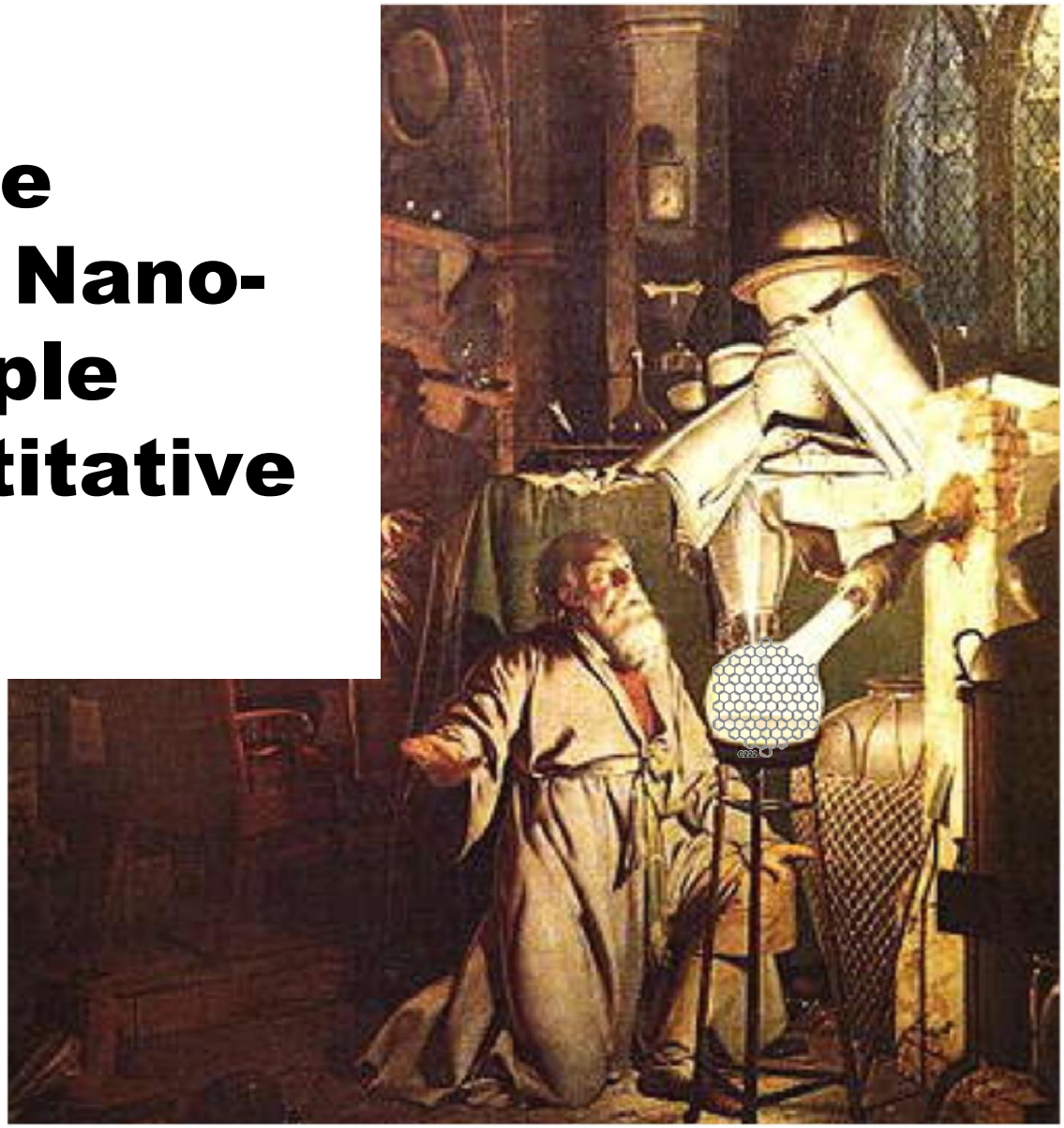
The Zero-Voltage Conductance of Nano-Graphenes: Simple Rules and Quantitative Estimates

Mayou, Zhou, Ernzerhof,
J. Phys. Chem. C, **2013**,
117 (15), pp 7870–7884



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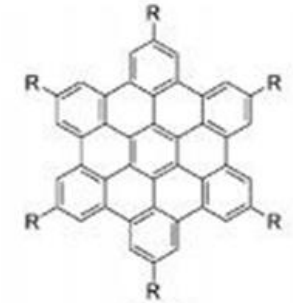
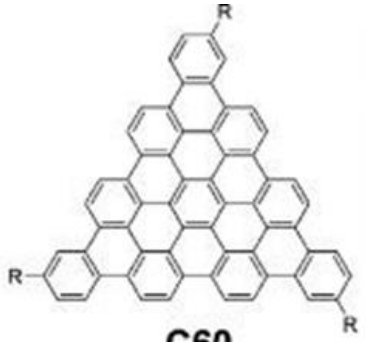
Polycyclic aromatic hydrocarbons (PAH), nowadays nano-graphene

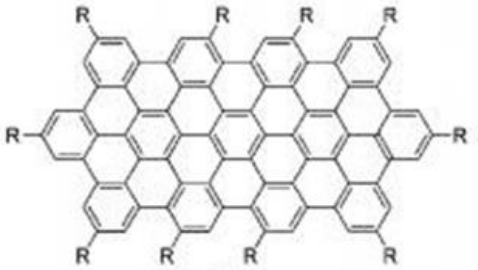
Kekulé molecules:



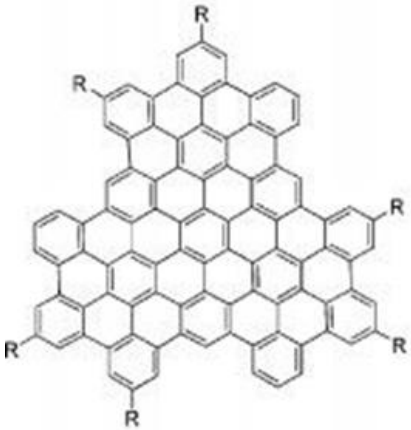
C42



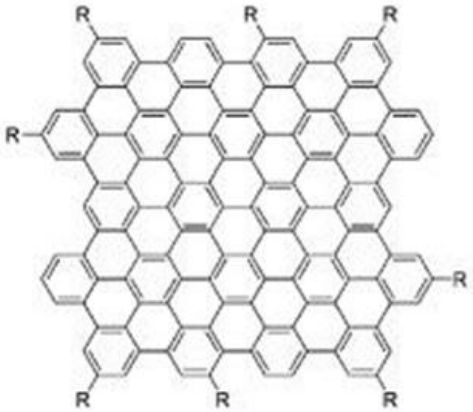
C60



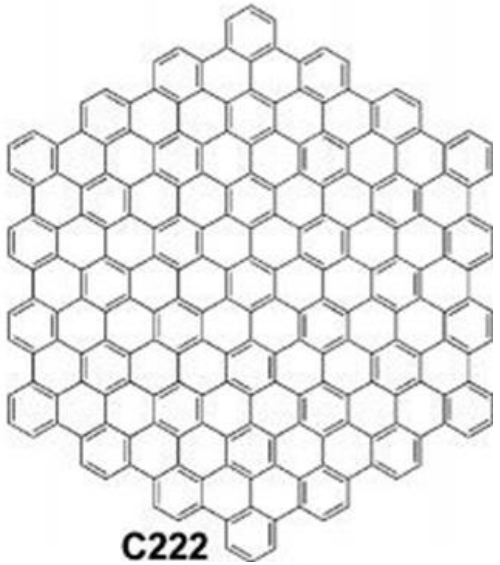
C78



C96



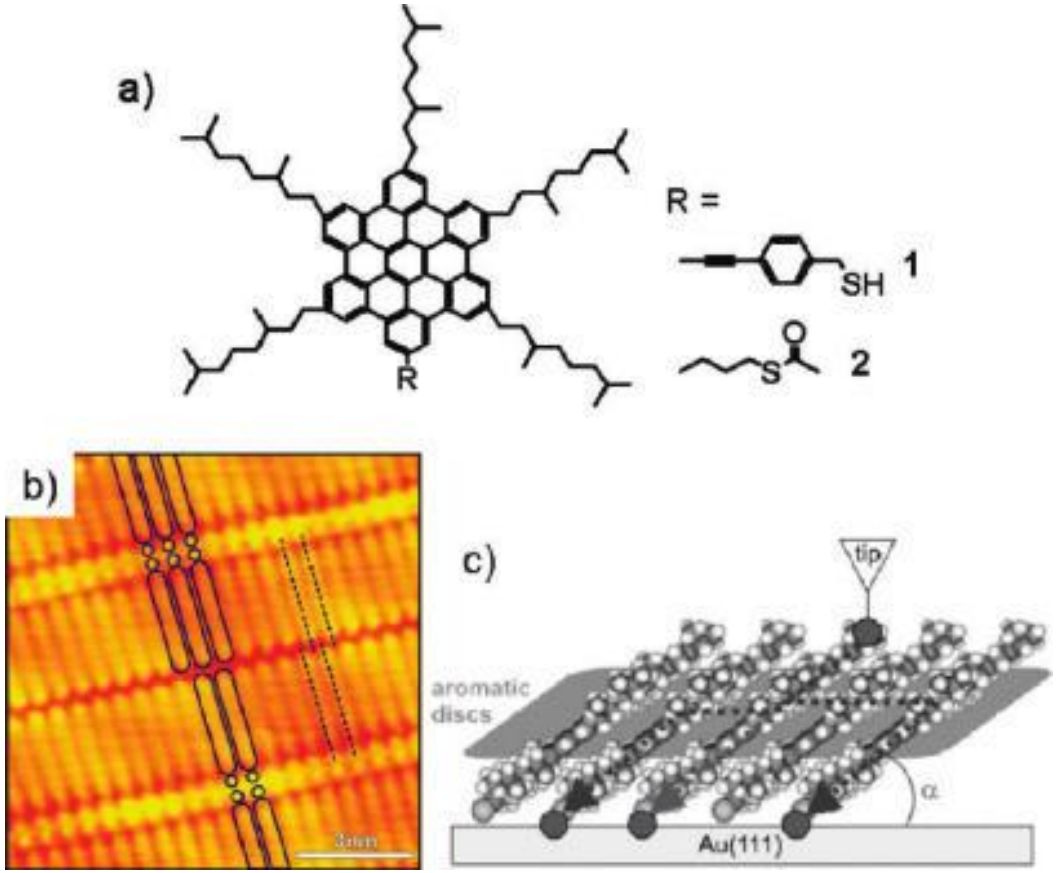
C132



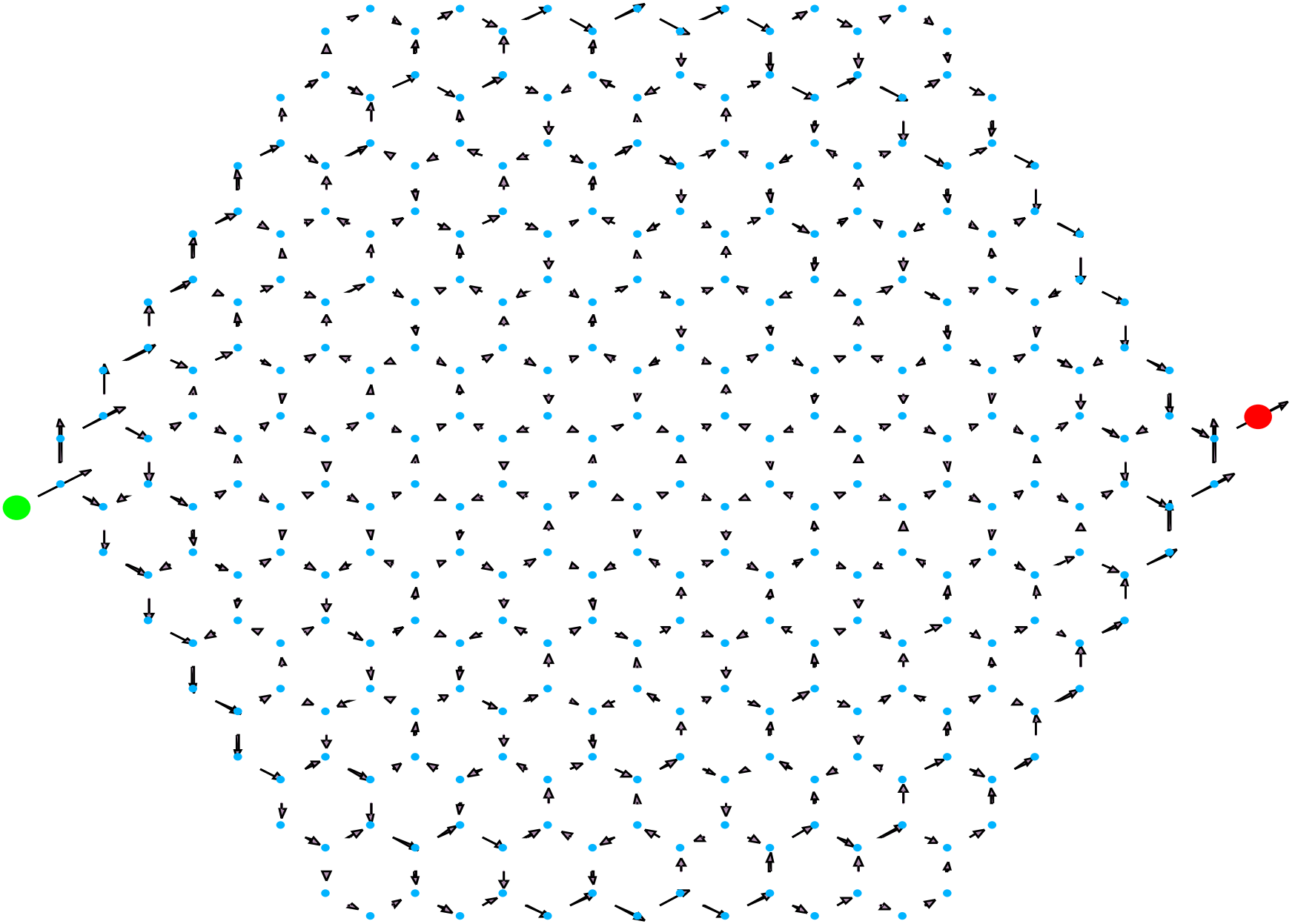
C222

Müllen group, Max Planck Institut, Mainz

Molecular electronics

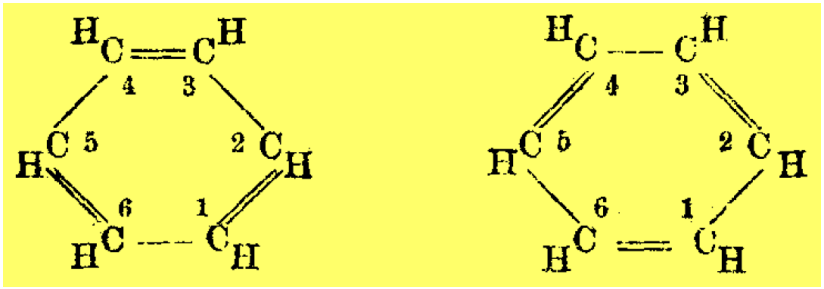


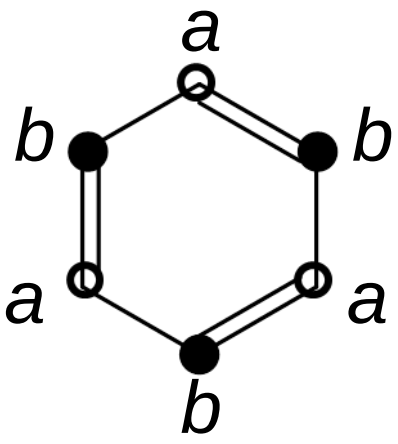
Käfer, Bashir, Dou, Witte, Müllen, Wöll, C. Adv. Mater. 2010, 22, 384.



Separation of Kekulé molecules into two types of carbons

Friedrich August Kekulé von Stradonitz (1829-1896).

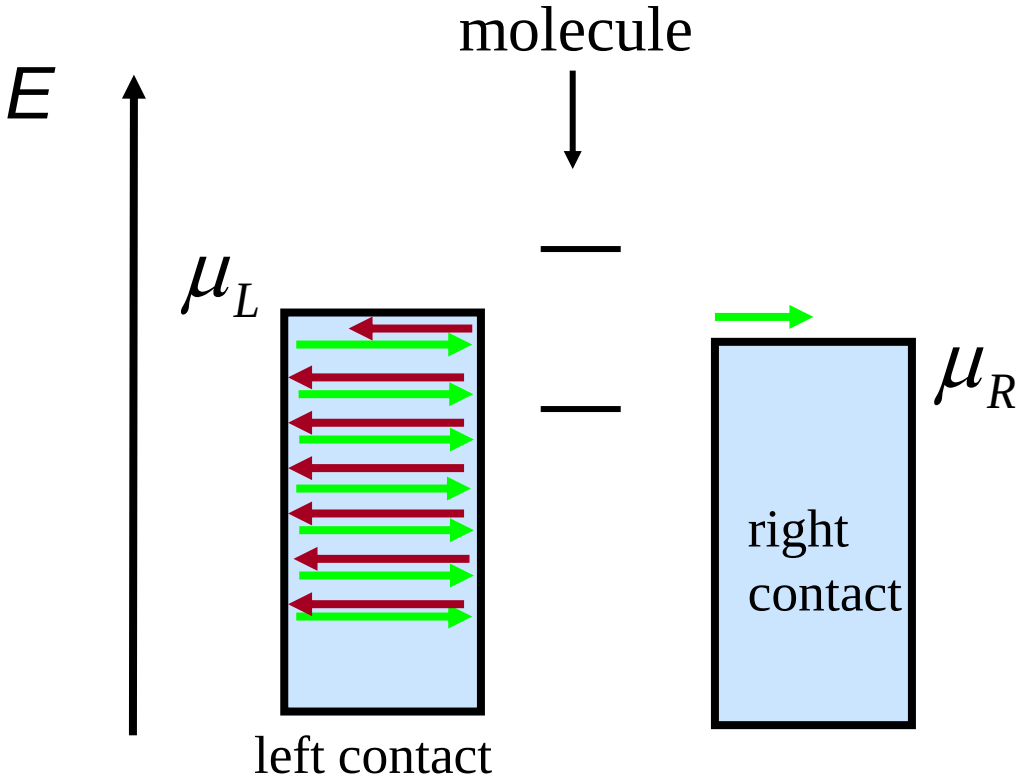




bipartite

Chemisches Institut, Universität Bonn

Landauer formula

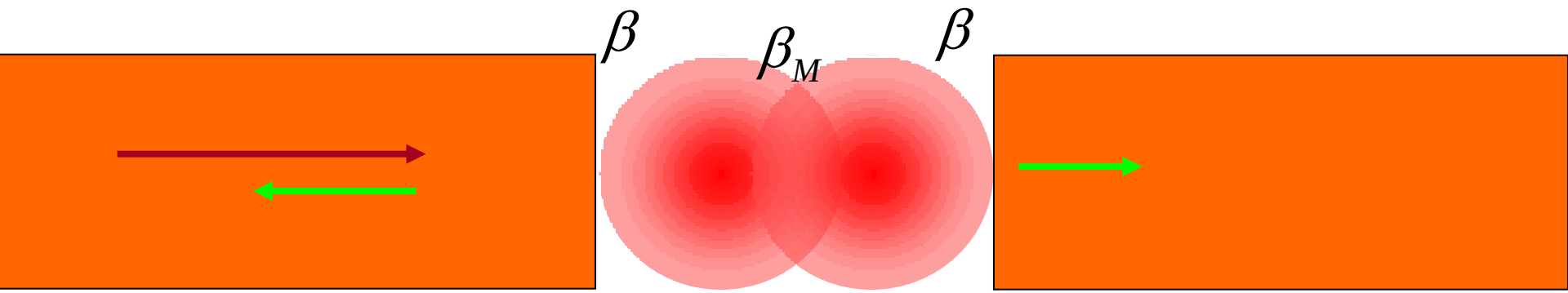


$$\Psi_L = \varphi^+ + r\varphi^- \qquad \Psi_R = t\varphi^+$$

$$\mathrm{T}(E) = |t(E)|^2 = 1 - |r(E)|^2$$

$$g(E) = \frac{e^2}{h} T(E)$$

The source-sink potential approach in tight binding (Hückel)



$$H^{eff}(r) = \begin{pmatrix} \Theta_L(r) & \beta_M \\ \beta_M & \Theta_R \end{pmatrix}$$

$$\Theta_L(r) = -i\beta\frac{1+r}{1-r}$$

$$\Theta_R = i\beta$$

Source and sink potential

Goyer, Ernzerhof, Zhuang, JCP, 126,144104 (2007): Ernzerhof, JCP 126,144104 (2007).

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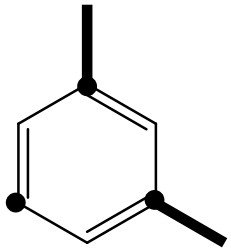
Simple theory for the conductance of conjugated systems (aa case)

*Contacts connected to two **a** atoms*



$$\mathrm{H} = \begin{pmatrix} \mathrm{H}_{AA} & \mathrm{M}_{AB} \\ \mathrm{M}_{BA} & \mathrm{H}_{BB} \end{pmatrix}$$

Reference energy of the atoms is set to 0

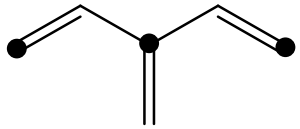
$$\mathrm{H}_A^{\mathrm{eff}} = \mathrm{H}_{AA} + \Theta_L(r) + \Theta_R - \mathrm{M}_{AB}\frac{1}{\mathrm{H}_{BB} - E}\mathrm{M}_{BA}$$

$\rightarrow \infty \quad \Rightarrow \quad$ no transmission

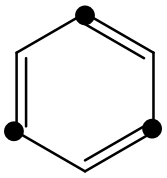
Simple theory for the conductance of conjugated systems (aa case)

Contacts connected to two a atoms

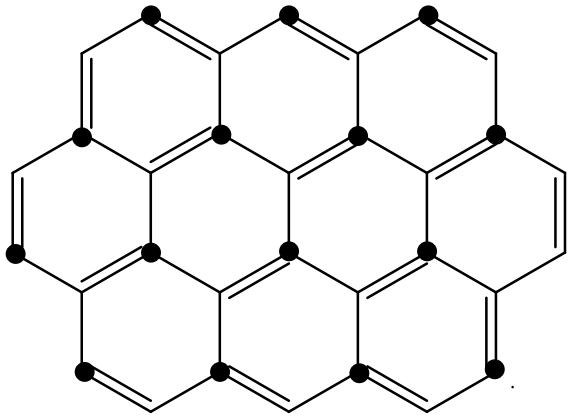
Cross-conjugation



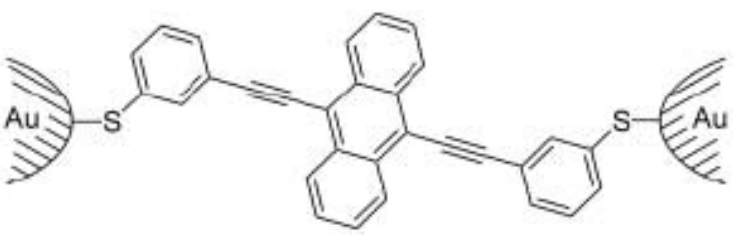
Meta vs. ortho & para connection

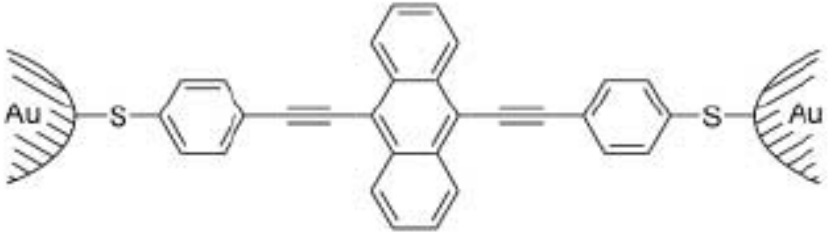


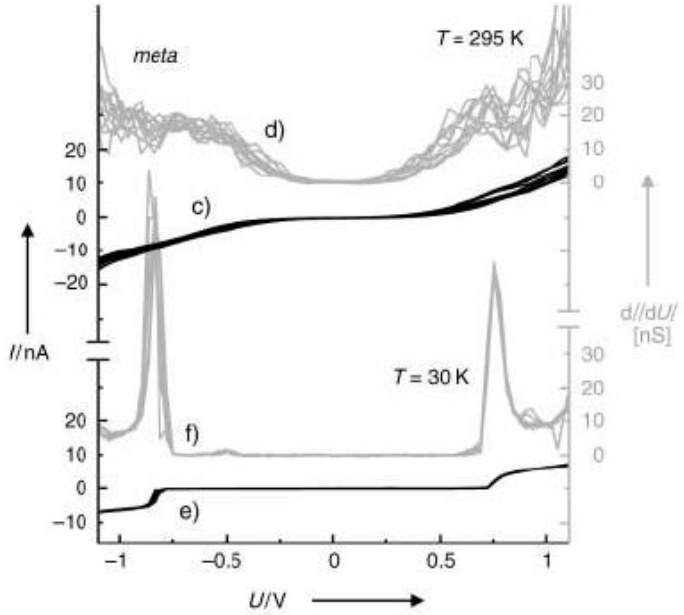
PAH

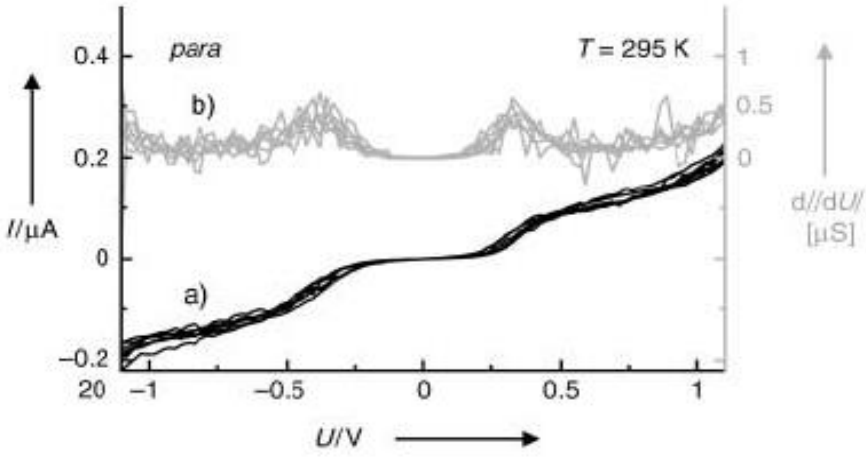


Impact of the position of the anchor group on molecular conductance









Mayor, Weber, Reichert, Elbing, von Hänisch, Beckmann, Fischer, Ang. Chemie Int. Ed., 42, 5834-5838 (2003)

nature nanotechnology

LETTERS

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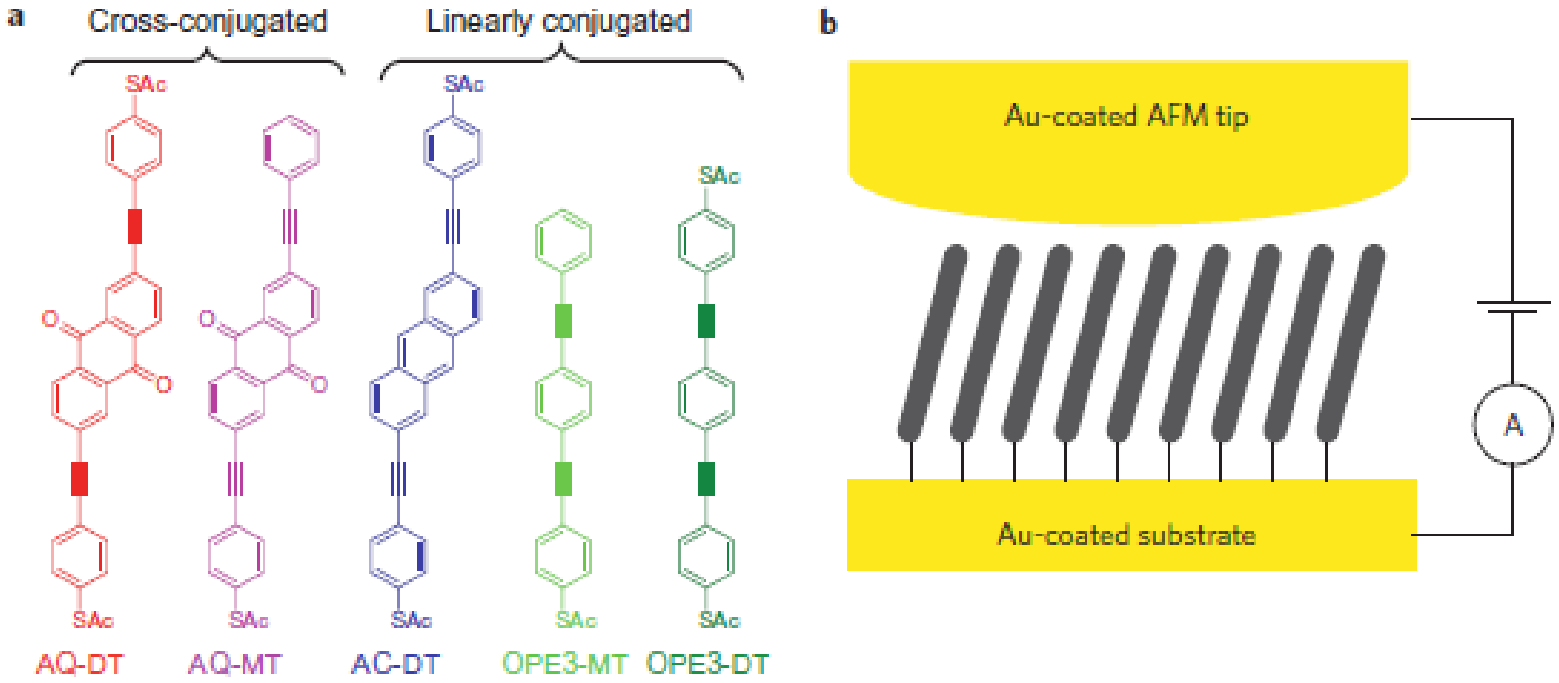
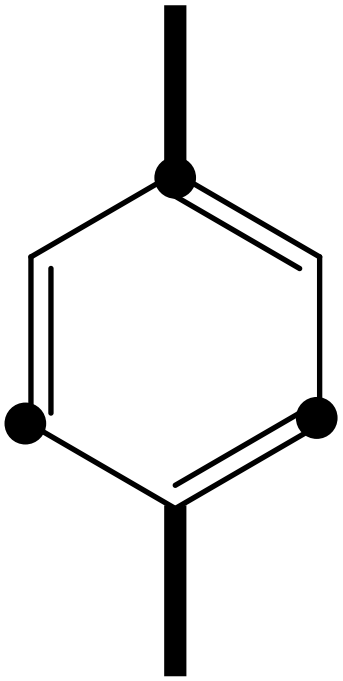
Observation of quantum interference in molecular charge transport

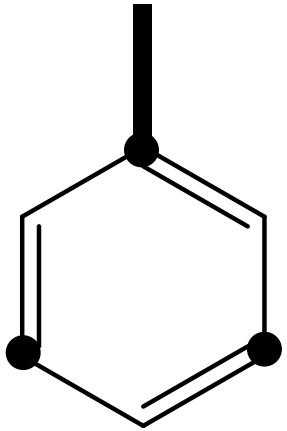
Constant M. Guédon[1†], Hennie Valkenier[2†], Troels Markussen[3], Kristian S. Thygesen[3], Jan C. Hummelen[2] and Sense Jan van der Molen[1*]

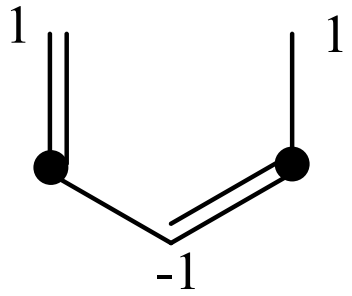


Ernzerhof, Zhuang, Rocheleau, JCP 123, 134704, (2005)

Simple theory for the conductance of conjugated systems (ab case)







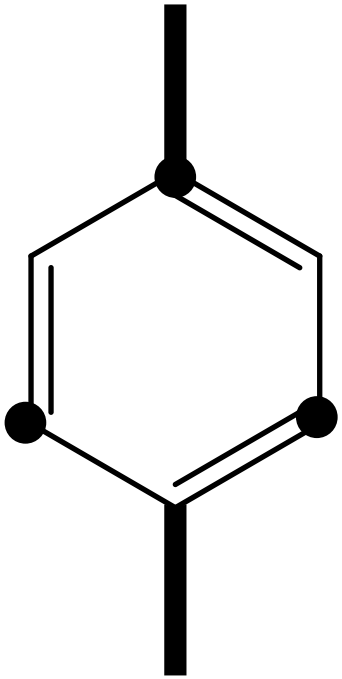
Longuet-Higgins, *J. Chem. Phys.* 1950, *18*, *265.*

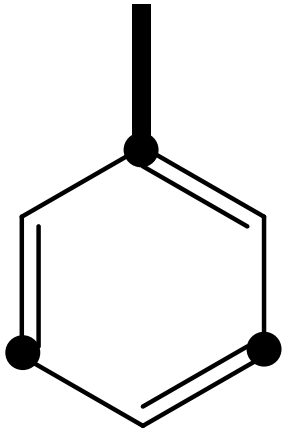
$$\mathbf{H}_{Ab}^{\text{eff}} = \mathbf{H}_{AA} + \mathbf{h}_{bb} + \Theta_L^b(r) + \Theta_R^a + \mathbf{M}_{Ab} + \mathbf{M}_{bA} - \mathbf{M}_{A\mathbb{C}b}\frac{1}{\mathbf{H}_{\mathbb{C}b\mathbb{C}b}}\mathbf{M}_{\mathbb{C}bA}$$

$$\mathbf{H}_{Ab}^{\text{eff}} = \begin{pmatrix} |c_a|^2\Theta_L(r) & t\sum_{l\in ad(b)} c_l \\ t\sum_{l\in ad(b)} c_l & \Theta_R \end{pmatrix}$$

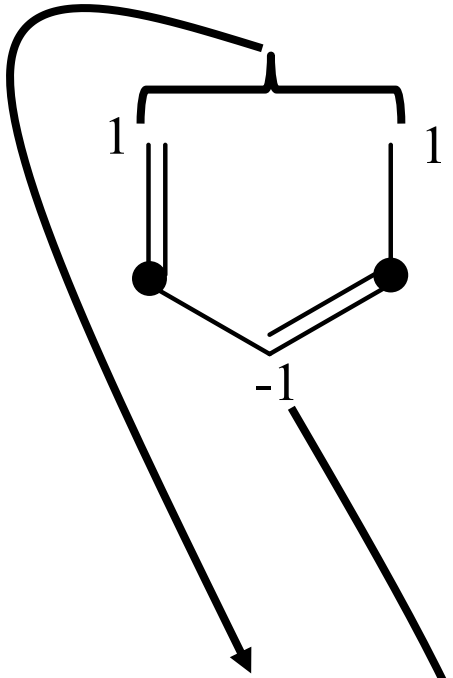
Simple theory for the conductance of conjugated systems (ab case)

*Contacts connected to an **a** and a **b** atom*





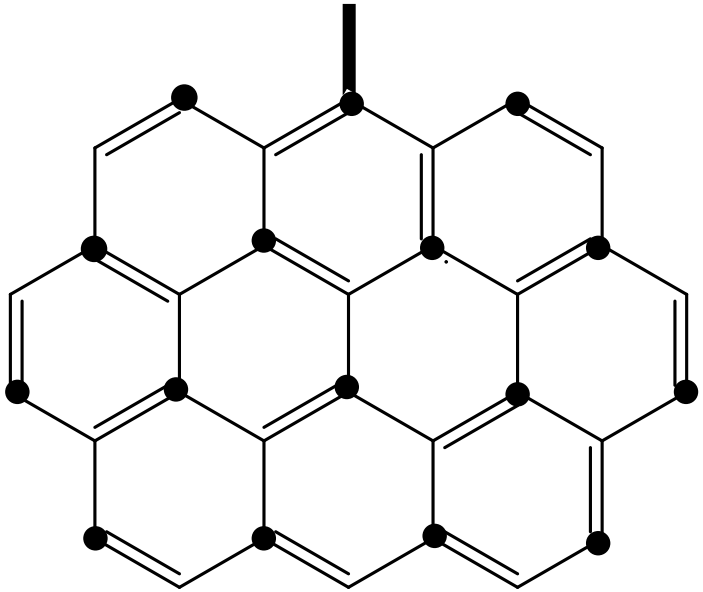
Defect state



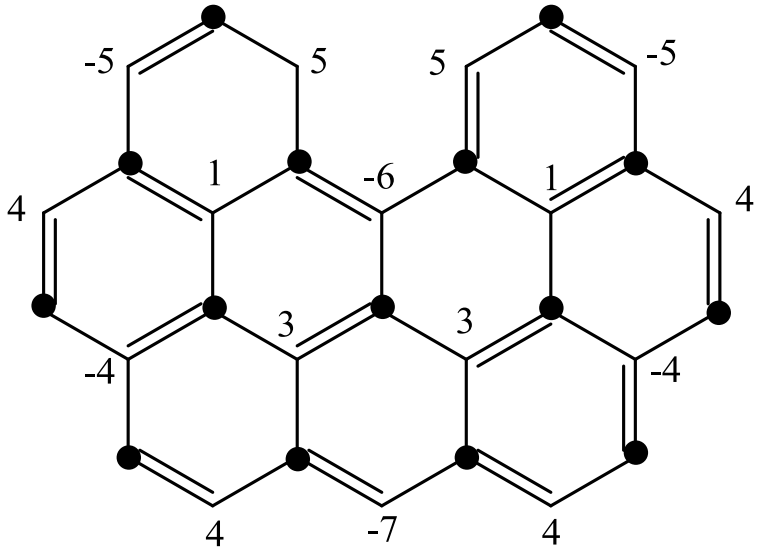
$$T(E=0) = 4s/(1+s)^2$$

$$s = \frac{t^2}{\beta^2} \frac{\left(\sum_{l \in ad(b)} c_l\right)^2}{|c_a|^2}$$

Ovalene

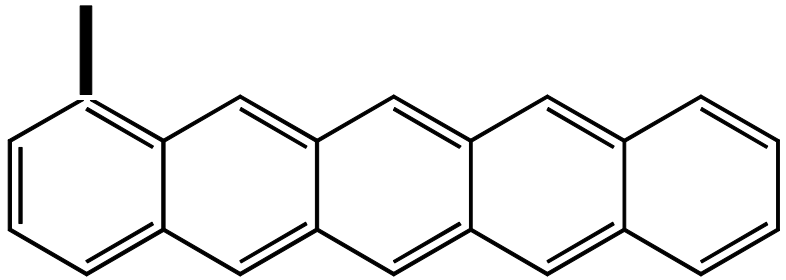


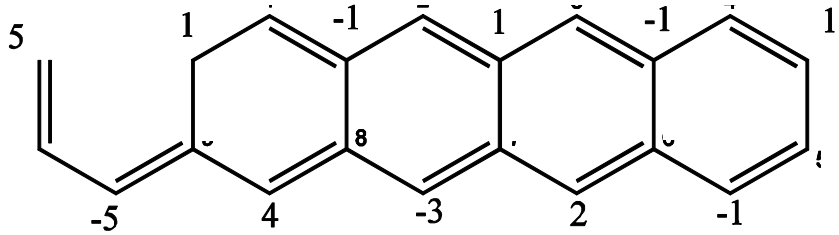
Delocalized defect state



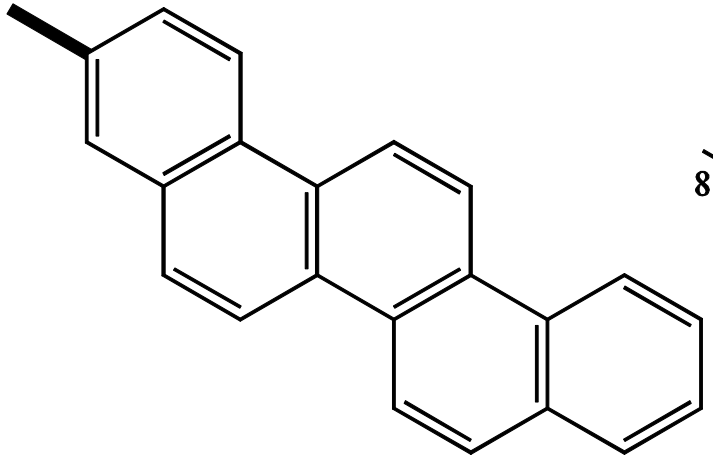
Pentacene & Picene

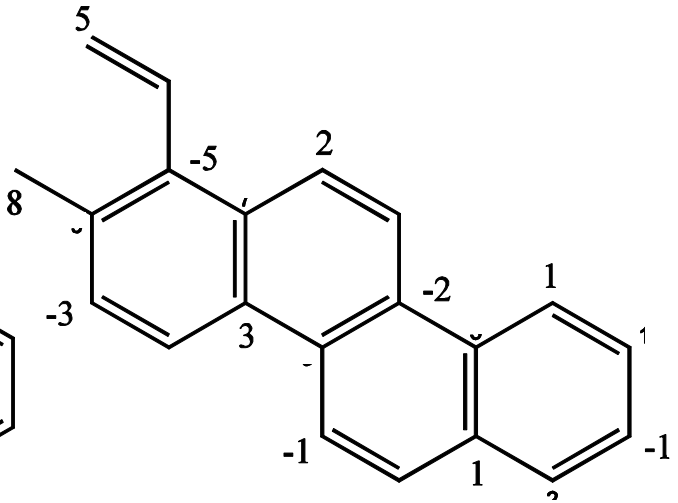
i



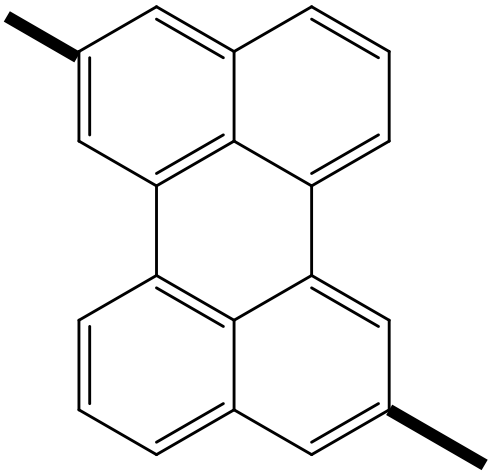


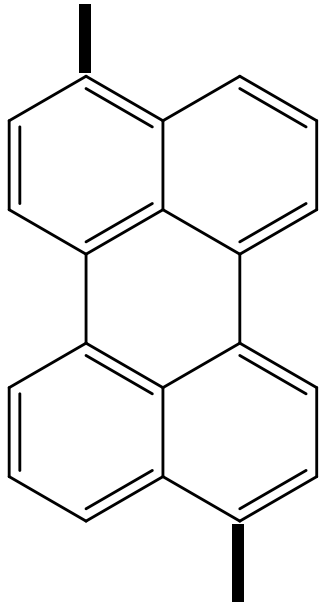
ii

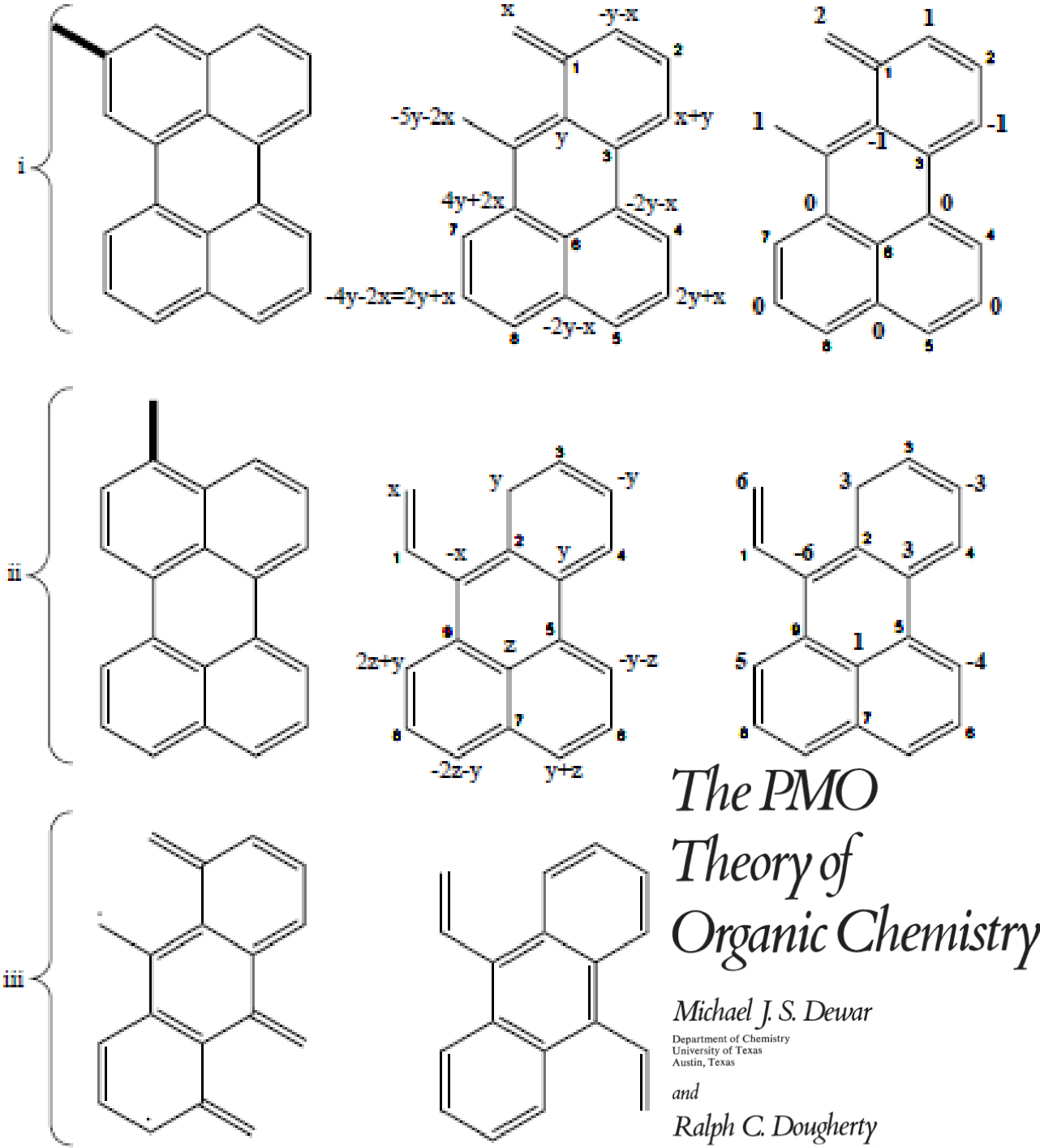




Perylene







The PMO Theory of Organic Chemistry

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Department of Chemistry
University of Texas
Austin, Texas

and

Ralph C. Dougherty

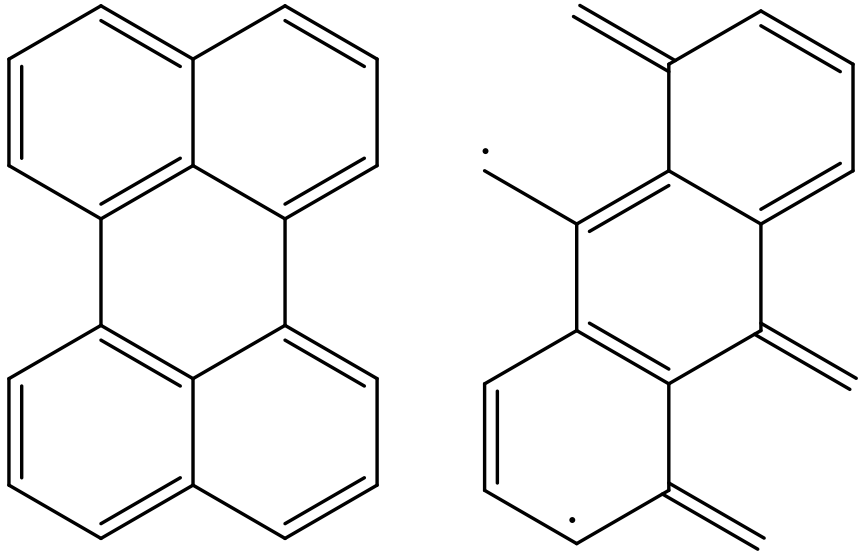
Conductance in terms of Kekulé structures

THE JOURNAL OF CHEMICAL PHYSICS 131, 244110 (2009)

Conduction in graphenes

P. W. Fowler,[1,a)] B. T. Pickup,[1,b)] T. Z. Todorova,[1,c)] and W. Myrvold[2,d)]
[1]*Department of Chemistry, The University of Sheffield, England S3 7HF, United Kingdom*
[2]*Department of Computer Science, University of Victoria, British Columbia V8W 3P6, Canada*

$$T(0) = \frac{4K_s^2 K_v^2 \tilde{\beta}^2}{(K_s^2 + K_v^2 \tilde{\beta}^2)^2},$$



Fowler, Pickup, Todorova, Myrvold, JCP, 131, 244110 (2009).

All electron DFT/Green's function approach