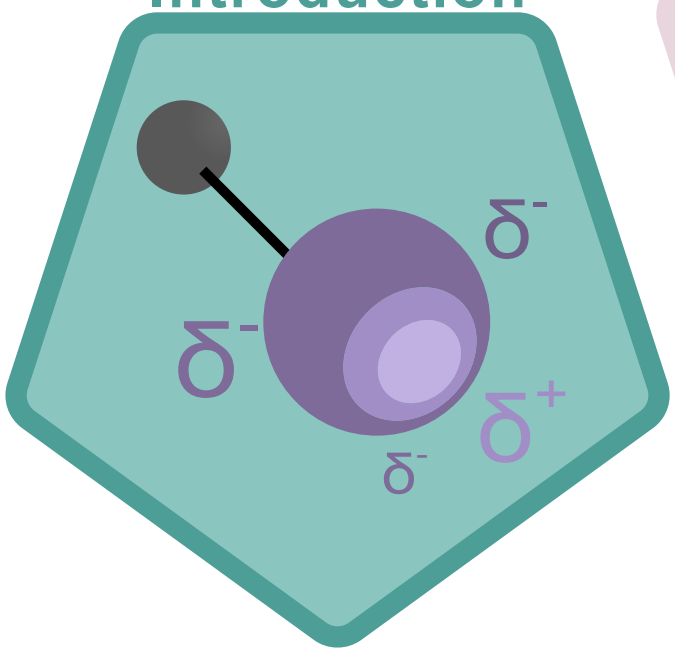
MANCHESTER 1824
The University of Manchester

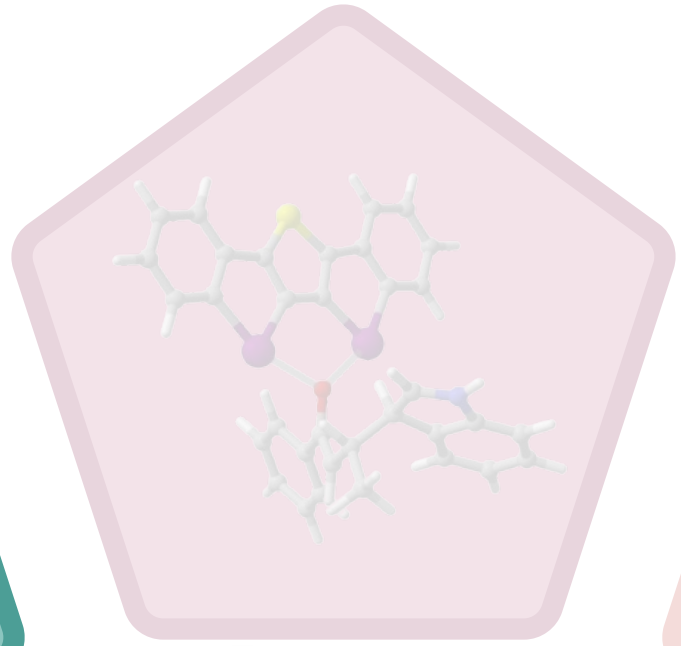
Computational Study on Bidentate Hypervalent Iodine-Based Catalysis

James O'Brien

Outline

Introduction





Results

Conclusions

1 Introduction: Halogen Bonding

Hydrogen bond:

LP (O) → BD* (Y^+-H)

Halogen bond (XB):

LP (O) → BD* (C-I)

T. Clark, M. Hennemann, J. S. Murray, P. Politzer, *J. Mol. Model.* **2007**, *13*, 291–296.

Introduction: Catalyst Rationale

Monovalent

<

Bivalent

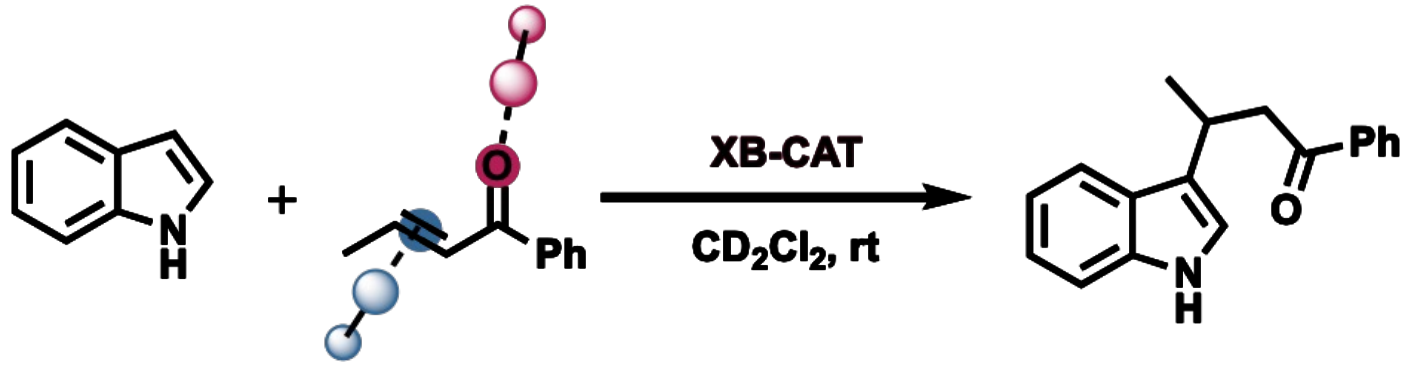
Monodentate

<

Bidentate

F. Heinen, E. Engelage, A. Dreger, R. Weiss, S. M. Huber, *Angew. Chem. Int. Ed.* **2018**, *57*, 3830–3833.
N. Melnyk, M. R. Garcia, C. Trujillo, *ACS Catal.* **2023**, 15505–15515.

3 Introduction: Reaction (Michael Addition)



J.-P. Gliese, S. H. Jungbauer, S. M. Huber, *Chem. Commun.* **2017**, *53*, 12052–12055.
R. Robidas, C. Y. Legault, *Angew. Chem.* **2023**, *135*, DOI 10.1002/ange.202301190.

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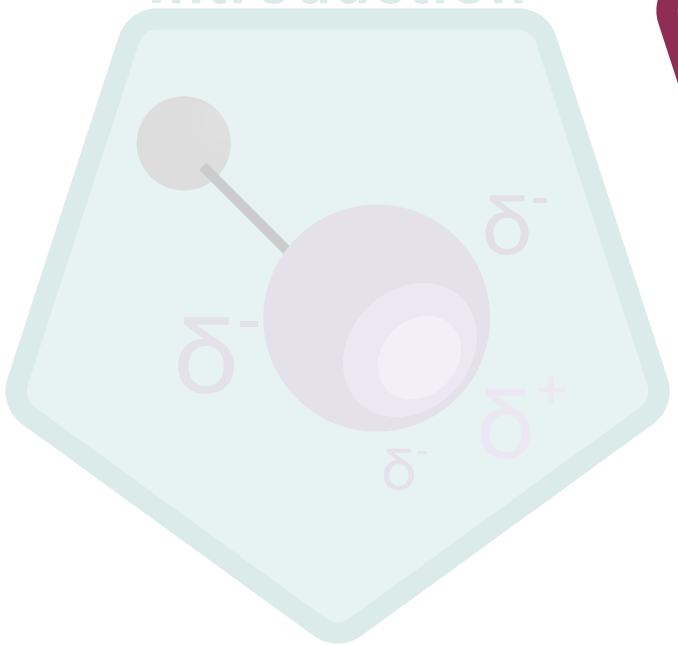

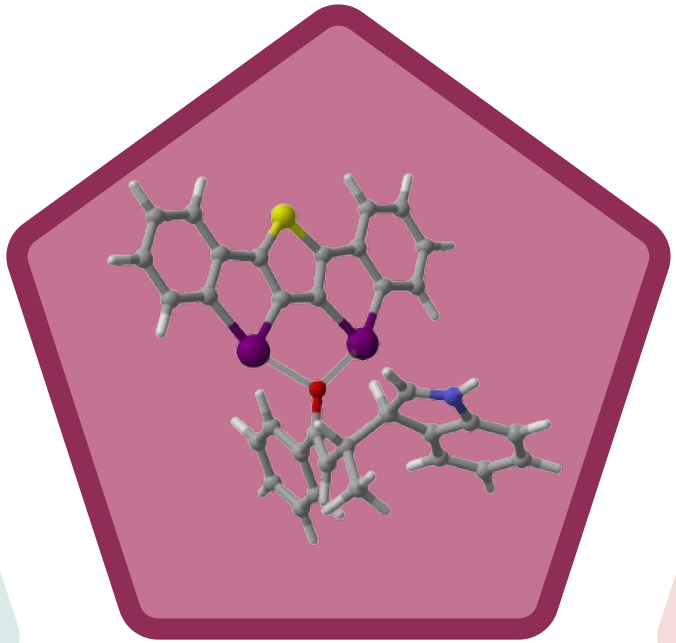

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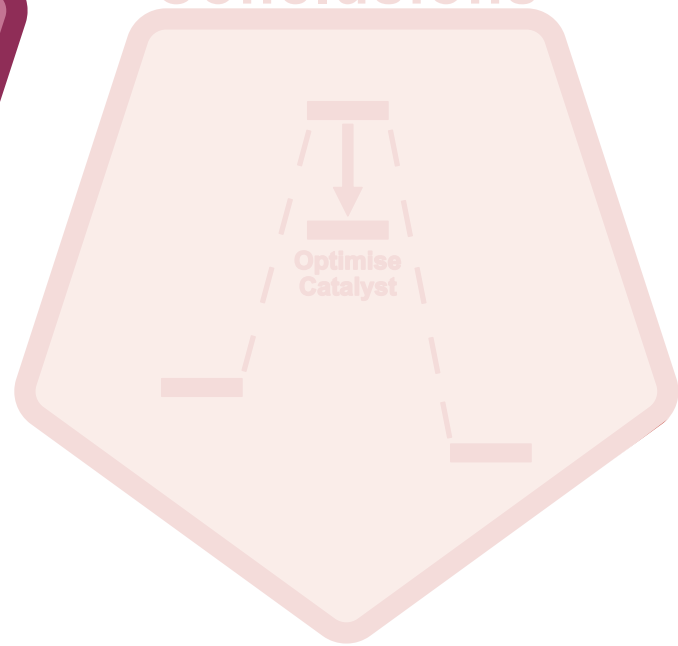


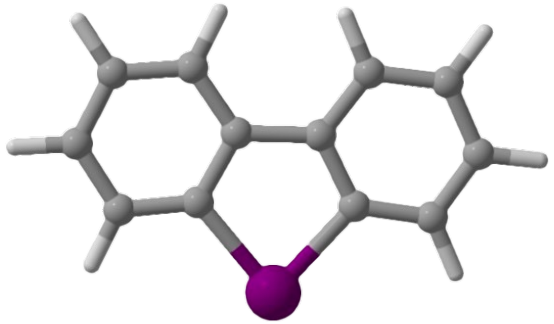
Results: Binding-Mode Investigation

CAT1

CAT2

ωb97xd/def2svp // ωb97xd/def2tzvp

Results: Binding-Mode Investigation



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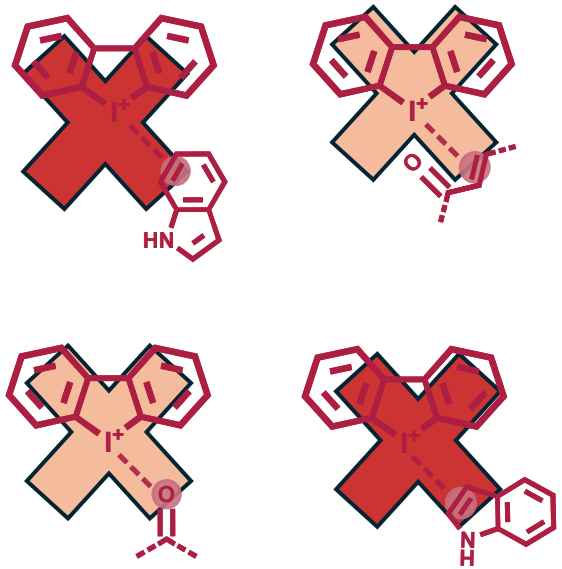
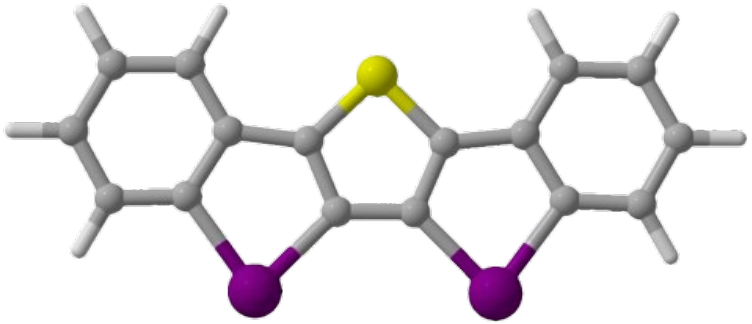
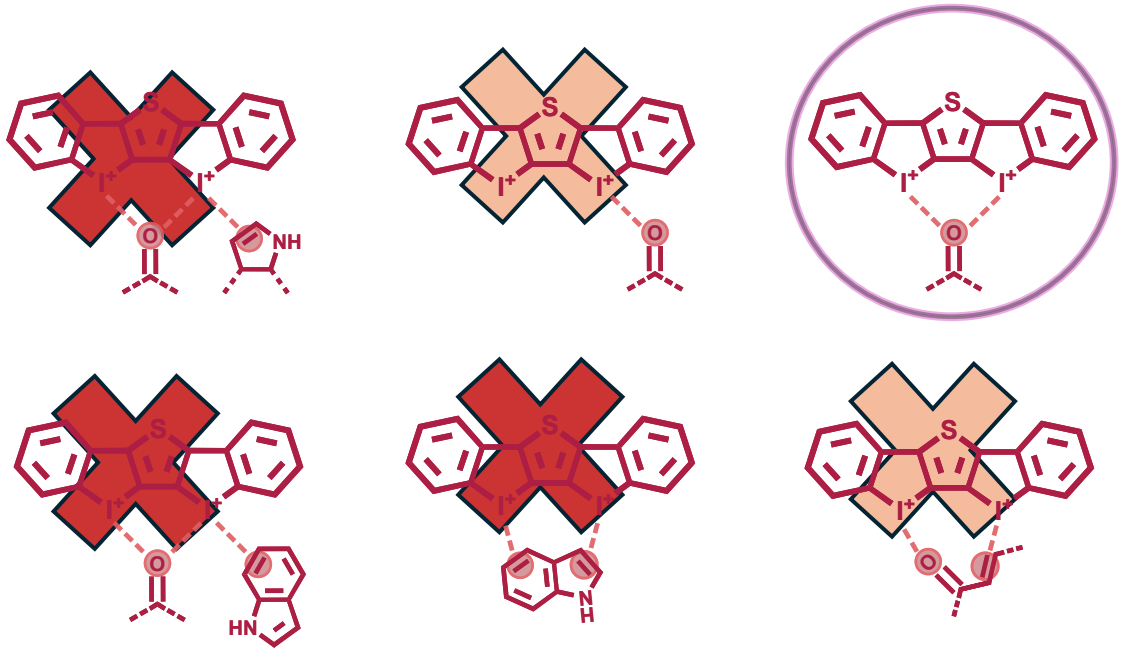




CAT2



ωb97xd/def2svp // ωb97xd/def2tzvp

Results: Functionalisation

ortho

ortho + para +

H

EWG CF_3 NO_2 CN

EDG CH_3 *t*Bu

Mix OH OMe

EWGs CF_3 NO_2 CN

H CF_3

ωb97xd/def2svp // ωb97xd/def2tzvp

Results: General Trends (–ΔG‡)

ωb97xd/def2svp // ωb97xd/def2tzvp

4 Results: Non-Covalent Interactions

Low $\nabla^2\rho$
$0 < \rho_{BCP} < 1$

Non-Covalent Interactions

ωb97xd/def2svp // ωb97xd/def2tzvp

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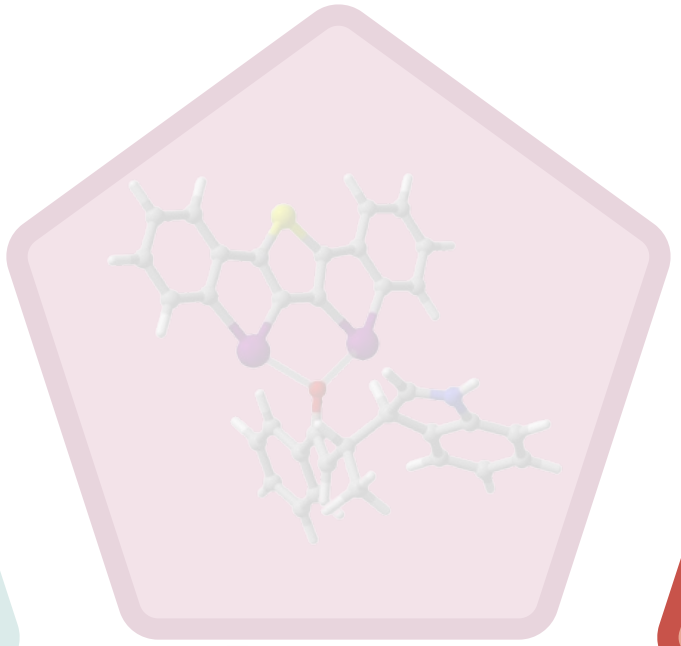

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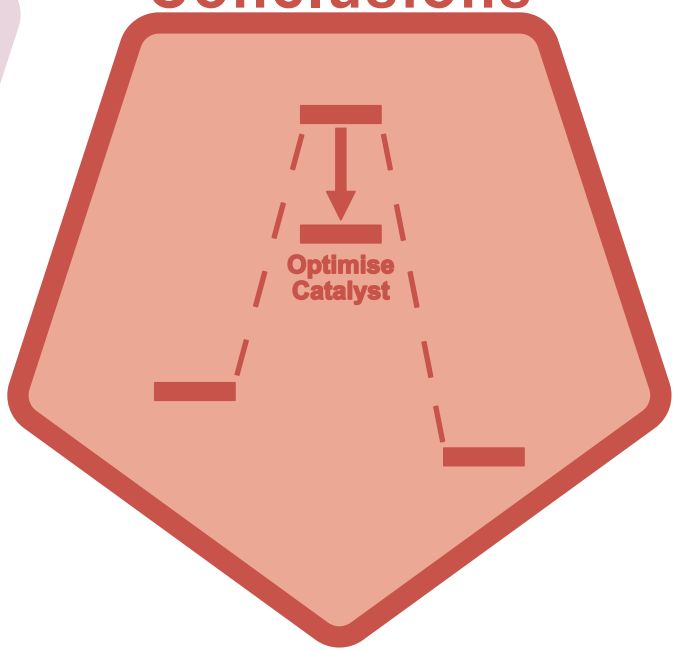

1 Conclusions

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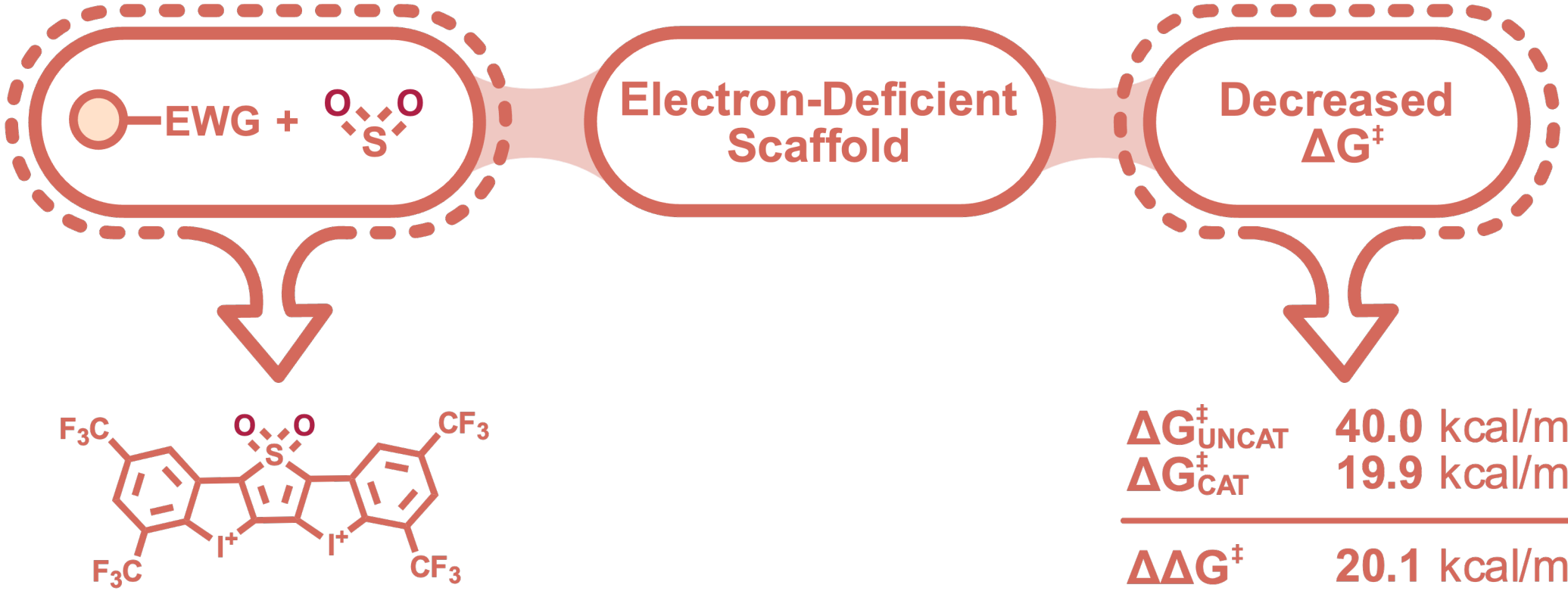

Thank You for listening & Thanks to:

People

Dr. Cristina Trujillo
Dr. Michael James
Dr. Iñigo Iribarren
Nika Melnyk
Rico Shing Lee
Tim Renningholtz
Diana Bura
Marina Díaz
Maxime Ferrer
Mauno Lius
Ethan Lim
Prof. Alberto Cruz

Organisations

University of Manchester
Computational Shared Facility
IT Services