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The octet rule and hypervalence: two misunderstood concepts

Ronald J. Gillespie [a,*], Bernard Silvi [b]

[a] *Department of Chemistry, McMaster University, Abb-267, Hamilton, Ont., Canada L8S 4M1*
[b] *Laboratoire de Chimie Théorique, Université Pierre et Marie Curie, 4, Place Jussieu, 75252 Paris cédex, France*

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Abstract

The octet rule proposed by Lewis states that the valence shell of an atom in a molecule always has eight electrons in its valence shell when each pair of shared electrons is counted as contributing fully and equally to the valence shell of both bonded atoms irrespective of the polarity of the bonds. However, as a result of attempts to allow for bond polarity an atom has been said to obey the octet rule if it has no more than eight electrons in its valence shell. This misinterpretation of the Lewis octet rule has led to much controversial discussion in connection with the concept of hypervalent molecules which have more than eight electrons in the valence shell of the central atom in their Lewis structures. Whereas hypervalent molecules clearly do not obey the Lewis octet rule it has been proposed that they do not violate the octet rule when it is expressed in its modified form because molecular orbital calculations of hypervalent molecules with strongly electronegative ligands, such as SF_6, have been interpreted to show that there are fewer than eight electrons in the valence shell of the central atom. The electron localization function (ELF) allows the populations of the bonding and nonbonding domains in a molecule to be determined to a reasonably good approximation in many cases. ELF calculations of hypervalent molecules with less electronegative ligands such as PMe_5, $PMe_3{=}CH_2$ $AsMe_5$, and $TeMe_6$, have shown that the population of the valence shell of the central atom is greater than eight, so these molecules do not obey the modified octet rule. We conclude that the octet rule is only valid in its original form as proposed by Lewis. We also conclude that hypervalence is not a useful concept as hypervalent molecules are not different in any significant way from Lewis octet molecules, except that in many, but not all, cases they have a coordination number higher than four.
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Keywords: Hypervalence; Octet rule; Lewis structures

1. The octet rule

Ever since Lewis proposed the octet rule in 1916 [1], it has become one of the most important concepts in any discussion of the electronic structure of molecules. Lewis noted that the vast majority of stable molecules have an even number of electrons and he was able to account for

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* Corresponding author. Tel.: +1-905-525-9140; fax: +1-905-522-2509
E-mail address: gillespi@mcmaster.ca (R.J. Gillespie).

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the formulas of these molecules by assuming that each bond corresponded to the sharing of two electrons or a pair, between the bonded atoms, and he called this the *rule of two.* He also noted that for the vast majority of stable molecules, when both shared pairs and unshared pairs of electrons are counted the central atom A of an AX_n molecule has eight electrons or four pairs in its valence shell. He called this the *rule of eight*. Langmuir later suggested that the rule of eight be called the *octet rule* [2] and this name was universally adopted. Even though Lewis realized that many bonds are polar he took no account of this, basing the octet rule on the assumption that each bonding pair of electrons contributes fully and equally to the valence shell of both bonded atoms. Lewis recognized that there are exceptions to the octet rule such as BF_3, PCl_5 and SF_6 but he did not regard the rather few exceptions that were known at the time as being of great importance. He considered that the rule of two, namely that electrons in stable molecules always appear to be in pairs, is of more fundamental importance. He had no explanation for this observation, but he was so convinced of its correctness and importance that he even suggested that Coulomb's law was not valid at very short distances. This suggestion is of course not correct but he was correct in emphasizing the importance of the electron pair which we now know is a consequence of the operation of the Pauli principle.

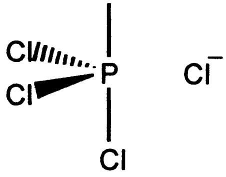
2. Hypervalence

Since Lewis's time many more exceptions to the octet rule have been found and they can no longer be regarded as minor, unimportant exceptions. Molecules which have Lewis structures with more than eight electrons in the valence shell of a central atom, such as PCl_5, with five pairs, and SF_6, with six pairs, are commonly called hypervalent, while those with fewer than eight, such as BF_3, are sometimes called hypovalent. As, over time, the octet rule came to be regarded more as a law of nature than as an empirical rule, hypervalent molecules, in particular, have received a great deal of discussion and attention. A hypervalent molecule was formally defined by Musher [3] as a molecule of the elements of Groups 15–18 in any oxidation state other than their lowest oxidation state. Thus PCl_5, SF_4, SF_6, ClF_3, ClF_5, and all the molecules of the noble gases, are examples of hypervalent molecules. They all have ten or more electrons in the valence shell of the central atom in the Lewis electron pair structure of the molecule.

It is interesting to note that chemists firmly held belief in the fundamental importance of the octet rule was largely responsible for the general acceptance for many years of the inertness of the noble gases. Only a few researchers in the 1920s and early 1930s speculated on the possible existence of hypervalent noble gas molecules such as XeF_6, for example, which might be expected as the final member of the series SbF_3, TeF_4, IF_5, XeF_6. Only a very few unsuccessful attempts were made to prepare such compounds and it was not until 1962 that the first noble gas compound '$XePtF_6$' was prepared by Bartlett [4].

3. Bonding in hypervalent molecules

In terms of the valence bond model and the concept of hybridization hypervalent molecules were at first accepted as true exceptions to the octet rule because it was believed the bonds could be described as being formed from sp^3d^n hybrid orbitals on the central atom. However, subsequent ab initio calculations showed that the contribution of d-orbitals to the bonding in hypervalent molecules, such as PCl_5 and SF_6 is very small, so this hybrid orbital description of hypervalent molecules was abandoned, although it is still seen in some text books. Attention then turned to showing that hypervalent molecules were not, in fact, exceptions to the octet rule. Since the majority of hypervalent molecules have ligands that are more electronegative than the central atom they have polar bonds. Such molecules can be described by resonance structures involving one or more ionic bonds. If we write structures with no more than four covalent (electron pair) bonds and one, two or three ionic bonds as in (1), (2) and (3).



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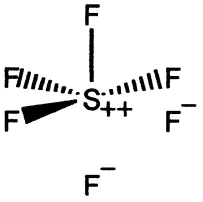

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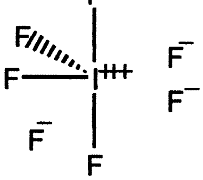
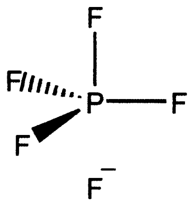


(3)

then these molecules appear to be consistent with the octet rule. However, as these structures are written to be in accordance with the octet rule they do not prove that the octet rule is obeyed.

The bonding in hypervalent molecules has alternatively been described in terms the 3-center 4-electron (3c-4e) bond using a simple qualitative molecular orbital model. This can be most easily discussed by using the PF_5 molecule as an example. Each of the three equatorial bonds is described as being formed from an sp^2-orbital on phosphorus and an appropriate ligand orbital. The two axial bonds are described in terms of a 3c-4e bond in which two ligand orbitals and a single 3p-orbital on the central atom are combined to give three molecular orbitals extending over all three atoms, a bonding orbital occupied by two electrons; a non-bonding orbital also occupied by two electrons; and an unoccupied anti-bonding orbital [5,6]. This model is equivalent to a description in terms of the two resonance structures **4** and **5** according to which each P–F (ax) bond may be described as a half-bond **6**. This model is said to be in agreement with the observation that the axial PF bonds are longer than the equatorial bonds. However, their difference in length (P–F_{ax} 157.7 pm; P–F_{eq} 153.4 pm) is substantially smaller than might be expected from the model. Moreover, this model implies that only the axial bonds are polar. A similar description of the bonding in a molecule such as SF_6 in which all the bonds are equivalent and equal in length necessitates the writing of three resonance structures **7**, **8**, and **9** each involving two 3c-4e bonds. This description is an unsatisfactory mixture of a molecular orbital model and valence bond resonance structures and as such is more confusing than enlightening.



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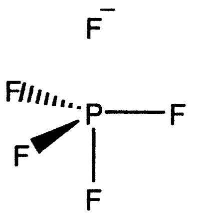

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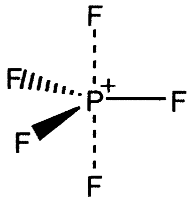

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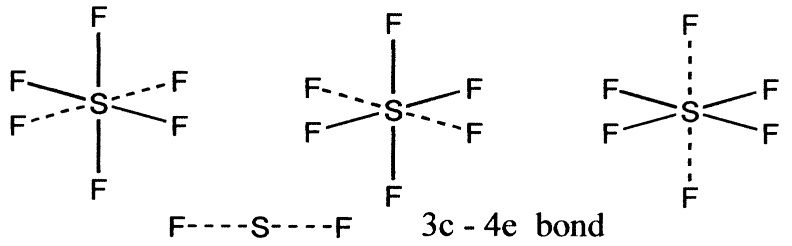
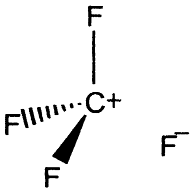


(7) (8) (9)

Another type of description of the bonding in hypervalent molecules has been given by Harcourt [7] in terms of his increased valence structures. But again these are valence-bond descriptions that can be written in accordance with the octet rule but they do not prove that the octet rule is obeyed.

4. The modified octet rule

Models involving polar bonds imply that the bonding electron pairs do not contribute equally and fully to the valence shells of both bonded atoms but contribute more to the valence shells of the ligands than to the valence shell of the central atom contrary to assumption made by Lewis in formulating the octet rule. Indeed, no molecule with polar bonds can have exactly eight electrons in the valence shell of the central atom except by chance. To emphasize this point, we note that CH_4 and CF_4 both obey the Lewis octet rule but if the polarity of the CF bonds is taken into account by writing resonance structures for CF_4 such as:



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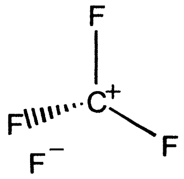


(11)

the carbon atom has fewer than eight electrons in its valence shell. Nevertheless CF_4 is regarded as obeying the octet rule. Thus a subtle change in the rule has occurred. It has been modified to mean that the central atom in an AX_n molecule may have eight, or fewer than eight, electrons in its valence shell but never more than eight. We call this rule the modified octet rule because it is not the Lewis octet rule. Whether or not a hypervalent molecule obeys the modified octet rule depends on the electronegativity of the ligands. In contrast no hypervalent molecule obeys the original Lewis octet rule, independently of the electronegativity of its ligands.

5. Determination of the electron population of the valence shell

To answer the question of whether or not a hypervalent molecule obeys the modified octet rule it is necessary to find just how many shared and unshared electrons are in the valence shell of the central atom of the molecule. On the basis of ab initio calculations it is possible, at least in principle, to find the electron population of the valence shell of an atom. However, we cannot obtain this information just from an ab initio calculation which gives only the wave function, geometry and energy of a molecule.

To obtain the information we need, namely the population of the valence shell of the central atom, two methods have been used: the molecular orbital method and the electron localization function (ELF) method. In the first the wave function of an AX_n molecule is expressed in terms of localized molecular orbitals and the contribution of each orbital to a given bond is found and hence the bond order. The total population of the valence shell of A is then $2n$(bond order AX). Reed and Schleyer [8] used natural population analysis (NPA) to obtain natural bond orders in a large number of four-coordinate hypervalent molecules. They found the central atom valence shell population to be 7.92 for H_3PS and to be smaller for the all the other molecules they studied which had more electronegative ligands, such as F and O. Cioslowski and Mixon [9] determined bond orders based on the atomic orbital overlap matrix (AOM). For SF_6 they found the SF bond order to be 0.64, so that the total bond order is 3.84 and there are 7.68 electrons in the valence shell of the sulfur atom. For ClF_4^+, including the lone pair electrons, they concluded that the total valence shell population slightly exceeds eight. In the light of these results it seems reasonable to conclude that with less electronegative ligands the electron population of the valence shell of a hypervalent atom might substantially exceed eight.

The possibility that hypervalent AX_n molecules with relatively weakly electronegative ligands might have more than eight electrons in the valence shell of A has been investigated recently by Noury, Silvi and Gillespie [10] using the ELF [11–13]. The ELF partitions the electron density distribution obtained from the wave function into regions where there is a high probability of finding a pair of electrons of opposite spin. Each region is called a basin and the average number of electrons in each basin can be found by integrating the electron density over the total volume of the basin. These basins are of three types, they are either core basins, or are valence shell basins that are connected to only one core (monsynaptic basins) or are connected to two or more cores (polysynaptic basins). Since the monosynaptic basins are associated with only one atom they are populated by electrons which have a nonbonding character, that is by the Lewis lone pair electrons. The polysynaptic basins are associated with two or more cores and are, therefore, populated by bonding electrons shared between these cores. Disynaptic basins which are associated with two cores are populated by the electrons of a normal 2-center bond whereas higher polysynaptic basins correspond to multicenter bonding such as the 3c-2e bonds in boranes. It is noteworthy that there are no examples of hypervalent molecules exhibiting a three center bond through a trisynaptic basin as might be expected from the 3c-4e model discussed earlier.

The mono and disynaptic basins in a molecule usually correspond very well in number and geometry with the domains of the VSEPR model as shown in Fig. 1 for the ClF_3 molecules.

Here, we see the isosurfaces of the basins for ELF = 0.65. They clearly indicate eight regions of electron localization: two monosynaptic chlorine basins corresponding to the two lone pairs on chlorine, a basin on each fluorine corresponding the three lone pairs on each fluorine, and three Cl, F disynaptic basins corresponding to the three bonding pairs. As is always the case for a

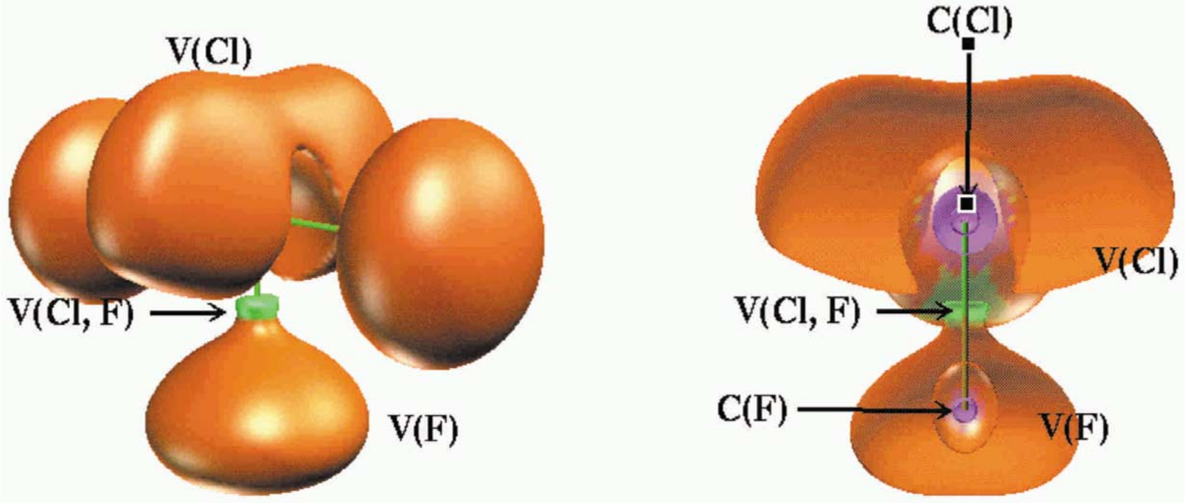


Fig. 1

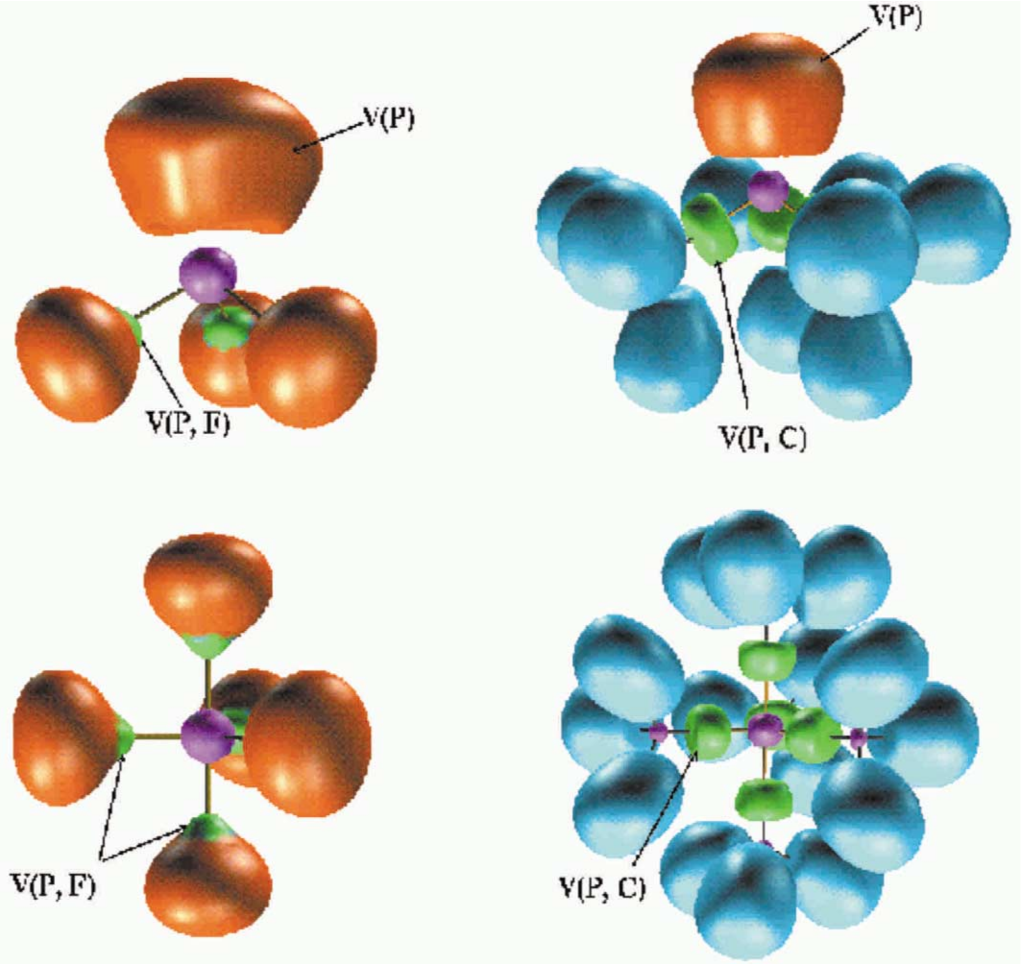


Fig. 2

Fig. 1. Localization domains of the ClF_3 molecule as shown by the ELF = 0.65 isosurfaces The red domains are the chlorine and fluorine nonbonding domains, the green domains are the Cl, F disynaptic bonding domains and the magenta domains are the core domains. The right hand part of the figure shows a view down the axial bonds of molecule that has been cut by a plane perpendicular to this axis so that the core domains can be seen.

Fig. 2. Localization domains of the molecules PF_3, PMe_3, PF_5, and PMe_5. The domains are colored as in Fig. 1. The blue domains are the disynaptic CH bonding domains. Since the hydrogen atom has a maximum of two electrons in its valence shell no distinction can be made between bonding and nonbonding electrons so that a CH disynaptic basin surrounds the hydrogen nucleus.

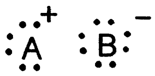
Table 1
Populations of the monosynaptic (non-bonding) and disynaptic (bonding) basins of some hypervalent molecules

	N(A, X)	Σ N(A, X)	N(X)	N(X)+N(A, X)
PF_5 (ax)	1.03	5.33	6.82	7.85
PF_5 (eq)	1.09		6.78	
PCl_5 (ax)	1.33	7.13	6.56	7.89
PCl_5 (eq)	1.49		6.43	
PMe_5 (ax)	1.86	9.42		
PMe_5 (eq)	1.90			
$PF_3{=}CH_2$ F	1.02	7.07	6.82	7.82
C	4.01			
$PH_3{=}CH_2$ H	2.01	8.52		
C	2.49			
$PMe_5{=}CH_2$ Me	1.94	8.41		
CH_2	2.59			
$AsCl_5$ (ax)	1.16	6.10	6.76	7.82
$AsCl_5$ (eq)	1.26		6.72	
$AsMe_5$ (ax)	1.90	9.68		
SF_6	1.03	6.18	6.80	7.83
SeF_6	0.36	2.18	7.54	7.90
$SeMe_6$	1.83	10.98		
$TeMe_6$	1.85	11.10		

N(A, X), population of each bonding basin; Σ N(A, X), valence shell population of A; N(X), population of the non-bonding basin of each X ligand; N(X)+N(A, X), valence shell population of each X ligand.

monatomic ligand the three lone pairs on each fluorine are not resolved from each other because they are not separately localized. At lower values of ELF these basins are larger and ultimately they touch, occupying all the molecular space. Integration of the electron density over these basins then gives the number of electrons in each of the bonding and non bonding regions However, the populations of these basins generally differ from the Lewis value of two. Only a disynaptic basin corresponding to a pure covalent bond has a population of two electrons while polar bonds have a smaller population depending on the electronegativity of the ligand. In a polar bond, some of the formally bonding electrons occupy the valence shell of the ligand as described, for example, by the two resonance structures **12** and **13**. Thus the population of the disynaptic (bonding) basin is less than two while the population of the monosynaptic (non-bonding) basin, that, in this case, is formally occupied by three lone pairs, is greater than six.

(12)



(13)

When the ligand X is more electronegative than A it will always have a total of eight electrons in its valence shell while the atom A may have any number from zero up to the number expected from a Lewis electron pair structure, namely eight for a Lewis octet molecule and up to ten, 12, or more for a hypervalent molecule. It is important to note that in this method of counting electrons, as in the Lewis method, the bonding electrons are counted twice, once for the ligand and once for the central atom.

Table 1 gives the populations of the valence shell basins for some of the molecules studied by Noury, Silvi and Gillespie [10]. We see that the valence shell population of the central atom increases with decreasing ligand electronegativity from values less than eight to values greater than eight as shown by the series PF_5 (5.33), PCl_5 (7.13), PMe_5 (9.42); by SeF_6 (2.18), and $SeCl_6$ (6.80), and by the molecules $PF_3{=}CH_2$ (7.07) and $PMe_3{=}CH_2$ (8.41). These populations are a consequence of the AX bond populations increasing from considerably less than two to very nearly two as expected for a weakly polar bond. In all the molecules with methyl or = CH_2 ligands the central atom valence shell population is greater than eight. So these molecules do not obey the modified octet rule which is, therefore, not a useful rule and has no fundamental significance.

Table 2
Populations of the monosynaptic (non-bonding) and disynaptic (bonding) basins in non-hypervalent (Lewis octet) molecules

	N(A, X)	N(A)	N(A)+%N(A, X)	N(X)	N(X)+N(A, X)
PF_3	0.84	2.12	4.64	6.97	7.81
PCl_3	1.28	2.13	5.96	6.59	7.87
PMe_3	1.90	2.16	7.86		
PH_2Me · H	1.97	2.11	7.88		
Me	1.83				
$AsCl_3$	0.99	2.35	5.32	6.90	7.89
$AsMe_3$	1.85	2.48	8.03		
SF_2	0.60	4.48	5.68	7.03	7.63
SCl_2	0.97	4.62	6.58	6.62	7.59
$SeCl_2$	0.90	4.78	6.58	6.75	7.48

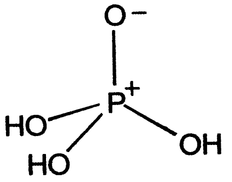
N(A), Population of the nonbonding basin on A. Other column headings as in Table 1.

Table 2 gives the bond and valence shell populations for some related nonhypervalent (Lewis octet) molecules. Fig. 2 shows isosurfaces of ELF for the PF_3 and PMe_3 molecules and for the corresponding hypervalent molecules PF_5 and PMe_5. All the expected P–F, P–C, and C–H disynaptic bonding basisn are observed together with the monosynaptic lone pair basin on the phosphorus atom in the nonhypervalent (Lewis octet) molecules PF_3 and PMe_3. Since the hydrogen atom has no core electrons the C–H bonding basin surrounds the H nucleus, these nuclei are not seen in Fig. 2. It has sometimes been thought that hypervalent molecules have a different kind of bonding from non-hypervalent molecules, such as the 3c-4e bond, but the bond basin populations show that they all have similar polar bonds. The disynaptic (bonding) basin populations are very similar in hypervalent and nonhypervalent molecules increasing with decreasing electronegativity of the ligand as in the following series of bonding basin populations, PF_3 (0.84); PCl_3 (1.28); PMe_3 (1.90) and PF_5 (1.07); PCl_5 (1.43); PMe_5(1.88). With the more electronegative ligands the bonds in the AX_5 molecules are a little less polar, and have a correspondingly slightly greater population, than in the corresponding AX_3 molecules as might be expected as a consequence of replacing a lone pair by two electronegative ligands. There is, therefore, no fundamental difference between the bonds in hypervalent molecules and in Lewis octet (non-hypervalent) molecules.

In our discussion, we have implicitly assumed that the ELF analysis of the electron density provides a partition of the electron density into bonding and nonbonding regions as is also assumed in the Lewis and VSEPR models. This is an approximation because in fact the continuous electron density distribution cannot be rigorously partitioned in this way. For many molecules, particularly those of the elements in the early periods of the periodic table which have relatively small cores, this partitioning appears to be a good approximation as the populations of both monosynaptic lone pair (nonbonding) basins and the disynaptic bonding basins of essentially pure covalent bonds such as a C–C or C–P bond are close to two electrons. For the heavier elements of Period 4 and beyond a clear separation between the bonding and nonbonding electrons cannot always be made [10]. Nevertheless, the calculated valence shell populations in the molecules, we have discussed exceed the value of eight by a substantial amount so that we consider that a our general conclusions are valid. In fact, the difficulty of obtaining an exact value for the population of a valence shell only further emphasizes that the modified octet rule is not a useful rule, based as it is on a precise counting of electrons.

6. Molecules with multiple bonds

In singly bonded hypervalent molecules the number of ligands X in an AX_n molecule is necessarily greater than four. However, there are a large number of molecules, such as H_3PO_4 and SO_2Cl_2, with multiple bonds that have only four ligands but are hypervalent according to Musher's definition [3]. Lewis did not regard these molecules as exceptions to the octet rule because he formulated them with bonds that were assumed to be 50% ionic and 50% covalent:



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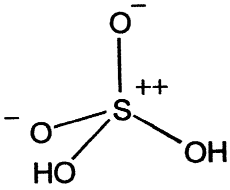
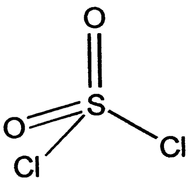


(15)

so as to be consistent with the octet rule. These structures have become widely accepted and are found in many introductory chemistry texts. They are analogous to the resonance structures of SF_6 with two ionic bonds (**2**) and there is no more justification for **14** and **15** than there is for **2.** It seems much more reasonable to describe them by structures with a number of bonds consistent with the oxidation state namely six for S in SO_2Cl_2 (**16**) and five in H_3PO_4 (**17**).



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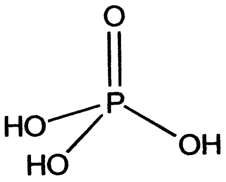
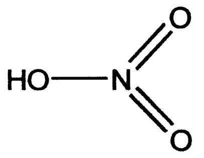


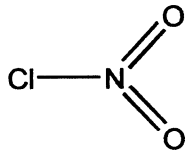
(17)

The double bonds are polar bonds just as the bonds in SF_6 are polar single bonds. But there is no reason to assume that their polarity is exactly that required to make them consistent with the modified octet rule.

Although they are not usually regarded as hypervalent, molecules of nitrogen in which it is in the +5 oxidation state, such as HNO_3, NO_2Cl and ONF_3 are hypervalent according to the Musher definition as shown in (18), (19) and (20).



(18)



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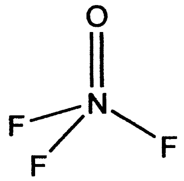
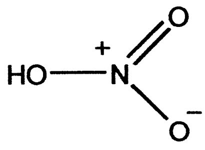
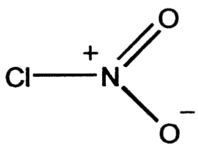


(20)

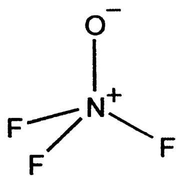
However, the electronic structures of these molecules are universally written in (21), (22) and (23):



(21)

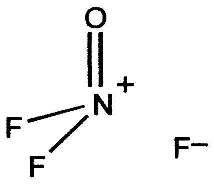


(22)



(23)

so as not to violate the octet rule. But there is no more reason to write these structures in this way than there is to write structure **14** for SO_2Cl_2 because they are based on the arbitrary assumption that an NO bond can be described as 50% ionic and 50% covalent. The molecule NOF_3 has been the subject of particular discussion because the NO bond has a length of only 115.8 pm which is essentially equal to the length of the NO bond in NO_2^+ (115 pm) which is universally regarded as a double bond. So in order to satisfy the octet rule the bonding is described in terms of resonance structures involving an NF ionic bond such as **24**.



(24)

But again these structures are written so as to be in accord with the octet rule. The NF bonds in this molecule which have a length of 143.1 pm are unexpectedly long compared with the NF bond in NF_3 which has a length of 136.5 pm. This unexpectedly long bond has been claimed to be consistent with the resonance structures **24** indicating that the NF bonds are polar. But a simple alternative explanation is that because the four ligands are close packed around the short NO distance necessarily increases the length of the NF bonds so that the O···F and F···F distances have the same length as in other close packed molecules of nitrogen [5,14]. The four-coordinated molecules of the Period 2 elements have been shown to generally have close packed ligands because of the small size of the Period 2 atoms [14–16]. The larger atoms of Period 3 and beyond may accommodate more ligands so that molecules with coordination numbers greater than four are rather common. These molecules are necessarily hypervalent so that there are many hypervalent molecules of these elements. In contrast the hypervalent molecules of nitrogen are confined to molecules with coordination numbers of four or less. Molecules such as NF_5 and NCl_5 are not known because of the difficulty of packing five ligands around the small nitrogen atom. So hypervalent molecules of nitrogen are much less common than the hypervalent molecules of the elements of Period 3 and beyond.

7. Do we need the term hypervalence?

So-called hypervalent molecules are very common and do not differ in any essential way from non-hypervalent molecules. The bonding in these molecules is very similar to that in non-hypervalent (Lewis octet) molecules, and although they are exceptions to the original Lewis octet rule, this rule is only an empirical rule without any firm theoretical foundation. There is, therefore, no reason to regard hypervalent molecules as belonging to a special class. There has, moreover, always been some doubt as to which molecules are hypervalent. For example, the Musher definition excludes molecules such a SiF_6^{2-} because Si is a Group 14 element and is in its normal stable oxidation state yet there are twelve electrons in the valence shell of silicon in its Lewis structure. The same considerations apply to the ion COF_3^- which has a structure analogous to the NOF_3 molecule. Again molecules such H_2SO_4 are so frequently assigned structures which obey the modified octet rule that they are often not regarded as hypervalent. Thus, not only is there no reason to regard hypervalent molecules as a special class, but the assignment of a particular molecule to this class is not always clear. Although we have, for convenience, used the term hypervalent throughout our discussion simply to distinguish those molecules which in their Lewis structures have more than eight electrons in the valence shell of the central atom, we have shown that there is no good reason to make this distinction, because these molecules are not in any other way different from Lewis octet molecules. As Lewis recognized his octet rule has exceptions and is less important than his rule of two. We conclude that the concept of hypervalence has ceased to be of any practical use and there is no longer any reason to classify any molecules as hypervalent.

8. Summary and conclusions

1) The Lewis octet rule states that there are eight electrons in the valence shell of any atom in a molecule (except hydrogen) when each bonding pair is regarded as contributing fully and equally to the valence shells of both bonded atoms.
2) Hypervalent molecules have been defined by Musher [1] as those molecules of the elements of Groups 15–18 in any of their oxidation states other than their lowest oxidation state. If following Lewis each bonding pair of electrons is considered to contribute equally to both of the valence shells of the two bonded atoms then the central atom in a hypervalent molecule has ten, 12 or even more electrons in its valence shell. In other words such molecules are exceptions to the Lewis octet rule.
3) Attempts to explain why hypervalent molecules do not obey the octet rule led to the polarity of the bonds in these molecules being taken into account. Resonance structures involving ionic bonds were chosen to describe bonding such that there are eight electrons in the valence shell of the central atom. Later molecular orbital calculations of bond orders led to the conclusion that in all the molecules studied, which had rather electronegative ligands, there are eight or fewer than eight electrons in the valence shell of the hypervalent atom. Hence it was concluded that these molecules obey the octet rule. However, they do not obey the octet rule as defined by Lewis but a modified rule that states that the valence shell of an atom may contain eight or fewer than eight electrons in its valence shell if the bond polarity is taken into account.
4) Recent work using the ELF has shown, however, that with sufficiently weakly electronegative ligands such as a methyl group the central atom in a hypervalent molecule may have more than eight electrons in its valence shell. So these hypervalent molecules do not obey either the modified octet or the original Lewis octet rule. Whether an atom in a hypervalent molecule obeys the modified octet rule or not is simply a function of the electronegativity of the ligands and it has no fundamental significance.
5) Comparison of the bonds in hypervalent molecules with those in analogous Lewis octet molecules shows that there is no fundamental difference in their nature. They are both polar bonds. The only small difference is that the bonds in the hypervalent molecules with electronegative ligands are a little less polar than those in nonhypervalent molecules.
6) All hypervalent molecules are exceptions to the Lewis octet rule and some of them are also exceptions to the modified octet rule. The modified octet rule, therefore, has no special significance. Provided it is recognized that it has exceptions the Lewis octet rule is still a useful pedagogical tool whereas the modified rule has no usefulness and there is therefor no reason to continue to use it. Lewis's rule of two is, moreover, still very useful for writing electron-dot structures of molecules. Lewis was correct in considering that the rule of two is more important than the rule of eight.
7) Whether or not an atom in a molecule may have more than four ligands, or more than a total of four ligands and lone pairs, as is the case for many hypervalent molecules, depends primarily on the size of the central atom.
8) As there is no fundamental difference between the bonds in hypervalent and non-hypervalent (Lewis octet molecules) there is no reason to continue to use the term hypervalent.

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