between states of positive and negative entropy. It was not until Priogine opened the debate on chemical reactions out of thermodynamic equilibrium that the issue came to have some respectability.

117. Of course some of these examples pose problems for any account of pure substance. Strictly speaking ruby and tourmaline are solid solutions, but this seems to stretch the notion of pure out of its common sense meaning. An even more extreme case are synthetic polymers, like nylon or polystyrene. In

practice, nylon is one compound, although strictly speaking every molecule with a different chain length is a different pure compound.

118. It is true that X-ray techniques give direct information about molecular structure, but chemically this is not very meaningful: at best it provides some ‘primary qualities’, which are of little value to the ‘interactive’ chemist.
119. Another issue that can be raised here is whether it makes sense to distinguish metaphysical (pre-Dalton), physical, *and* chemical atoms (Benrath, 1953; Gavroglu and Simoes, 1994) and what it means to refer to the shape of a molecule (Amann, 1992, 1993, 1996; Woolley, 1978, 1986; Ramsey, 1997). Gascoigne (1961) has argued that molecules, atoms, electrons, and bonds score very differently when the question of realism is raised. Molecules (and crystals) refer to concrete things which can exist by themselves. Atoms, ions, and electrons are essentially parts of things and normally, at least not in ordinary terrestrial contexts, do not exist by themselves. Bonds refer to abstract geometrical entities. Molecules and crystals are not, in fact, built or formed from atoms; chemical substances are not made from atoms, but from other chemical substances. But Gasgoigne’s molecules that ‘can exist by themselves’ would seem to be a rare phenomenon.
120. See contributions of Beatty, Brandon, and Sober in *Philosophy of Science*, 64 (Proceedings): S432–S467.
121. See, for example, Rosenberg (1994) and McIntyre’s (1997) discussion of Gould’s views.
122. See for recent discussions of chemical laws Psarros (1994); and for related issues Bhushan and Rosenfeld (1995), Röhler (1962), Trindle (1984) and Zhdanov (1963) on models, Hofmann (1990) and Hoffmann et al. (1996) on models and Ockham’s razor in chemistry and Mainzer (1997) on symmetry and complexity.
123. *Cf.* the earlier observations of Caldin (1959) and MacDonald (1960) in section 3.
124. Alternatively, the selection rules are laws. Given millions of colliding molecules selection rules determine (within limits) which complexes survive.
125. For some arguments and references to other literature see van Brakel (1999).
126. The form that was introduced in the philosophy of mind by Davidson (1970); *cf.* van Brakel (1999).

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