WHAT COMES AFTER STABLE OCTET? STABLE SUB-SHELL!

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Previous research has shown that students' existing conceptions are critical to subsequent learning because there is interaction between the new knowledge that the students encounter and their existing knowledge from previous lessons. Taber (1999a) found A-level students in the UK had difficulty in understanding the principles determining the magnitude of ionisation energy because of their pre-existing octet rule framework. In a related study, Tan et al. (2005) explored the conceptions of ionisation energy of A-level students in Singapore, and found that these students also applied the octet rule framework to decide if an isolated sodium ion would recombine with an electron to reform the sodium atom, and whether another electron could be removed from the sodium +1 (Na^+) ion. In addition, the study found that there appeared to be an offshoot of the octet rule framework, the 'stable fully-filled and half-filled sub-shell' thinking, which the students in Singapore used to explain the trend of ionisation energies across Period 3.

INTRODUCTION

Research has shown that the learner's existing knowledge has significant effects on new learning (Driver, 1995; Duit, 1995; Johnstone, 1999; Osborne & Wittrock, 1985; Pintrich, Marx, & Boyle, 1993). The learner's stored knowledge influences the selection of, and the attention given to, the various aspects of the learning task. The learner then generates links between the task and what he/she already knows, retrieves information from memory to make sense of the task, tests the validity of the task, and subsumes his/her constructions of the task into his/her depository of knowledge. If a person tries to learn something new and cannot find existing knowledge with which to link it, he/she may try to 'bend' the knowledge to fit somewhere (cf. Gilbert, Osborne, & Fensham, 1982), and this gives rise to erroneous ideas (Johnstone, 2000).

Osborne, Bell and Gilbert (1983) state that students often misinterpret, modify or reject scientific viewpoints based upon the way they really think about how and why things behave, so it is not surprising that research shows that students may persist almost totally with their existing views (Treagust, Duit, & Fraser, 1996). When the students' existing knowledge prevails, the science concepts are rejected or there may be misinterpretation of the science concepts to fit or even support their existing knowledge. If the science concepts are accepted, it may be that they are accepted as special cases, exceptions to the rule (Hashweh, 1986), or in isolation from the students' existing knowledge, only to be used in the science classroom (de Posada, 1997; Osborne & Wittrock, 1985) and regurgitated during examinations. Additional years of study can result in students acquiring more technical language but still leave the alternative conceptions unchanged (de Posada, 1997).

OCTET RULE FRAMEWORK

Taber (1997, 1998, 1999b) found that students commonly used an alternative conceptual framework derived from the octet rule to 'understand' bond formation and chemical reaction. The octet rule, a consequence of the effect of electrical interactions in the quantized atom, is a useful 'rule of thumb' (Taber, 2001) when students first learn about chemical bonding in O-level chemistry. It helps them to work out the electronic configuration of an ionic or a covalent compound, and the chemical formulae of the compounds. For example, they can work out that the sodium ion (Na^+) has an electronic configuration of 2.8 and the chloride ion (Cl^-) would have the configuration 2.8.8, and thus, sodium chloride would have the formula, NaCl. However, students tend to "over-generalise the rule from being a way of identifying likely stable species, to become a general purpose explanations for why reactions occur" (Taber, 2001, p. 146) – students who adopt the octet rule framework believe that "chemical reactions take place, and bonds form, to allow atoms to have full outer shells" (Taber, 1999b, p. 136). A consequence of the octet rule framework is that students see covalent bonding as simply the sharing of electrons, and ionic bonding as electron transfer, to achieve full outer shells, rather than electrostatic interactions between particles. Other examples of alternative conceptions of bonding arising from the octet rule framework (Taber 1998, Tan & Treagust, 1999) include:

- the number of ionic bonds formed is determine by the number electrons an atom gains or loses to achieve a full octet structure,
- ionic compounds contain ion-pair molecules,
- in ionic lattices, there are two types of interactions, ionic bonds with the ion-pair molecules, and forces between them,
- atoms are less stable than their ions.

For example, students may think that sodium only forms one ionic bond with chlorine since it donates one electron to chlorine to form the sodium ion and chloride ion. This can lead to the idea that sodium chloride exists as sodium ion-chloride ion pairs of molecules since each sodium ion can only form one bond with one chloride ion. Students who adopt the octet framework are able to make sense of secondary chemistry, "albeit to understand chemistry differently from the teacher" (Taber, 2001, p. 142). The octet rule framework is significant because it can block the learning of scientific explanations for bonding, and research suggest that alternative frameworks are resistant to changes and difficult to 'unlearn' (Driver & Easley, 1978; Duit & Treagust, 1995; Fetherstonhaugh & Treagust, 1992; Taber, 1998). It can also affect the future learning of other related chemistry concepts as students may look at the new learning material "through the lenses of their preinstructional conceptions" (Duit & Treagust, 1995, p. 47) and misinterpret the new concepts to fit or even support their existing octet rule framework.

STUDIES ON IONISATION ENERGY

In related studies, Taber (1999a, 2003) found that A-level students in England had difficulty in understanding the principles determining the magnitude of ionisation energy. Several alternative conceptions he determined from the results were:

- the sodium atom would be more stable if its 3s electron is removed,
- if 3s electron of sodium is removed, it will not return because the sodium ion achieves a stable electronic configuration,
- only one electron can be removed from sodium because of the stable configuration of the sodium ion,
- sodium 7- ion (Na^{7-}) is more stable than the sodium atom.

Taber believes that the four alternative conceptions arose because the students based their explanations on the octet rule framework. For example, the students learned that energy was required to remove an electron from an isolated sodium atom, so the atom should be considered as stable in comparison with the separated ion and electron. However, from their octet rule framework perspective, the sodium atom would not be considered as stable as it did not have a full outer shell. Similarly, the students believed that only one electron can be removed from the sodium atom since the full outer shell electron configuration of the Na^+ ion would be lost if more electrons were removed – this is despite having studied the trend of successive ionisation energies.

Tan, Goh, Chia and Taber (2005) carried out a study to determine if A-level (Grade 11 and 12) students in Singapore had similar alternative conceptions and explanatory principles of the factors influencing ionisation energy as their A-level counterparts in the United Kingdom, as well as to explore students' conceptions of the trend of ionisation energy across different elements in the Periodic Table. They developed a two-tier multiple-choice diagnostic instrument on ionisation energy, the Ionisation Energy Diagnostic Instrument (IEDI), using procedures defined by Treagust (1995). Examples of items in the IEDI are given in the Appendix. The IEDI was administered to 777 Grade 11 (17 years old) and 202 Grade 12 (18 years old) students from eight out of a total of 17 A-level institutions in Singapore, in June and July 2003 (see Tables 1 and 2). The schools were selected on the basis of the willingness of the teachers in the schools to participate in the study. The intention of the study was to determine the A-level students' performance on the IEDI as a group, so the sex of the students, the different sample sizes of the two year groups of students as well as the schools these two groups of students came from were not important variables. Thirty-two students were interviewed, either in pairs or in groups of four, using the IEDI as the protocol to determine if there was any ambiguity in the items and to further probe the thinking behind their answers. These students were chosen by their teachers. Each interview lasted between 40 minutes to an hour. Table 3 describes the composition of the various groups interviewed and the schools from which they came.

Table 1
Distribution of the A-level students over schools

School	Grade	Female	Male	Total
81	12	76	71	147
82	11	72	57	129
83	11	35	40	75
84	11	81	66	147
85	11	77	80	157
86	12	31	22	53
87	11	110	75	185
88	11	17	29	46
Total		499 (53.1%)	440 (46.9%)	939 (100%)

Note: 40 students did not state their gender

Table 2
Types of schools involved in the study

Type of school	School	Total number of students (%)
Top rung	81, 83, 86, 88	325 (33.2)
Middle rung	84, 85	319 (32.6)
Lower rung	82, 87	335 (34.2)

Table 3
Students interviewed using the IEDI as the interview protocol

School	Students	Number of students (%)
82 (lower rung)	(1,2), (3,4), (5,6), (7,8)	8 (25)
83 (top rung)	(9,10,11,12), (13,14,15,16)	8 (25)
84 (middle rung)	(25,26,27,28), (29,30,31,32)	8 (25)
85 (middle rung)	(17,18,19,20), (21,22,23,24)	8 (25)

Note: The numbers in a bracket in the 'Students' column denote the students in each interview group, for example, (1,2) denotes that Students 1 and 2, from School 82, were interviewed together.

Table 4 describes the percentage of the A-level students selecting each response combination for selected items in the IEDI. The results for an item will not add up to 100% if there were students who did not select a response to both parts of the item, selected an answer combination which was beyond the options given in the item, or selected more than one answer combination. Alternative conceptions are considered significant and common if they existed in at least 10% of the student sample (Peterson, 1986). Table 5 summarises the relevant significant common alternative conceptions of the A-level students.

Table 4
The percentage of the A-level students (n=979) selecting each response combination for selected items in the IEDI

Item	Content option	Reason option					Total
		(1)	(2)	(3)	(4)	(5)	
4	A	*15.6*	*18.0*	**48.1***	3.6	-	85.3
	B	.1	.3	.7	1.6	-	2.7
	C	5.3	.3	.1	0	-	5.7
	D	.1	.1	0	0	-	0.2
5	A	1.2	2.2	2.9	*22.0*	4.2	32.5
	B	13.1	9.1	29.2*	9.3	2.2	62.9
	C	.1	.1	.2	0	0	0.4
6	A	6.2	*48.1*	2.9	**5.4***	5.5	68.1
	B	.9	7.2	8.5	1.8	8.3	26.7
	C	.1	.1	.1	.1	.1	0.5
8	A	3.9	4.5	7.6	5.8	-	21.8
	B	5.5	24.9	4.6	34.0*	-	69.0
	C	.3	.1	.1	.2	-	0.7
9	A	2.7	3.9	*19.6*	7.4	**32.1***	65.7
	B	6.8	1.6	3.5	10.4	4.3	26.6
	C	.2	.1	.3	.4	0	1.0

Note: Figure in bold and with an asterisk indicates the correct answer.
Figure in italics indicate a major alternative conception (>10%)

Table 5
Relevant alternative conceptions determined from the administration of the IEDI

Alternative conception	Choice combination	Percentage of students with the alternative conception
Octet rule framework		
The second ionisation energy of sodium is higher than its first because the stable octet would be disrupted.	Q4 (A1)	16
Stable fully-filled or half-filled sub-shells		
The first ionisation energy of sodium is less than that of magnesium because magnesium has a fully-filled 3s sub-shell.	Q5 (B1)	13
The first ionisation energy of silicon is less than that of phosphorus because the 3p sub-shell of phosphorus is half-filled.	Q8 (B2)	25
The first ionisation energy of phosphorus is greater than that of sulphur because the 3p sub-shell of phosphorus is half-filled, hence it is stable.	Q9 (A3)	20

Tan et al. (2005) found that the Singapore students also used the octet rule framework to justify why the second ionisation energy of sodium was greater than its first ionisation energy (Item 4, A1, 16%). This differs from the curriculum model, which states that the removal of the second electron from sodium involves removing an electron from an inner (second) shell. The electrons in the second shell are more strongly attracted to the nucleus as they are closer to the nucleus and experience shielding/screening from only two electrons in the first shell, so the second ionisation energy of sodium is higher than its first ionisation energy. When asked during interviews why an octet configuration gave the sodium ion "stability", several students either stated that they were taught so, or that it was because the outermost shell of the sodium ion was filled so it could not gain or lose any electrons.

P6: Because it is already stable…I mean you know…the outermost shell…it's like eight electrons…so…if it attracts another electron…then it will become unstable…so…it's more likely to stay stable than form (the atom).

I: Why do you say that the octet structure gives it stability?

P6: That's what we are taught right…octet structure is supposed to be stable.

I represents the interviewer; P6 represents student 6; … represents pauses

P15: I put B4 (item 3)…because with sodium (ion) right … you have the…octet configuration so it will be more stable…whereas sodium as an atom…only has…is not fully filled in the outermost shell…so it is not so stable.

I: Ok…can you explain why the fully filled outermost shell is stable?

P15: Because the teacher taught so.

I: Why will the ion be more stable?

P14: Because octet…stable octet configuration.

I: Why is an octet configuration stable?

P14: Because it has eight electrons in the outermost shell already…so no electrons will go in no electrons will go out…then it is very stable…to achieve a stable configuration…stable octet structure you need to have all your…shells filled… outermost shell filled.

STABLE FULLY-FILLED OR HALF-FILLED SUB-SHELLS

In item 5, 13% stated that magnesium had a higher first ionisation energy than sodium because magnesium had a fully-filled 3s orbital/sub-shell which gave it stability (B1), while in items 8 and 9, 25% (B2) and 20% (A3), respectively, indicated that phosphorus had a higher first ionisation energy compared to silicon and sulphur because the 3p sub-shell of phosphorus was half-filled, hence it was stable. The excerpt of an interview below illustrates this 'stable fully-filled or half-filled sub-shell' thinking:

P14: I put B1 (item 5)…because the magnesium…the last orbital…the 3s orbital is fully filled so it will tend to be more stable…and when an orbital is either half or fully filled it will be more stable…so since sodium has only one electron in the…so when fully filled will be more stable…sodium has only one electron in the s orbital…so to be more stable it will tend…it will be easier to remove…that electron and so the ionisation energy will be lower than that of magnesium.

I: So you are saying that the first ionisation energy of magnesium is higher?

P14: It is more stable.

I: Because of the…

P14: It's fully filled orbital.

I: So why is this fully filled orbital stable…the $3s^2$?

P14: Just like in the shell…I mean…to achieve the octet structure…must have eight electrons…so when you have eight electrons in the outer shell…will be more stable… so when the orbital is fully filled then… more stable… because there's…like…more stable.

I: So stability comes with filled orbitals?

P14: Fully filled and half filled…but fully filled will have higher stability.

I: And the reason for the stability is?

P14: Reason for the stability…I'm not so sure.

I: Ok, what about you, P30?

P30: I choose B2 (item 8).

I: Why B2?

P30: Because it's like…phosphorous is $3p^3$ so that means there's the last…they are half-filled so they are more stable.

I: Why is half-filled more stable?

P30: Half-filled because they are all filled singly throughout, that's why it is more stable.

P14 and P30 believed that a fully-filled or half-filled sub-shell was stable because both were analogous to a 'stable octet' – there was no conflict between the octet rule framework and the 'stable fully-filled or half-filled sub-shell' thinking, in fact, the former seemed to lead 'naturally' to the latter, from shell to sub-shell. In the curriculum model, magnesium has a higher first ionisation energy than sodium because its greater nuclear charge outweighs the repulsion between its 3s electrons. A similar reason accounts for the higher first ionisation energy of phosphorus compared to silicon. However, sulphur has lower first ionisation energy than phosphorus even though sulphur has a greater nuclear charge. This is because the repulsion between the paired 3p electrons in sulphur outweighs its greater nuclear charge. The greater shielding of the 3p electron by the inner shell electrons as well as the 3s electrons explains why aluminium has a lower first ionisation energy compared to magnesium. It has to be noted that students will have great difficulty answering questions on ionisation energy trends if they cannot either remember whether increased nuclear charge or increased repulsion/shielding between electrons is more important in specific cases or recall the shape of the trend graph, and so work out which factors must be more important in each case. Thus, it is not a matter of grave concern if students cannot decide between, for example, A4 or B3 in item 5, or A5 or B4 in item 9. However, it is problematic when students think that a fully-filled 3s sub-shell gives magnesium its stability, and hence higher first ionisation energy compared to aluminum, while phosphorus, with its 3p sub-shell half-filled, is more stable than sulphur and hence has higher first ionisation energy than sulphur.

Tan et al. (2005) believe that, similar to the octet rule framework, the 'stable fully-filled or half-filled sub-shell' thinking arises from its use as a heuristic by teachers, this time to help students remember the anomaly in the trend of ionisation energy across Periods 2 and 3. Unfortunately, students (and even teachers) adopt it as an explanation for the trend of ionisation energy. Cann (2000) also commented that this 'half-filled (and also completely-filled) shells having intrinsic stability' reason was common and could be found in textbooks, but it offered "no explanation in terms of electrostatic or quantum mechanical interactions within the atom" (p. 1056). An example of the use of both the octet rule framework and stable fully-filled or half-filled sub-shells in a text book is given below:

"The values for Ne and Ar are the highest in their periods because it requires a great deal of energy to break *a stable filled shell of electrons*. There are several irregularities. The high values for Be and Mg are attributed to the *stability of a filled s shell*. The high values of N and P indicate that *a half-filled p level is also particularly stable*. The values for B and Al are lower because removal of one electron leaves *a* *stable filled s shell*, and similarly with O and S *a stable half-filled p shell* is left" (Lee, 1977, p.96, *present authors' emphasis*)

In summary, it was not surprising that students readily accepted the 'stable fully-filled or half-filled sub-shell' thinking as it was an 'offshoot' from the octet rule framework. Furthermore, as it was also used by teachers in their lessons and stated in some textbooks, students would think that the 'stable fully-filled or half-filled sub-shell' thinking was a legitimate explanation for the anomaly in the trend of ionisation energy across Periods 2 and 3.

CONCLUSION

The only times students encounter the concepts on ionisation energy are in formal science lessons. Thus, it is likely that the alternative conceptions arise from the way bonding and ionisation energy is taught and learnt (Taber, 2004; Tan et al., 2005). The use of the octet rule heuristic in teaching and learning of bonding, and the use of the 'stable fully-filled and half-filled sub-shell' heuristic in the teaching and learning of the trend of ionisation energy across Periods 2 and 3 can give rise to alternative conceptions in ionisation energy. Thus, teachers need to be wary of using such heuristics in their teaching, and to challenge students' use of the heuristics as explanations for the trend of successive ionisation of an atom, and the trend of ionisation energies across a period.

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APPENDIX: EXAMPLES OF ITEMS IN THE IEDI

Sodium atoms are ionised to form sodium ions as follows:

$Na(g) \rightarrow Na^{+}(g) + e$

4. After the sodium atom is ionised (i.e. forms Na^{+} ion), more energy is required to remove a second electron (i.e. the second ionisation energy is greater than the first ionisation energy) from the Na^{+} ion.

   A True.

   B False.

   C This should not happen as the Na^{+} ion will not lose any more electrons.

   D I do not know the answer.

   Reason:

   (1) Removal of the second electron disrupts the stable octet structure of Na^{+} ion.

   (2) The same number of protons in Na^{+} attracts one less electron, so the attraction for the remaining electrons is stronger.

   (3) The second electron is located in a shell which is closer to the nucleus.

   (4) The second electron is removed from a paired 2p orbital and it experiences repulsion from the other electron in the same orbital.

5. Sodium, magnesium and aluminium are in Period 3. How would you expect the first ionisation energy of sodium ($1s^2$ $2s^2$ $2p^6$ $3s^1$) to compare to that of magnesium ($1s^2$ $2s^2$ $2p^6$ $3s^2$)?

   A. The first ionisation energy of sodium is greater than that of magnesium.

   B. The first ionisation energy of sodium is less than that of magnesium.

   C. I do not know the answer.

   Reason:

   (1) Magnesium has a fully-filled 3s sub-shell which gives it stability.

   (2) Sodium will achieve a stable octet configuration if an electron is removed.

   (3) In this situation, the effect of an increase in nuclear charge in magnesium is greater than the repulsion between its paired electrons in the 3s orbital.

   (4) The paired electrons in the 3s orbital of magnesium experience repulsion from each other, and this effect is greater than the increase in the nuclear charge in magnesium.

   (5) The 3s electrons of magnesium are further from the nucleus compared to those of sodium.

6. How do you expect the first ionisation energy of magnesium ($1s^2\ 2s^2\ 2p^6\ 3s^2$) to compare to that of aluminium ($1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^1$)?

   A. The first ionisation energy of magnesium is greater than that of aluminium.

   B. The first ionisation energy of magnesium is less than that of aluminium.

   C. I do not know the answer.

   Reason:

   (1) Removal of an electron will disrupt the stable completely-filled 3s sub-shell of magnesium.

   (2) The 3p electron of aluminium is further from the nucleus compared to the 3s electrons of magnesium.

   (3) In this situation, the effect of an increase in nuclear charge in aluminium is greater than the repulsion between the electrons in its outermost shell.

   (4) In this situation, the effect of an increase in nuclear charge in aluminium is less than the repulsion between the electrons in its outermost shell.

   (5) The paired electrons in the 3s orbital of magnesium experience repulsion from each other, whereas the 3p electron of aluminium is unpaired.

8. Silicon, phosphorus and sulphur are in Period 3. How would you expect the first ionisation energy of silicon ($1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^2$) to compare to that of phosphorus ($1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^3$)?

   A The first ionisation energy of silicon is greater than that of phosphorus.

B The first ionisation energy of silicon is less than that of phosphorus.

C I do not know the answer.

Reason:

(1) Silicon has less electrons than phosphorus, thus its 3p electrons face less shielding.

(2) The 3p sub-shell of phosphorus is half-filled, hence it is stable.

(3) The 3p electrons of phosphorus are further away from the nucleus compared to that of silicon.

(4) In this situation, the effect of an increase in nuclear charge in phosphorus is greater than the repulsion between its 3p electrons.

9. How would you expect the first ionisation energy of phosphorus ($1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^3$) to compare to that of sulphur ($1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^4$)?

A The first ionisation energy of phosphorus is greater than that of sulphur.

B The first ionisation energy of phosphorus is less than that of sulphur.

C I do not know the answer.

Reason:

(1) More energy is required to overcome the attraction between the paired 3p electrons in sulphur.

(2) 3p electrons of sulphur are further away from the nucleus compared to that of phosphorus.

(3) The 3p sub-shell of phosphorus is half-filled, hence it is stable.

(4) In this situation, the effect of an increase in nuclear charge in sulphur is greater than the repulsion between its 3p electrons.

(5) In this situation, the effect of an increase in nuclear charge in sulphur is less than the repulsion between its 3p electrons.