Second Laureate
Applied Research

Project Title: Antiaromaticity proved by the anisotropic effect in 1H NMR spectra
Researcher: Prof. Erich Kleinpeter
Country: Germany
Field: Chemistry
Scientific Affiliation: University of Potsdam

Abstract:

The spatial magnetic properties (through-space NMR shieldings, or TSNMRSs) of the antiaromatic -9oxaanthracene anion 12^- and of the corresponding -9dimeric dianion 11^{2-} have been calculated by the gauge-invariant atomic orbitals (GIAO) perturbation method employing the nucleus independent chemical shift (NICS) concept and visualized as iso-chemical-shielding surfaces (ICSSs) of various size and direction. The TSNMRS values, thus obtained, can be employed to indicate antiaromaticity by paratropic ring currents of the anionic compounds of 11^{2-} and 12^- studied and other neutral and ionic antiaromatic molecules from previous studies because anisotropic effects of functional groups in 1H NMR spectra have quantitatively proven to be the molecular response property of theoretical spatial nucleus independent chemical shieldings (NICS).

Biography:

70-1965 studied Chemistry at the University of Leipzig; diploma thesis: "NMR spectroscopic characterization of azaindolizines"

74-1970 Assistant at the same Department of Chemistry; Dr. rer. nat. thesis: "Investigation of the electronic state of dyes and dye intermediates by NMR and quantum-chemical calculations"

82-1974 Senior assistant at the same Department of Chemistry

1981 Habilitation: "Determination of configuration, conformation and intramolecular flexibility of organic compounds by NMR and quantum-chemical calculations"

85-1982Associated Professor of Organic Chemistry, Addis-Ababa University, Ethiopia

92-1985Docent of Spectroscopy (from 1988 on Professor of Chemistry), Martin-Luther-University Halle-Wittenberg; from 92-1989 Head of the Department of Analytical Chemistry

Since 1993 Professor of Analytical Chemistry; University of Potsdam; Head of the Department of Chemistry

2011 Honorary Doctor of the University of Szeged (SZTE), Hungary

Publication: over 400 papers, reviews, full books; more than 80 invited lectures.