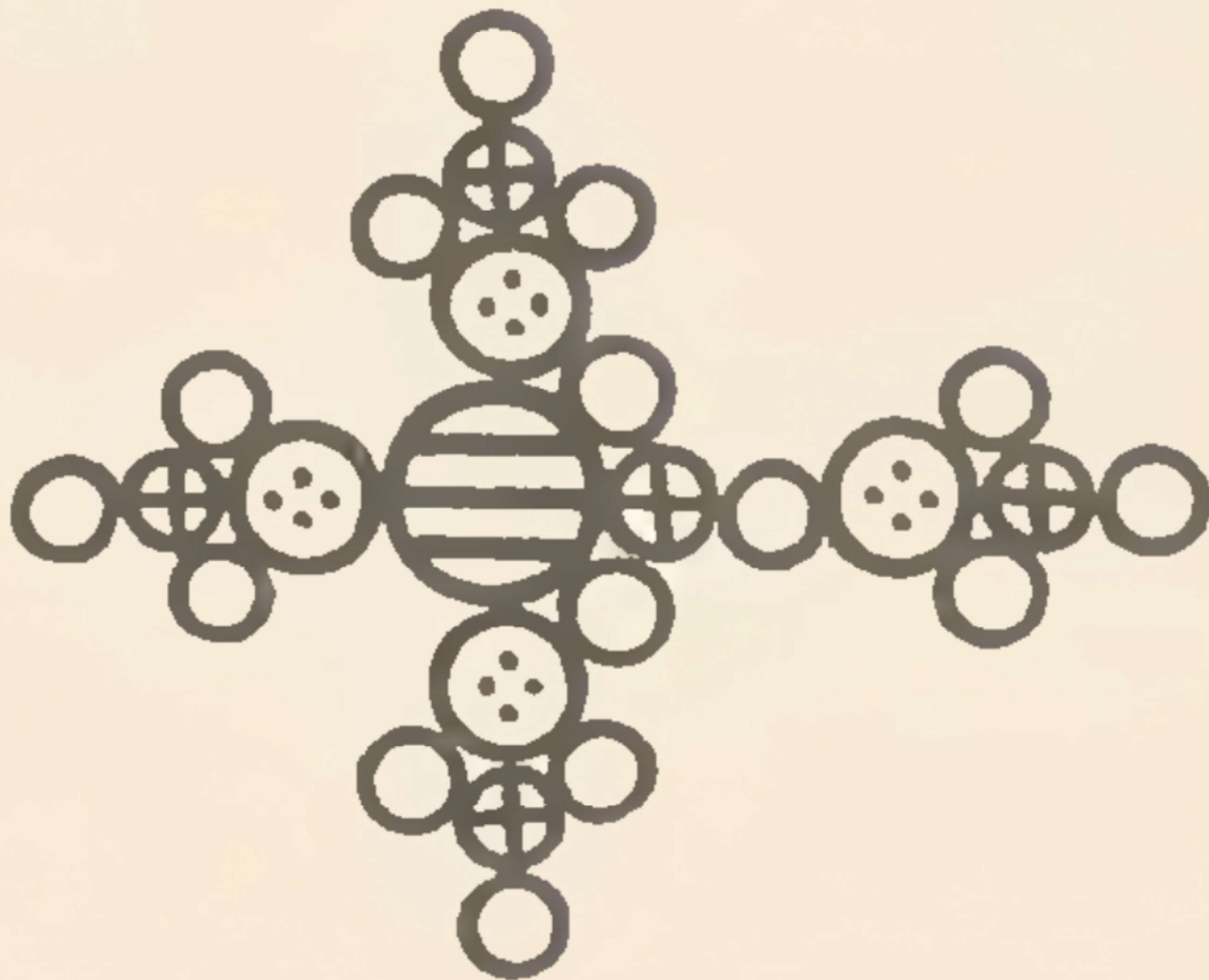


# **Indescribable structure: finding words for the future**

Jonathan M Goodman

Department of Chemistry,  
University of Cambridge



A  
NEW SYSTEM  
OF  
CHEMICAL PHILOSOPHY.

---

PART I.

---

BY  
JOHN DALTON.

---

REPRODUCED IN FACSIMILE

BY

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# ELEMENTS

Platz 4

## *Simple*



## *Binary*



## *Ternary*



*Quaternary*

30



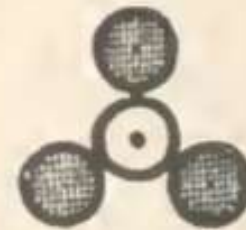
31



32



33

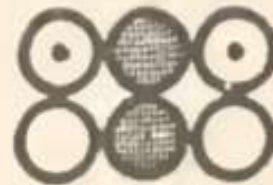


*Quinquenary & Sextenary*

34

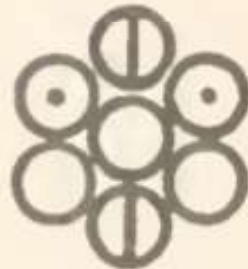


35

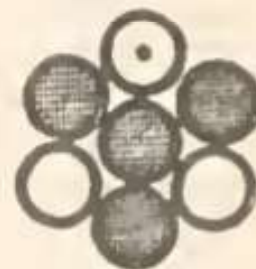


*Septenary*

36



37

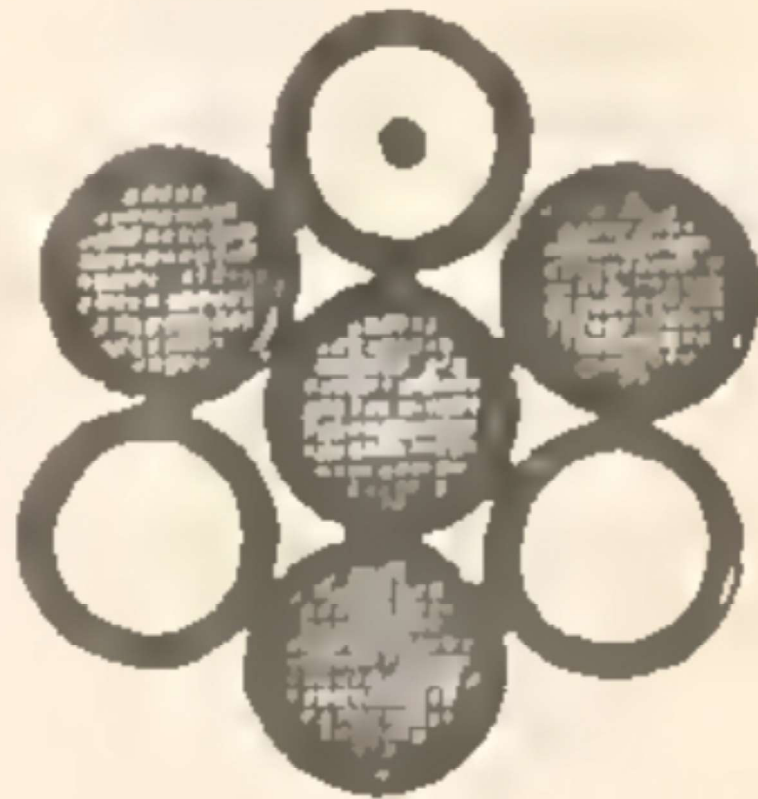


WHEN any body exists in the elastic state, its ultimate particles are separated from each other to a much greater distance than in any other state; each particle occupies the centre of a comparatively large sphere, and supports its dignity by keeping all the rest, which by their gravity, or otherwise are disposed to encroach up it, at a respectful distance.

An atom of sugar,

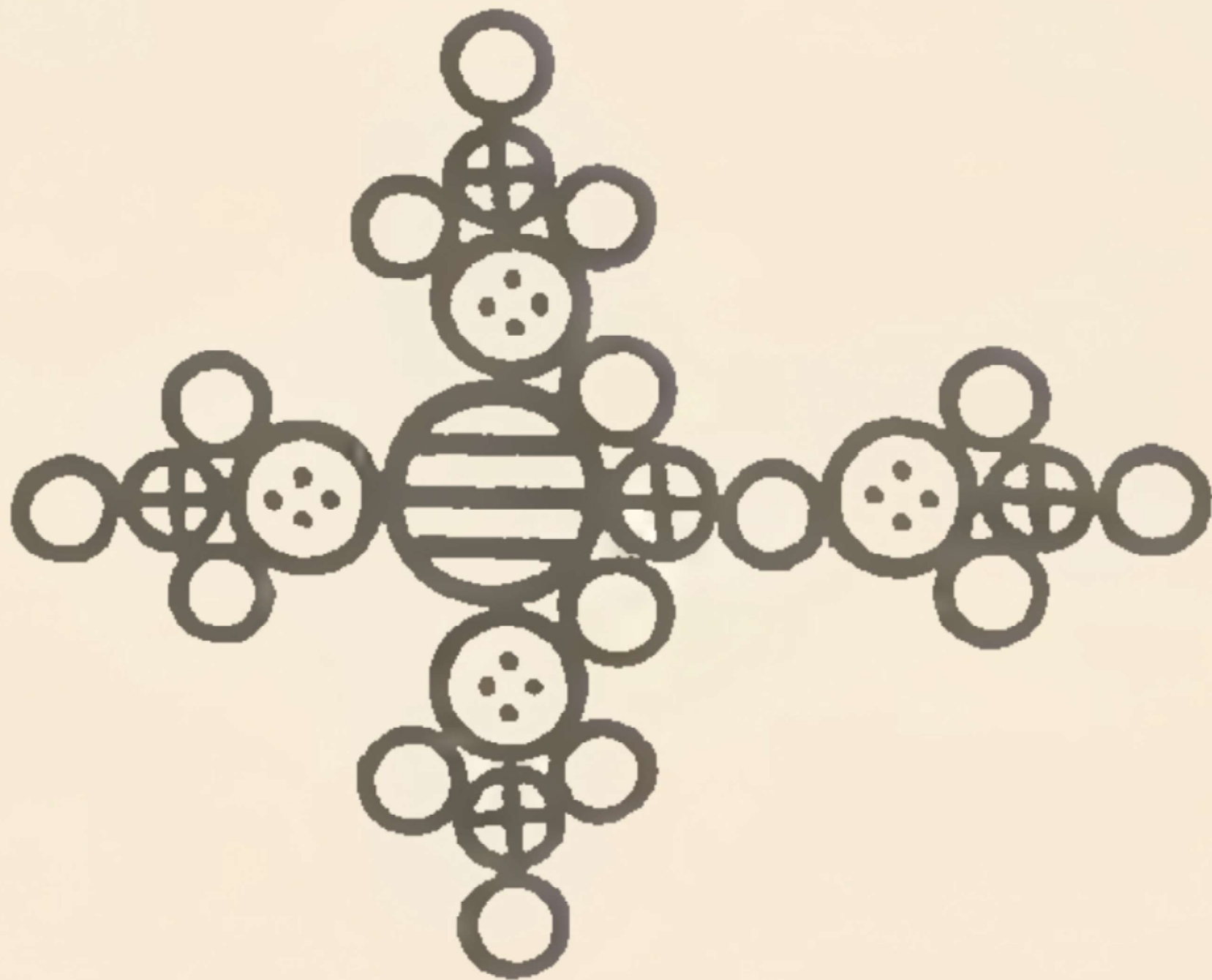
1 alcohol + 1 carbonic acid

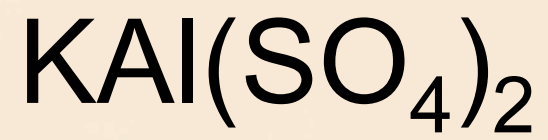
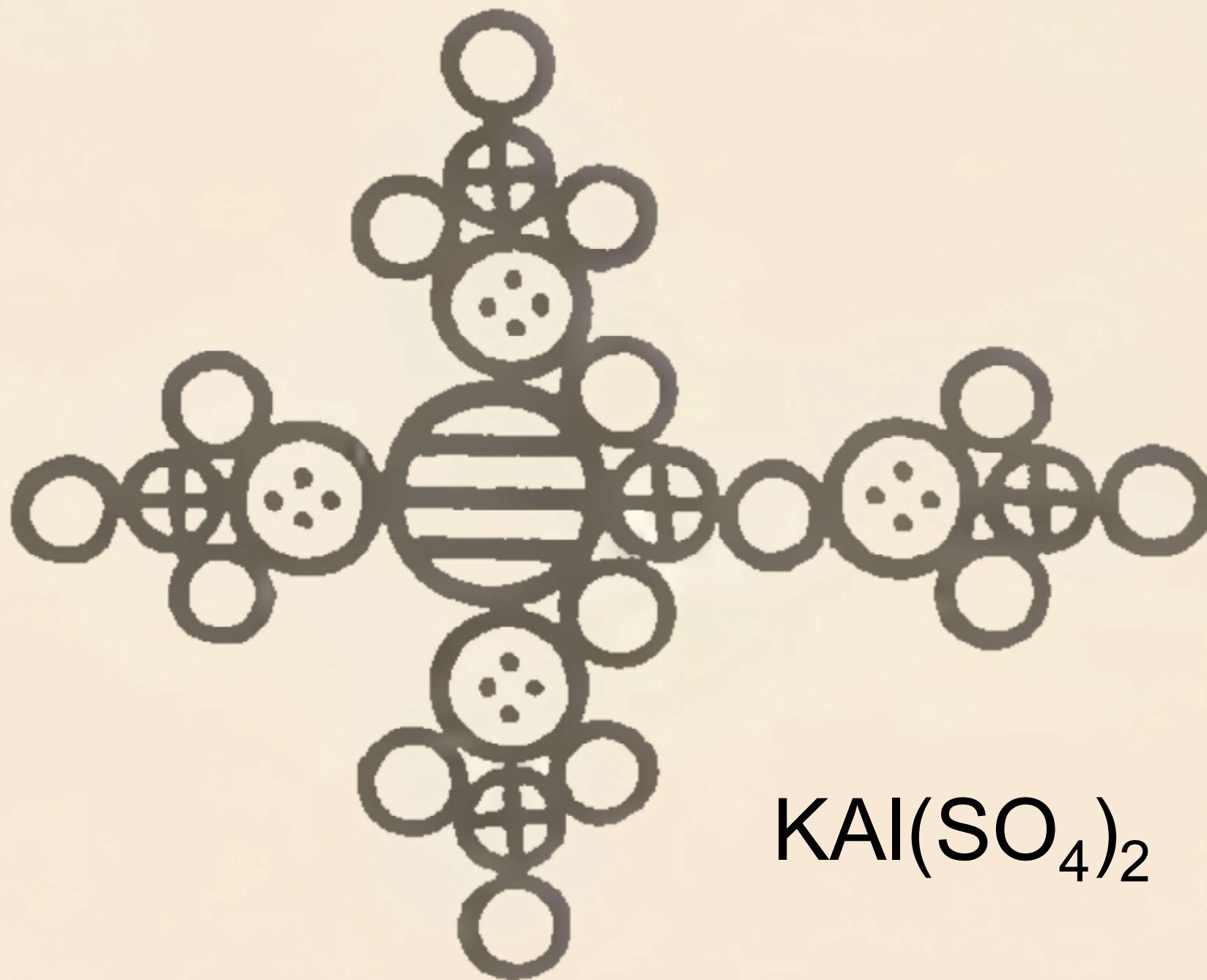
*Septemary*



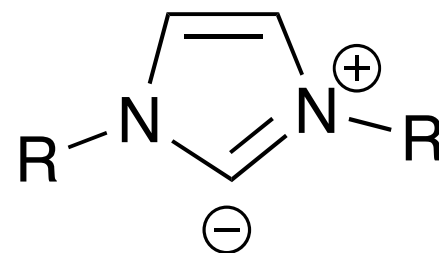
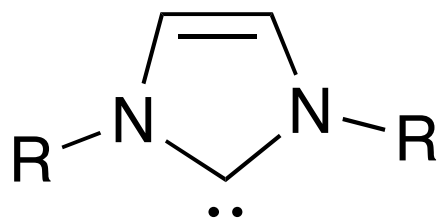
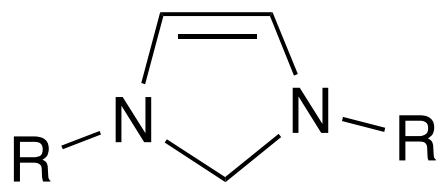


Now it is one great object of this work, to shew the importance and advantage of ascertaining *the relative weights of the ultimate particles, both of simple and compound bodies, the number of simple elementary particles which constitute one compound particle, and the number of less compound particles which enter into the formation of one more compound particle.*

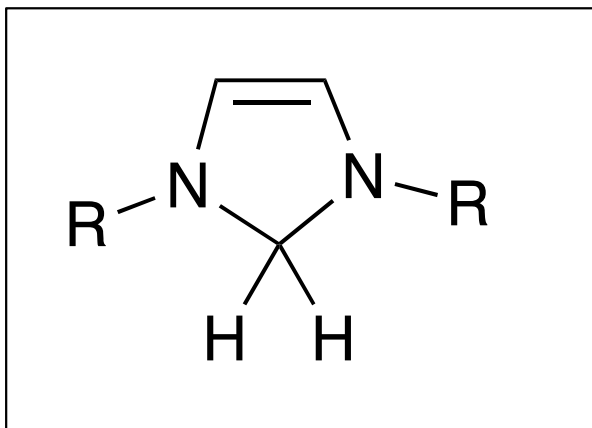
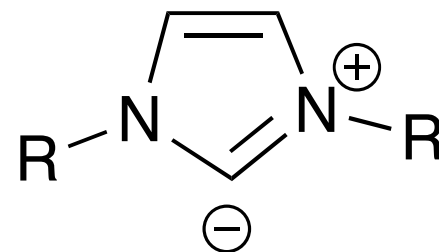
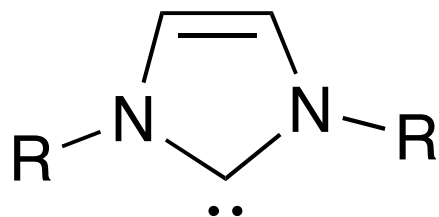
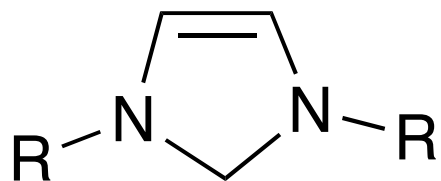




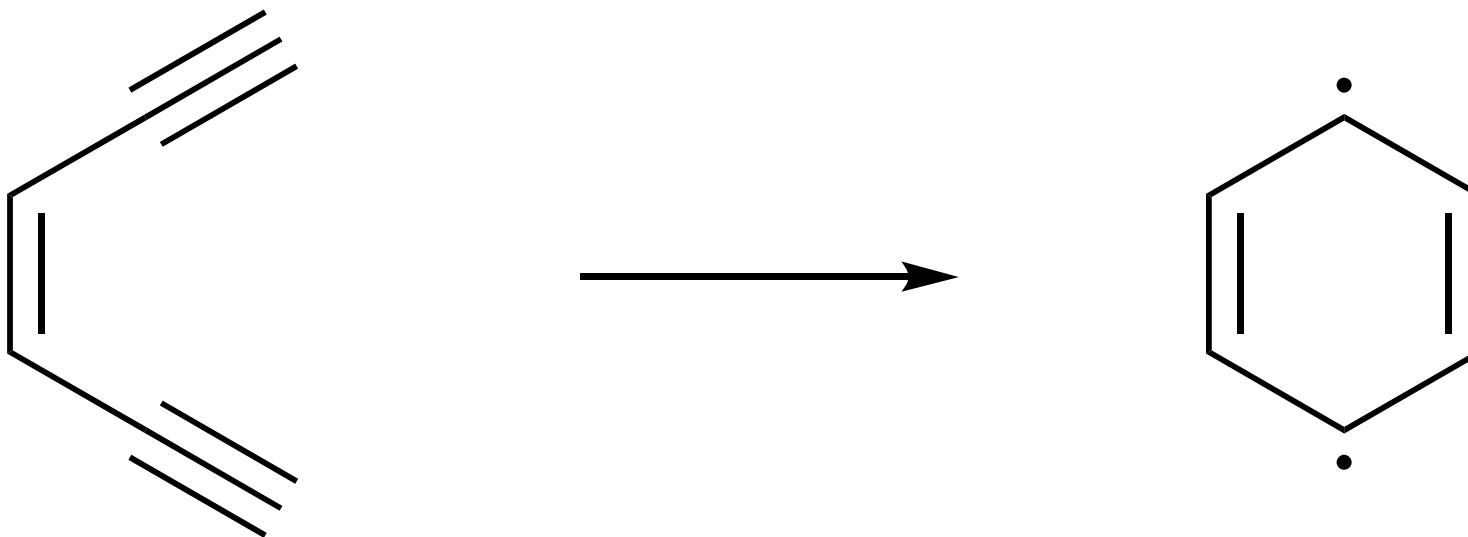
## N-Heterocyclic Carbenes



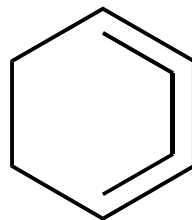
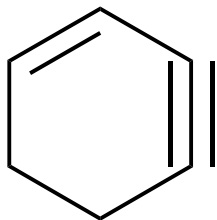
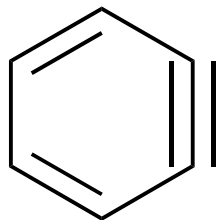
## N-Heterocyclic Carbenes



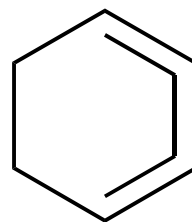
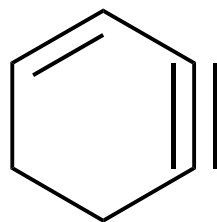
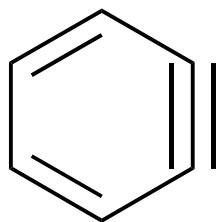
## Bergman Cyclisation



Benzyne

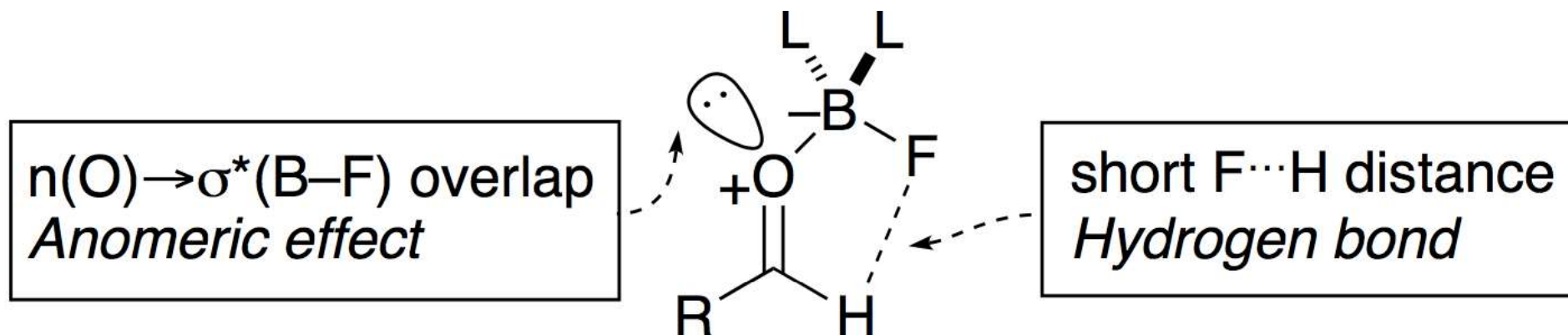


Benzyne



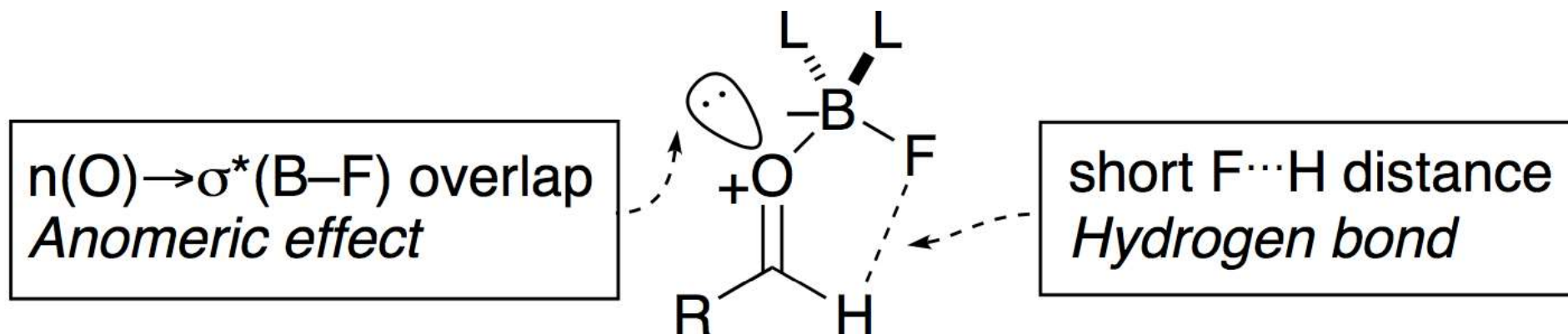
William C Shakespeare **DOI:** 10.1021/ja00179a050



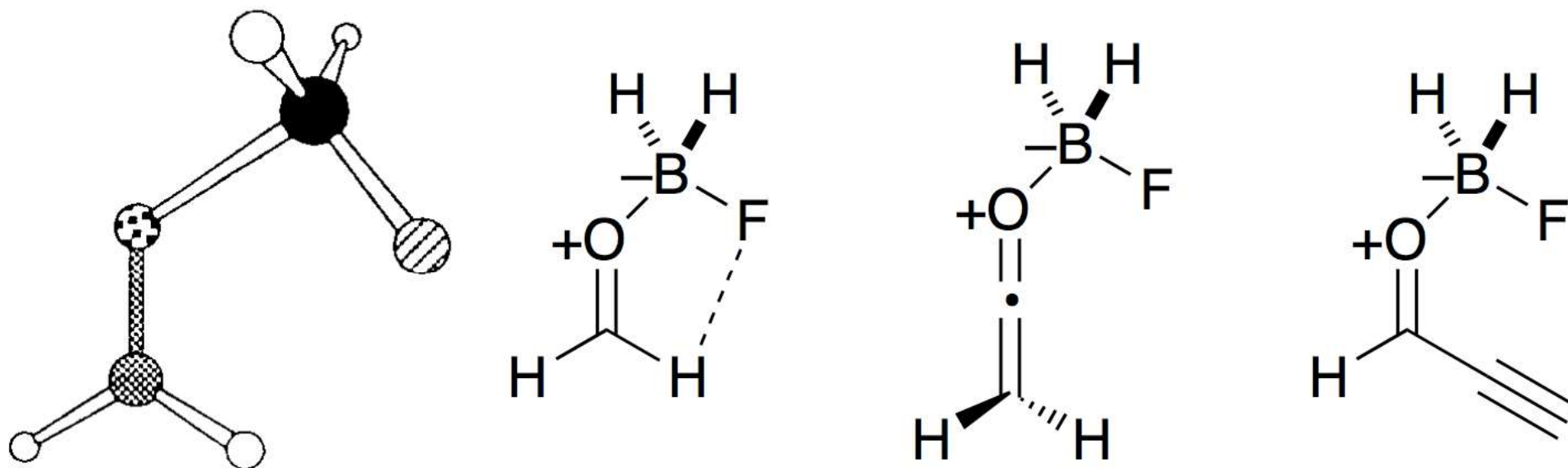


Carbonyl  $\text{H}_2\text{BF}$  complexes: anomeric effect and hydrogen bond

M. D. Mackey, J. M. Goodman *Chem. Comm.* 1997, 2383-2384.  
DOI: [10.1039/a706288e](https://doi.org/10.1039/a706288e)

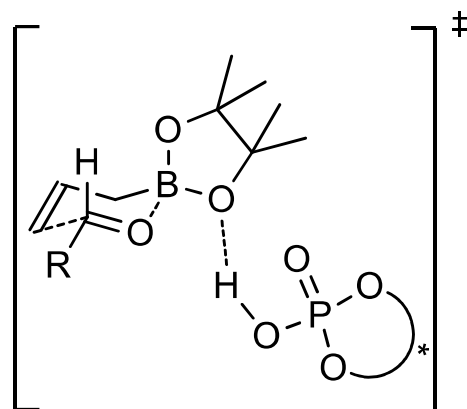
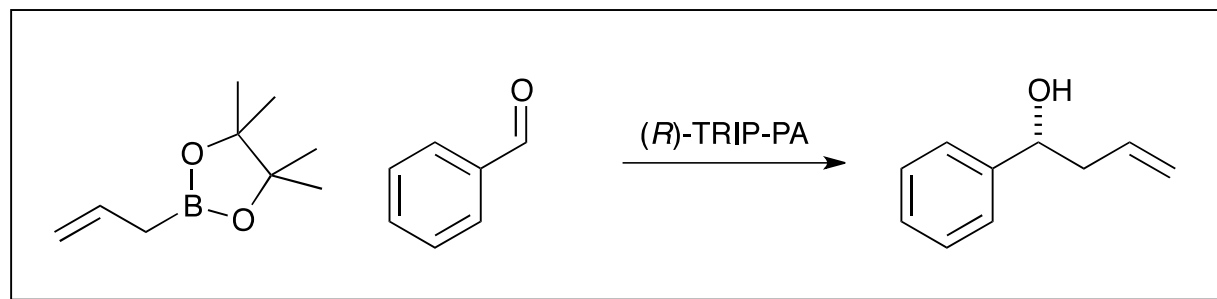
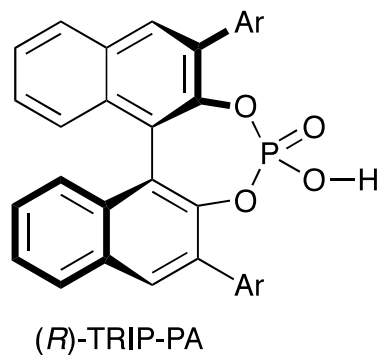


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 DOI: [10.1039/a706288e](https://doi.org/10.1039/a706288e)

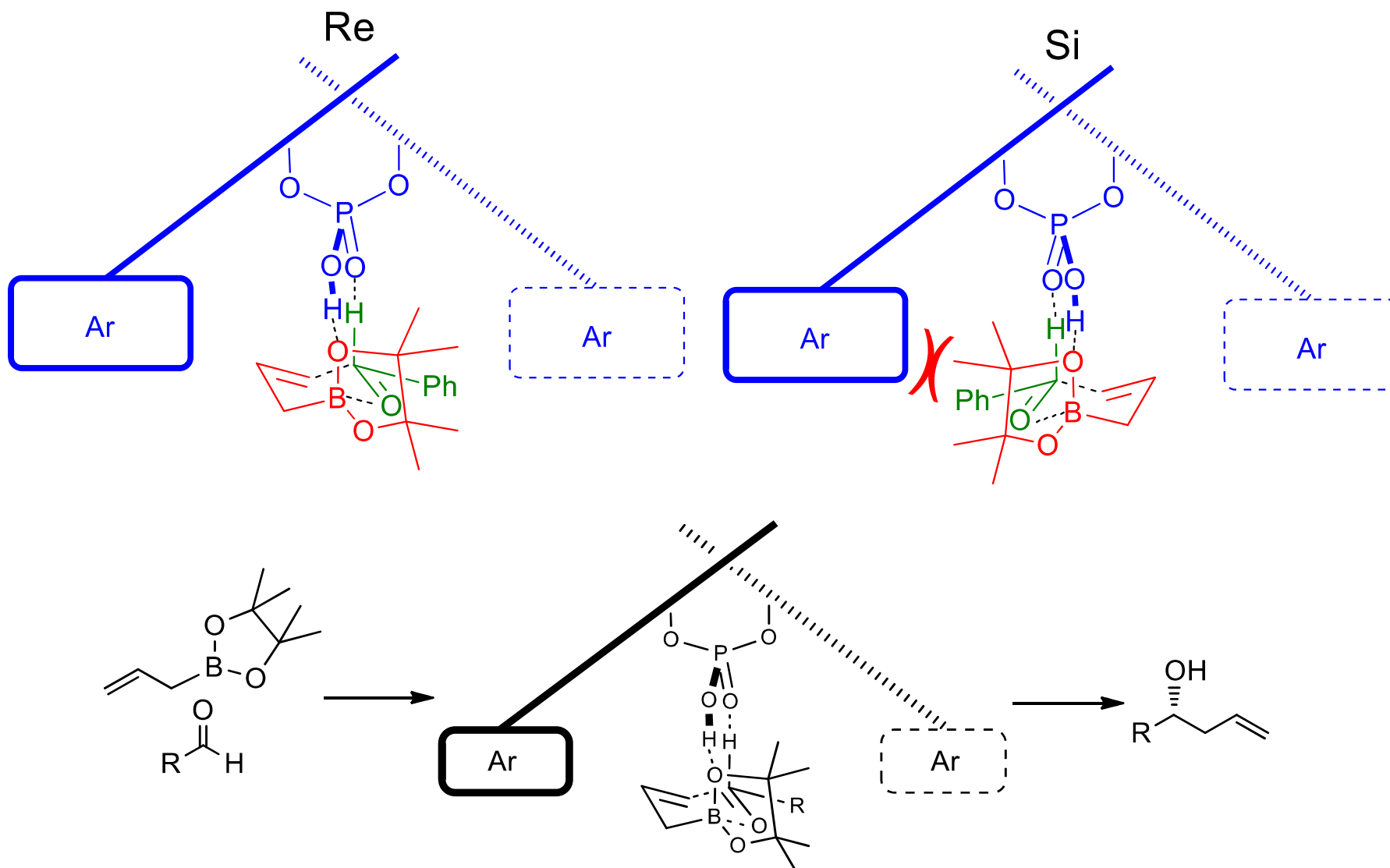
# Allylboration of Aldehydes

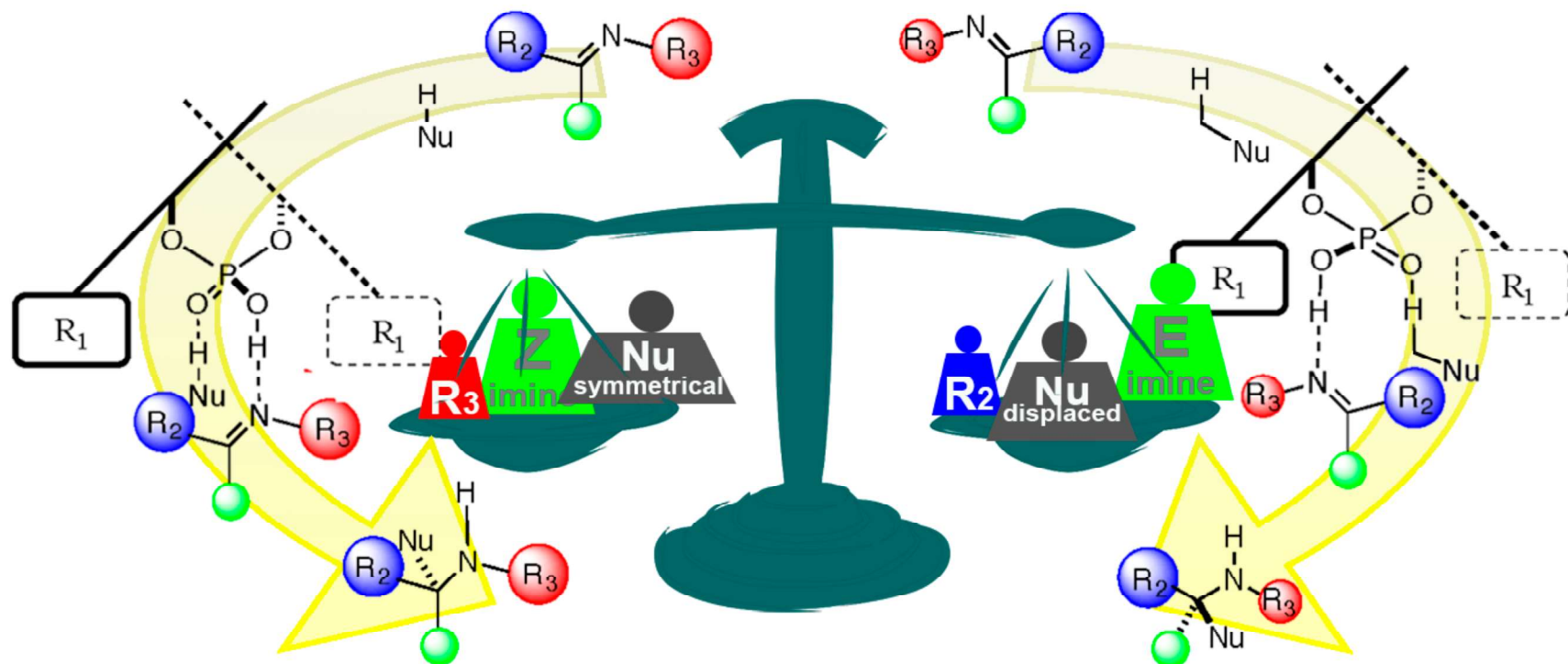


Antilla's Model

R	Yield	ee
Ph	99 %	98 %
4-ClC <sub>6</sub> H <sub>4</sub>	98 %	99 %
1-naphthyl	93 %	98 %

# Allylboration Model



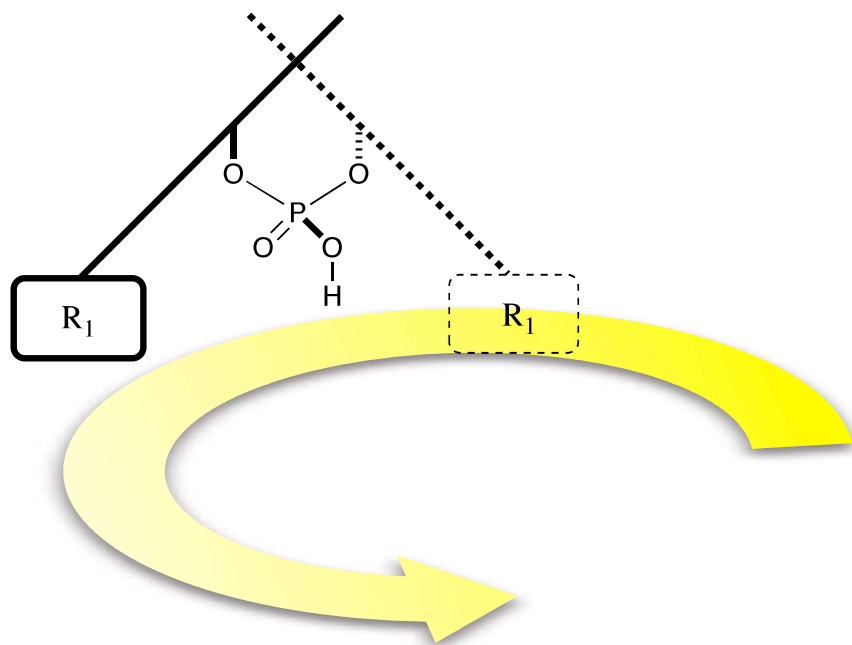


# A Practical Guide for Predicting the Stereochemistry of Bifunctional Phosphoric Acid Catalyzed Reactions of Imines

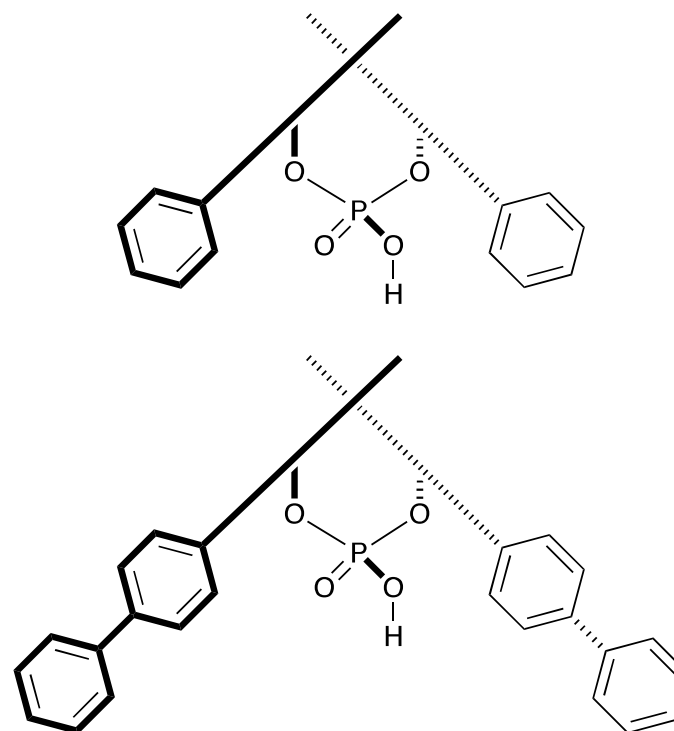
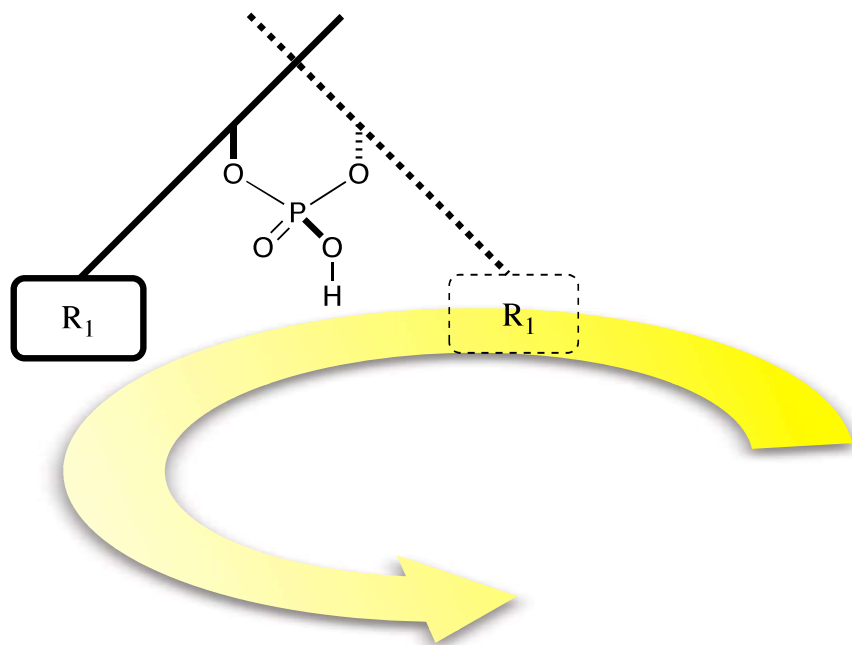
J. P. Reid, L. Simon and J. M. Goodman

*Acc. Chem. Res.* 2016, **49**, 1029-1041.

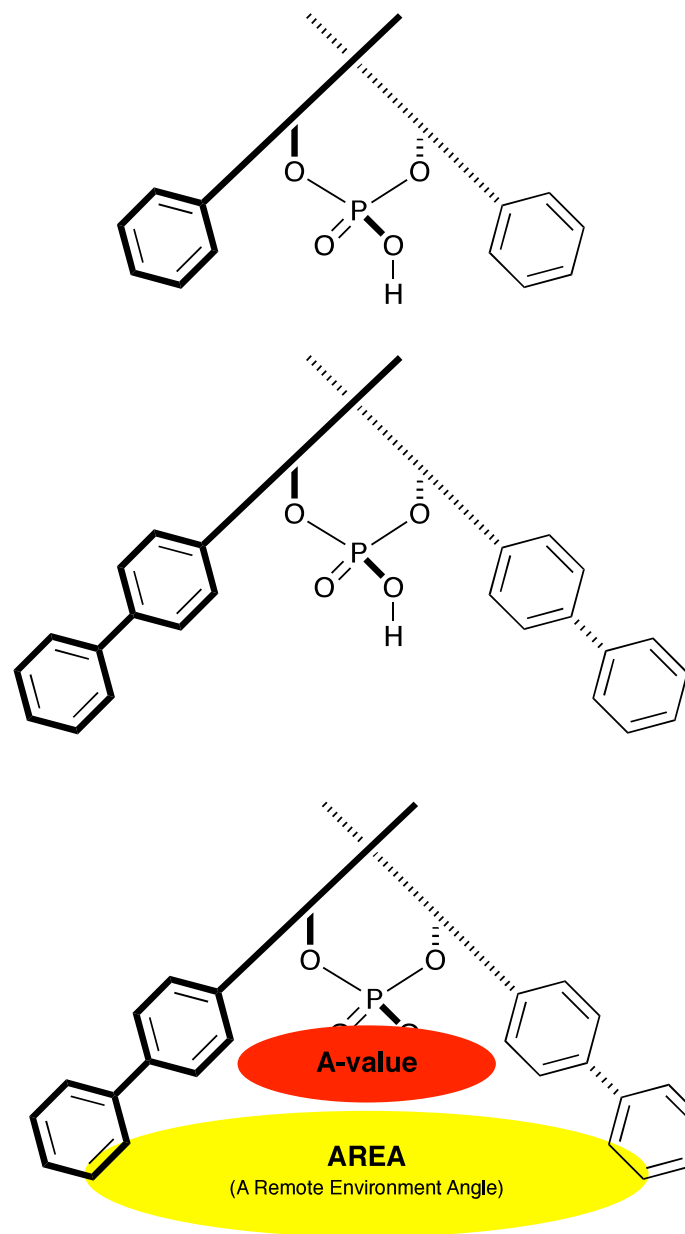
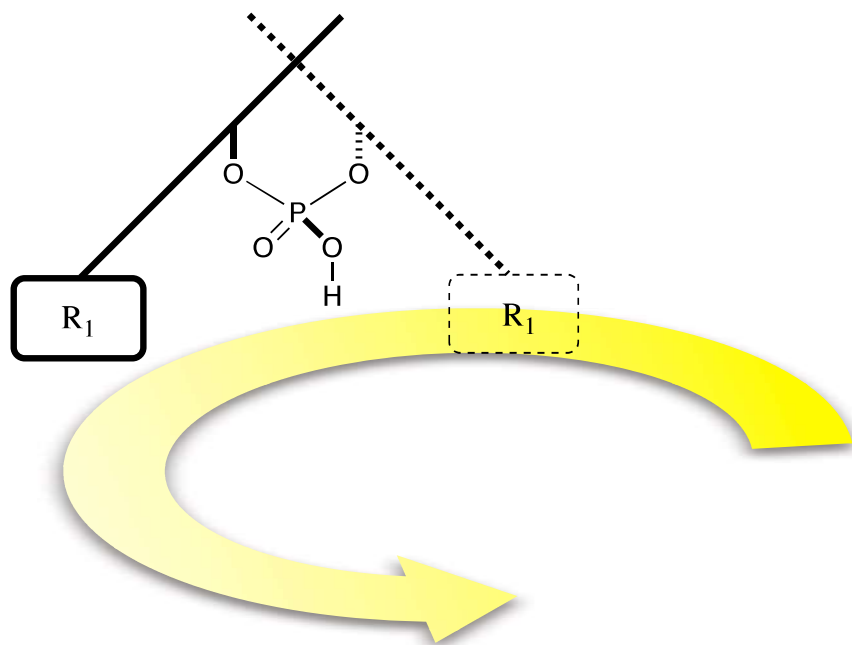
DOI: [10.1021/acs.accounts.6b00052](https://doi.org/10.1021/acs.accounts.6b00052)



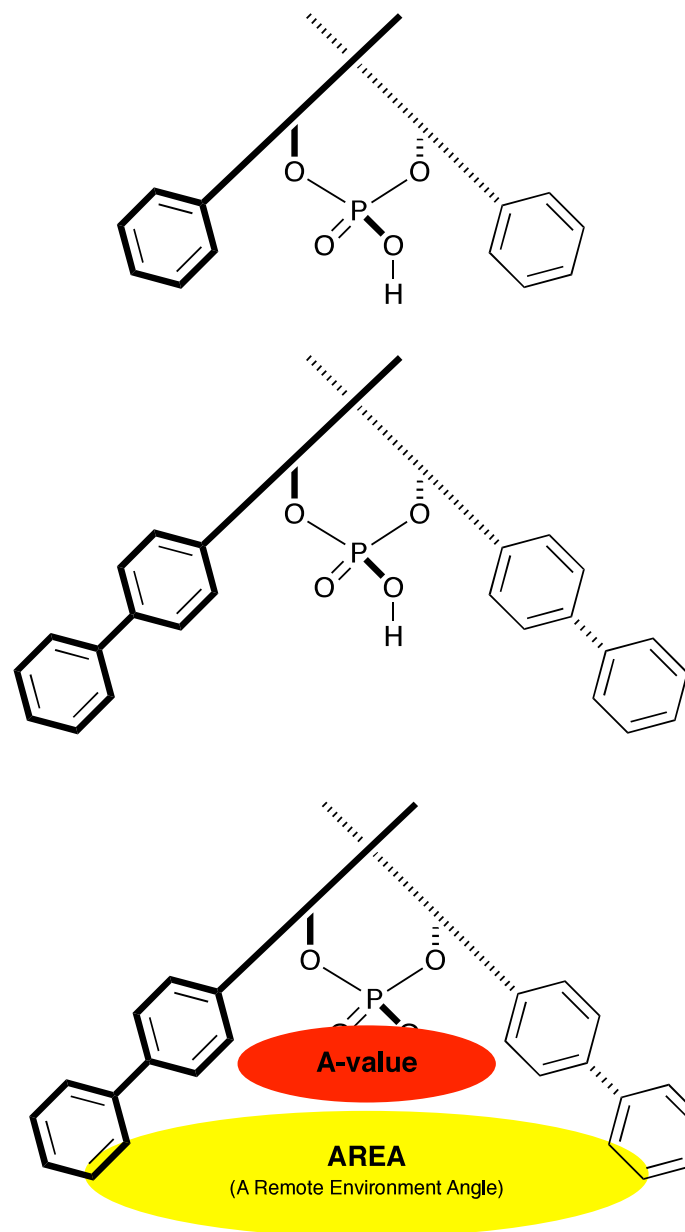
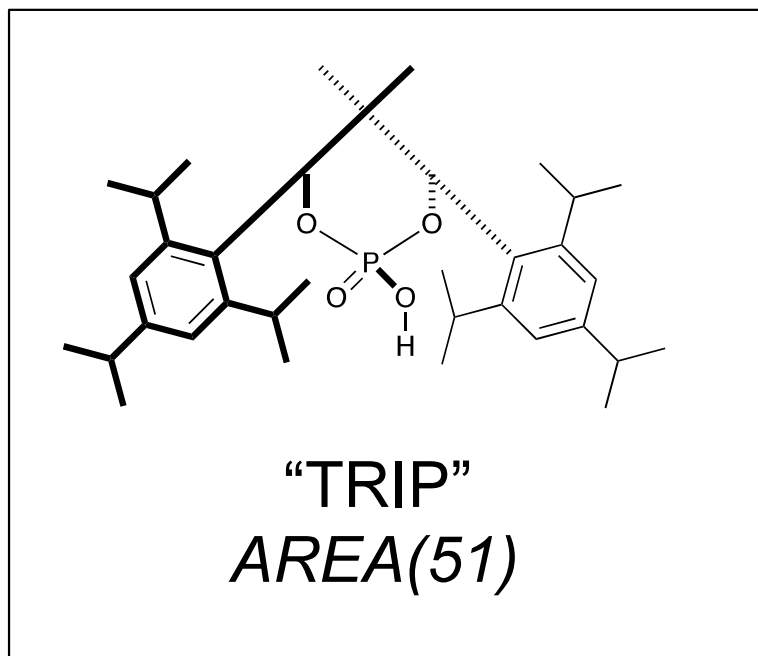
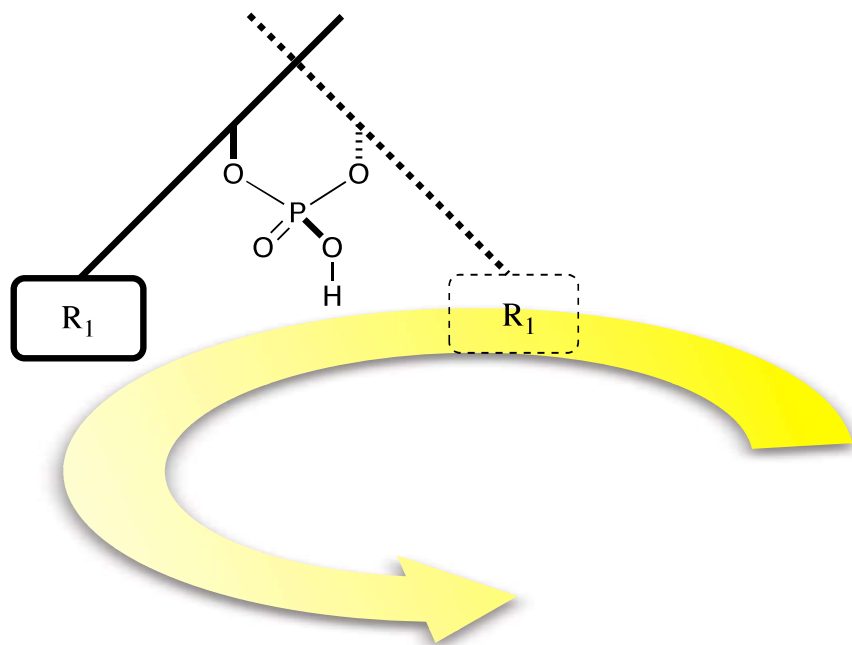
J. P. Reid and J. M. Goodman  
*J. Am. Chem. Soc.* 2016, **138**, 7910-7917.  
DOI: [10.1021/jacs.6b02825](https://doi.org/10.1021/jacs.6b02825)

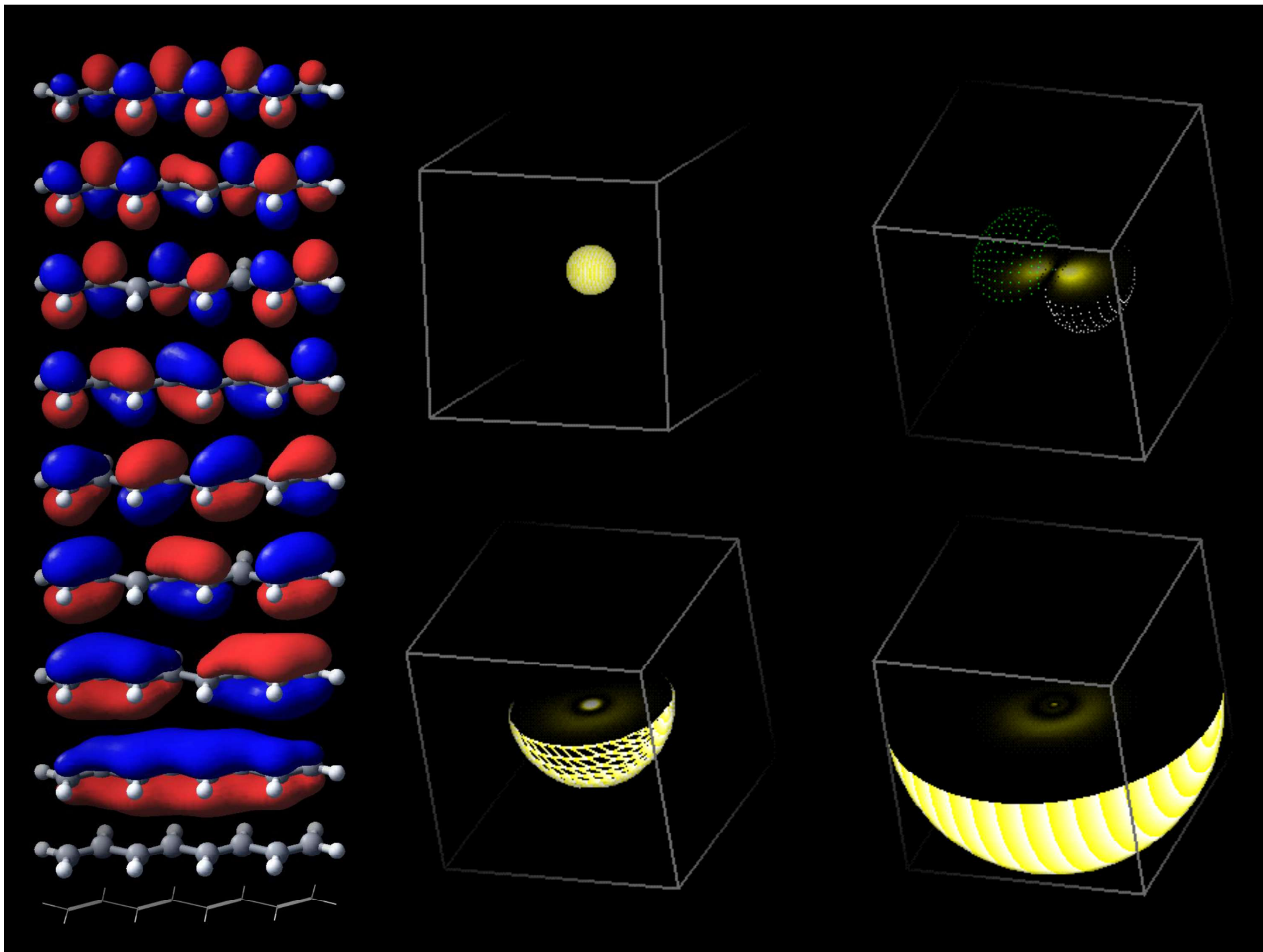


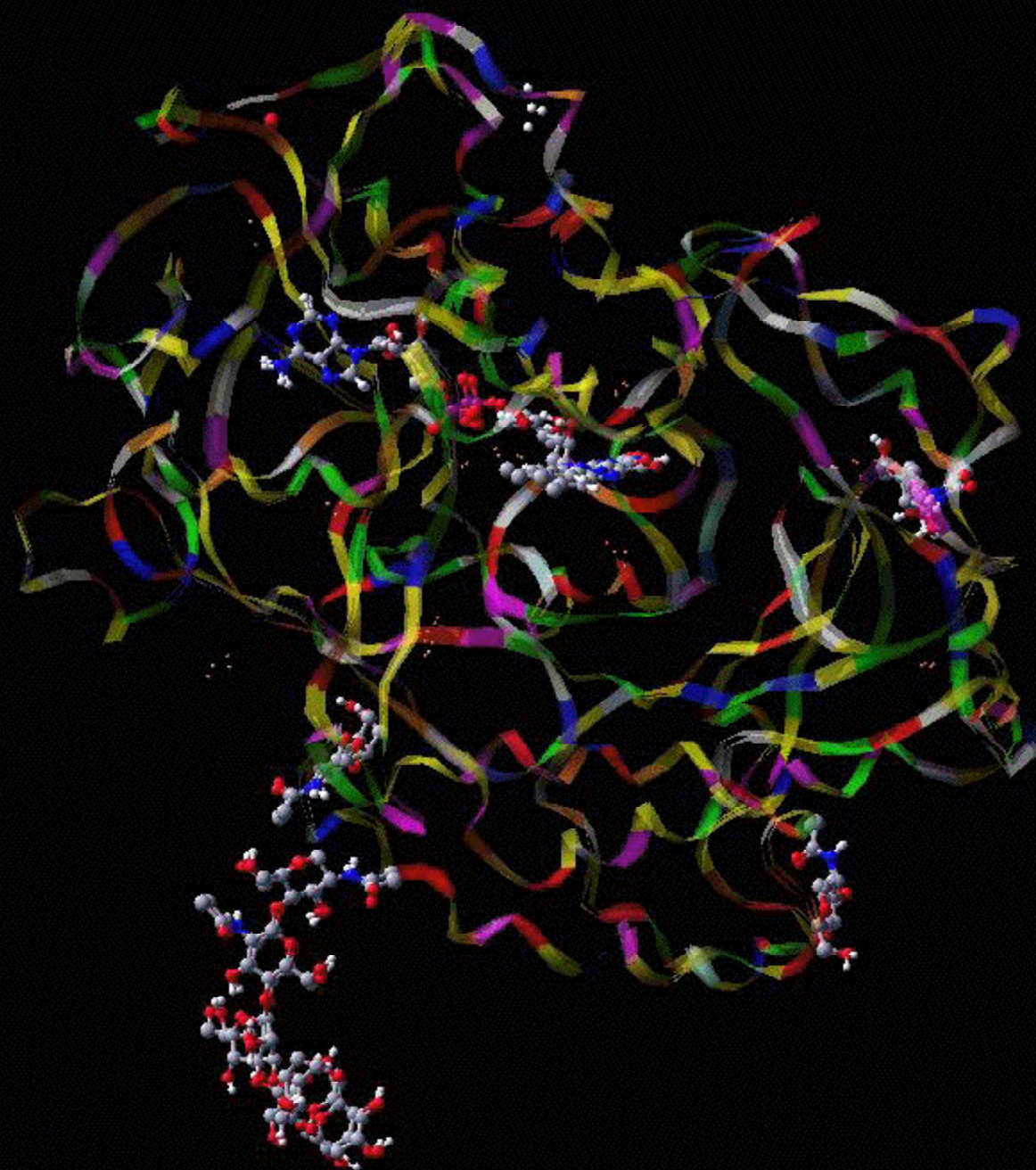
J. P. Reid and J. M. Goodman  
*J. Am. Chem. Soc.* 2016, **138**, 7910-7917.  
 DOI: [10.1021/jacs.6b02825](https://doi.org/10.1021/jacs.6b02825)







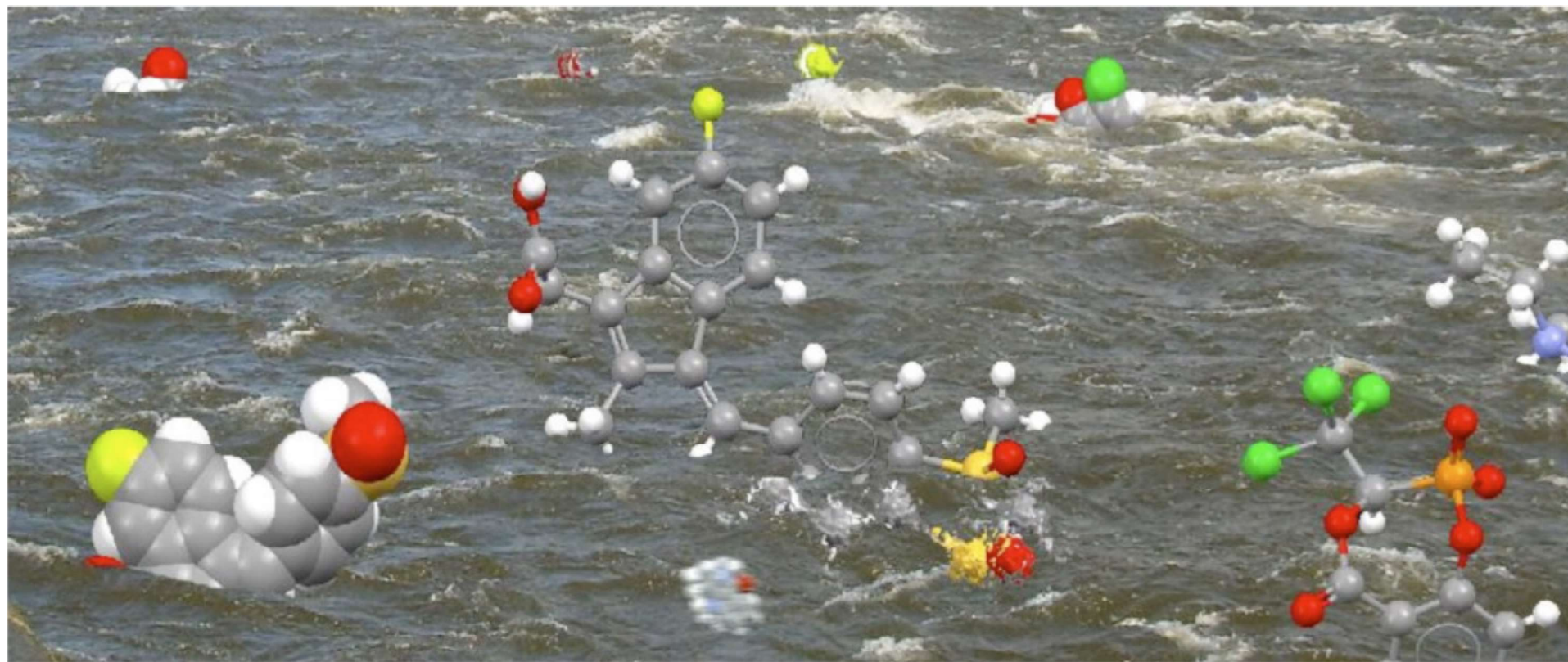






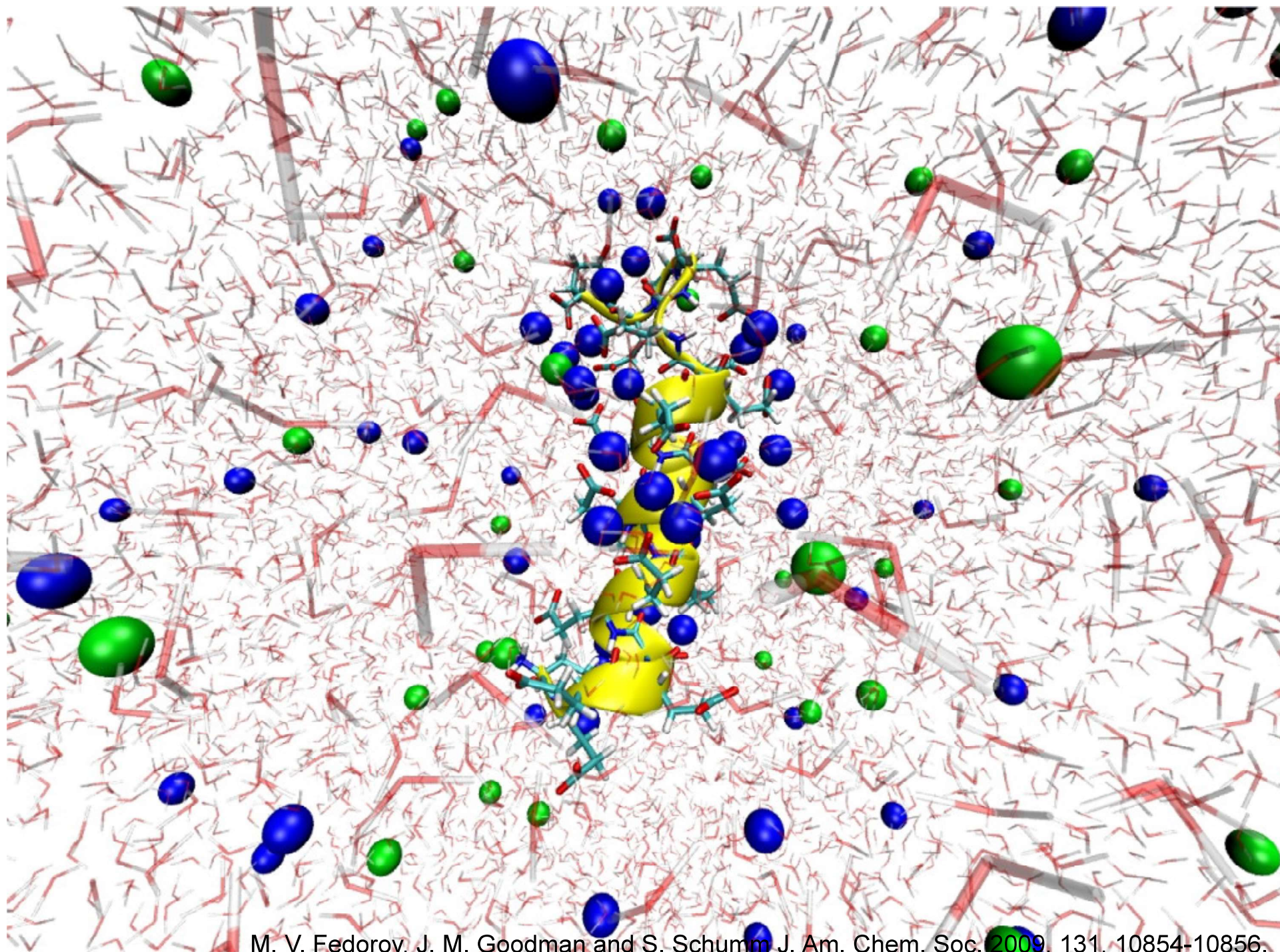
# Solubility Challenge

Can You Predict Solubilities of Thirty-Two Molecules  
Using a Database of One Hundred Reliable Measurements?



*J. Chem. Inf. Model.* 2008, **48**, 1289-1303.

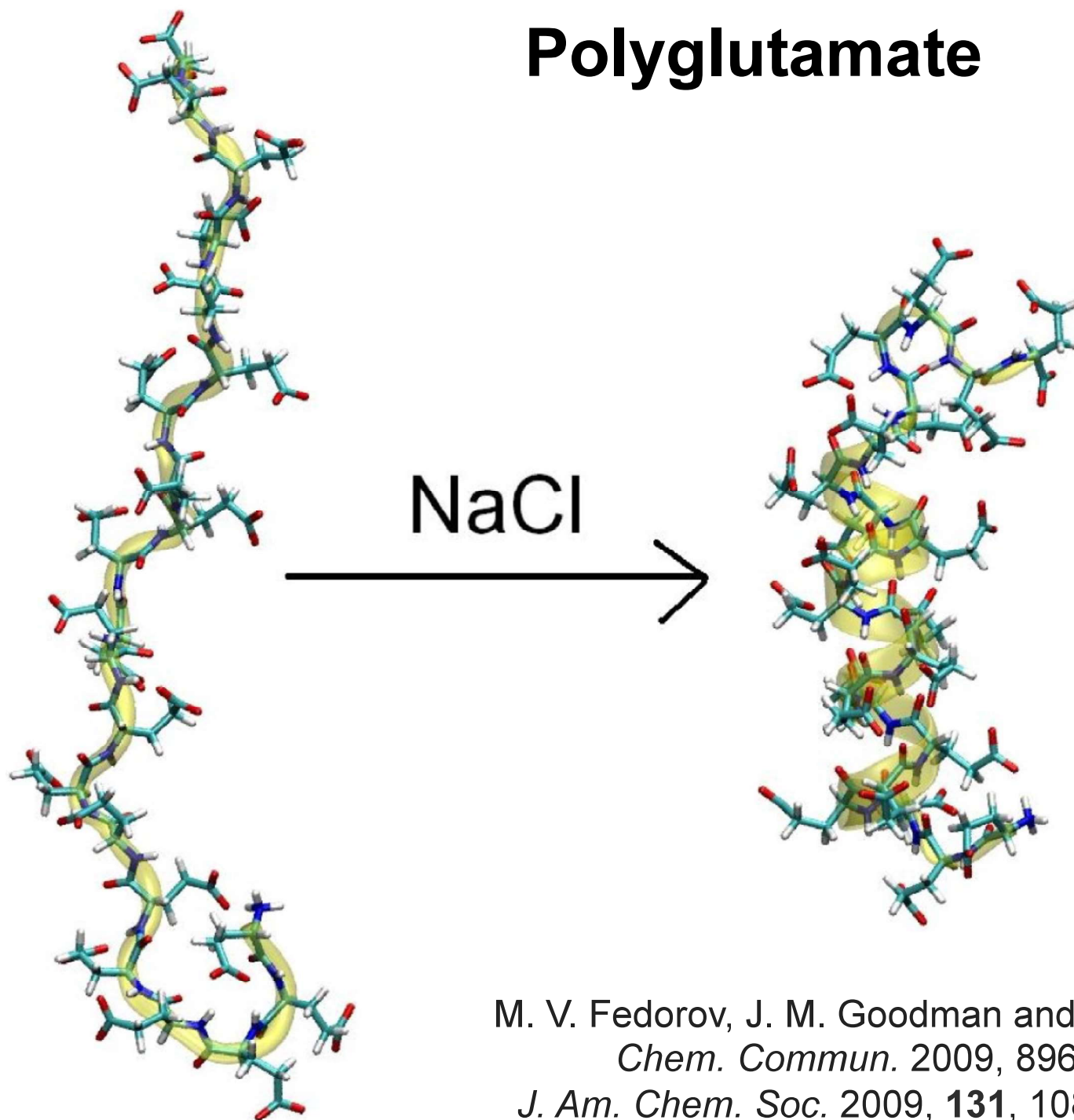




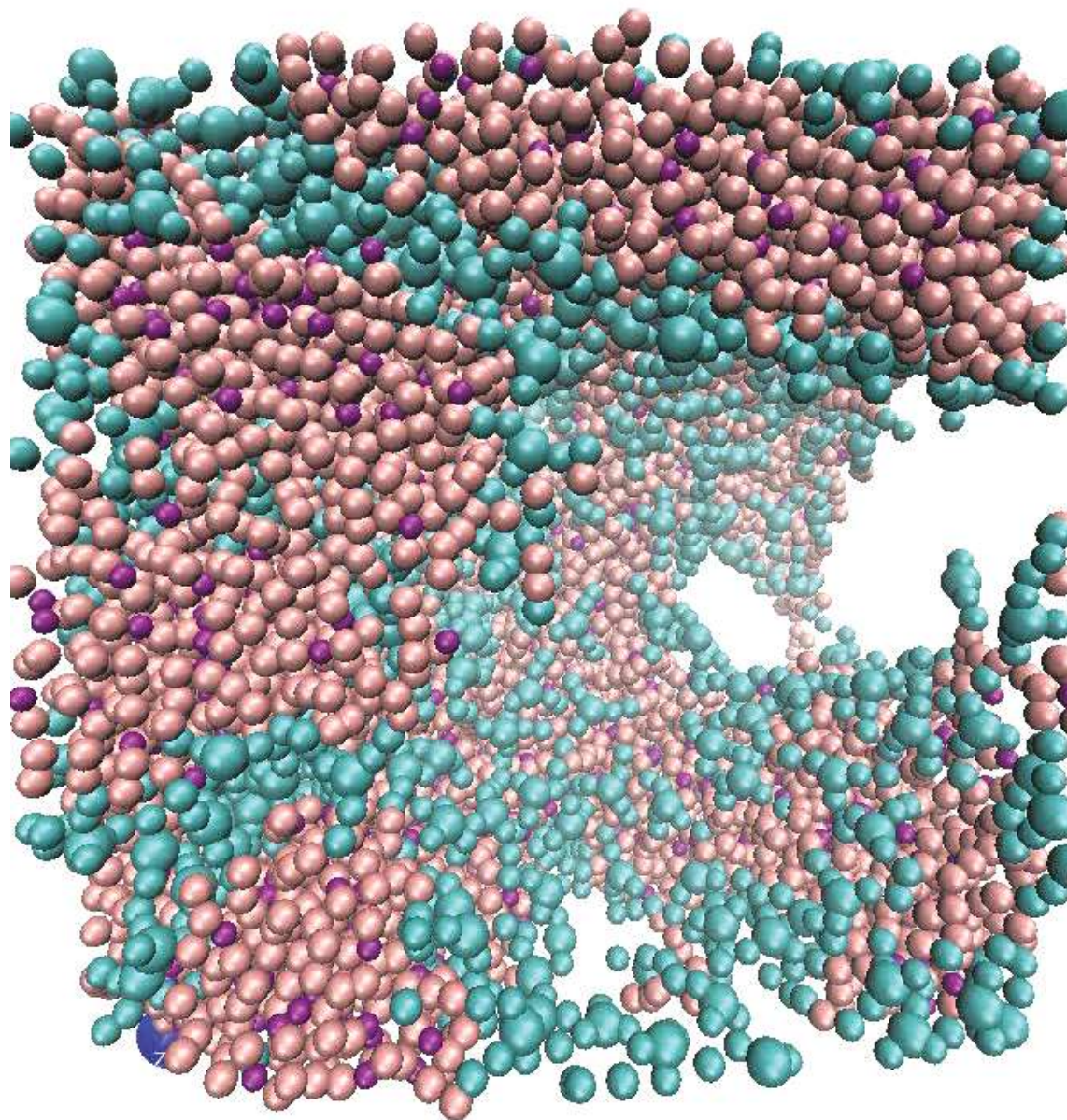
M. V. Fedorov, J. M. Goodman and S. Schumm J. Am. Chem. Soc. 2009, 131, 10854-10856.

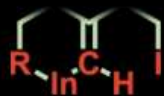


# Polyglutamate



M. V. Fedorov, J. M. Goodman and S. Schumm  
*Chem. Commun.* 2009, 896-898.  
*J. Am. Chem. Soc.* 2009, **131**, 10854-10856.



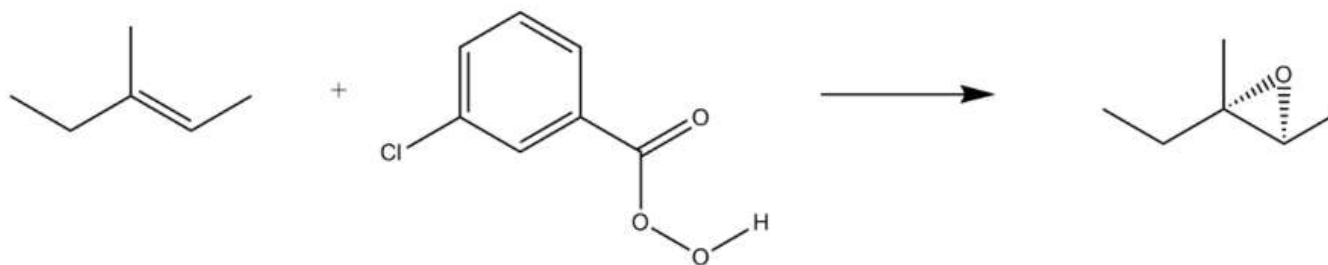


## The RInChI Project

The aim of the RInChI project, in the same vein as InChI, is to create a unique data string to describe a reaction. Reaction InChIs, or RInChIs, are such data strings. They use the InChI software and from an rxn input file a RInChI can be created. The tools for doing this are below, and some helpful information is given in the [help](#) pages.

### RInChI Versions

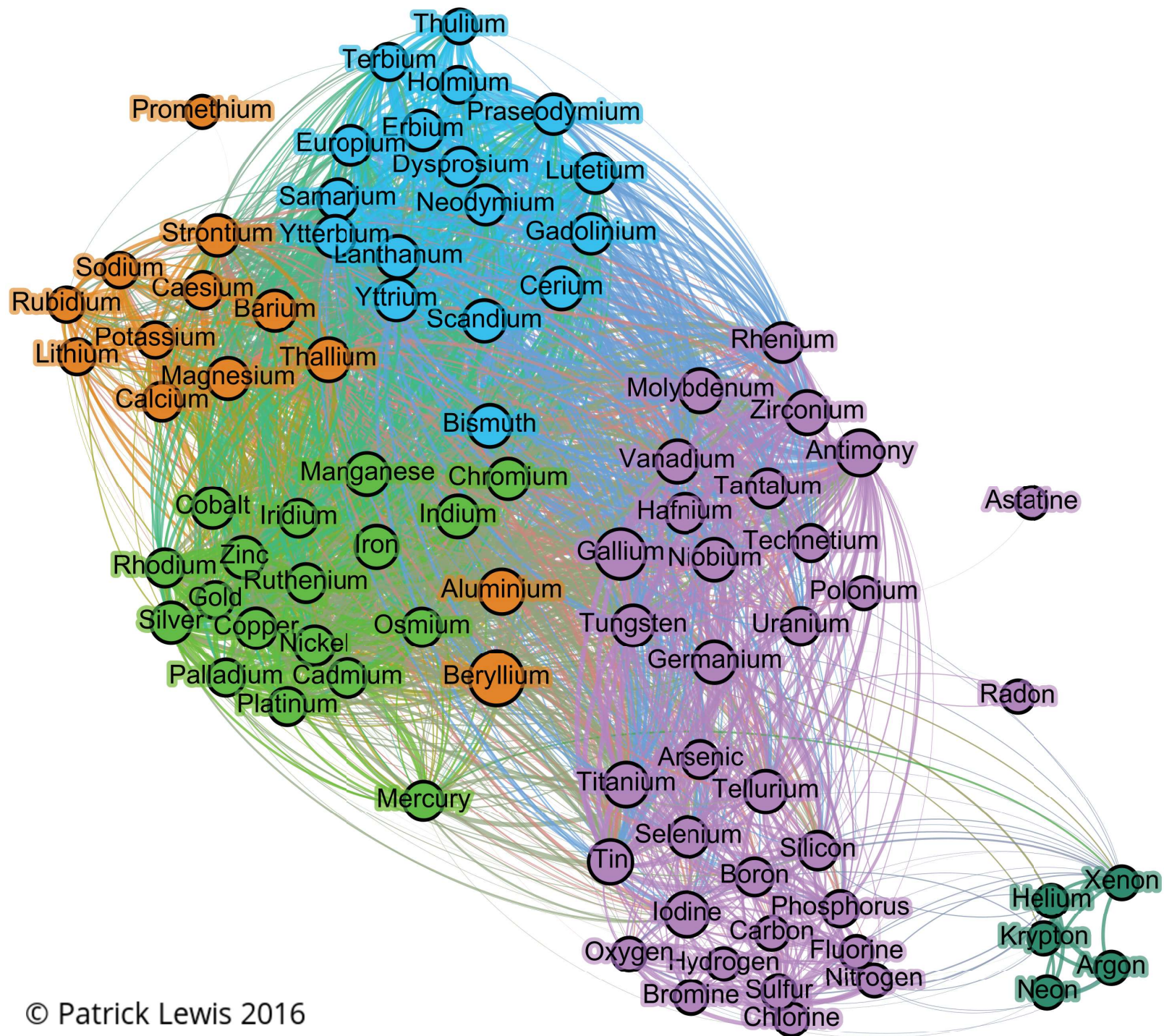
Tools on this site work with RInChI v1.00 unless otherwise stated. All tools run with Python 3



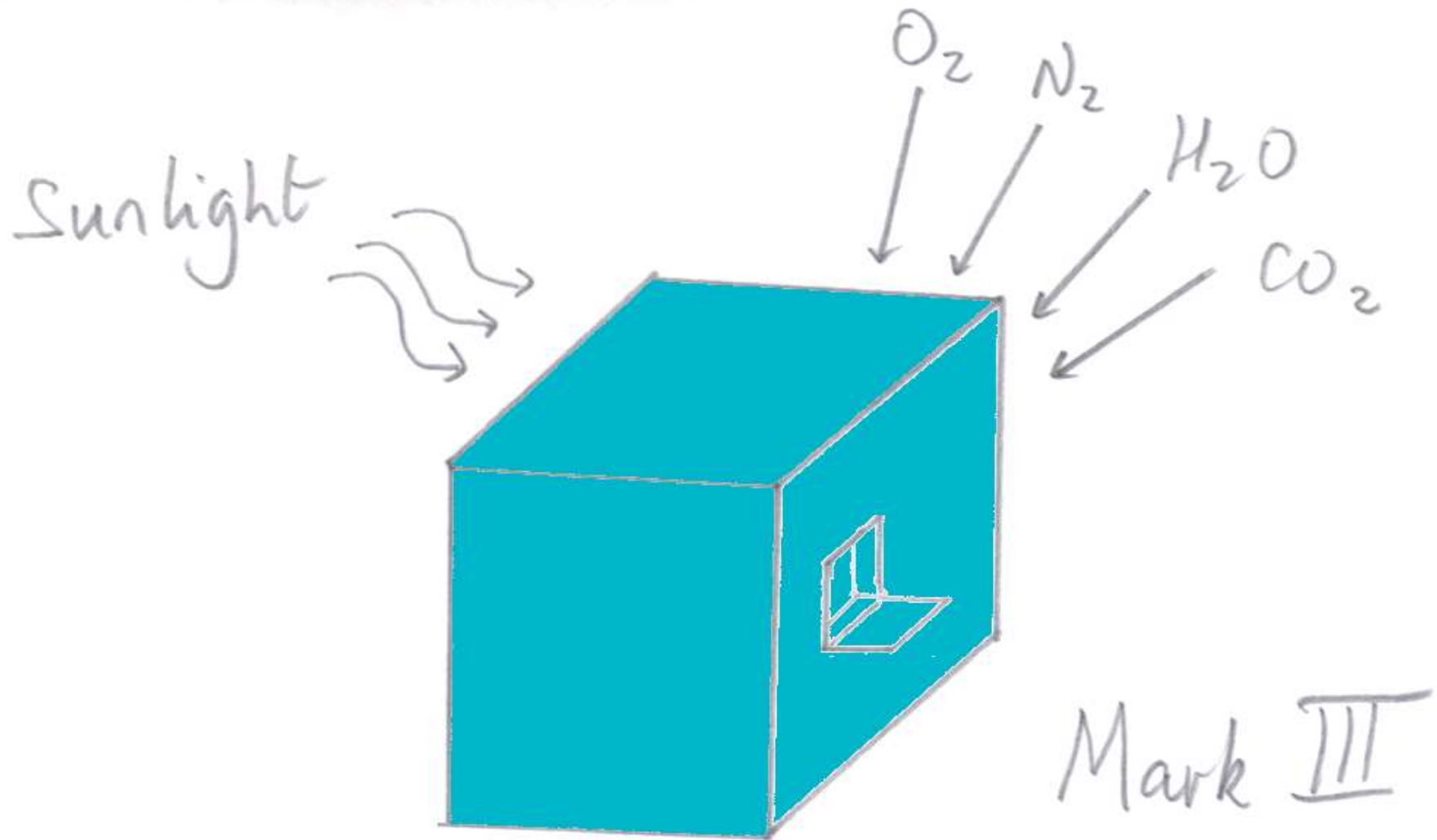
RInChI=1.00.1S/C6H12/c1-4-6(3)5-2/h4H,5H2,1-3H3/b6-4+!C7H5ClO3/c8-6-3-1-2-5(4-6)7(9)11-10/h1-4,10H<>C6H12O/c1-4-6(3)5(2)7-6/h5H,4H2,1-3H3/t5-,6-/m0/s1/d+

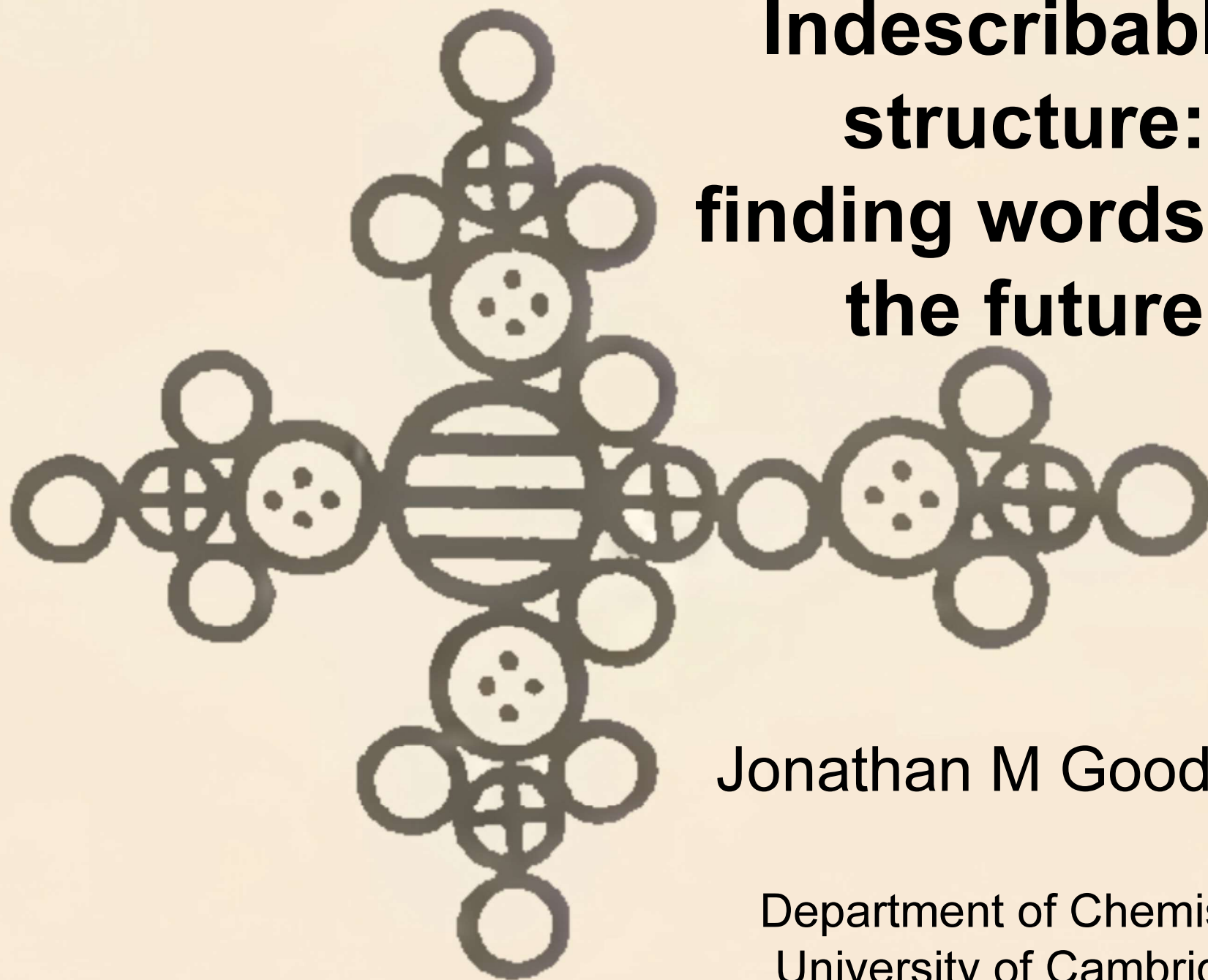
Example of a RInChI v1.00





# Dial a Molecule





# **Indescribable structure: finding words for the future**

Jonathan M Goodman

Department of Chemistry,  
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