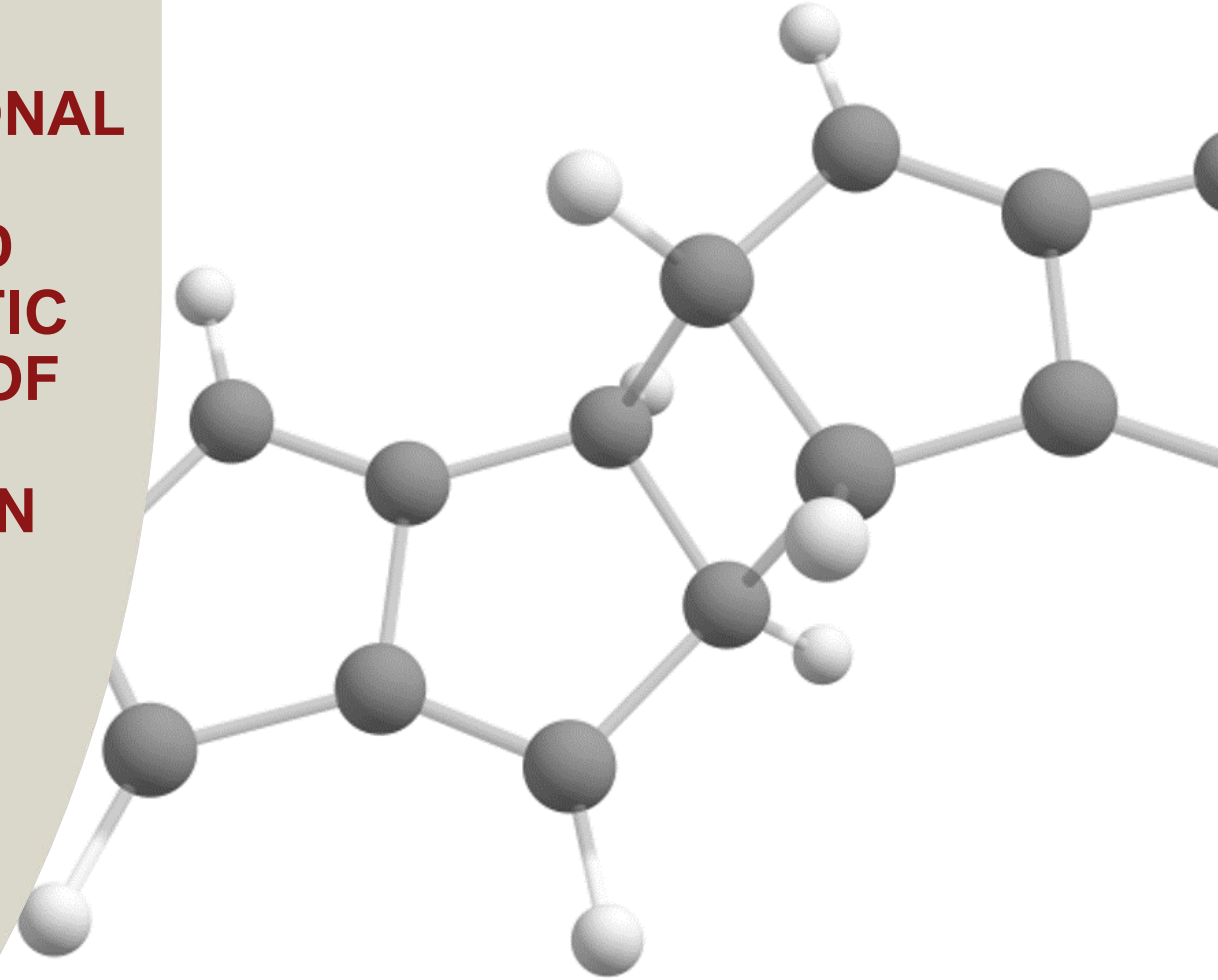
COMPUTATIONAL QUEST FOR CONTROLLED ANTIAROMATIC REACTIVITY OF PENTALENE DIMERIZATION



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Girona Seminar
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High …tteries†

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Molecular engineering of antiaromatic orangarin-based sensitizers for high-performance dye-sensitized solar-cell applications …ed

Swati Singh Rajput‡, Samarth Razdan‡, Tejendra Banana, Neelam Chandravanshi and Md Mehboob Alam*

Department of Chemistry, Indian Institute of Technology Bhilai, Durg, 491001, Chhattisgarh, India. E-mail: mehboob@iitbhilai.ac.in

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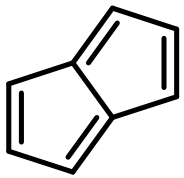
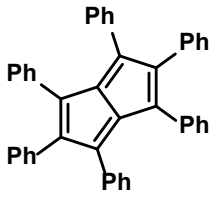
Introduction



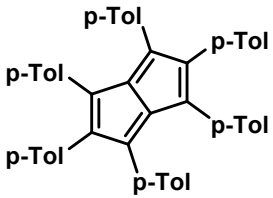
Pentalene (C_8H_6)

- 8 π-electrons → **ANTIAROMATIC**
- Not isolated neither spectroscopic observation until 1997
- Challenging molecule (high reactivity)

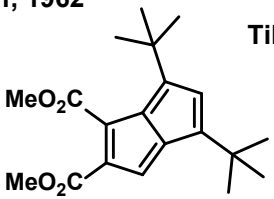
STERIC PROTECTION



Le Goff, 1962

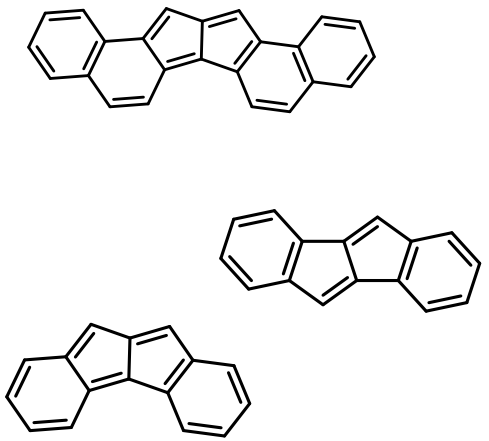


Tilley, 2009

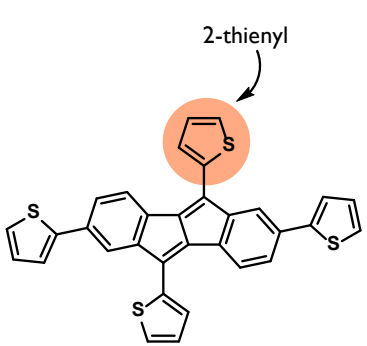


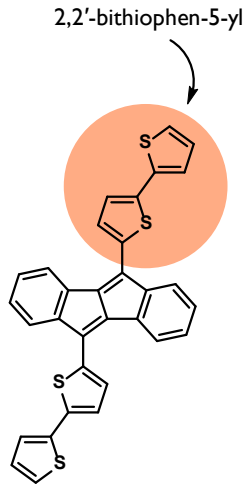
Hafner,1977

ELECTRONIC STABILIZATION

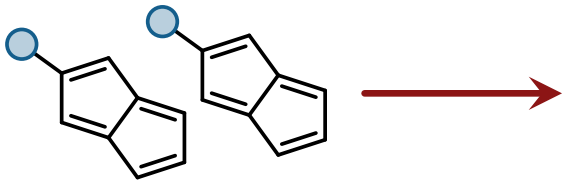


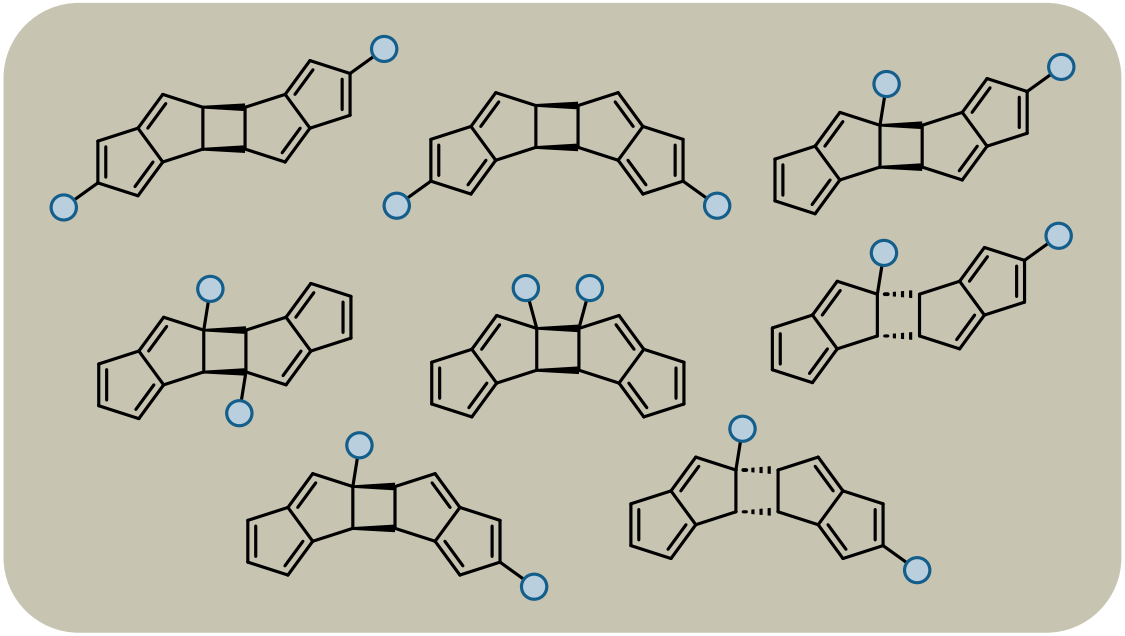
PUSH-PULL SUBSTITUTION

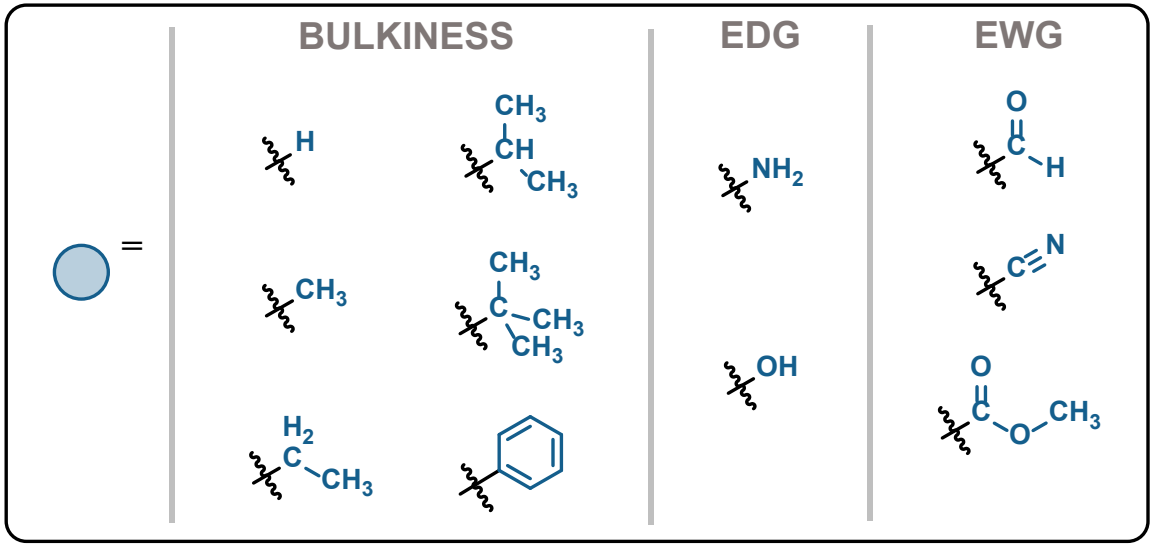




Procedure

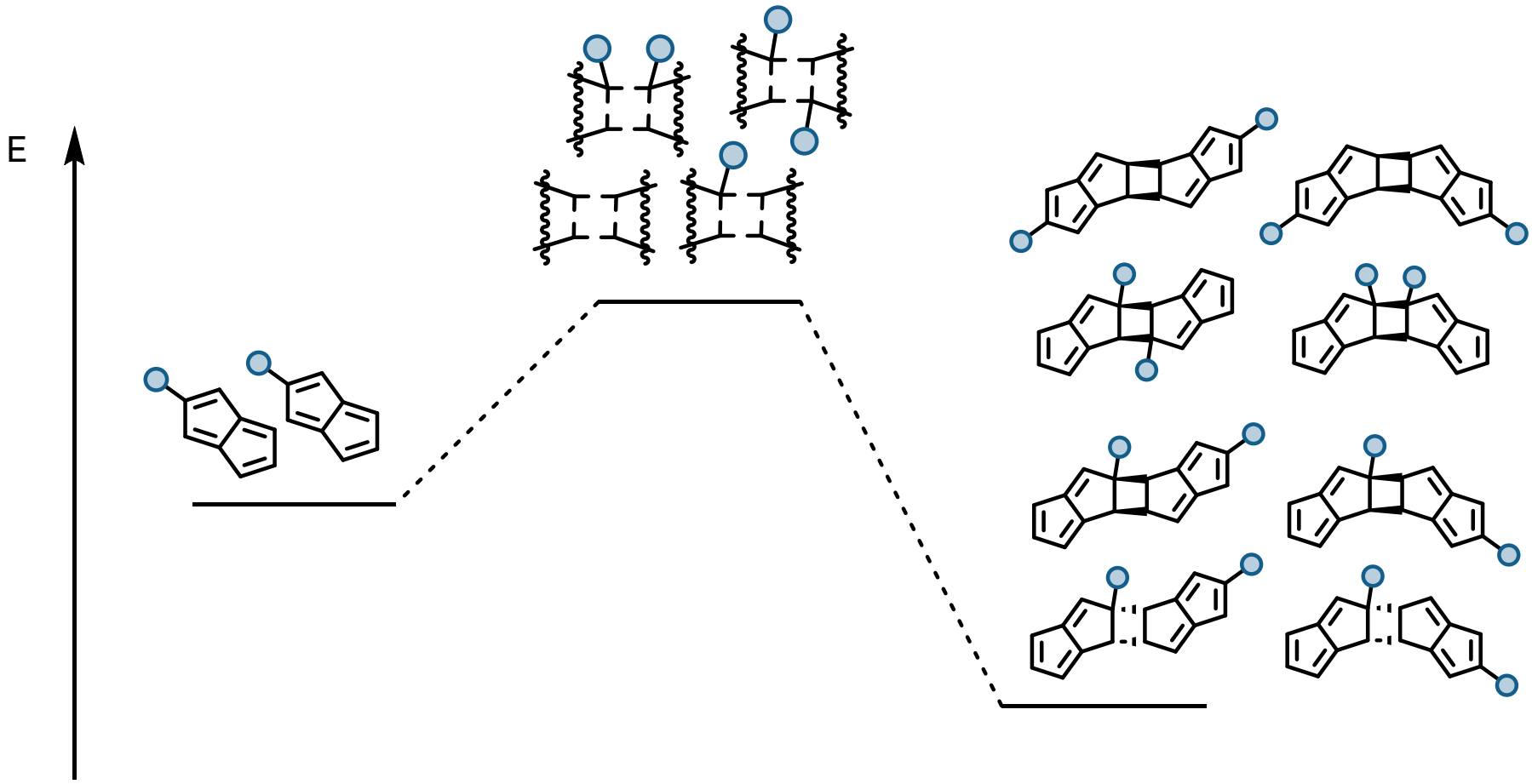




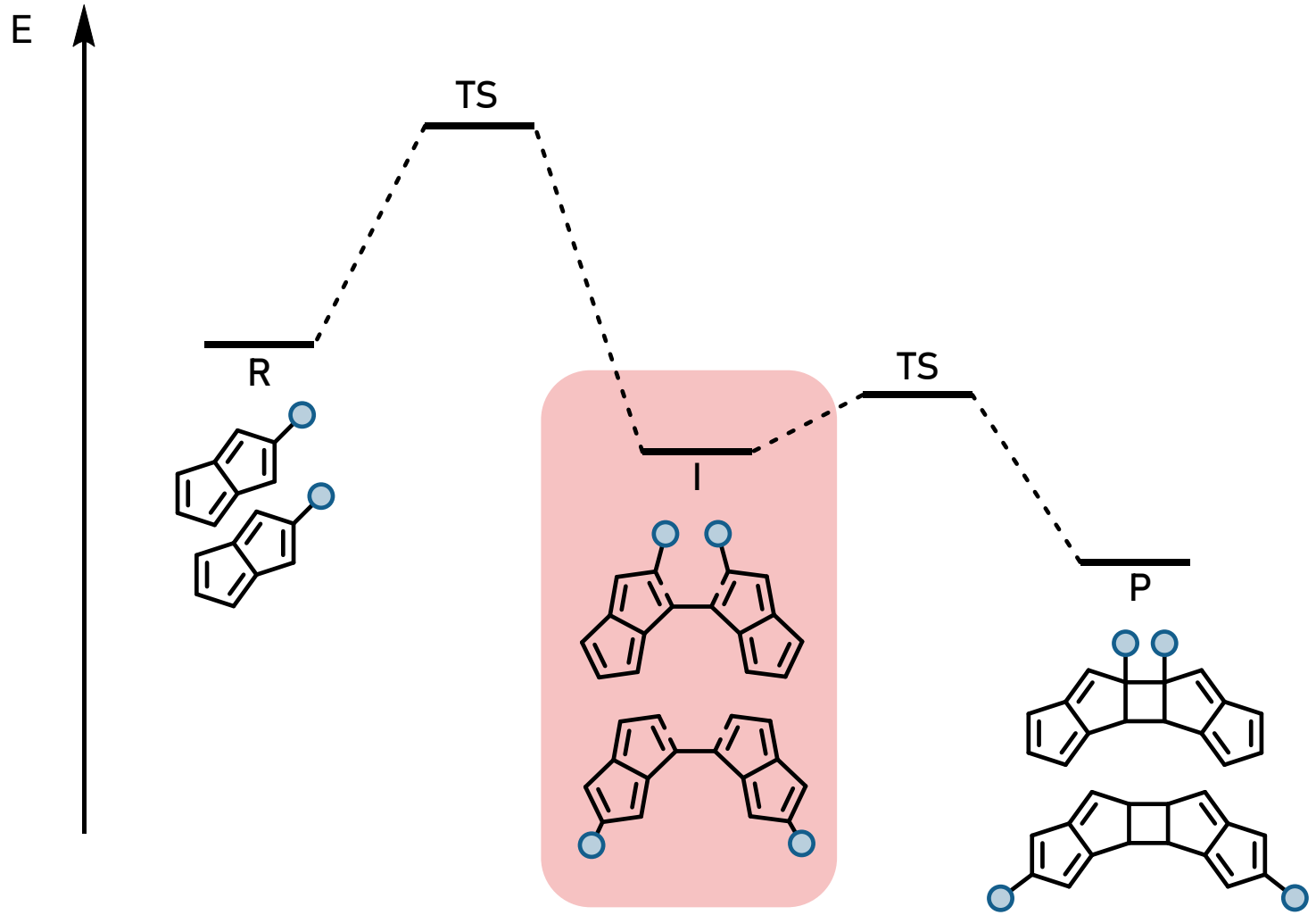


B3LYP-D3(BJ)/6-311++G(d,p)

Reaction framework



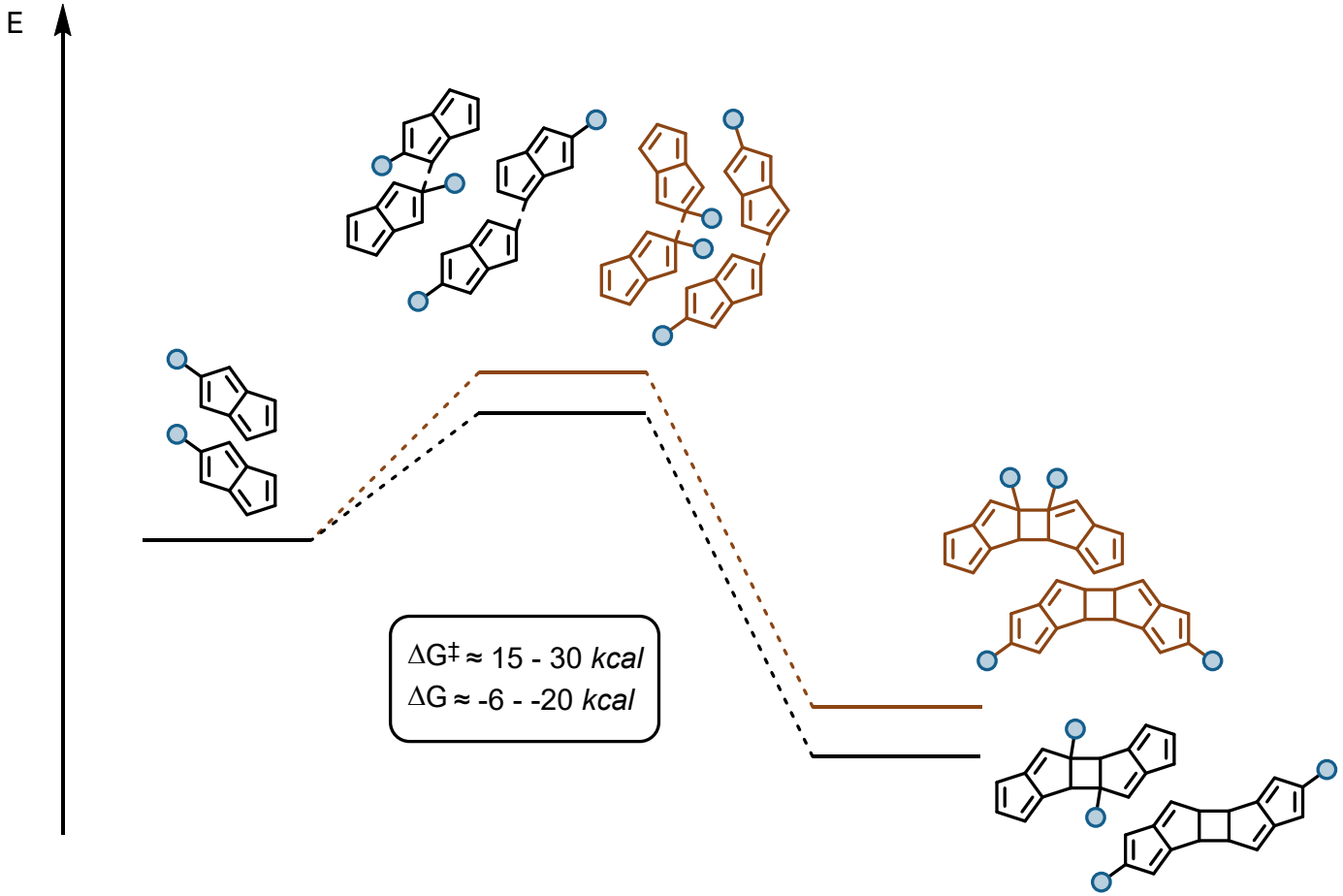
Reaction framework (special case)



Results

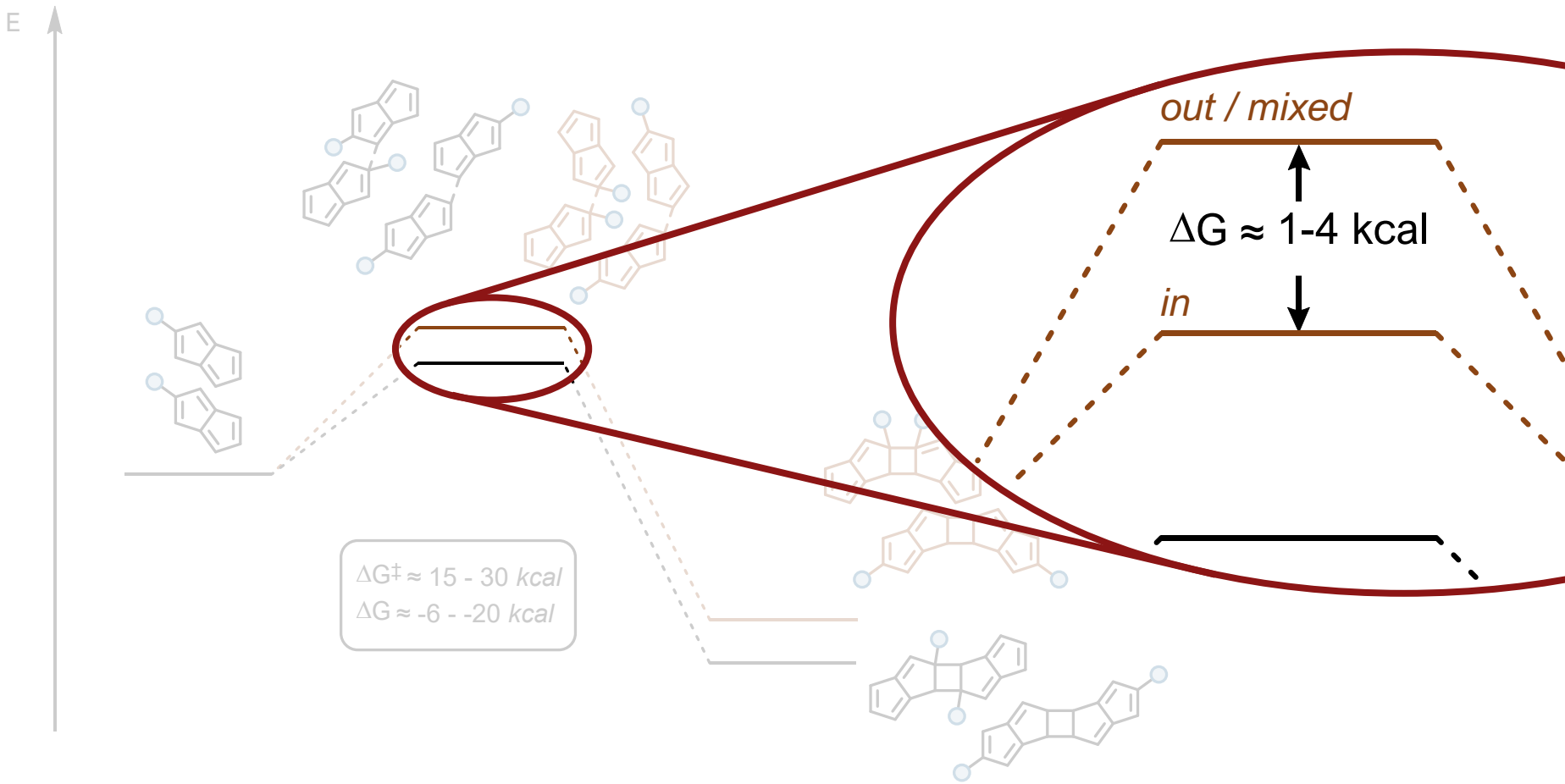
- TOPOLOGY
- ELECTRONIC EFFECTS
- BULKY EFFECTS

Results – TOPOLOGY



» *cis* conformation tends to have higher energy barriers than *trans* ones (≈ 3-4 *kcal*).

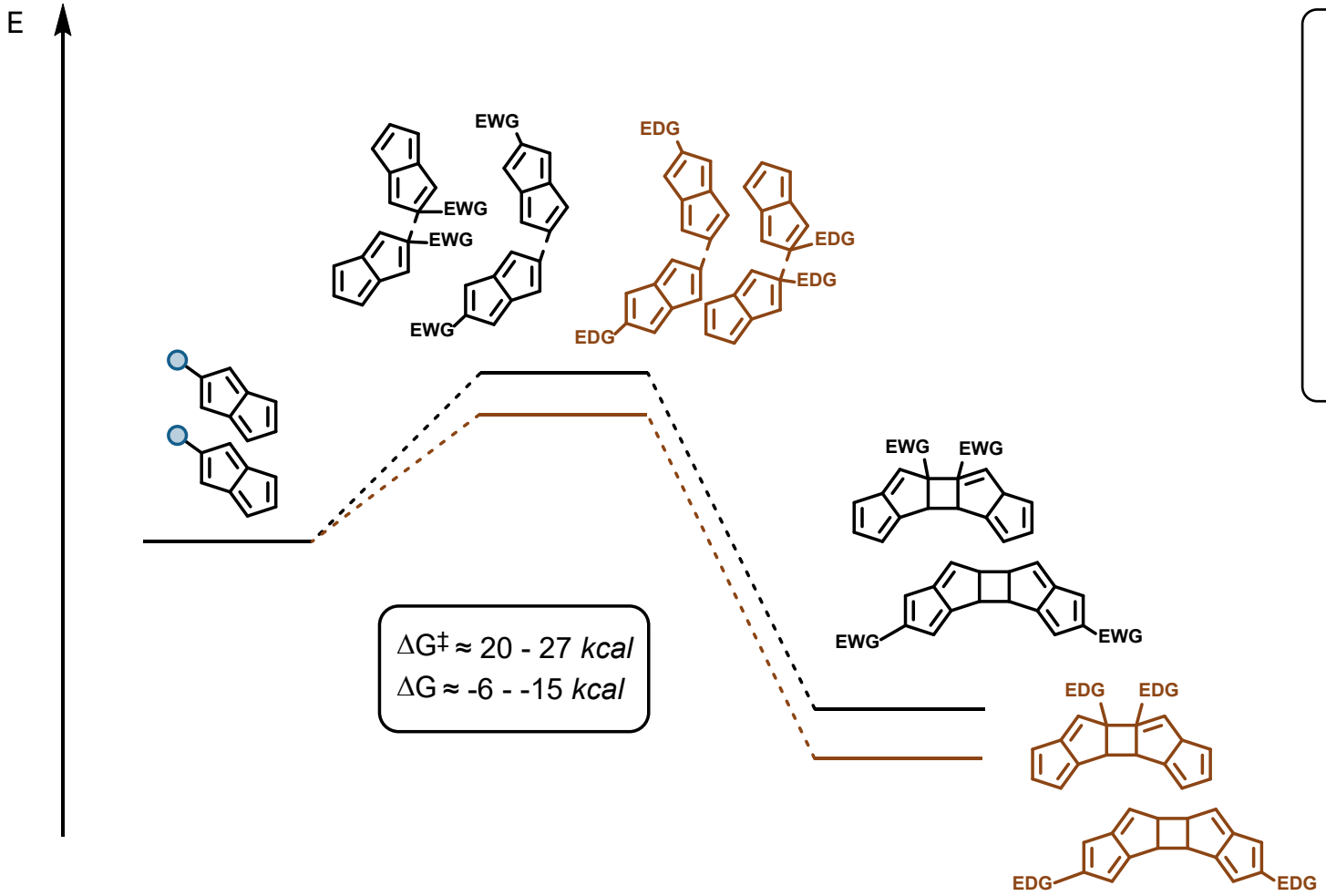
Results – TOPOLOGY

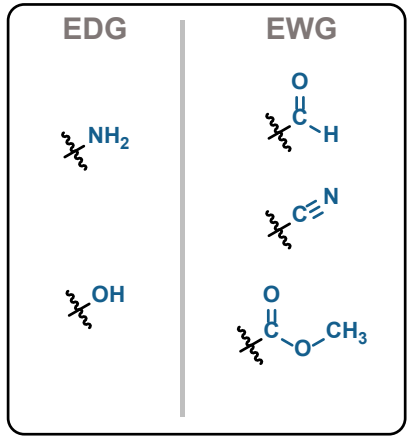


» *cis* conformation tends to have higher energy barriers than *trans* ones (≈ 3-4 *kcal*).

» The *out* and *mixed* orientation of the substituent results in higher energy barriers and greater stability (≈ 4-5 *kcal*).

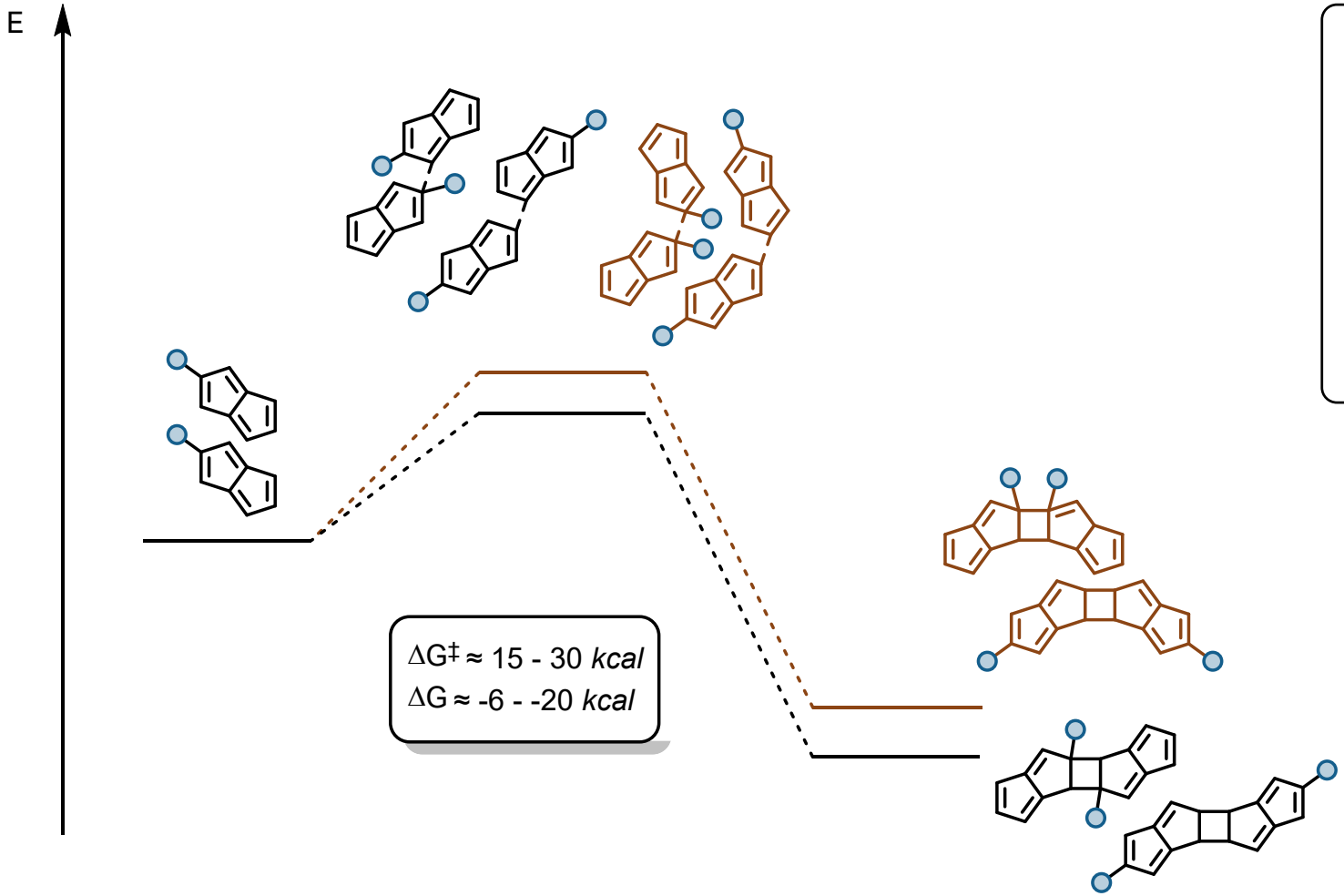
Results – ELECTRONIC EFFECTS

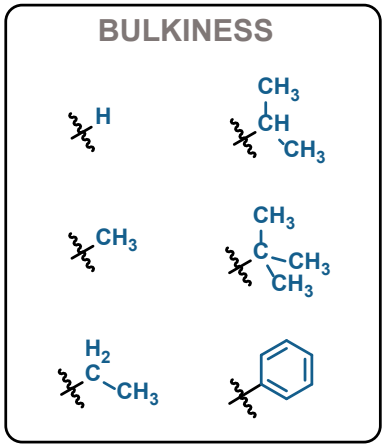




» *Electron-withdrawing groups* (EWG) tend to increase energy barriers (≈ 1-4 *kcal*), whereas *electron-donating groups* (EDG) lead to more stable systems (≈ 5 *kcal*).

Results – BULKY EFFECTS





» The results generally follow the expected trends based on steric hindrance, although some deviations are observed (i.e. *Ph*), indicating that this effect alone is not sufficient to explain the behavior.

Acknowledgements

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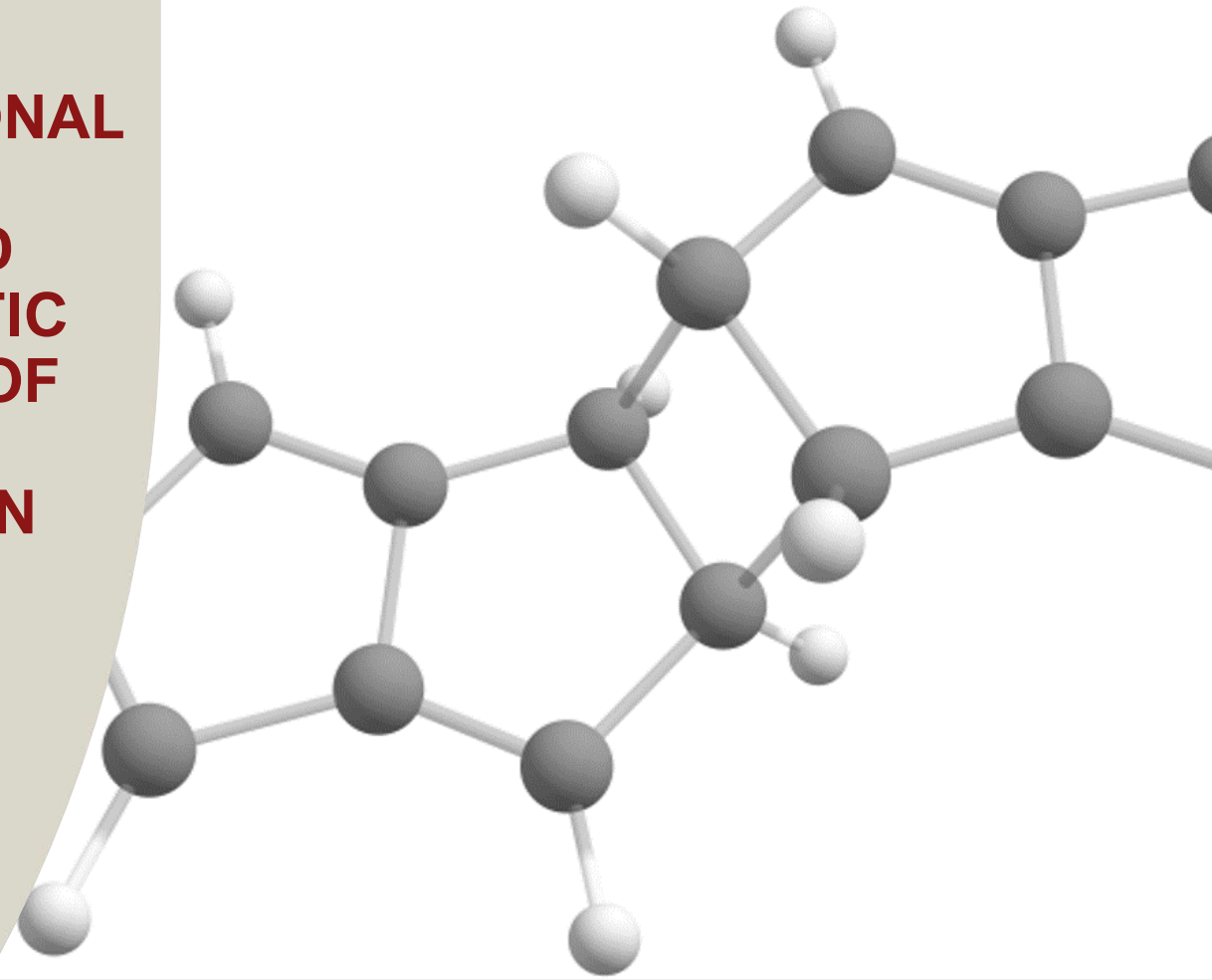

Thank you!

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