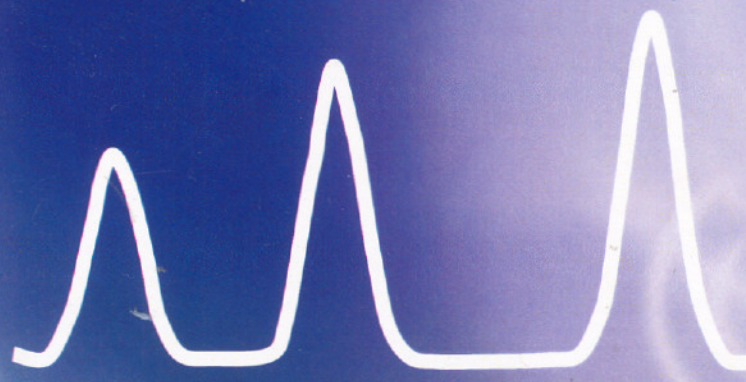

AMPERE NMR School

19 – 28 June 2008
Poznań, Wierzba
Poland

ABSTRACTS

Edited by S. Jurga

UNDER THE AUSPICES OF THE AMPERE GROUP
& ADAM MICKIEWICZ UNIVERSITY, POZNAŃ

CEI
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SoftComp
SOFT MATTER COMPOSITES

PROGRAMME AMPERE NMR SCHOOL, WIERZBA 2008

	SUNDAY	MONDAY		TUESDAY		WEDNESDAY	THURSDAY	FRIDAY	SATURDAY
8.00-9.00		BREAKFAST		BREAKFAST		BREAKFAST	BREAKFAST	BREAKFAST	BREAKFAST
9.00-9.45		***R. Kimmich*** From the basic equation of motion of molecules to NMR measurands: The harmonic radial potential theory of polymers		***J. Fraissard*** NMR of Physisorbed ^{129}Xe Used as a Probe to Investigate Porous Solids		***Sh. Vega*** New Aspects of Proton Decoupling in Solid State NMR	***F. Fujara*** Spacially resolved NMR in heavy ion irradiated ionic crystals	***C.A. de Lange*** Scope and limitations of accurate structure determination using liquid-crystal NMR	
9.45-10.30		***R. Wasylishen*** Probing nuclear spin-spin coupling tensors in solids		***D. Michel*** NMR on ferroelectric materials with very small sizes and on particles confined in nanoporous matrices		***A. Wong*** Application of solid-state NMR spectroscopy to low gamma quadrupolar nuclei	***E. Rössler*** Molecular Dynamics in Soft and hard confinement – a playground for ^{31}P NMR	***E. Burnell*** What NMR of solutes in liquid-crystalline solvents can tell about the ordering potential	
10.30-11.00		COFFEE BREAK		COFFEE BREAK		COFFEE BREAK	COFFEE BREAK	COFFEE BREAK	
11.00-11.45	ARRIVAL AND REGISTRATION	Parallel sessions ***J. Blicharski*** Rotational Magnetic Resonance and possibilities of a detection	***S. Stapf*** Spatially resolved monitoring of catalytically activated hydrogen peroxide decomposition – a test case for reaction monitoring by NMR	Parallel sessions ***M. Schönhoff*** Pulsed Field Gradient NMR studies of molecular exchange in colloidal systems	***R. Böhmer*** Deuteron NMR studies of the dynamics in clathrates	***M. Ernst*** Spin Diffusion in MAS Solid-State NMR	***K. Müller*** Order and dynamics in disordered solids as evaluated by solid state NMR spectroscopy	***J. Stepišnik*** Constrained molecular self-diffusion in the bulk water measured by NMR	DEPARTURE
11.45-12.30		***D. Kruk*** Various ways to enhance NMR signals: recent theoretical progress	***M. Vogel*** Mechanisms of Ion Transport in Solid-State Electrolytes: Insights from NMR Multi-Time Correlation Functions	***F. Grinberg*** Diffusion and Structure in Self-assembling Systems Studied by NMR	***B. Geil*** Correlation of primary relaxation and high-frequency modes in supercooled liquids. A Deuteron NMR study	Oral presentations ***B. Grünberg*** ***S. Naumov*** ***F. Poli***	Oral presentations ***Y.S. Postolenko*** ***K. Jasiński*** ***G. Woźniak***	Oral presentations ***M. Grbić*** ***M. Simčič*** ***W. Węglarz***	
12.30-15.00		LUNCH		LUNCH		LUNCH	LUNCH	LUNCH	
15.00-17.00		Oral presentations ***I. Rostykus*** ***S. Dekarchuk*** ***T. Mykhailova*** ***S. De Santis***		Oral presentations ***B. Blicharska*** ***J. Tritt-Goc*** ***S. Poberezhets*** ***L. Lalowicz*** ***L. Latanowicz***		Social event	Poster presentations (1-23)	Poster presentations (1-22)	
17.00-19.30		**Workshop** ***M. Giersig*** Nanomaterials and their Applications in Electronic and Biomedicine	**Workshop** ***F. Fujara, D. Kruk, E. Rössler*** Perfect recipe for dealing with strange relaxation data	**Workshop** ***R. Wasylishen, D. Michel*** NMR of Quadropolar Nuclei	**Workshop** ***E. Burnell, C.A. de Lange*** NMR of Ordered Liquids		Poster session I	Poster session II	
19.30-20.30	DINNER	"ALL TOGETHER PARTY"		DINNER		DINNER	DINNER	DINNER	

ARYLDIKETO ACIDS COMPLEXATION ABILITY AND KETO-ENOL TAUTOMERS RATIO IN PRESENCE OF MG^{2+}. UV/VIS AND NMR SPECTROSCOPY STUDY IN NONAQUEOUS MEDIA

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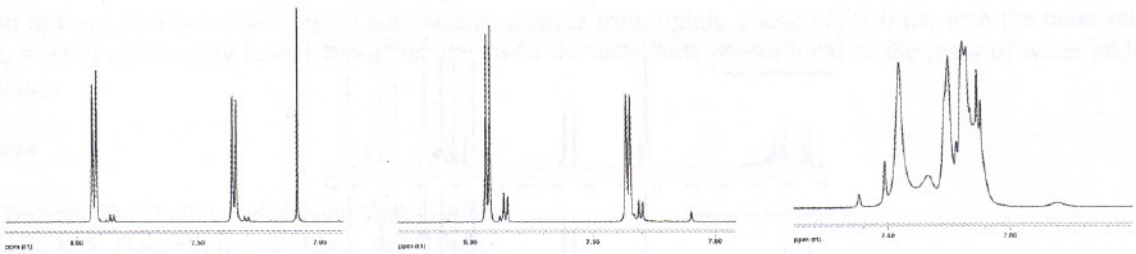
4-Aryl/heteroaryl-2,4-dioxobutanoic acid (ADK) derivatives exert widespread biological activities. Targeting HIV-1 integrase, the enzyme responsible for integration of viral DNA in host genome, is among the most important ones [1]. ADK–Mg^{2+} complex formation in the active site is postulated as an important factor that determinates degree of enzyme inhibition [2]. Congeneric set of 4-; 3,4- and 2,5-phenyl substituted ADK was synthesized. During routine characterization, mass spectra obtained by liquid chromatography-electrospray ionization (LC-ESI MS) showed presence of 2M–1 and 2(M–1)+Na ions for all compounds. It was observed that 2(M–1)+Na are more intensive than 2M–1 peaks in spectra of compounds with 3-alkyl substituents, despite substitution in other positions on the phenyl ring. In turn, in MS spectra of all other studied compounds 2M–1 peaks are more intensive. This could indicate significantly better complexation ability of 3-alkyl substituted derivatives and might have pharmacological implications.

We have found that there is no significant complexation ability between ADK and Mg^{2+} in aqueous solutions (pH range 1-8). To check potential differences in complexation ability between 3- and 4- phenyl substituted ADK, ^1H and ^{13}C NMR spectra were recorded in CD_3OD with and without Mg^{2+} ion. ^1H NMR spectra of 4-(4-Methylphenyl)-2,4-dioxobutanoic acid and 4-(2,5-Dimethylphenyl)-2,4-dioxobutanoic acid in presence of Mg^{2+}, are shown on Figure 1 a) and b).



a) b) c)

Fig.1. Regions of ^1H NMR spectra of 4-(4-Methylphenyl)-2,4-dioxobutanoic acid alone (a), 4-(4-Methylphenyl)-2,4-dioxobutanoic acid (b) and 4-(2,5-Dimethylphenyl)-2,4-dioxobutanoic acid (c) forty minutes after Mg^{2+} was added to ADK in 1 : 2 (M : L) molar ratio; recorded in CD_3OD.

As can be seen on selected spectra regions, there is no significant complexing ability of 4-Me- comparing to 2,5-di-Me- substituted derivative. Another interesting observation, considering spectra of 4-Me- derivative, is that keto-enol ratio is significantly changed when Mg^{2+} ion is present in solution. This was not observed in DMSO-d_6.

Job's spectrophotometric method [3, 4] was used to confirm the complex stoichiometry (M:L = 1:2) and to compare abilities of 4-; 3,4-; 2,5-phenyl and β-naphthyl substituted derivatives to complex with Mg^{2+}.

References

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Acknowledgements

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