Synthesis and Characterization of Organothio-Substituted Pentacenes

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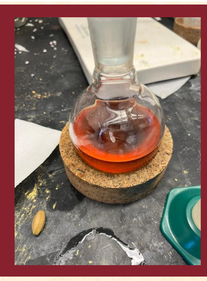

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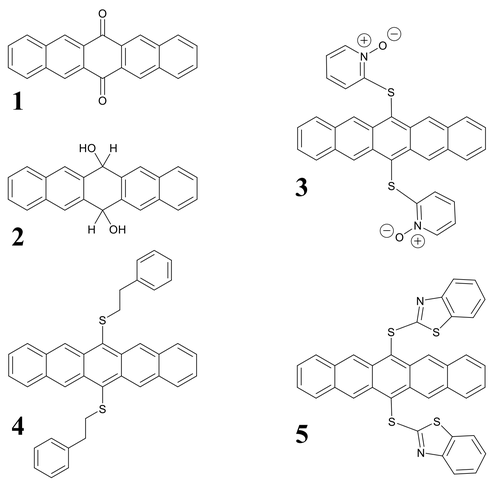
Abstract

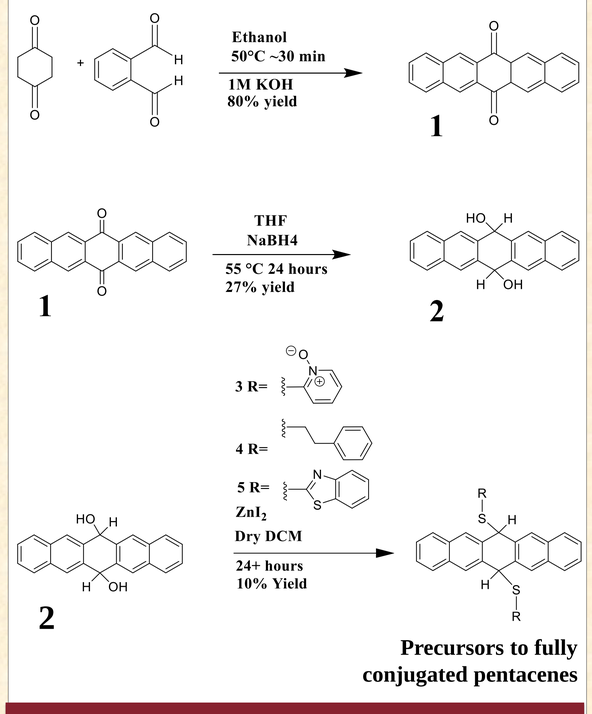
Organic semiconductors, such as pentacene-based molecules, provide advantages over inorganic silicon-based semiconductors including reduced costs, lower toxicity and adjustable properties. Pentacene derivatives are proven for devices like transistors, solar cells, and displays.



Objectives

- Synthesize and purify new organic semiconductor compounds based on pentacene (pentacene derivatives)
- Characterize new compounds using NMR (nuclear magnetic resonance) & UV-vis spectroscopies plus cyclic voltammetry
- Calculate structures and energetics of new compounds, including HOMO-LUMO gaps, using computational software (Spartan, Level of theory = B3LYP/6-311+)

Reactions



Computational Results

Table 1. Spartan calculated values

Substituent	Energy/au	LUMO/eV	HOMO/eV	HOMO-LUMO gap/eV	UV wavelength max/ nm
6,13-Quinone **(1)**	-996.309747	-2.88	-6.58	3.7	397.41
6,13-Diol **(2)**	-998.699391	-1.82	-6.25	4.43	308.57
2-Mercaptopyridine N-oxide **(3)**	-2288.08465	-3.28	-5.35	2.07	706.41
Phenylethanethiol **(4)**	-2262.921	-2.89	-4.95	2.06	697.94
2-Mercaptobenzothiazole **(5)**	-3086.62086	-3.22	-5.27	2.05	714.02

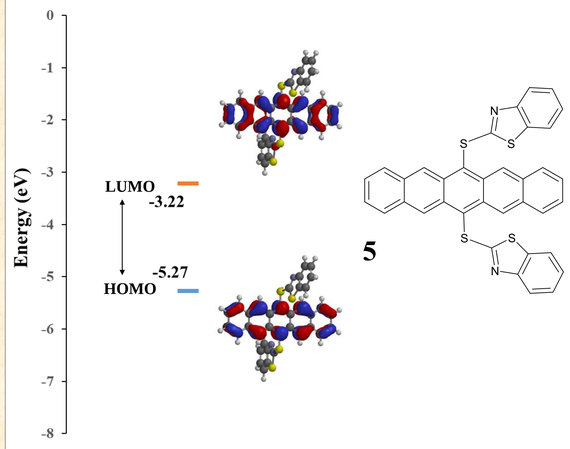
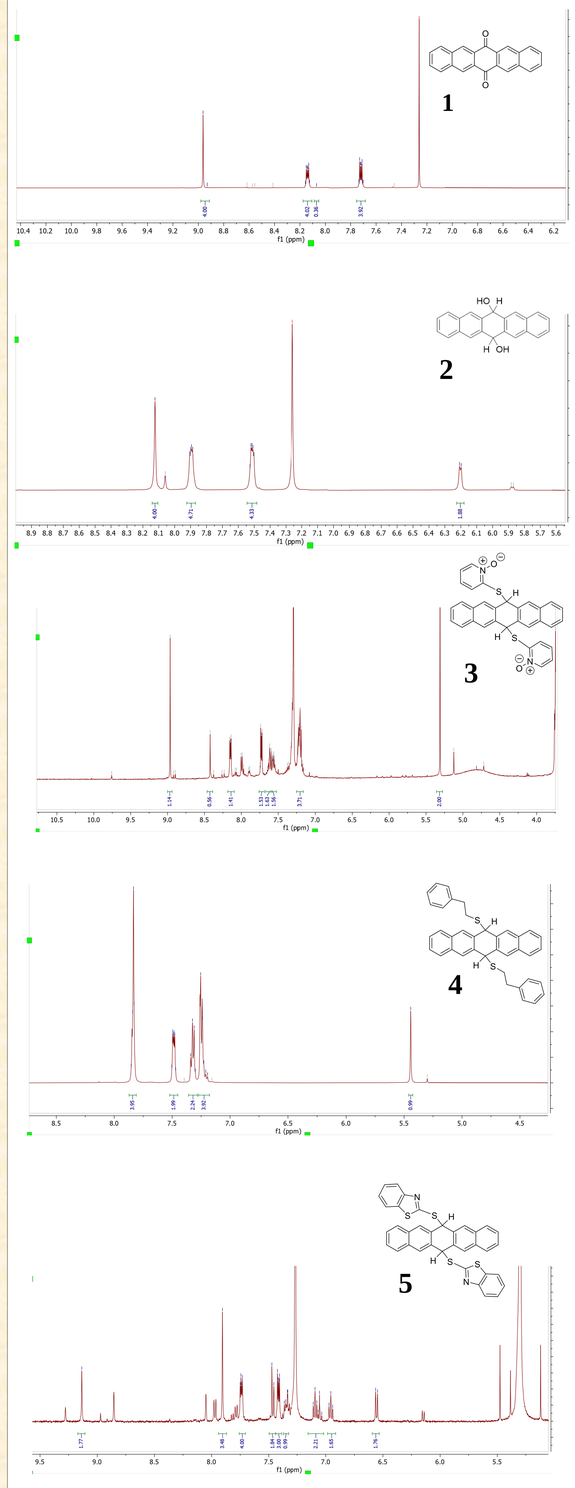


Figure 1. Frontier molecular orbitals of **5**

Spectroscopic Characterization



Summary

- New Pentacene based organic semiconductors and their precursors have been synthesized, purified and characterized
- Quantum mechanical calculations indicate that our target pentacenes possess small HOMO-LUMO gaps of approximately 2 eV

Next Steps

- Perform final synthetic step to fully aromatize the new pentacene derivatives
- Characterize new organic semiconductors by UV-vis spectroscopy and cyclic voltammetry to experimentally determine HOMO-LUMO gaps
- Publish results in a chemistry journal

References

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