STUDIES OF HYDROGEN-BONDED SYSTEMS: USING MODELS – ADVANTAGES AND LIMITATIONS*

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The scientist is practically *forced* to use models – physical, conceptual and/or mathematical. The models simplify the interpretation of the experimental facts and facilitate the acceptance of more or less abstract ideas. On the other hand, the models are *not* the reality but, rather, its simplified representation. A disregard of the latter fact and a blind confidence in the employed models may lead to serious errors. Depending upon our needs in any given case, either simple or more refined models may be used but what is always needed is the full knowledge of the inherent limitations of the utilized model. The simple models are easier to handle than the more sophisticated ones, but the consequences drawn from them are apt to be less reliable. Examples (mainly taken from the author's own work on various hydrogen-bonded systems) are given of the usefulness of even the simplest possible models but also of the perils accompanying the uncritical use of some commonly utilized models.

Key words: hydrogen bonding; models; infrared spectra; crystallohydrates; scientific methodology.

INTRODUCTION

Any scientific study has, as its final goal, the search for truth and, in the case of the exact (or natural) sciences, the understanding of the nature or the investigated part of it. Since the whole of the nature is much too large and much too complicated to study and comprehend, it is necessary to choose a certain part of it (that is, to define a system) and limit the scope and concentrate the efforts to the investigation of the *system*, rather than the entire nature. Since even the systems and their behavior are complicated, in trying to understand them and interpret the experimental facts, the system is often replaced by a *model* for it. The present paper is devoted to the discussion of the advantages of using models and the limitations which must be kept in mind. The examples which are to be discussed will come mainly from the field of vibrational spectroscopy (particularly the studies on hydrogen-bonded systems), but the general ideas about both the advantages and the limitations are, hopefully, of more general nature.

GENERAL CONSIDERATIONS

Generally speaking, the models can be physical, conceptual or mathematical.

The *physical* models are schemes, maquettes or other physical objects which *represent* real objects – from atoms and molecules to engines or spacecrafts and are used in many fields of human endeavor, especially in education and industry. They are useful also in the course of the *scientific* studies as a visualization of the essential features of the studied system or some of its properties. The *conceptual* models are mental constructs based, as a rule, on common or specialized knowledge in the given area or in areas which have close relation to the studied system. A good conceptual model makes it easier to comprehend the nature and the principal properties of the system under investigation. Finally, the *mathematical* models are sets of mathematical expressions designed to represent the experimentally determined or postulated relations between various properties of the system and to predict its behavior under untested circumstances. The advent of the computers and the improvement of their performance, on the one hand, and the developments of the theoretical basis of mathematical modeling, on the other, make these models an extremely valuable scientific tool.

Although different, all types of models have *common* features of which the most important one is the fact that the model contains (or reflects) only a

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subset of the properties of the real system. Thus, as already mentioned, the model (be it physical, conceptual or mathematical) is *not* an *exact* substitute for the system.

If a *small* subset is used, *i.e.* if only the *most essential* properties are included, the model is a simple one. If, on the other hand, a *large* or *very large* subset of properties is included, a *complicated* or *very complicated* model results.

Irrespective of the amount of properties included in the model:

- the model is only a *model*;
- it must include *the most important* features of the system;
- it is based on our knowledge of the system;
- it should be useful;
- it should be logical;
- it should be intuitively acceptable.

A *prerequisite* is, of course, our *knowledge* of the properties of the system and this, unfortunately, is rarely quite the case.

Among the main *advantages* of using the models, the following could be mentioned :

- it is possible to treat cases which are, otherwise, unmanageable;
- even when this is not so, we can finish our job in an *easier*, *cheaper* or in some other way *more acceptable* manner.

Among the *limitations*, the following are important to remember (some have been previously mentioned) :

- we are never sure whether *all the essential* properties of the system **are** indeed included in the model;
- the simpler the model, the more likely it is that the conclusions drawn from it will be *deficient*, if not outright *erroneous*;
- the complicated models are difficult to use.

In what follows, a brief revue will be given of some work done by the author and his collaborators where models of various complexities were used. Some further examples of the use of models in areas close to the author's research interest will be discussed.

EXAMPLES

Molecular vibrations

When treating molecular vibrations, one deals with complex motions in a *quantum-mechanical* system. Even in relatively simple molecules these motions are elaborate and hard to visualize and in the case of polyatomic molecules the treatment becomes intolerably complex.

To facilitate the task, often used are simple models in which the atoms are likened to balls and the chemical bonds between the atoms to springs connecting the balls (Fig. 1 shows a representation of such a model for a diatomic AB molecule). A further approximation is frequently added, namely it is supposed that the vibrations are *harmonic* in character.
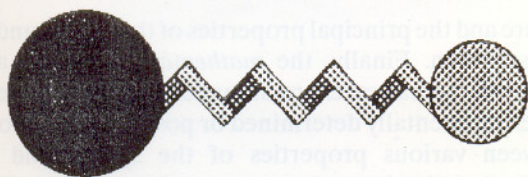

Fig. 1. A simple ball-and-spring model
for a diatomic molecule

Obviously, the model is quite crude and far from being an exact replica of the real system since the atoms are *not* balls and the bonds are *not* springs. The model is not exact, but it is helpful, even in its simplest form. Namely, it is close to our everyday experience and thus

it is acceptable. Moreover, the strength of the spring reflects the strength of the chemical bond and the stronger the spring (*i.e.* the bond) is, the higher the frequency of the vibration is expected to be. The harmonic approximation adds to the ease of handling the model since only one force constant is needed to describe the oscillatory motion of the diatomic molecule.

If the system under study is a *triatomic* molecule (*e.g.*, H_2O), the above-described model can be easily modified and the triatomic oscillator[*] can be treated as being composed of two coupled diatomic oscillators (Fig. 2). Under such assumptions, two motions of the resulting oscillator are easily envisaged – one in-phase and one out-of-phase motion. As previously, the model is *not* exact, and this time it is only *partly* useful since we know that there should be *three* vibrational motions: two stretchings and one bending. Even disregarding the quantum-mechanical nature of the vibrational motions, the model must be refined by introducing one additional force constant in order to bring it to a better agreement with the properties of the real system. Actually, the two above-mentioned motions (the in-phase and out-of-phase ones) are the two *stretching* vibrations of the triatomic oscillator[**]. As long as the molecule is free and symmetric, it is not advisable to revert to the model of coupled oscillators. If, however, the molecule is unsymmetrically *bonded* (*e.g.*, by hydrogen bonds of considerably different

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[*]   It should be noted that if the oscillator is indeed a water molecule, its geometry is only approximately reproduced in Fig. 2.

[**] Actually, even in the case of an ABA molecule such as water, the symmetric stretching mode involves some bending and *vice versa*.

strength) or if the two end-atoms are different (as in HOD), the model becomes useful in treating the *stretching* vibrations since we then talk of *uncoupled* oscillators (see below).
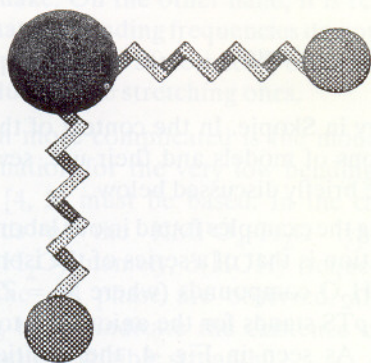

Fig. 2. A simple model for a triatomic oscillator treated as being composed of two diatomic oscillators sharing a common atom

As the number of atoms in the molecule increases, more and more force constants (including interaction ones) are required in order to describe the molecular motions, to reproduce the vibrational frequencies and to visualize the form of the normal modes of the isolated molecule. Such tasks are not possible to accomplish without the use of suitable computer programs but nowadays this is not a serious obstacle, at least as long as the vibrations are treated as harmonic and reliable values of force constants could be chosen or transferred from previously treated similar system. An additional requirement is the proper choice of the force filed meaning that it is necessary to choose between different possible models. In the case of complicated molecules, the process of adding force constants to the force field frequently leads to a high degree of arbitrariness since a given set of experimental frequency values could be reproduced equally well by using different sets of force constants.

At any rate, the vibrations of a polyatomic molecule involve *all* the atoms. In order to facilitate the treatment (especially in the case of organic molecules) a much simpler model is often employed based on the concept of *group vibrations*. If, namely, the mass of one of the vibrating atoms is much less than that of the rest of neighboring atoms (such is the situation with hydrons bound to carbon, nitrogen or oxygen atoms) or if one of the force constants is much larger than the remaining ones (*e.g.*, when two atoms are bound by double or triple bonds) some of the vibrations become localized in only a given part of the molecule (see, for example, [1]). Such vibrations can then be treated in much the same vein as those of a diatomic molecule. The model is appealing and often works so well that it is easy to forget that, strictly speaking, it does not

properly represent the real situation. The concept is further extended by introducing the notion of *coupled vibrations* which represents an even further deviation from the reality.

The models describing the molecular vibrations can be refined by supposing that the vibrations are *anharmonic*. Additional constants must be introduced but they are not easily transferable and, moreover, we have to choose the form of the anharmonic force field. All this makes the model more complicated and more difficult to grasp thus reducing its usefulness.

Summarizing the above-mentioned characteristics of the models describing the molecular vibrations, it can be said that the simple models are easily understandable and useful in reproducing the main features of the systems composed of vibrating and non-interacting molecules (such as those in gasses) as long as the molecules are of moderate complexity[*]. On the other hand, the more complicated models can, in principle, reproduce the properties of the vibrating molecules in a better way but they are more complicated to use and their consequences (*e.g.* the results of the *normal-coordinate treatment*) largely depend on the choices made. Among the latter, the choice of the force field, of the force-constant values, of the number and character of interaction force constants etc. can be mentioned in addition to the choice whether to treat the vibrations as harmonic or as anharmonic.

Hydrogen-bonded systems

In the case of a more involved system such as a hydrogen-bonded group of atoms R–X–H···Y, the ball-and-spring model can be modified depicting the hydrogen atom as being bound simultaneously by two springs[**] (Fig. 3). Since the participation of the hydron in two bonds must result in a redistribution of the electron density, the original X–H bond must be weakened and the value of the corresponding force constant accordingly diminished. Clearly, this would then lead to a decrease of the corresponding stretching frequency. On the other hand, the bending of the system must be more difficult than when the additional spring (*i.e.*, force) is absent, so that the bending force constant is expected to increase and the R–X–H bending frequency should become higher than in the case of the non-hydrogen bonded R–X–H group. The stronger the hydrogen bond, the larger the shifts of the X–H stretching mode (*towards lower* values) and of the R–X–H bending mode (*toward higher* frequency values) are expected to be. These expectations are easy to remember and they are a natural consequence of the accepted model.

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[*] The existence of rotational structure of the vibrational bands is, for the moment, ignored.

[**] The R–X–H group is often not linear but this is of no immediate consequence for our present purposes.

Fig. 3. A simple model for the hydrogen-bonded R–X–H · · · Y system

The experimental results most of the time bear out the expectations and, as a rule, the hydrogen bonding does indeed shift the stretching and bending vibrations (*e.g.*, those of water in crystallohydrates) in the expected directions. If there are no reasons to believe that this is not so, one could rather safely look for water bending bands at high frequencies if the stretching bands are found at relatively low wavenumber values and *vice versa*.

However, what is true *most of time* is not true always and the attempt to correlate the O–D stretching and H–O–D bending frequencies of half-deuterated water in crystallohydrates [2] resulted with such a scatter that no meaningful correlation could be found. On the other hand, some quite unexpected cases have been encountered in the course of the systematic studies on crystallohydrates performed by the members of the Structural Chemistry Group at the Institute

of Chemistry in Skopje. In the context of the general considerations of models and their use, several such cases will be briefly discussed below.

Among the examples found in our laboratory, the first to mention is that of a series of the isomorphous $M(pTS)_2 \cdot 6H_2O$ compounds (where M = Zn, Co, Ni or Mg and pTS stands for the anion of p-toluenesulfonic acid). As seen in Fig. 4, the position of the centroid of the complex band in the water stretching region is found [3] at frequencies increasing in the order Zn < Co < Ni < Mg but the centroid of the bands in the HQH bending region also *increases* in the same order. The simple model is, therefore, inadequate and inapplicable and must be modified. Apparently, even in the case of isomorphous compounds, the position of the water stretching bands depends not only on the hydrogen bond strength, but also of the strength of the metal-to-water interactions and the
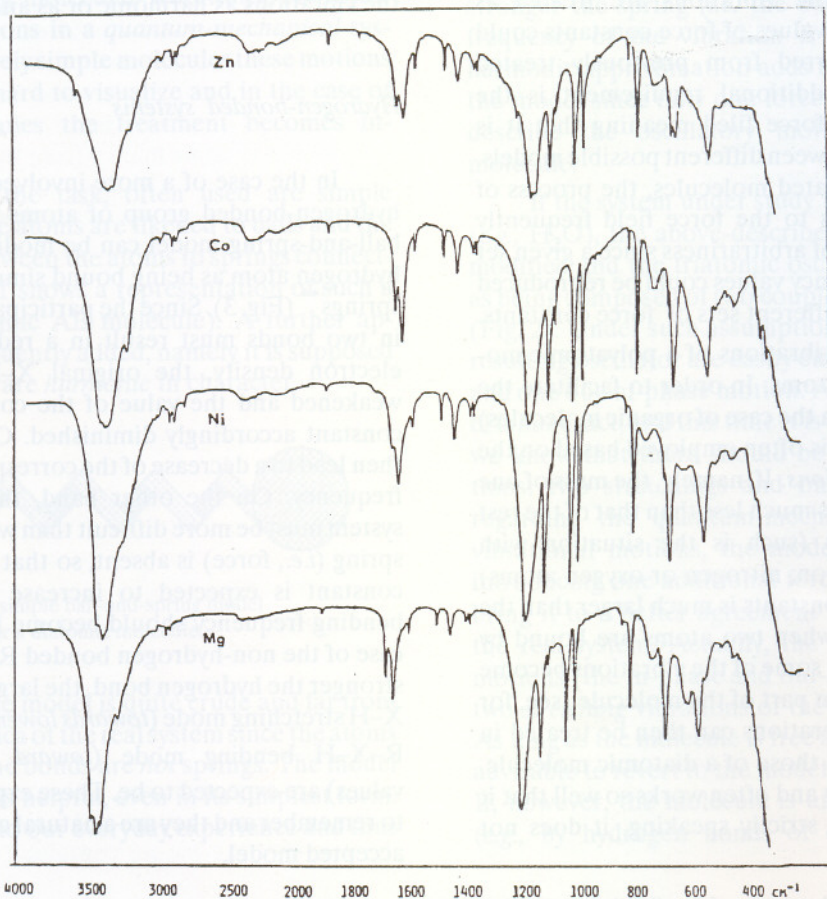

Fig. 4. Infrared spectra of compounds of the $M(pTS)_2 \cdot 6H_2O$ type

observed position of the bands is a compromise between the two factors. Such an explanation is reasonable but it alters the simple model, makes it more complicated and the predictions are more difficult to make. On the other hand, it is reasonable to assume that the bending frequencies do not depend (or do not depend to the same extent) on the same factors which influence the stretching ones.

Even more complicated is the model on which the explanation for the very low bending HOH frequencies [4, 5] must be based. In the case of solid compounds of the $KMPO_4 \cdot H_2O$ type (*e.g.*, in $KNiPO_4 \cdot H_2O$), namely, $\delta(HOH)$ frequencies lower than in the gas phase are observed, although the stretching bands indicate the existence of hydrogen bonds of non-negligible strength.

As mentioned, such an experimental finding requires an even more drastic change in the accepted model than that previously discussed. The explanation which has been given [4, 5] takes into account the crystallographic results for the isomorphous compound $KMgPO_4 \cdot H_2O$ [6] which show that in the crystal the water molecules are situated in the vicinity of two metal ions (Mg^{2+} and K^+) and *four* potential proton acceptors. Such a situation is thought to assist the H–O–H bending vibration, causing a lowering of its frequency below the gas-phase value. Irrespective of the plausibility of the given explanation, the fact remains that the simple model has been considerably altered and made much more complicated.

Among the factors which certainly influence the hydrogen bond strength is the electric charge on the acceptor atom. Thus, hydrogen bonds characterized by comparable X–H · · · Y distances will be stronger if the acceptor atom is, for example, an oxygen atom from an OH^- group then a sulfate oxygen bearing only a fraction of the electric charge of the same type of atom in the previous case. Such a conclusion is based on the model according to which the electrostatic contribution is of considerable importance for the hydrogen bond strength [7]. Such a model is easily extendible to cover acceptor atoms from closely related polyatomic ions (*e.g.*, tetrahedral AB_4^{2-} anions such as SO_4^{2-}, SeO_4^{2-} or BeF_4^{2-}) bearing the same overall charge but differing in the electronegativities of either A (as in the sulfate – selenate pair) or both A and B (as in the sulfate – tetrafluoroberyllate pair). The studies of isomorphous pairs of sulfates and selenates [8, 9] showed that almost invariably the water stretching bands are found at lower frequencies in the selenates than in the sulfates. One of the best such examples was found in the case of the $CaSO_4 \cdot 2H_2O$ – $CaSeO_4 \cdot 2H_2O$ pair

[10] to which the probably isomorphous $YPO_4 \cdot 2H_2O$ was added*. The consistently lower water stretching frequencies in the case of the selenates were interpreted on the basis of a model in which it was assumed that owing to the lower electronegativity of selenium (as compared to sulfur) the electron density in the region of the oxygen lone pairs should be higher and thus the conditions for hydrogen bonding would be more favorable.

Since beryllium is much less electronegative than either sulfur or selenium, whereas fluorine is more electronegative than oxygen, the model would predict that the partial negative charge on the fluorine atoms in BeF_4^{2-} ions would be higher than that on the oxygen atoms in SO_4^{2-} or in SeO_4^{2-} anions**. Consequently, the tetrafluoroberyllate ions would be much better proton acceptors than either the sulfate or the selenate ones and the water stretching frequencies should be found at considerably lower frequencies than in the case of the counterparts containing oxoanions. However, this model apparently fails when the hydrates of tetrafluoroberyllates which are isomorphous (or at lest, isotypical) with those of the corresponding sulfates were studied [13–15]. In no case, namely, the water stretchings had appreciably lower frequency in the tetrafluoroberyllate than in the sulfate or selenate, no good explanation being proposed so far for this unexpected finding. Irrespective on whether the model is fallacious or some important factor has not been taken into account, the fact is that an intuitively appealing model can not explain all the related findings.

Should we, then, always take into account the interactions between water molecules and the neighboring metal ions, the exact arrangement of the surrounding proton-acceptors or the partial electric charge on them? The answer is that if the experimentally determined or assumed structure does not require it, it is not practical to abandon the simple and intuitively more easily acceptable model. In other words, there should be clear physical reasons for the substitution of the simple models by more complicated ones. However, the examples given above (as well as those which follow) should alert the investigator that in situations when we do not know the exact physical nature of the studied system, the simple model *might not* be a satisfactory representation of the true situation (although it often *is*).

Isotopically isolated HOD molecules in crystals

Among the procedures quite often used in the study of crystallohydrates is that known as *isotopic isolation*. When this technique is applied, the first step

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* The water bands in the latter compound were found at frequencies lower than in the two calcium salts, obviously as a consequence of the higher partial charge on the phosphate oxygen atoms compared with that of the sulfate or selenate oxygens.

** A calculation of the partial charges on the fluorine atoms in BeF_4^{2-} ions [12] lent support to such a notion. The calculation, namely, yielded a value of –0.56 for the partial relative charge on the fluorine atoms in the tetrafluoroberyllate anions, as compared with the values of –0.415 and –0.409 [13] for the sulfate and selenate oxygens respectively.

is to prepare samples in which the molecules of one water isotopomer (as a rule, HOD) are practically entirely surrounded by molecules of another isotopomer (H_2O or D_2O) and then study the spectra in the O–H or O–D stretching region depending on whether the HOD molecules are isotopically isolated by D_2O or H_2O molecules respectively. The isotopic isolation eliminates or reduces the effects which are due to the vibrational interactions between identical oscillators and thus simplifies the spectra. Structural inferences are made based on the number and/or position of the bands in the studied regions.
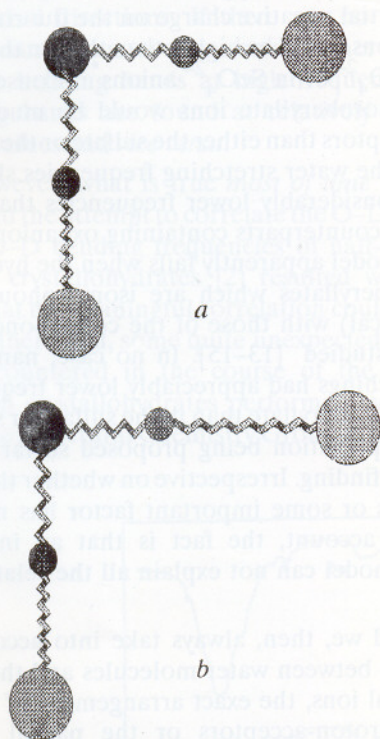

Fig. 5. A schematic representation of a HOD molecule hydrogen bonded by two identical (a) and two unlike (b) hydrogen bonds

Because of the considerable difference in the masses of the two hydrons, the HOD stretching vibrations are thought to be *uncoupled* so that one almost pure O–H (at higher frequencies) and one O–D stretch (at lower frequencies) result.

Taking into account the character and strength of the hydrogen bonds, two possibilities exist: the two acceptors and the two hydrogen bonds may be either identical or different. These two situations are approximately represented[*] in Fig. 5.

If the bonds are completely alike (i.e., if the water molecule is located on a symmetry element such as a two-fold symmetry axis or a mirror plane bisecting the H–O–H angle) as in Fig. 5a, it does not matter which

hydron is a proton and which is a deuteron and only one O–D stretching band is expected (and, indeed, observed).

If, on the other hand, the two acceptors and the hydrogen bonds are not identical (as in Fig. 5b), it is important which hydron is a proton and which is a deuteron and two O–D stretching band are expected (and, usually, observed). A simple example of this kind is found in the case of $Rb_2[MnCl_4(H_2O)_2]$ in the structure of which, as shown by the crystallographic data [16], all water molecules are of the same type and are hydrogen-bonded by two crystallographically nonequivalent O$\cdots$Cl bonds. As seen in Fig. 6, two bands of approximately equal intensity are observed [17] in the O–D and the O–H stretching regions of the spectrum of HOD molecules isotopically isolated by H_2O molecules (a) or by D_2O molecules respectively (b). If we denote by H_1 (or by D_1) the hydron involved in the weaker hydrogen bond and by H_2 (or by D_2) that which forms the stronger H-bond, the bands at higher frequency could be attributed to the O–D_1 or the O–H_1 stretching vibrations while those at lower frequency should originate from the O–D_2 or the O–H_2 stretchings.
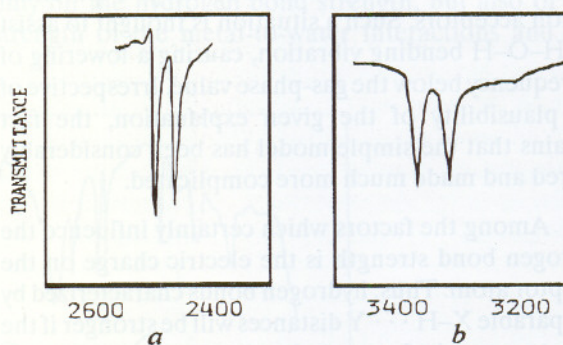

Fig. 6. The O–D (a) and the O–H (b) stretching regions of the spectra of isotopically isolated HOD molecules in $Rb_2[MnCl_4(H_2O)_2]$

The model implicitly assumed in such an interpretation is based on the supposition that the X–H$\cdots$Y bonds which are longer are, at the same time, weaker and *vice versa*[**]. Such an assumption lies *behind the attempts (e.g.,* that in Ref. 18) to correlate the O–D stretching frequency of isolated HOD molecule with the crystallographically determined X$\cdots$Y distances. The resulting plot, however, showed a considerable scatter of the points around the regression line, the deviations being much larger than warranted by the experimental uncertainities. Further tests even on groups of closely related compounds [19–21] showed that the two-parameter regression curves are hardly siuitable for prediction purposes. The situation

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[*] As in Fig. 2, the geometry of the molecule is not properly reproduced.

[**] It is even customary to speak of *hydrogen bond strenght* when the X$\cdots$Y distance is meant which may be grossly inadequate since the degree of linearity of the hydrogen bonds may vary considerably and nominally shorter bonds may, in fact, be weaker than some of those characterized by longer X$\cdots$Y distances.

could be improved if a multiple regression is carried out, taking into account the effects of some of the interactions enumerated above (especially those between the water molecules and the metal ions). However, this requires a knowledge of the parameters to be included (*e.g.*, the *effective ionic radii* [22, 23], the partial relative electric charges etc. which themselves are not directly measurable quantities) and complicates the model.

Understandably, the situation is more perplexing if several types of water molecules are present in the structure. If the number of non-equivalent hydrogen bonds is n and the probability of isotopic substitution of each proton by a deuteron is practically equal, then the simple model would predict the appearance, in the corresponding region of the spectra of samples containing isotopically isolated HOD molecules, of n O–D or O–H stretching bands of comparable intensity. The expected number of bands is indeed *often* found in the spectra of crystallohydrates containing more than one type of hydrogen bonds although even in these cases the intensities are not always as expected. Thus, in the case of the monohydrates of sodium thiosaccharinate [24] and of lead saccharinate [25] the O–D stretching band found at higher frequency is considerably less intense than that appearing slightly lower. Two possible explanations were given, one involving the preferential deuterium-for-proton substitution at sites where the hydrons are involved in stronger hydrogen bonding and the other based on the assumption [26] that the form of the normal modes is different in the case of asymmetrically bonded HOD molecules when they acquire one of the two possible orientations (H–O–D $\cdots$ O and D–O–H $\cdots$ O, respectively). Each of these explanations, however, represents a breach with the simple model.

As for the assignment of the individual bands in the O–D stretching region, the simplest procedure is to assign the band at the highest frequency to the vibration of the uncoupled O–D oscillator whose deuteron takes part in the weakest hydrogen bond and to associate the bands at progressively lower frequencies with the O–D oscillators involved in gradually stronger and stronger hydrogen bonds. The model enabling us to do so is simple and appealing. On the other hand, it must be pointed out that quite a few cases exist when such an uncomplicated and, at first sight, logical procedure is simply not working.

A striking case of this type (and one for which a reasonable explanation was proposed) is the appearance of the O–D stretching bands in the spectrum

of partially deuterated $Cu(pTS)_2 \cdot 6H_2O$. Six non-equivalent hydrons exist in the structure of this compound [27] and, consequently, six bands would be expected.
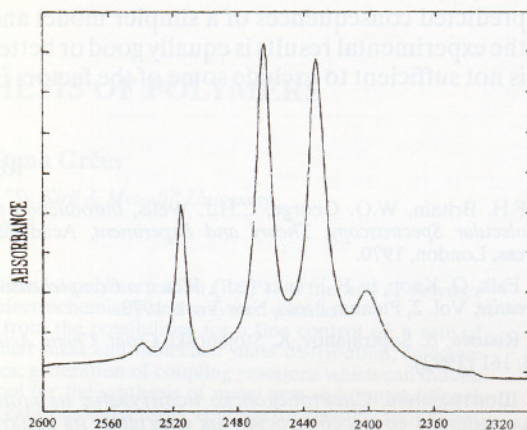

Fig. 7. The O–D stretching region in the FTIR spectrum of $Cu(pTS)_2 \cdot 6H_2O$

However, as seen in Fig. 7 [28], only three prominent bands of unequal intensity are observed in the FTIR spectrum with one additional much weaker band at around 2400 cm^{-1}. Neither the number of bands nor their intensity correlate well with the experimentally found O $\cdots$ O distances. As discussed in Ref. 28, in order to explain the discrepancies, it is necessary to assume that the position of the bands is determined not only by the O $\cdots$ O distances and by the partial electric charge on a given acceptor atom but also by the number of hydrogen bonds in which it participates. Such an explanation (plausible as it is), however, deviates significantly from the simple model of one-to-one correspondence of bands and distinct hydrons and of the major role which the O $\cdots$ O distances play in determining the position of the bands.

The enumeration of examples could, of course, continue practically indefinitely and they can be chosen from practically any field of study. It is to be believed that the majority of investigators are familiar with the problem of choosing a model and the limitations posed by the selected model. We all, however, tend to forget sometimes about the limitations and to disregard them. The purpose of the present paper is to remind the reader not only of the necessity and usefulness of using models but also of the perils related to their uncritical use.

CONCLUSIONS

The following suggestions stem from what has been said above:
• we are *destined* to use models;
• use the simple models as long as you can;

• be aware that the predicted results or the drawn conclusions may not be correct;
• if it turns out that the results/conclusions are unacceptable, *modify* the model (perhaps, make it more complicated) or *abandon* it altogether;

- if a mathematical model is used, include as many factors as warranted by the physical considerations of the system;
- if a model involving many factors is used in one case, the mere fact that the fit between the predicted consequences of a simpler model and the experimental results is equally good or better is not sufficient to exclude some of the factors in

another case; there should, rather, be sound physical reasons for doing so;
- never use models beyond the limits of their applicability;
- do not try to test the validity of the model within the model itself;
- try to fit the model to the reality; do **not** try to force the reality into the model.

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Р е з и м е

ИЗУЧУВАЊА НА ВОДОРОДНО СВРЗАНИ СИСТЕМИ: УПОТРЕБА НА МОДЕЛИ – ПРЕДНОСТИ И ОГРАНИЧУВАЊА

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Клучни зборови: системи со водородни врски; модели; инфрацрвени спектри; кристалохидрати; научна методологија.

Научниците се речиси *принудени* да употребуваат модели – физички, концептуални или математички.

Моделите го поедноставуваат интерпретирањето на експерименталните факти и го олеснуваат прифаќањето на идеи од кои некои може да бидат и апстрактни. Од друга страна, моделите *не се реалност*, туку нејзина поедноставена претстава. Пренебрегнувањето на овој последен факт и слепата доверба во употребуваниот модел може да доведат до сериозни грешки. Во зависност од нашите потреби, за секој даден случај моделите може да бидат едноставни или комплексни, но секогаш е потребно колку што е можно поцелосно познавање на инхерентните ограничувања на

употребуваниот модел. Едноставните модели се полесни за употреба од оние што се пософистицирани, но постои поголема веројатност дека заклучоците што се изведуваат врз основа на едноставните модели ќе имаат ограничено важење, а може да бидат и сосема погрешни. Дадени се примери (предимно избрани од трудовите на авторот и неговите соработници посветени на изучувањето на водородно-сврзани системи) за корисноста од употребата на едноставните модели, но и за опасностите што во себе ги крие користењето на модели од кои некои вообичаено се употребуваат.