Chemical Structure Recognition: A Rule-based Approach

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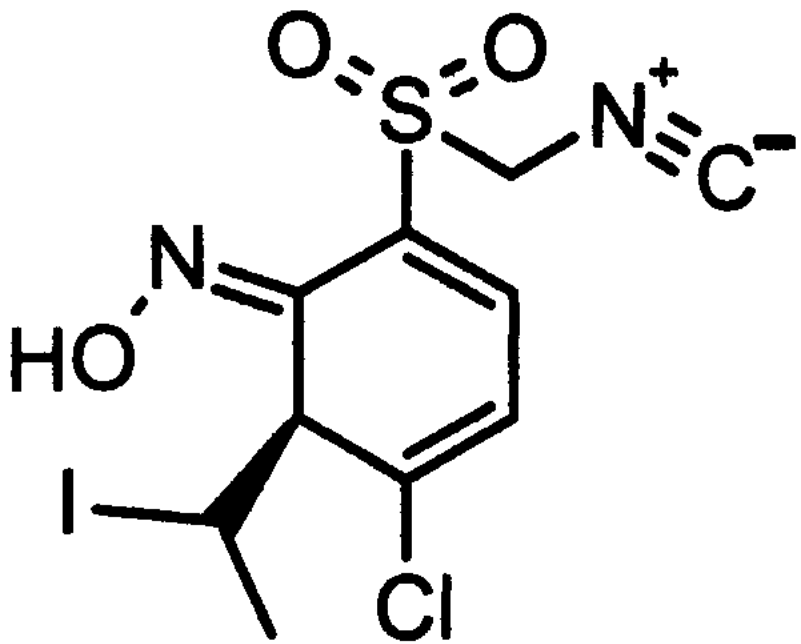
Motivation

- Chemical literature contains much information in molecule diagrams
  research articles, patent specs, catalogues, etc.
- Diagram recognition can make information accessible
  visually impaired readers, search, chemical software
- There are a number of academic and commercial approaches
  mostly following a traditional procedural method
  details often only vaguely described

We present a clearly defined rule based approach.

Problem



Recognising molecular diagrams requires:

- Basic image analysis
- Shape recognition
- Contextual discrimination of many cases
- Strategy to manage cases

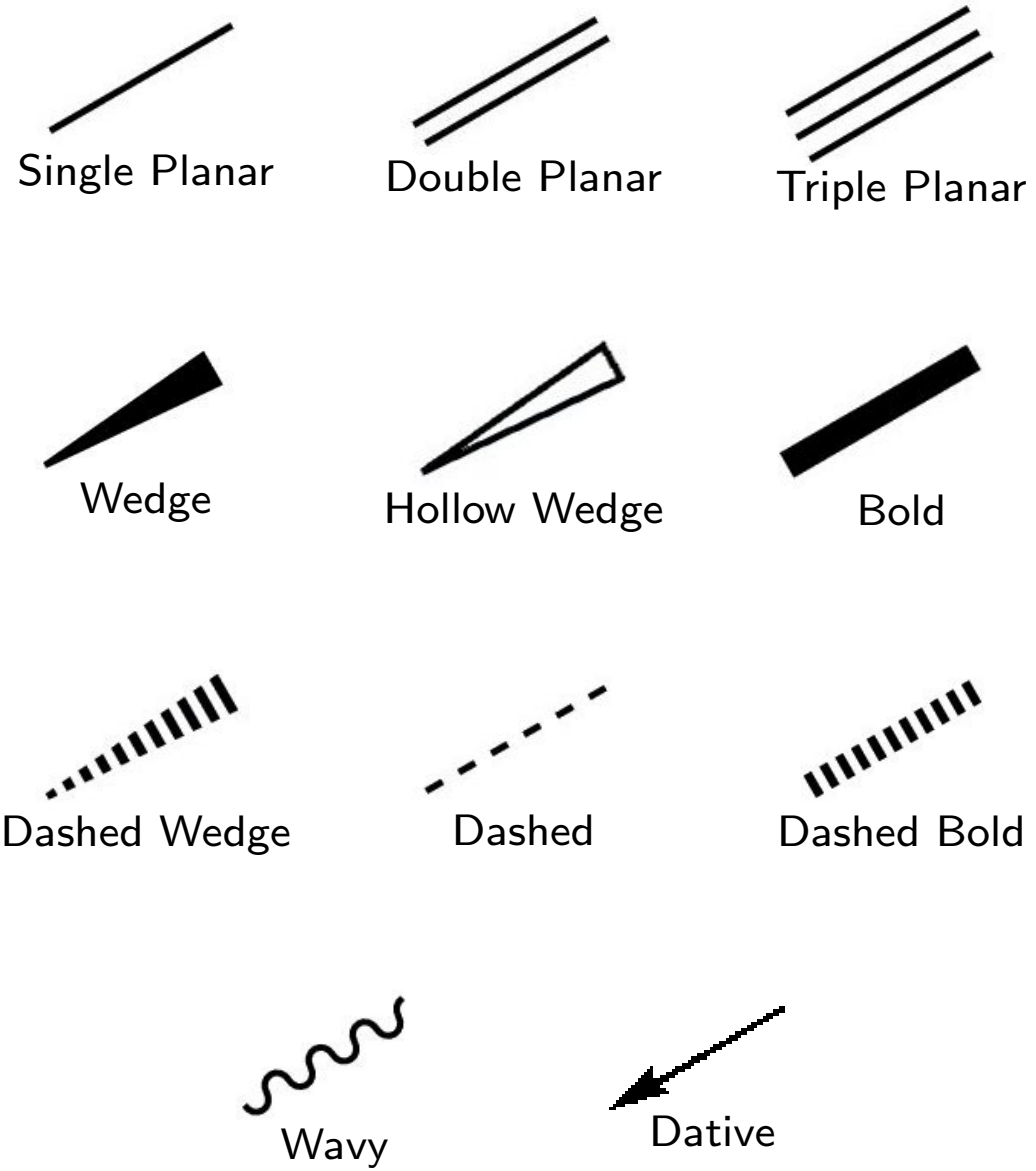
Diagram Elements

Single Planar

Double Planar

Triple Planar

Diagram Elements



Extra Complexities

Implicit Nodes in Bond Sequences

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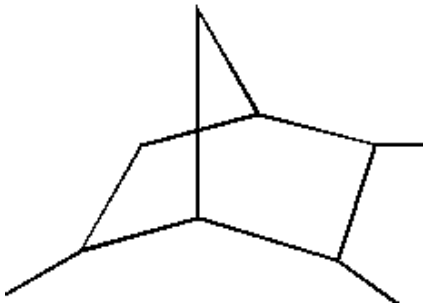
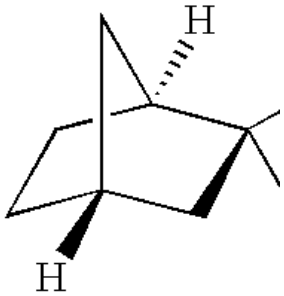


Closed Bridge Bond



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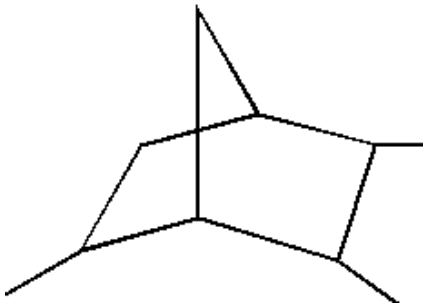

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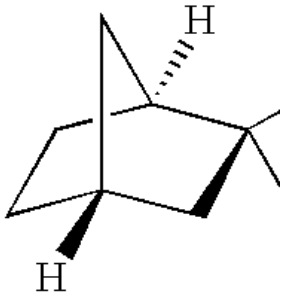

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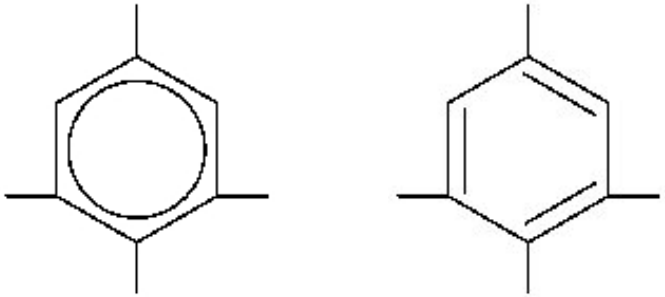
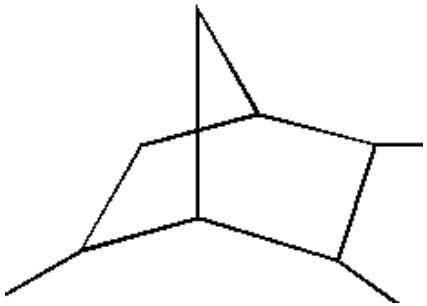


Aromatic Rings

Extra Complexities

Implicit Nodes in Bond Sequences



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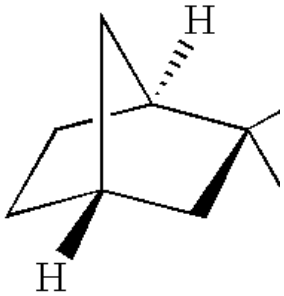
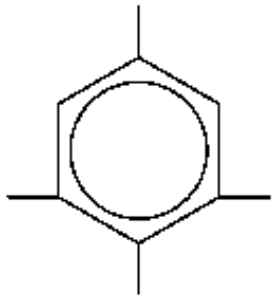
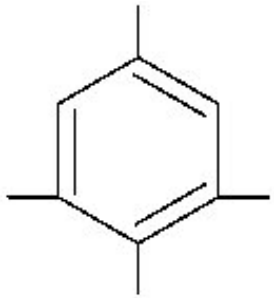
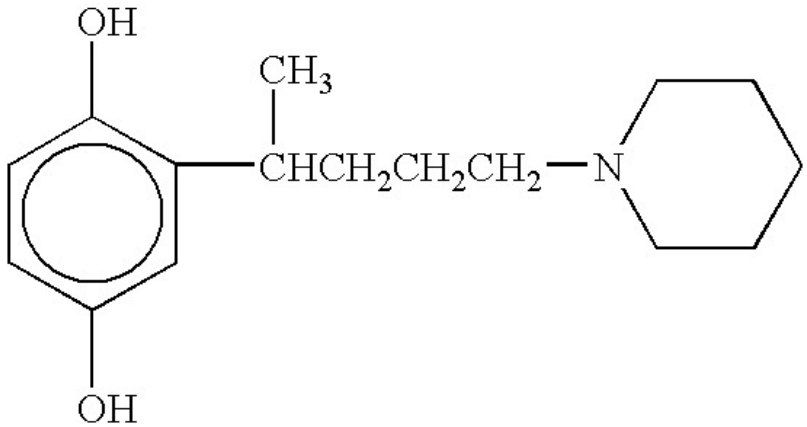


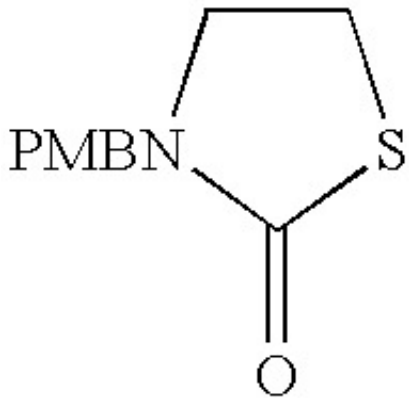
Open Bridge Bond





Aromatic Rings





Superatoms

Overall Procedure

- Preprocessing
  Noise removal, binarise, connected-component analysis
- Simple OCR & Character Grouping
- Detection of geometric primitives:
  Line segments, Arrows, Circles, Triangles, Character Groups
- Rewrite primitives into a directed graph using rule-based System
- Disambiguation and graph correction
- Produce output from graph (e.g. MOL, SMILES)

Rule Based System

Input: Set of well defined geometric primitives:
Line segments, Arrows, Circles, Triangles, [Character Groups]

Output: Directed graph representing a molecule

- 18 rules defined in terms of

  Preconditions: Find and remove appropriate primitives

  Postconditions: Add to output graph and possibly new primitives
- Mutually exclusive pre-conditions (except 2 bridge bond rules)
- Order of application is irrelevant
- A number of fuzzy parameters allow for some training.

Some Concepts and Parameters

- Approximate Collinearity/Dash Neighbouring
  - Radius of collinearity *rc*
  - Dash length *dl*
  - Dash separation *ds*

- Approximately Parallel with separation *bs* and overlap *ol*, $\|_{bs}^{ol}$

Bond Rules I

Single Planar Bond

1. l is a line segment.
2. There is no line segment l' such that $l \parallel^{ol}_{bs} l'$.

Consequence l is a single bond with endpoints of l

Bond Rules II

Double Planar Bond

1. $L = \{l_1, l_2\}$ is a set of two line segments.
2. $length(l_1) > wb$ and $length(l_2) > wb$.
3. $l_1 \parallel^{ol}_{bs} l_2$.
4. There is no line segment $l \notin L$ such that $l_1 \parallel^{ol}_{bs} l$ or $l_2 \parallel^{ol}_{bs} l$.

Consequence Cutting(l_1, l_2) will yield a double bond as well as at most two new line segments.

Bond Rules III

Triple Planar Bond

1. $L = \{l_1, l_2, l_3\}$ is a set of three line segments.
2. for every $l \in L$ we have $length(l) > wb$.
3. $l_1 \parallel^{ol}_{bs} l_2$ and $l_2 \parallel^{ol}_{bs} l_3$ and $l_1 \parallel^{ol}_{2*bs} l_3$.
4. There is no line segment $l \notin L$ such that $l_1 \parallel^{ol}_{bs} l$ or $l_2 \parallel^{ol}_{bs} l$ or $l_3 \parallel^{ol}_{bs} l$.

Consequence Cutting(l_1, l_2, l_3) will yield a triple bond as well as at most four new line segments.

Bond Rules IV

Dashed Bond

1. $L = \{l_1, \ldots, l_n\}$, where $n \geq 3$, is a set of line segments,
2. L is approximately collinear.
3. Every element of L has length of approximately dl.
4. No two elements of L have a separation distance of less than the minimum of ds.
5. Two elements of L, called the *end elements*, dash-neighbour wrt. ds precisely one other element of L. All other elements of L, called *internal elements*, dash-neighbour wrt. ds precisely two other elements of L.

Consequence L forms a dashed bond with endpoints given by the endpoints of the minimal line segment that contains $l_1, \ldots, l_n$.

Results I

- OSRA's benchmark dataset of 5735 images:

	OSRA Succ.		OSRA Failed		Total	
MolRec Succ.	4277	(74.58%)	796	(13.88%)	5037	(88.46%)
MolRec Failed	152	(2.65%)	510	(8.89%)	662	(11.54%)
Total	4429	(77.23%)	1306	(22.77%)	5735	(100%)

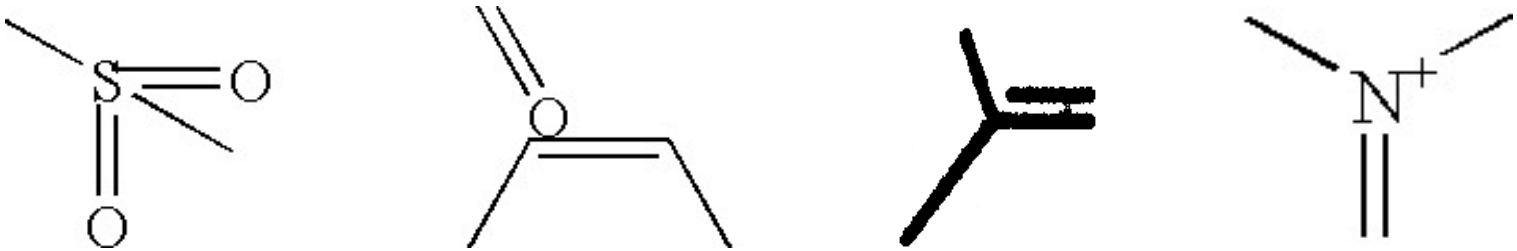
- Our dataset of 5740 images from Maybridge catalogue:

	OSRA Succ.		OSRA Failed		Total	
MolRec Succ.	3823	(66.72%)	981	(17.12%)	4804	(83.84%)
MolRec Failed	335	(5.85%)	591	(10.31%)	926	(16.16%)
Total	4158	(72.57%)	1572	(27.43%)	5730	(100%)

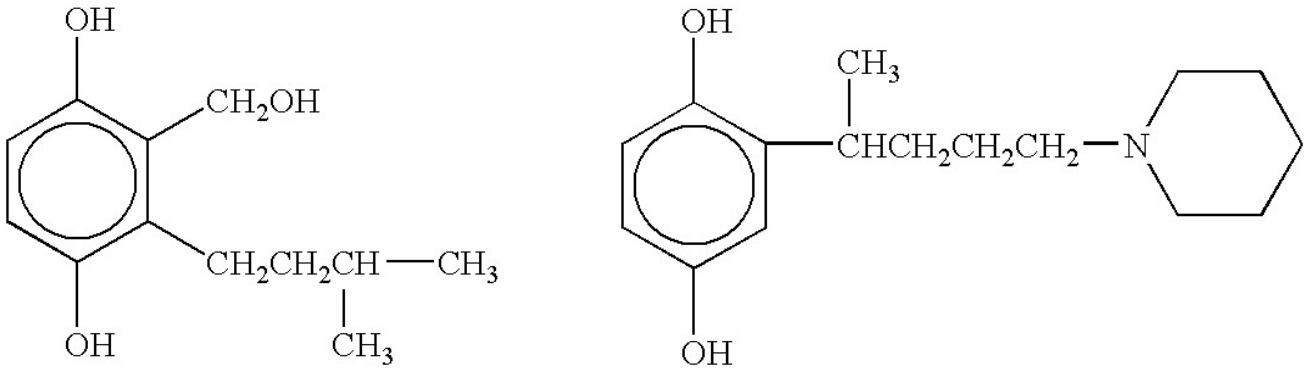
- TREC's Image2Structure Task:
  Achieved highest recognition rate (95%) on 1000 test images.

Reasons for Failure I

- Image has touching components:

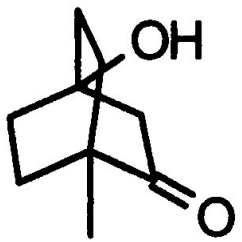


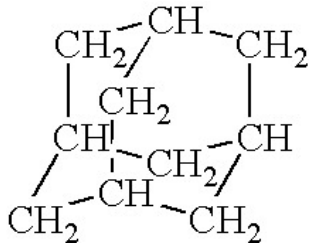
- Incorrect superatom connectivity:



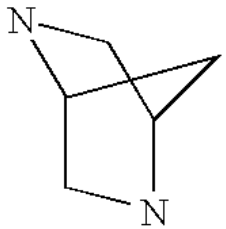
Reasons for Failure II

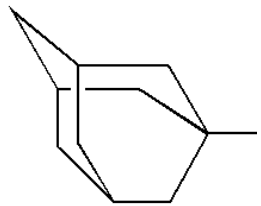
- Ambiguous Images:





- Problematic bridge bonds:





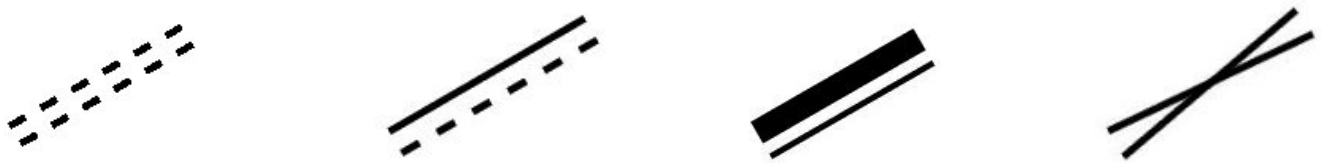
Reasons for Failure III

- Incorrect stereochemistry:

  - Our heuristics for guessing direction based on size of character group/complexity of structure at each end of the bond
  - Needs deeper domain knowledge to improve
- Dashed wedge bonds mis-identified:
  - Short dashes at narrow end mis-recognised as a dashed bond
  - Long dashes at wide end mis-recognised as dashed wedge or dashed bold bond
  - Result: dashed bond mis-recognised as 2 connected bonds

Conclusions and Future Work

- Clearly defined rule based approach to molecule recognition
- Some robust techniques to identify primitives
- First implementation yields good experimental results
- Flexible approach that can be easily extended
  Aromatic bonds, Tautomeric bonds, Double bond with stereo



- Better disambiguation for bridge bonds
- More chemical information to solve connection permutation problem for superatoms