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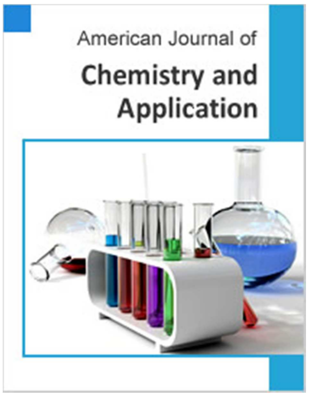

Interaction of Elements in Binary Compounds of Hydrogen

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Abstract
The calculations of the electron concentration (C_{electr}, mol/cm^3) and coefficient of consolidation (Buying) for the source of the chemical elements and their binary compounds with hydrogen on the basis of reference data on the density of matter in the condensed state. It is proposed to use the electron density as the structural characteristics of materials.

1. Introduction

Chemical interaction and phase transformations are traditionally characterized by thermodynamic parameters and state diagrams. Transformation of substances, accompanied by heat effects and volume changes. Density, an important characteristic of substances is the result of two factors: 1) the mass that is concentrated in the nuclei of atoms and 2) the volume formed by electron shells. The formation of new structures of matter is determined by the interaction of electronic shells of atoms and molecules. Chemical processes are reactions occurring with the formation of a new connection.. The act of chemical interaction is the formation of new electron (molecular) orbitals. Chemical bond between atoms is due to overlapping electron clouds. The transformation of substances is determined by the interaction of electronic shells of atoms and molecules.

Thermal processes are examined in detail in numerous papers on chemical thermodynamics and information on changes is not sufficient.

Works [1 – 5] present the normalized value of the volume changes in chemical reactions (coefficient of consolidation), which correlates with thermodynamic properties. As the volume formed by the electrons that enter the value of the "concentration of electrons" which can be used as the structural characteristics of the substance.

The aim of this work was to identify the possibility of using a standard value of volume change characteristics, allowing to estimate the intensity of the interaction between dissimilar atoms, and the electron concentration is determined in units of mol/cm^3, as the amount for assessing the structure of the material.

2. Methods

In the papers (Molchan, Fertikov, Seguru 2015, 2016, 2017) the formula for determining the concentration of elemental substances electrons on the basis of reference data (JCPDS PCPDFWIN, 2002; NPO «Professional», 2007; Babichev et al., 1991) according to their density in the condensed state is presented [6 – 11]:

$$C_{electron} = \frac{d}{M} Z \quad (1)$$

where $C_{electron}$ is for the concentration of electrons in a unit of volume, mole/cm^3;

d is for substance density in the condensed state, g/cm^3;

M is for molecular weight, g/mole;

Z is for the ordinal number of the element in the Periodic table.

For chemical compounds the electron density is determined through the following expression:

$$C_{electron} = \frac{number\ of\ electros\ in\ compound\ (in\ one\ mole)}{volume\ of\ mole\ of\ compound\ (condenced\ state)} \quad (2)$$

A_aB_b type compound has a concentration of electrons

$$C_{electron} \approx \frac{a Z_A + в Z_B}{M/d} \quad (3)$$

where a is for the subscript of element A,

Z_A is for the ordinal number of element A,

b is for the subscript of element B,

Z_B is for the ordinal number of the element B,

Metal alloys are not simple mixture of various components, but represent different chemical compounds of the elements forming the alloy.

To estimate the depth of interaction between atoms it is convenient to compare the volumes of substances before the reaction ($V_{component}$) and the volumes of substances after the reaction ($V_{product}$). The value obtained is then standardized to the finished product volume. The result (in %) characterizes the change in the volume of the substances in the course of reaction. This value can be designated as a coefficient of consolidation:

$$K_{consolidation.} = \left(\frac{\Sigma V_{компон.} - V_{прод.}}{V_{прод.}} \right) \times 100\% \quad (4)$$

The coefficient of consolidation be positive or negative. It means that the reaction product may have a volume which is smaller than the sum of volumes of the initial elements, and can be greater than the sum of the initial volumes (loosening of the electron shells).

3. Results

When comparing the connection of δ-TiH and TiH_2, it is necessary to bear in mind that a mole of atoms of titanium has a volume of 10.55 cm^3, a mole of hydrogen atoms in the condensed state has a volume of 13.3 cm^3 mol δ-TiH has a volume of 12.17 cm^3 mol TiH_2 has a volume of 12.25 cm^3.

Table 1 shows the characteristics of the chemical elements interacting with the hydrogen, and the resulting compounds.

Table 1. *The thermodynamic parameters, the compaction and concentration of electrons for binary hydrides.*

	-ΔHº298 kJ/mole	**-ΔGº298 kJ/mole**	**Coefficient of consolidation (Kconsolidation), %**	**Concentration of electrons in the compound (Celectron), mole/cm^3**	**Concentration of electrons in the element forming the hydride (Celectron), mole/cm^3**
LiH	90	68	160.5	0.396	0.231
NaH	52	32	110.7	0.685	0.466
KH	55	37	108.4	0.711	0.420
RbH	59	-	109.3	1.15	0.663
CsH	50	29	115.0	1.43	0.775
HF	-	-	90.9	0.831	0.931
HCl	-	-	24.3	0.726	0.970
HBr	-	-	36.6	1.26	1.36
HI	-	-	4.1	1.44	2.06
δ-TiH	-	-	95.9	1.89	2.09
CuH	-	-	98.7	2.92	4.07
ZrH	-	-	61.6	2.42	2.84
NbH	-	-	94.7	3.39	3.78
RhH	-	-	122.3	4.74	5.42
BeH_2	19	-16	115.3	0.411	0.821
MgH_2	77	37	120.3	0.760	0.859
CaH_2	175	136	138.4	1.00	0.773
SrH_2	180	141	122.8	1.46	1.10
BaH_2	190	152	93.4	1.73	1.466
H_2S	-	-	48.5	0.635	1.03
ScH_2	-	-	152.3	1.40	1.41
VH_2	-	-	200.0	2.15	2.76
H_2O	292	234	117.5	0.644	1.11
TiH_2	144	105	203.3	1.96	2.09
CrH_2	-	-	290.8	3.00	3.31
ZrH_2	163	123	144.8	2.53	2.84
NbH_2	-	-	163.2	3.02	3.78
H_2Se	-	-	30.8	1.09	2.06
YH_2	-	-	118.6	1.93	1.96

	$-\Delta H^o 298$ kJ/mole	$-\Delta G^o 298$ kJ/mole	Coefficient of consolidation (Kconsolidation), %	Concentration of electrons in the compound (Celectron), mole/cm^3	Concentration of electrons in the element forming the hydride (Celectron), mole/cm^3
H_2La	-	-	79.2	2.15	2.52
PrH_2	-	-	90.7	2.45	2.84
EuH_2	-	-	120.2	2.57	2.17
ErH_2	-	-	127.1	3.53	3.68
YbH_2	-	-	135.5	3.30	2.82
LuH_2	-	-	130.7	3.79	3.99
HfH_2	-	-	151.8	4.66	5.37
AcH_2	-	-	78.9	3.32	3.96
ThH_2	-	-	89.6	3.61	4.15
PuH_2	140	102	67.8	4.14	7.64
NH_3	70	-	242.2	0.641	0.517
AlH_3	12	-46	145.4	0.787	1.30
PH_3	-	-	41.0	0.476	1.11
AsH_3	-	-	34.2	0.912	2.52
UH_3	127	73	137.3	4.30	7.36
PuH_3	-	-	107.1	3.85	7.64
BkH_3	-	-	135.9	4.17	5.81
V_2H	-	-	67.0	2.62	2.76
Cr_2H	-	-	62	2.85	3.31
Ni_2H	-	-	68.7	3.63	4.24
Ta_2H	-	-	46.2	6.13	6.70
C_7H_{12}	-	-	122.3	0.610	1.12
$C_{36}H_{18}$	-	-	37.3	0.745	1.12
$MnH_{0.85}$	-	-	124.7	3.02	3.39
$MoH_{1.19}$	-	-	135.5	4.04	4.48
$TcH_{0.69}$	-	-	69.7	4.19	5.05
$TcH_{0.45}$	-	-	59.1	4.77	5.05
$PbH_{0.64}$	-	-	76.2	8.39	4.49
$Pb_{1.5}H_2$	-	-	137.2	7.44	4.49
$La_4H_{12.19}$	-	-	138.3	2.27	2.52
$La_8H_{18.4}$	-	-	96.4	2.19	2.52
$CeH_{2.53}$	-	-	138.6	2.66	2.80
$CeH_{2.29}$	-	-	198	3.51	2.80
H_5Nd_2	-	-	124.5	2.61	2.91
Sm_3H_7	-	-	120.8	2.79	3.12
$EuH_{1.9}$	-	-	109.5	2.51	2.17
$H_{2.87}Tm$	-	-	157.0	3.28	3.81
$TaH_{0.93}$	-	-	92.5	6.12	6.70
$PaH_{1.67}$	-	-	104.3	5.09	6.05
Si_4H	-	-	165	1.11	1.21
B_4H_{10}	-	-	105.5	0.407	1.08
B_5H_{11}	-	-	93.4	0.411	

4. Discussion

Determination of correlation between selected characteristics in table 1 indicates that there is no correlation. For example, for a number of compounds LiH, NaH, KH, RbH and CsH correlation coefficient between ΔH^o_{298} and ΔG^o_{298} equal to 0.997 (critical correlation coefficient at 0.95 confidence probability is equal to 0.805). The correlation coefficient between ΔH^o_{298} and compression ratio for that row is equal to 0.954.

The correlation coefficient between ΔG^o_{298} and compression ratio for that row is equal to 0.957.

The correlation coefficient between ΔG^o_{298} and concentration of electrons in the elements forming this series of hydrides that is equal to -0.813.

The correlation coefficient between the concentration of electrons in hydrides and concentration of electrons in the elements forming this series of hydrides that is equal to 0.987.

For a number of compounds BeH_2, MgH_2, CaH_2, SrH_2 and BaH_2 correlation coefficient between ΔH^o_{298} and ΔG^o_{298} equal to 0.999 (critical correlation coefficient for five pairs at 0.95 confidence probability is equal to 0.805). The correlation coefficient between ΔH^o_{298} and concentration of electrons in hydrides for this series is equal to 0.901.

The correlation coefficient between ΔG^o_{298} and concentration of electrons in hydrides of this series equal to 0.903.

The correlation coefficient between coefficient of consolidation and concentration of electrons in the elements forming this series, equal breakout of -0.827.

The correlation coefficient between the concentration of electrons in hydrides and concentration of electrons in the elements forming this series, equal to 0.860.

For a number of compounds of δ-TiH, CuH, ZrH, NbH, RhH correlation coefficient between the concentration of electrons in hydrides and concentration of electrons in the elements forming this series, equal to 0.963.

For a number of 20 compounds H_2S... PuH_2 the correlation coefficient between the concentration of electrons in hydrides and concentration of electrons in the elements forming this series, equal to 0.868 when critical correlation coefficient with a probability of 0.9995 equal to 0.679.

For a number of compounds NH_3, AlH_3, PH_3, AsH_3, UH_3, PuH_3, BkH_3 the correlation coefficient between the concentration of electrons in hydrides and concentration of electrons in the elements forming this series, is equal to 0.964 (critical probability equal to 0.95 0.679).

Comparing the connection of δ-TiH and TiH_2, it is necessary to bear in mind that a mole of atoms of titanium has a volume of 10.55 cm^3, a mole of hydrogen atoms in the condensed state has a volume of 13.3 cm^3 mol δ-TiH has a volume of 12.17 cm^3 mol TiH_2 has a volume of 12.25 cm^3.

A mechanical model of interaction of titanium with hydrogen can be represented as: having a similar size of atoms, the hydrogen nucleus (proton) falling on the electronic shell of titanium and a single electron obsessed with 22 electrons in titanium, the amount of connections is approximately equal to the volume of Titan. To connect TiH_2, where one mole of titanium have two moles of hydrogen, both the hydrogen proton sit on shell of titanium and socialized are 24 electrons, keeping the amount of titanium.

Comparing compaction ratios for compounds CrH_2 and Cr_2H, it becomes clear that the protons of hydrogen atoms sit on the electronic shells of atoms of chromium and compress volumes of hydrogen, which are formed by one electron.

The same considerations are valid when comparing pairs of compounds VH_2 and V_2H, or ZrH and ZrH_2, NbH and NbH_2, or.

A comparison of the volumes of the substances before the reaction and after allows you to better reveal the interaction of atoms and molecules than it can make heat effects.

5. Conclusions

1. It is proposed to use density as one of the variables, able to characterize the interaction of atoms in condensed system to evaluate the properties of substances.
2. The correlation between the value of the enthalpy of reaction energy with the calculated compaction.
3. Compaction ratios can be used as relative chemical potentials for the elements included in chemical compounds.
4. It is proposed to use the concentration of electrons of an element or compound defined in units of mol/cm^3, as a structural characteristic of the material.
5. The correlation between the enthalpy of hydride formation of one-, two - and three-and tetravalent metals with the concentration of electrons in the source metal.
6. To assess the degree of interaction of initial components in the formation of compounds is proposed to use the coefficient of consolidation.

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