

Q) ベンゼンの分子軌道を簡単に調べる方法は？

<http://m.hulis.free.fr/hulis.html>

The screenshot shows the HuLiS HTML5 interface in a browser window. The page title is "HuLiS HTML5 is a Huckel and Lewis program for tablets and smartphones". Below the title, there is a description: "This version is optimized for tablets and Google Chrome. The classic Java version is runnable on the website of HuLiS". A link to an "online tutorial" is provided.

The interface is divided into several sections:

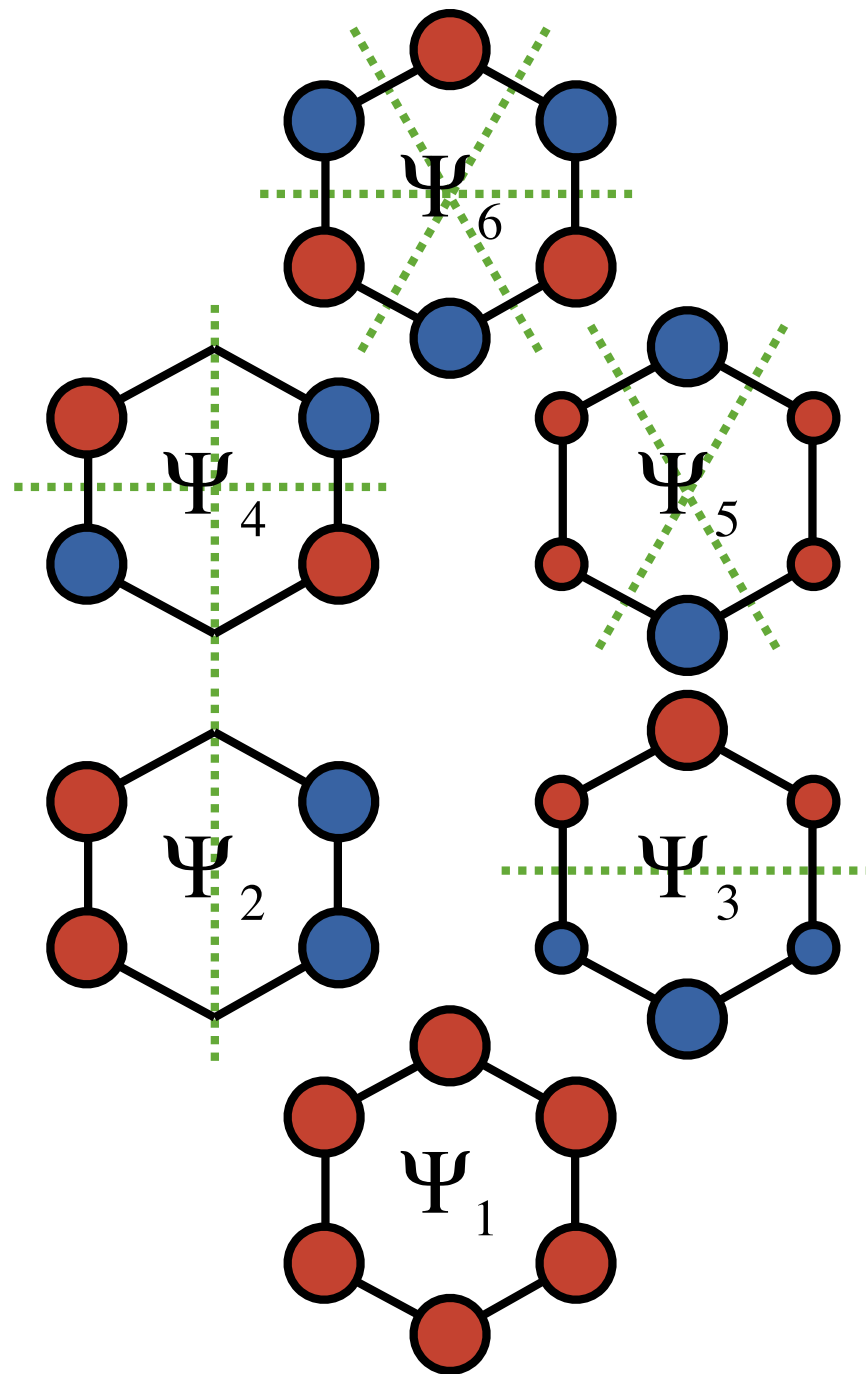
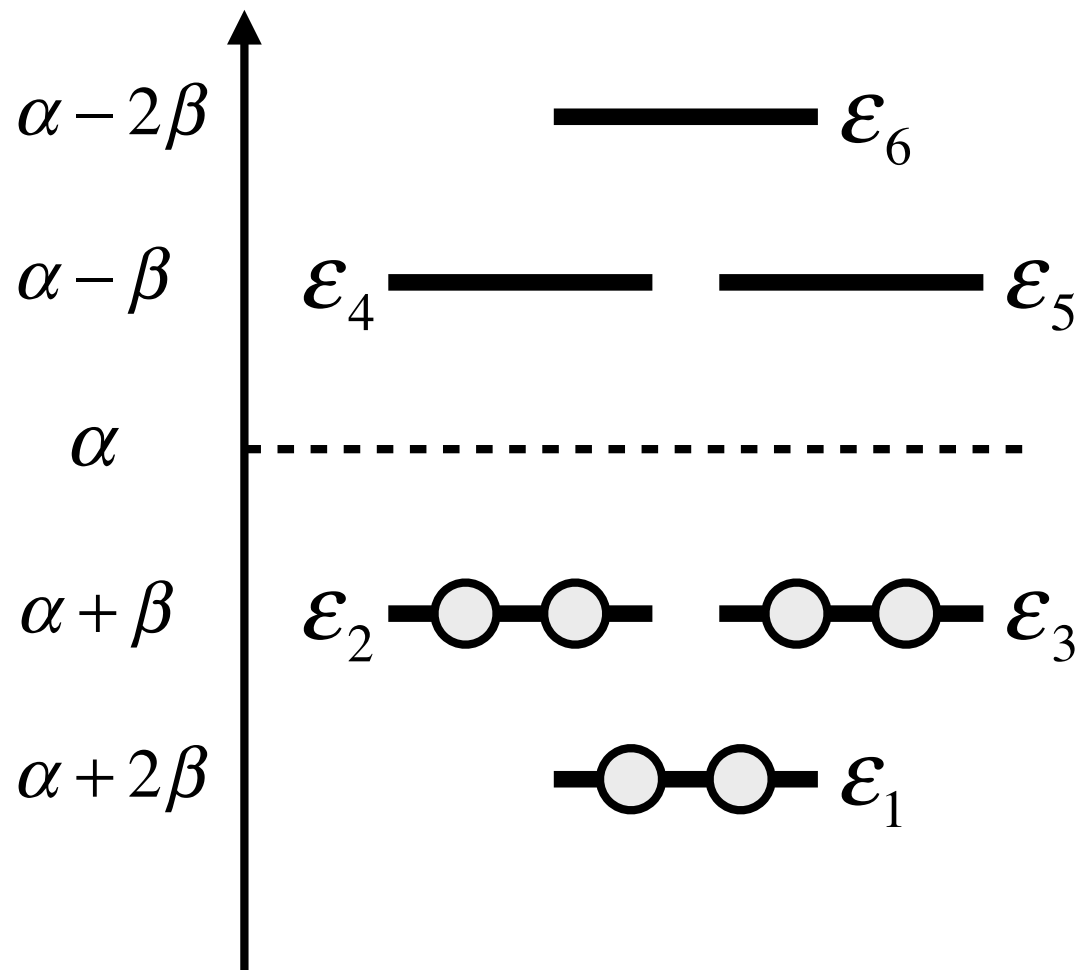
- Huckel** (left panel, blue header): Contains controls for zooming, sorting, and selecting orbitals. Buttons include "Sort", "i", "hij", " Ψ_i ", "qi", "Results", and "Erase all".
- Central Panel**: A large empty area for displaying molecular orbitals, with a vertical energy scale on the right ranging from -5 to 5. Below the scale is a "Charge" control with a slider set to 0.
- Lewis Mesomery** (right panel, orange header): Contains buttons for "Generate all", "Create", "Results", "Erase 1", and "Erase mesomery", along with a percentage input field.

Below the main interface, there is a section for "Choose the number of structures" with a slider set to $n=0$. At the bottom left, there is a small blue box containing the text:

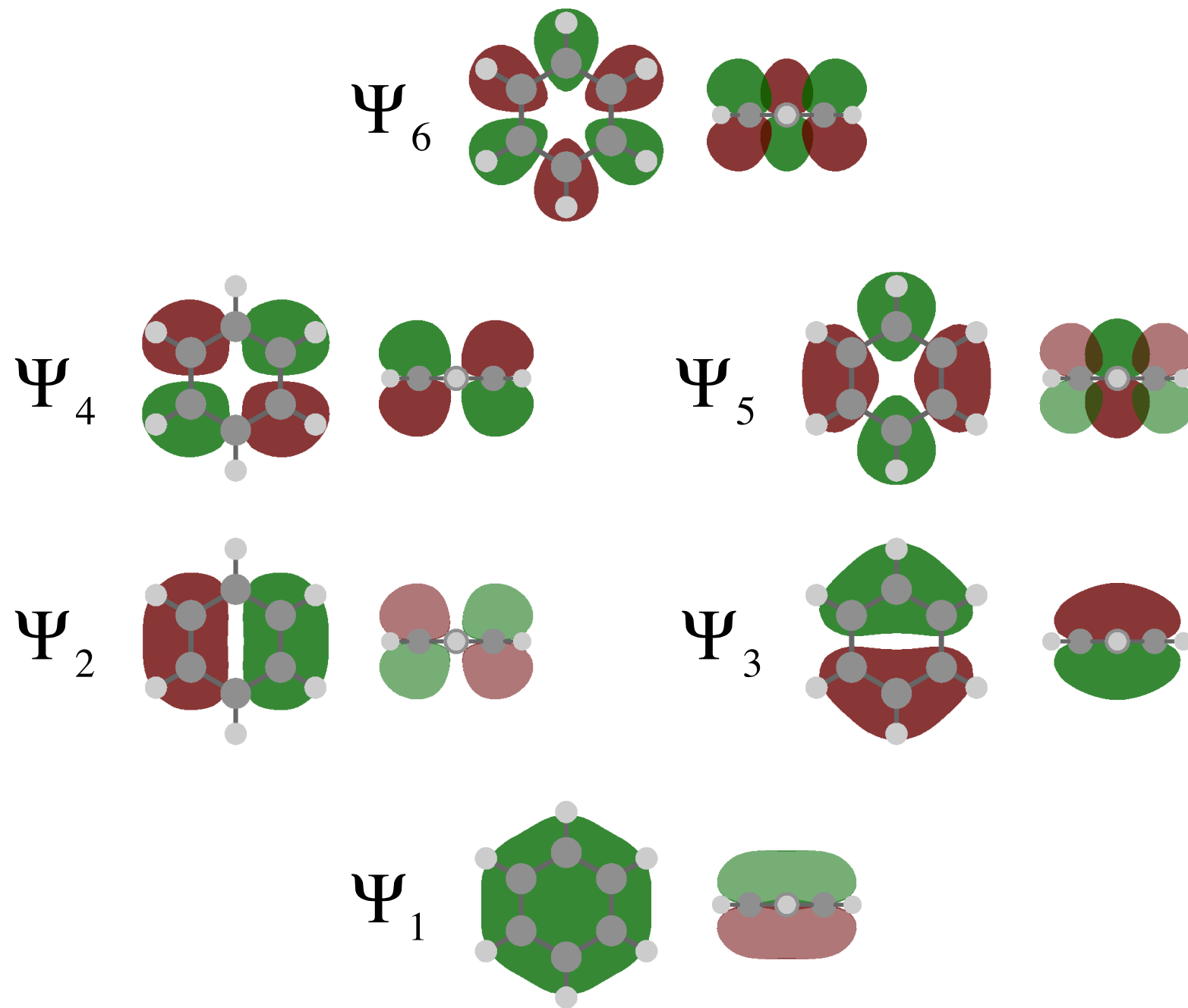
$$\Psi_{\text{tot}}$$
$$E_{\text{tot}} = 0\beta$$

At the bottom of the page, there is a link to visit the full version (Java) at the HuLiS website.

Q) ベンゼンの π 電子状態は？

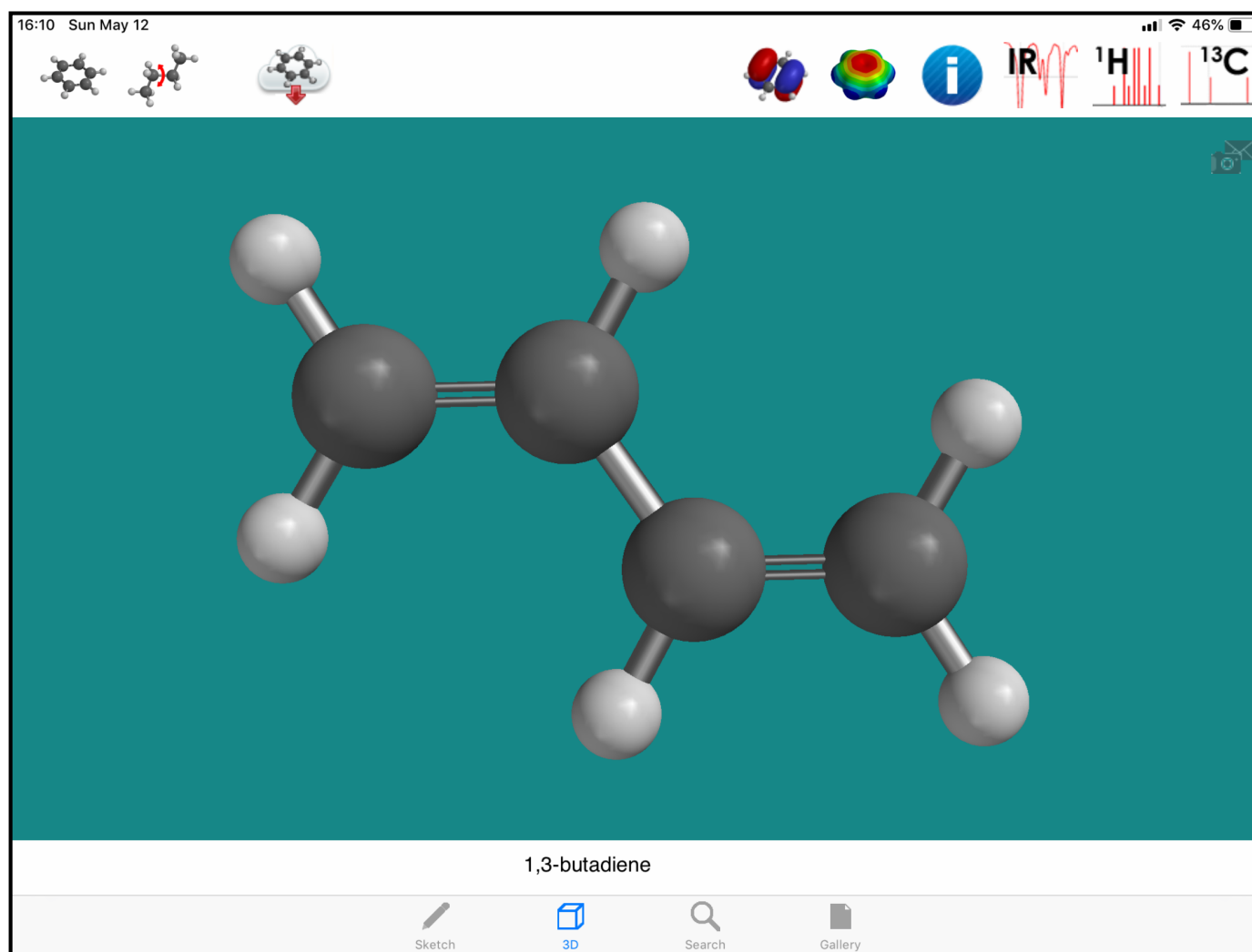
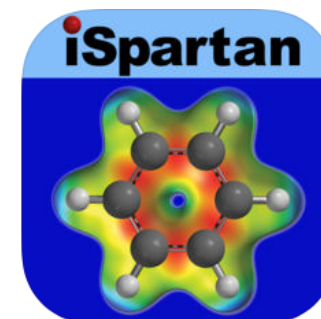


Q) もっと高精度な量子化学計算と比較すると？

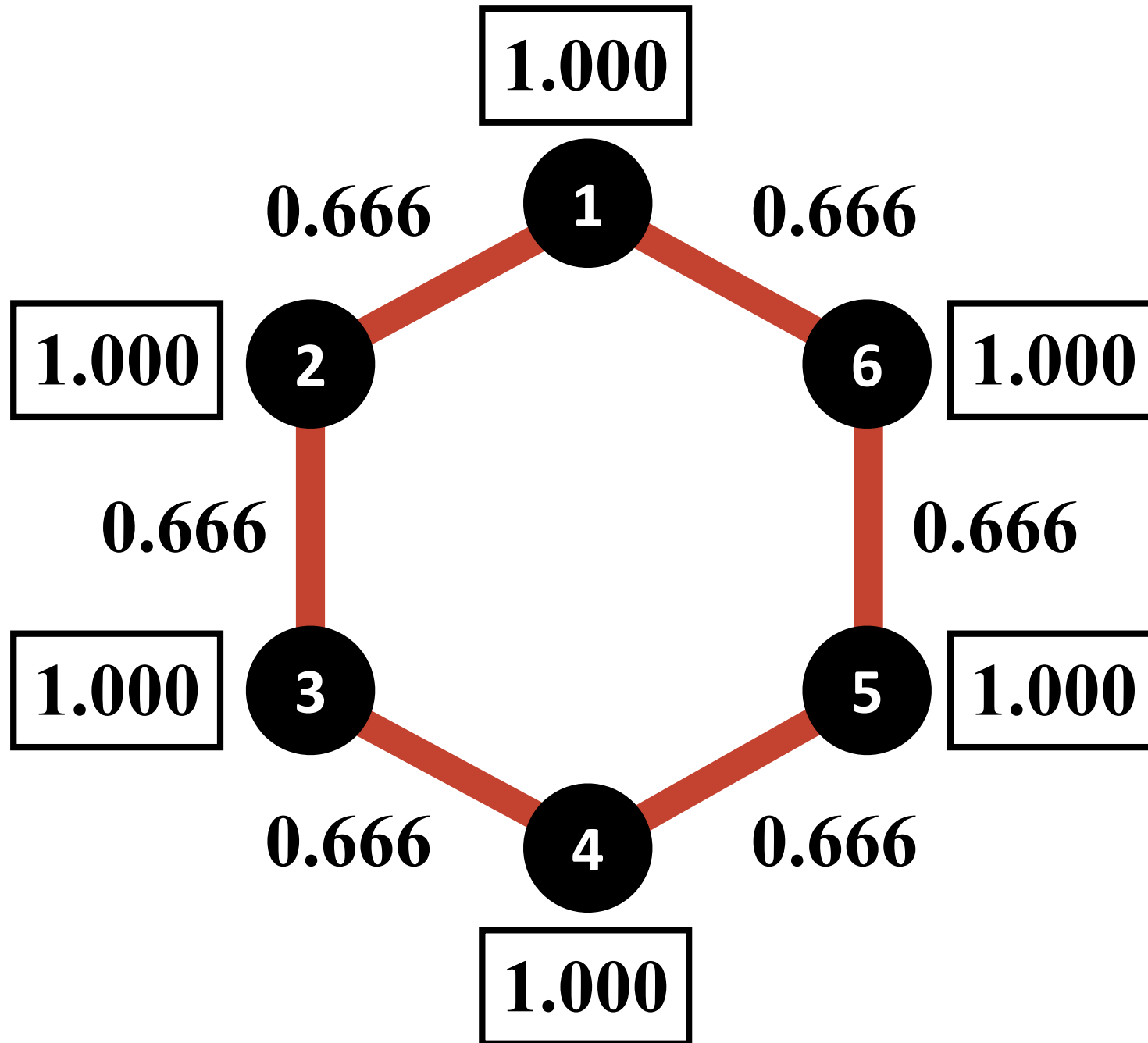


Q) iPadで量子化学計算できる？

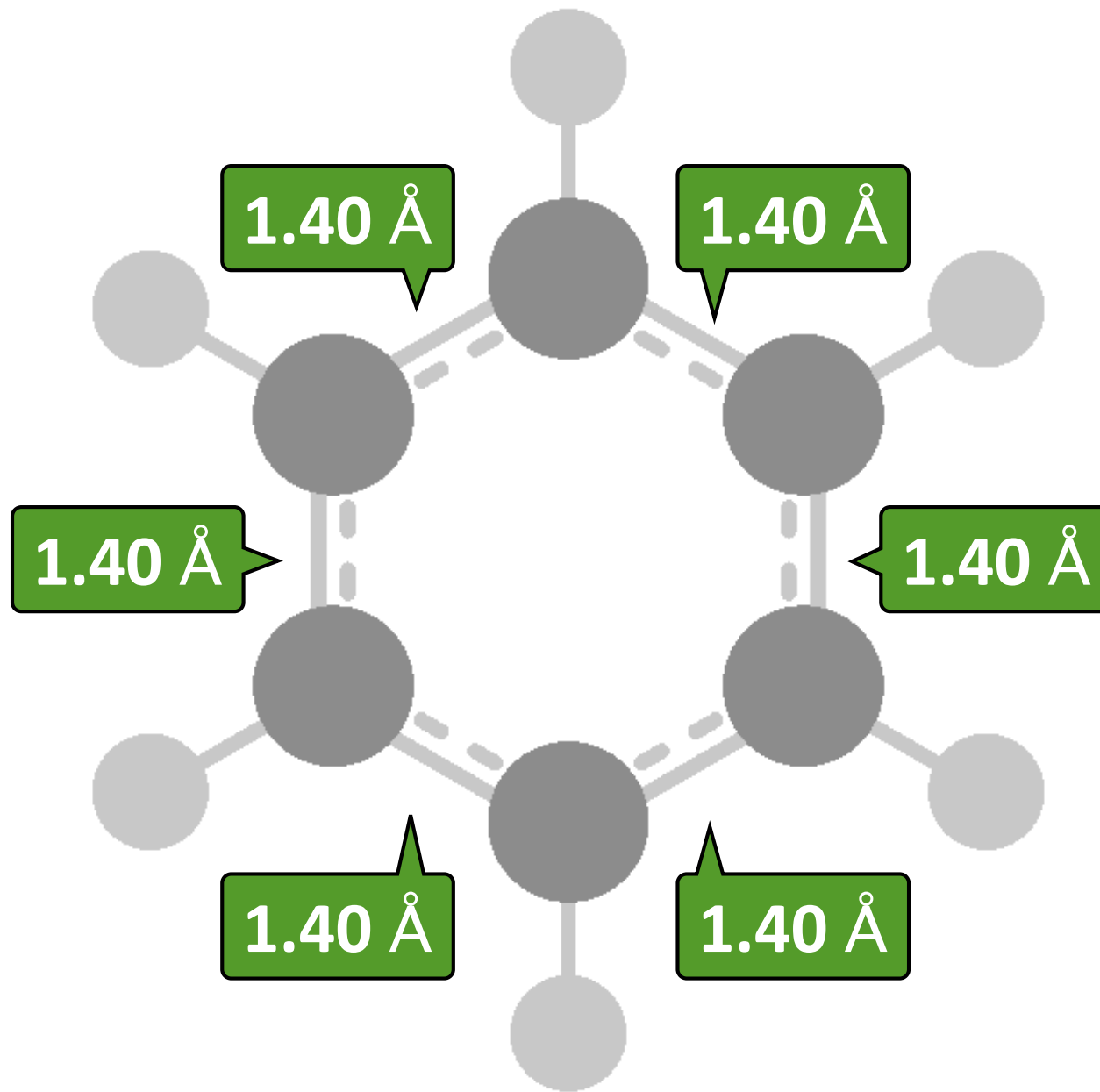
A) iSpartan (2,400円) がおすすめ



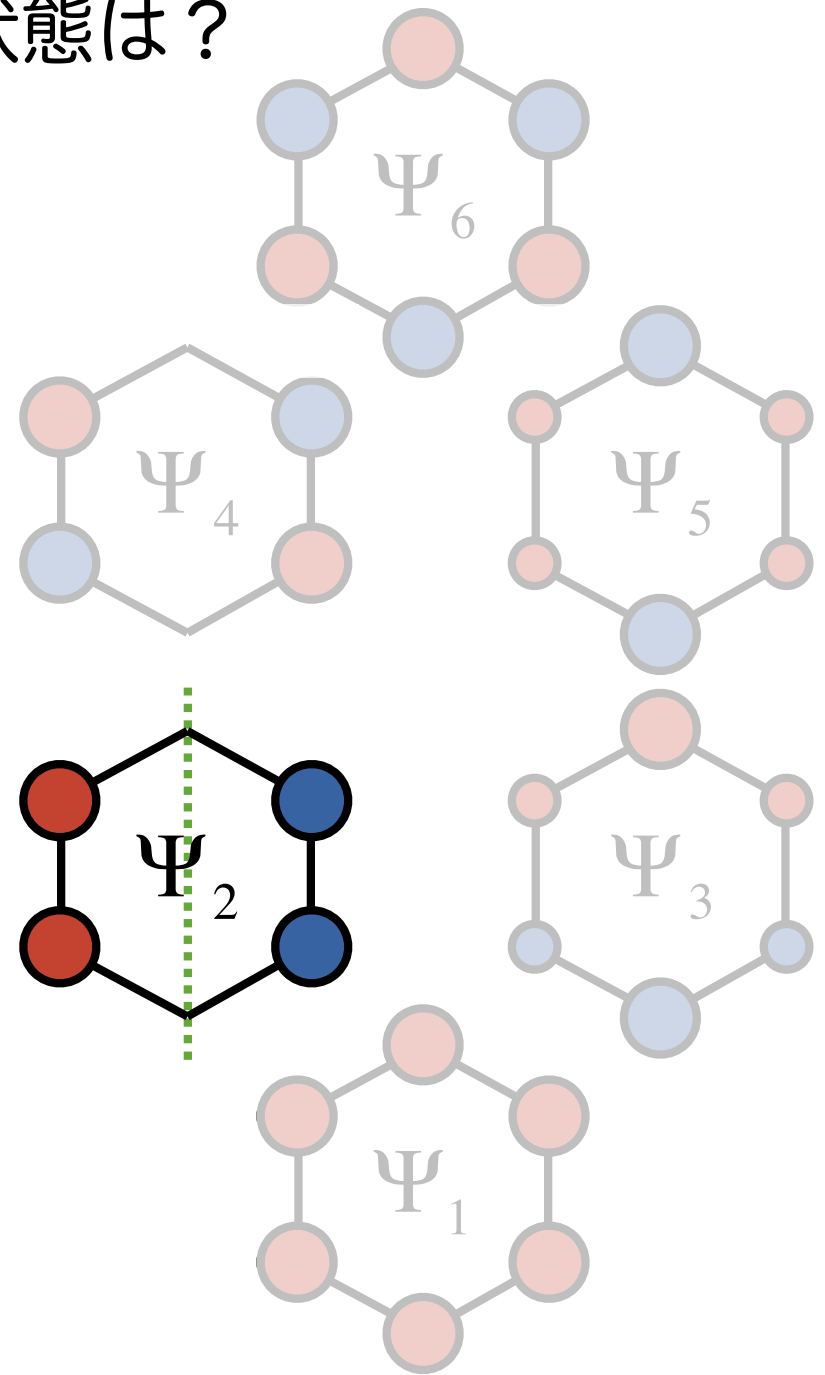
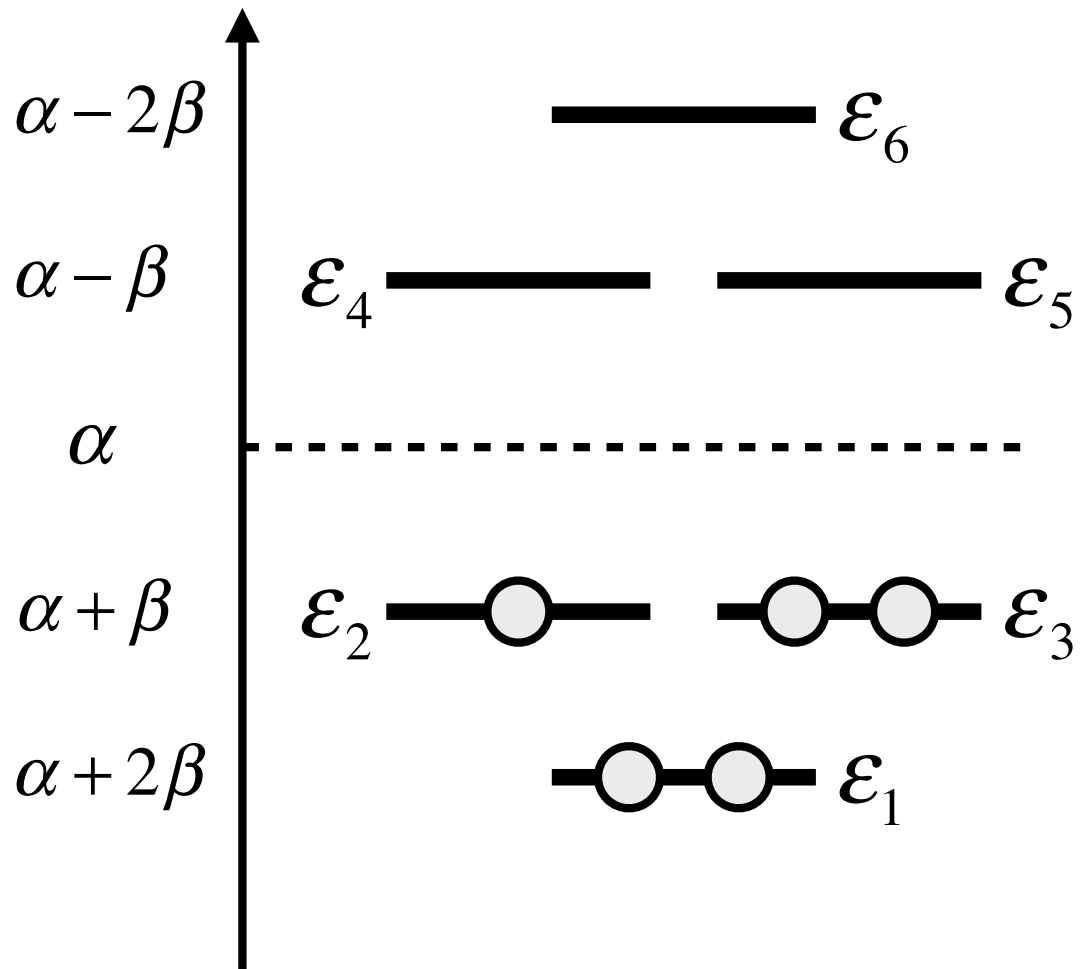
ベンゼンの電子密度・結合次数



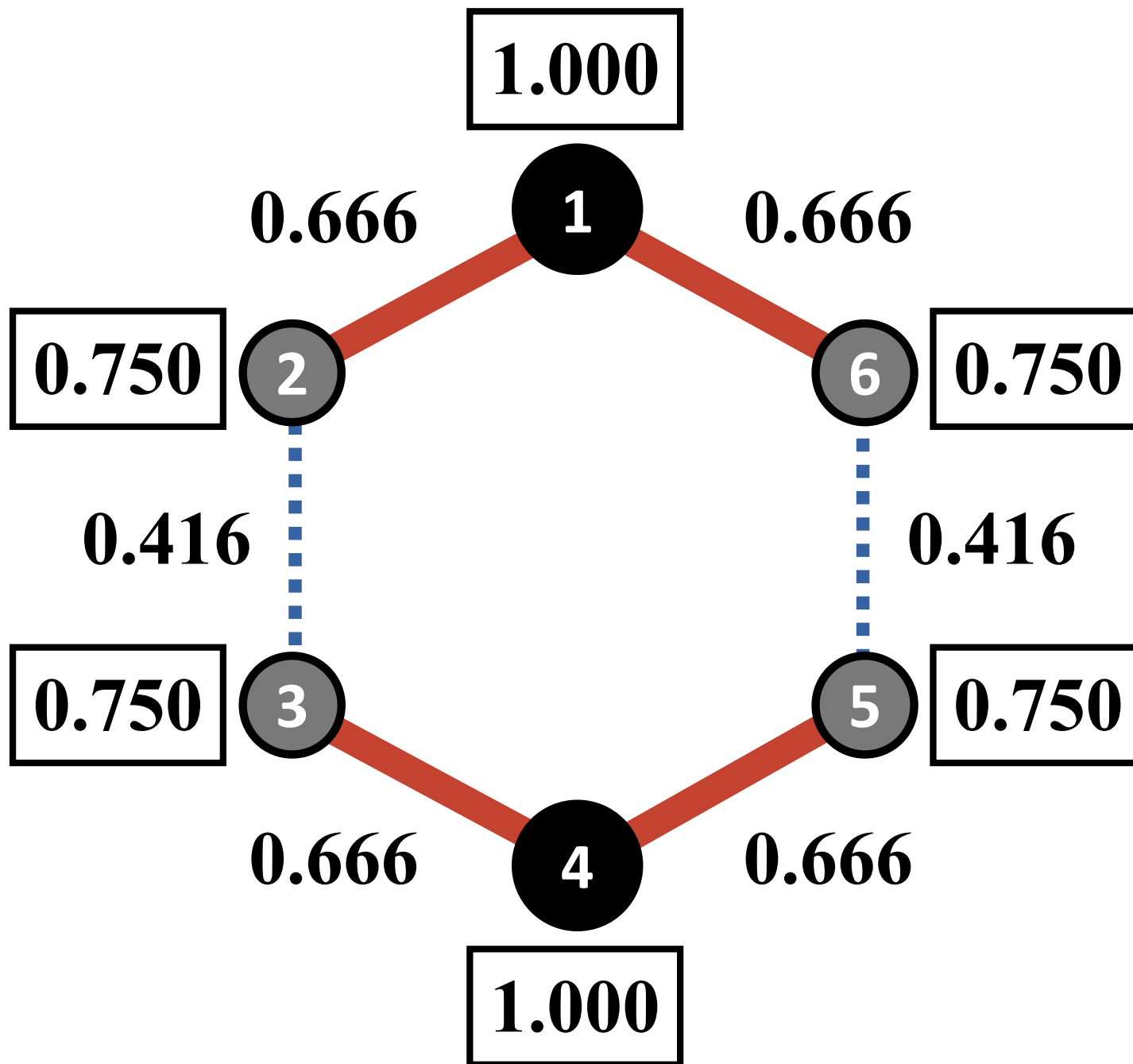
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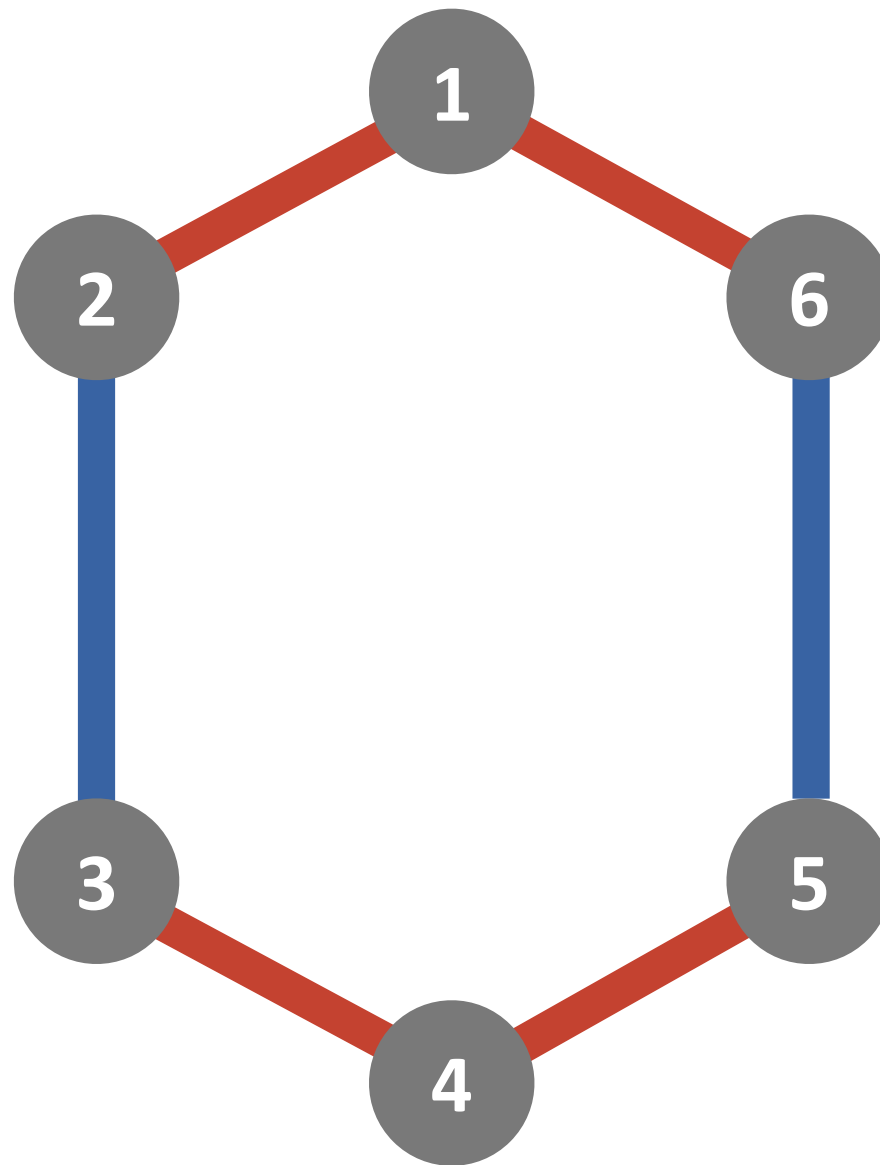
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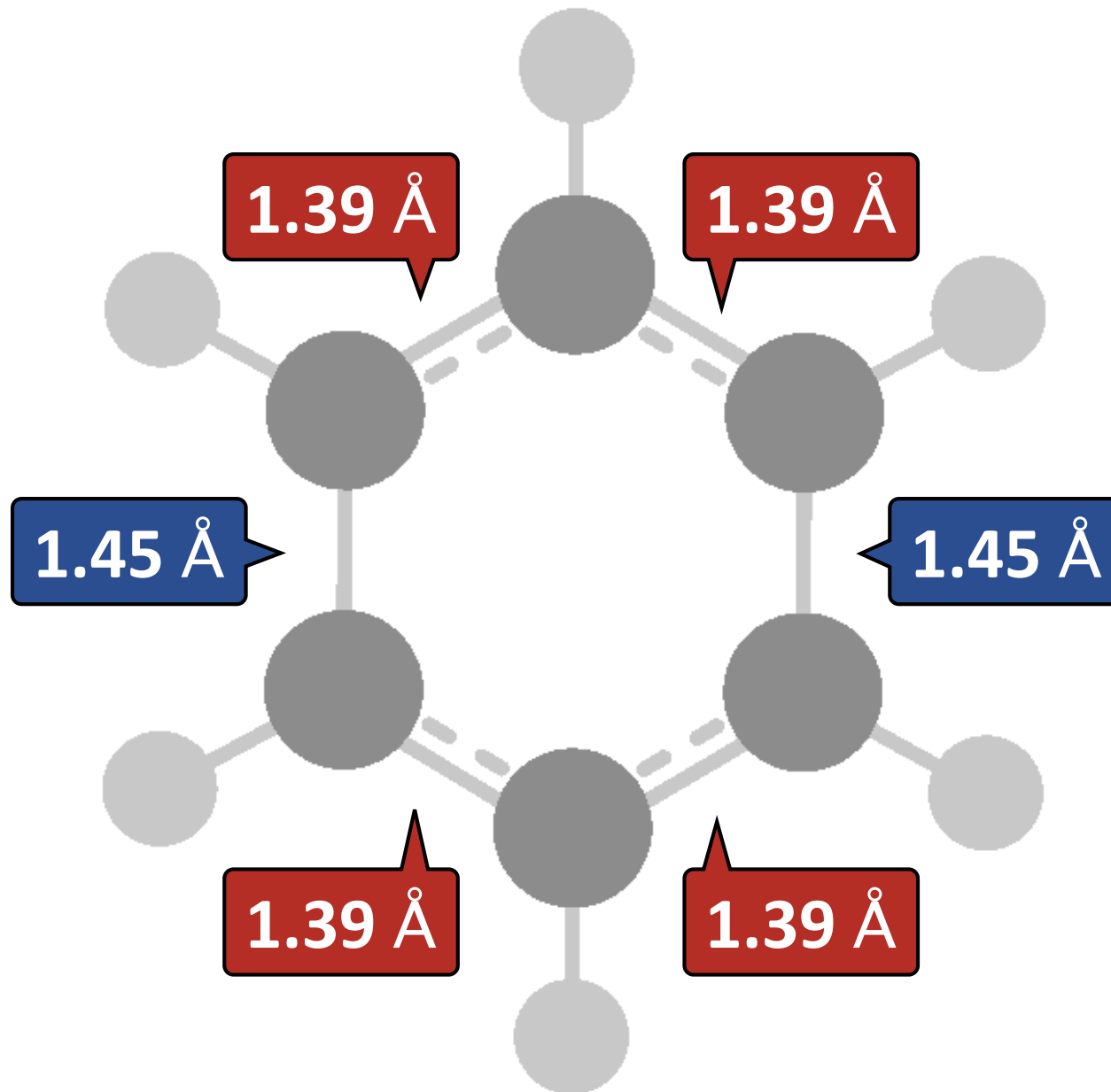
ベンゼンカチオンの電子密度・結合次数



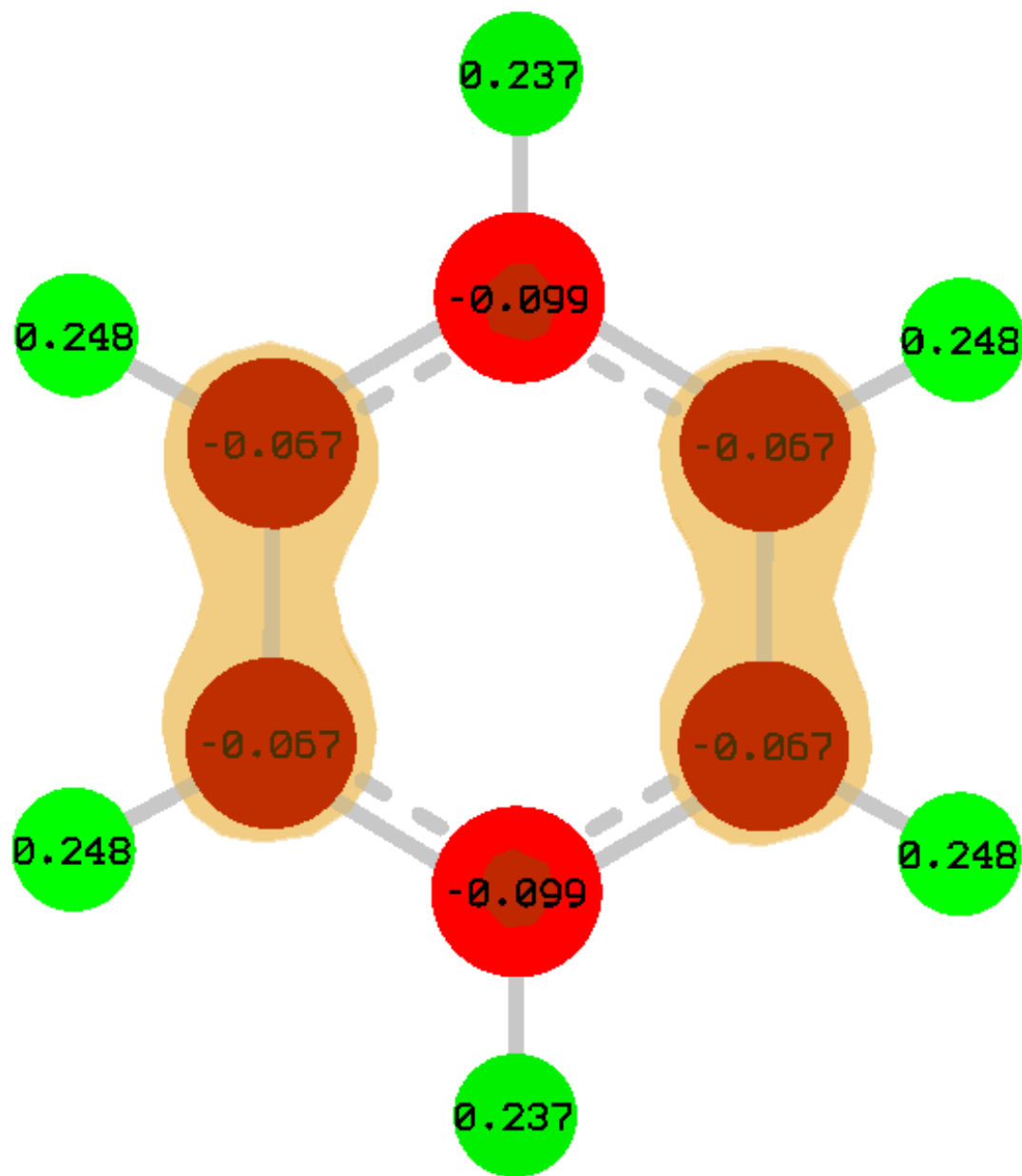
ベンゼンカチオンの分子構造



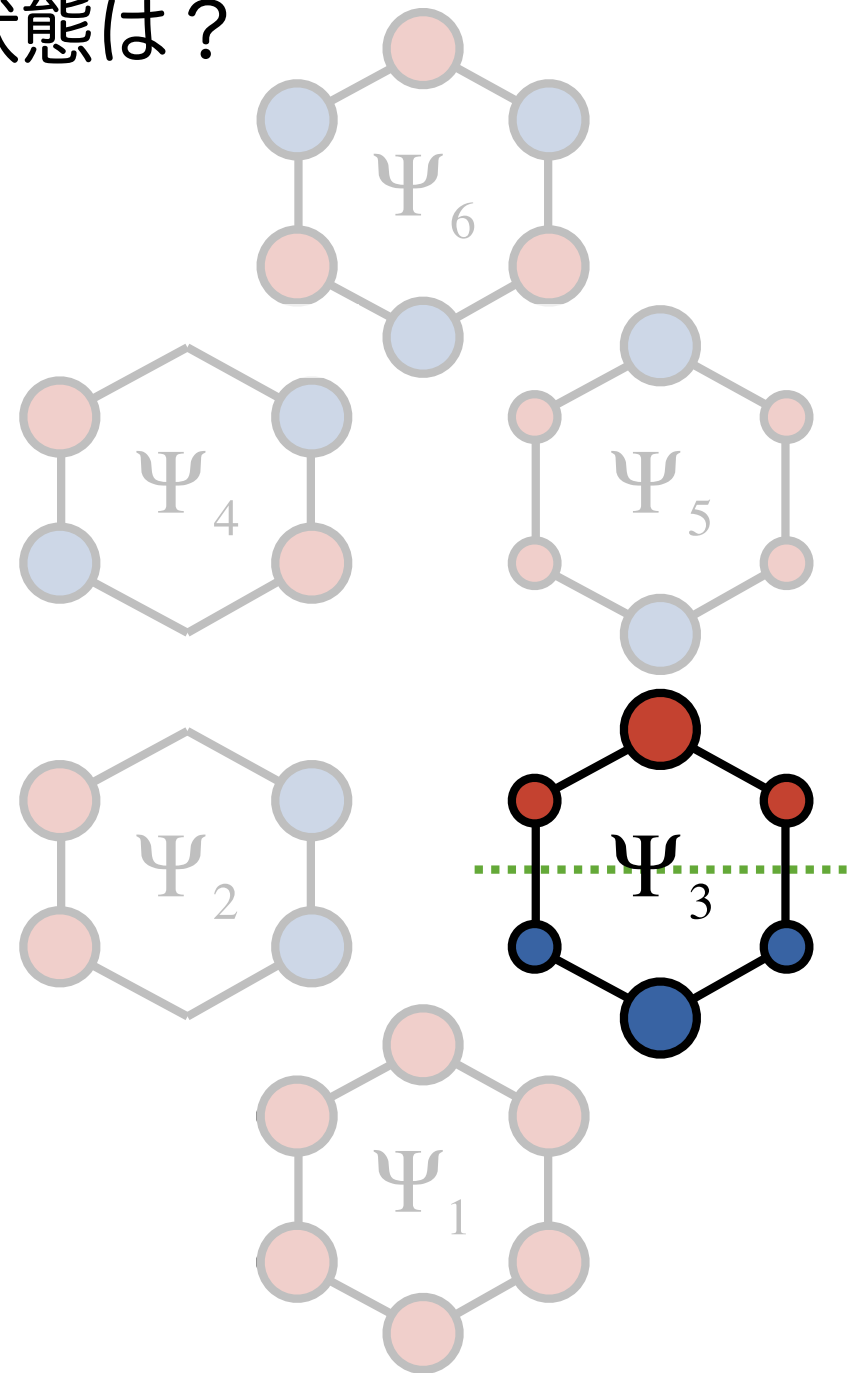
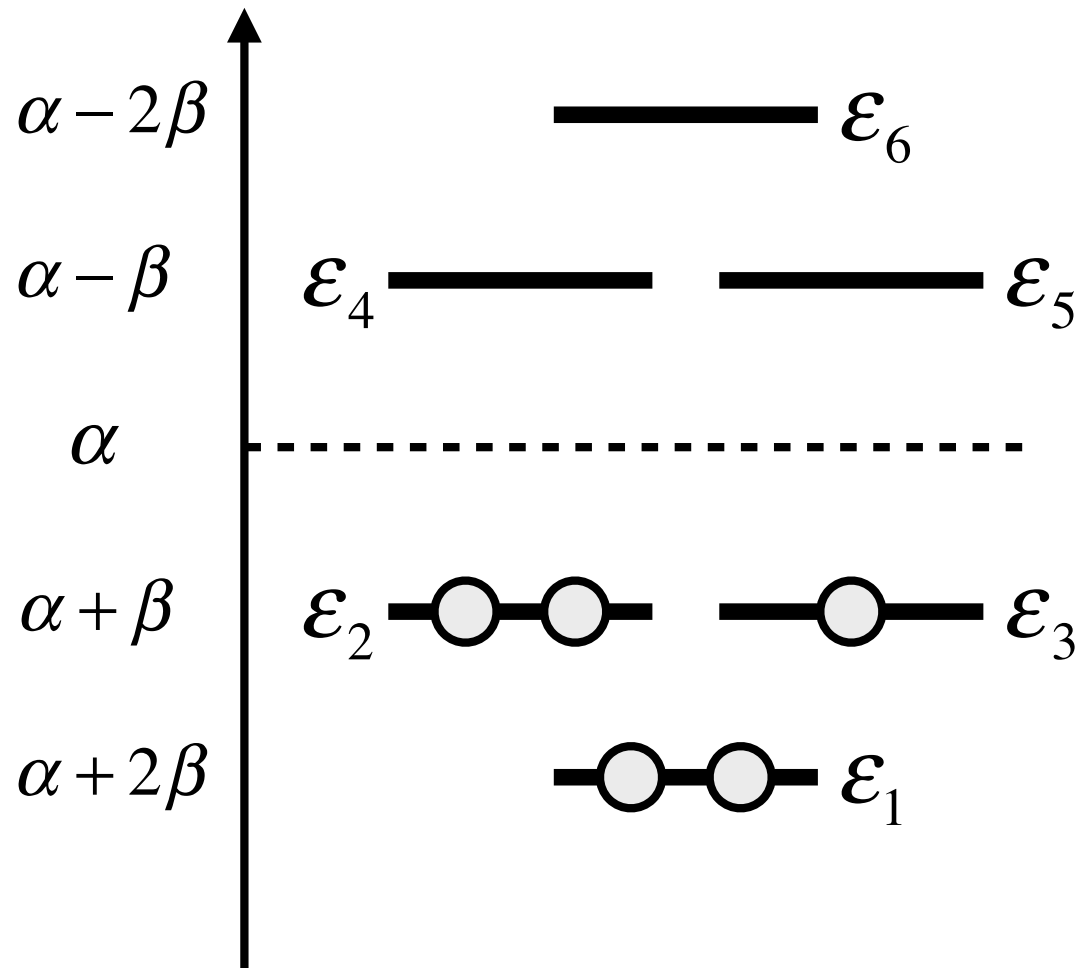
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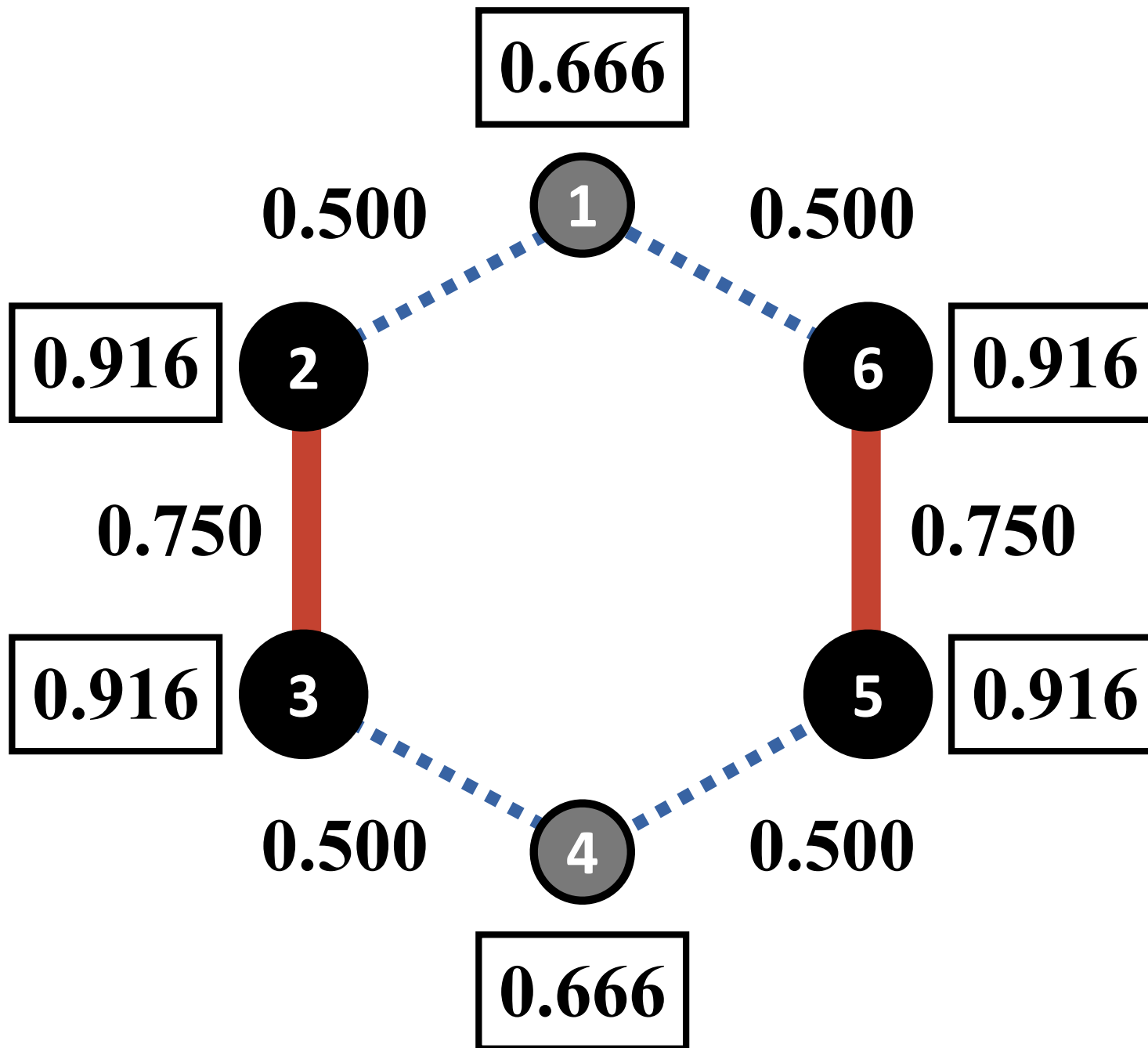
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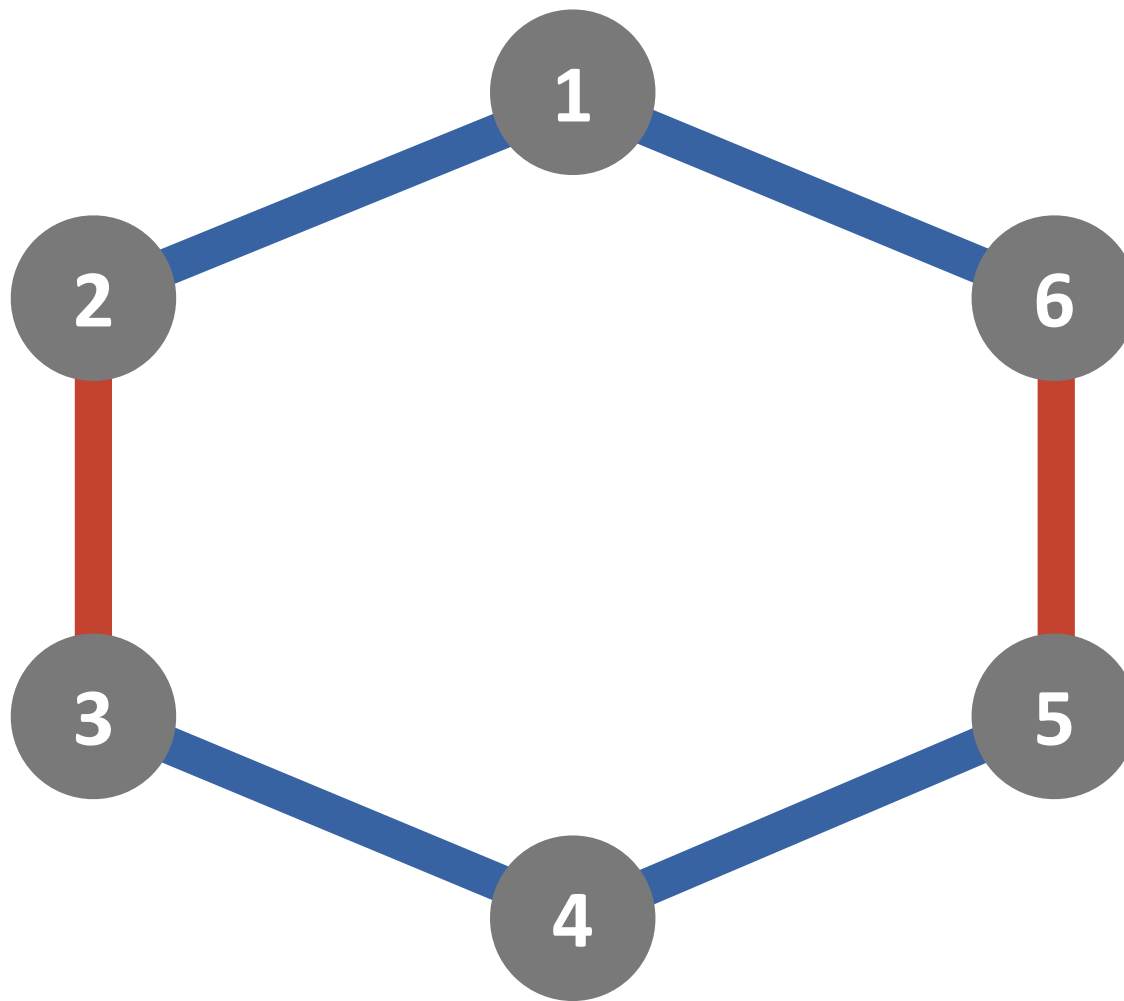
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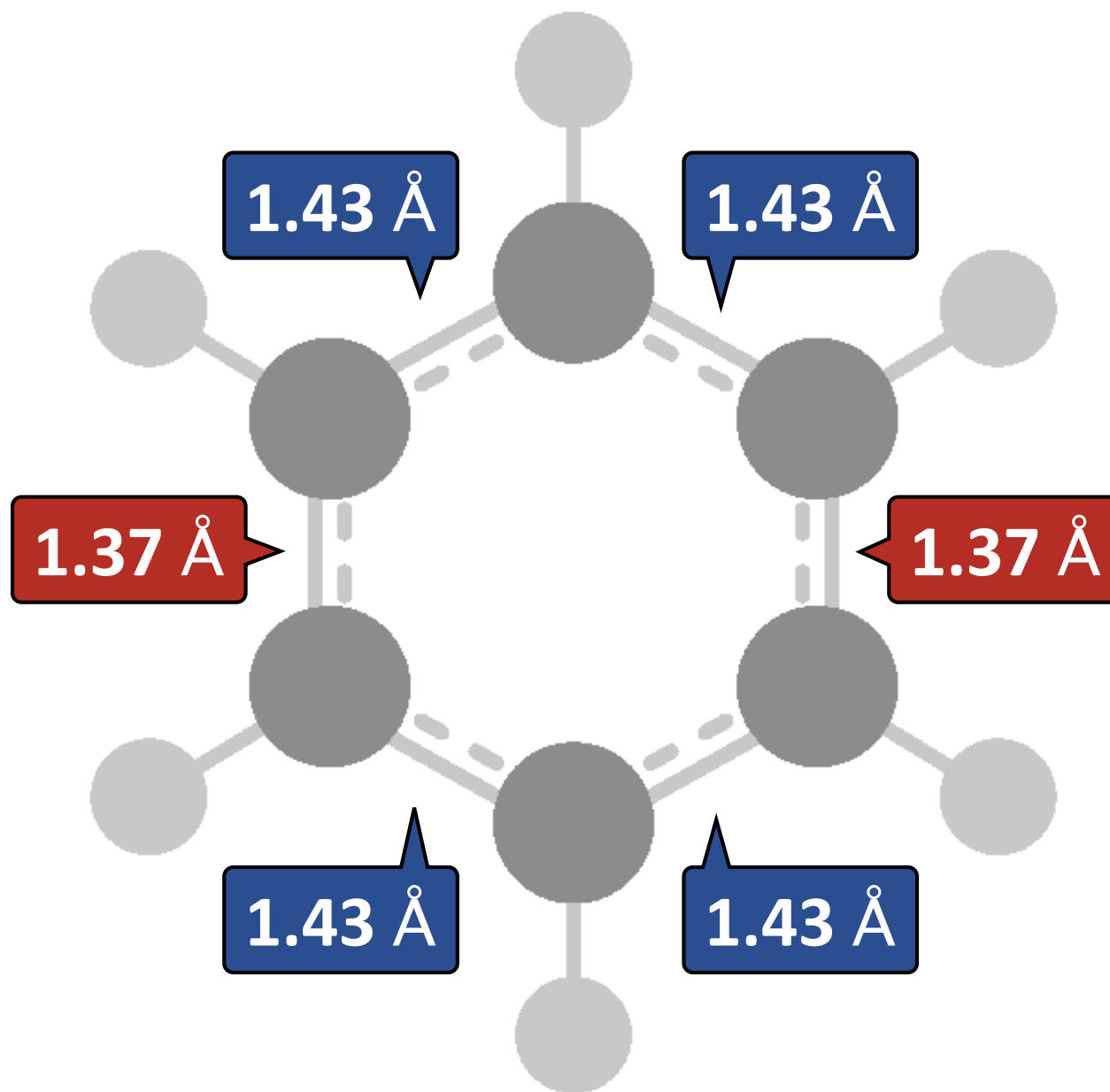
ベンゼンカチオンの電子密度・結合次数



ベンゼンカチオンの分子構造



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