MAGIC 2026

Book of Abstracts

Magnetically Induced Aromaticity, Gauge Invariance, and Currents

— Joseph Black Building, University of Glasgow— West End, Glasgow

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01

Aromaticity & Metastability in the Open Shell

Cate S. Anstöter

University of Glasgow, UK

Radical anions are the workhorse intermediates of single-electron-transfer and reductive chemistry. In the solution phase they are stabilised by their environment, sitting safely within the bound-state world that conventional quantum chemistry is built to describe. Remove the solvent and many of these anions become unbound. These states are metastable electronic resonances that fall outside this remit, posing an open challenge: how to capture their properties at all, from the lifetime of the metastable state itself to its aromaticity?

Ring currents, mapped with the ipsocentric (CTOCD-DZ) approach, are the natural probe of aromaticity, but the method has so far been formulated only for closed-shell systems. Taking the three $C_{10}H_8$ isomers — naphthalene, azulene and fulvalene — as a testbed, I will show how connectivity alone governs both whether the anion binds an electron (electron affinities spanning ~1.6 eV) and how its aromaticity responds to added charge. Combining XMCQDPT2 energies and characters, ipsocentric current densities, and complex-energy lifetimes, I will explore how aromaticity and metastability in the open-shell may be related.

02

Orbital Contributions to Magnetic Shielding of Cyclo[2n]carbons (n = 3–12)

Marija Baranac-Stojanović

University of Belgrade – Faculty of Chemistry, Belgrade, Serbia · mbaranac@chem.bg.ac.rs

The π-electron contribution to the out-of-plane component of the magnetic shielding tensor is widely used to assess diatropicity and paratropicity of rings with conjugated bonds, and thus to support their aromaticity or antiaromaticity. This work shows that the commonly used natural chemical shielding (NCS) analysis within the natural bond orbital (NBO) program gives unreliable contributions for the core, sigma and in-plane π-electron systems of cyclo[2n]carbons and proposes another way to estimate the contribution of the in-plane π electrons.

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03

Transmission As a Diagnostic of Orbital Topology

Alexander Barnett
University of Manchester, UK

The particle-on-a-ring model provides a simple framework for understanding the stability, magnetic properties, and topology of π-conjugated systems. When a weak perpendicular magnetic field is applied to this model, the quantisation of angular momentum reveals the Hückel 4n+2 rule and ring currents, resulting in aromaticity; at larger magnetic fields, the same physics gives rise to Aharonov–Bohm oscillations, producing a Berry phase.

Orbital topology offers an alternative, field-free handle on the Berry phase: twisting a carbon macrocycle into an e.g. Möbius geometry modifies the boundary conditions experienced by the delocalised electrons, acting as a synthetic gauge field encoded by molecular structure, which has consequences for aromaticity and electronic structure.

This talk explores this connection in a series of helical carbon macrocycles spanning Hückel, Möbius, and the recently-introduced half-Möbius topologies. The geometric phase introduced by molecular twist is encoded in the electronic structure, and evolves with ring size and topology.

Quantum transmission is proposed as a diagnostic for this physics. Computed within the Landauer–Büttiker formalism, the transmission function is sensitive to the same phase information that governs aromatic character, and unlike diagnostics such as NICS, can in principle be measured by single-molecule conductance experiments. Preliminary results illustrate how transmission responds to changes in orbital topology, and discuss the equivalence between applied magnetic flux and geometric twist in their effect on electron transport.

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04

Conjugated Circuit Models for Altans

Nino Bašić

University of Primorska, Slovenia · Institute of Mathematics, Physics and Mechanics, Slovenia

Conjugated-circuit (CC) models are used in chemical graph theory to estimate aromatic stabilisation, resonance energy, and, of interest here, maps of ring currents in conjugated hydrocarbons.

Let P be a patch, i.e., a plane chemical graph whose degree-2 vertices are all incident with the external face. A cycle C in P is a conjugated circuit if C is of even length and $P - C$ contains a perfect matching (Kekulé structure).

Altanisation originated in the chemical literature as a formal device for constructing generalised coronenes from smaller structures. An altan of a patch P is a patch obtained in the following way: let h be the number of degree-2 vertices along the perimeter of P. A new cycle of length $2h$ is inserted in the outer face, and every second vertex of this cycle is joined by a spoke to a former degree-2 vertex along the perimeter, in the obvious manner.

Naïve discovery or enumeration of all conjugated circuits tends to be computationally inefficient. We show how the properties of altans and iterated altans can be exploited to compute the map of ring currents for every generation of an altan in the CC model efficiently from that of the parent patch. These maps can be used to comment on the annulene-within-an-annulene model.

This is joint work with Patrick Fowler.

05

A Challenge to the Buckingham–Stephens Model

Daniel Blasco[a], Jan Novotný[a], James R. Asher[b], Raphael J. F. Berger[c], Stanislav Komorovský[b], Radek Marek[a]

[a] CEITEC – Central European Institute of Technology, Masaryk University, Brno, Czechia
[b] Institute of Inorganic Chemistry, Slovak Academy of Sciences, Bratislava, Slovakia
[c] Department of Chemistry and Physics of Materials, Paris Lodron University of Salzburg, Salzburg, Austria

The remarkable upfield shift of the NMR signal of the H ligand in transition-metal hydrido-complexes is highly sensitive to the coordination environment of the metal and, in particular, to the electronic nature of the ligand in the trans position relative to H. In 1964, Buckingham and Stephens proposed that the local paratropic currents sustained by the partially filled valence d-shell of the transition-metal atom were the source of the large NMR shielding of H. Thus, minute variations in the metal–hydrogen bond length due to the different σ-donor/π-acceptor capabilities of the trans ligand modulate the NMR shift of H. The paratropic character of the transition-metal atomic vortex has been inferred by examining the anisotropy of the NMR shielding tensor of bonded H in a series of early transition-metal carbonyl complexes. However, magnetically induced currents have not yet been directly studied.

In this contribution, the electronic nature of the ligand trans to H and its effect on the strength and topology of the magnetically induced current in a selection of d-block-metal hydrido-complexes is analysed from a computational perspective. The non-negligible contribution due to electron spin–orbit coupling is isolated and studied, and turns out to be the factor determining the observed trend. Our results refute the previously proposed governing role of the atomic current around the metal atom (as in the Buckingham–Stephens model), associated with trans-ligand induced variations in the metal–hydrogen bond length, in determining the characteristic ^{1}H NMR shifts of ligand H.

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06

Magnetically Induced Current Densities in Benzene and Cp Rings in Sandwich Compounds – What Happens upon Cation Binding?

Katarina A. Ćeranić[1], Slavko Radenković[2], Slađana Đorđević[2], Dušan P. Malenov[3]

[1] Innovative Centre of the Faculty of Chemistry, Studentski trg 12–16, Belgrade, Serbia
[2] University of Kragujevac, Faculty of Science, P.O. Box 60, Kragujevac 34000, Serbia
[3] University of Belgrade – Faculty of Chemistry, Studentski trg 12–16, Belgrade, Serbia

Aromatic rings coordinated in sandwich compounds have been shown to form significantly stronger cation–π interactions compared to uncoordinated benzene. In this work, we analysed the effect that the formation of the cation–π interaction has on the aromaticity of these systems. Cation–π complexes of ferrocene and bis(benzene)chromium with alkali (Li^+, Na^+, K^+) and alkaline earth (Be^{2+}, Mg^{2+}, Ca^{2+}) cations were optimized at the B3LYP-D3/def2-TZVP level, and Magnetically Induced Current Densities (MICD) were calculated by the diamagnetic-zero variant of the continuous transformation of the origin of the current density (CTOCD-DZ) method.

The calculated MICDs show that cation–π interactions with an uncoordinated benzene ring prompt a reduction of aromatic character, while with sandwich compounds an increase in aromaticity is observed. The trends in the MICD values were further compared with two electron delocalization aromaticity indexes: the Electron Density of Delocalized Bonds (EDDB) and the Multi-Center Index (MCI).

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07

About Analytic Continuation of Discrete Graph Spectra. The Case of Current-Sustaining Cycles.

Remi Chauvin

As very basic features, adjacency or Laplacian spectra of finite chemical graphs are discrete and real-valued. After the issue of non-real eigenvalues of directed cyclic graphs and underlying directed topological resonance "energy" (DTRE) was addressed at MAGIC 2024, the formal possibility of embedding indexed real graph spectra into bounded or periodic continuous complex extensions through a general functional operator will be addressed at MAGIC 2026 using tools of umbral calculus.

08

Exploring the Aromatic Limit of Cyclocarbons

Beren Dempsey
University of Manchester, UK

Cyclocarbons (C_N), covalently bonded ring allotropes of carbon, provide an excellent testbed for studying aromaticity. According to Hückel's rule, they can be classified as doubly aromatic (N = 4k+2, where k is an integer, e.g. C_{22}) or anti-aromatic (N = 4k, e.g. C_{20}), depending on the number of atoms in the ring. However, the maximum ring size for which aromatic stabilisation can persist remains unclear, with previous theoretical studies suggesting that aromaticity may be limited to rings up to approximately C_{18}.

This work investigates the aromaticity of large cyclocarbons. Using tip-induced chemistry, we prepared and characterised cyclocarbons up to N = 88 and analysed their transport gaps. When N is small, formally aromatic (N = 4k+2) cyclocarbons have larger gaps than the formally anti-aromatic (N = 4k) ones, and this difference becomes smaller as N increases, indicating a transition towards non-aromatic behaviour. These measurements are compared with theoretical predictions from (a) tuned density functional theory and (b) large active-space approximate configuration interaction calculations performed on both classical and quantum hardware. Both computational approaches show strong agreement with experimental observations, indicating that the answer to the question of the limit of cyclocarbon aromaticity is 42.

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09

Fat Goblets and Whether Patches Really Matter

Timothy Dickens
University of Cambridge, UK

This talk will explore two themes. First, after a short recap on unpaired electrons in triangulene, distorted triangulene, and Clar Goblet-like structures, a nomenclature will be proposed to help label these structures. Results will then be presented on 'fat goblets' — structures that are wider than the conventional goblets which have a simple six-membered central ring.

The second part of the talk will focus on exploring what effect the central patch has in systems with altan rings attached, and how changing the shape of the patch and varying the oxidation state affects the ring currents calculated using a variety of computational techniques.

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Beyond π Systems: σ-Aromaticity in Halogenated Cycloalkane Dications

Slađana Đorđević, Slavko Radenković
University of Kragujevac, Serbia

Aromaticity has long been the domain of π-conjugated systems, yet σ-delocalization offers a compelling alternative for stabilizing cyclic structures. This study investigates the transition of halogenated cycloalkanes from non-aromatic precursors to σ-aromatic dications. Through the lens of magnetically induced current densities (MICD), the electron density of delocalized bonds (EDDB), and aromatic stabilization energy (ASE), significant aromatic character is demonstrated in halogen units, reminiscent of the iconic $C_6I_6^{2+}$ system.

Notably, these findings challenge the universality of Hückel's rule in σ-systems, highlighting the critical role of orbital selection rules in determining aromaticity. This research expands the boundaries of aromatic theory, demonstrating how oxidation can fundamentally redefine the bonding nature of halogenated frameworks.

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11

Aromaticity Signatures in the UV-vis Absorption Spectra of (Sub)Phthalocyanines

Sílvia Escayola

Novel synthetic methods have expanded the possibilities for engineering porphyrin and phthalocyanine derivatives with tailored electronic and optical properties. Here, we investigate the UV-vis absorption spectra of substituted phthalocyanines and their contracted analogues, subphthalocyanines, which display nonplanar, bowl-shaped geometries. These macrocycles contain extended π-conjugated systems that govern their characteristic electronic response and make them relevant to materials science and catalysis.

We examine how structural changes affect aromaticity and spectroscopy. By combining experimental UV-vis data with electronic aromaticity descriptors and analysis of magnetically induced ring currents, we identify a correlation between external conjugated pathways and the Q bands. These results provide molecular-level insight into how structural modifications tune the optical properties of porphyrinoid systems.

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Patterns of Ring Current in Altans

Patrick Fowler
University of Sheffield, UK

Abstract to follow.

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Global Aromaticity in Paramagnetic Open-Shell Oxidation States of Porphyrin Nanorings

Lene Gödde
University of Oxford, UK

Several butadiyne-linked porphyrin nanorings *c*-P_N (where N is the number of porphyrin units) have been synthesized in the Anderson group and their global (anti)aromaticity has been studied extensively using NMR spectroscopy. Until now, N has generally been an even number. Here we report the template-directed synthesis of a butadiyne-linked 9-porphyrin ring *c*-P9 and study the effects of an uneven number of building blocks on the electronic properties.

The nine-legged template T9 binds *c*-P9 and locks it into a cylindrical geometry. The template furthermore serves as a probe for global ring currents around the nanoring and enables investigation of aromaticity in oxidation states with odd numbers of π-electrons. The odd number of porphyrins makes *c*-P9 very suitable for probing charge delocalization by EPR spectroscopy, for example when the nanoring is in the 9^+ oxidation state.

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Defying Antiaromaticity — The Curious Case of Pentalenopentalenes

Amrita Gogoi

Technion – Israel Institute of Technology, Israel

Antiaromatic molecules offer attractive electronic properties but are intrinsically unstable. Annelation with arenes can stabilize antiaromatic cores, yet often suppresses the very properties of interest. Here, we investigate the (anti)aromatic character of two families of pentalenopentalene-based polycyclic hydrocarbons — bisbenzannelated and biscycloheptatriene-annelated — in both the S_0 and T_1 states.

Despite exhibiting markedly different symmetry, open-shell character, and magnetic response, all systems follow a single unifying principle: a persistent preference for preserving local aromatic subunits. In T_1, the same behavior emerges through localization of spin density, maintaining local aromaticity and inducing a local reversal of aromatic character. Resonance structure analysis combined with the Randić conjugated circuit model provides a general framework for rationalization and a direct connection between behavior and topology.

These findings underscore that neither Hückel nor Baird rules can be naïvely applied to polycyclic (anti)aromatic systems and offer design principles for persistent antiaromatic molecules.

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Exalted Diamagnetism in Transition Metal Complexes with Bi_3^{3-}

Antun Habajec

Aromaticity is traditionally discussed in the context of organic molecules. In recent years, research in all-metal aromaticity has attracted interest, with claims of striking complexity, often with differing contributions from σ-, π-, δ- or ϕ-electrons. Additionally, metalloaromatic molecules were shown to exhibit exalted diamagnetism.

A popular way to characterise the (anti)aromaticity of a molecule is by analysing the ring current induced by a perpendicular external magnetic field. In the ipsocentric approach, the ring current is a sum of diatropic (aromatic) and paratropic (antiaromatic) contributions which arise from spin-allowed transitions from occupied to virtual orbitals, and are governed by well-understood selection rules.

In this work, we use the ipsocentric approach to understand the aromaticity and magnetic susceptibility in a series of transition metal complexes with a Bi_3^{3-} ring sandwiched between two f-block metals stabilised by organic scaffolding. The ring current of Bi_3^{3-} remains constant in all complexes, showing that it remains aromatic. In contrast, f-electrons provide a paratropic contribution to the magnetic susceptibility, which can be explained by a minimal model counting the number of allowed f-block transitions.

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16

Ring Currents in Metallic Sandwich Compounds

Remco Havenith
University of Groningen, Netherlands

The delocalised nature of the electrons in the $Ti(P_5)_2^{2-}$ complex has been studied using a ring current analysis, to deduce the oxidation state of the Ti atom. We show that this complex can be considered as a Ti(IV) ion encapsulated in a $(P_5)_2^{6-}$ cage. Furthermore, an unusual ring current is induced, leading to 'pancake' aromaticity. This is further explored for other metals and ligands.

Chemical Reactivity in Magnetic Fields: A Perspective from Symmetry, Current-DFT, and Conceptual DFT

Bang C. Huynh[†*], Meilani Wibowo-Teale[‡], Andrew M. Wibowo-Teale[‡], Frank De Proft[§], Paul Geerlings[§]

[†] Physical and Theoretical Chemistry Laboratory, Department of Chemistry, University of Oxford, Oxford OX1 3QZ, UK
[‡] School of Chemistry, University of Nottingham, Nottingham NG7 2RD, UK
[§] Research Group of General Chemistry (ALGC), Vrije Universiteit Brussel (VUB), Pleinlaan 2, B-1050 Brussels, Belgium
[*] Presenting author

Magnetic fields have been known to induce unexpected chemical behaviours in atoms and molecules. However, interpreting these effects with quantum-chemical theories is often challenging as magnetic fields inevitably introduce complex phases into wavefunctions, thereby obfuscating their interpretation.

In this talk, it will be shown how symmetry provides a route through this difficulty. In particular, by using group, representation, and corepresentation theories via QSym², a program for Quantum Symbolic Symmetry, complex-valued quantum-chemical quantities can be interpreted with intuition closely analogous to that used for real-valued quantities. This framework is then applied to current-density-functional theory and conceptual density-functional theory calculations to obtain chemically meaningful predictions for molecular behaviours in strong magnetic fields.

To illustrate its generality, the unitary and magnetic symmetries of important DFT quantities — frontier molecular orbitals, electron densities, and Fukui functions — are analysed for several small molecules in external magnetic fields. The obtained insights motivate the concepts of modular symmetry breaking and phasal symmetry breaking, which formalise the connection between the macroscopic constraints on the electric dipole moment imposed by time reversal and the microscopic symmetry properties of wavefunction- and density-based quantities.

Finally, this symmetry-based perspective sheds light on unusual magnetic-field-induced chemical phenomena: the orbital-driven reversal of electric dipole moments, the inability of magnetic fields to induce enantioselectivity, and the spin-controlled alteration of regioselectivity in ambident nucleophiles.

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18

Recent Calculations of the Magnetic Response in Conjugated Molecules

Guglielmo Monaco

University of Salerno, Italy

The magnetic response can be computed effectively nowadays by several approaches and codes. Using SYSMOIC, we have computed it in several interesting cases that will be presented here. We will also discuss how a divergence-free current can be obtained out of finite basis set calculations.

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(Anti)aromaticity of Same-Symmetry Singlet and Triplet ππ* States: Same–Same but Different, or Totally Different?

Henrik Ottosson

Uppsala University, Sweden

It has earlier been observed in computational studies that Baird's rule for the lowest ππ* triplet states (T_1) — i.e., the 4nπ-electron count for aromaticity and (4n+2)π-electron count for antiaromaticity — is often extendable to the lowest singlet ππ* states (S_1). This is puzzling as, e.g., the S_1 state of benzene is of different symmetry than the T_1 state. There is also no clear-cut theoretical explanation of why Baird's rule would be applicable to the lowest singlet excited state of ππ* character.

We report results from a study of C_{2v} symmetric heteroaromatics for which we analyse the aromatic and antiaromatic character of the lowest few pairs of analogous triplet and singlet excited states. We observe in computations of MICDs and NICS values that states with the same spatial symmetry (either A_1, A_2, B_1 or B_2) but different multiplicities (singlet or triplet) are mostly of opposite tropicities. The observation can be rationalized by the Steiner–Fowler rules as there is a difference in which virtual transitions are accessible in analogous singlet and triplet ππ* states. Yet, there is not always an agreement with electronic (anti)aromaticity descriptors. The cause for this deviation will be discussed.

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Magnetic Properties of 2D-Ising Lattices from Transition Metal Complexes

Christian Pachl
Karlsruhe Institute of Technology (KIT), Germany

In molecular chemistry, the magnetic properties of transition metal compounds are usually defined only by the molecular structure. The local electronic structure of the transition metal ions as well as intramolecular interactions to other spin centers suffice to describe the bulk magnetic properties. When investigating a series of Zn(II) and Co(II) radical complexes, we found that the local spins are coupled to neighbouring molecules in a 2-dimensional Ising-type lattice.

The ligand system has been investigated by itself with DFT and Current Density methods, and the magnetic properties simulated using an in-house developed Complete Active Space Spin Orbit Configuration Interaction (CASOCI) program as well as Broken-Symmetry DFT and Monte Carlo simulations. This revealed an interconnected disordered net of magnetic coupling constants.

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Fused 3D/2D Magnetically Aromatic System Achieved through Carbon–Carbon to Boron–Nitrogen Isosterism

Jordi Poater
University of Barcelona, Spain

The realization of genuine 3D/2D aromatic systems through fusion of BN/CC isosteric azaborines with carborane clusters has been systematically examined using magnetic response analysis. Current density maps, bond current strengths, and DIAL surfaces demonstrate that magnetic descriptors provide the most sensitive criterion for multidimensional aromaticity. Although all isolated azaborines are aromatic, the magnitude and uniformity of their diatropic ring currents strongly depend on the number and relative positioning of BN units, with consecutive BN incorporation attenuating and polarizing the circulation.

Fusion studies reveal that neither benzene nor mono-BN azaborine sustains integrated 3D/2D aromaticity due to a strong paratropic current localized at the fusion bond. In contrast, systems containing two consecutive BN/CC isosteres — particularly 1,4-diaza-2,3-diborine and 1,4-diaza-2-borine — exhibit a continuous diatropic ring current across the interface, consistent with effective magnetic communication between the planar ring and the boron cage. Electronic and energetic analyses support these findings but are less discriminating than magnetic criteria. Overall, this work establishes magnetic response properties as decisive tools for identifying viable 3D/2D aromatic systems and defines structural requirements for their design.

22

Foundations of Electron Counting in σ-Aromatic Systems

Slavko Radenković

University of Kragujevac, Serbia

Electron-counting rules of aromaticity, such as the Hückel and Baird rules, have long been used to predict both aromatic character and the tropicity of magnetically induced current density (MICD) in conjugated cyclic molecules. Originally formulated for annulenes, these rules were later extended to a broader class of monocyclic π-conjugated systems. More recently, it has been shown that Hückel and related aromaticity rules can also be successfully applied to σ-conjugated cyclic systems.

In this work, we demonstrate a fundamental limitation of these electron-counting rules in cyclic systems containing tangentially oriented p atomic orbitals engaged in σ-type bonding. While the rules correctly predict MICD tropicity for systems with an even number of atoms in the ring, they fail for odd-membered rings, yielding incorrect predictions of aromatic and antiaromatic behavior. To illustrate this limitation, magnetically induced current densities were calculated for a series of periodo-annulenes at the B3LYP/def2-TZVP level of theory.

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A Molecule with Half-Möbius Topology

Igor Rončević

University of Manchester, UK

π-Conjugated systems are fascinating because their electrons are highly delocalised, while remaining bound by their orbital basis. In π-conjugated rings a key phenomenon is aromaticity, or the presence of a ring current in a magnetic field, which demonstrates that the electronic wavefunction is coherently delocalised around the whole molecular ring. Topologically trivial π-conjugated rings with ring currents obey Hückel's rule: they are aromatic if they have 4N+2 π-electrons, and anti-aromatic if they have 4N π-electrons, where N is an integer.

In rings that resemble a Möbius strip — a body with a single edge — Hückel's rules are reversed. This reversal is a consequence of a 180° twist in their orbital basis upon one circulation of the ring.

This talk presents recent work on the characterisation of a molecule with half-Möbius topology, in which the orbital basis twists by 90° upon one circulation of the ring.

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24

Spin-Selective Aromaticity in the n,π* Excited States of Heteroaromatic Molecules

Miquel Solà
Universitat de Girona, Spain

The photochemistry of heteroaromatic compounds depends on the character of their lowest electronically excited states, which are of either n,π* or π,π* type. For species with 4n+2 π-electrons, the n,π* type of states have an odd number of π-electrons, leading to an unclear character spanning from aromatic to antiaromatic.

We analyze here the n,π* excited states of (4n+2)π-electron heteroaromatics with in-plane lone-pairs applying Mandado's 2n+1 rule for aromaticity of separate spins. After excitation of an electron from n to π*, a (4n+2)π-electron species has 2n+2 alpha π-electrons and 2n+1 beta π-electrons (or vice versa), and becomes alpha π-antiaromatic and beta π-aromatic. Yet, the antiaromatic alpha π- and aromatic beta π-components seldom cancel, leading to residuals with aromatic or antiaromatic character. Having (anti)aromatic residuals influences the relative stability of the n,π* states. We discuss which factors determine which type of vertical excited state (n,π* or π,π*) is the lowest in energy for various heteroaromatics.

Investigating NMR Properties via Magnetically Induced Current Density: From Spin-Spin Coupling Maps to Relativistic Effects in Paramagnetic Systems

Francesco Ferdinando Summa
University of Salerno, Italy

This contribution highlights the versatility and predictive power of the magnetically induced current density approach, evaluated via time-independent standard response equations at both Hartree–Fock (HF) and Density Functional Theory (DFT) levels, as a central tool for modeling and interpreting Nuclear Magnetic Resonance (NMR) properties. Two distinct applications are discussed.

1. Visualizing Through-Bond and Through-Space J-Couplings. The first part of the talk introduces a novel method for calculating nuclear spin-spin coupling density functions entirely in the atomic orbital basis. By going beyond the standard Fermi contact approximation to include all four Ramsey terms, this methodology utilizes the current density induced by nuclear magnetic dipoles as its leading motif. The resulting coupling density functions provide an intuitive, pictorial tool to visualize the transmission pathways of nuclear coupling, allowing a clear spatial differentiation between interactions mediated through chemical bonds and those transmitted through space.

2. Relativistic Formulation for Paramagnetic NMR (pNMR). The second part of the talk focuses on the computation of nuclear magnetic shielding and magnetizability tensors in open-shell, paramagnetic molecules. Scalar and field-free spin-orbit relativistic corrections are introduced into the current density framework using a Zeroth-Order Regular Approximation (ZORA) formulation. This approach ensures variational stability at the nuclear coordinates, successfully capturing heavy-atom effects on light-atom shieldings (HALA effect). Furthermore, it demonstrates full thermodynamic consistency with the general Van Vleck formulation, recovering the temperature-dependent Curie contribution through explicit integration of the magnetically induced spin current density, without requiring the intermediate calculation of EPR g-tensors or Zero-Field Splitting (ZFS) Hamiltonians.

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Toy Models Reveal Intrinsic Biases in NICS: Insights to Verify NICS Interpretations

Emiel Vanden Berghe

Ghent University, Belgium

The nucleus-independent chemical shift (NICS) as an aromaticity index rests on the premise that the NICS value can be interpreted to infer those aspects of a system's current-density susceptibility (J) that are relevant to magnetic aromaticity. While the shielding density acts as an intermediary in the inferential relation between NICS and J, the complexity of shielding-density patterns in molecular systems hinders the extraction of generalisable insights.

To address the complexity introduced by molecular systems, we introduce toy models designed to isolate inherent features of the NICS–J relationship and to separate intrinsic NICS behaviour from aromaticity. We find that NICS provides an inherently biased reflection of J, resulting in artifacts that could be misinterpreted to yield conclusions that conflict with the magnetic aromaticity criterion upon which the NICS methodology is justified. This work establishes a foundation for using toy models as a means to gain the insight needed to verify NICS interpretations with respect to the underlying J in molecular systems.