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Interparticle interaction in condensed media: some elements are 'more equal than others'

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Contents

Abstract. Some aspects of interparticle and intermolecular interaction in condensed media are discussed, with special emphasis on hydrogen bonding (intermolecular interaction involving hydrogen atoms) and chemical bonds between carbon atoms. The intermediate strength of hydrogen bond is due to the hydrogen atom having no inner-shell electrons ('zero-sized ion'). Hydrogen-bonded substances exhibit a large number of modifications and aggregate states at or near normal temperature and pressure conditions. The diversity of carbon structures and the uniquely strong interatomic interaction they exhibit is determined by the position of carbon in the Periodic Table (the middle of the second period). The simultaneous presence of hydrogen and carbon atoms in substances leads to a huge variety of possible states (including metastable ones) for organic substances. The region of existence of 'complex' organics lies in a rather narrow temperature–pressure range of 100–1000 K and 0–1 GPa.

1. Introduction

One of the most beautiful and fruitful discoveries ever made in physics and chemistry, Mendeleev's Periodic Table of Elements, is remarkable, among other things, in that the very positions of the elements in it tell us much about interatomic chemical bonds and the properties of the condensed media the elements form. Although each element is, of course, unique, there are physical phenomena for which some elements are of particular importance. It is two such elements, hydrogen and carbon, which are at the focus of this note. In many compounds, including biological substances, hydrogen gives rise to what is called hydrogen bond, an interaction of intermediate strength between strong (covalent, metallic, and ionic) and weak (molecular and van der Waals) bonds. Carbon, whether in elementary substances or compounds, forms a wide variety of structures, including those with extremely high elastic moduli (for example, diamond or lonsdaleite), in which it varies in valence and is involved in various types of bonding. It is interesting that the reason why hydrogen and carbon behave in this special way can be explained in a rule-of-thumb manner by simply noting the positions they occupy in the Periodic Table.

Various aspects of interparticle interaction in condensed media are discussed in considerable detail in many chemistry textbooks, as well as in the context of chemical bonding theory [1], and much of what will be discussed here is quite familiar to chemists, even though expressed in a different language from theirs. However, such 'simple' objects as elementary substances do not attract much attention of chemists, thus raising the hope that this paper may be of interest to them as well. Add to this the fact that quantum mechanics, which underlies the chemical bond theory, was created by physicists, after all.

Given the Periodic Table copies currently in use, in which most elements are painted black or red, it is a self-suggesting question to ask a school or a college student which two elements are the only ones usually painted blue. It is not our two 'heroes' hydrogen and carbon: their respective colors are also red and black. The correct answer is mercury (Hg) and bromine (Br), and what makes them that special is that their associated elementary substances are liquid under normal conditions, whereas all the other elementary substances are either solid (black color) or gaseous (red color).

That so few elements are liquid under normal conditions is in strong contrast to the fact that we see dozens of liquids every day, water, oil, and hydrocarbons being just the first examples that come to mind. Why is it then that liquids are so rare among elementary substances under normal conditions, while at the same time being numerous and diverse among

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compounds, especially organic ones? To understand this, let us first take a look at how particles interact in various classes of substances.

2. 'Strong' interatomic interaction in condensed media

Each chemical bonding is ultimately underlain by an electromagnetic interaction. If atoms have some of their inner electron shells unfilled, then the partial delocalization of electrons from different atoms decreases the energy of the system — or, in other words, chemical bonding occurs. Comparing interatomic covalent and metallic bonds, in the former collectivized electrons mainly concentrate along interatomic directions, whereas in the latter their density distribution is more uniform. Compounds made up of different atoms may experience ionic bonding, which involves the collectivization of electrons and in which the electron density partially shifts from one kind of atoms to another.

There is currently no doubt that chemical bonding in molecules and condensed media can be described to any degree of accuracy using quantum mechanical calculations. The reality is, however, that even with the most powerful modern computer clusters accurate *ab initio* calculations can be made only for a few dozen light atoms with few inner-shell electrons. Note that the concept of chemical bond in condensed media is itself only loosely defined. In physical terms, what the concept is about reduces to calculating the energy of the ion lattice system with the corresponding electron density distribution, and in many cases (for example, in metals) the term 'chemical bond' is not really of much use.

At the qualitative level, however, the binding (or cohesive) energy of atoms can always be tentatively viewed as consisting of several contributions, the dominant one being the Coulomb interaction (in the general sense of the term, that includes the electron exchange interaction due to the quantum nature of electrons). For metals and covalent systems, this is, loosely, the Coulomb interaction between electrons and ions, whereas for ionic materials this is, again loosely, the interaction between ions of opposite signs. The natural unit with which to measure the Coulomb interaction is the rydberg ($\mathrm{Ry} = me^4/2\hbar^2 = 13.6$ eV), the ionization energy of the hydrogen atom. Because the effective sizes of most atoms are several times larger than the Bohr radius and because interatomic interaction comprises several terms of different signs, the binding energy per atom in materials with metallic, ionic, and covalent types of interatomic interaction turns out to be several times smaller than Ry and ranges between 1 and 10 eV. Heating a material causes the thermal excitation of the atomic vibrations which, on reaching some atom-specific critical values, leads first to the melting and then to the vaporization of the material. Binding energies of as much as 1 – 10 eV per atom (see Fig. 1) lead to high values for the critical liquid–gas transition point ($\sim 10^4$ K), the boiling point ($\sim 10^3 - 10^4$ K), and, usually, the melting point ($\sim 10^3$ K) (Fig. 2). Accordingly, under normal conditions most materials with strong interatomic bonds (metallic, covalent, and ionic) should be solid — which is indeed the case. Mercury (Hg) makes here the sole exception. Apart from mercury, caesium (Cs) and gallium (Ga) also have melting points close to room temperature. There are two factors which explain these relatively low melting points.

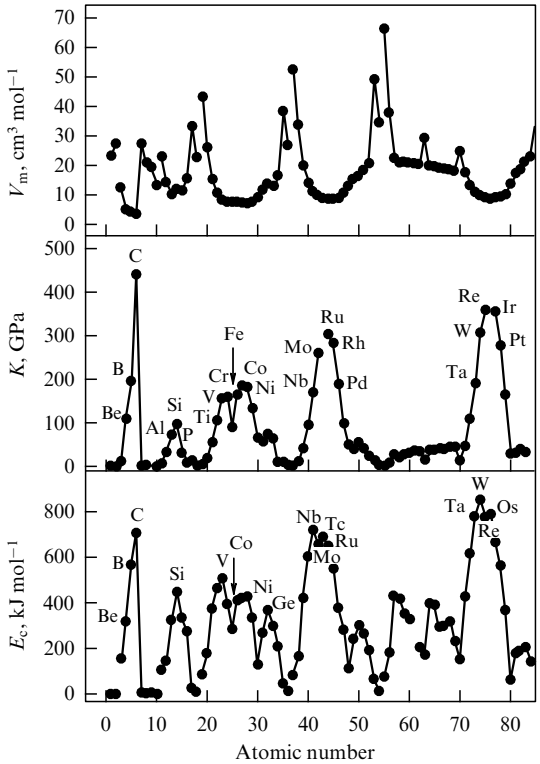

Figure 1. Molar volume, modulus of dilatation, and binding energy as functions of atomic number for some elementary substances.

First, Hg and Cs have lower binding energies than most metals. The electronic subshells of mercury atoms are filled (the electronic configuration of the Hg atom is as follows: [Xe] $4f^{14}5d^{10}6s^2$), so that they are in a sense more neutral than those of most other metals, and the delocalization of valence electrons in condensed phases of mercury is rather insignificant. In addition, because of the large size of the Hg and Cs ionic cores and due to the strong screening of their nuclei by the f electrons, the interatomic interaction in Hg and Cs is much weaker than in most metals, with the result that for Hg the critical temperature for the liquid–gas transition is $T_c \sim 1750$ K, compared to as much as $T_c \sim 5 \times 10^3 - 10^4$ K for most metals and covalent and ionic compounds.

Another reason for the relatively low melting points in a number of metals is the strongly noncentral interatomic interaction and, as a result of this, the softening of the spectrum of atomic vibrations along certain directions. 'Soft' directions — the factor which causes crystal to melt — are sometimes due to the anisotropic structure of the crystal (as, for example, in Ga, Bi, and to some extent Hg), but, quite unusually, can also be found (with increasing temperature) in isotropic lattices — due again to the fundamentally noncentral interaction in metals. A nice example is the anomalous softening of the elastic modulus of C_{44} in a strongly compressed face-centered cubic (fcc) Na lattice and the anomalously low melting point of Na ($T_m \sim 300$ K) at $P \sim 100$ GPa [2, 3].

Summing up, the melting points (and even more so, the boiling points) of most metals and covalent and ionic substances should be considerably above room temperature; exceptions, usually due to a random coincidence of factors, are few and merely confirm the rule.

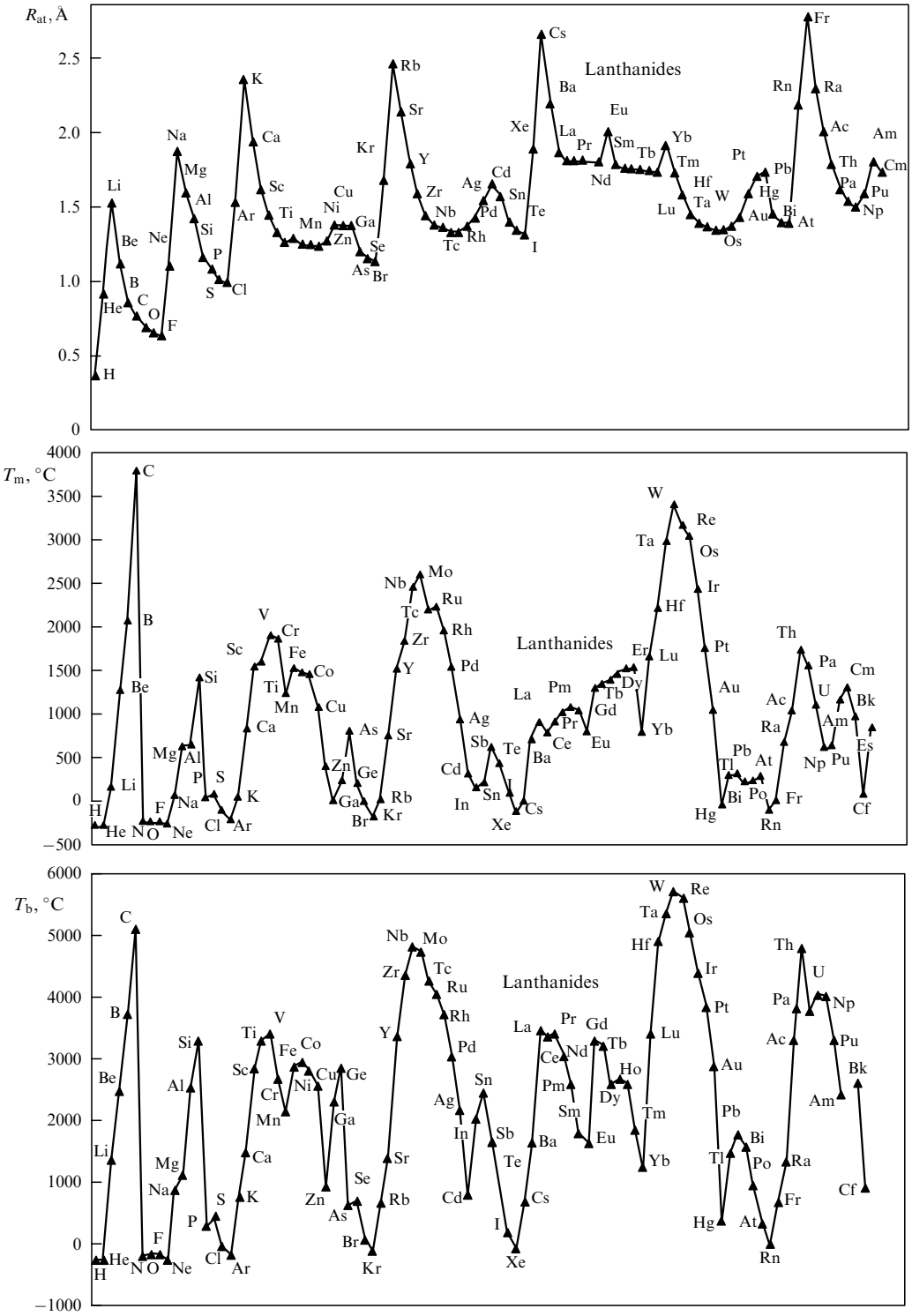

Figure 2. Effective atomic radius R_{at}, melting point T_m, and boiling point T_b for elementary substances.

3. 'Weak' interatomic interaction in condensed media

Let us next turn to weak interparticle interaction. If the outer electron shells of atoms are filled (rare gases), bringing the atoms closer together has no electron collectivization effect, and there is no Coulomb interaction between the particles in the system. Nor is the dipole–dipole interaction present if the particles are spherically symmetric. It is only in the next order of perturbation theory where interaction — namely, the fluctuation dipole–dipole (or van der Waals) interaction — comes about, with the attractive potential of the form $U(R) \sim r_0^5/R^6$, where r_0 is the effective size of the atom, and R is the interatomic distance, being less than the Coulomb interaction potential by a factor of $(r_0/R)^5$. For rare gases, one has $R/r_0 \sim 3$, so that their attractive potential and binding energy are 2–3 orders of magnitude less than the strong Coulomb interaction potential, i.e., the binding energy ranges 0.01–0.1 eV per atom (see Figs 1 and 3). Often groups of a few neighboring atoms held together by strong covalent

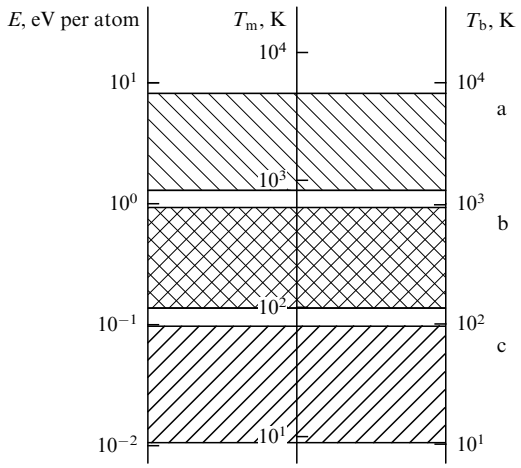

Figure 3. Ranges of per-atom binding energies and corresponding ranges of melting and boiling points for differently bonded substances: (a) 'strong' (covalent, metallic, ionic) bond; (b) hydrogen bond; (c) 'weak' (molecular, van der Waals) bond.

bonds are in turn linked together by weak dipole–dipole or fluctuation dipole–dipole bonds. Such groups of bound atoms are then called molecules and the bonds between them, molecular.

For nonpolar molecules like H_2, N_2, and O_2, weak intermolecular interaction has a similar nature to the van der Waals interaction. Polar molecules like HCl, with their dipole moments, exhibit dipole–dipole interaction, the corresponding attractive potential being $U(R) \sim r_0^2/R^3$. The intermolecular interaction energy, which is usually two orders of magnitude less than the Coulomb interaction energy in the case of strong interatomic bond, amounts to ~ 0.1 eV per atom.

As a result, rare gases and most molecular substances have boiling points (and critical liquid-to-gas transition temperatures) of as low as $\sim 10^2$ K and correspondingly low melting points of $\sim 10-10^2$ K (see Figs 2 and 3). Under normal conditions these substances are in a gaseous state. The only exceptions among elementary molecular substances are Br_2 and I_2, which under room conditions reside in the liquid and solid states, respectively. The reason for this is the large sizes of the Br and I atoms and, hence, of the molecules Br_2 and I_2. For large-sized molecules, the atoms in the molecule are about as close to each other as to their counterparts in the neighboring molecules, thus invalidating the view of a substance as a collection of molecules. For small-sized molecules like H_2 or N_2, where covalent bonds within the molecules are two orders of magnitude as large as those between the molecules, molecules look almost spherical at distances where the interatomic interaction potential has a minimum, and the intermolecular interaction is similar to the van der Waals interaction. For large molecules like Br_2 and I_2, the interaction becomes stronger because of the contribution from the interaction with the atoms of the neighboring molecules.

In fact, with the intramolecular interaction only several fold greater than the intermolecular, the very subdivision of the substance into molecules is rather questionable. This is even more true for numerous covalent and ion-covalent compounds, such as SiO_2, MgO, and As_2S_3, in which dividing the material into molecules is acceptable only as a way to describe the structure of a material but by no means as a tool for estimating the binding energy. Notice once more that as far as the interatomic interaction is concerned, the binding energy is larger for light elements with small atomic radii because in this case the Coulomb interaction is stronger; for intermolecular bonding the situation is the reverse — bond is stronger between large molecules (because their dipole moment, induced or permanent, is larger) — and even the concept of a molecule as an individual structural unit is too loose to be of value. The intramolecular bond is, of course, again stronger for molecules made up of light elements with small atomic radii (like N_2, CO and some others).

Hence, for most molecular substances the boiling point (and even more so, the melting point) are much below room temperature, the exceptions (which are rare) being due to the fact that interparticle interactions can no longer be considered molecular. As a result, chemical bond in the condensed phases of Br_2 and I_2 is intermediate between the strong and weak bonds.

Thus, we now see why so few elementary substances are in the liquid state under normal conditions. Referring to Fig. 2, this is clearly reflected in the way the melting and boiling points of substances depend on the atomic number. On the other hand, as already noted, we see lots of liquids around us in our everyday life. And one thing which is common to almost all of them is hydrogen bond.

4. Hydrogen bond

It is hydrogen bond which is intermediate between the strong (covalent, metallic, ionic) and weak (van der Waals and molecular) bond types. The hydrogen binding energy is typically in the range of 0.1 to 1 eV per molecule, exactly corresponding to the boiling and melting point ranges of 10^2-10^3 K (see Fig. 3). The special feature of hydrogen bonding is that a hydrogen atom in one molecule forms a second, weaker bond with an atom in another molecule. This latter atom (normally, F, O, or N) should be highly electronegative and have an unshared electron pair, i.e., a pair not involved in the intramoleculr chemical bonding. Typical examples of hydrogen-bonded substances are water, HF, alcohols, and glycerin (Fig. 4). While originally thought

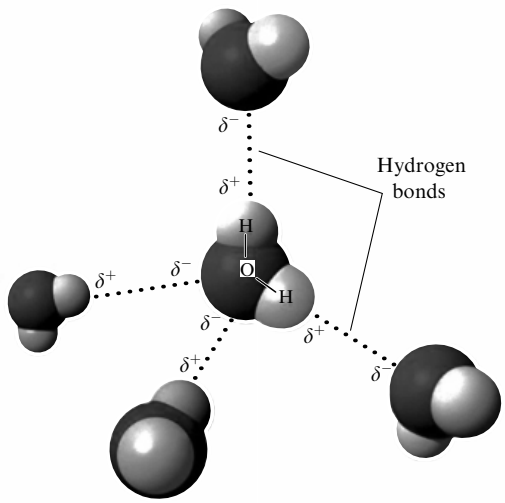

Figure 4. Hydrogen bonds between water molecules.

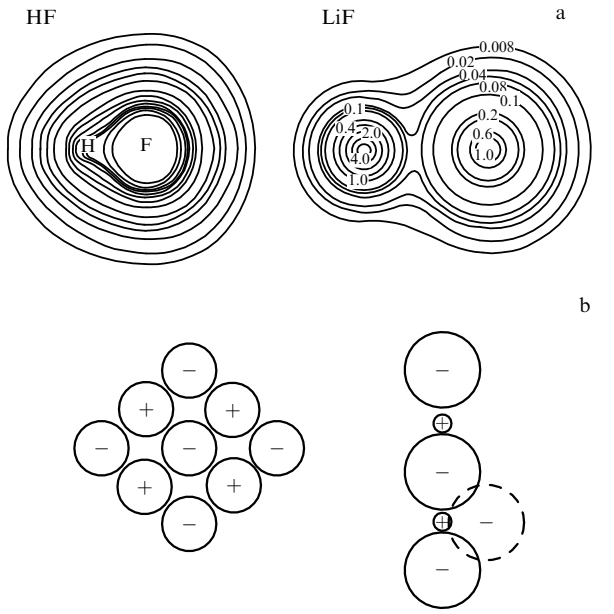

Figure 5. (a) Qualitative electron density distribution in HF and LiF molecules, and (b) the 'geometric' factor in the formation of ionic crystals and H-bonded chain structures.

of as primarily an electrostatic bond between molecules, it was later demonstrated that hydrogen bonding is heavily dependent on the donor–acceptor mechanism, in which charge is partially transferred from the unshared electron pair of an electronegative atom of one molecule to the 1s orbital of the H^+ ion [4–6].

Hydrogen bond is currently considered as intermediate between the polar covalent, ionic, and dipole–dipole molecular bond types [4–6] and can to the first approximation be regarded as the limiting case of dipole–dipole bond, which is much stronger than the usual molecular bonds due to the small size of the hydrogen atom and extremely (in fact, vanishingly) small size of the hydrogen ion (in fact, a proton).

Helium aside, hydrogen is the only element that has no inner electron shell, with the result that hydrogen-containing molecules may approach one another close enough to form intermediate-strength bonds. An additional feature of the hydrogen atom — the higher ionization potential compared to most other atoms — results in no noticeable amount of charge being transferred from the hydrogen atom to the anion in the molecule. Further, the small size of the hydrogen atom creates pure geometric reasons why it cannot effectively interact with more than two of its neighbors because, due to the Coulomb repulsion, no additional anion can come close to the hydrogen ion (Fig. 5). As a result, hydrogen bond can never become 'real' ionic bond.

For example, whereas hydrogen bonding between HF molecules cannot produce anything more than a chain, Li and Na combine with fluorine into an ionic crystal in which Li and Na ions form ionic bonds with the whole of their environment of fluorine ions (see Fig. 5). The result is that, although Li and Na atoms are larger than the hydrogen atom, the binding energies of LiF and NaF crystals are higher than that of HF. The polar nature of hydrogen bond, combined with the fact that hydrogen atoms can enter only two (weak and strong) types of bonding, leads to a large diversity of loosely packed network structures based on molecules containing H, O, F, N, etc. atoms.

It should be noted that at ultrahigh pressures, when intermolecular and intramolecular separations become comparable, hydrogen atoms can form an ion sublattice. In particular, H_2O ice at pressures of around 100 GPa actually transforms into an ionic crystal in which oxygen atoms are at the sites of a body-centered cubic (bcc) lattice, and hydrogen ions are located midway between neighboring oxygen atoms [7]. Also, ammonia (NH_3) can transform into an ionic crystal state at megabar pressures [8].

To reemphasize, what makes hydrogen bonding unique is the unique feature of the hydrogen atom — the absence of an inner electron shell. Helium, the only other element without an inner electron shell, has a filled valence s shell and forms weak van der Waals bond between atoms in a condensed state at low temperatures. Because of the absence of an inner electron shell in the atom, the compressibility of solid and liquid helium is higher than that of other rare gases, and the metallization pressure of solid He is lower than that of solid Ne [9].

Thus, it is because of the intermediate energy of hydrogen bond that H-bonded substances make transitions between their various modifications and between all three aggregate states at temperatures and pressures close to normal. So, if you find under terrestrial conditions a liquid you never knew of before, chances are high that this is a hydrogen-bonded substance.

Hydrogen bonding plays a fundamental role in biological substances like proteins and genetic code carrying DNA. In particular, it is this bond which links the bases of the opposite DNA strands. At room temperature this bond is easy to break — thus allowing the transmission of information — but not easy enough that this could become a background process (which would make information storage impossible).

5. Diversity of carbon structures

Turning to carbon — the second element of the two 'more equal than others' — there are many respects in which it is unique. First, carbon atoms exhibit a diversity of valence and electronic hybrid states when participating in forming covalent bonds (sp, sp^2, sp^3 hybridization) (Fig. 6), thus leading to a tremendous diversity of crystalline and amorphous carbon structures with carbon coordination numbers of 2, 3, 4 or any other (on the average) in this range. Along with strong covalent interatomic bonds, weak van der Waals interaction can take place between certain groups (molecules) of carbon atoms. For example, weak interaction in graphite occurs between carbon planes; in carbynes, between atomic chains, and in fullerenes, between closed carbon molecules. As a result, the structures carbon can form are three-dimensional (diamond, lonsdaleite), quasi-two-dimensional (graphite), quasi-one-dimensional (carbyne), intermediate between the last two (nanotubes), and quasi-zero-dimensional (fullerites). Not that the above list of carbon modifications is comprehensive, though: there are in fact an infinite number of both real and hypothetic structures of this kind (Figs 7 and 8).

Another remarkable feature of carbon is that carbon–carbon covalent bond is one of the strongest. As a result, the carbon modifications — diamond and lonsdaleite — have the highest elastic moduli and the best mechanical properties among all substances known [18].

The unique behavior of carbon in forming condensed phases stems from its unique position in the Periodic Table of

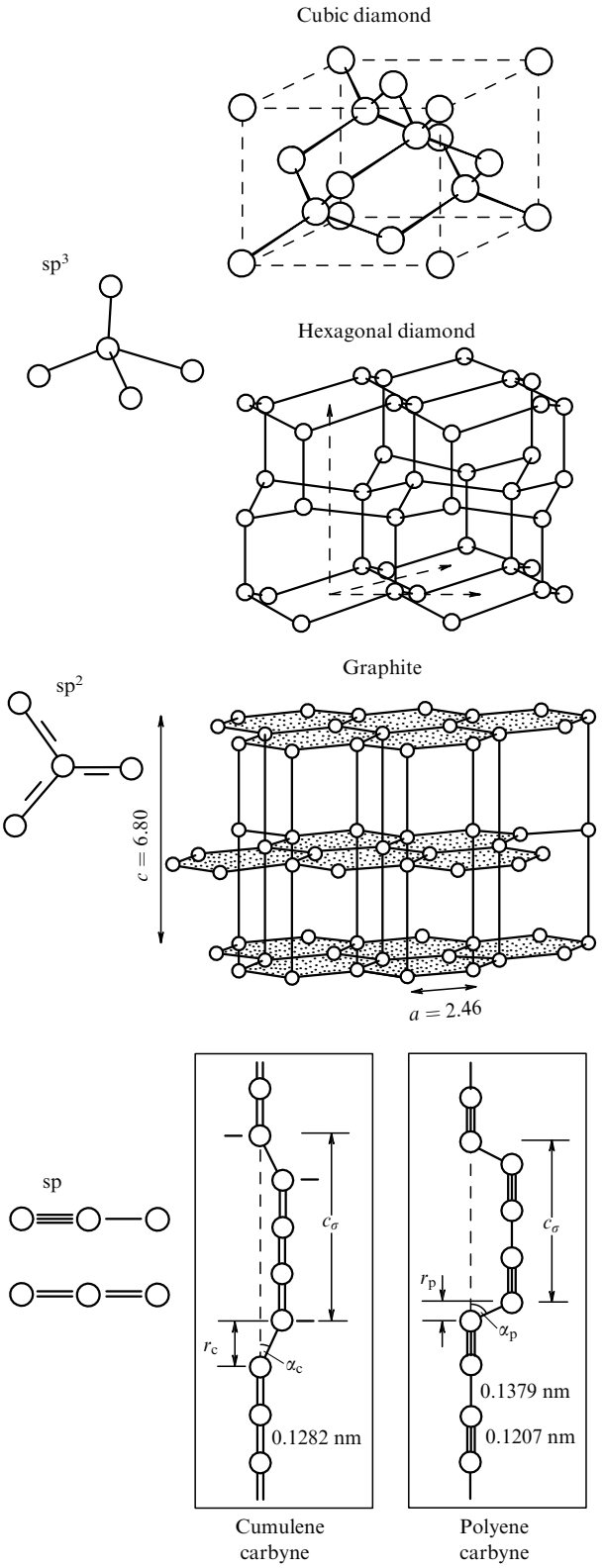

Figure 6. Illustration of different hybridization types and various valencies in carbon structures.

Elements, in the mid-second period (see Figs 1 and 2). Accordingly, carbon has a very small ion size (there are only two electrons in the inner shell) and at the same time has a large number of electrons — four — ready to take part in forming chemical bonds (the maximum number possible, in fact, because N and O, the second-period elements that follow carbon, obey the '$8 - N$' rule when forming bonding orbitals).

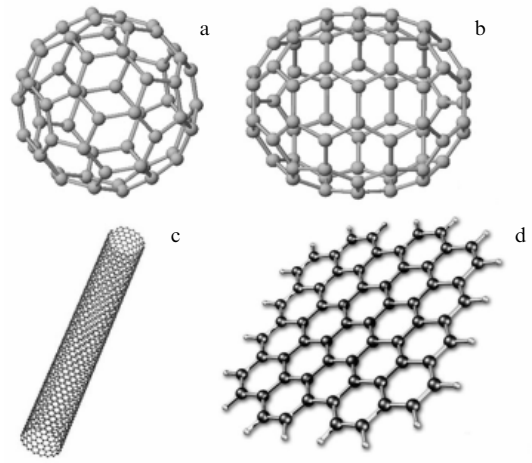

Figure 7. 'Unconventional' carbon modifications: (a) C_{60} fullerene molecule; (b) C_{70} fullerene molecule; (c) nanotube, and (d) carbon plane (graphene).

Thus, because of their small size, carbon ions are held together by extremely strong covalent bond, resulting in three-dimensionally bonded carbon phases (diamond and lonsdaleite) being superior to all known substances in terms of atomic density and, moreover, in terms of density per valence electron [19]. It is this which explains the record high values of elastic moduli, cohesion energies, and melting and boiling points in carbon phases (see Figs 1 and 2). A further consequence of the small size of the carbon ion is the very strong covalent bond between carbon atoms at various types of hybridization of electronic states. For π-bonds, the strong overlap of the electron clouds of neighboring atoms, located on both sides of the chemical bond axis, results in the energy of π-bond being not much less than that of σ-bond (where orbitals overlap along the bond axis) (Fig. 9). This, in turn, leads to much stronger and shorter sp- and sp^2-bonds as compared to the sp^3-bonds and also results in nearly the same binding energies per carbon atom in different modifications with a different coordination and valency of carbon atoms.

For example, the binding energy per atom in graphite exceeds that in diamond by a mere 0.02 eV (note that the binding energy itself is 7.2 eV). At the same time, without taking into account the zero-vibration energy of the atoms, the cohesion energy of diamond is 0.01 eV higher than that of graphite (also per atom) [20]. For carbon's subgroup neighbors, silicon and germanium, the situation is quite the opposite. Because in silicon and germanium atoms inner electron shells (and hence ions) are larger in size than those in carbon, the only bonds efficient enough for them are σ-bonds; π-bonds do not form, and any structures with sp- and sp^2-states have much lower energies than the diamond-like phases of Si and Ge, with their sp^3-atoms. As a consequence, Si and Ge do not exhibit graphite- or fullerite (Si_{60}, Ge_{60})-like modifications because these would have a very low binding energy and poor stability. Thus, carbon's unique position in the Periodic Table enables it to form a wide diversity of carbon structures and leads to record high values of binding energies and elastic moduli in a number of carbon modifications.

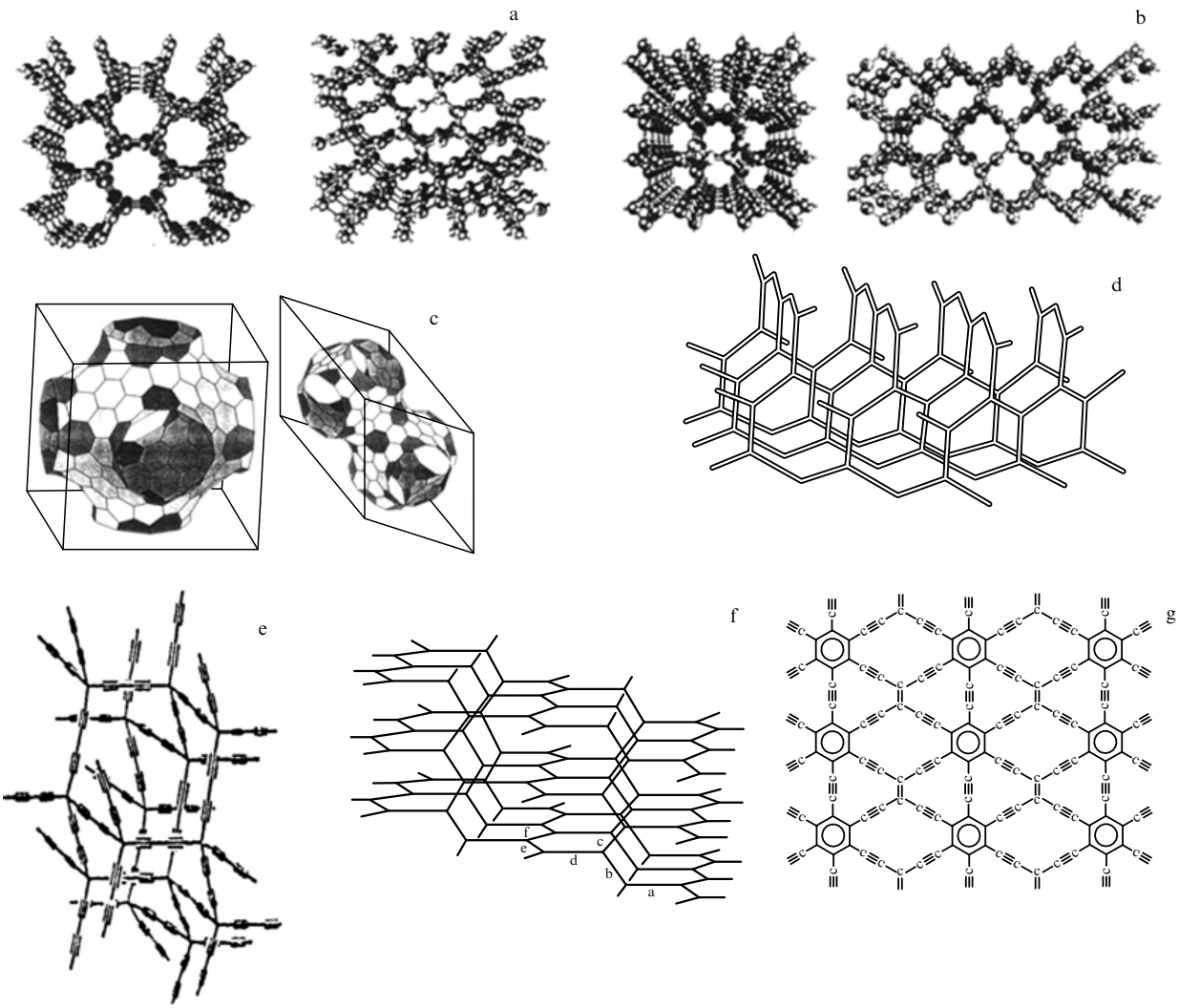

Figure 8. Hypothetical carbon structures: (a) R6-sp^2-structure [10]; (b) BCT-8-sp^2-structure [10]; (c) carbon schwartzites [11–13]; (d) H6-sp^2-structure [14, 15]; (e, f) three-dimensional combined sp-sp^2-structures [16], and (g) quasi-two-dimensional combined sp-sp^2-structures (graphynes [17].

6. Organic materials: 'hydrogen-bonded carbon structures'

The diversity of carbon structures complements the packing behavior diversity of H-bonded molecules when the substances contain both carbon and hydrogen atoms. If molecules contain oxygen and/or nitrogen along with carbon and hydrogen, then condensed phases can simultaneously exhibit exceptionally strong intramolecular covalent bond between carbon atoms; moderately strong intramolecular carbon–hydrogen bond, and intermediate-strength intermolecular hydrogen bond. Importantly, one and the same chemical composition can in fact exhibit an infinite diversity of molecular structures with similar cohesion energies. Carbon atoms in such structures form various types of 'rigid skeletons' made of chains, rings, and quasi-two- and quasi-three-dimensional sections, whereas nitrogen and oxygen atoms, also with a small-sized inner electron shell, are in a sense no less important in that they can build themselves into such skeletons at various points and so give rise to effective hydrogen bonding in certain directions.

It thus becomes clear how 'complex' organic chemistry is evolved from 'simple' inorganic chemistry. Where the highest diversity of similar-energy structures (most of them metastable!) occurs [21] is precisely in light-element molecular compounds which — a necessary condition — contain carbon and hydrogen. Known organic compounds, i.e., hydrocarbon derivatives, currently number more than 30 million, whereas inorganic substances — whatever other atoms they comprise — number in the 'mere' hundreds of thousands.

Closely related to the issue of the diversity and complexity of organic materials is the issue of the complexity of biological objects, for which the infinite diversity of structures with similar energies is a point of fundamental importance. The simple arguments and estimates given above, in fact, rule out an alternative — i.e., other than hydrocarbon-based — biological substances like those from silico-organic life. Similar-energy structures based on Si or other elements would be infinitely less diverse than carbon- and hydrogen-based organic compounds. While silicon and other elements can, of course, be present in considerable amounts in biological objects, their structure forming role is negligible.

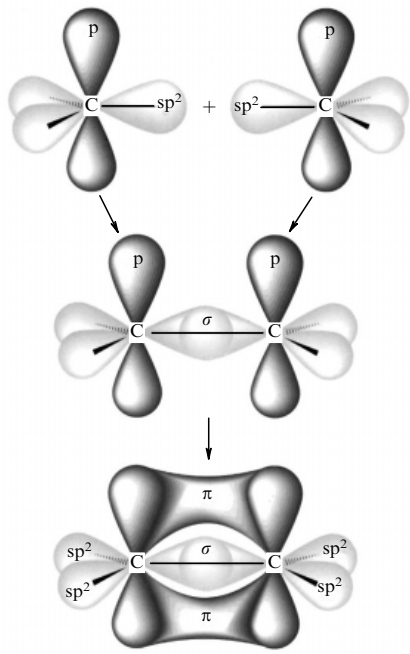

Figure 9. Schematic formation of σ- and π-bonds in sp^2-hybridized carbon modifications (graphite, nanotubes, fullerenes). Note that π-bonding works only at small interatomic distances.

As already noted, transitions between various modifications (in particular, aggregate states) of H-bonded substances occur in the temperature range $10^2 - 10^3$ K. The corresponding pressure range for organic substances to reversibly transform from one state to another is from 0 to 1 GPa [21]. Thus, what we call 'complex' biological life can exist only in the narrow temperature–pressure range of $10^2 - 10^3$ K and 0 – 1 GPa. For temperatures beyond or pressures above this range, the number of possible structures and states with similar energies falls of by a factor of as high as several thousand.

It should be noted, though, that conditions that gave rise to complex organic compounds and indeed to living objects themselves is a broad and rather controversial topic which is beyond the scope of this note. On the other hand, of interest is the very fact that — with a closer look at the Periodic Table of Elements — even very complex and important things can be discussed in such a 'simple' way.

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