Decorating Phenalene: An Approach Towards Benzannulated Peropyrenes

Jordyn Gunderson, Marc R. MacKinnon*,
Department of Chemistry and Biochemistry, University of Regina, Regina, Canada
Email: marc.mackinnon@uregina.ca

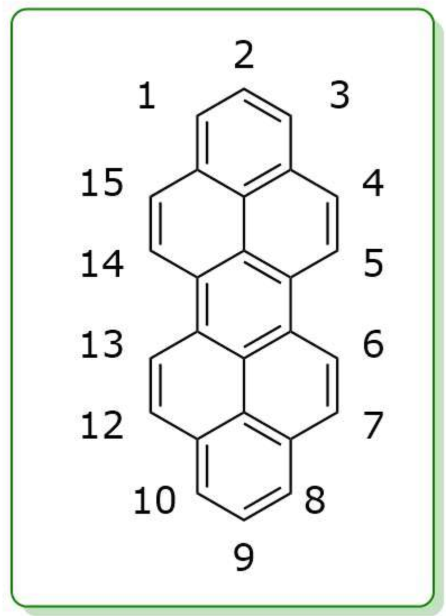
Introduction: Polycyclic Aromatic Hydrocarbons and Peropyrene

- Polycyclic aromatic hydrocarbons (PAHs) are molecules that contain at least 2 aromatic rings usually fused together
- Found naturally in crude oil and soil and also as products from incomplete combustion (soot)

- Historically these molecules were of interest to the dye industry and later as model compounds for studies into the nature of aromaticity

- More recently, interest in these compounds has been renewed due to their optoelectronic and photophysical properties

- One such compound, **peropyrene** is of particular interest due its advantageous photophysical properties:



1. Highly structured absorption (λ_{max} = 445 nm in CH_3CN) and emission (λmax = 450 nm in CH_3CN) spectra[1]
2. High fluorescence quantum yields ≈ 0.90 in most solvents[1]
3. Potential for singlet fission ($E(S1)$ = 2.79 eV, $E(T1)$ = 1.36 eV)[2]

- However, synthetic access to peropyrene cores is hindered by limited routes

- One of the best approaches is by dimerization of 2 phenalene units under oxidative conditions

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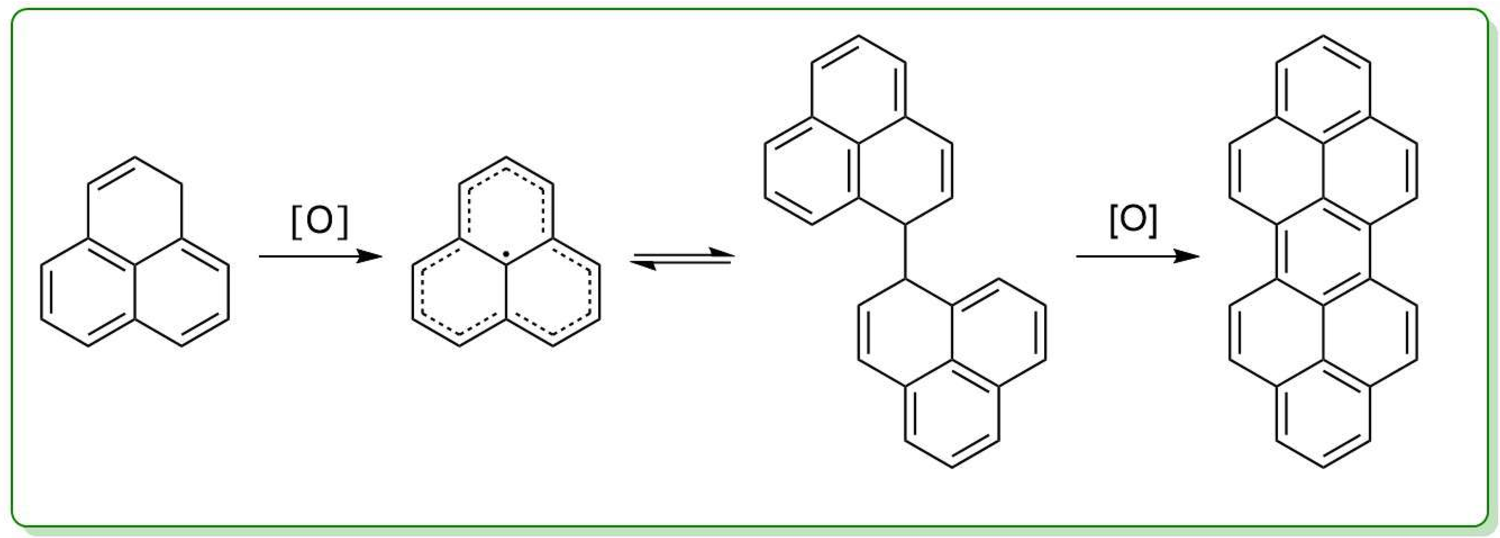
References: 1) Wenzel, U.; Löhmannsröben, H. G. *J. Photochem. Photobiol. A* **1996**, *96*, 13-18. 2) Nichols, V. M.; Rodriguez, M. T.; Piland, G. B.; Tham, F.; Nesterov, V. N.; Youngblood, W. J.; Bardeen, C. J. *J. Phys. Chem. C* **2013**, *117*, 16802-16820. 3) Uchida, K,; Kubo, T.; Yamanaka, D.; Furube, A.; Matsuzaki, H.; Nishii, R.; Sakagami, Y.; Abulikemu, A.; Kamada, K. *Can. J. Chem.* **2017**, *95*, 432-444.

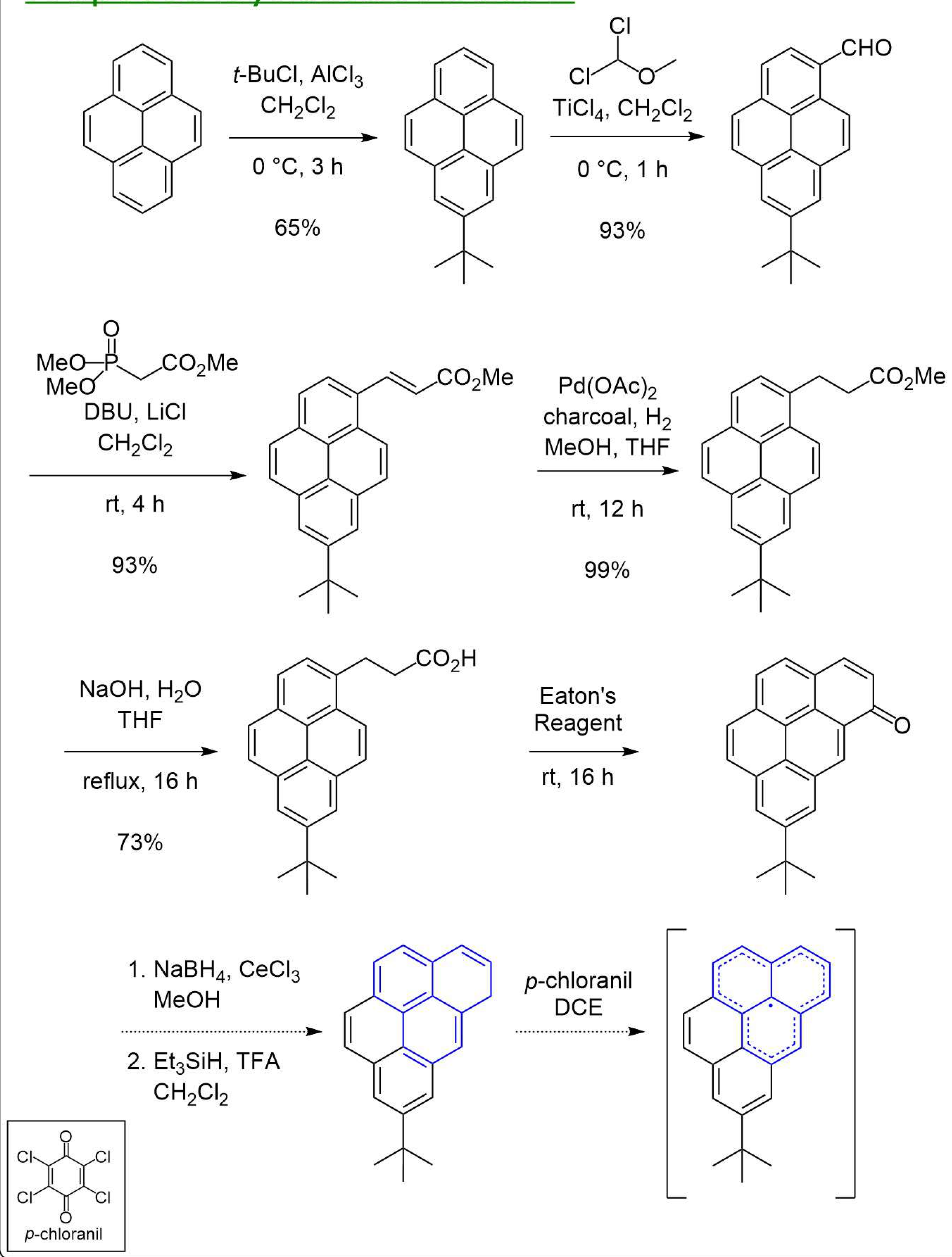
Phenalene and Phenalenyl Radicals

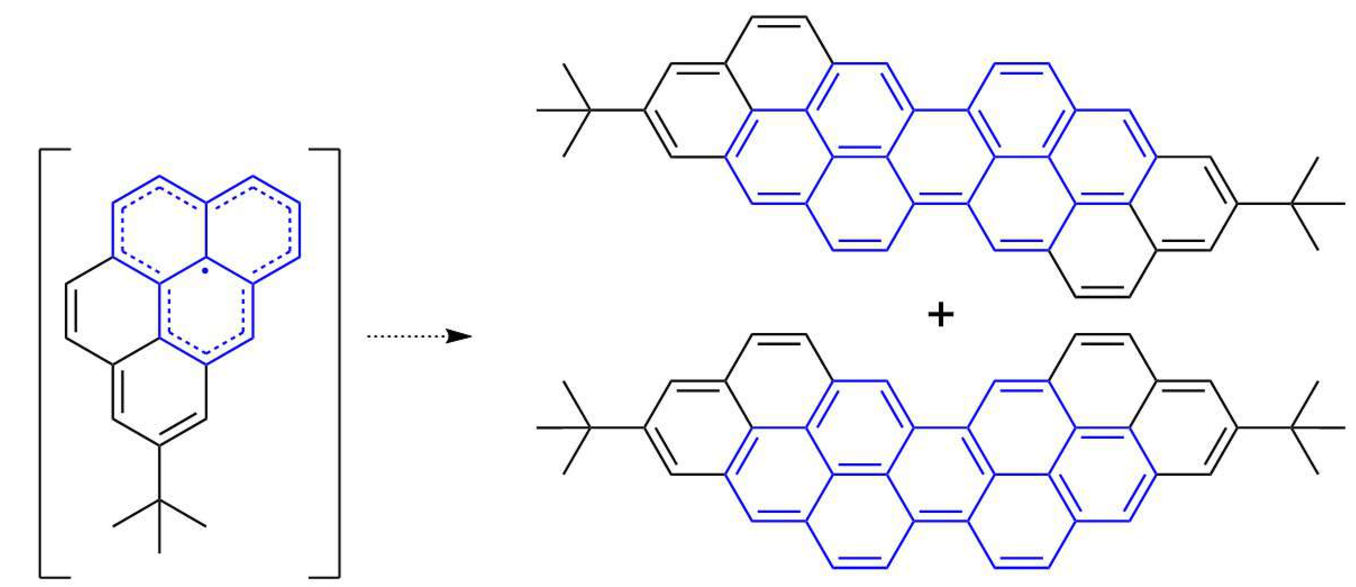
- Phenalene is readily oxidized to the phenalenyl radical when treated with an oxidant[3]



- This project aims to utilize this ability of phenalenes and phenalenyl radicals to construct benzannulated peropyrene systems

Proposed Synthetic Route 1





Benzannulated peropyrene target molecules

Alternative Target Molecule