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ARCHITECTURE OF THE SÃO CARLOS 2.0 TESLA NMR TOMOGRAPH

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A Nuclear Magnetic Resonance (NMR) tomograph is a sophisticated and versatile pulsed NMR Fourier spectrometer being more and more used for Medical diagnostic purpose. We developed in São Carlos (IFQSC/USP) an NMR spectrometer and a control system based on modules destined to: generate RF and field gradient tailored pulse shapes; event synchronism; data acquisition, digitalization and averaging of NMR signals; devices for image viewing; generation and detection of RF signals; NMR probes. The system has enough flexibility to operate under control of a great variety of computers.

At present, the control system works with the 280-based microcomputer MicroLIE (developed in our labs) and is being tested with a spectrometer prototype developed to operate with a VARIAN 12" iron core resistive magnet at 0.6 Tesla.

The system we describe in this paper is designed to operate later with a solenoidal superconductive magnet, with 31 cm bore and magnetic field strength up to 2.0 Tesla, with a gradient coil set fully time and gradient orientation controlled.

With the resistive prototype we obtained our first images of phantoms, small fruits and vegetables limited to about 3 cm diameter. The techniques used for image reconstruction are two-dimensional convolution/retroprojection and 2DFT, both with slice selection of less than 9 mm thickness. The images obtained will be shown in poster exposition.

A-5

CARBON-PROTON COUPLING CONSTANTS AND CARBON SHIELDING CONFORMATIONAL EFFECTS IN VERATROLE AND METHYLENEDIOXYBENZENE DERIVATIVES

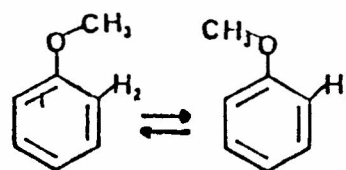
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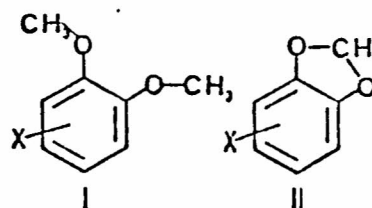
The barrier to inner rotation about the C(sp²)-O bond in anisole in solution is known to be notably larger than kJ at room temperature but not large enough to prevent rapid interconversion between the two coplanar rotamers [J. Goulon, U. Canet, H. Evans, and G.J. Davies, Mol. Phys. 30, 973 (1975)].



In ortho-substituted anisoles the steric hindrance between the two adjacent groups defines a methoxy group conformation which is cis to the proton in ring position 6.

The consequences of this preferred conformation on ¹³C-NMR parameters are being studied both from an empirical and a theoretical viewpoints.

For this purpose several veratrole (I) and methylenedioxybenzene (II) derivatives were synthesized and their proton coupled and decoupled spectra were analysed in order to determine C-H spin-spin couplings as well as carbon chemical shifts.



The effect of the conformational change of the methoxy group on ¹³J(CH) was studied and results thus obtained were compared with similar effects of the methoxy group in vinyl derivatives [R.J. Koole, H.J. A. de Aie, P.E. Hansen, Org. Magn. Reson. 22 (3), 146 (1984)].

In order to obtain a deeper understanding of factors originating the ¹³J(CH) cis/trans difference, IPPP-INDO calculations were carried out [A.R. Engelmann and R.H. Contreras, Int. J. Quantum Chem. 23, 1033 (1983)].

Empirically, the additivity rule of substituent effects was applied looking for a quantitative estimation of the influence of a side-chain conformational change on carbon shieldings.

In order to correlate ¹³C chemical shifts to atomic electron densities, INDO calculations were performed in the studied compounds. Mulliken population analyses were carried out at the INDO optimized geometries.

Campo	Dado
*****	Documento 1 de 1
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Autor Secundário	Torre Neto, A. (*)
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Autor Secundário	Bonagamba, Tito José (*)
Autor Secundário	Beckmann, Nicolau (*)
Autor Secundário	Slaets, Jan Frans Willem
Autor Secundário	Panepucci, Horácio Carlos
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Localiz.Eletrônica	"Clicar" sobre o botão para acesso ao Currículo Lattes de Alberto Tannus -- http://buscatextual.cnpq.br/buscatextual/visualizacv.do?id=K4783286H5
Localiz.Eletrônica	"Clicar" sobre o botão para acesso ao Currículo Lattes de Mateus José Martins -- http://buscatextual.cnpq.br/buscatextual/visualizacv.do?id=K4786514T3&dataRevisao=null
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