# 第261回化学コロキウムのお知らせ

日時： 7月 25日（月）16:30−

場所： 8号棟303号室

演者： Henrik Ottosson准教授

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演題： Exploiting the “Mr. Hyde” Character of Benzene for New Photochemistry

**Abstract:** Aromaticity is a core concept in the electronic ground state ($S_0$), as given by Hückel’s rule. Yet, in the lowest ππ* triplet state ($T_1$) the rule for aromaticity and antiaromaticity is reversed, as shown theoretically by Baird in 1972. Today, Baird’s rule has been confirmed by a range of quantum chemical computations as well as supported by spectroscopic evidence. We recently described benzene as a molecular “Dr. Jekyll and Mr. Hyde” with its antiaromatic character in the first ππ * excited states being its “Mr. Hyde” character. This antiaromatic character of the excited benzene ring has now been used to identify and develop new photoreactions that are difficult or impossible in the $S_0$ state. Moreover, in polycyclic molecules with certain connectivities, *e.g.*, biphenylene, the excited state antiaromatic character of the benzene ring is alleviated and can lead to an excited state aromatic character. Taken together, Baird’s rule is used far too seldom for the development of new photochemical reactions and for the design of novel photoactive molecules.

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