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DIELECTRIC PROPERTIES OF WATER-MIXED SODIUM BORHYDRATES

Abstract

The dielectric properties of sodium borohydride mixed with water were studied using molecular dynamics simulations. Various concentrations of water and sodium borohydride were used in the model system. The values of dielectric permittivity and excess permittivity of solutions were calculated. Dielectric parameters was compared according to different concentrations of water and sodium borohydride in solutions. These studies were carried out using the GROMACS software package. According to the studies, at x ~ 0.2 molar concentrations of sodium borohydride, excess values of the dielectric constant were observed, and in a binary mixture of sodium borohydride - water, heteromolecular structures with the largest number of hydrogen bonds were formed.

INTRODUCTION

Hydrogen has enormous efficiency as an alternative energy source. Currently, the use of renewable energy sources is one of the main problems. In order to use hydrogen for different purposes, it is first necessary to find a solution to the question of its storage, transportation, distribution and safety. The requirements for hydrogen storage systems are determined by the nature of its application. It is more convenient to store hydrogen with a compound than to store itself. The volume and mass fraction of hydrogen in a compound are important in this. Matall hydrides or clathrate structures are the same term for storing large-share and large-mass hydrogens [1, 2]. Among hydrides, sodium borohydrate occupies a special place due to its high content of H2 and stability. This ensures that the catalytic hydrolysis of the compound produces hydrogen under controlled conditions.It can also be said that sodium borohydrate is the best remedy for keeping the vodo-rod in a solid state. In 2012, early marota-ba was successfully used to store, separate and re-release hydrogen under medium conditions, even though it does not produce any temperature and pressure conditions [3].

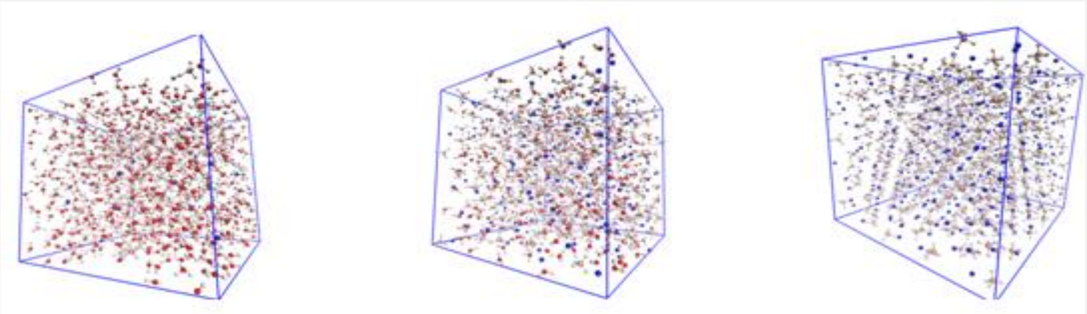
Sodium borohydrate, also known as sodium tetragidridoborate, and sodium tetrogidro - borate. It is an inorganic compound with the formula NaBH4. Usually sodium borohydrate is a substance in the form of a white powder (fig. This compound was introduced in the 1940s by H. I. Discovered by Schlesinger [4].

1-fig. Appearance of sodium borohydrate in powder form

We compare the dielectric absorption-solutes of binary solutions with the molecular dynamics method, share the excess dielectric constants and determine the structures with the most hydrogen bonds. The results obtained indicate at what concentration of liquid-liquid the most clathrate structures were formed. As a result, we predict the optimal mixture of water and sodium borohydrate, in which hydrogen can be stored.

Metod

The research was carried out on the Ubuntu system in the GROMACS program. The calculation was carried out using the thermostatic control algorithms of Berendsen in a cubic box filled with sodium borohydrate and water molecules. The research was carried out at constant pressure($P=10^7$ Pa) and temperature(t=300 K at room temperature) [5]. The equations of motion were solved using theverlet algorithm in the time step of 1.0 fs. The Coulomb action forces between molecules were calculated using the Evald method with an accuracy of $1\cdot10^{-6}$kl/mol. The calculation process was repeated at concentrations of 0.1÷1.0 of the solution. The isothermal compressive strength of water was obtained at a value of $4.5\cdot10^6$ Pa. With an increase in the concentration of sodium borohydrate in the mixture, changes in the sequence of hydrogen bonds occur between water-water, water–solution, solution–solution.



2-fig. a) 10% $NaBH_4$ and 90% H_2O box , b)50% $NaBH_4$ and 50% H_2O box, c) when water is not addedNaBH$_4$ the box view of

Using the molecular dynamics method, dielectric absorption of sodium borohydrate and water mixtures over the entire concentration range was studied. Their ε^E the value of excess dielectric constants (1) is calculated by the formula [6]:

$$\varepsilon^E = (\varepsilon_A - \varepsilon_{A\infty}) - [(\varepsilon_S - \varepsilon_{S\infty})(1-x) + (\varepsilon_{NaBH4} - \varepsilon_{NaBH4\infty}) \cdot X \qquad (1)$$

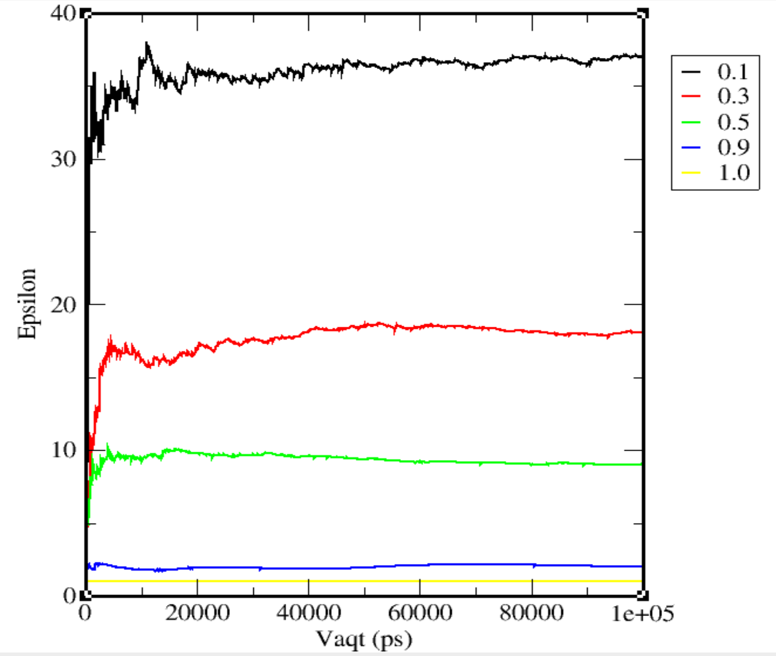
In here ε_A – dielectric absorption of the mixture, ε_S – dielectric absorption of water, ε_{NaBH_4} – dielectric absorption of sodium borohydrate x– concentration of sodium borohydrate.

DISCUSSIONS AND RESULTS

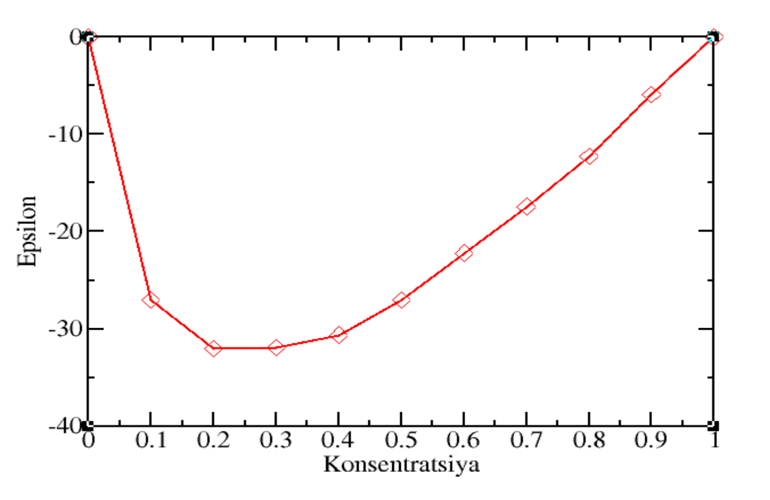
Determine the dielectric absorption of a mixture of water and sodium borohydrate, as we noted above, and at the same time the excess dielectric absorption-dik(Table 1).

Concentration	X_{NaBH4}	Y_s	E	ε^E
0	0	1000	71.09	0.09
0.1	100	900	37.06	-27.0244
0.2	200	800	25.04	-32.0388
0.3	300	700	18.13	-31.9432
0.4	400	600	12.45	-30.6176
0.5	500	500	9.05	-27.012
0.6	600	400	6.854	-22.2024
0.7	700	300	4.65	-17.4008
0.8	800	200	2.786	-12.2592
0.9	900	100	2.135	-5.9046
1	1000	0	1.034	0

1-table: Dielectric absorption ε and excess dielectric absorption of water and sodium borohydrate mixtures of different concentrations ε^E values of Lars. In this placeX_{NaBH_4} – Sodium borohydride and Y_s – number of water molecules

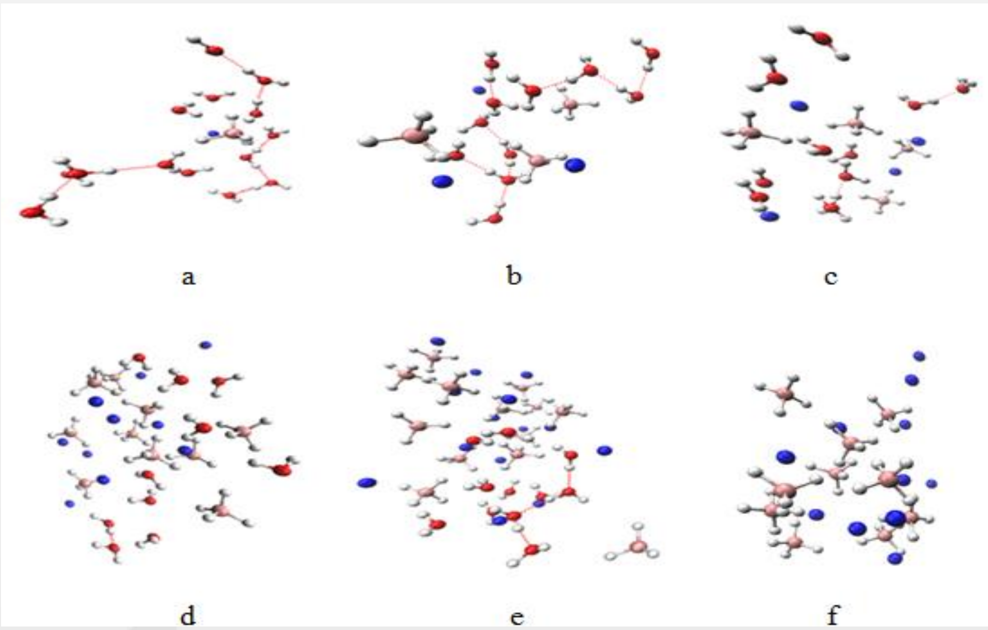


3-fig. Dielectric absorbency of different concentrations of water vanatrium borohydrate



4-fig. Excess dielectric sing-resistance of sodium borohydrate and water solutions of different concentrations

The dielectric absorbents of the solution according to the different concentrations of water and sodium borohydrate in its composition were compared (Figure 4).According to comparisons, dielectric absorption ε was highest in solution with a concentration of 0.1 mol, and epsilon began to decrease as the concentration of sodium borohydrate in solution increased. According to studies carried out to determine the value of the excess dielectric constant, the results sought were observed at a concentration of x~0.2 moles of sodium borohydrate, in which heteromolecular structures with the most hydrogen bonds were formed in the sodium borohydrate–water binary mixture.



5- fig.(A)10% of sodium borohydrate; (b) 20%; (c) 40%; (d) 50%; (e) 60%; (f) 100%

image of heteromolecular structures of sodium borohydrate – water binary mixtures with hydrogen bond at their relative concentrations

CONCLUSION

When sodium borohydrate is placed in the water, its dielectric absorption is low. In this case, with an increase in the concentration of sodium borohydrate in the mixture, the dielectric absorption of the binary fluid began to decrease. Solutions were produced in the range of concentrations 0.1÷1.0. In this range, it was found that the structures with the most hydrogen bonds are formed in a sodium borohydrate– water mixture with a concentration of x~0.2 mol. Hence, the most effective borohydrate water mixture for hydrogen storage was predicted using theoretical studies. In the future, scientists who will experiment with our results will be able to use as a roadmap.

REFERENCES

1. Nilufar Axmedova, Jamoliddin Razzokov "Role of sodium borohydrates in hydrogen storage"."JOURNAL OF NEW CENTURY INNOVA-TIONS IN ALL AREAS" 2022-y.
2. Olga V. Netskina, Oksana V. Komova, Valentina I. Simagina, Anna G. Gntsler, Yekatrina D. Grayfer "SODIUM BOROHYDRIDE IS A SOURCE OF PURE HYDROGEN FOR PORTABLE FUEL CELLS" Russian 2006-y.
3. Masimov, E. and H. Abbasov, Refractometry determination of the hydration number of ions in diluted aqueous solutions of magnesium sulfate. Russian Journal of Physical Chemistry A, 2012. 86(3): p. 399-401.
4. *Banfi, Luka; Narisano, Enrika; Riva, Renata; Stiasni, Nikola; Xieremann, Martin; Yamada, Tru; Tsubo, Tatsuyuki (2014), "Natriy Borohidrid", Organik sintez uchun reaktivlar entsiklopediyasi, John Wiley & Sons, 1-13 betlar,* doi:10.1002 / 047084289x.rs052.pub3, ISBN 9780470842898
5. Grubmüller, H., et al., Generalized Verlet algorithm for efficient molecular dynamics simulations with long-range interactions. Molecular Simulation, 1991. **6**(1-3): p. 121-142.

6. Ramana.C.V et al. Generalized and excess dielectric constants in non polar+ polar binary liquid mixtures of toluene with alcohols at 303, 313 and 323 K. Thermochimica Acta, 2013. 566: P. 130-136.