

Provisional Report on Discussions on Group 3 of The Periodic Table

by Eric Scerri

The following article is intended as a brief progress report from the group that has been tasked with making recommendations to IUPAC about the constitution of group 3 of the periodic table (<https://iupac.org/project/2015-039-2-200>). It is also intended as a call for feedback or suggestions from members of IUPAC and other readers.

In the course of many discussions held by the task group we have concluded that there is no objective means to adjudicate between group 3 consisting of Sc, Y, La and Ac or as Sc, Y, Lu and Lr. This situation makes it more important that IUPAC should make a ruling on the question which in the final analysis is one of convention rather than one that can be decided on objective scientific grounds. What has also become apparent is that this question cannot be treated independently of that of the form of the periodic table as a whole.

As Jeffrey Leigh reminded readers of this magazine not long ago, IUPAC does not officially support any particular form of the periodic table even though the organization frequently publishes a period table with the label of "IUPAC periodic table" [1].

Attempts to resolve the group 3 conundrum have focused on chemical and physical properties and also on microscopic properties such as the electronic configurations of the atoms concerned [2]. However, none of these criteria provide a clear-cut resolution of the question. Moreover, it becomes increasingly clear that there may not be any such thing as one optimal table in a purely objective sense.

There is a well-developed literature in the philosophy of science that concerns itself with classification and with the question of natural kinds, that is to say sets of objects which are related to each other through what might be said to be purely objective properties. For example, until recently biological species were believed to be natural kinds in biology. For an animal to be classified as a tiger, for example, would require the specification of the genetic characteristics of this species.

Natural kinds are distinguished from so-called artificial kinds for which classification depends rather on human choices and not on an independently existing reality. The typical example of an artificial system of classification is the classification of library books.

No one library system such as that of the Library of Congress can be said to be more correct than its competitors. The way in which these library systems classify books involves non-objective criteria as to how to demarcate books on chemistry, for example, from those on biology.

In the 1970s and 80s a theory was developed by philosophers Kripke and Putnam who sought to define natural kinds through their essences or their objective properties [3]. A favorite example of a natural kind in this literature has been that of a chemical element, which according to Kripke and Putnam can be specified by stipulating its atomic number. Needless to say, Kripke and Putnam were not the first to propose such an identification. That distinction belongs to Van den Broek and Moseley [4]. What Kripke and Putnam did was to fully adopt the scientific definition of element-hood in order to identify elements as natural kinds.

For an atom of an element to be gold for example requires that the atom should have an atomic number of 79. In addition, if an atom is found to have atomic number 79 this uniquely identifies it as being an atom of gold. Said in the jargon of philosophers, the possession of an atomic number of 79 is both necessary and sufficient for the identification of a particular atom as being a gold atom.

The Kripke-Putnam approach to natural kinds has come under various forms of criticism in the years since it was first proposed. In the case of species, like tigers, it has been pointed out that evolution spoils the picture, since the very essence of what it is to be a tiger is bound to change as time evolves. However, this objection could not be raised as far as elements are concerned, since broadly speaking atoms of any particular element do not evolve into other atoms over time, apart from those that decay radioactively.

A more general objection to the Kripke-Putnam approach to thinking of natural kinds has been the realization that, whatever kinds are being considered, there is always a certain degree of interest dependence that enters the stipulation of sets of entities be they tigers, galaxies or elements [5]. The new approach recognizes that epistemological considerations, having to do with our knowledge of the world, should also be taken into account when discussing the classification of scientific entities.

If we are to believe what the experts on the philosophy of classification and natural kinds have to tell us we should renounce the notion that we will ever arrive at a truly optimal periodic table, since any system of classification must inevitably remain interest dependent. Of course this state of affairs should not

Project Place

negate the attempts to resolve such questions as the membership of group 3 of the periodic table but it should remind us of the fact that any resolution must concede a certain degree of conventionality, or choice, on the part of the scientific community. We should accept that a degree of convention must be utilized in selecting a periodic table that can be presented as the best compromise table that combines objective factors as well as interest dependence.

A very brief history of forms of the periodic table

As is well-known, the earliest periodic tables contained eight columns and were based on the assumption that all periods were of equal lengths. Such tables, which have survived to this day in some countries, have the advantage of simplicity of form and display the fact that most group numbers correspond to the maximum oxidation state of the element in question. However, Mendeleev and other early discoverers of the periodic system began to use medium-long form tables consisting of 18 groups. This tendency became the norm as a result of tables published by Deming in 1923 and due to the increasing use of quantum mechanics to explain the form of the periodic table. The 18-column table corresponds to two elements in the s-block, ten in the d-block and six in the p-block to reflect precisely the maximum number of electrons that can be accommodated into a set of s, d and p orbitals respectively, starting with period four. Meanwhile, the inner transition elements of f-block are generally represented as a disconnected footnote consisting of either 14 or 15 elements, depending on which particular table one consults.

Herein lies the variation which is closely connected with the question of the constitution of group 3 of the periodic table. There are a total of 3 possible forms of the 18-column table, each of which corresponds to a particular group 3 assignment. In the tables shown in figures 1 to 3, group 3 is shown as containing either Sc, Y, La and Ac or Sc, Y, Lu and Lr or just Sc and Y.

While the first two options seem to be equally plausible on an 18-column representation, there is one difference that this

Group #:

		1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
H																			He
Li	Be													B	C	N	O	F	Ne
Na	Mg													Al	Si	P	S	Cl	Ar
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr		
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe		
Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn		
Fr	Ra	Ac	Rf	Db	Sg	Bh	Hs	Mt	Ds	Rg	Cn	Nh	Fl	Mc	Lv	Ts	Og		

Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu
Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr

		1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
H																			He
Li	Be													B	C	N	O	F	Ne
Na	Mg													Al	Si	P	S	Cl	Ar
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr		
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe		
Cs	Ba	Lu	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn		
Fr	Ra	Lr	Rf	Db	Sg	Bh	Hs	Mt	Ds	Rg	Cn	Nh	Fl	Mc	Lv	Ts	Og		

La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb
Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No

1	2											13	14	15	16	17	18		
H																		He	
3	4													5	6	7	8	9	10
Li	Be													B	C	N	O	F	Ne
11	12													13	14	15	16	17	18
Na	Mg													Al	Si	P	S	Cl	Ar
19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36		
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr		
37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54		
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe		
55	56		72	73	74	75	76	77	78	79	80	81	82	83	84	85	86		
Cs	Ba		Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn		
87	88		104	105	106	107	108	109	110	111	112	113	114	115	116	117	118		
Fr	Ra		Rf	Db	Sg	Bh	Hs	Mt	Ds	Rg	Cn	Nh	Fl	Mc	Lv	Ts	Og		

57	58	59	60	61	62	63	64	65	66	67	68	69	70	71
La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu
89	90	91	92	93	94	95	96	97	98	99	100	101	102	103
Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr

Figure 1-3: Variations of the 18-column table with group 3 shown as containing either Sc, Y, La and Ac (top) or Sc, Y, Lu and Lr (middle) or just Sc and Y (bottom).

The figure shows two periodic tables side-by-side, both with 32 columns. The top table (Figure 4-5 top) shows group 3 elements as Sc (21), Y (39), Lu (71), and Lr (103). The d-block is a continuous sequence of 10 elements from Ti (22) to Zn (30). The bottom table (Figure 4-5 bottom) shows group 3 elements as Sc (21), Y (39), La (57), and Ac (89). The d-block is split into two blocks: one with 9 elements from Ti (22) to Cu (29), and another with 11 elements from Zr (40) to Hg (80).

Figure 4-5: 32-column table with group 3 shown as Sc, Y, Lu, Lr. (top) 32-column table with group 3 shown as Sc, Y, La, Ac and split d-block.

representation masks somewhat. This difference is far more apparent if the periodic table is displayed in an even more expanded 32-column format which incorporates the f-block into the main body of the table.

If Lu and Lr appear in group 3, as they do in figure 4, the d-block consists of a continuous sequence of 10 elements. On the other hand, if group 3 consists of Sc, Y, La and Ac, as it does in figure 1, the d-block rows now appear to be split in a very uneven fashion (fig 5). For example, in period 6 we find La (considered as a d-block element) followed by a sequence of 14 f-block elements from Ce to Lu followed by a sequence of nine d-block elements from Hf to Hg.

The periodic table that is sometimes labeled as “IUPAC periodic table” as shown in figure 3 avoids assigning the 3rd and 4th members of group 3 altogether, by simply leaving empty spaces below Sc and Y. As a result, the f-block then appears to contain two rows of 15 elements, and thereby violates the simple one-to-one correspondence between orbital capacity as required by the elementary quantum mechanical account of the periodic table.

The only 18-column table that appears to avoid the drawback in the split of the d-block while also maintaining a 14-element-wide f-block is the one shown in figure 2. Needless to say, the assignment of elements to these blocks is approximate, just as the assignment of

electronic configurations to atoms also represents an approximation. Moreover, one may readily concede that an element such as thorium does not actually possess any f-orbital electrons and yet it is classified as being among the f-block elements in all five of the periodic table representations shown in figures 1 to 5.

A student looking at the table shown in figure 3 is bound to wonder whether there is some scientific reason for making the f-block have a width of 15 elements. Neither a student, nor his/her instructors, would probably realize that the table in question has been designed by practitioners of specialized branch of relativistic quantum mechanics concerned with the properties of super-heavy elements [6]. Such interest-dependence should not, in our view, dictate how the periodic table is presented to the general chemical and scientific community.

Perhaps a compromise could be reached on the table depicted as figure 2 since it achieves three *desiderata*. First, it displays all the elements in order of increasing atomic number. Secondly, it avoids splitting the d-block into two highly uneven portions, and thirdly, it depicts all the blocks of the periodic table in accordance with the underlying quantum mechanical account of the periodic table which calls for 2, 6, 10 and 14 orbitals to occur in the extra-nuclear electron-shells.

Historical developments have shown that quantum

mechanics provides an explanation for the periodic table even if it does not provide a full and exact reduction of the periodic table. It appears that some practitioners of relativistic quantum chemistry uphold the grouping together 15 rather than 14 elements in the f-block of the table. However, any such findings should not be imposed on the majority of users of the periodic table and should not, in our view, dictate how the periodic table is presented to the widest possible audience of chemists, chemical educators and chemistry students.

For more information and comments, contact Task Group Chair Eric Scerri <scerri@chem.ucla.edu> | <https://iupac.org/project/2015-039-2-200>

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Development of a Machine Accessible Kinetic Databank for Radical Polymerizations

Machine learning is a young discipline in the chemical sciences that has nonetheless led to significant changes in research approaches in a relatively short-time span. Any machine-assisted research approach requires training sets and machine-readable databases to retrieve information from. A standardization of notations allows for data exchange between computer systems and softwares. As an example, the recently introduced BigSMILES (simplified molecular-input line-entry system) notation (Lin *et al.* *ACS*

Cent. Sci. 2019, 5, 9, 1523-1531; <https://doi.org/10.1021/acscentsci.9b00476>) allows the exchange of structural data for polymer across computer systems.

The IUPAC working party on Modelling of Polymerization Kinetics and Processes has collated significant kinetic data on free radical polymerization in recent years, and published a series of benchmark papers on the topic. While generally available, still many researchers do not make full use of these data sets. A database will increase awareness and foster better use of the data. More importantly, a machine-readable database will allow for direct and automated exchange of data. For example, kinetic models can always retrieve the latest and most updated kinetic data for specific monomers. In machine-learning approaches, algorithms can make use the data for deep learning and interconnection with other data such as molecular characteristics, physical properties or further kinetic data. This can range from prediction of materials properties to automated process control in synthesis.

The kinetic database will consist of all IUPAC benchmarked kinetic data for free radical polymerization. A further selection of reliable kinetic data will be made to also include monomers that have not yet been critically assessed. For these monomers, the database can serve as a future starting point for data collection. While not part of this project, the same database could later be extended by other parameters, such as overall time conversion relations, molecular weights, and physical properties of the resulting polymers from polymerization. The database will be designed in a fashion to allow facile extension to either direction.

First versions of the database will be hosted via Monash University. Source codes will be published open access and long-term migration of the database to central servers is envisaged.

For more information and comments, contact Task Group Chair Tanja Junkers <Tanja.Junkers@monash.edu> | <https://iupac.org/project/2019-045-1-400>

Assessment of Absolute Isotope Ratios for the International Isotope Delta Measurement Standards

Currently, isotope delta measurements are reported relative to an international measurement standard that forms the zero-point of the scale and the base of the traceability chain.

The absolute isotope ratios of these measurement standards are the fundamental values which allow

Project Place

conversion of isotope delta values to other expressions of isotopic composition such as isotopic abundances, absolute isotope ratios or atomic weights that are often used in studies involving stable isotopes as tracers. At least some of the discrepancies between laboratories in these measurements is due to application of different values for the absolute isotope ratio of the zero-point materials. These isotope ratios are also the quantities which link the isotope delta scale to the international system of units.

The currently-recommended values of these absolute isotope ratios are derived from publications reporting measurement results, however in some instances there are multiple publications each reporting different values. Absolute values underpinning carbon or silicon isotope delta scales, for example, are not consistent and uniform recommendations are needed. Collating these measurement results and assessing them will allow new best-estimates of these absolute isotope ratios to be determined that reflect all previous measurements, rather than selecting a single publication as the source of the recommended value.

Considerations during such assessment include the nature of the calibration employed during measurement as well as the uncertainty budget. The new best estimates will be distributed in the form of an IUPAC Technical Report and will be available on the website of IUPAC Commission on Isotopic Abundances and Atomic Weights, CIAAW.org, in machine-readable form.

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Development of a Metadata Schema for Critically Evaluated Solubility Measurement Data

The IUPAC Solubility Data Series (SDS) is an important asset of IUPAC. Originally conceived as a series of printed volumes, the SDS transitioned to the Journal

of Chemical and Physical Reference data in 1998. Today, the publication of critically evaluated solubility data is more appropriately disseminated in digital form and this project is a critical step to enabling accurate exchange in the global digital arena. Given the work by NIST to digitize some the SDS volumes in the late 1990's (<https://srdata.nist.gov/solubility/>) and the more recent work by the task group chair, reimagine the NIST data as a modern RESTful website, [1] there is now significant interest in the digitization of the SDS to create a digital asset and leverage the significant amount of time and effort invested by the members of the IUPAC Subcommittee on Solubility and Equilibrium Data (SSED).

This project therefore will focus on the development of metadata schema for accurate capture and representation of solubility data reported in the SDS volumes, both in terms of the curated literature values (SDS compilations) and the subsequent critical evaluation of systems with sufficient reported values (SDS evaluations). Understanding the needs for the accurate reporting of critically evaluated data will inform the development of general guidance on reporting of experimental data.

The work of this task group will be disseminated in a technical report in *Pure and Applied Chemistry* and as a reference document for the two schemas to be used by the SSED. This work will flow into the work of the Interdivisional Subcommittee on Critically Evaluated Data (ISCED) and potentially other critical evaluation activities in IUPAC.

Reference

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For more information and comments, contact Task Group Chair Stuart Chalk <schalk@unf.edu> | <https://iupac.org/project/2020-018-1-024>