Saint Petersburg State University
Faculty of Physics
Department of Quantum Magnetic Phenomena

International Symposium and Summer School in Saint Petersburg

Nuclear Magnetic Resonance in Condensed Matter

10th meeting: "NMR in Life Sciences"
July 8 – 12 2013

Book of Abstracts

an AMPERE event

Saint Petersburg, Russia
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NMRCM 2013
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Conformation preference of ibuprofen in chloroform by 2D-3D NMR and GIAO quantum chemistry calculation

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1. Introduction

Our studies are dedicated to conformational details for drugs in solutions. It is well known that polymorphism of drug compounds affects the solubility and plays an important role in the production of pharmaceuticals. In turn, properties of polymorphs are connected with molecular structures of compounds and their ability to exist in different conformational forms in the solvent, from which recrystallization occurs. Therefore, search for new polymorphic forms of drug is closely associated with the study of the conformational state of drugs in solutions.

We are now studying (S)-ibuprofen is the active enantiomer of ibuprofen. Ibuprofen (Fig. 1) is a nonsteroidal anti-inflammatory drug (NSAID) used for reduce fever and treat pain or inflammation.

2. Results and discussion

We performed a proper assignment of lines in the ^{1}H and ^{13}C NMR spectra with the aid of experiments 2D HMBC, 2D NOESY, HSQC, TOCSY; NOESY , INADEQUATE and 3D HMQC-TOCSY.

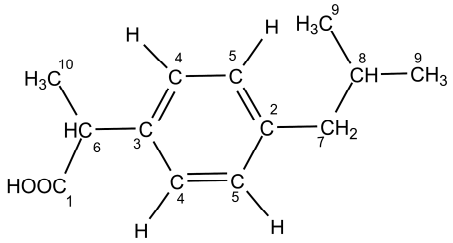

Figure 1. Structure of ibuprofen

In our case, the HSQC and HMBC showed similar patterns for aromatic protons in ibuprofen. In order to obtain unambiguous assignment of proton and carbon resonances, we decided to record (13C,13C)-INADEQUATE spectrum (Fig. 2).

It allows us to trace the connectivities of carbon atoms: 9-8-7-2-5-4-3-6 (atom numbering is as in Fig. 1). Evidently, signals of carbons 4 and 5 are interchanged, as compared to the AIST database [1].

M.L. Vueba,M.E. Pina,and L.A.E. Batista de Carvalho in 2007 published the result of a theoretical study of ibuprofen using density functional theory (DFT) calculations[2]. Eight different geometries were found to be energy minima. Might assume that the NMR measurements and the DFT conformer structures are accurate, but that the populations conformers are not.

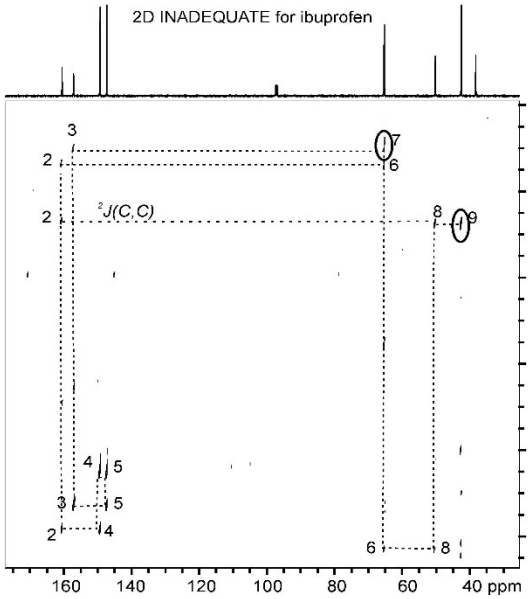

Figure 2. 2D INADEQUTE for ibuprofen in chloroform

Comparing the chemical shifts ^{13}C (δ (R) = TrσTMS− Trσ(R)) of the calculations GIAO and experimental determination ^{13}C, we obtain estimates of the conformational preferences (fig 3) by partial correlation method.

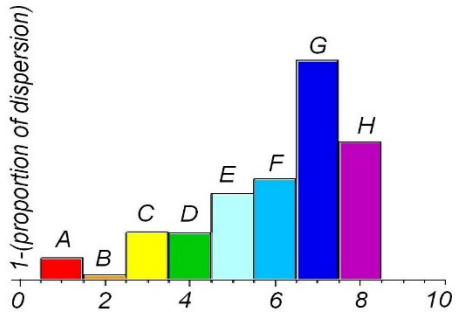

Figure 3. Conformational preferences of ibuprofen in chloroform

Evidently, conformer G and H predominate, are E and F also present but to a lesser extent than conformer G and H. Conformers proportion of A,B,C,D is relatively small. Such conformers preference because the concentration of ibuprofen in chloroform saturated.

References

[1] Spectral Database for Organic Compounds SDBS. http://sdbs.riodb.aist.go.jp
[2] M.L. Vueba,M.E. Pina,L.A.E. Batista de Carvalho. – *J Pharm Sci.*, **97(2)**, 845-859 (2007).