Unraveling the Enigma of Craig-Type Möbius-Aromatic and Other Recent GIMIC Studies

Dage Sundholm

Department of Chemistry,
Faculty of Science,
University of Helsinki,
Finland

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- Aromaticity and antiaromaticity
- The GIMIC method
- Current-density strengths
- Twist and writhe
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- Tropicity
- Craig-type Möbius aromatic molecules
- Craig-type Möbius aromatic 10-Platinacorrole

Aromaticity and Antiaromaticity

What is aromaticity?

IUPAC states that cyclic molecular systems are aromatic when

- they are energetically stabilized due to electron delocalization
- they are structurally more stable than nonaromatic molecules when undergoing chemical transformations Energy
- They have a small bond-length alternation (BLA) Structure
- Aromatic molecular rings sustain a net diatropic ring current when they are exposed to an external magnetic field
- NMR signals of protons on the outside of an aromatic ring are shifted to larger chemical shifts (smaller magnetic shielding constants) Magnetic

https://doi.org/10.1351/goldbook.A00442
V. I. Minkin, Pure Appl. Chem. 71 (1999) 1919–1981
G. Merino, M. Solá, I. Fernández, C. Foroutan-Nejad, P. Lazzeretti, G. Frenking, H. L. Anderson, D. Sundholm, F. Cossío, M. A. Petrukhina, J. Wu, J. I. Wu, A. Restrepo, Chem. Sci. 14 (2023) 5569-5576.
H. Ottosson, Chem. Sci. 14 (2023) 5542-5544.
I. Agranat, Struct. Chem. 35 (2024) 715-720.

What is antiaromaticity?

- Antiaromatic molecules have larger BLA than aromatic ones
- They have a smaller BLA than nonaromatic rings Structure
- They sustain a net paratropic ring current when they are exposed to an external magnetic field
- Paratropic ring currents shift the NMR chemical shifts of outer hydrogens to smaller values (larger magnetic shielding constants) Magnetic
- They are energetically more stable than nonaromatic molecule Energy
- The lower energy prevents them from becoming nonaromatic
- They are energetically less stable than aromatic ones
- Antiaromatic molecules are rare

The gauge-including magnetically induced currents method (GIMIC)

The GIMIC method

The elements of the nuclear magnetic shielding tensor are the same regardless whether they are calculated as the second derivative or obtained by integrating the Biot-Savart expression

$$\int \sum_{\mu\nu} D_{\mu\nu} \frac{\partial^2}{\partial m_\alpha^I \partial B_\beta} \left[\chi_\mu^*(\mathbf{r})\hat{h}\chi_\nu(\mathbf{r})\right] \mathbf{dr} + \int \sum_{\mu\nu} \frac{\partial D_{\mu\nu}}{\partial B_\beta} \frac{\partial}{\partial m_\alpha^I} \left[\chi_\mu^*(\mathbf{r})\hat{h}\chi_\nu(\mathbf{r})\right] \mathbf{dr}$$
$$= -\int \frac{\partial \mathbf{A}_I^{\mathbf{m}}(\mathbf{r})}{\partial m_\alpha^I} \cdot \frac{\partial \mathbf{J}_\gamma(\mathbf{r})}{\partial B_\beta} \mathbf{dr}$$

The spatial contributions to the elements of the nuclear magnetic shielding tensor are also the same with the two approaches

Since gauge-including atomic orbitals (GIAO basis functions) are used

$$\chi_\mu(\mathbf{r}) = \exp(-\frac{i}{2}(\mathbf{B} \times [\mathbf{R}_\mu - \mathbf{R}_O] \cdot \mathbf{r})\chi_\mu^{(0)}(\mathbf{r})$$

the current density is gauge independent

J. Jusélius, D. Sundholm, J. Gauss, J. Chem. Phys. 121 (2004) 3952

The current-density susceptibility expression

$$\mathcal{J}^{\tau}_{\gamma}(\mathbf{r}) = \sum_{\mu\nu} D^{\kappa}_{\mu\nu} \frac{\partial \chi^{*}_{\mu}(\mathbf{r})}{\partial B_{\tau}} \frac{\partial h(\mathbf{r})}{\partial m^{K}_{\gamma}} \chi_{\nu}(\mathbf{r}) + \sum_{\mu\nu} D^{\kappa}_{\mu\nu} \chi^{*}_{\mu}(\mathbf{r}) \frac{\partial h(\mathbf{r})}{\partial m^{K}_{\gamma}} \frac{\partial \chi_{\nu}(\mathbf{r})}{\partial B_{\tau}} +$$

$$\sum_{\mu\nu} \frac{\partial D^{\kappa}_{\mu\nu}}{\partial B_{\tau}} \chi^{*}_{\mu}(\mathbf{r}) \frac{\partial h(\mathbf{r})}{\partial m^{K}_{\gamma}} \chi_{\nu}(\mathbf{r}) - \sum_{\gamma} \epsilon_{\gamma\tau\delta} \left[\sum_{\mu\nu} D^{\kappa}_{\mu\nu} \chi^{*}_{\mu}(\mathbf{r}) \frac{\partial^{2} h(\mathbf{r})}{\partial m^{K}_{\gamma} \partial B_{\delta}} \chi_{\nu}(\mathbf{r}) \right]$$

where $\chi_{\mu}(\mathbf{r}) = \exp(-\frac{i}{2}(\mathbf{B} \times [\mathbf{R}_{\mu} - \mathbf{R}_{O}] \cdot \mathbf{r}) \chi^{(0)}_{\mu}(\mathbf{r})$ are the GIAOs

- GIMIC input data are:
  - The unperturbed AO density matrix
  - The first-order perturbed AO density matrices
  - Basis-set information
- An NMR shielding calculation is necessary
- Spin-currents when κ is spin up (α) or spin-down (β)
- Can be calculated at DFT, MP2, CCSD(T), CASSCF, . . . levels of theory
- It is interfaced to CFOUR, GAUSSIAN, QCHEM, FERMIONS++ and TURBOMOLE
- github.com/qmcurrents/gimic and zenodo.org/record/8180435

J. Jusélius, D. Sundholm, J. Gauss, J. Chem. Phys. 121 (2004) 3952
D. Sundholm, H. Fliegl, R. J. F. Berger, WIREs Comput. Mol. Sci. 6 (2016) 639-678

Ring-current strengths and aromaticity

Aromaticity and ring currents

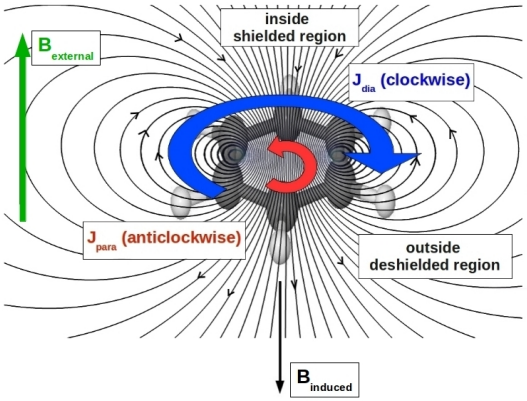
Aromatic molecules sustain net diatropic (in classical direction) ring currents

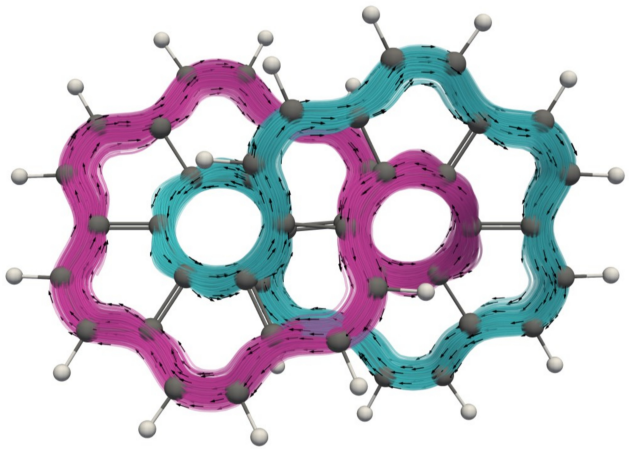
Antiaromatic molecules sustain net paratropic ring currents

The degree of aromaticity can be estimated by integrating ring-current strengths

Aromatic pathways of multiring molecules are obtained by integrating the current density passing chosen chemical bonds

Ring currents and their strengths can be calculated with GIMIC





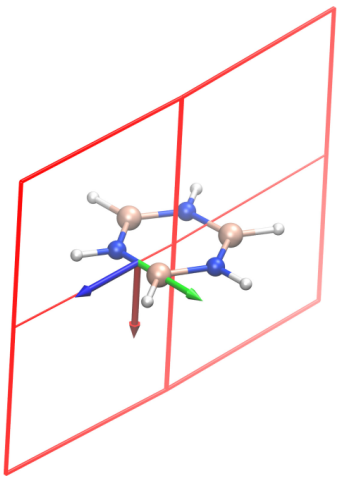
M. Dimitrova, D. Sundholm, Chapter 5 in Aromaticity: Modern Computational Methods and Applications, Ed. I. Fernández López, Elsevier (2021) pp. 155-194. http://arxiv.org/abs/2105.04902
D. Sundholm, H. Fliegl, Handbook of Porphyrin Science, Vol. 46, Eds K. M. Kadish, K. M. Smith and R. Guilard, World Scientific (2022)

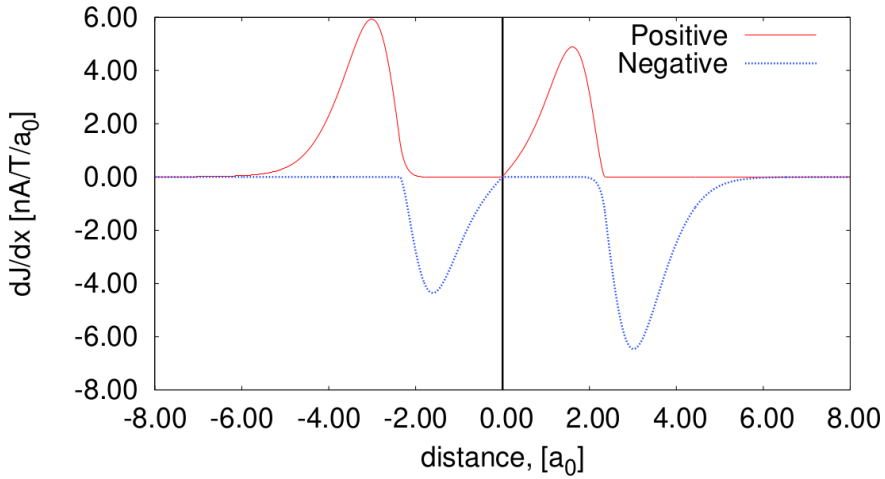
Ring-current strengths

The current strength passing the plane **S** is obtained by integrating the flux through it.

The current-density flux is obtained by contracting the magnetically induced current density with an external magnetic field normalized to one.

$$I = \int_S \sum_\beta \frac{B_\beta}{|\mathbf{B}|} \frac{\partial \mathbf{J}_\gamma(\mathbf{r})}{\partial B_\beta} \cdot \hat{\mathbf{n}}\, d\mathbf{S}$$





The ring-current profile is obtained by integrating differential contributions of the current density passing through the plane.

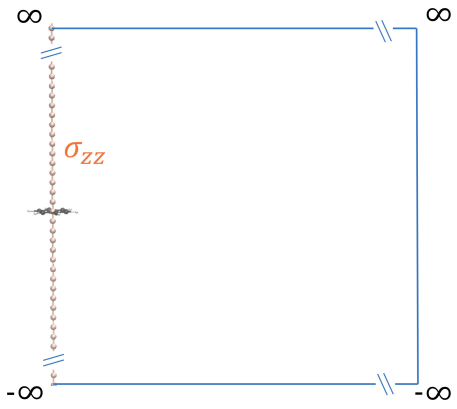
J. Jusélius, D. Sundholm, J. Gauss, J. Chem. Phys. 121 (2004) 3952

Maxwell-Ampère's Law

The Maxwell-Ampère's law states that the current strength of a vortex can be determined by integrating the induced magnetic field around the current flux.

The ring-current strength of a molecular ring can determined by integrating the induced magnetic field along the center of the vortex from $-\infty$ to ∞, since far away from the molecule the induced magnetic field vanishes.

The induced magnetic field declines very slowly with the distance, whereas the current density declines exponentially as the electron density



$$\iint_S \mathbf{J} \cdot \mathrm{d}\mathbf{S} = \frac{1}{\mu_0} \oint_\ell \mathbf{B}_{\text{induced}} \cdot \mathrm{d}\boldsymbol{\ell},$$

$$\mathbf{B}_{\text{induced}} = -\boldsymbol{\sigma}\mathbf{B}_{\text{external}}$$

The induced magnetic field is proportional to the magnetic shielding tensor σ

R. J. F. Berger, M. Dimitrova, R. T. Nasibullin, R. R. Valiev, D. Sundholm, Phys. Chem. Chem. 24 (2022) 624-628.

Twist and Writhe

Twisted Topology

The topology of twisted molecules are characterized by:

- Linking number (L_k), which is an integer times π, (usually π is omitted)

$$L_{\mathrm{k}} = \frac{1}{2\pi}\oint \mathrm{d}s \oint \mathrm{d}s' \left(\frac{\mathrm{d}\vec{r}_1(s)}{\mathrm{d}s} \times \frac{\mathrm{d}\vec{r}_2(s')}{\mathrm{d}s'}\right) \cdot \frac{\vec{r}_1(s) - \vec{r}_2(s')}{|\vec{r}_1(s) - \vec{r}_2(s')|^3}$$

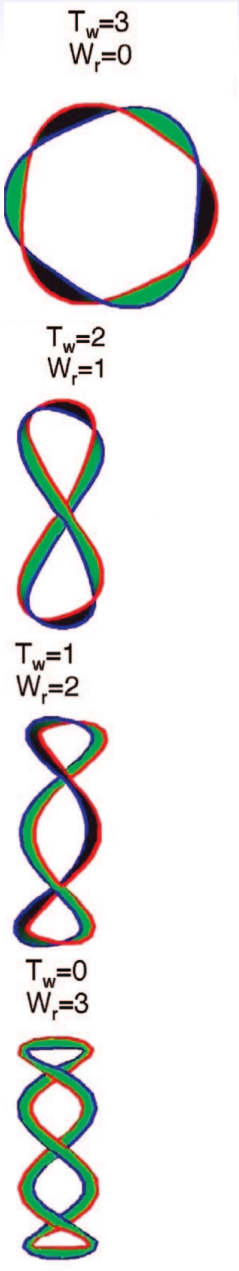
- Twist (T_w) is a sum of local rotation angles

$$T_{\mathrm{w}} = \frac{1}{\pi}\oint \mathrm{d}s [\hat{t}(s) \times \hat{t}_1(s)] \cdot \frac{\mathrm{d}\hat{t}_1(s)}{\mathrm{d}s}$$

- Writhe (W_r) is a nonlocal property representing the curvature of the loop.

$$W_{\mathrm{r}} = \frac{1}{2\pi}\oint \mathrm{d}s \oint_{s \neq s'} \mathrm{d}s' \left(\frac{\mathrm{d}\vec{r}_1(s)}{\mathrm{d}s} \times \frac{\mathrm{d}\vec{r}_1(s')}{\mathrm{d}s'}\right) \cdot \frac{\vec{r}_1(s) - \vec{r}_1(s')}{|\vec{r}_1(s) - \vec{r}_1(s')|^3}$$

They are related through $L_k = T_w + W_r$



S.M. Rappaport, H.S. Rzepa 130 (2008) 7613-7619

Aromaticity rules of twisted rings

The aromaticity rules depend on the molecular topology and the number of occupied conjugated orbitals of the ring

A molecular ring with an even L_k number (including zero) is aromatic when it has odd number of occupied conjugated orbitals in the ring

This is the combined Hückel aromaticity rule for singlet states and for states with higher spin multiplicity

A molecular ring with an odd L_k number is aromatic when it has even number of occupied conjugated orbitals in the ring

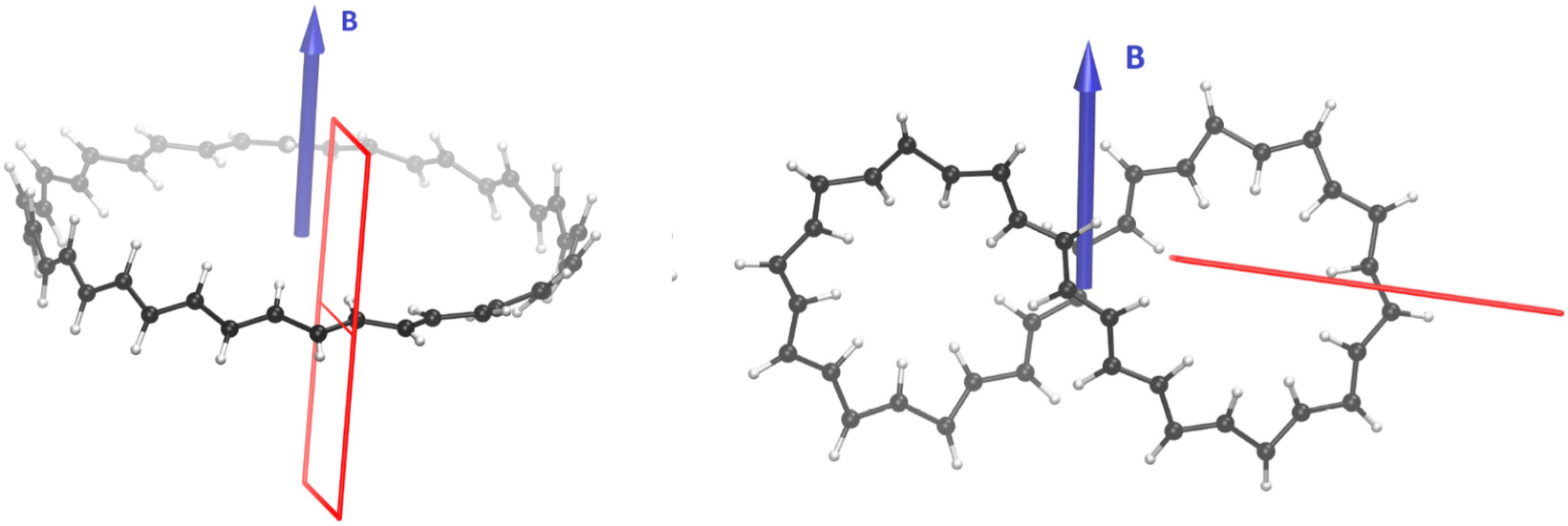
An even L_k value and an even number of orbitals leads to antiaromaticity

An odd L_k value and an odd number of orbitals leads to antiaromaticity

P. W. Fowler and H. S. Rzepa, PCCP 8 (2006) 1775-1777.
R. R. Valiev, T. Kurtén, L. I. Valiulina, S. Yu. Ketkov, V. N. Cherepanov,M. Dimitrova, D. Sundholm, PCCP 24 (2022) 1666-1674.

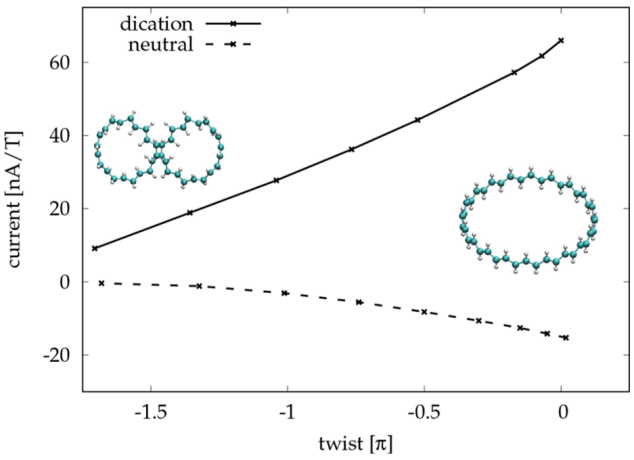
Aromaticity of twisted $C_{40}H_{40}$

- The magnetic field direction with the largest projection area is chosen
- The projection area seen along the B field has only one loop
- The perpendicular direction would not induce any current in molecular ring in the right picture

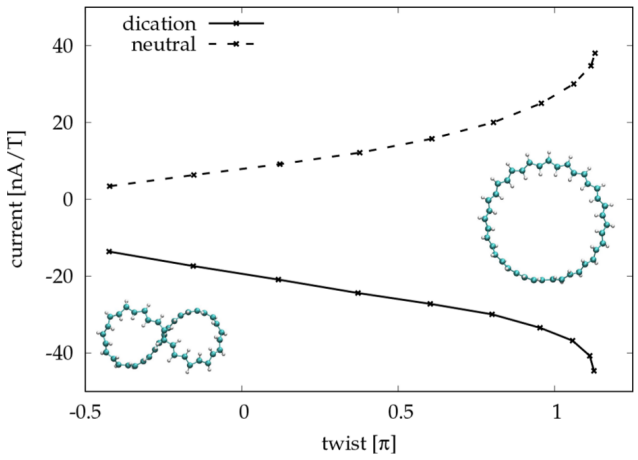


L. N. Wirz, M. Dimitrova, H. Fliegl, D. Sundholm, J. Phys. Chem. Lett. 2018, 9, 1627-1632

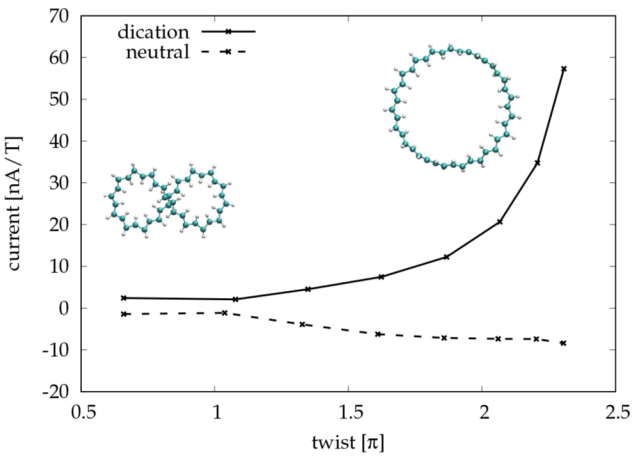
Current strengths of $C_{40}H_{40}$ as a function of T_w and W_r



L_0



L_1



L_2

The tropicity of the ring-current is determined by L_k and the number of occupied orbitals in the conjugated ring

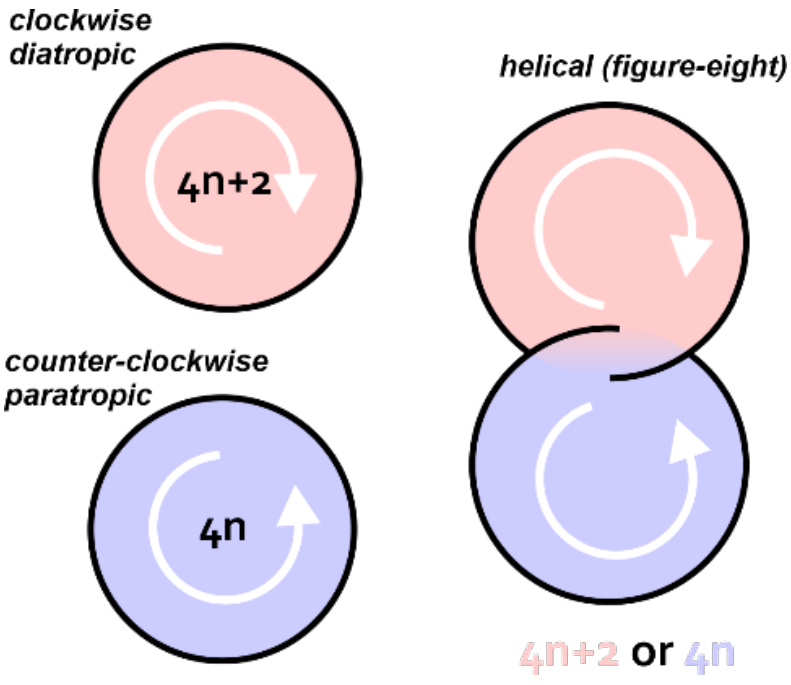
The ring-current strength decreases with increasing W_r

The local twist T_w has a smaller influence on the ring-current strength

L. N. Wirz, M. Dimitrova, H. Fliegl, D. Sundholm, J. Phys. Chem. Lett. 2018, 9, 1627-1632

Doubly-twisted 8-shaped molecules

The ring-current pathway of 8-shaped molecules



Diatropic ring current is assumed to flow in the clockwise direction

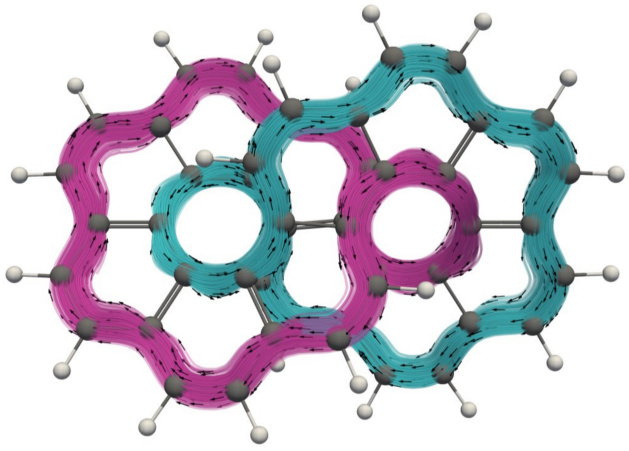
Paratropic ring current is assumed to flow in the anticlockwise direction

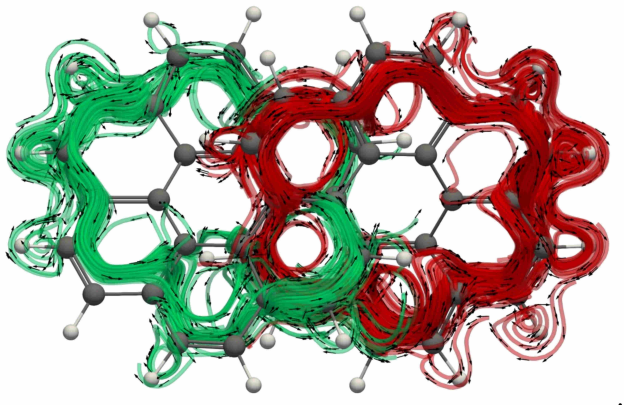
The eight-shaped structure can be considered as a combination

The two loops have conflicting aromatic character

The current pathway must take another route or stop leading to nonaromaticity

Ring-current pathways of [12]infinitene





Neutral [12]infinitene has two independent (purple and green) diatropic ring currents.

The green loop in the paratropic direction to the left is smaller than the diatropic loop to the right.

The diatropicity wins over paratropicity

Neutral [12]infinitene is globally aromatic.

The ring current of the [12]infinitene dication makes a shortcut at the crossing point

[12]infinitene dication has a through-space ring current with two (green and redish) independent coronene-like pathways

The [12]infinitene dication is antiaromatic

M. Orozco-Ic, R. R. Valiev, D. Sundholm, Phys. Chem. Chem. Phys., 2022, 24, 6404.

Tropicity

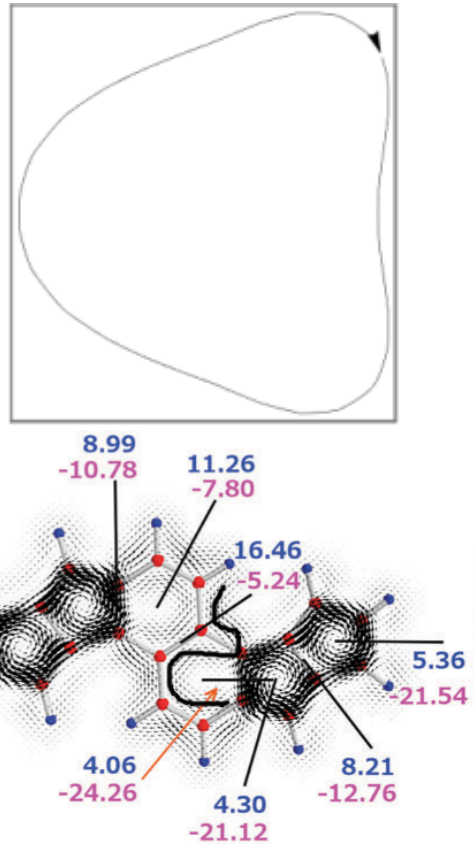
Tropicity of current-density vortices

The tropicity is the circulation direction of the current density with respect to the direction of the external magnetic field.

The current density can be separated into diatropic and paratropic vortices

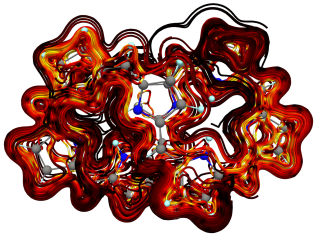
Tropicity is a global property that can be determined by following the current density around the whole vortex using the Runge-Kutta method

The diatropic current density in naphthalene annelated with two pentalene units has a similar route as the paratropic current density in naphthalene

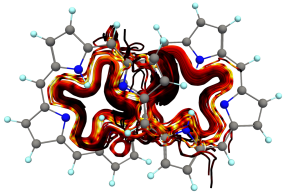


D. Sundholm, R. J. F. Berger, H. Fliegl, Phys. Chem. Chem. Phys. 18 (2016) 15934-15942
Q. Wang J. Pyykkö, M. Dimitrova, S. Taubert, D. Sundholm, Phys. Chem. Chem. Phys. 25 (2023) 12469-12478.

Separated diatropic and paratropic contributions



Diatropic



Paratropic

Trajectories of the current-density vector field are obtained by using the Runge-Kutta method

$$\vec{a}_{n+1} = \vec{a}_n + \frac{1}{6}\left(\vec{k}_1 + 2\vec{k}_2 + 2\vec{k}_3 + \vec{k}_4\right)$$

$\vec{k}_1 = h\vec{v}(\vec{a}_n)$,
$\vec{k}_2 = h\vec{v}(\vec{a}_n + \frac{1}{2}\vec{k}_1)$,
$\vec{k}_3 = h\vec{v}(\vec{a}_n + \frac{1}{2}\vec{k}_2)$, and
$\vec{k}_4 = h\vec{v}(\vec{a}_n + \vec{k}_3)$

h is the step length.

The cross product $\vec{v}(\vec{a}_n) \times \vec{v}(\vec{a}_{n+1})$ is calculated for each step along the trajectory.

The tropicity (τ) of the current density in the chosen starting point is calculated as the scalar product with the vector of the external magnetic field.

The contributions from each trajectory step around the whole vortex are added.

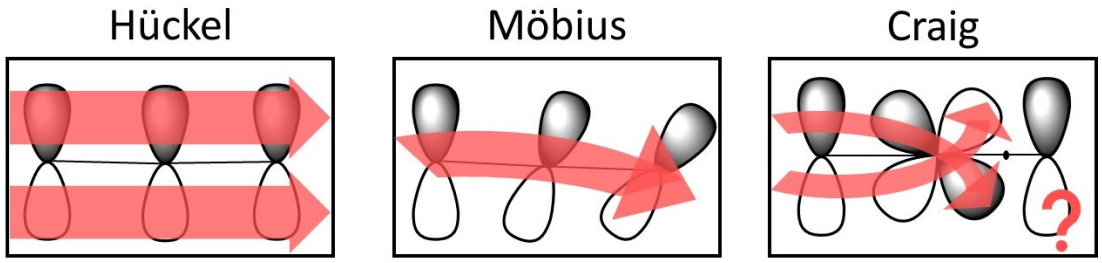
$$\tau = \sum_n \vec{B}_{\text{external}} \cdot \left(\vec{v}(\vec{a}_n) \times \vec{v}(\vec{a}_{n+1})\right)$$

Q. Wang J. Pyykkö, M. Dimitrova, S. Taubert, D. Sundholm, Phys. Chem. Chem. Phys. 25 (2023) 12469-12478.

Craig-type Möbius aromatic molecules

Craig-type Möbius (anti)aromatic rings

A planar ring is thought to possess Möbius topology because the orbital phase has Möbius twisted topology obeying the corresponding aromaticity rules.



This is called Craig-type Möbius aromaticity sustaining a diatropic ring current and Craig-type Möbius antiaromaticty sustaining a paratropic ring current

D. P. Craig and N. L. Paddock, Nature 181 (1958) 1052-1053

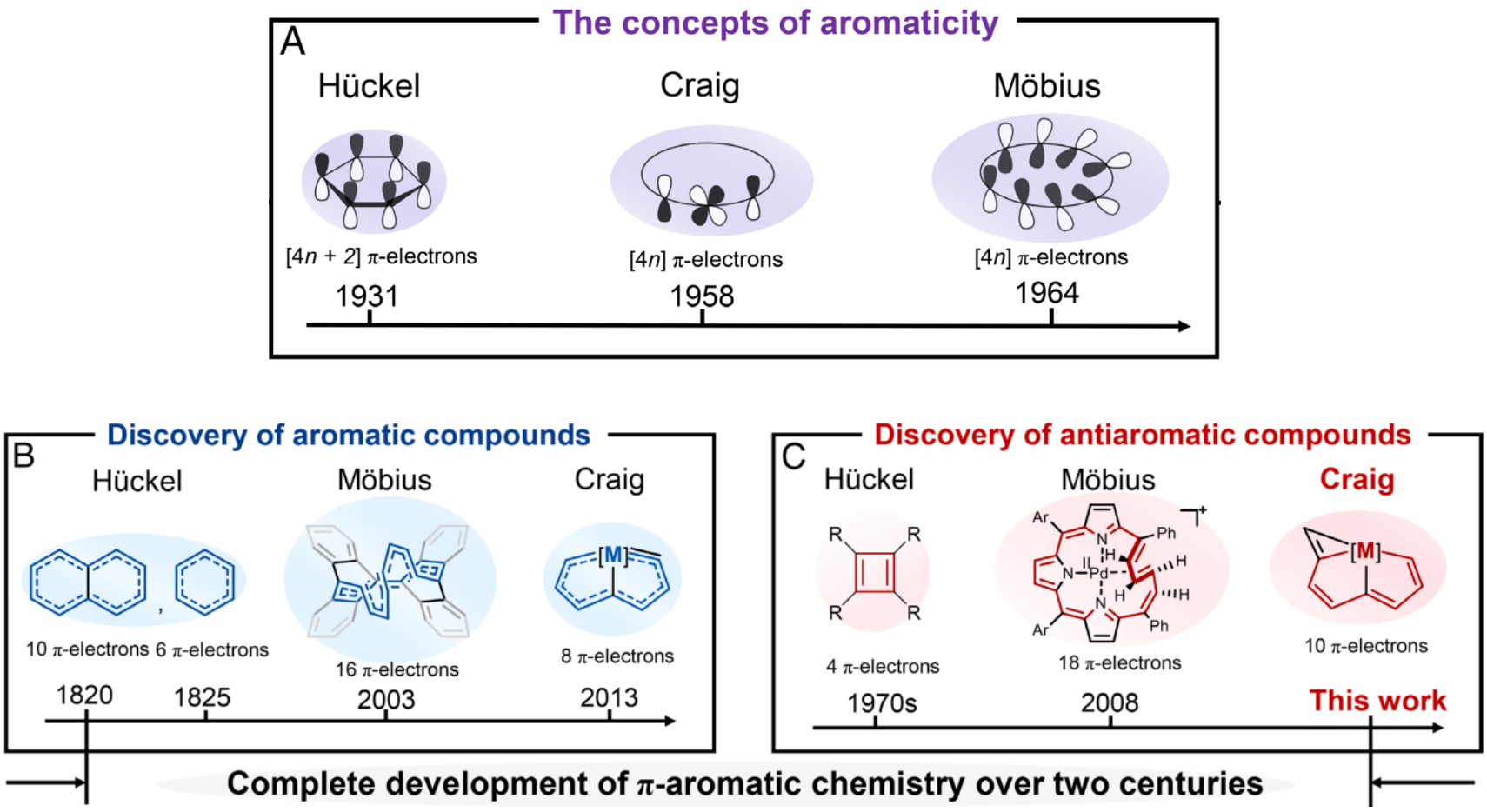
Osmium containing rings have been suggested to be Craig-type Möbius aromatic

C. Zhu, S. Li, M. Luo, X. Zhou, Y. Niu, M. Lin, J. Zhu, Z. Cao, X. Lu, T. Wen, Z. Xie, P. v. R. Schleyer and H. Xia, Nat. Chem., 5 (2013) 698-703.
C. Zhu, M. Luo, Q. Zhu, J. Zhu, P. v. R. Schleyer, J. I.-C. Wu, X. Lu and H. Xia, Nat. Commun., 5 (2014) 1-7.
Y. Cai, Y. Hua, Z. Lu, Q. Lan, Z. Lin, J. Fei, Z. Chen, H. Zhang and H. Xia, Proc. Natl. Acad. Sci. USA, 118 (2021) e2102310118.

At least an osmium containing molecular ring has been suggested to be Craig-type Möbius antiaromatic

L. Chen, L. Lin, A. R. Nath, Q. Zhu, Z. Chen, J. Wua, H. Wang, Q. Li, W.-F. Lin,J. Zhu, H. Xia, Proc. Nat. Am. Soc. 120 (2023) e2215900120

Craig-type Möbius (anti)aromaticity



L. Chen, L. Lin, A. R. Nath, Q. Zhu, Z. Chen, J. Wua, H. Wang, Q. Li, W.-F. Lin,J. Zhu, H. Xia, Proc. Nat. Am. Soc. 120 (2023) e2215900120

E. Hückel, Z. Physik 70 (1931) 204-286
D. P. Craig and N. L. Paddock, Nature 181 (1958) 1052-1053
E. Heilbronner, Tetrahedron Lett. 5 (1964) 1923-1928

Craig-type Möbius aromatic ring

In a Craig-type Möbius aromatic molecule the diatropic ring current is assumed to have Möbius topology, *i.e.*, the ring current makes two laps before it reaches the starting point. However, the L_k number must be even.

1	Ring	ECP	X2C	SO-X2C
	A	5.29	5.38	5.31
	B	6.85	6.89	6.65

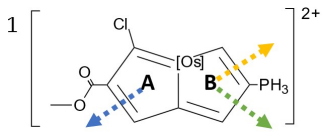
1 is weakly aromatic with a ring-current strength of c. 6 nA/T

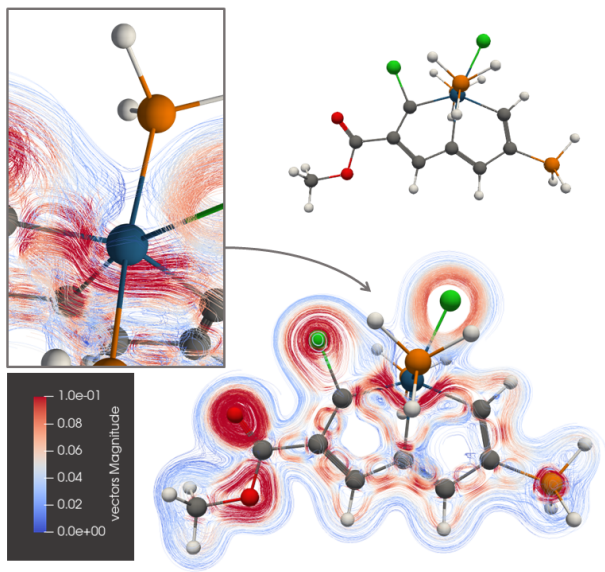
The equal ring-current strength of A and B suggest a global ring current

The ring current avoids the osmium atom on the inside

Osmium sustains a strong paratropic atomic current

No Möbius topology of the ring current is seen





Current-density analysis of molecule **1**

It is not Craig-type Möbius aromatic

A. Rabe, Q. Wang, D. Sundholm, Dalton Trans. 53 (2024) 10938
Y. J. Franzke and C. Holzer, J. Chem. Phys., 159 (2023) 184102.
Y. Cai, Y. Hua, Z. Lu, Q. Lan, Z. Lin, J. Fei, Z. Chen, H. Zhang and H. Xia, Proc. Natl. Acad. Sci. USA, 118 (2021) e2102310118.

Craig-type Möbius antiaromatic ring

Molecule **4** is suggested to be the first Craig-type Möbius aromatic molecule sustaining a paratropic ring current

4	Ring	ECP	X2C	SO-X2C
	A	-0.62	-0.57	-0.68
	B	1.35	1.33	1.25
	C	12.14	12.24	12.13

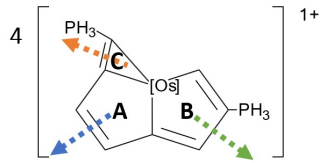
Rings A and B of **4** do not sustain any ring currents

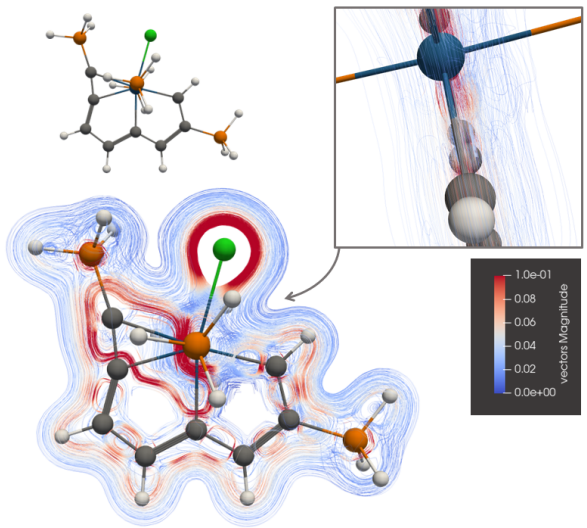
Ring C sustains a diatropic ring current of 12 nA/T

The ring current avoids the osmium atom on the inside

Osmium sustains a strong paratropic atomic current

The ring current has no Möbius topology



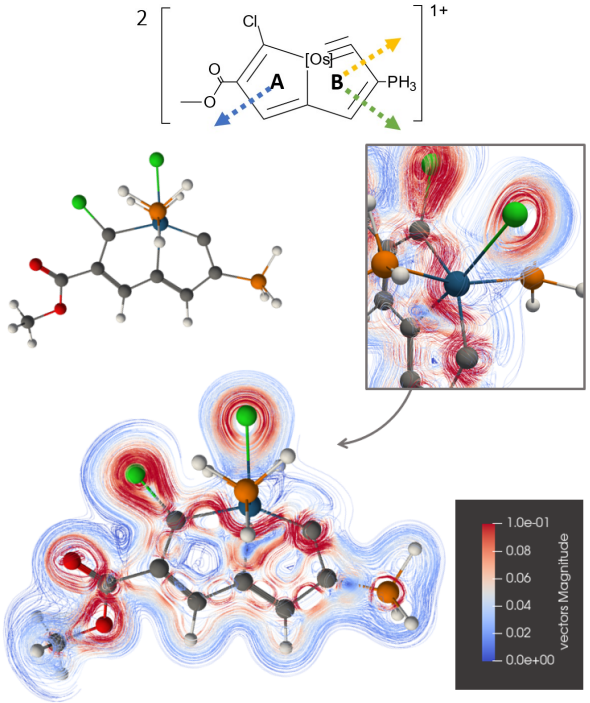


Current-density analysis of molecule **4**

It is not Craig-type Möbius antiaromatic

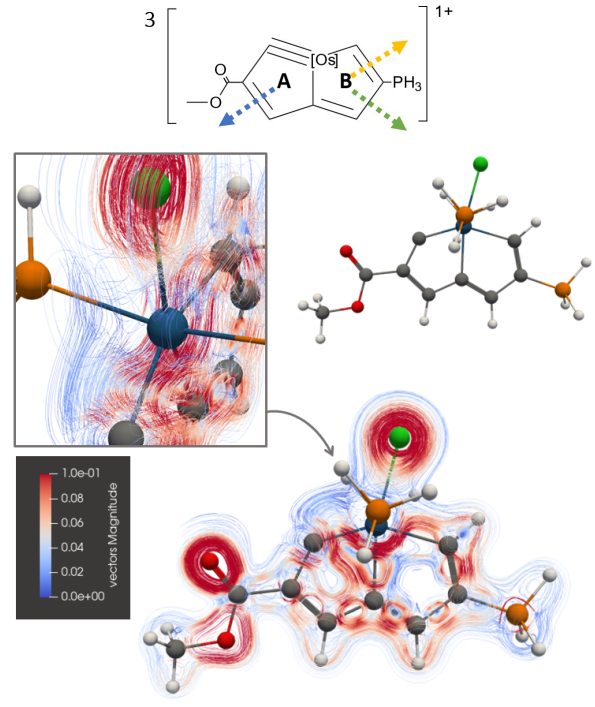
A. Rabe, Q. Wang, D. Sundholm, Dalton Trans. 53 (2024) 10938
Y. J. Franzke and C. Holzer, J. Chem. Phys., 159 (2023) 184102.
L. Chen, L. Lin, A. R. Nath, Q. Zhu, Z. Chen, J. Wua, H. Wang, Q. Li, W.-F. Lin,J. Zhu, H. Xia, Proc. Nat. Am. Soc. 120 (2023) e2215900120

*Current density of molecules (**2**) and (**3**)*



Molecule (**2**)

(**2**)	Ring	ECP	X2C	SO-X2C
	A	5.91	5.91	5.90
	B	0.96	0.98	0.96



Molecule (**3**)

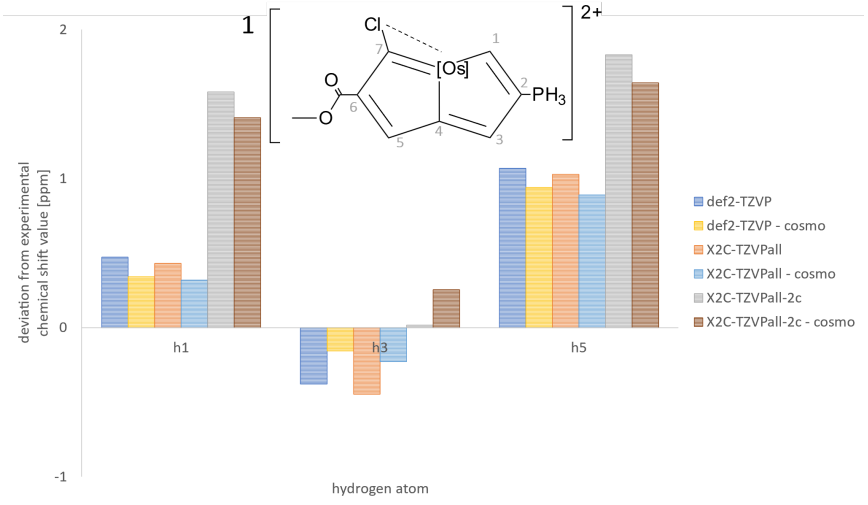
(**3**)	Ring	ECP	X2C	SO-X2C
	A	4.71	4.72	4.78
	B	7.96	8.03	7.81

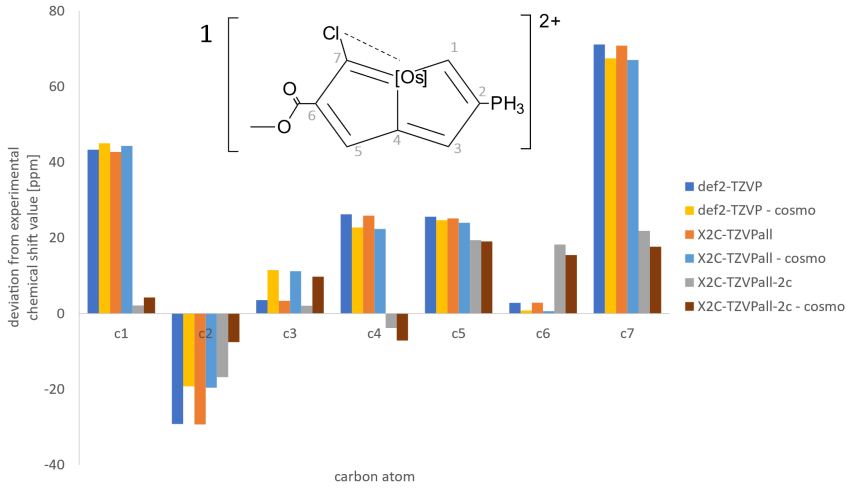
A. Rabe, Q. Wang, D. Sundholm, Dalton Trans. 53 (2024) 10938
Y. J. Franzke and C. Holzer, J. Chem. Phys., 159 (2023) 184102.
Y. Cai, Y. Hua, Z. Lu, Q. Lan, Z. Lin, J. Fei, Z. Chen, H. Zhang and H. Xia, Proc. Natl. Acad. Sci. USA, 118 (2021) e2102310118.

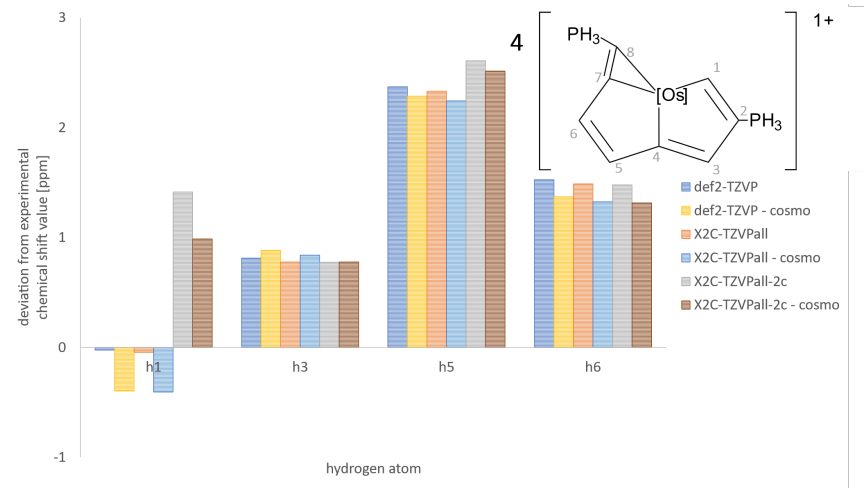
^{1}H NMR and ^{13}C NMR chemical shifts of (**1**) and (**4**)

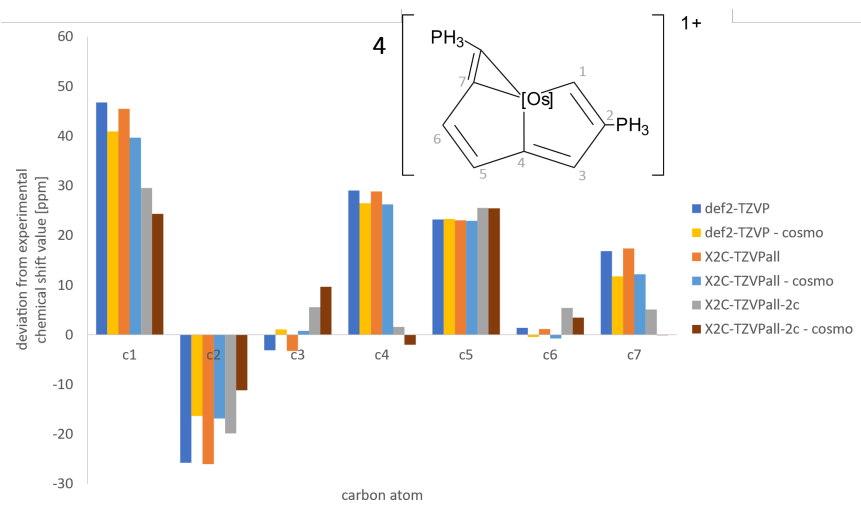
The difference between calculated and measured chemical shifts

A. Rabe, Q. Wang, D. Sundholm, Dalton Trans. 53 (2024) 10938







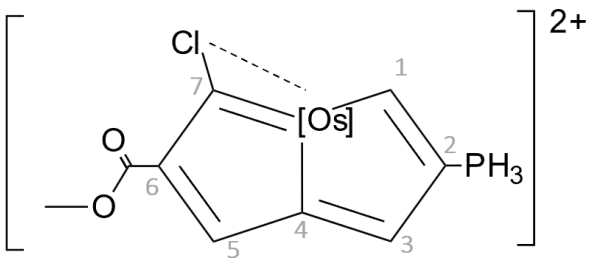


^{13}C NMR and ^{1}H NMR chemical shifts of (**1**)

1	ECP def2-TZVP	ECP def2-QZVP	X2C x2c-TZVPall	SO-X2C x2c-TZVPall-2c	Exp.
C1	269.73	273.84	268.98	228.50*	226.4
C2	109.48	111.05	109.25	121.90	138.7
C3	166.38	168.93	166.03	164.85	162.8
C4	214.95	217.50	214.47	184.90*	188.7
C5	190.77	193.57	190.18	184.60	165.2
C6	152.93	155.46	152.81	168.33	150.1
C7	297.47	301.59	297.04	248.23*	224.6

1	ECP def2-TZVP	ECP def2-QZVP	X2C x2c-TZVPall	SO-X2C x2c-TZVPall-2c	Exp.
H1	14.07	14.21	14.03	15.18*	13.60
H3	9.16	9.18	9.09	9.56	9.54
H5	10.01	10.03	9.97	10.77	8.94

1

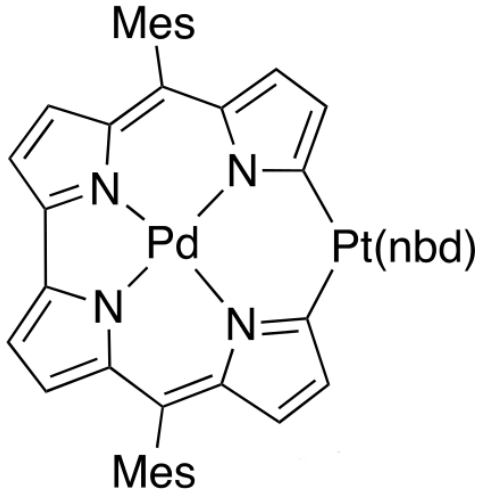


* indicates atom next to Os

Craig-type Möbius Antiaromatic 10-Platinacorrole

Aromaticity of 10-Platinacorrole

10-platinacorrole with a norbornadiene (NDB) ligand has a planar corrole ring



NMR spectroscopy shows that it is antiaromatic

Counting the electrons suggests that it has (4n+2) conjugated electrons

Odd number of conjugated orbitals suggests aromatic nature

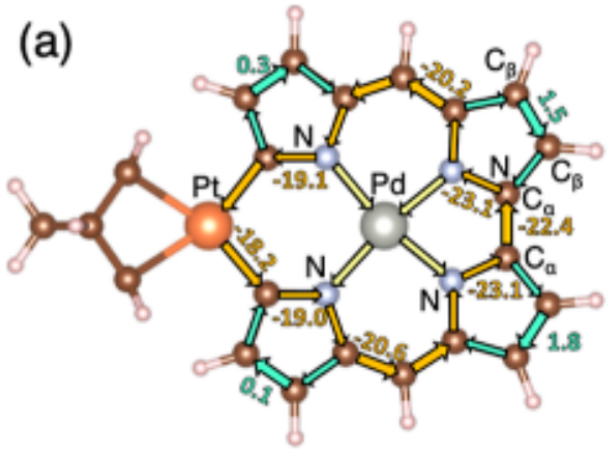
What to blame, Craig-type Möbius?

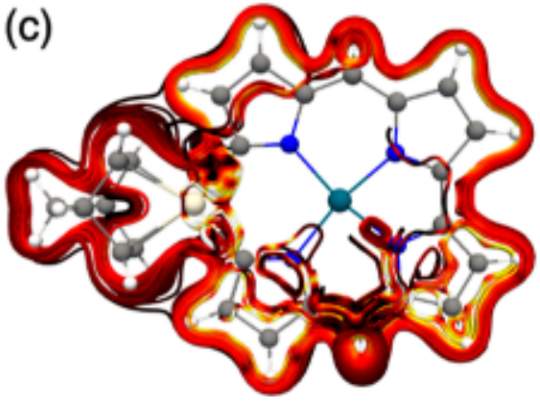
Cannot we calculate the number of electrons?

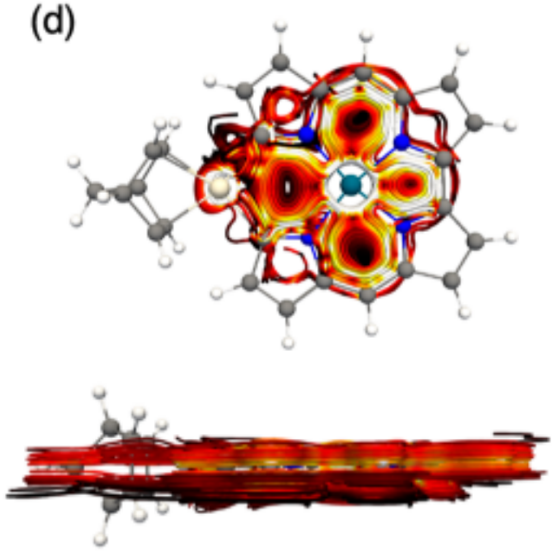
or cannot we trust the Hückel rules?

K. Miwa, T. Yokota, Q. Wang, T. Sakurai, H. Fliegl, D. Sundholm, H. Shinokubo, J. Am. Chem. Soc. 146 (2024) 1396-1402.

Current-density of 10-Platinacorrole







No Möbius topology of the ring current

The pyrrole rings contribute 5 electrons (20 electrons)

The meso-carbons contribute 1 electron (2 electron)

The charge of the ring is -2 (2 electrons)

Pt contributes 2 orbitals (d_{xz} and d_{yz} or 4 electrons)
(alternatively: The charge of Pd is +1 and Pt contributes 1 electron, 24 electrons

Even number of orbitals (4n electrons) leads to antiaromaticity.

K. Miwa, T. Yokota, Q. Wang, T. Sakurai, H. Fliegl, D. Sundholm, H. Shinokubo, J. Am. Chem. Soc. 146 (2024) 1396-1402.

Summary

- GIMIC is a powerful tool for studies of magnetically induced current-density (MICD)
- Features to interpret the MICD have been and will be implemented in GIMIC
- The aromaticity concept is difficult to understand
- MICD provides information about it
- All (anti)aromatic molecules sustain a net (para)diatropic ring current
- All molecules sustaining a ring current are not necessarily (anti)aromatic
- Electron delocalization as well as diatropic and paratropic ring currents stabilize molecular rings
- Craig-type Möbius aromaticity should be abandoned because there is no reason for retaining it
- More kinds of aromaticity can probably have the same fate when we know more about their properties
- We should try to reduce the number of members in the aromaticity family instead of inventing new ones

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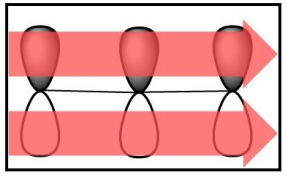
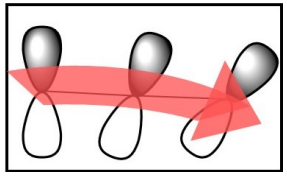
- Tomoya Yokota (Nagoya)

AECC Beijing Institute of Aeronautical Materials supports our participation in MAGIC 2024

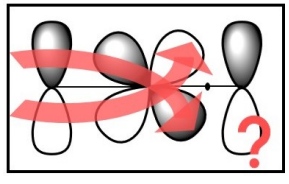
Hückel



Möbius



Craig



That's All Folks

Thank You for Your attention