emergence occurs in the desert iguana, *Dipsosaurus dorsalis*, in late morning several hours after sunrise and at a time when the animal can achieve optimal body temperature levels. Similar observations have been made on horned lizards (*3*). Certainly, the animal's problem of securing safe nocturnal shelter without losing activity time in the morning is met by this mechanism (*4*).

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20 August 1962

Binding of Inert Gas Halogenide Molecules

Abstract. An electronic explanation of the existence of noble gas halides and predictions of the properties to be expected of these compounds is presented.

Formation of XeF_4 and XeF_2, recently reported (*1*), invalidates one of chemistry's oldest and most widely accepted rules.

The traditional model of a rare gas atom envisions a series of shells completely filled through ns^2np^6 (Ne, $n = 2$; A, $n = 3$; Kr, $n = 4$; Xe, $n = 5$; Rn, $n = 6$). Each one-electron orbital is occupied by one electron with α spin and another with β spin, and each shell as well as the atom as a whole is spherically symmetric. By virtue of the Pauli exclusion principle, this model adequately describes the instantaneous electron-electron correlation between electrons with the same spin but not that between electrons with antiparallel spin. Correlation between antiparallel pairs of electrons produces a separation between them and causes a slight distortion of the atom. It is the small, time-averaged, spatial separation of these antiparallel electron pairs which gives the possibility of a shared electron (*2*). As in most chemical problems, the one-electron orbitals decrease rapidly with distance, and only the outer *ns* and *np* shells contribute to binding. The number of antiparallel *ns* and *np* pairs in rare gas atoms is four. Thus a maximum of four halide atoms may be bound. The spatial separation of antiparallel spin pairs does not prevent us from setting up a many-electron wave function which is a singlet for either the atom or the molecule (*3*). For both the two-halogen and four-halogen species half of the halogen atoms will have α spin and half β spin, and we expect the molecules to have no net magnetic moment.

A rather complete and detailed picture of the electron configuration in the atom and molecule can be constructed. First, the *ns* shell will be inside the *np* shell by a small amount, and the two ionization potentials are quite different (*4*). This does not imply any chemical discontinuity in the periodic table as the *ns* shell is completed, but it does mean that hybridization between the *s* and *p* orbitals of the conventional sort present in carbon is not favored. Another important fact is the absence of correlation coupling between *s* and *p* shells (*5*), which allows the shells to act independently of one another. Second, Unsöld's theorem (*6*) states that for the undistorted noble gas atoms the three np^{α} electrons and three np^{β} electrons are each spherically symmetrical. The correlation distortion will have radial and angular components. Figure 1 shows schematically the radial correlation separation for α, β pairs. Figure 2 is a sketch of the xenon $5p$ and fluorine $2p$ radial functions in the binding region. Similar figures may be drawn for the $5s$ radial functions and for other combinations of noble gas and halogen atoms. Binding is achieved by the difference in the overlap between the α and β functions and the fluorine $2p$ orbitals. Because of the spherical symmetry of the three undistorted np^{α} and np^{β} electrons, these two groups of three electrons will be angularly separated as far as possible from one another, thereby giving a high probability to an approximate octahedral distribution of electrons. The two *ns* electrons will tend to be on opposite sides of the nucleus and form an ellipse. Angular correlation produces a separation of α and β spins in angle and a differential overlap effect similar to the radial displacement of Fig. 2.

The obviously high symmetry of the noble gas atoms and a preliminary infrared absorption spectrum (*1*) indicate a tetrahedral or planar configuration for the four halide atoms in tetrahalide molecules. I predict a planar configuration. The electrons forming the *np* octahedron may be pictured as follows: there are four equidistant electrons (two α and two β) on the equator of a sphere, and the spins alternate around the equator. One pole has an electron of α spin, the other an electron of β spin. Four halogen atoms may become associated with the four equatorial electrons, deriving three-fourths of their binding from the *np* shell and one-fourth from the *ns* shell. Bonding of the four equatorial atoms is enhanced by a large average separation of antiparallel spins, and this favors an orientation of the *ns* double ellipsoid with its long axis on a line joining the two polar electrons. Closer proximity of the *ns* electrons to the two polar *np* electrons reduces the average spin separation and discourages binding to the polar electrons. The effective radii for the halogen atoms may be approximately equal to the smallest nonbonded radius if the fluorine does not penetrate deeply into the xenon. If the xenon radius is taken directly from the observed interatomic distances in crystals, the bond length in XeF_4 may be as great as $1.90 + 0.85 = 2.75$ Å (*7*). This prediction does not follow from any fundamental aspect of the model, and it could be considerably less. Preliminary Raman

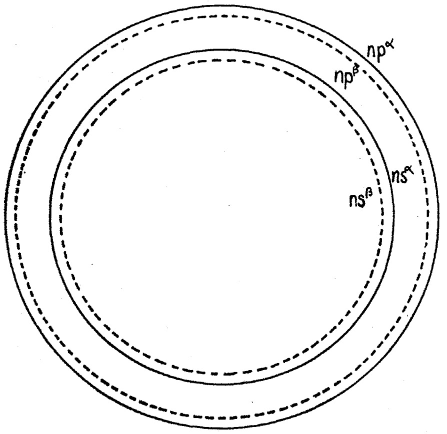

Fig. 1. Radial separation of antiparallel spin pairs in rare gas atoms.

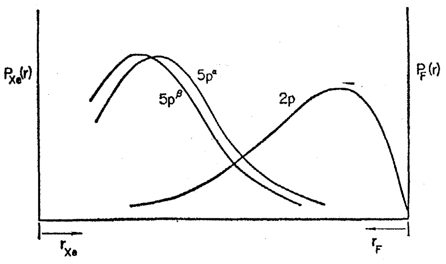

Fig. 2. Radial wave functions in binding region for XeF_4 or XeF_2. [$P^2(r) \equiv r^2R^2(r)$ = proportional to radial charge distribution]

spectra measurements of solid XeF_4[1] show the pattern of lines characteristic of a planar configuration (*1*), but this experiment on the solid is not nearly so indicative of the molecular configuration in the gas phase as is usually the case in chemical problems because the small binding energy may be comparable to the energy difference between two closely related crystal structures. If future gas phase electron diffraction studies or other experiments prove that XeF_4 is tetrahedral rather than planar, we will be forced to treat *s* and *p* shells as a single entity of eight electrons composed of two interpenetrating four-electron tetrahedra with opposite spins. Lennard-Jones (*8*), Linnett (*9*), and Pauling (*10*) have discussed this type of electron arrangement.

Linear dihalide molecules are also predicted by the model. We start with the same octahedral *np* distribution as before, but now the two halide atoms are attached at the polar positions. In contrast to the binding to equatorial electrons, binding to the polar electrons is enhanced by angular antiparallel spin correlation. Each polar electron is left relatively isolated by two surrounding pairs of almost cancelling antiparallel spin pairs. Circular symmetry in the equatorial plane and the increase in binding produced by antiparallel spin separation constrains the *ns* electron distribution to a nearly spherical shape. Binding through the polar position may allow the halogen atom to penetrate deeper into the noble gas atom, leading to a slightly more completed shell for the halogen, a slightly larger binding energy, and a shorter bond length (*11*).

The various symmetries inherent to the model exclude the possibility of an unambiguous stable trihalide molecule. As suggested by the experiment (*1*), the observed species of this form are probably transitory. The same argument holds true for any odd number of halogen atoms. Stable hexahalides should also be excluded. One of the postulates of the model is the potentiality for binding one halogen atom for every participating antiparallel spin pair. I believe that this is essentially correct and that a hexahalide molecule is not likely to be found, but because of the possibility of contributions from inner shells and the large angular separation of antiparallel spins in the *np* shell there is a definite probability that they exist.

No detailed attempt at present has been made to understand the apparently stable $XeOF_3$ and $XeOF_4$ species. But when the asymmetry of a third type of atom is introduced, a large variety of new electronic configurations become possible, each a small perturbation of the basic di- and tetrahalide configurations. In $XeOF_3$ the oxygen atom may be a direct substitution for a fluoride, being satisfied by the partial sharing of a single electron. A more nearly complete 2*p* shell is possible for oxygen in XeF_3OF, and xenon retains four bonds.

These predictions and discussion apply equally to all inert gas halogenide molecules, but there are other standard chemical effects which make it unlikely that the whole series will be observed as readily XeF_4 and XeF_2. In addition to the electron-sharing type of binding I have hypothesized there will be attractive dispersion forces between the atoms. The two forces may well be of comparable magnitude. Since the dispersive force is directly proportional to the polarizability of the noble gas atoms and since the polarizability decreases with decreasing atomic number for the inert gases (*12*), we may expect the probability of finding these molecules to decrease in similar fashion. The other controlling factor is the relative electronegativity of the halogenide atoms. Higher electronegativity favors binding and since electronegativity decreases along the sequence F, Cl, Br, I (*7*), we expect the probability of formation for inert gas halogenide molecules also to decrease along this sequence (*13*).

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13. I have had a helpful conversation with Professor C. P. Smyth.

17 October 1962

Second Order Neurons in the Acoustic Nerve

Abstract. In silver-stained preparations of the rat auditory system large neurons were distributed over the whole length of the acoustic nerve. These neurons received many synaptic endings which arose from collaterals of the acoustic fibers. The axons of the neurons ascended toward the cochlear nuclei. Similar neurons were found in the mouse, but not in the bat or cat.

In a variety of mammals, including the rat, mouse, guinea pig, cat, dog, and some bats, the lower auditory system is generally represented as consisting of an acoustic nerve which terminates in the several divisions of the cochlear nucleus. While the literature contains references to nerve cells extending from the cochlear nucleus into the acoustic nerve, these cells are usually considered as belonging to the ventral cochlear nucleus and as being confined to the head of the acoustic nerve. An example of this arrangement is to be found in the distribution of the cells of the interstitial division of the cochlear nucleus in the upper part of the acoustic nerve in the cat as described by Lorente de Nó (*1*).

In the course of a series of anatomical experiments on the auditory system of the albino rat (Sprague-Dawley) we found that the acoustic nerve contained a number of very large neurons scattered throughout its length. The general appearance of the acoustic nerve and its contained neurons is shown in Fig. 1*A*. Acoustic nerve neurons have been found in all the animals (50) we have ex-