The actual problem of producing materials with given properties cannot be solved before several auxiliary questions that are, moreover, of an independent, purely scientific, importance have been clarified. Such a question is first the relationship between the physical and chemical properties of compounds (molecules and solids) and their chemical structure; the second problem is to find the nature of the chemical structure of the substance, i.e., ultimately, the nature of the chemical bond. It should be noted that the second problem is an independent one, but the first cannot be solved without successful solution of the second.

The problems concerning the nature of the chemical bond have recently been worked out to a considerable extent both in theoretical and semiempirical investigations. Quantum-mechanical concepts, zone theory, the method of molecular orbitals, ideas on the donor-acceptor properties of transition metals, electronegativity, etc. play an important role in these studies.

The electronegativity concept was introduced by Pauling [1] and worked out in several papers [2–4]; it is now represented by a parameter, the electronegativity of atoms, that is expressed in nominal units and indicates the capacity of atoms to capture or donate so-called bond electrons. Although definite progress has been made with the theory of electronegativity, there still remain a few shortcomings that are related to the specific properties and the compound classes examined.

Fig. 1. Dissociation energy of diatomic molecules $D$ (drawn line) and the correlated activity $\alpha$ of the elements (dashed line). The electron structure of the normal atoms is indicated in parentheses above the line; the electron structure of excited atoms from which the reported $\alpha$ values were derived are given below the activity line.

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Among the shortcomings, or, rather difficulties, in the theory of electronegativity we may mention the following ones:

1. Although electronegativity fairly well explains the properties of ionic compounds, it gives a much poorer description of the properties of compounds with a large fraction of covalent bonds, especially if the bonds have a metallic character.

2. The theory of electronegativity is difficult to apply to compounds of transition metals characterized by a variable valence, and also to intermetallic compounds with an undefined valence.

3. The electronegativity values determined from different properties usually differ. It is interesting to note that the values differ not only in numerical magnitude but also in dimension.

In this respect it is convenient to introduce another parameter system that permits us to find the structure of molecules and solids, albeit to a first approximation, and is free of the shortcomings of the theory of electronegativity. The parameter system to be introduced should meet the following requirements: 1) it must be determined not only by the properties of compounds consisting of given elements but also by the properties of the elements themselves; 2) it must determine not only the degree of transfer of bond electrons from one element to another, but also the number of electrons participating in the bond, i.e., the valence of the elements in the compound considered; 3) it must make allowance for the fact that the bond electrons transferred from one element to another not only constitute the ionic fraction of the bond but participate together with transferred electrons in covalent and metallic bond types.

Starting from energetic and spectroscopic data, we attempt to introduce a set of parameters that might satisfy the above-mentioned requirements and characterize the formation of compounds.

We start from the excitation energies of the atoms from which the compound is formed. It is evident that atoms characterized by a high activity (in the usual meaning) have to be relatively weakly excited to form compounds; on the other hand, more inert atoms can form bonds only if the excitation energy is higher. If excitation of atoms is compared with the changes in the ground electron state that give rise to excited p-electron states (or increase the number of p-electrons), and these electrons stimulate the formation of bonds between the atoms (assumption by the authors), it becomes probable that a definite criterion that characterizes the activity of excited atoms in the formation of chemical bonds may be introduced. It should be borne in mind that the ionization energy of atoms is a definite stability criterion, as is illustrated by the group of noble gas atoms. Starting from these assumptions, we may state that it is convenient to introduce the dimensionless parameter $\phi$ as a criterion characterizing the activity of atoms in the formation of chemical bonds; this parameter is defined as the ratio between the excitation energy that generates p-electrons in the electron configuration on the atom and the first ionization energy of the atom.