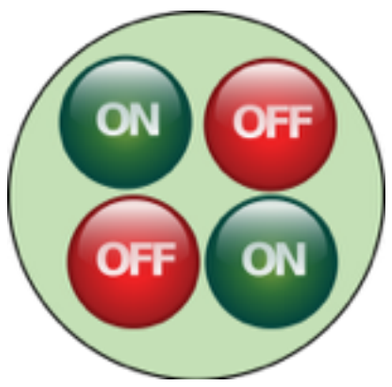
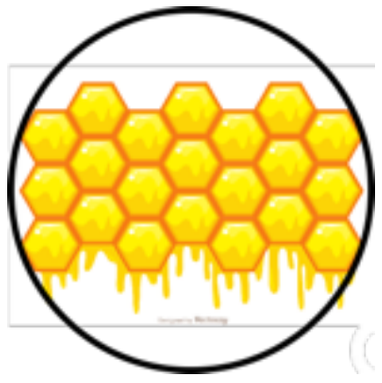
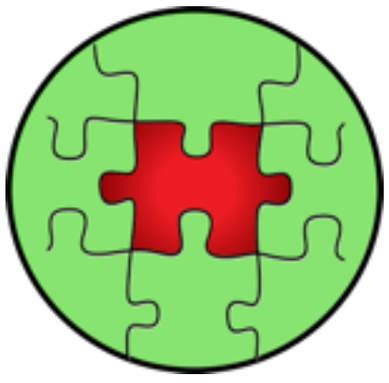
2D Cöördgen

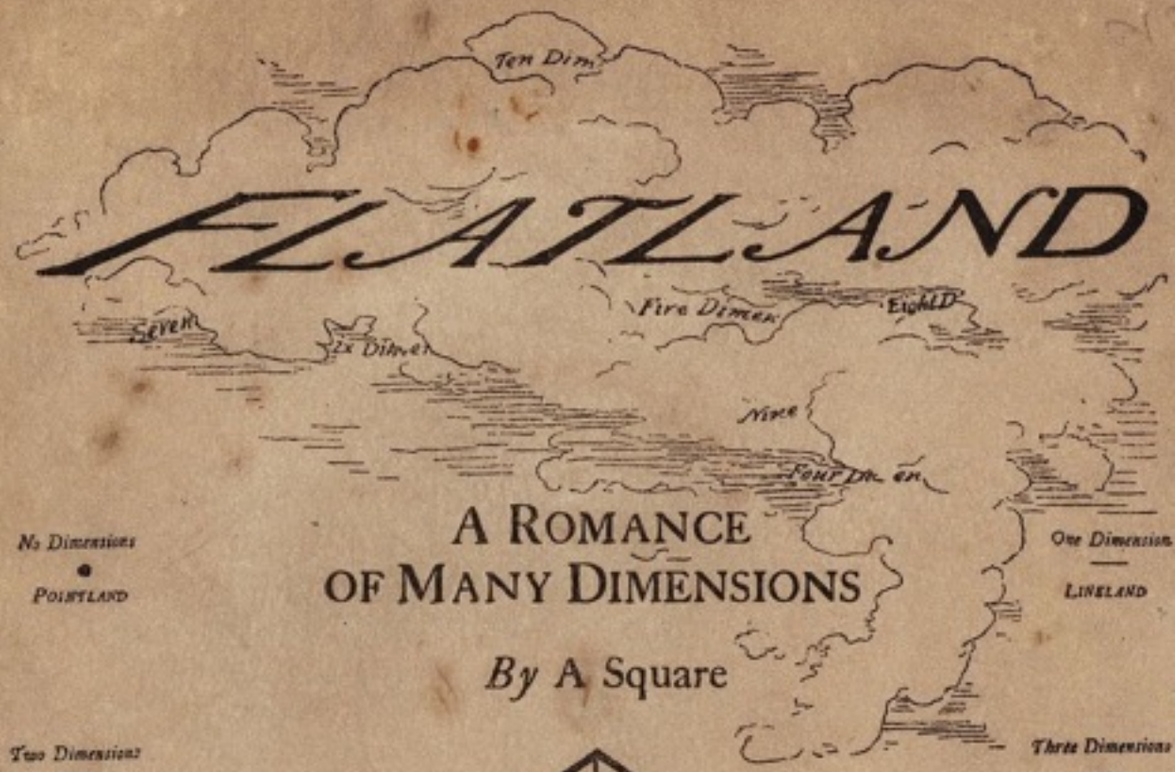
Chemistry in Plane View



Nic Zonta - Schrödinger

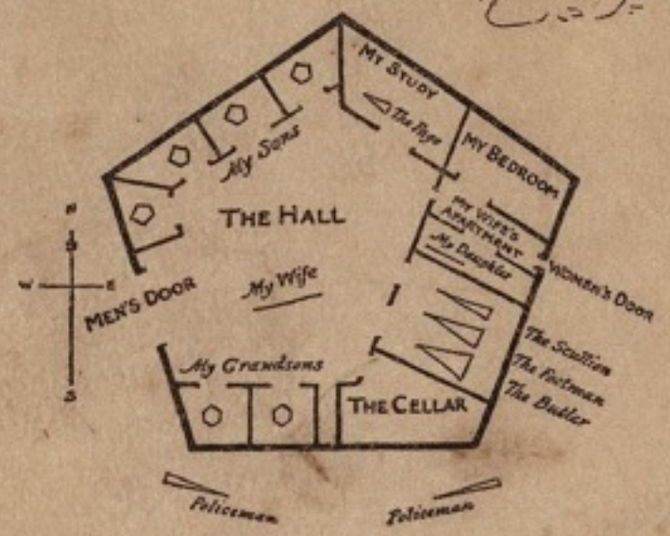
"O day and night, but this is wondrous strange"



FLATLAND

A ROMANCE OF MANY DIMENSIONS

By A Square

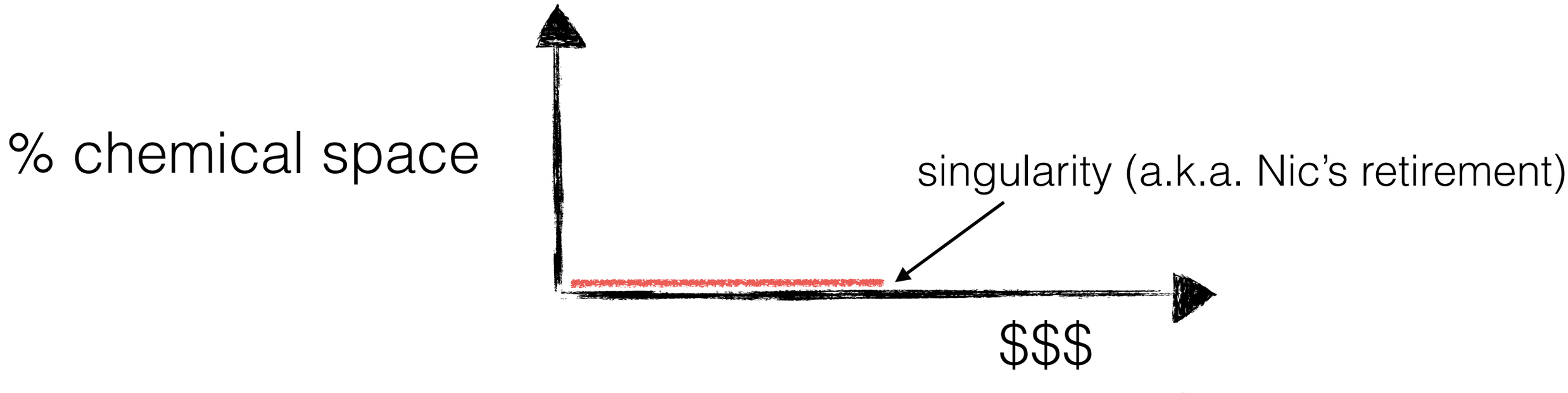


LONDON
SEELEY & Co., ESSEX STREET, STRAND
Price Half-a-crown

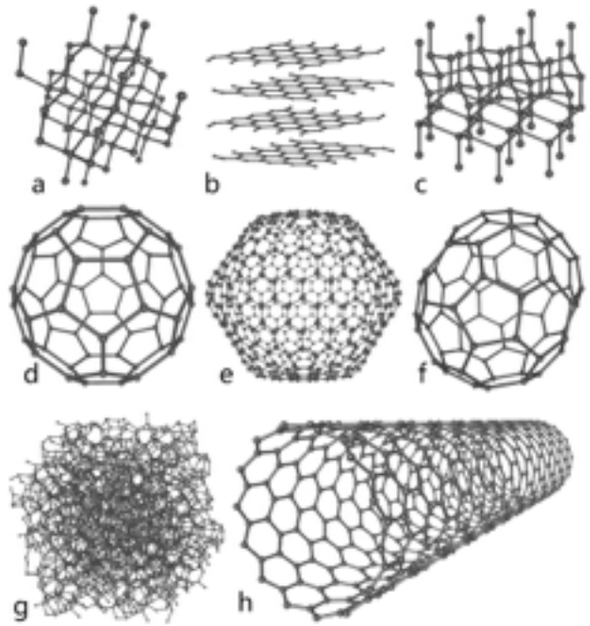
"And therefore as a stranger give it welcome"

Goals I

Specificity VS Simplicity



Schrodinger's law: no matter how complicated the problem is, the guys in MatSci have a worse one for you



maintaining code is a cost. **Simplify**

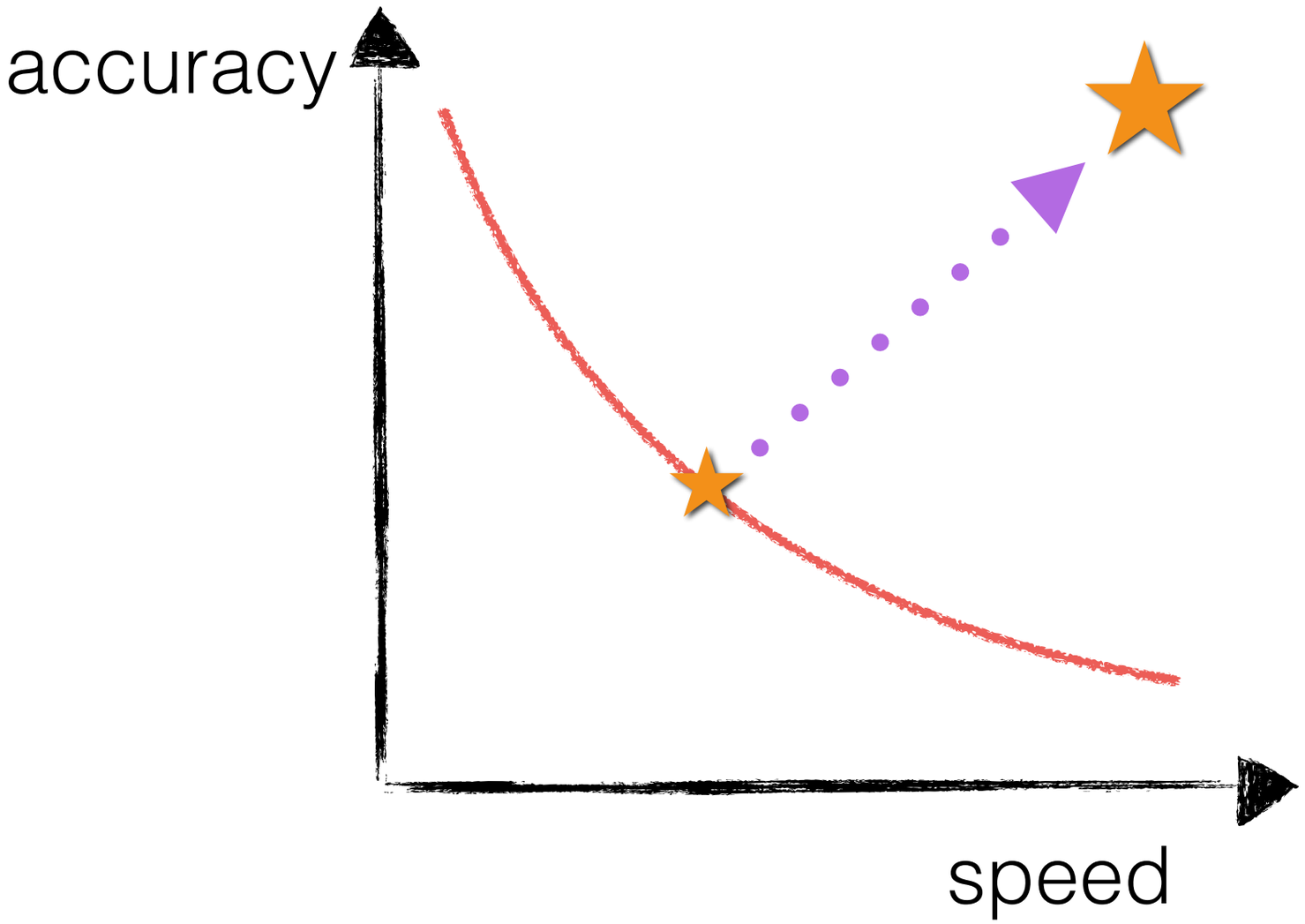
Goals II

Accuracy VS Speed

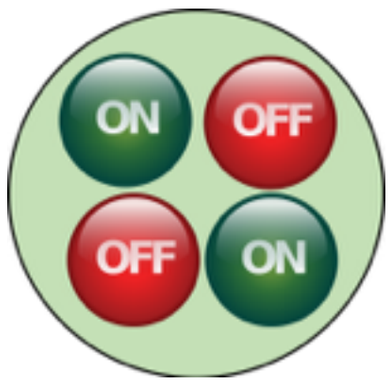
no right answers

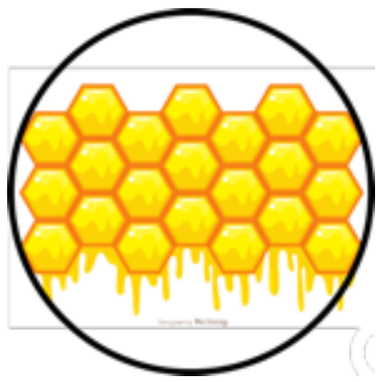
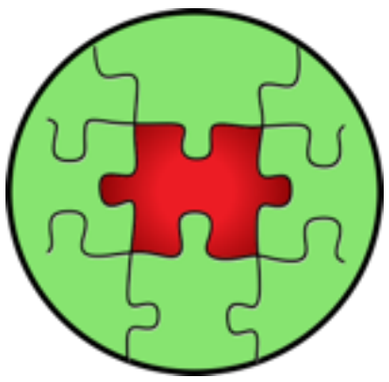
Great starting point Nic!

now just make it faster and more accurate



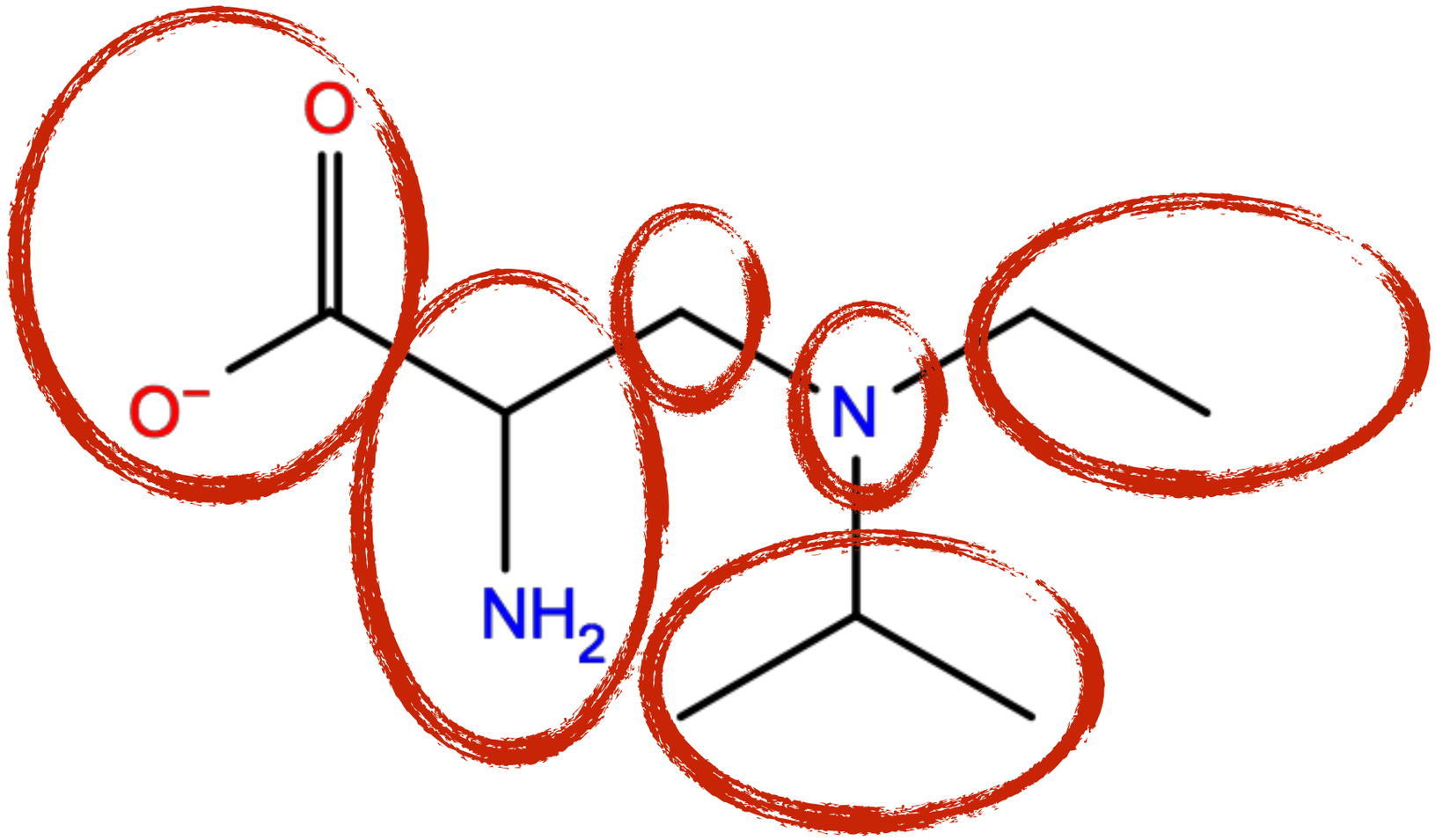
Lets play 2D Coordgen!



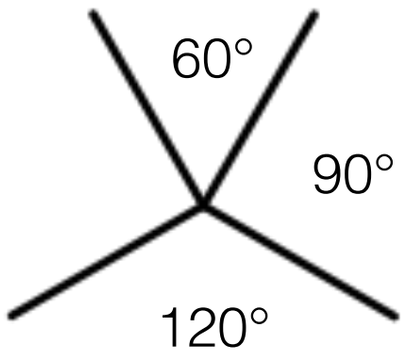



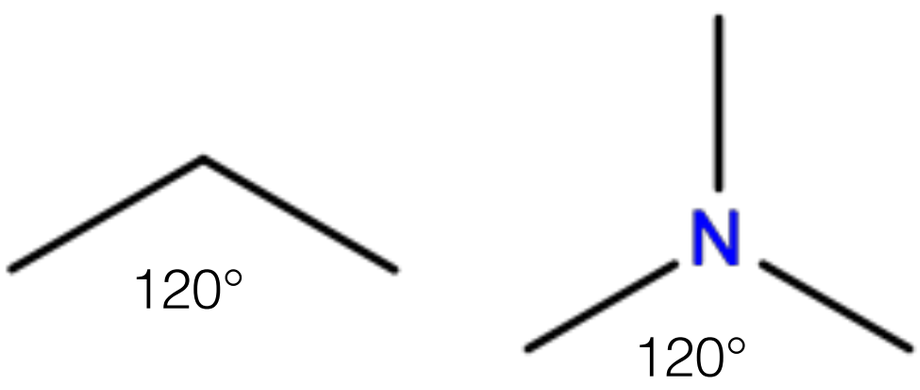
lvl1 - bonds

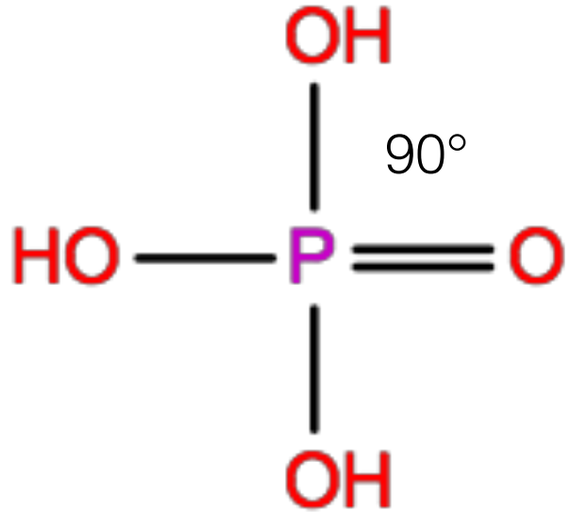
Divide…



…and conquer

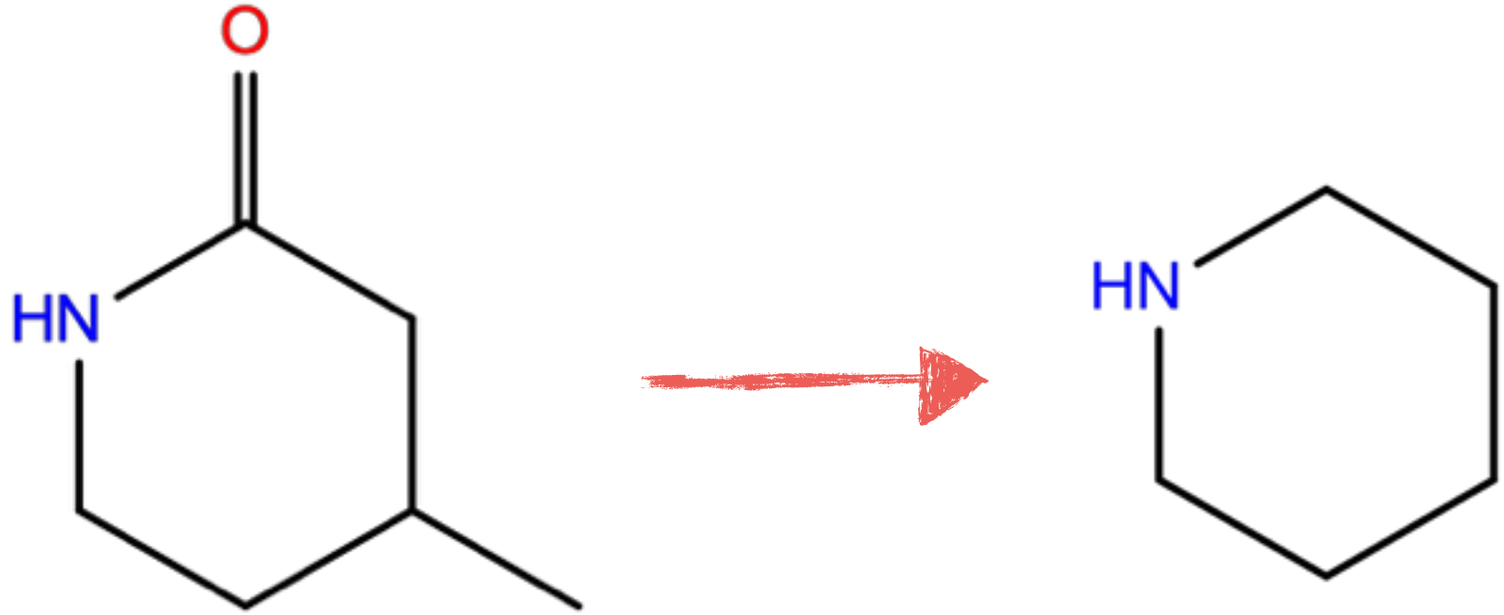




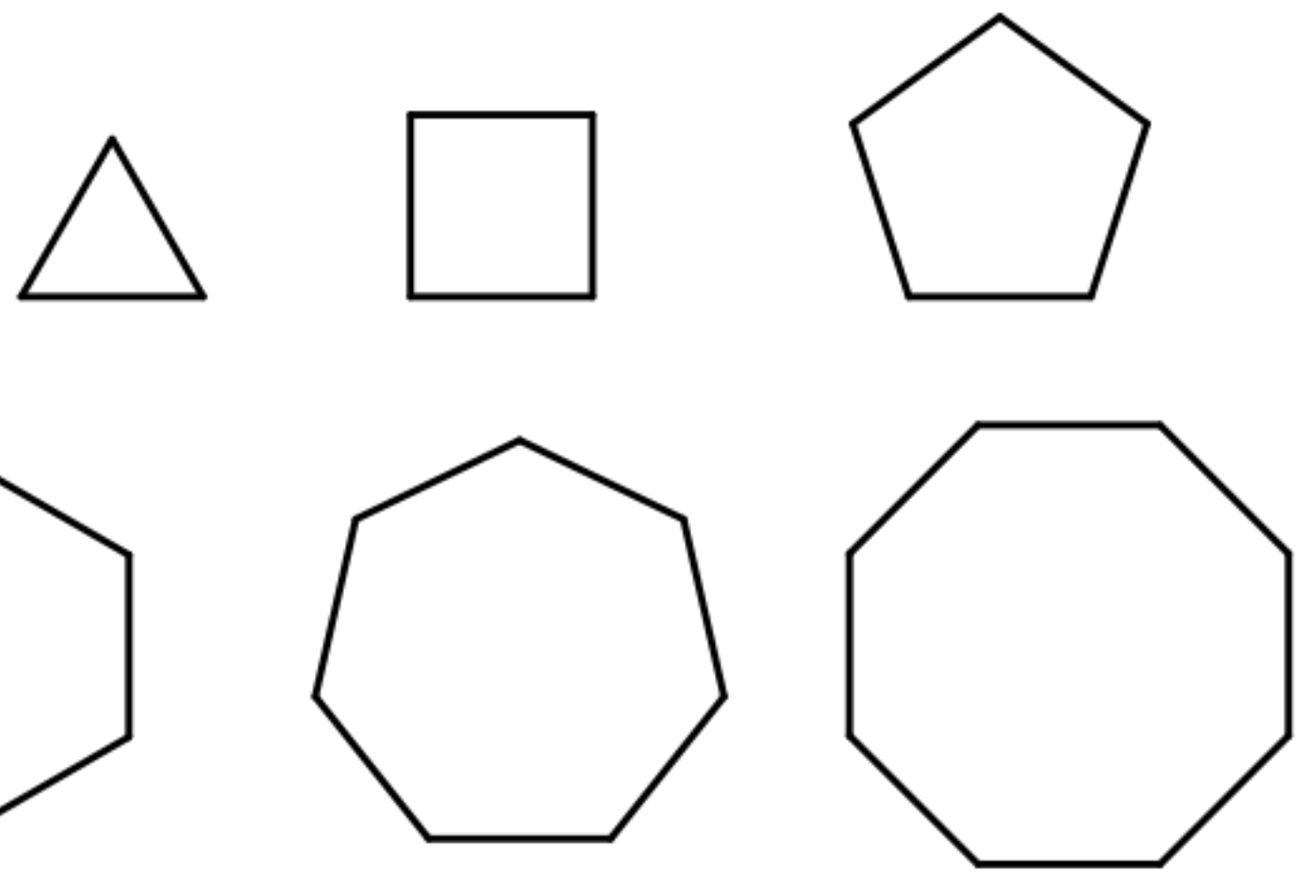


lvl 2 - rings

Divide…

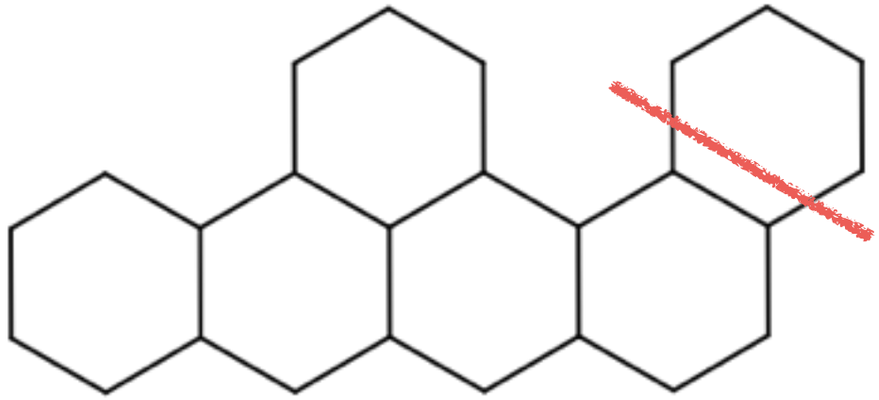


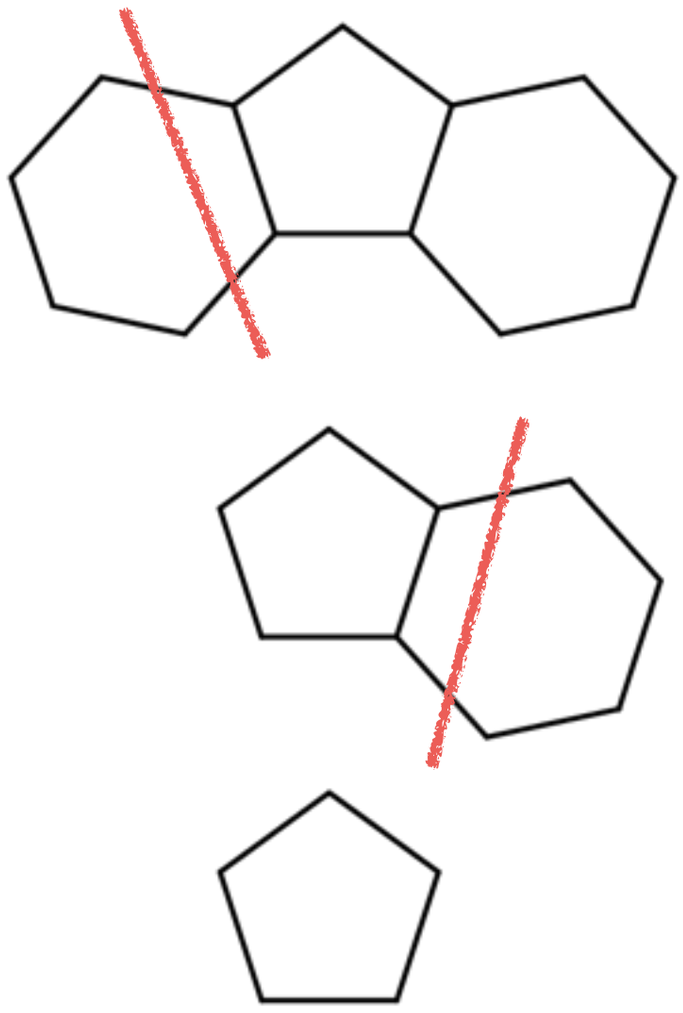
…and conquer

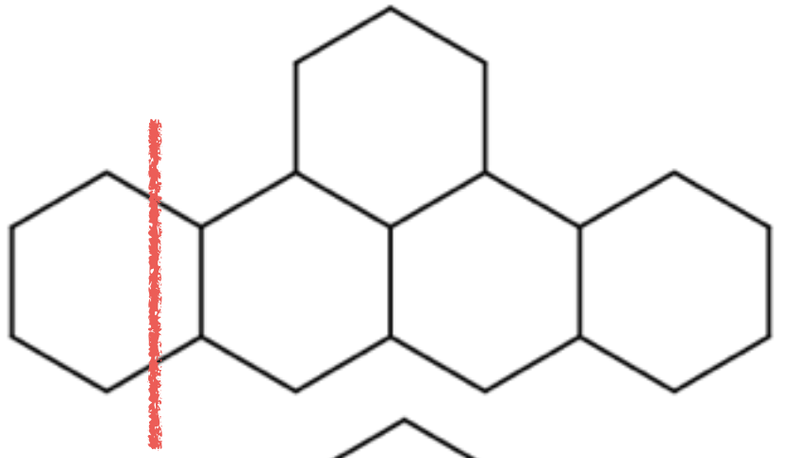


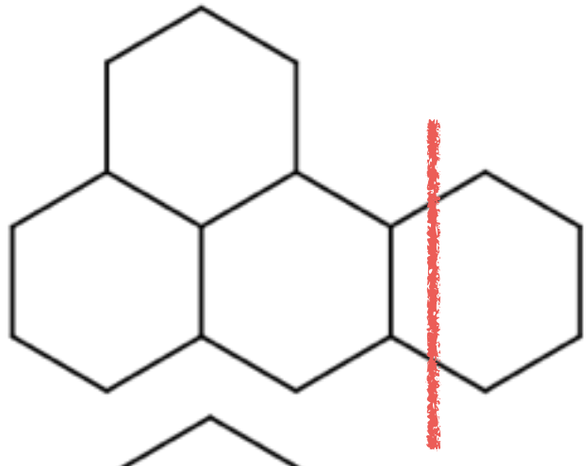
lvl 3 - ring systems

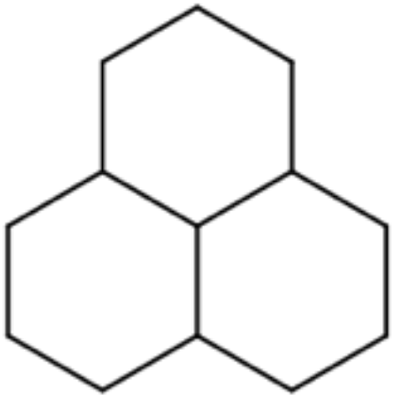
Divide…



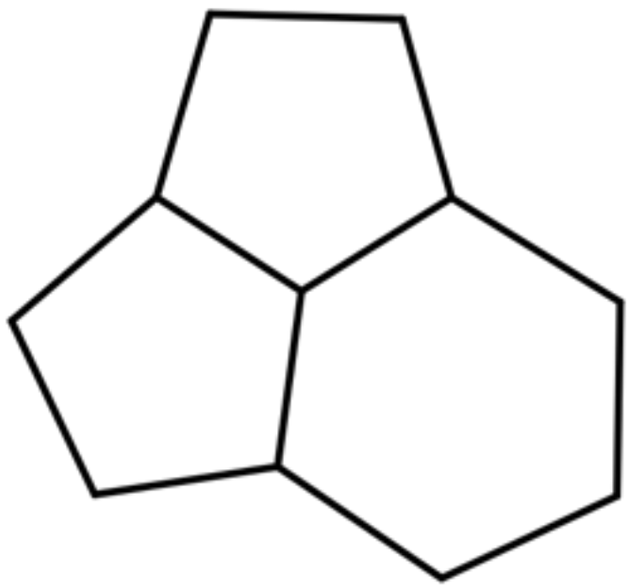


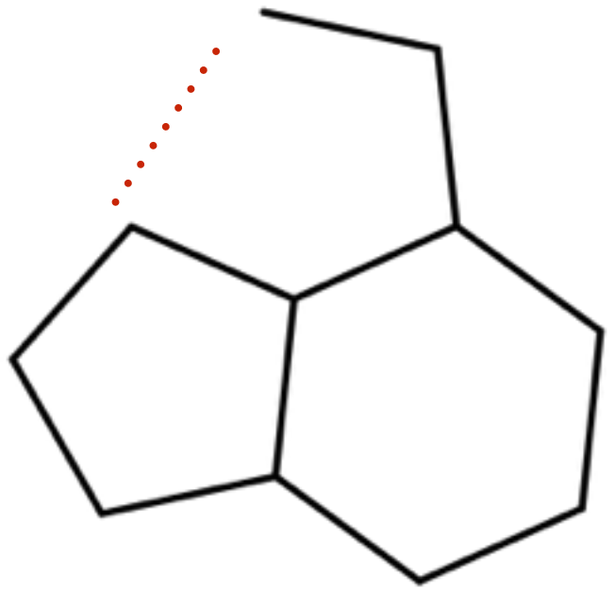


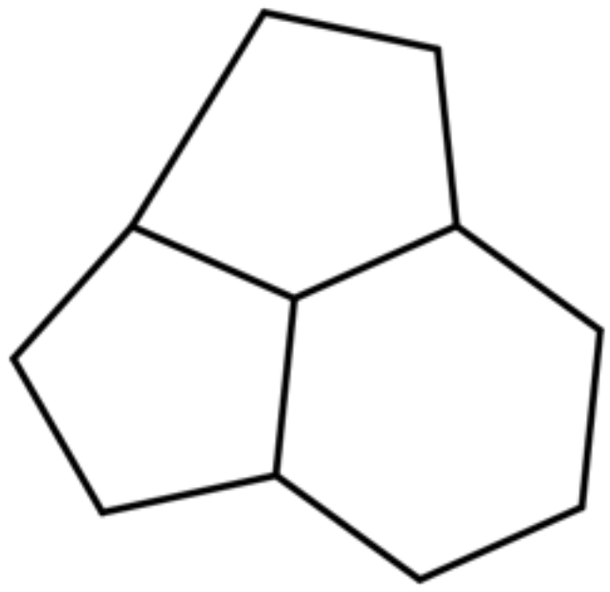


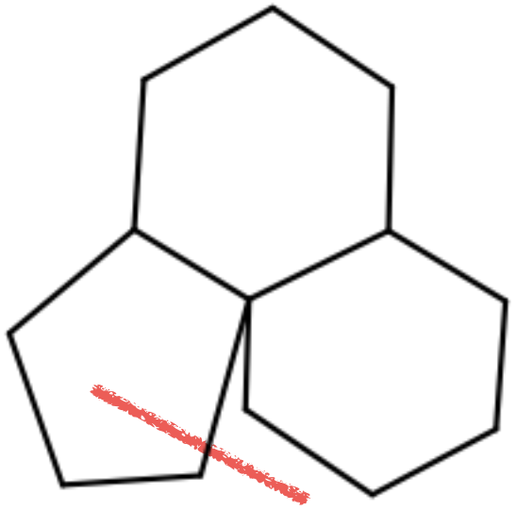


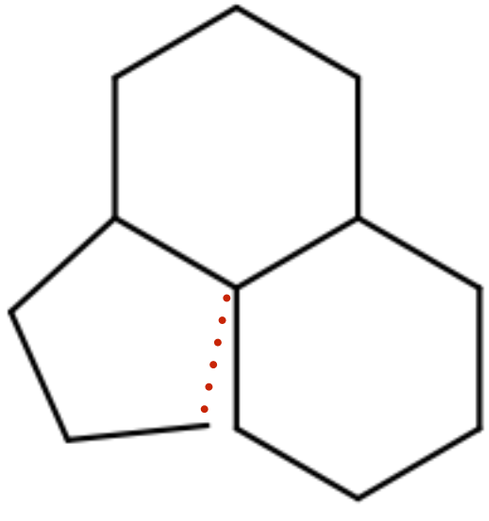
Divide…

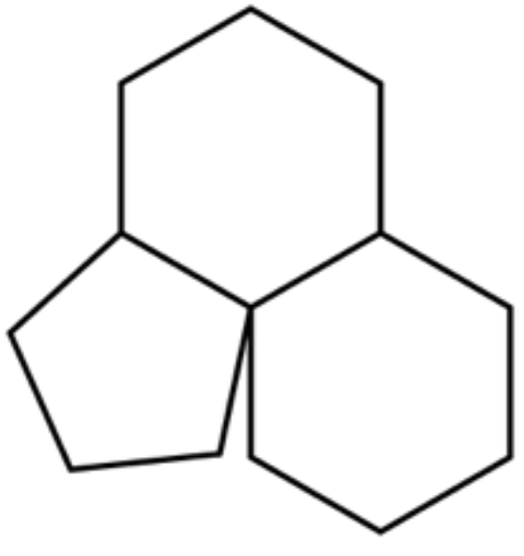




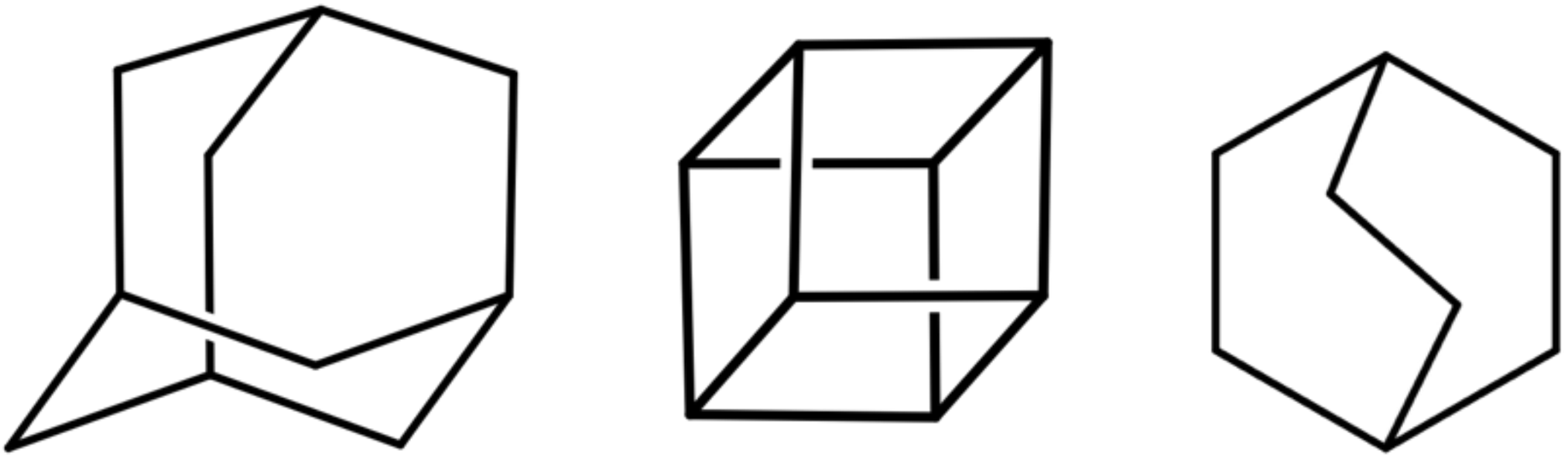






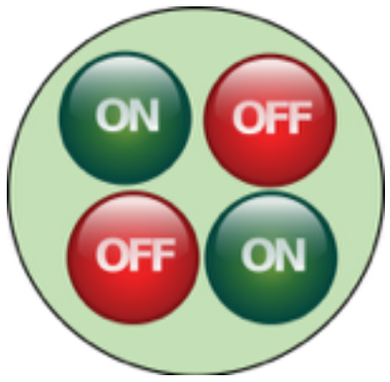


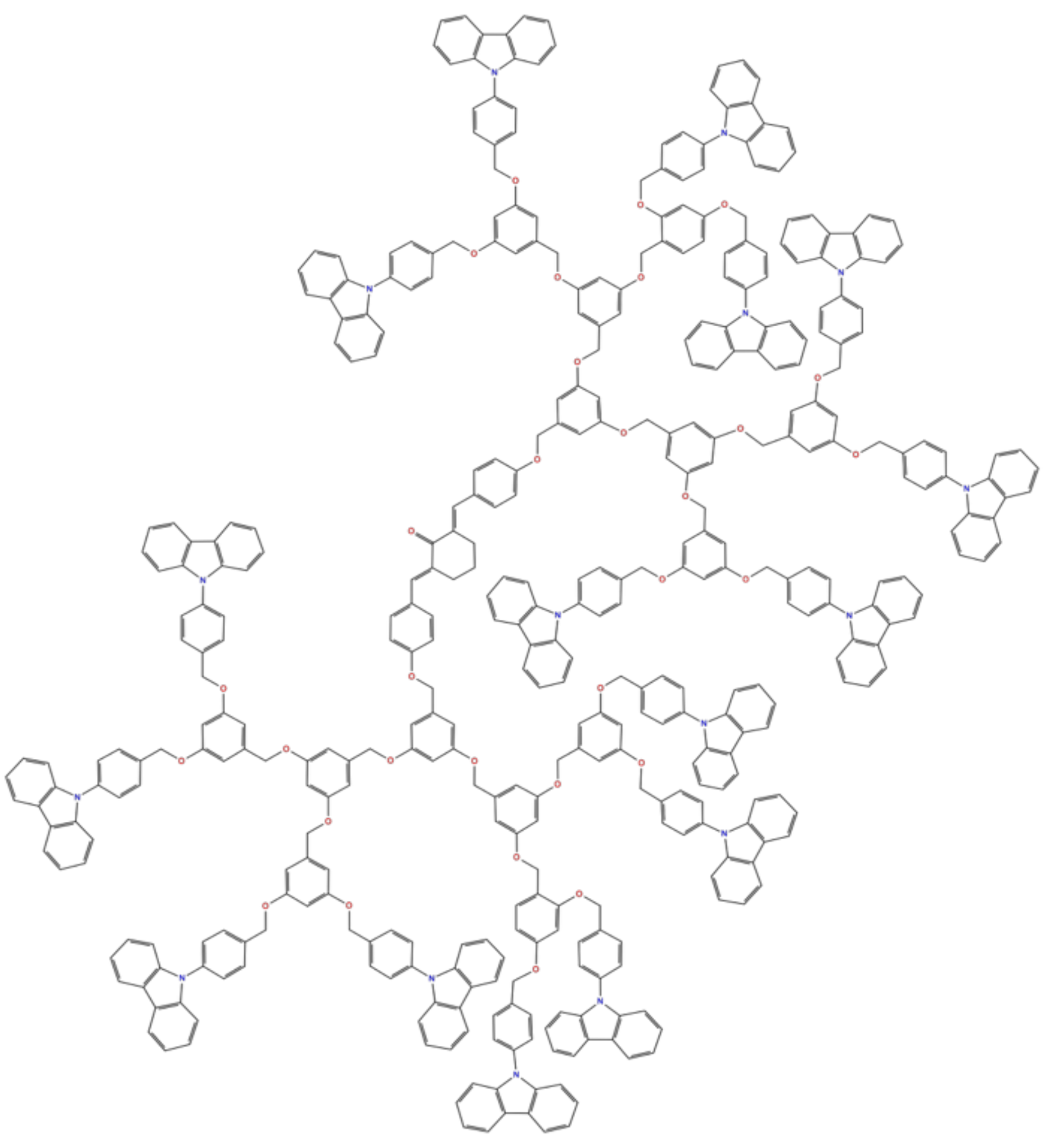
…and conquer

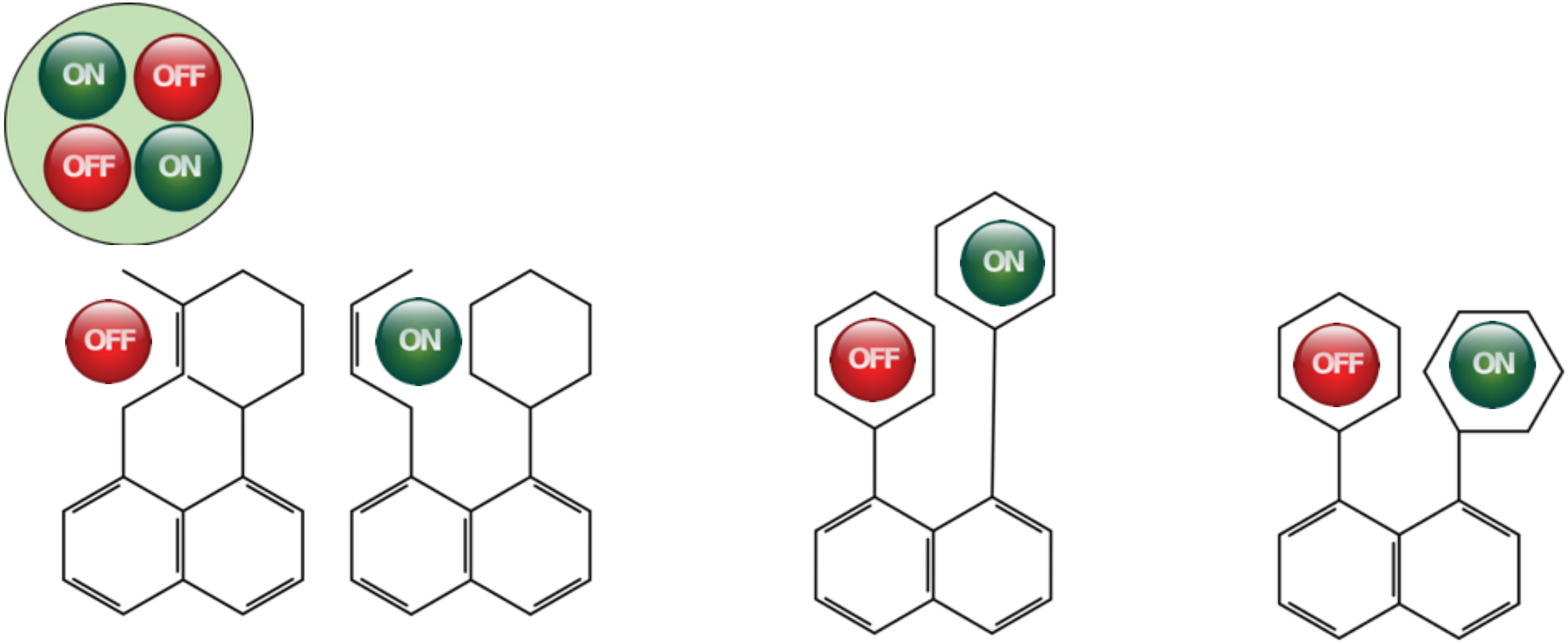


.mae format. Users can specify add their own

lvl 4 - clashes

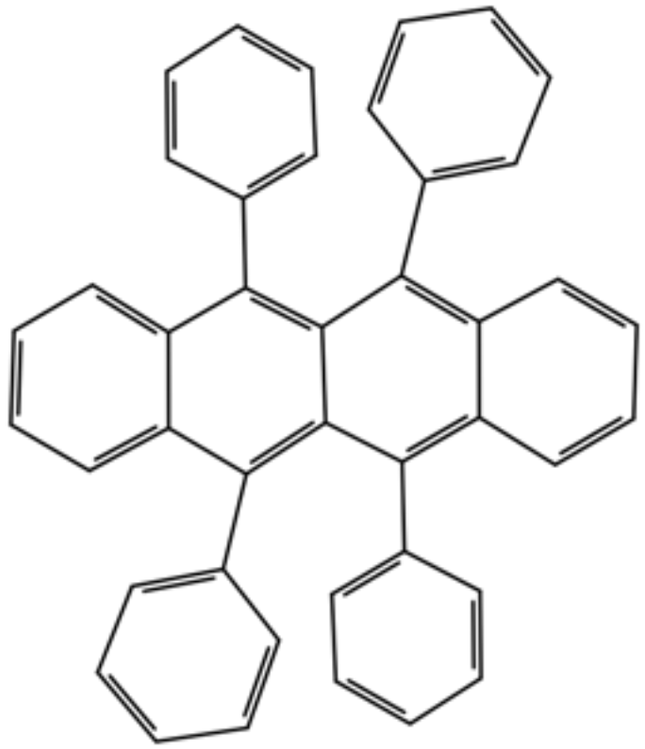


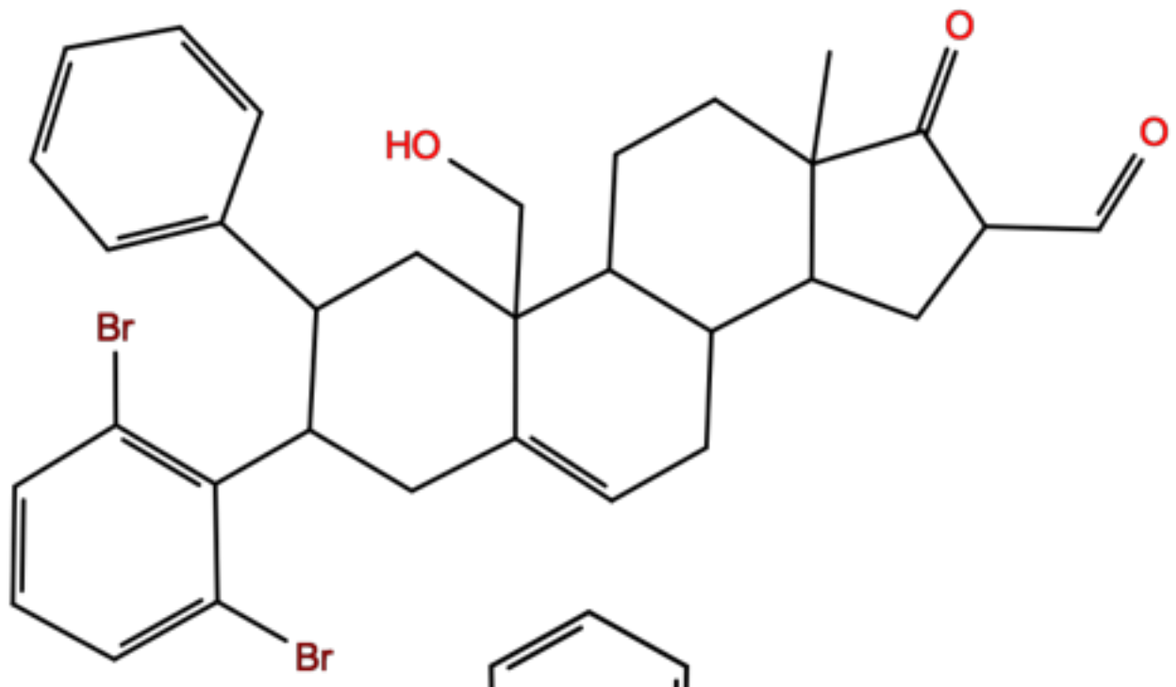


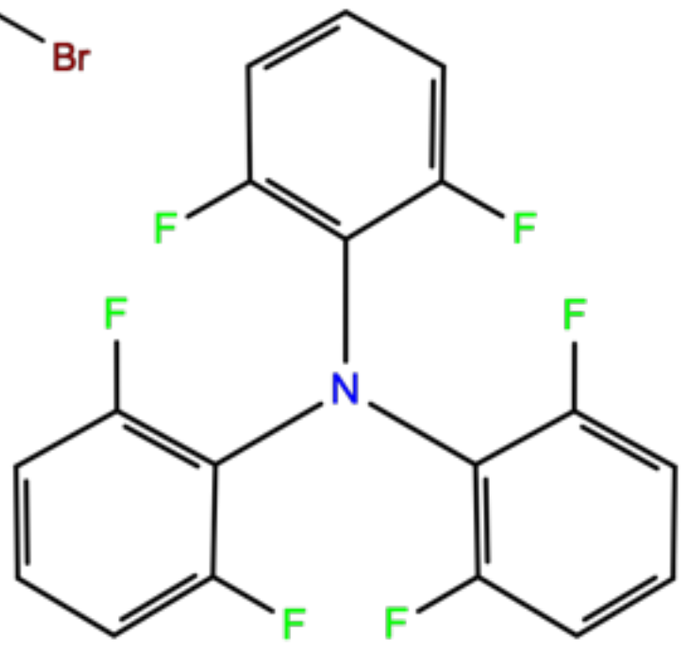


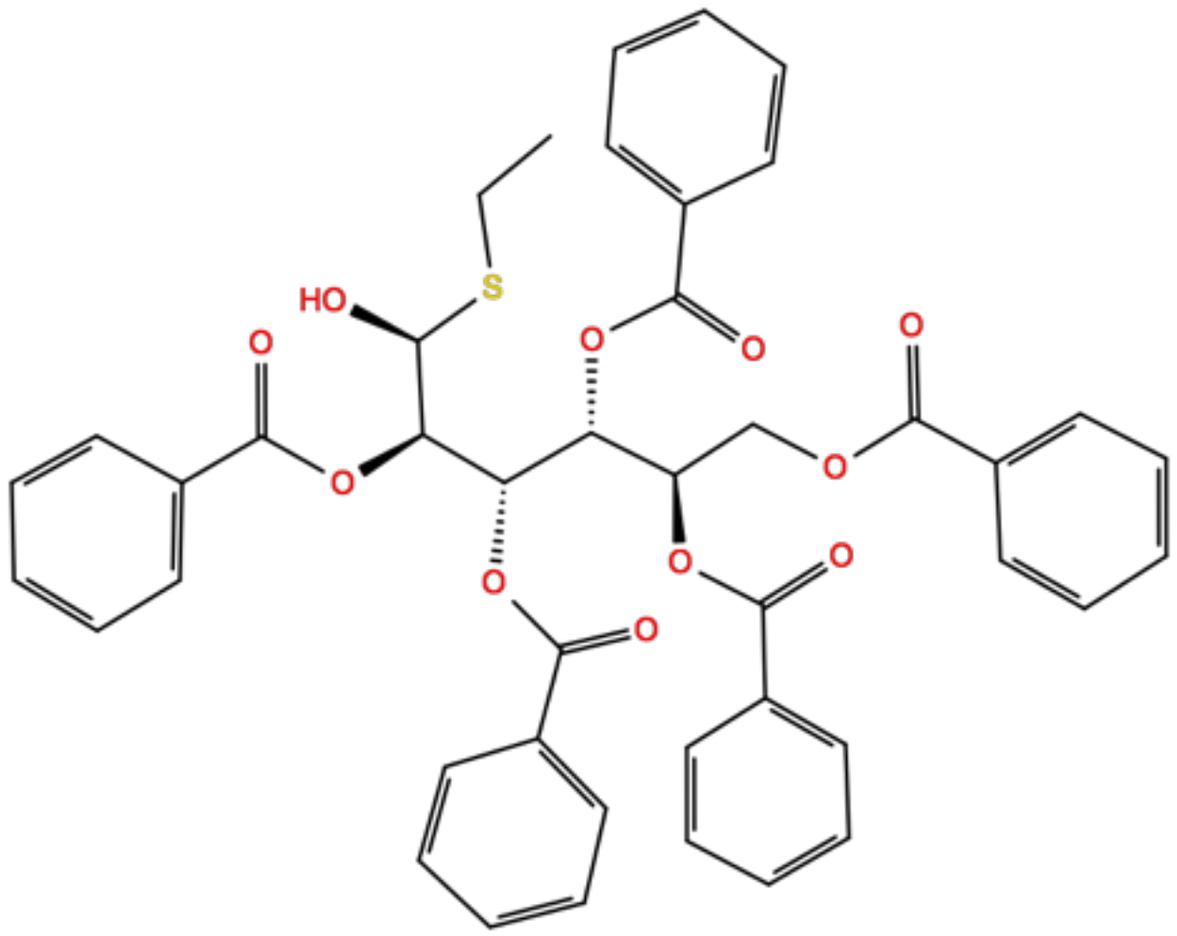
flip stretch pivot

FF minimisation

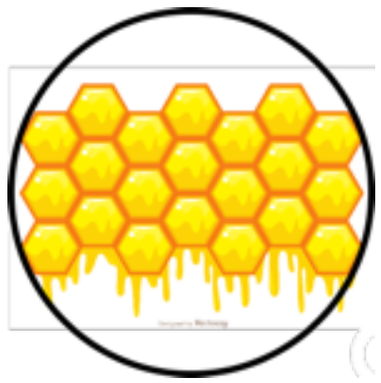




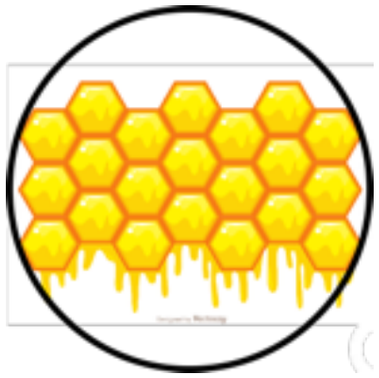




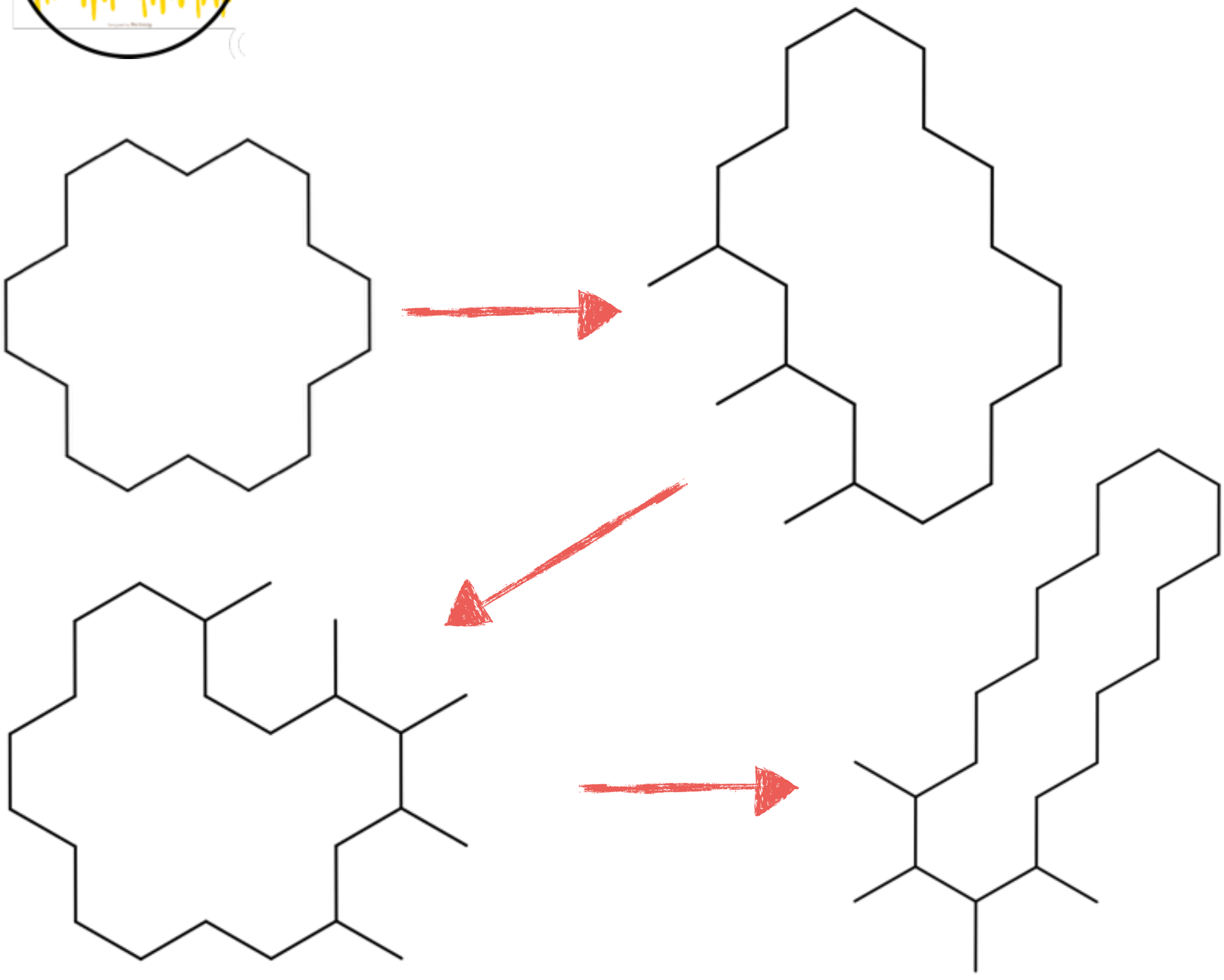
lvl 4 - macrocycles

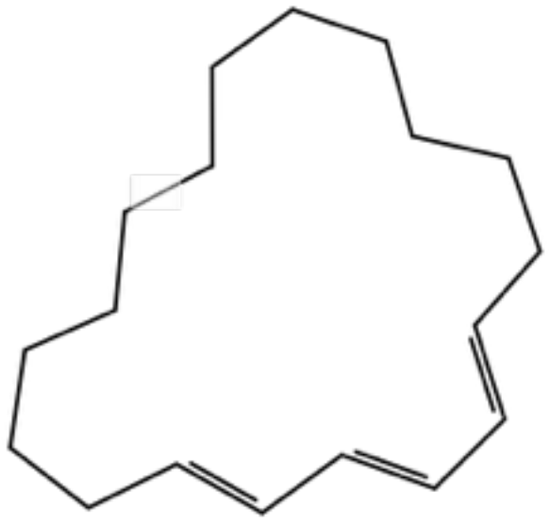


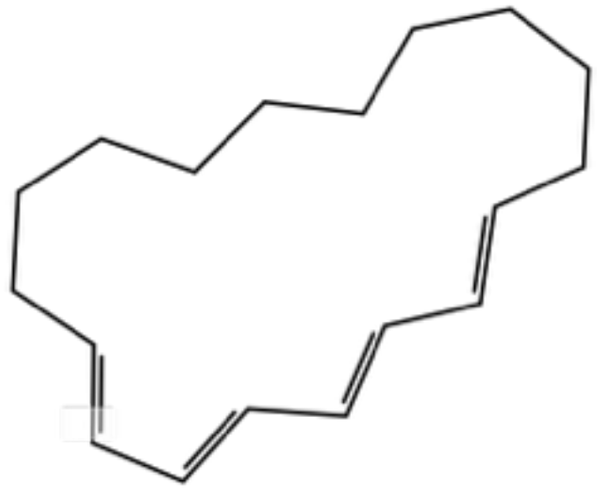
Hexagonal polyominoes

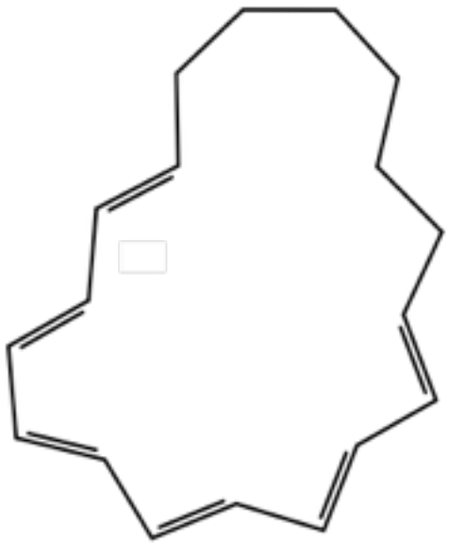


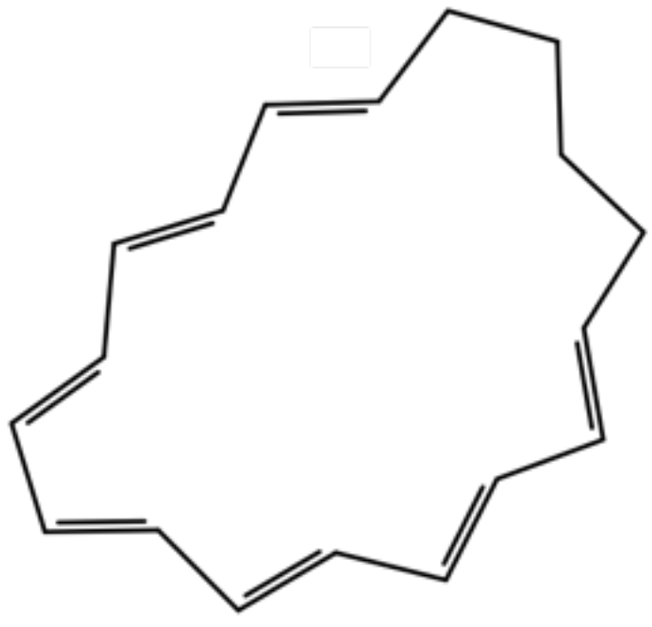
Honeycomb tetris

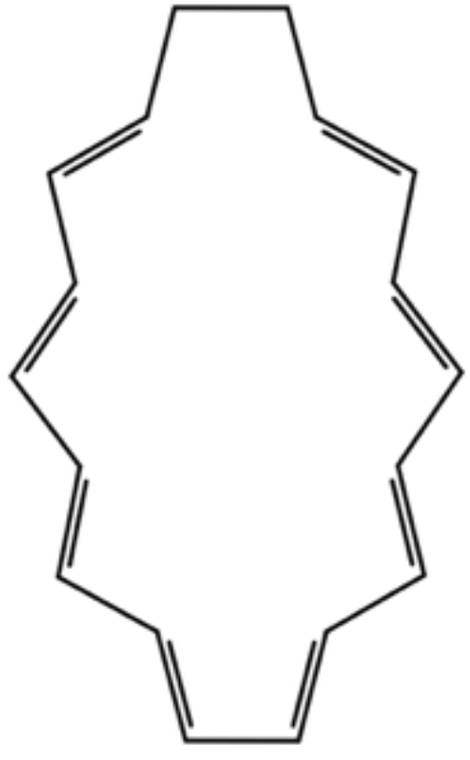




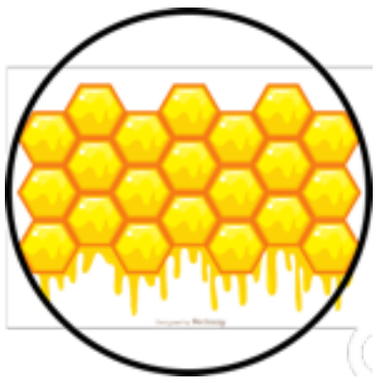


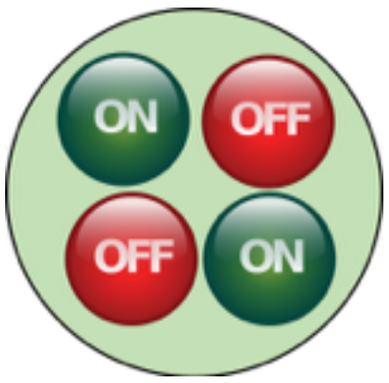


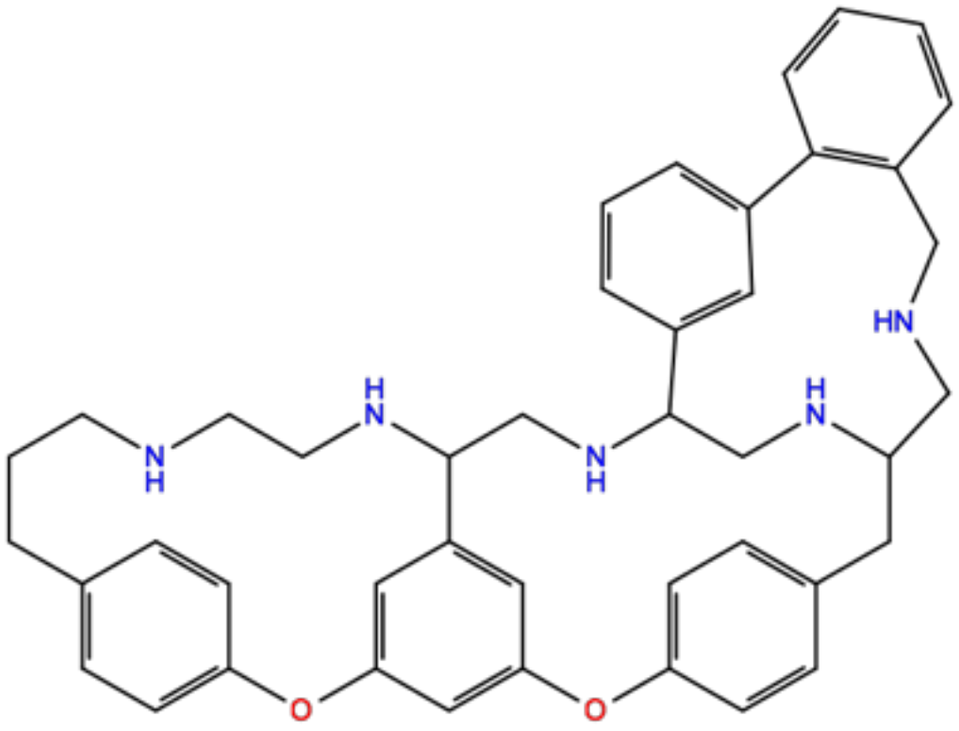




lvl 5 - macrocycle systems



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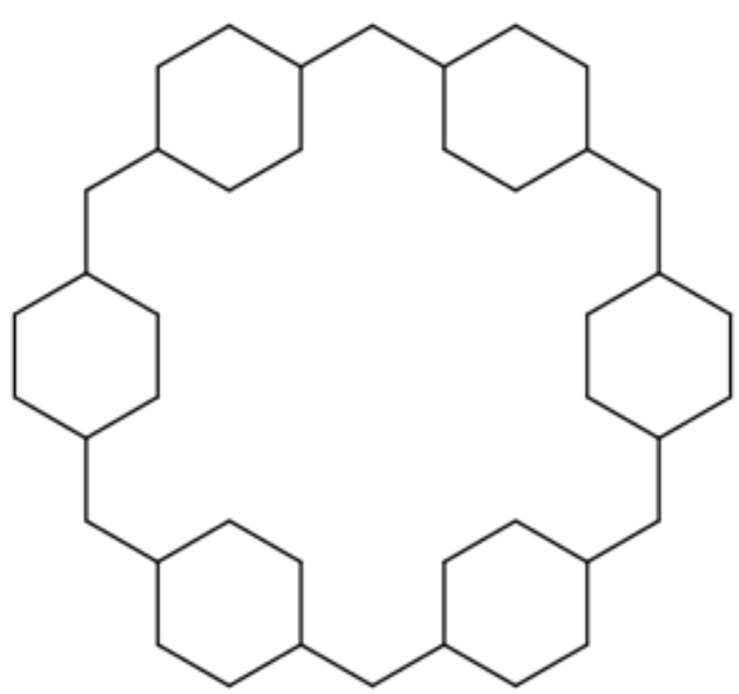
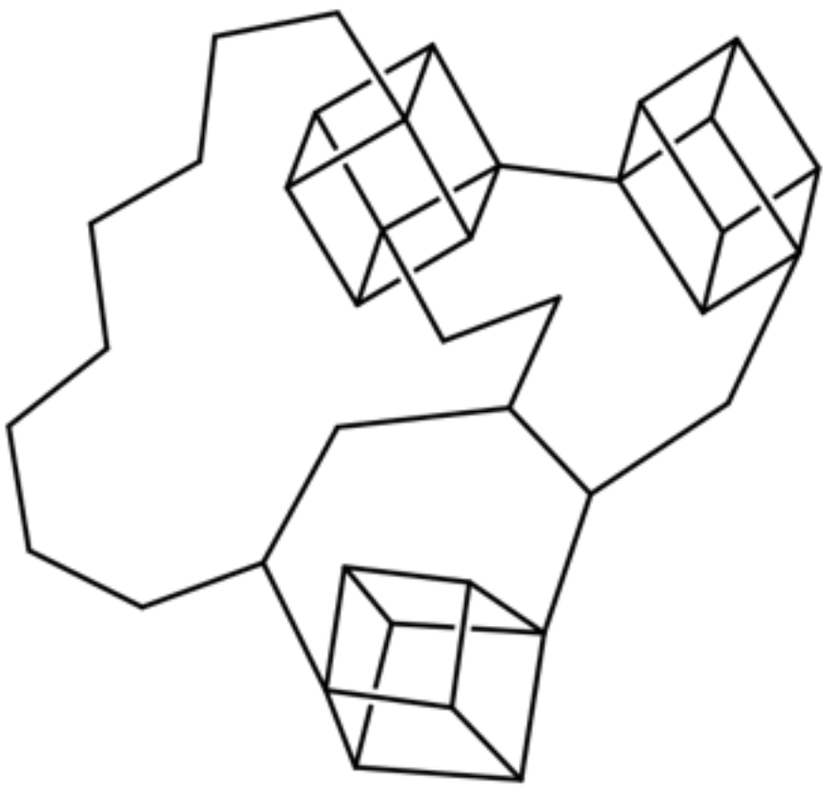
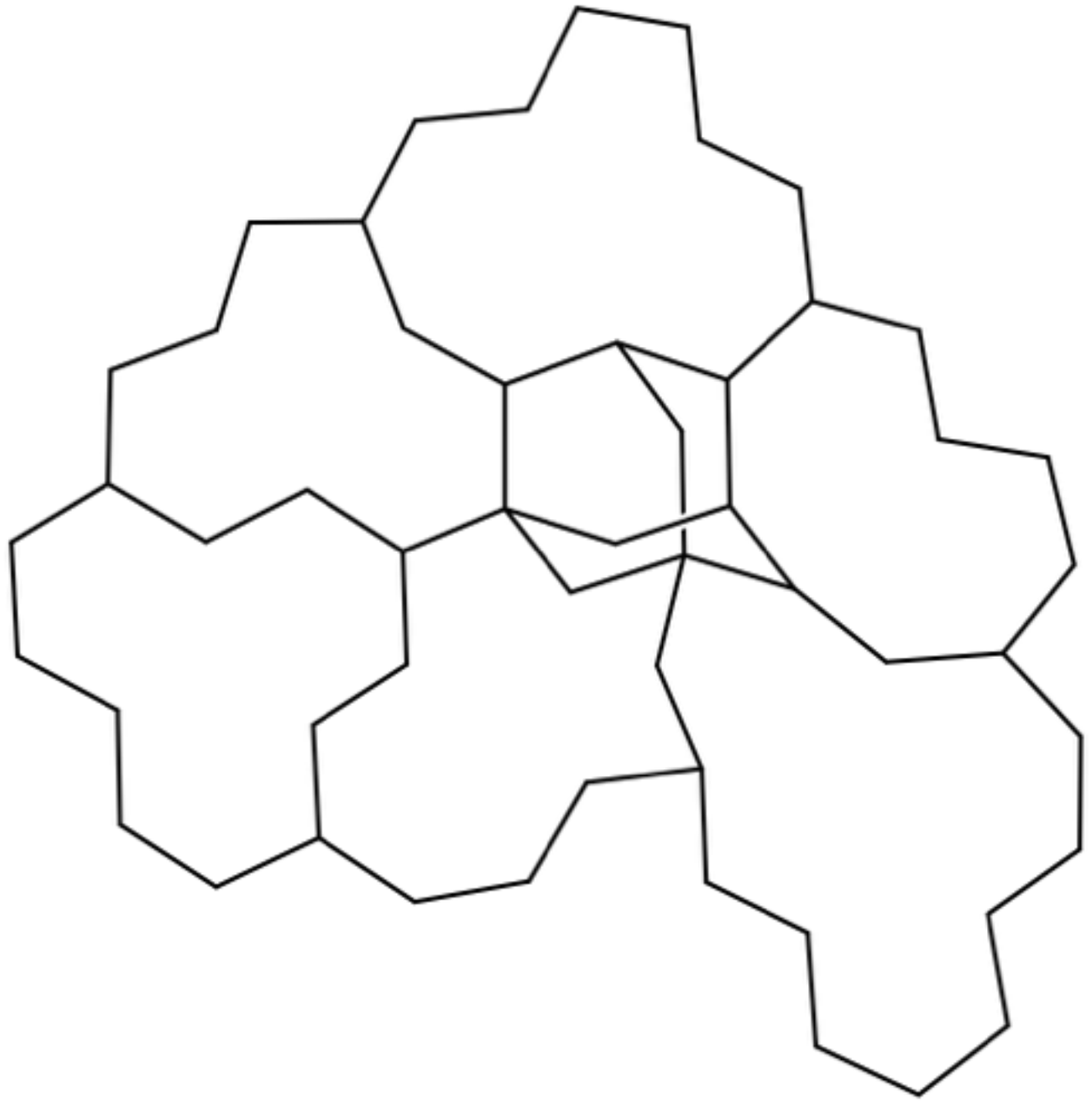
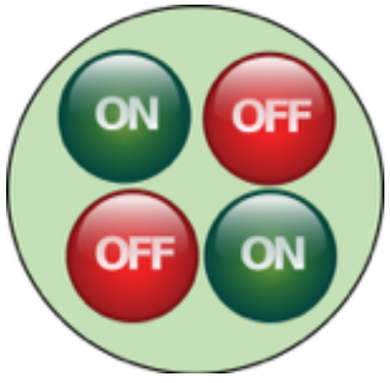


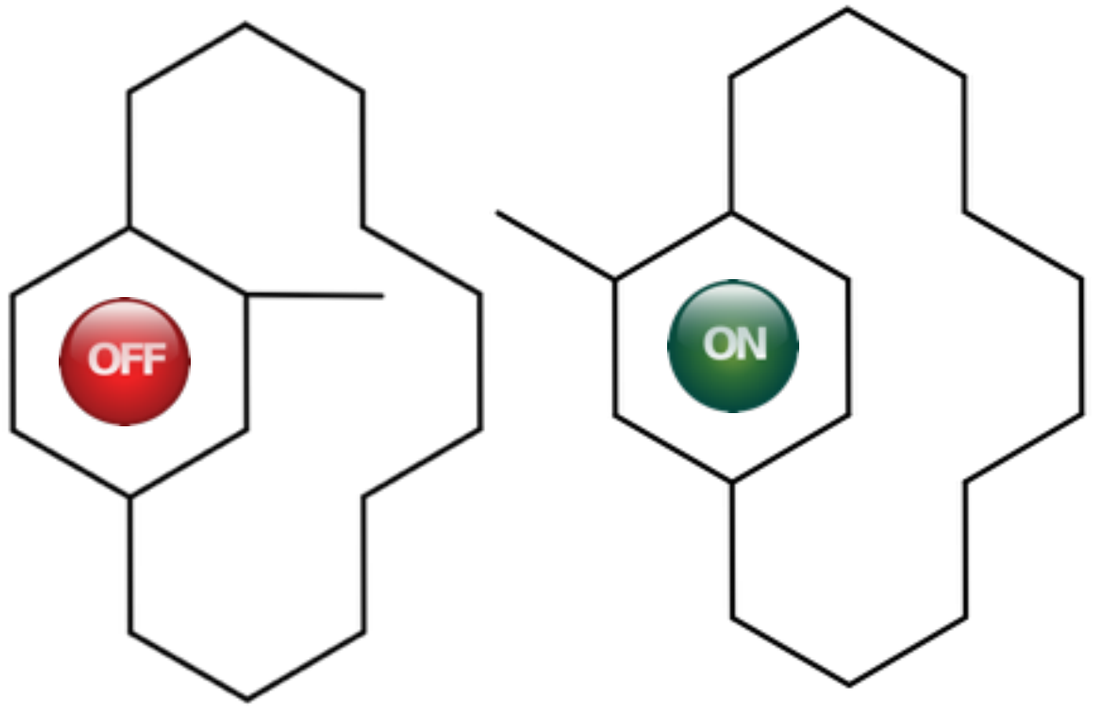




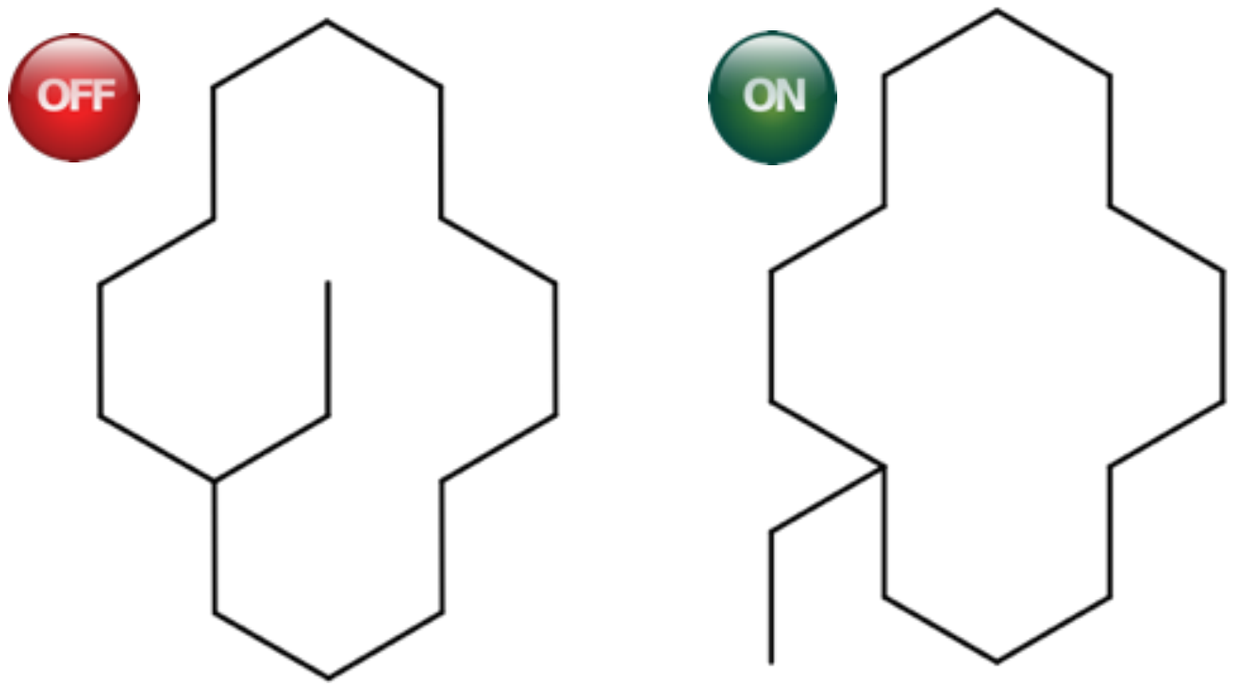
Fantachemistry

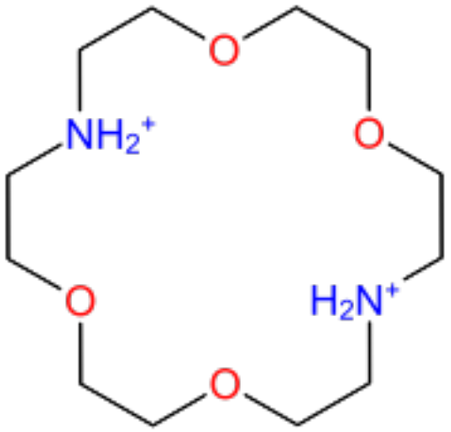


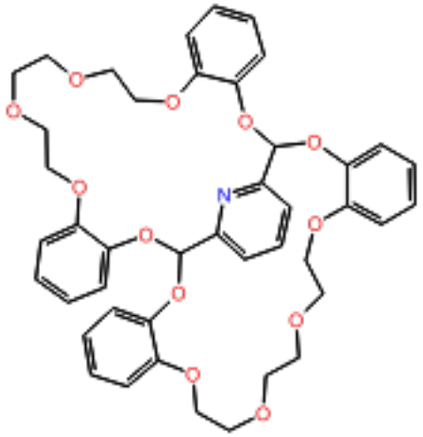
ring flip

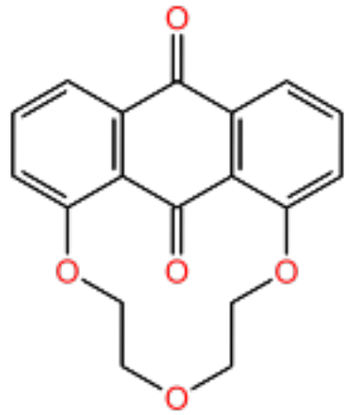


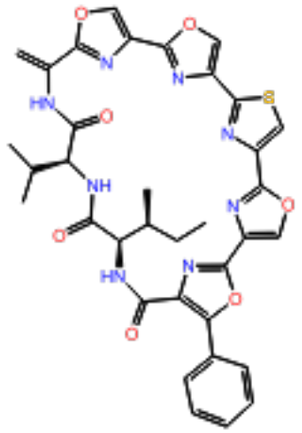
mirror

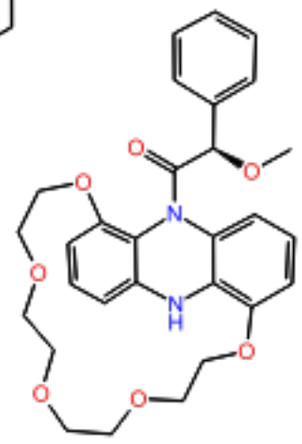


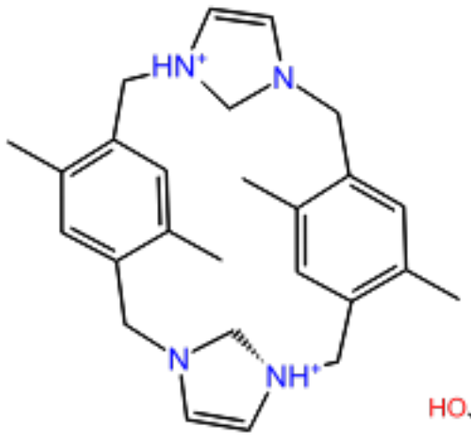


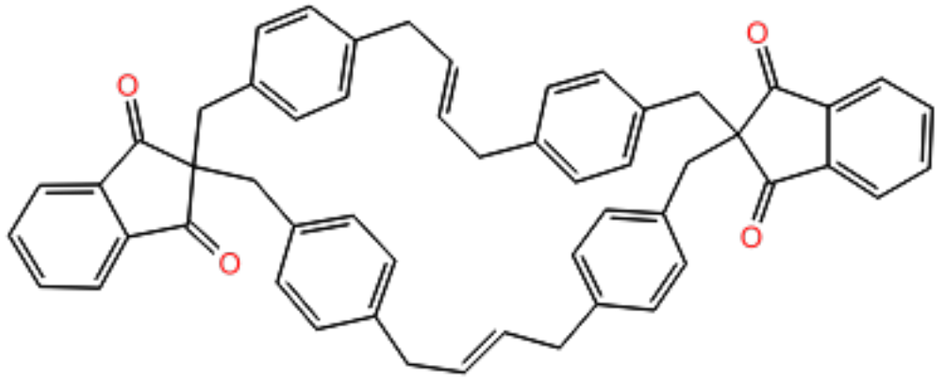


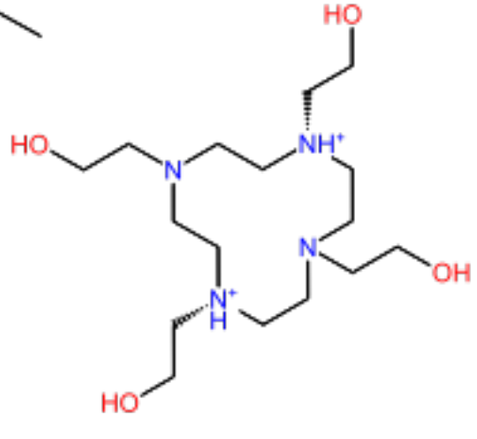


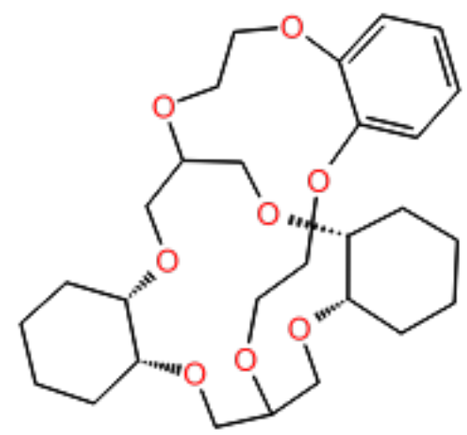




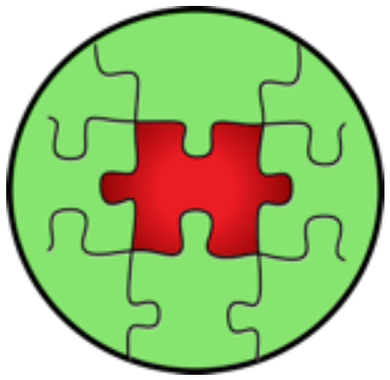


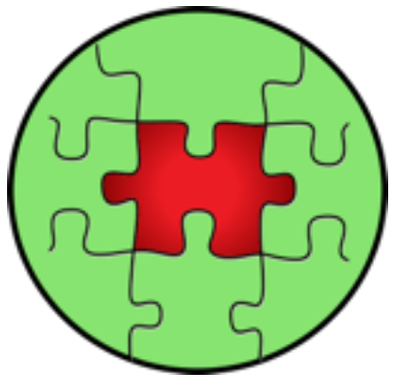




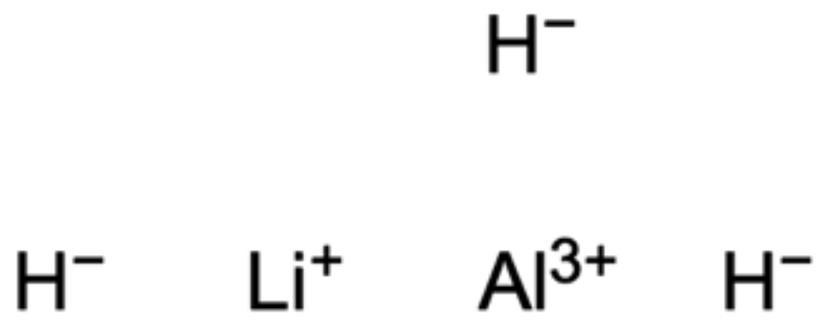


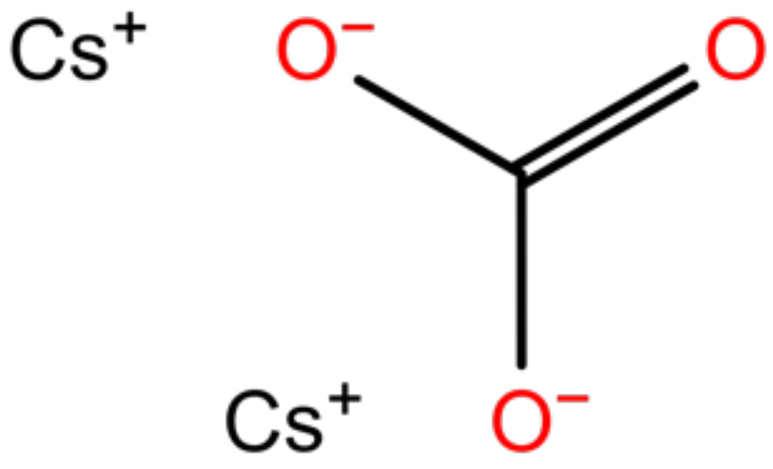
lvl 8 - molecular systems

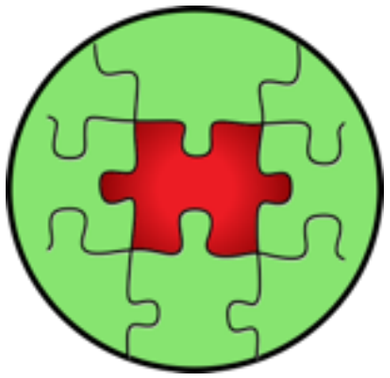




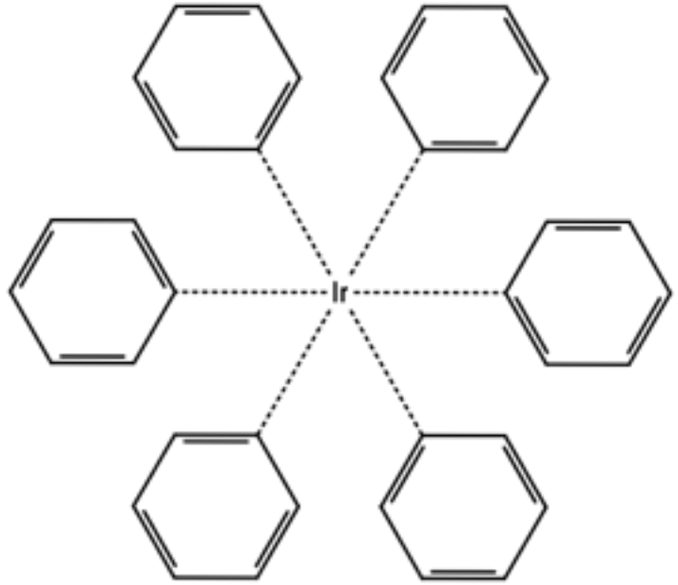
Counterions

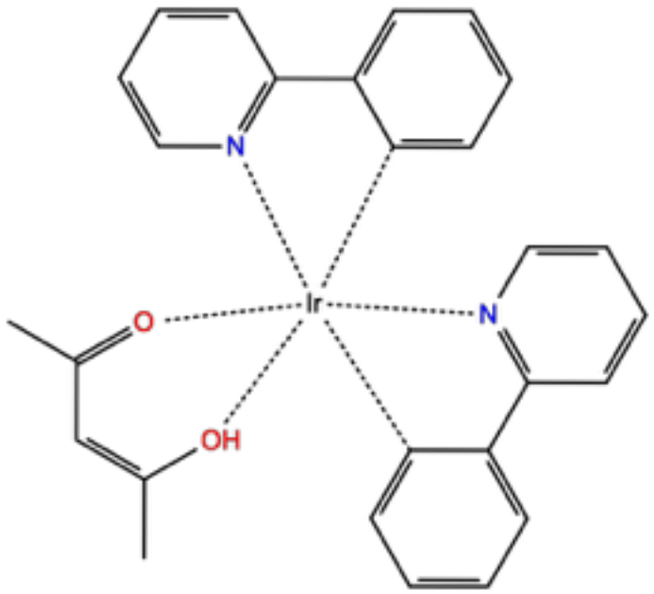


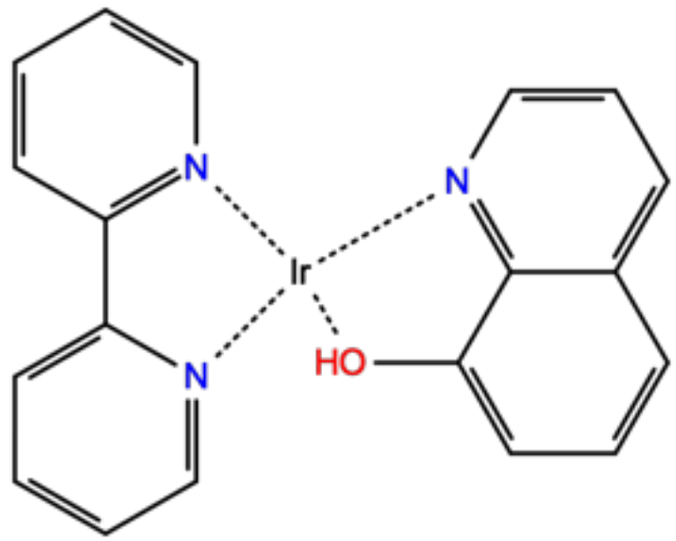


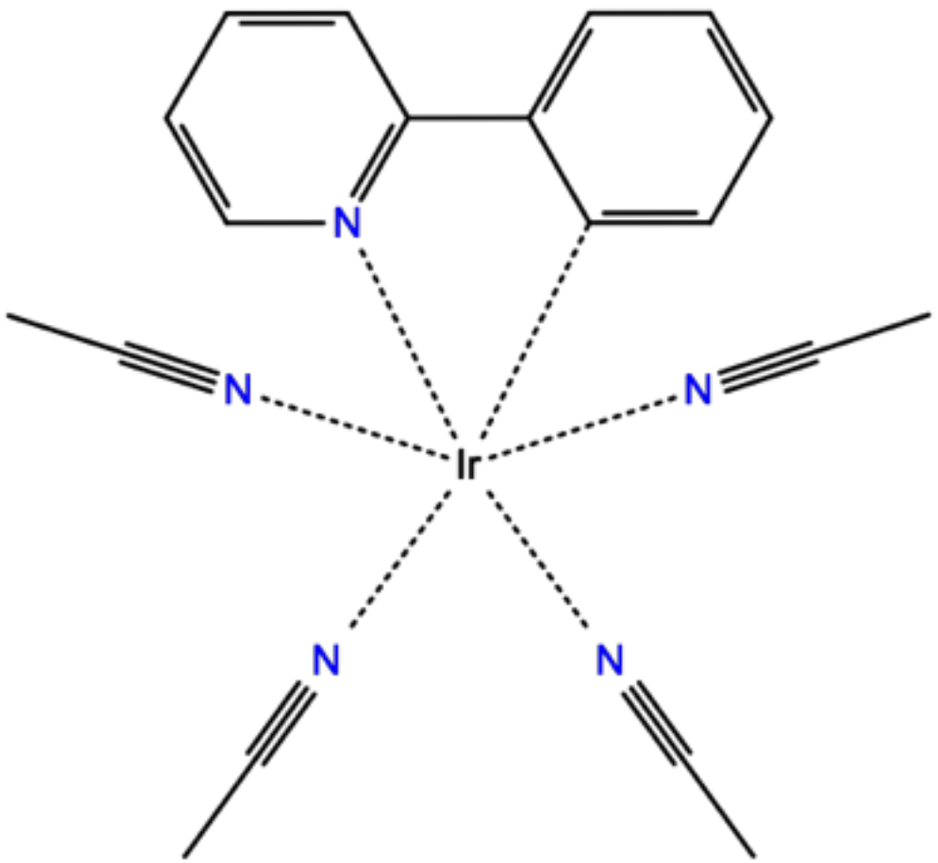


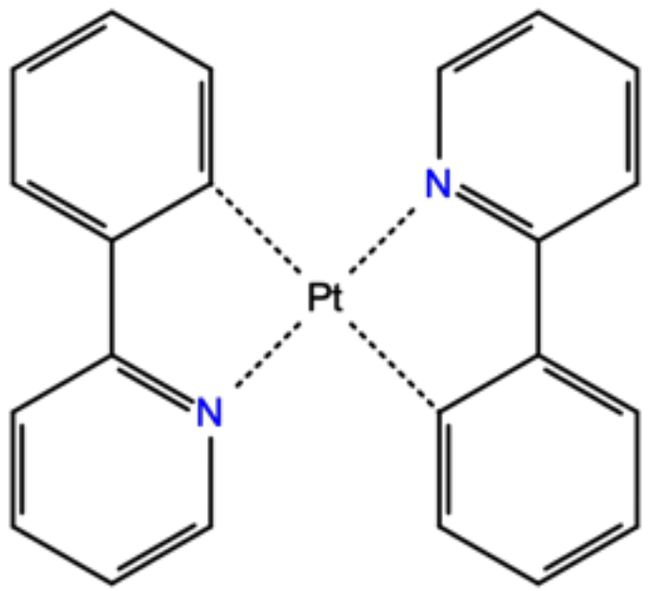
Metal coordination

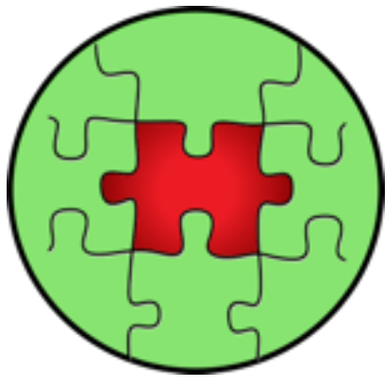






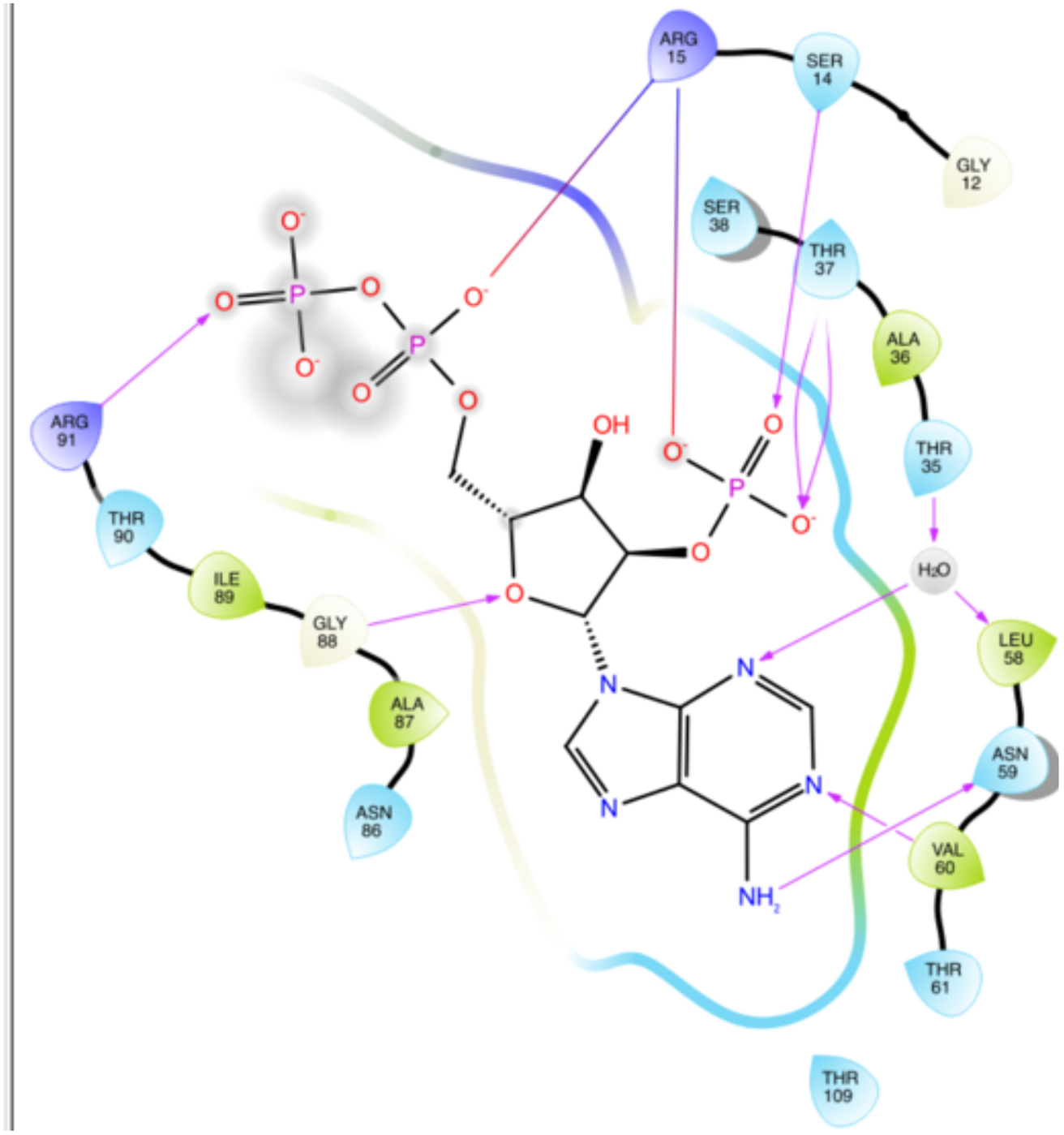






Residues

1q7c



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Thank you very much!

Any Questions?