Classifying Chemicals Using Description Graphs and Logic Programming

Despoina Magka, Boris Motik and Ian Horrocks

Department of Computer Science, University of Oxford

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Outline

1 Motivation

2 DGLPs, Implementation and Overview

Modelling Chemicals with OWL

- OWL used for the representation of molecular structures

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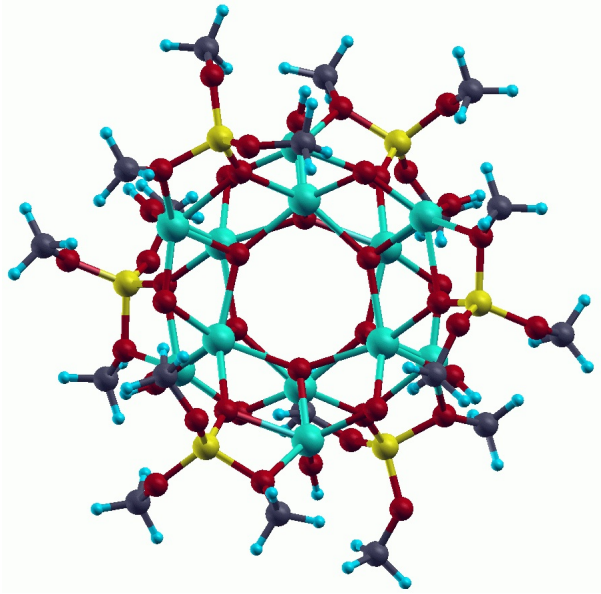

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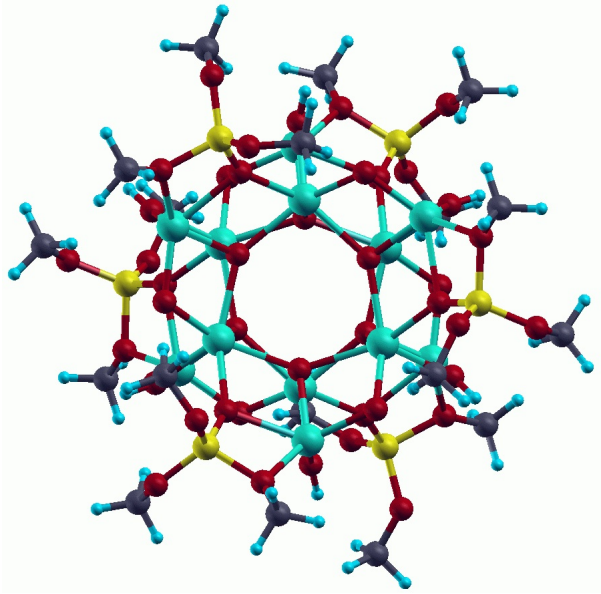

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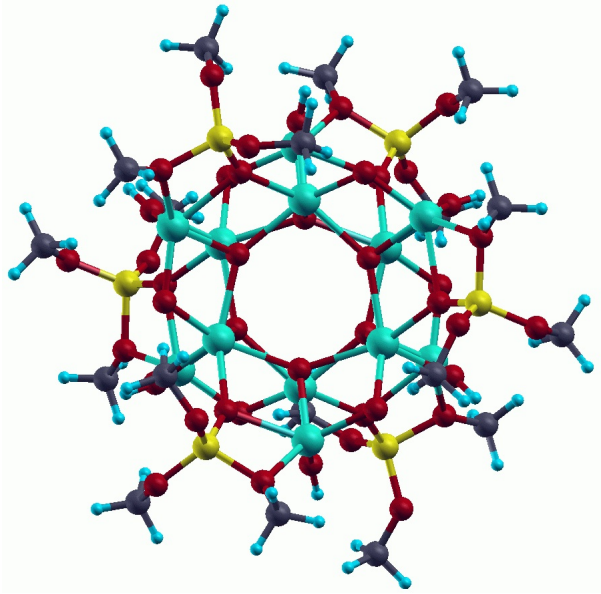

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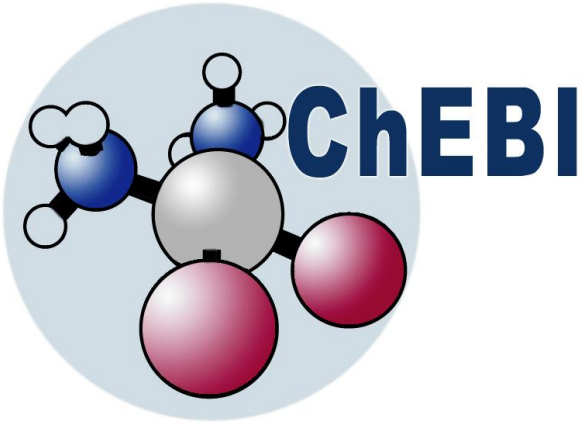
- Subsumptions between molecules and chemical classes
  [Hastings et al., OWLED, 2010]

THE CHEBI ONTOLOGY

- OWL ontology Chemical Entities of Biological Interest



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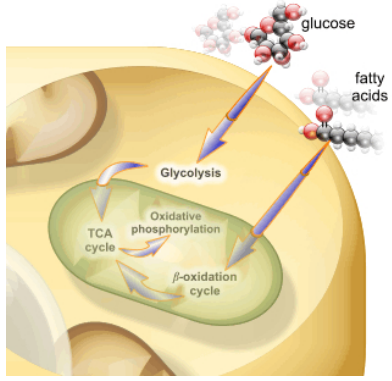

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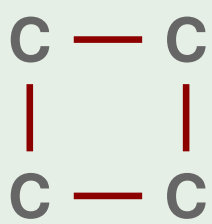

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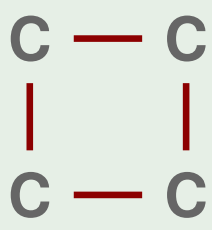

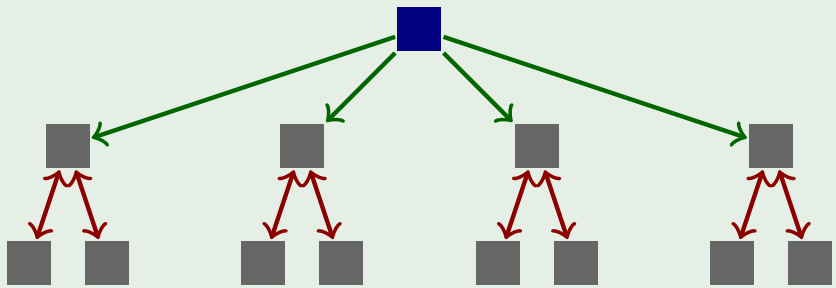

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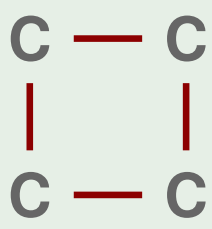

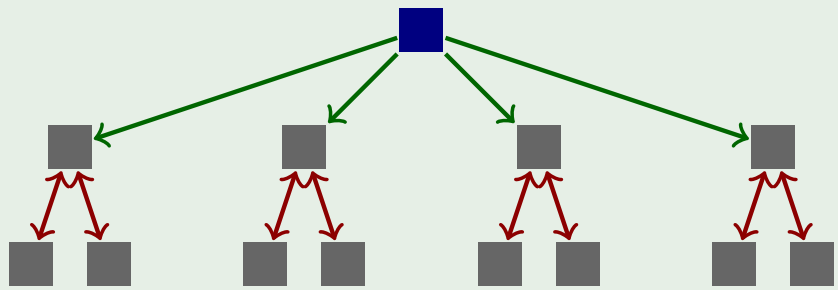

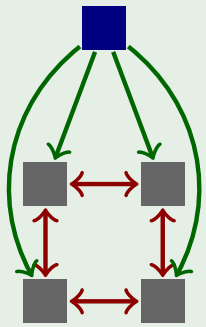

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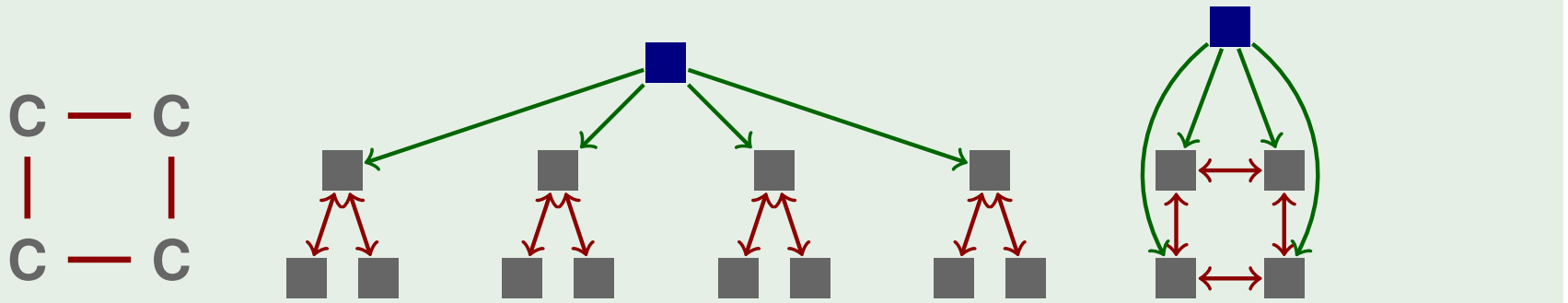

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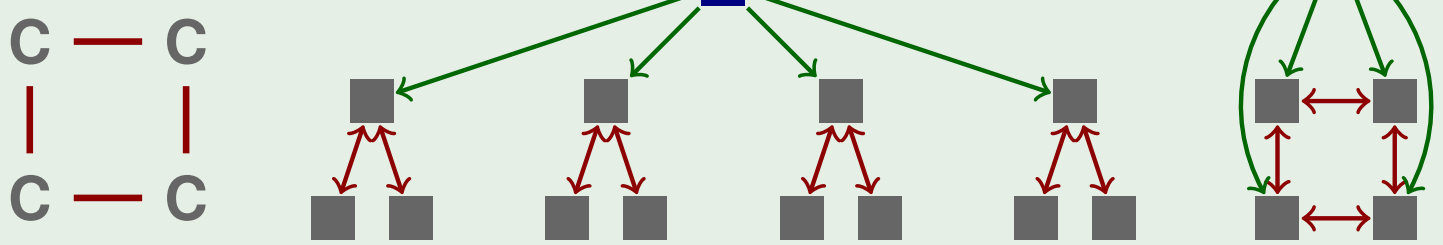

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  - Does cyclobutane contain a four-membered ring? ✘
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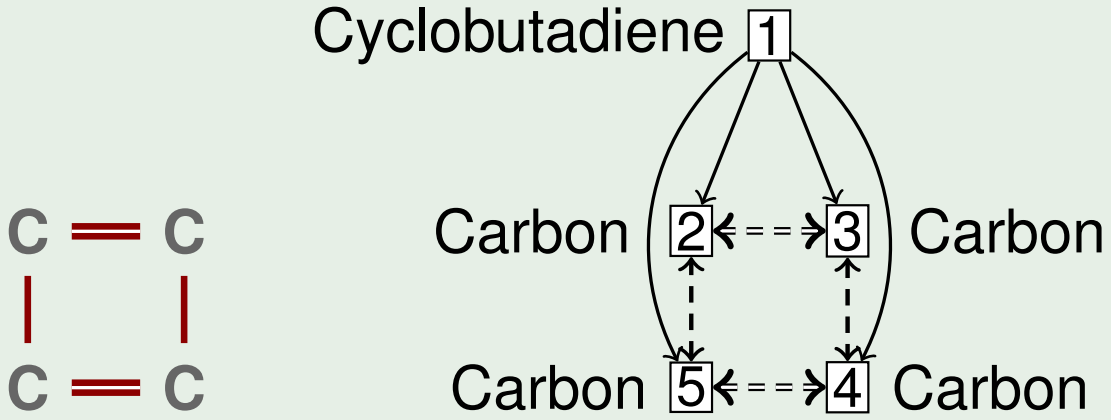

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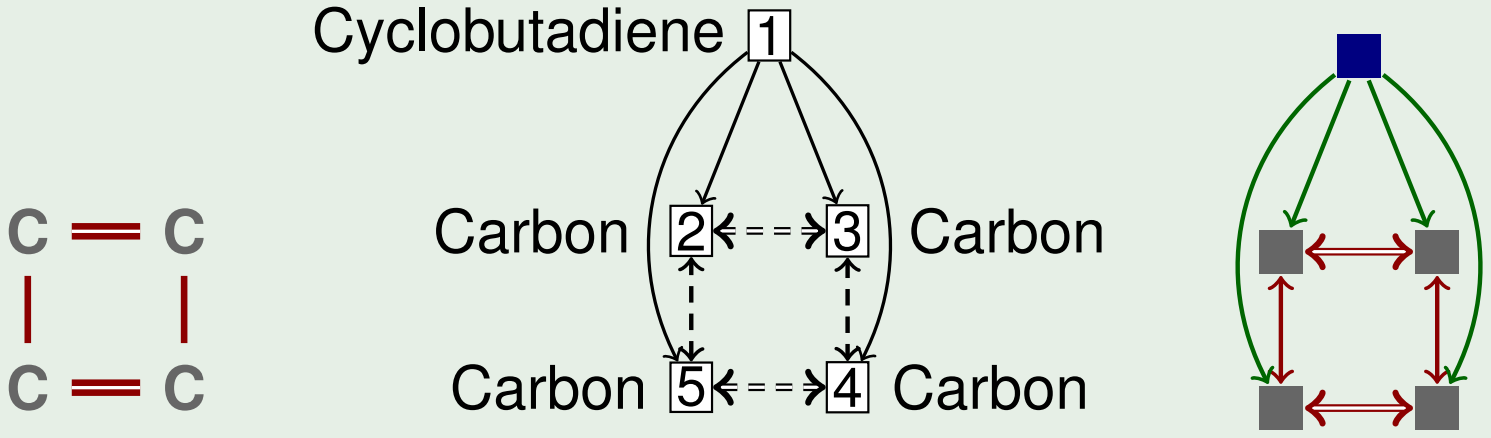

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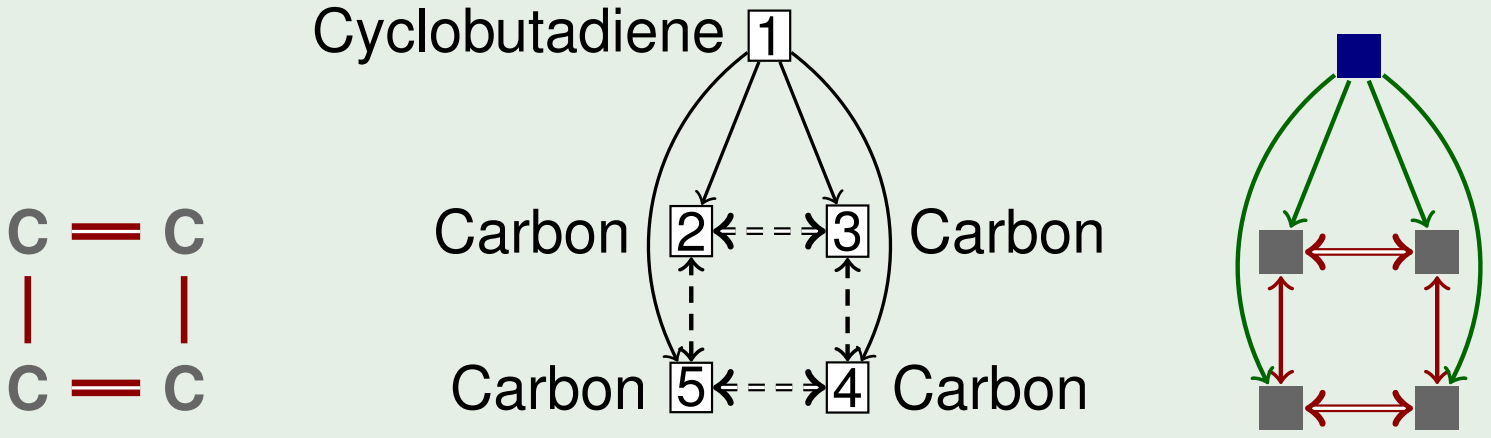

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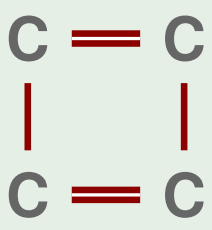

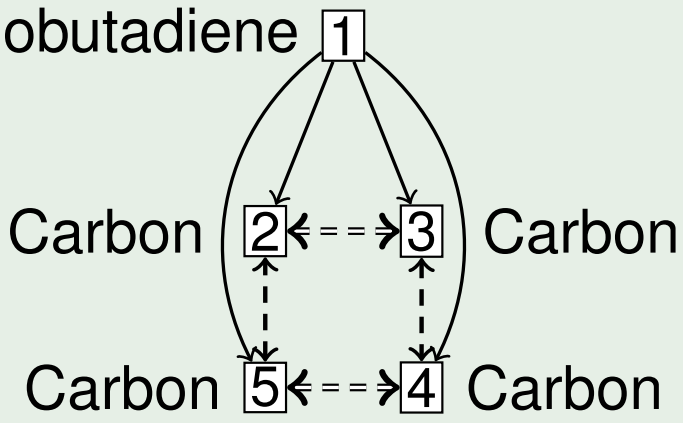

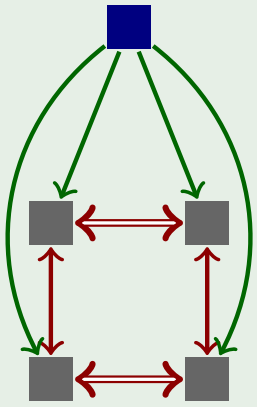

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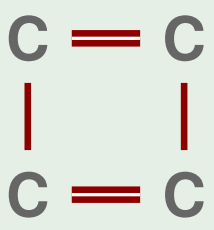

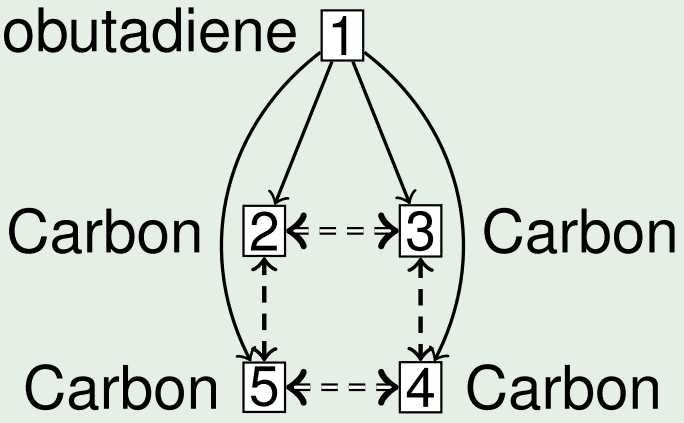

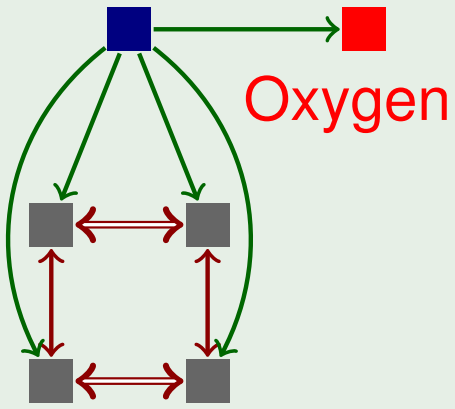

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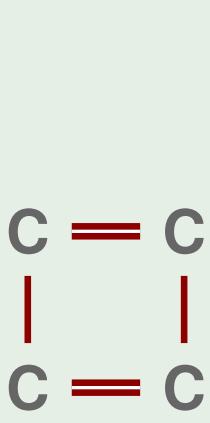

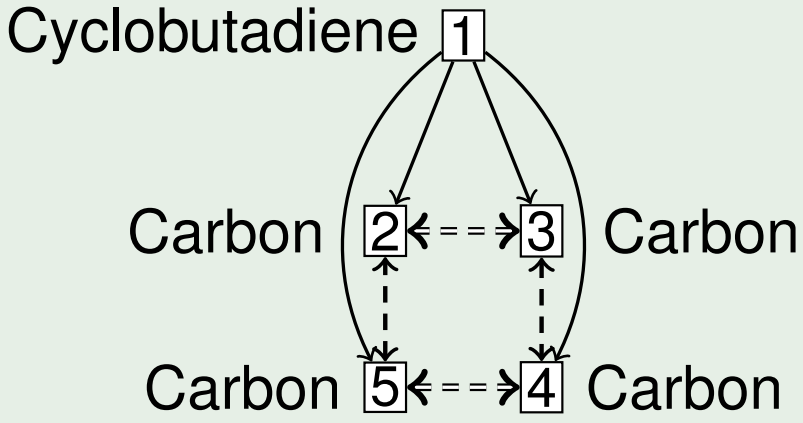

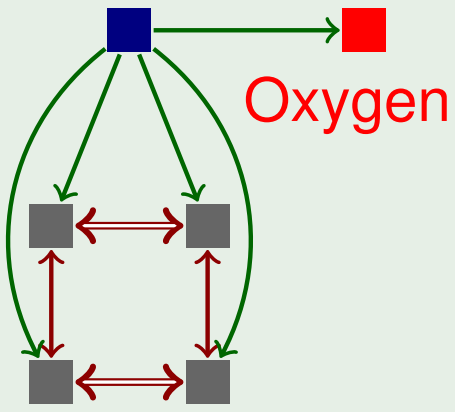

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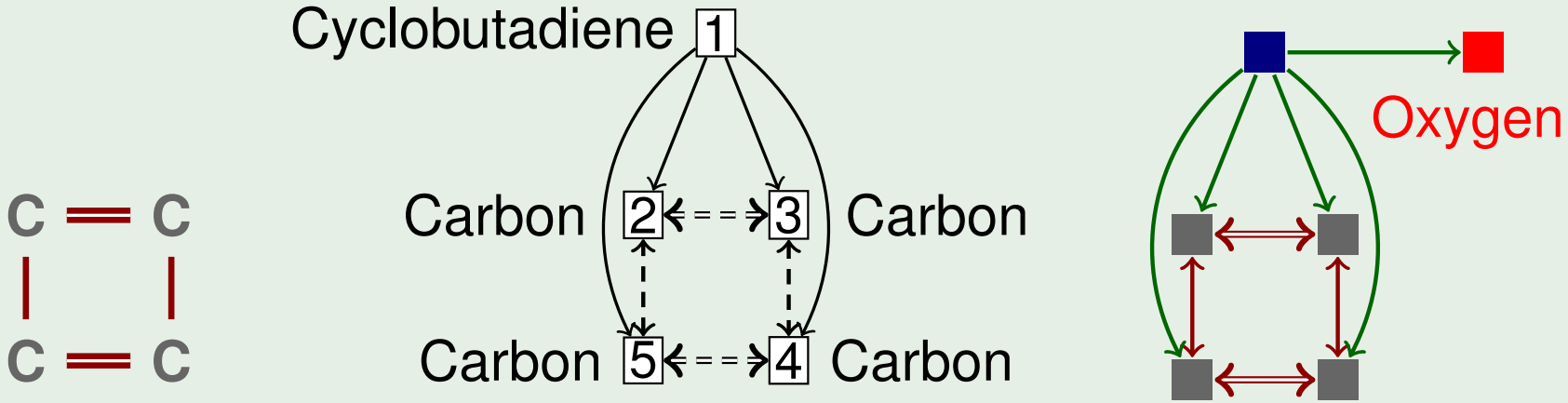

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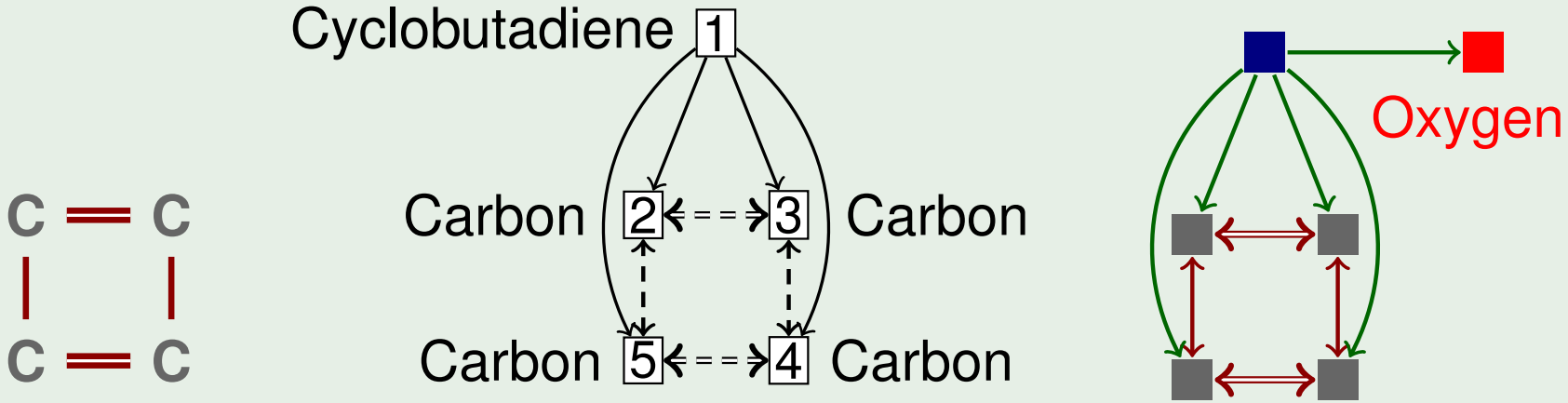

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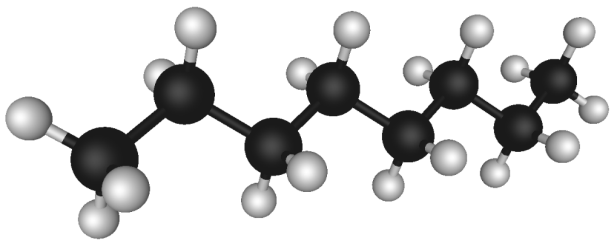

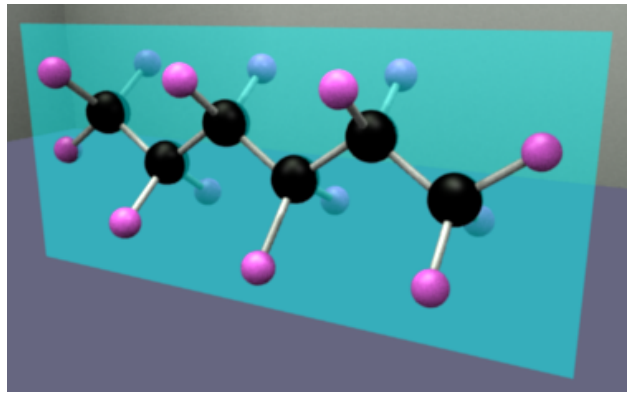

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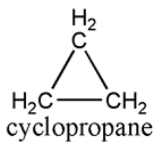

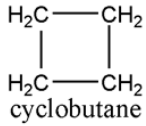

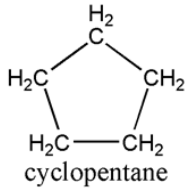

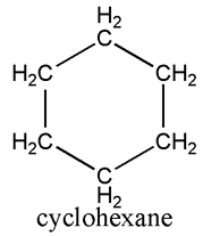

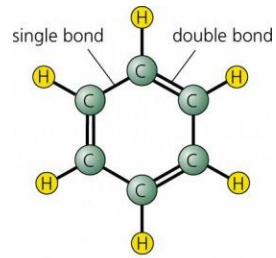

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- Prototypical implementation of a logic-based chemical classification software

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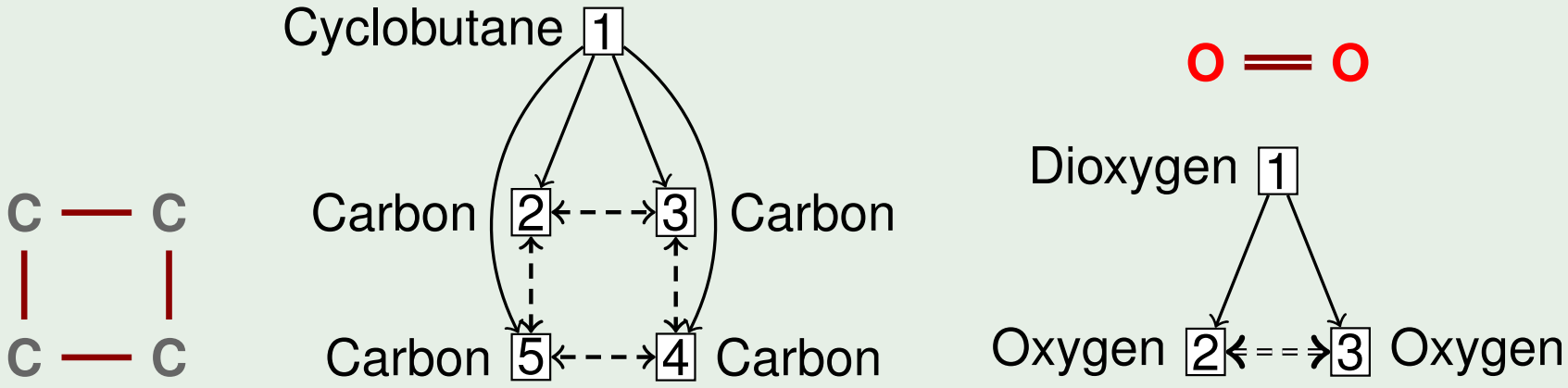

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$$\text{Cyclobutane}(c_1), \quad \text{Dinitrogen}(c_2), \ldots$$

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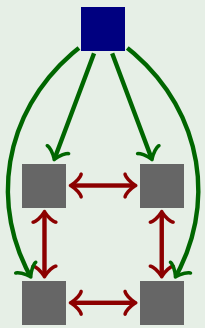

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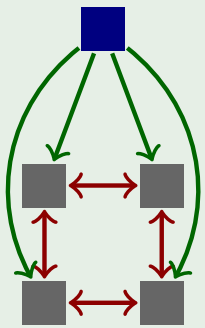

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\text{Cyclobutane}(x) &\rightarrow G_{cb}(x, f_1(x), f_2(x), f_3(x), f_4(x)) \\
G_{cb}(x, y_1, y_2, y_3, y_4) &\rightarrow \text{Cyclobutane}(x) \wedge \\
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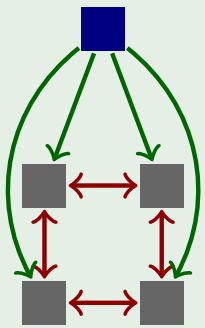

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- Function symbols allow for schema-level reasoning

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Example

$$\text{Molecule}(x) \wedge \text{HasAtom}(x, y) \wedge \textbf{not}\ \text{Carbon}(y) \wedge \textbf{not}\ \text{Hydrogen}(y) \rightarrow \text{NotHydroCarbon}(x)$$

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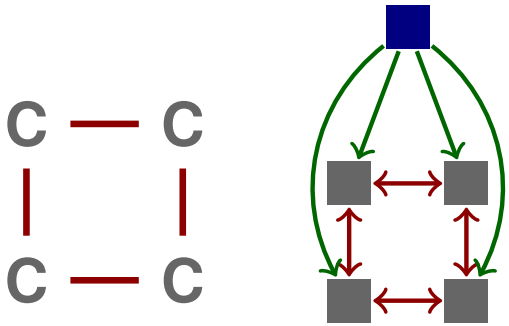

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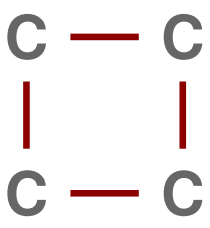

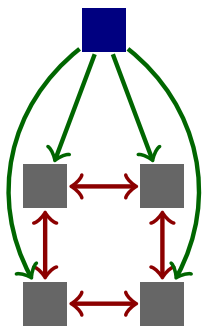

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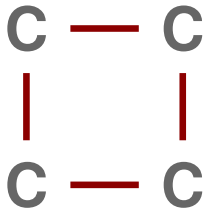

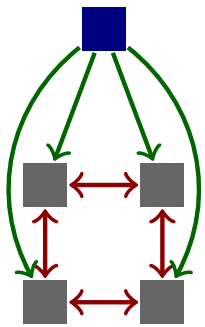

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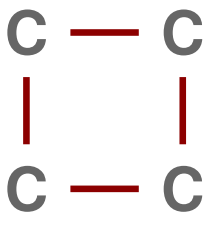

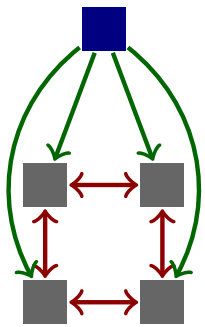

- Does cyclobutane contain a four-membered ring? ✓

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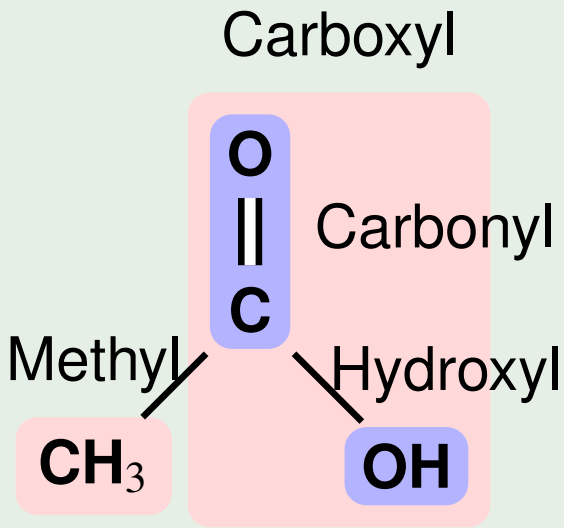

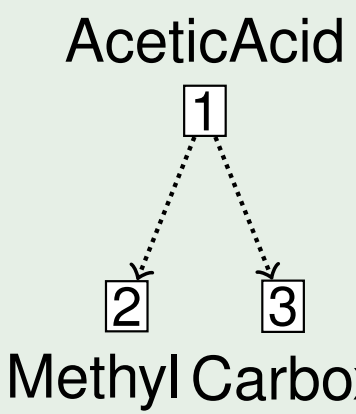

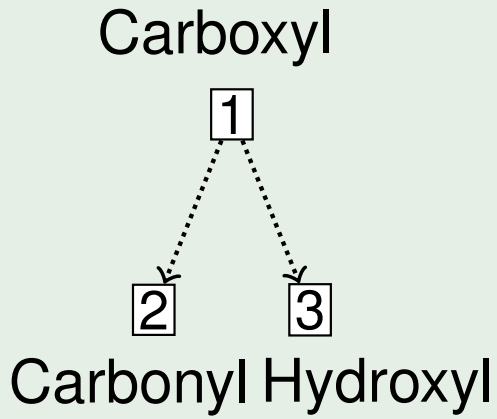

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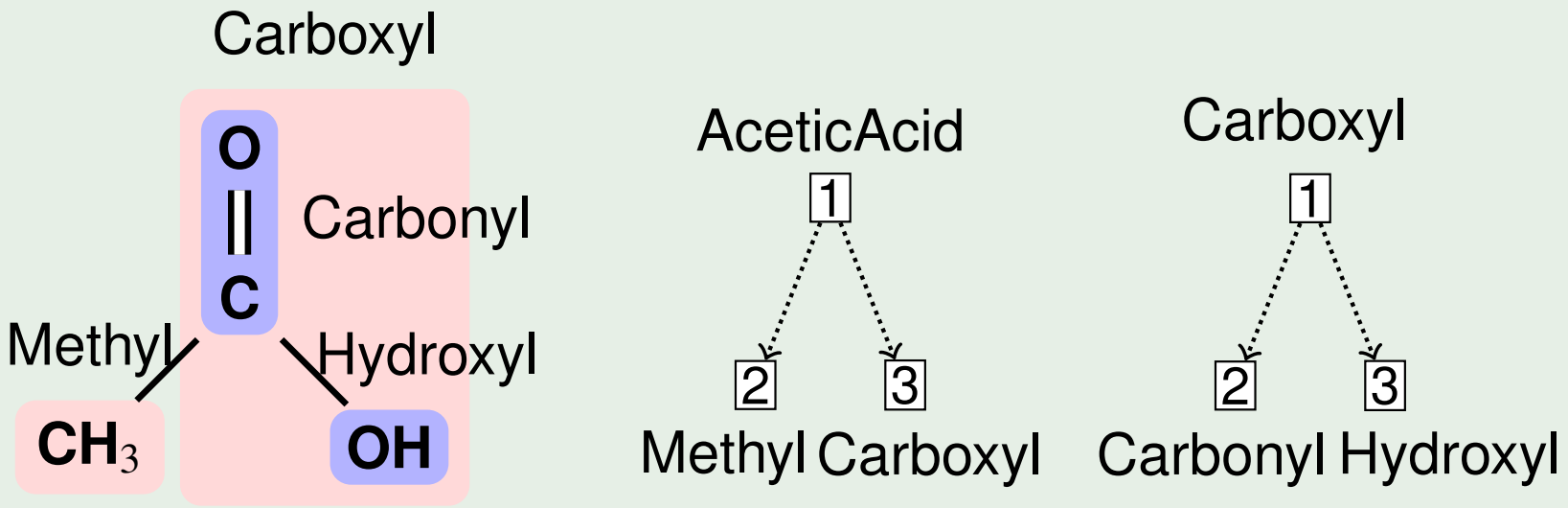

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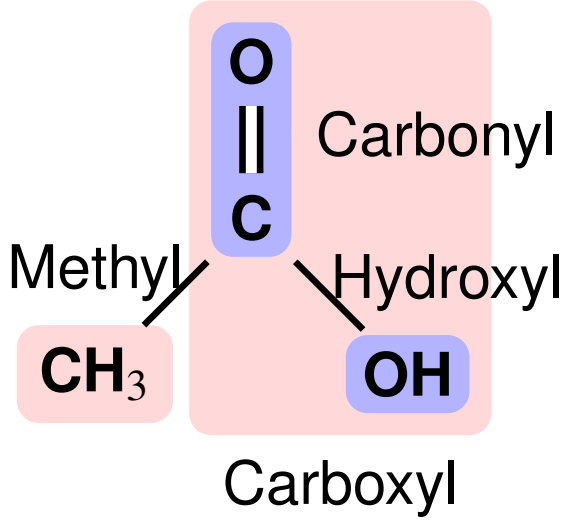

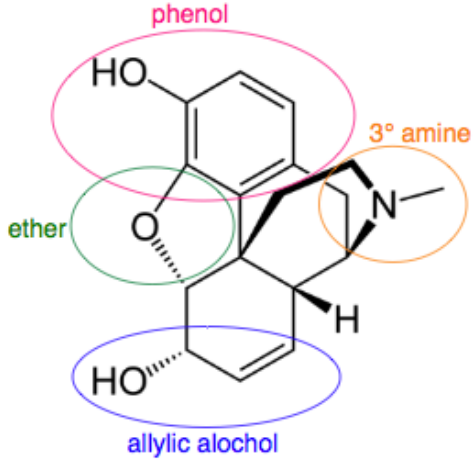

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- Thank you for listening. Questions?