

## **ESF Workshop: New perspectives on Aromaticity: Scientific report.**

Reporters: Patrick Fowler (Exeter), Francesco Zerbetto (Bologna), John Sandall (Exeter).

The ESF workshop “New Perspectives on Aromaticity”, held at the Crossmead Centre, University of Exeter, Exeter, UK, from July 5 to July 9, 2003 under the auspices of the European Science Foundation, had participation from 32 scientists working in the chemical and physical sciences, and drawn from research groups across Europe.

In keeping with the interdisciplinary nature of the topic, a mixture of experimental and theoretical talks were presented, in a schedule that gave ample opportunity for discussion. The meeting was characterised by excellent presentations, some involving films and demonstrations, and lively discussion sessions in which a number of controversial issues were aired and through which, by the end of the meeting, a large amount of scientific common ground was established. The workshop atmosphere, in which all participants were accommodated on site in secluded surroundings encouraged the continuation of discussions well outside the formal sessions, and was a major factor in establishing agreement and promoting future research collaborations on remaining contentious issues.

The scientific sessions were designed to move between various strands of the topic, deliberately mixing experimental and theoretical talks, conceptual with applied theory, and periodically returning to discussion of implications for synthetic chemistry. This helped to ensure that the expert audience was exposed to thinking from other disciplines, and it stimulated genuine exchange of information and views. Many participants commented favourably on this aspect of the workshop.

The workshop started with a short presentation on ESF from the representative, Professor Judith Howard. Scientific sessions began with a wide-ranging presentation *Assessment Of Aromaticity via Molecular Response Properties* by Prof. Paolo Lazzeretti (Modena) on the basic theory, philosophical and computational aspects of properties associated with aromaticity, which raised questions about the use of NICS (Nucleus-Independent-Chemical-Shift) as an aromaticity index. This provoked a spirited defence by Prof. Paul Schleyer of the NICS concept in the ensuing discussion, which set the scene by introducing a number of themes of definition, interpretation and explanation of aromaticity that were to recur over the next three days. The discussion was followed by *Ring Current and Magnetic Properties Of C<sub>48</sub>N<sub>12</sub> aza-fullerenes*, a talk on the application of the theory to some novel fullerene derivatives, by Prof. Riccardo

Zanasi (Salerno) which illustrated the versatility and economy of ring-current mapping methods for large systems.

The second session of the first day was devoted to presentation of some experimental properties of aromatic and related systems. Dr. N. McKeown, (Manchester), discussed *Nanoporous Materials Derived From Phthalocyanines and other Aromatic Species*, showing the role of serendipity in the initiation of this field of chemistry, its connections with current thinking on aromaticity and conjugation, and pointing to ways of exploiting intermolecular interactions of conjugated systems to create nanoporous materials. Prof. Petra Rudolf (Gröningen) in her talk *Electron delocalisation detected by electron spectroscopies* gave an overview of solid-state spectroscopic experiments that reflect on electron delocalisation, and hence probe a property that is a pre-requisite of aromaticity. The morning ended with a short talk by Prof. Andre Rassat (ENS, Paris), *Steric Effects On Mesomerism*, on the conceptual links between aromaticity and the time-honoured Woodward-Hoffmann rules of organic chemistry.

The afternoon session began with a talk from Prof. Paul von R. Schleyer (Erlangen), probably the world's leading proponent of the magnetic criterion for aromaticity. Under the general title *Aromaticity Evaluations* he developed arguments for the usefulness of the NICS value in different systems, particularly examining the onset of bond alternation in annulenes and the relationship between NICS and Clar structures in graphenes. Much ensuing discussion centred on the relationship between the NICS value at the centre of a ring and the current density flowing in or around that ring. Questions that emerged were the extent of the experimental foundation for ring-current effects in proton shieldings, relationship of isotropic NICS values to tensor components, and inferability of current pattern from single-point shieldings.

In the next, two-part paper *Delocalized Electrons In Molecules: The ACID Method; Synthesis of Moebius aromatics* Prof. Rainer Herges (Kiel) combined a discussion of his own theoretical method with some exciting new synthetic chemistry. He discussed his ACID method for determining the extent of electron delocalisation in molecules and then informed the audience of his group's successful synthetic realisation of the first Möbius aromatic compound, a functionalised  $4n$  cycle given aromatic character by a single twist. This remarkable tour de force, reinforced by the use of a giant molecular model, was appreciated by all present and provoked excited discussion of the possibilities for generalising the synthesis, and the magnetic characteristics to be expected of such a molecule; the latter being an introduction to one of the lectures later in the afternoon session.

Prof. Frank De Proft (Brussels) in a talk entitled *Conceptual And Computational Density Functional Theory: Applications In The Study Of Aromaticity* discussed the application of

density functional theory to the study of aromaticity, and in particular the extraction of qualitative interpretation for the computed results by employment of the conceptual framework of global and local hardness and softness which fits naturally with DFT. As a concrete example, he examined transition states for cyclo-addition reactions, showing how predictions based on NICS values can go awry when polar structures are involved. Dr. Henry Rzepa returned to the theme of Möbius compounds in *Aromaticity With A Twist*, giving an orbital analysis of the 4n annulenes and using the computed NICS values of a number of series of hypothetical structures to validate Heilbronner's original suggestion. Challenges to visualisation and experimental realisation of these predictions were taken up in the discussion session.

In the final talk of the day Prof. Mircea Diudea (Cluj, Romania) spoke on *Stability Of Tubulenes: A Second Cylinder Rule*, looking at factors such as open/closed shell electronic structure, HOMO-LUMO gap and overall stability of series of structures based on fullerenes and nanotubes, developing systematics for closing the end of cylinders in a stable fashion and showing how simple principles might inform future molecular design in this area.

The second day started with a paper presented by the workshop chair, Prof. Patrick Fowler (Exeter) on *Mapping And Understanding Ring Currents*, demonstrating mapping of ring current density in a variety of aromatic systems, giving an understanding at the orbital level of molecular response to an applied magnetic field in terms of activity of just a few frontier electrons. Special methods for large graphene systems were introduced and shown to contradict conclusions inferred from the NICS approach. Ensuing discussion centred on the source of this difference, identifying a problem with the way that orbital contributions are defined in other approaches.

Dr. Remco Havenith (Warwick) also used iposcentric techniques, amongst others, in *Different Views On Aromaticity: Ring Currents And Resonance Energies* to examine the nature of aromaticity in systems such as  $\alpha,\omega$ -bicyclopentadienylpolyacenes, Al<sub>42</sub><sup>-</sup> and cyclooctatetraene. Physical conclusions on the changeover from anti-aromatic to aromatic current patterns on the first series, existence of  $\sigma$ -rather than  $\pi$ -currents in the Al<sub>42</sub><sup>-</sup> species, and orbital explanations of current survival and quenching in COT, were drawn. Prof. Leonardus Jenneskens (Utrecht) *Non-alternant cyclo-penta and cyclo-hepta fused PAH vs. closed carbon Surfaces* returned to an experimental perspective by comparing electrochemical properties of non-alternant fused polycyclic aromatic hydrocarbons with fullerenes. Remarkable correlations of band-gap with reduction potential and of reduction potential between parent and cyclopentafused species is clarified by examination of orbital models.

The final session of the morning began with a presentation from Christopher. Simpson (Mainz) on *Giant Polycyclic Aromatic Hydrocarbons as Processable Graphite* discussing the work of the Muellen group on the chemical synthesis of giant polycyclic aromatic hydrocarbons that correspond to graphitic-type structures of definite composition amenable to characterisation and property investigation, as an essential precursor to the manufacture of useful devices. The talk was replete with targets for theoretical investigation and hints of future progress on the experimental side. The molecules being discussed are, for well characterised species, simply enormous: one fourth generation species contains the same number of carbon atoms (1812) as there are isomers of 60-fullerene. Prof. Roger Taylor (Sussex) gave the next talk with the tongue-in-cheek title of *How To Make Fullerenes Aromatic*, showing how the site and pattern of addition in fullerenes and azafullerenes is in many cases guided by the aromaticity of the product, which has a signature of minimal bond-length alternation and implications for magnetic properties. The concept of aromaticity is here also guiding the intuition of synthetic chemists in their exploration of fullerenes as chemical building blocks.

The session ended with a talk on *Ring Currents In Annulenes* from A. Soncini (Exeter) who used a specific example of the size-dependent changes in properties along the series of  $4n+2$  annulenes to compare the apparently discordant predictions of the NICS and ipsocentric orbital models to show that in fact, when the consequences of symmetry breaking are rightly understood, the two approaches are mutually consistent.

On the final day of the meeting, Prof. Marek Krygowski (Warsaw) re-introduced non-magnetic criteria for aromaticity and in his talk *Two Faces of the Structural Aspects Of Aromaticity* re-focused the discussion on empirical, geometry-related models for description of aromaticity. The talk and the following discussion established some degree of compatibility between the geometric and magnetic criteria, but pointed to a real area of disagreement in the aromaticity literature. The next talk was given from the physicist's perspective by Prof. Gotthard Seifert (Dresden) under the title *Ring Currents, Nuclear Magnetic Shielding And Aromaticity*. He gave a short account of the basic quantum mechanics of magnetic response properties in a DFT model and advocated calculation of orbital contributions to NICS using a formalism developed between the Dresden and Erlangen groups. This thoughtful presentation stimulated a long and intense discussion session that brought out the essentials of the different approaches to orbital contributions, which were to be further explored later in the day at the general discussion session. This lecture set closed with a contribution from Prof. Bernard Silvi (Paris) on *How Topological Partitions Of Electron Distributions Reveal Delocalisation*. This

gave an introduction to the electron localisation function (ELF) which was to be used in later talks (Sola, Lepetit) as a probe of aromatic patterns in electronic structure.

In the second session of the day, Prof. Arnout Ceulemans (Leuven) moved the discussion from linear response properties to the description of the behaviour of systems under large magnetic fields and in *Magnetic Vortices And Aromaticity* presented, with powerpoint movies, applications of a phenomenological Hamiltonian, generally used to describe superconductivity, to aromatic molecules. Then Dr. Miquel Solá (Girona) made a case for *The Para-delocalisation Index as an Electronic Index of Aromaticity* as a way of estimating aromaticity using the ELF method described earlier, and made comparisons with both NICS and geometric criteria.

The afternoon session contained the final three lectures of the workshop. Prof. Andreas Hirsch (Erlangen) described some electron-counting ideas for three-dimensional aromatic cage structures in his approach to *Spherical Aromaticity*, which gave a useful insight into a conceptual modelling process that exploits traditional chemical intuitions to link together 2D and 3D structures. In this picture a structure such as  $P_4$  is an aromatic. Dr. Christine Lepetit (Toulouse) in *Aromaticity And Homoaromaticity In Carbomeric Structures* described a series of formal and in some cases chemically realised expansions of traditional aromatic structures into ‘carbomers’ and proposed the aromaticity and possible homoaromaticity of these systems, backed up by ELF calculations. Finally Prof. Philippe Hiberty connected simple and not-so-simple theories to show how *Distortive tendencies of  $\pi$  electrons in  $\pi$ -delocalised systems* link the problems of existence and destruction of aromaticity to the competition between  $\sigma$  and  $\pi$  electrons. All three lectures evoked numerous questions from the audience.

The final official session of the workshop was a scheduled general discussion, for which all delegates had been invited to prepare formal questions and flash presentations tying together key points from their own presentations, comments that had arisen in the question-and-answer sessions, and topics that had become major talking points over the three days. More than 20 substantive comments were made, and the discussion lasted well beyond the allotted hour and a half. A large degree of consensus was reached on what had become the main issues of the meeting – the magnetic criterion for aromaticity, its connection with the NICS model and the role and interpretation of current density mapping. A brief summary of that consensus might be as follows:

The ability of a cyclic system to support a diatropic induced current in the presence of an external field is a workable criterion for aromaticity. The NICS (nucleus-independent chemical shift) concept has given a readily calculated index which when interpreted carefully gives insight

into the existence of such currents. However, practicable distributed-gauge methods for efficient calculation and visualisation of induced current density are also now available and the new maps give a more direct picture of aromaticity that avoids many of the pitfalls of a single-number index approach. The ipsocentric approach gives an interpretation of ring currents at the orbital level in terms of a small subset of frontier electrons. Orbital contributions from this method are advocated as a route to qualitative and quantitative understanding of magnetic aromaticity. Further work to harmonise calculation of orbital contributions between different methods is also advocated. A huge variety of systems and types of aromaticity is now open for exploration.

As always at successful meetings, a number of bilateral and multilateral projects for collaboration were established. In particular it is intended for a joint paper clarifying the role of orbital contributions to be submitted to an international journal by a combination of proponents of NICS and ipsocentric approaches. This should serve the wider community by establishing a standard methodology for tackling magnetic aromaticity from the theoretical perspective.

### **Publication**

The discussions at this meeting will be given a more permanent form as a result of negotiation between the organisers and the UK Royal Society of Chemistry. The workshop proceedings in the form of full manuscripts from speakers, to be peer-reviewed in the normal way, will be submitted for a special issue of *Physical Chemistry Chemical Physics*. The deadline for submission is in September 2003, and the special issue is expected to appear in Spring 2004. The workshop chair, co-chair and a member of the organising committee (Fowler, Zerbetto, Jenneskens) will assist PCCP as Guest Editors. About 15 – 20 papers are expected.

Many of the participants are also likely to submit papers to a special issue of *Chemical Reviews* (American Chemical Society) on Aromaticity and Delocalisation, edited by Prof. Schleyer for publication in 2004/5. Following on the heels of the earlier special issue of the same journal on Aromaticity, this initiative instances the continuing fascination of this area for researchers in all branches of chemistry and on several continents.

### **Future Prospect**

There was much progress at this meeting, but there is clearly scope for much more, and now that some of the obscurities of the disagreements on technical theoretical details have been cleared up, there is a need for a period of consolidation, intense research on specific systems and organization of a larger meeting to bring the fruits of this activity to the wider chemistry and physics community. It is hoped that support for such a meeting could be arranged under the auspices of the ESF. Collaborations started at this meeting are also likely to feed into applications to Framework programmes of the EC.

## ESF Workshop: New perspectives on Aromaticity

### FINAL PROGRAMME:

<b>Saturday 5 th July 2003</b>	
From <b>16.00</b>	REGISTRATION, CROSSMEAD CONFERENCE CENTRE
<b>19.30</b>	BUFFET DINNER

<b>Sunday 6 th July 2003</b>	
<b>08.00</b>	BREAKFAST
<b>Session 1</b>	Chair: Patrick <b>Fowler</b> (Exeter)
<b>09.15</b> <b>09.25-09.40</b>	Opening remarks Presentation on behalf of ESF <b>Judith Howard</b> (Durham)
<b>09.40-10.20</b>	<b>Paolo Lazzeretti</b> (Modena) <i>Assessment Of Aromaticity via Molecular Response Properties</i>
<b>10.20-11.00</b>	<b>Riccardo Zanasi</b> (Salerno) <i>Ring Current &amp; Magnetic Properties Of C<sub>48</sub>N<sub>12</sub> aza-fullerenes</i>
<b>11.00-11.15</b>	COFFEE
<b>Session 2</b>	Chair: T Marek <b>Krygowski</b> (Warsaw)
<b>11.15-11.55</b>	<b>Neil McKeown</b> (Manchester) <i>Nanoporous Materials Derived From Phthalocyanines and other Aromatic Species</i>
<b>11.55-12.35</b>	<b>Petra Rudolf</b> (Groningen) <i>Electron delocalisation detected by electron spectroscopies</i>
<b>12.35-12.55</b>	<b>Andre Rassat</b> (ENS, Paris) <i>Steric Effects On Mesomerism</i>
<b>13.00</b>	LUNCH
<b>Session 3</b>	Chair: Leo <b>Jenneskens</b> (Utrecht)
<b>14.30-15.10</b>	<b>Paul von Rague Schleyer</b> (Erlangen/Georgia) <i>Aromaticity Evaluations</i>
<b>15.10-15.50</b>	<b>Rainer Herges</b> (Kiel) <i>Delocalized Electrons In Molecules: The ACID Method; Synthesis of Moebius aromatics</i>
<b>15.50-16.10</b>	TEA

<b>16.10-16.50</b>	Frank <b>De Proft</b> (Brussels) <i>Conceptual And Computational Density Functional Theory: Applications In The Study Of Aromaticity</i>
<b>16.50-17.30</b>	Henry <b>Rzepa</b> (Imperial College) <i>Aromaticity With A Twist</i>
<b>17.30-17.50</b>	Mircea <b>Diudea</b> (Cluj, Romania) <i>Stability Of Tubulenes: A Second Cylinder Rule</i>
<b>19.30</b>	DINNER

<b>Monday 7 th July 2003</b>	
<b>From 07.30</b>	BREAKFAST
<b>Session 4</b>	Chair: Riccardo <b>Zanasi</b> (Salerno)
<b>09.00-09.40</b>	Patrick <b>Fowler</b> (Exeter) <i>Mapping And Understanding Ring Currents</i>
<b>09.40-10.20</b>	Remco <b>Havenith</b> (Warwick) <i>Different Views On Aromaticity: Ring Currents And Resonance Energies</i>
<b>10.20-11.00</b>	Leonardus <b>Jenneskens</b> (Utrecht) <i>Non-Alternant Cyclo-Penta And Cyclo-Hepta Fused PAH vs. Closed Carbon Surfaces</i>
<b>11.00-11.15</b>	COFFEE
<b>Session 5</b>	Chair: Petra <b>Rudolf</b> (Groningen)
<b>11.15-11.55</b>	Christopher <b>Simpson</b> (Mainz) <i>Giant Polycyclic Aromatic Hydrocarbons as Processable Graphite</i>
<b>11.55-12.35</b>	Roger <b>Taylor</b> (Sussex) <i>How To Make Fullerenes Aromatic</i>
<b>12.35-12.55</b>	Alessandro <b>Soncini</b> (Exeter) <i>Ring Currents In Annulenes</i>
<b>13.00</b>	LUNCH
FREE AFTERNOON - Discussions	
<b>19.30</b>	DINNER



<b>Tuesday 8 th July 2003</b>	
<b>From 07.30</b>	BREAKFAST
<b>Session 6</b>	Chair: Francesco <b>Zerbetto</b> (Bologna)
<b>09.00-09.40</b>	T Marek <b>Krygowski</b> (Warsaw) <i>Two Faces of the Structural Aspects Of Aromaticity</i>
<b>09.40-10.20</b>	Gotthard <b>Seifert</b> (Dresden) <i>Ring Currents, Nuclear Magnetic Shielding And Aromaticity</i>
<b>10.20-11.00</b>	Bernard <b>Silvi</b> (Jussieu, Paris) <i>How Topological Partitions Of Electron Distributions Reveal Delocalization</i>
<b>11.00-11.15</b>	COFFEE
<b>Session 7</b>	Chair: Paolo <b>Lazzeretti</b> (Modena)
<b>11.15-11.55</b>	Arnout Ceulemans (Leuven) <i>Magnetic Vortices And Aromaticity</i>
<b>11.55-12.35</b>	Miquel <b>Solà</b> <i>The Paradelocalisation Index as an Electronic Index of Aromaticity</i>
<b>13.00</b>	LUNCH
<b>Session 8</b>	Chair: Arnout <b>Ceulemans</b> (Leuven)
<b>14.10-14.50</b>	Andreas <b>Hirsch</b> (Erlangen) <i>Spherical Aromaticity</i>
<b>14.50-15.30</b>	Christine <b>Lepetit</b> (Toulouse) <i>Aromaticity And Homoaromaticity In Carbomeric Structures</i>
<b>15.30-16.10</b>	Philippe <b>Hiberty</b> (Orsay) <i>Distortive tendencies of pi electrons in pi-delocalised systems</i>
<b>16.10-16.30</b>	TEA
<b>Session 9</b>	Chair: John <b>Sandall</b> (Exeter)
<b>16.30-18.00</b>	General Discussion
<b>19.30</b>	DINNER

<b>Wednesday 9 th July 2003</b>	
<b>From 07.30</b>	BREAKFAST & DEPARTURE

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'New Perspectives on Aromaticity', Exeter, July 5-9 2003**

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