

## LITHIUM – HYDROGEN – OXYGEN

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By the example of spectra of hydrogen and deuterium we notice the small ~0.03 % distinction of wavelengths in the same series. This regularity should be observed also concerning other elements and their isotopes.

Natural lithium consists of two stable isotopes:  ${}^6\text{Li}$  – 7.52% and  ${}^7\text{Li}$  – 92.48%. We have checked up spectra of lithium in three databases, but have not found any hint on distinction of wavelengths  ${}^6\text{Li}$  – 7.52% and  ${}^7\text{Li}$ , in spite of the fact, that wavelengths in these databases are resulted within the tenth share of picometer, i.e. accuracy is not worse than 0.001%.

In polytronic model of atom, spectral series of isotopes can be used for exact calculation of diameters of polytrons and crystallographic angles in atoms. Thus, available experimental data can be used only for definition of the approximate sizes of atom of lithium.

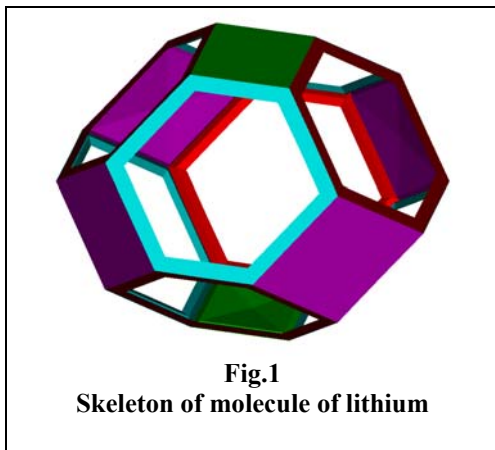
The second way for definition of the sizes of atoms and their geometry is based on using of parameters of crystal lattice, which also are determined with spectroscopic methods. It is considered to be, that these methods possess the highest accuracy.

We shall try to determine quantitatively accuracy of a spectral method concerning crystal lattices of lithium.

Lithium is very ductile metal. Temperature of melting is 453.69K; temperature of boiling is 1620K. At temperature higher 77K lithium shows volume-centered cubic lattice with parameter  $a=351.00\text{pm}$  ( $\alpha$ -Li). The volume for one atom is equal  $V_{\text{at}}=21.622 \text{ \AA}^3$ . At temperature lower 77K lithium shows face-centered cubic lattice with parameter  $a=437.9\text{pm}$  ( $\beta$ -Li). Volume for one atom  $V_{\text{at}}=20.993 \text{ \AA}^3$ . In some handbooks the information is sited, that at temperature lower 77K lithium shows hexagonal close-packed lattice with parameters  $a=308\text{pm}$ ,  $c=482\text{pm}$ . The volume for one atom is equal  $V_{\text{at}}=19.799 \text{ \AA}^3$ . Density of liquid lithium at temperature of melting is equal  $515\text{kg/m}^3$ . The corresponding calculation gives average volume for one atom in a mix of liquid lithium 7.52%( ${}^6\text{Li}$ ) + 92.48%( ${}^7\text{Li}$ )  $V_{\text{at}}=22.380\text{ \AA}^3$ .

As to solid lithium, in various handbooks the density of solid lithium from 533 up to 539  $\text{kg/m}^3$  is given. Thus, the average volume for one atom in solid литии is in limits from 21.624 up to  $21.384 \text{ \AA}^3$ . The error of calculation of the linear sizes of atom at the given method makes 0.3%. Solid lithium possesses high temperature linear expansion coefficient  $56 \times 10^{-6} \text{ 1/K}$ . If we shall accept, that the above-stated parameters are measured at temperature 77K, then at temperature 273K ( $0^\circ\text{C}$ )  $\alpha$ -Li will have volume-centered cubic lattice with  $a=351 \times (1+196 \times 56 \times 10^{-6}) = 354.85\text{pm}$ . Accordingly,  $\beta$ -Li at temperature of absolute zero will have parameter of face-centered cubic lattice  $a=437.9 \times (1-77 \times 56 \times 10^{-6})=436.01\text{pm}$ . Thus, in the specified range of temperatures the error can achieve 1%.

On the basis of the aforecited data we have found diameter of lithium polytron  $D_{\text{Li}}=252.6\text{pm}$ .



Gaseous lithium consists of diatomic molecules  $\text{Li}_2$ .

Energy of dissociation of molecule of lithium is equal  $99.0 \text{ kJ/mol} = 1.026 \text{ eV/molecule}$ . We have not any bases to consider, that at temperature lower, then temperature of evaporation, lithium has atomic structure. Therefore, we have made modeling of crystal of lithium from diatomic molecules. For more evident representation, we shall represent molecule of lithium as skeleton of truncated bipyramid (fig.1).

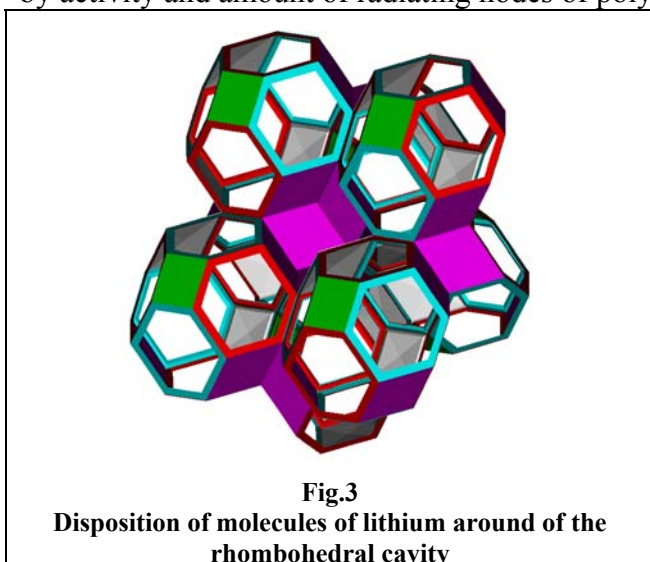
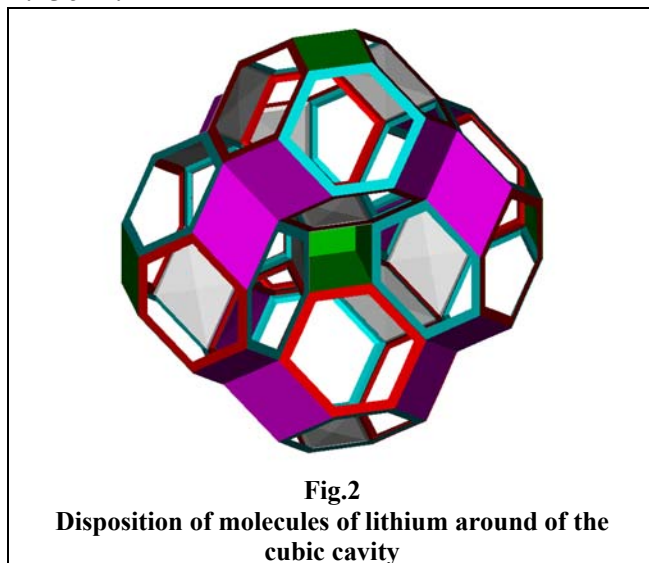
Bipyramid has 8 six-angle sides, four rhombic sides and two square sides. The main axis of symmetry passes through square sides of bipyramid. Molecules of lithium are connected with each other in the crystal by six-angle

sides in such a manner, that the main axes of any neighboring molecules are perpendicular each other. At such connection in the crystal, the cavities of two kinds are formed. In figs.2 and 3 the disposition of molecules of lithium around of the specified cavities is shown.

The volume of the cubic cavity in fig.2 is equal  $2.236\text{\AA}^3$ .

The cavity in fig.3 represents the regular polyhedron, which is formed by twelve rhombuses. The big diagonal of the rhombus is equal to static diameter of lithium polytron (252.6pm). The distance between two opposite rhombuses in 12-hedron also is equal to static diameter of polytron. The volume 12-hedron is equal  $11.398\text{\AA}^3$ . The net volume of truncated bipyramid is equal  $34.194\text{\AA}^3$ . Accordingly, one atom of lithium occupies in molecule the volume  $17.097\text{\AA}^3$ .

At temperatures higher and lower 77K, lithium shows various types of crystal lattices – cubic and hexagonal. Apparently, this property of a crystal of lithium is conditioned by activity and amount of radiating nodes of polytrons in cavities of that and other type.

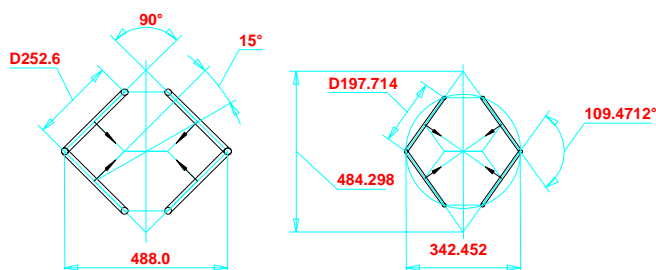


Liquid lithium, at temperature 900-1000K and at the increased pressure, actively reacts with molecular hydrogen  $H_2$  and with molecular deuterium  $D_2$ . As a result of this reaction, the lithium hydride (LiH) and the lithium deuteride (LiD) are formed. Enthalpy of formations is  $\Delta H^0_{\text{solid}} = 90.7 \text{ kJ/mol} = 0.94 \text{ eV/molecule}$ .

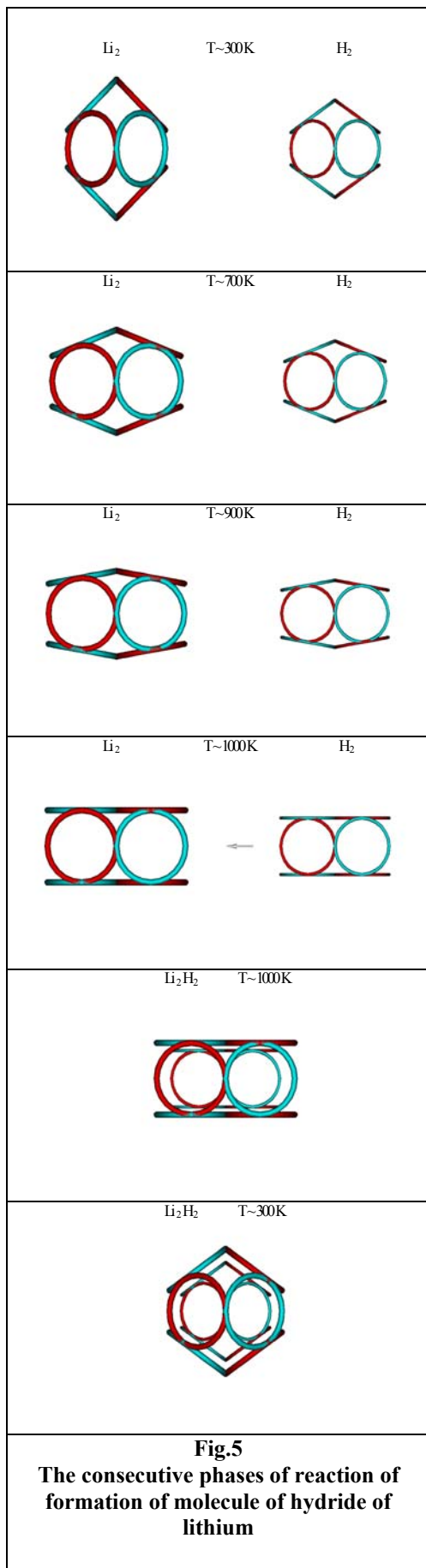
Hydride of lithium has temperature of melting 965K, i.e. on 511K higher, than temperature of melting of lithium. Solid hydride of lithium has cubic face-centered lattice with parameter  $a=408.3\text{pm}$ . Density of crystal of hydride of lithium is  $780 \text{ kg/m}^3$ .

Corresponding calculations show, that volume of the crystal, falling at one molecule of hydride of lithium under formula LiH, is in limits  $V_{\text{mol}}=17\pm 0.05\text{\AA}^3$ , i.e. the volume of diatomic molecule of hydride of lithium is little bit less than volume of atom of lithium.

In fig.4 the dispositions of polytrons in the molecule of lithium (the left drawing) and in the molecule of hydrogen (the right drawing) schematically are shown.



**Fig.4**  
**Disposition of polytrons in molecule of lithium (the left drawing) and in a molecule of hydrogen (the right drawing)**



In fig.5 the consecutive phases of reaction of formation of four-atomic molecule of hydride of lithium from one molecule of lithium and one molecule of hydrogen in the atmosphere of molecular hydrogen are shown.

The high temperature and high pressure promote for fast penetration of molecule of hydrogen into molecule of lithium. Reaction proceeds with absorption of energy.

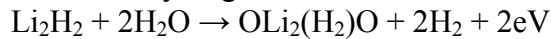
Decomposition of hydride of lithium on molecular hydrogen and molecular lithium occurs upside-down.

Reaction of decomposition proceeds also at high temperature, but in an inert atmosphere or in vacuum.

In fig.6 the crystal lattice of hydride of lithium is shown.

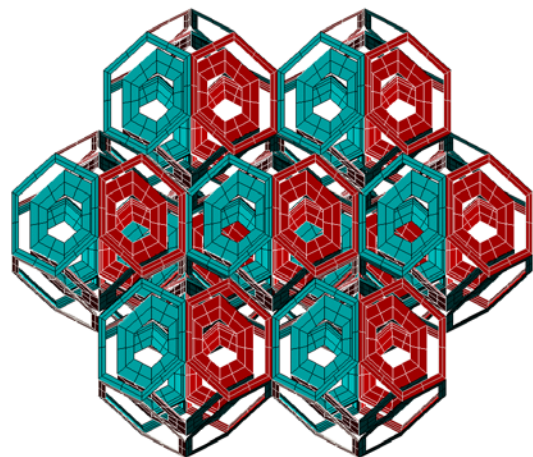
This close-packed lattice can show as cubic, and hexagonal structure.

Under normal conditions the hydride of lithium reacts with water and decomposes on hydroxide of lithium and molecular hydrogen:



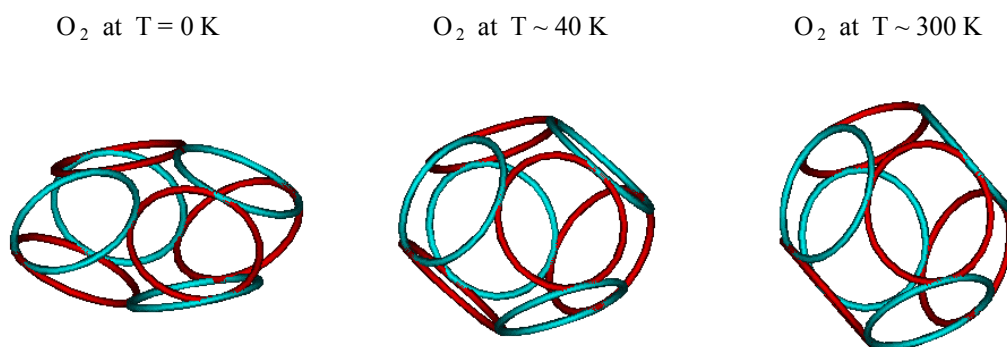
At interaction of 1kg of hydride of lithium with water it is generated 2.82 m<sup>3</sup> or 0.2535kg of molecular hydrogen.

By the example of hydride of lithium we have shown, that as a result of reaction of association of two molecules, the external molecule (Li<sub>2</sub>) gets crystallographic angles of an internal molecule (H<sub>2</sub>). In this case, crystallographic angle in the molecule of hydride of lithium is equal 109.4712°, i.e. same, as well as in molecule of hydrogen.



**Fig.6**  
The crystal lattice of hydride of lithium  
Кристаллическая решетка гидроксида лития  
(axonometric projection)

Change of temperature in crystal always causes the change of crystallographic angles in atoms and molecules. The polytronic model explains this effect by that, at change of temperature, the amount of nodes in polytrons and spatial position of the connected nodes are change. Oxygen is one of elements, which possesses abrupt nonlinear dependence of crystallographic angles from temperature. On fig.7 three molecules of oxygen are shown at various temperatures. The left molecule has a dihedral angle at top of bipyramid equal  $132.4708^\circ$ , the average molecule –  $90^\circ$ , the right molecule –  $70.5288^\circ$ .



**Fig.7**  
**Forms of molecule of oxygen at various temperatures**

At atmospheric pressure, the temperature of melting of oxygen is equal  $54.8\text{K}$ .

At temperature lower  $23.8\text{K}$  oxygen has monoclinic lattice with parameters  $a=540.3\text{pm}$ ,  $b=342.9\text{pm}$ ,  $c=508.6\text{pm}$ , the angle  $\beta=132.53^\circ$ . The cell contains three molecules. The design volume of crystal for one molecule is equal  $23.1\text{\AA}^3$ .

At temperature from  $23.8\text{K}$  up to  $43.8\text{K}$  oxygen has tetragonal (rhombohedral) lattice with parameters  $a=330.7\text{pm}$ ,  $c=1125.6\text{pm}$ . The cell contains five molecules. The design volume of crystal for one molecule is equal  $24.6\text{\AA}^3$ .

At temperature higher  $43.8\text{K}$  oxygen has a cubic lattice with parameter  $a=683\text{pm}$ . The cell contains six molecules. The design volume of crystal for one molecule is equal  $26.5\text{\AA}^3$ .

At temperature  $283\text{K}$  and at pressure  $9.6\text{GPa}$  ( $100$  thousand atmospheres) solid oxygen has a rhombic lattice with parameters  $a=421.51.3\text{pm}$ ,  $b=295.67\text{pm}$ ,  $c=668.97\text{pm}$ . The cell contains four molecules. The design volume of crystal for one molecule is equal  $20.8\text{\AA}^3$ .

We have executed the geometrical modeling for set forth above crystallographic structures and have calculated diameter of the oxygen polytron  $D_0=202.534\text{pm}$ .

Oxygen can form with lithium two simple oxides –  $\text{Li}_2\text{O}$  and  $\text{Li}_2\text{O}_2$ . Reaction is put into practice at heating of lithium in air above  $500\text{K}$ , and the basic product of reaction is  $\text{Li}_2\text{O}$ , whereas  $\text{Li}_2\text{O}_2$  is formed in microscopic amounts.

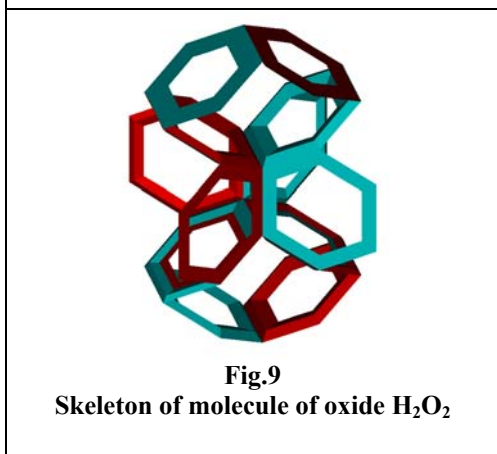
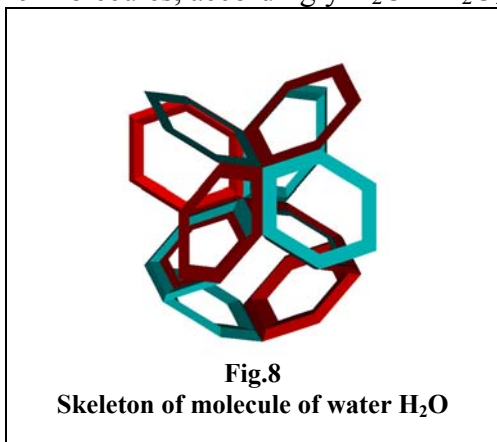
Reaction of joining of molecules of oxygen with molecules of lithium occurs under the same pattern, as well as at formation of hydride of lithium. But molecule of oxygen is more hardly (fatter), than molecule of hydrogen, therefore the molecule of lithium can "swallow" only half-molecule of oxygen. Oxide  $\text{Li}_2\text{O}_2$  can be formed only in those rare cases when one molecule of lithium simultaneously from two sides is attacked with two molecules of oxygen.

Oxide of lithium  $\text{Li}_2\text{O}$  has cubic close-packed lattice with parameter  $a=462.8\text{pm}$ . The melting temperature is  $1726\text{K}$ . Density  $d=2013\text{kg/m}^3$ . At temperature higher  $1300\text{K}$  it is sublimated. In a gaseous condition at temperature higher than melting temperature,  $\text{Li}_2\text{O}$  partially dissociates into  $\text{Li}$  and  $\text{O}_2$ . Corresponding calculation shows, that volume of molecule  $\text{Li}_2\text{O}$  is in limits  $24.72\pm 0.07\text{\AA}^3$ . The dihedral angle at top of truncated bipyramid is approximately equal  $135^\circ$ , i.e.



it is close to parameter of monoclinic lattices of oxygen. Unfortunately, we have not found in reference books the data for a crystal lattice  $\text{Li}_2\text{O}_2$ .

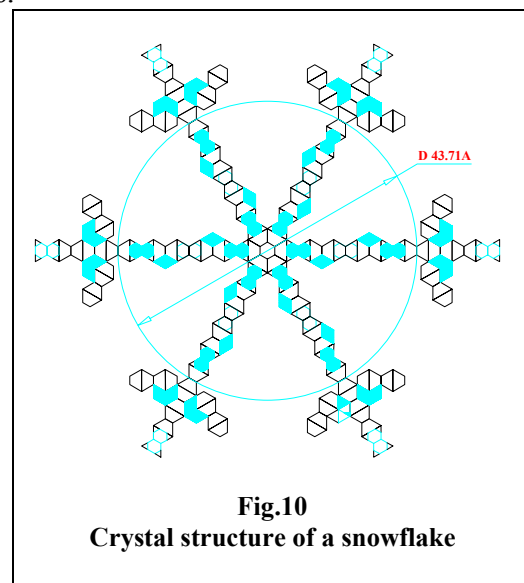
Hydrogen and oxygen can form two simple compounds – water (oxide of hydrogen  $\text{H}_2\text{O}$ ) and peroxide of hydrogen ( $\text{H}_2\text{O}_2$ ), but the scheme of joining of atoms of oxygen with molecules of hydrogen differs from the of joining of atoms of oxygen with molecules of lithium. In fig. 8 and 9 molecules, accordingly  $\text{H}_2\text{O}$  и  $\text{H}_2\text{O}_2$ , are shown.



The hydrogen and oxygen polytrons have approximately identical diameters, therefore atoms of oxygen and hydrogen can incorporate only with external sides and edges.

It is well known, that in comparison with compounds of other elements, water possesses exclusive properties. Neither the standard theory of structure of atoms, nor other theories and models, till now could not explain anomalous properties of water. We have closely studied all data about crystallographic angles and internuclear distances in a molecule of water and came to the conclusion, that the most authentic answers can be found in structure of a snowflake (see fig.10).

Atoms of hydrogen are represented in figure as trapezes. Each beam of snowflake represents as the shank from molecules of hydrogen. Atoms of oxygen (blue color) are wrapped around of hydrogen shanks as left-spiral or right-spiral chains.



We consider, that in structure of a snowflake the nature of DNA molecule and secret of the living matter is concealed.

The anomalous properties of water and others oxygen-containing compounds are caused by the anomalous temperature characteristic of atoms and molecules of oxygen. For example, among the high-temperature superconductors there is a class of complex oxides, which contain chains of oxygen up to 10 atoms.

For example,  $\text{HgBa}_2\text{Ca}_2\text{Cu}_3\text{O}_{8+\delta}$  passes into superconducting condition at 153K.

In superconductors of this class, the conductivity is provided with atoms and molecules of oxygen. And at that, atoms of oxygen should have strictly determined crystallographic angles. Other elements are intended for preservation of crystal structure of compound.

The further development of the polytronic theory opens the way for more purposeful search of new materials with necessary physical and chemical properties.