Classifying Chemicals Using Description Graphs and Logic Programming

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Outline

Modelling Chemicals with OWL

- OWL used for the representation of molecular structures

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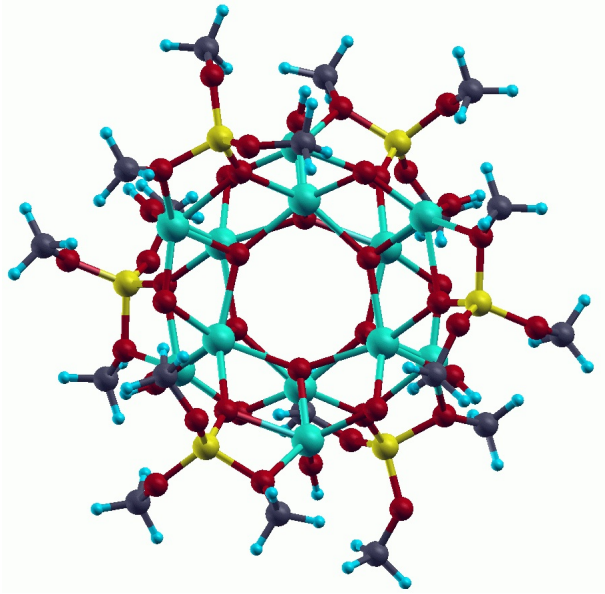

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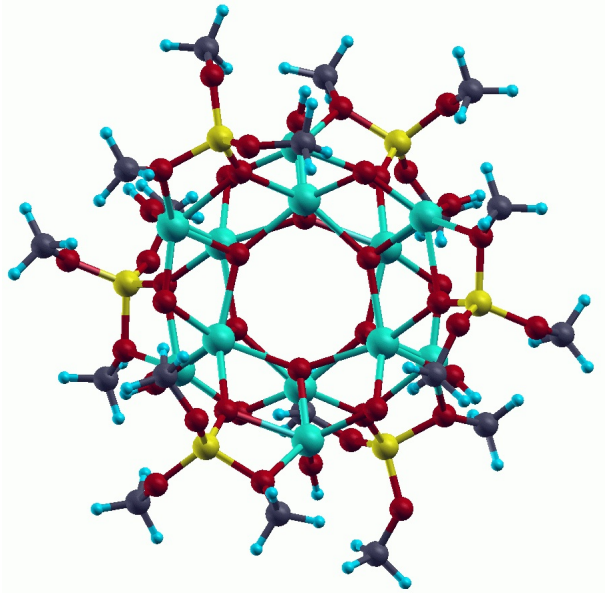

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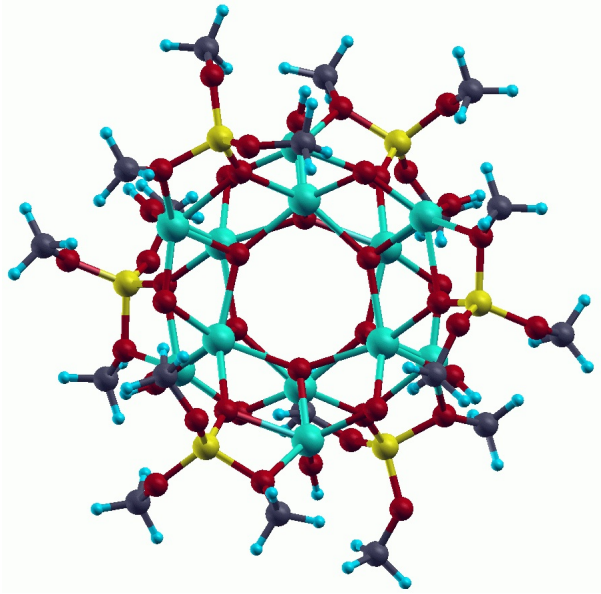

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- Subsumptions between molecules and chemical classes
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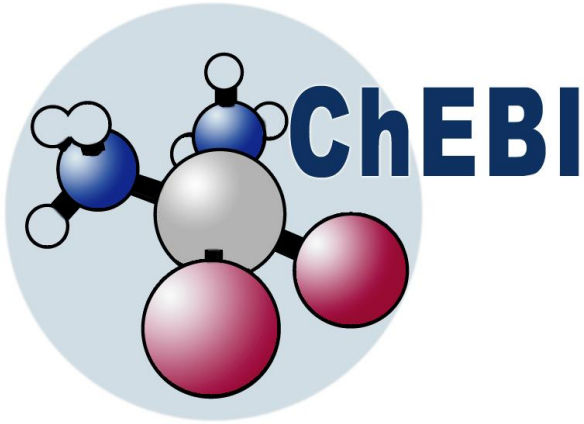
THE CHEBI ONTOLOGY

- OWL ontology Chemical Entities of Biological Interest



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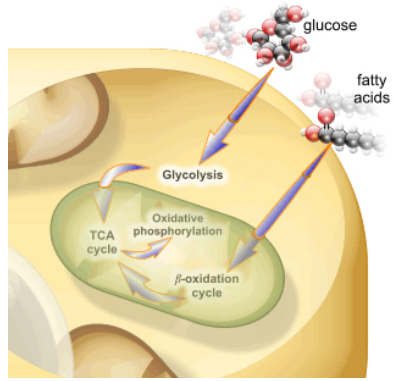

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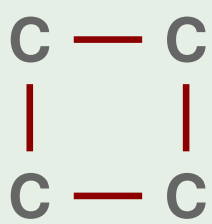

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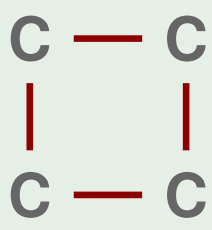

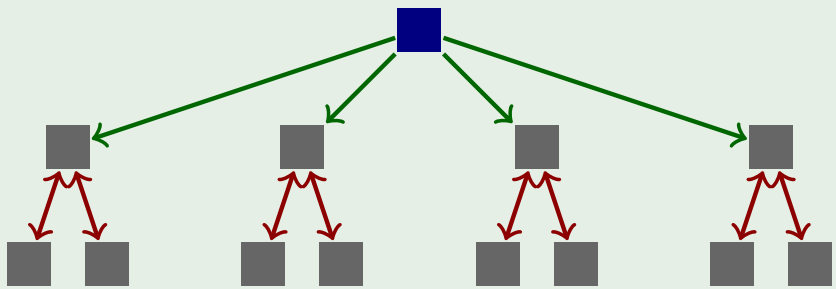

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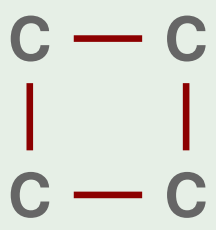

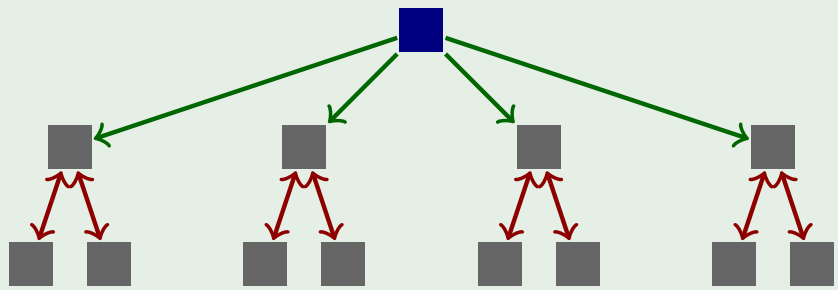

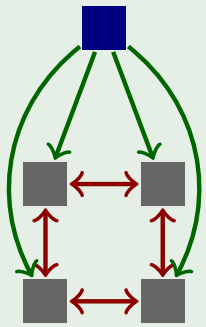

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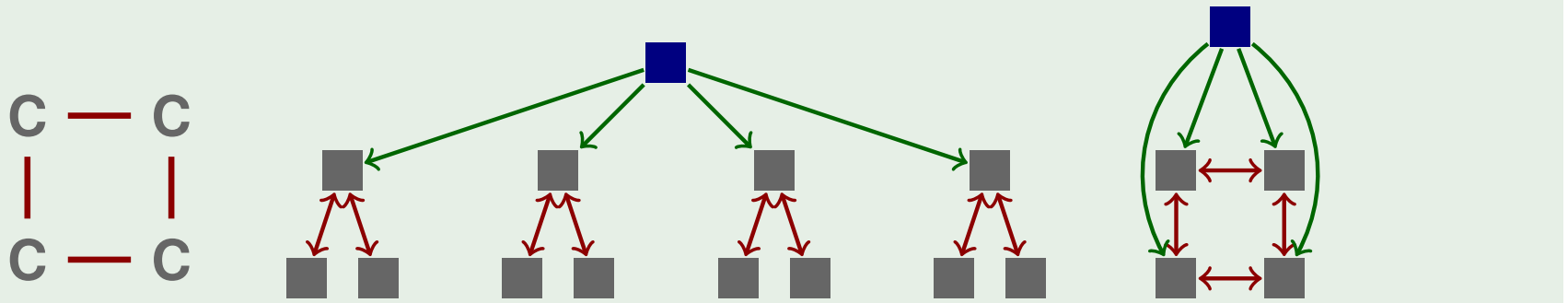

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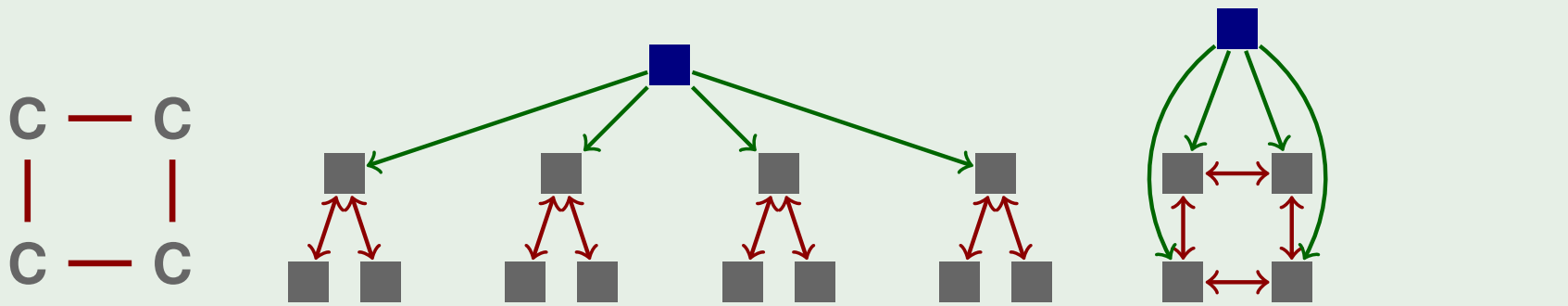

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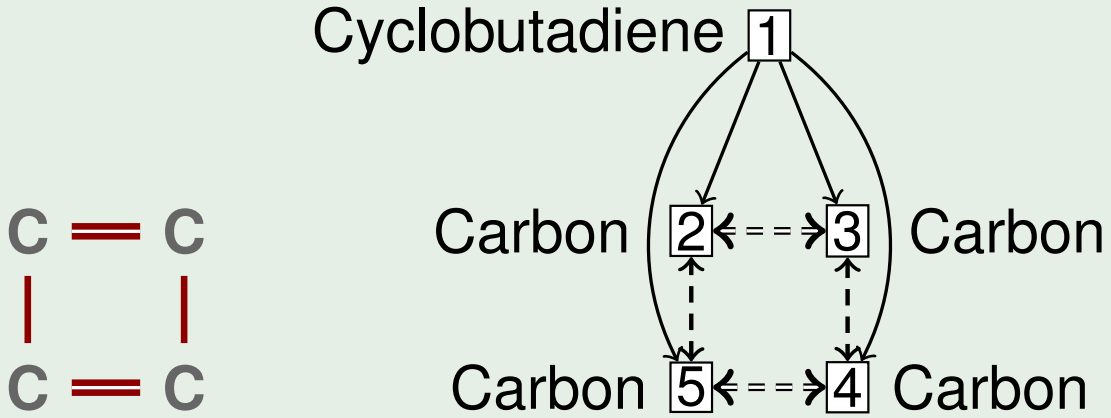

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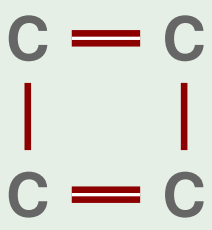

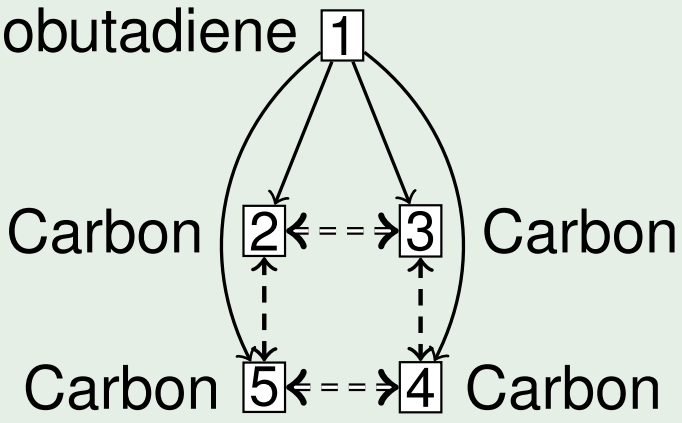

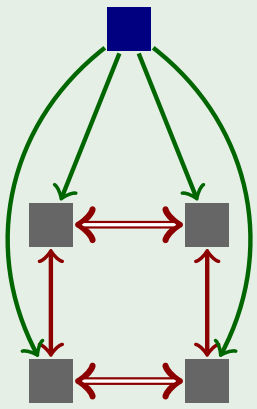

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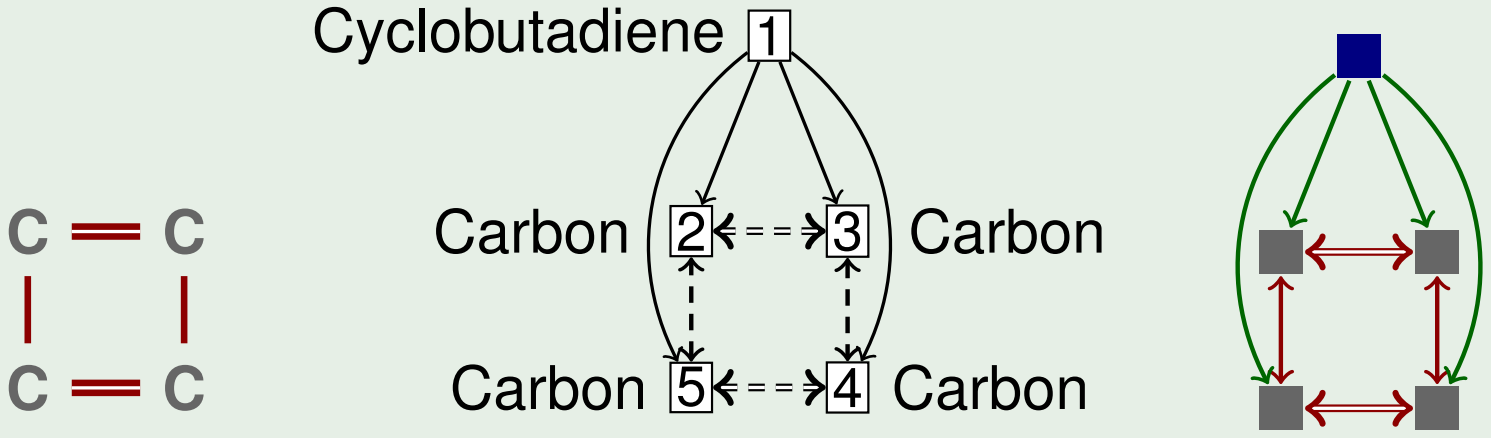

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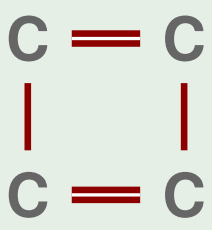

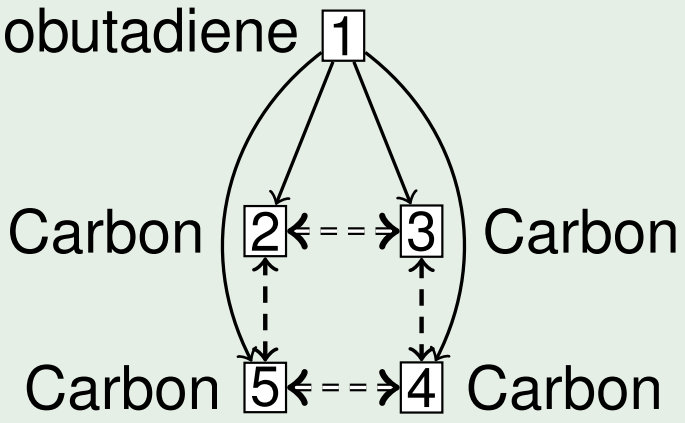

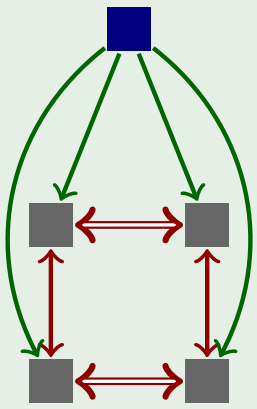

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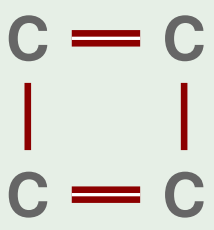

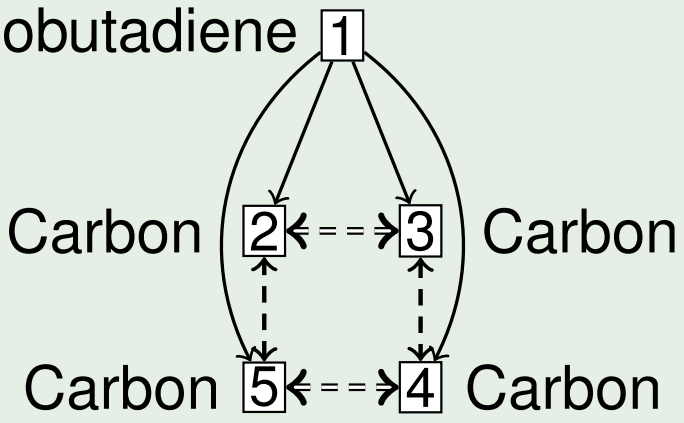

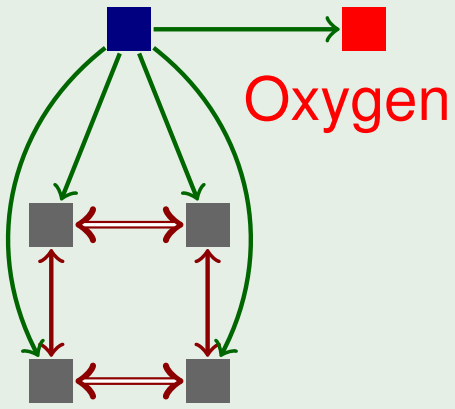

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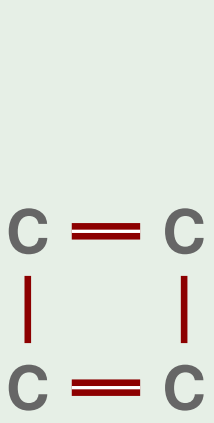

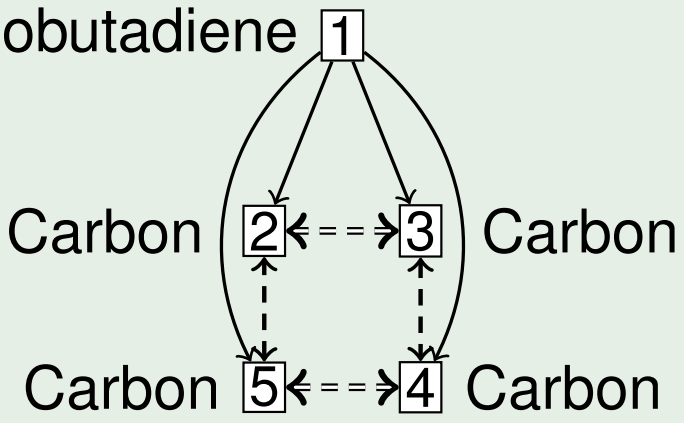

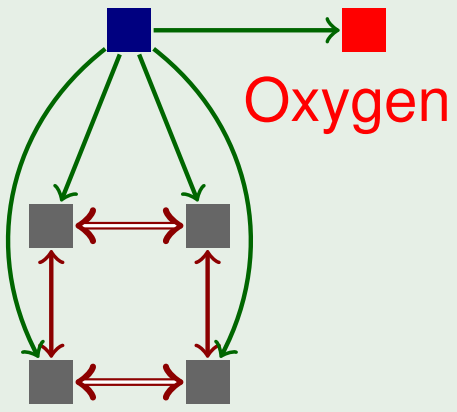

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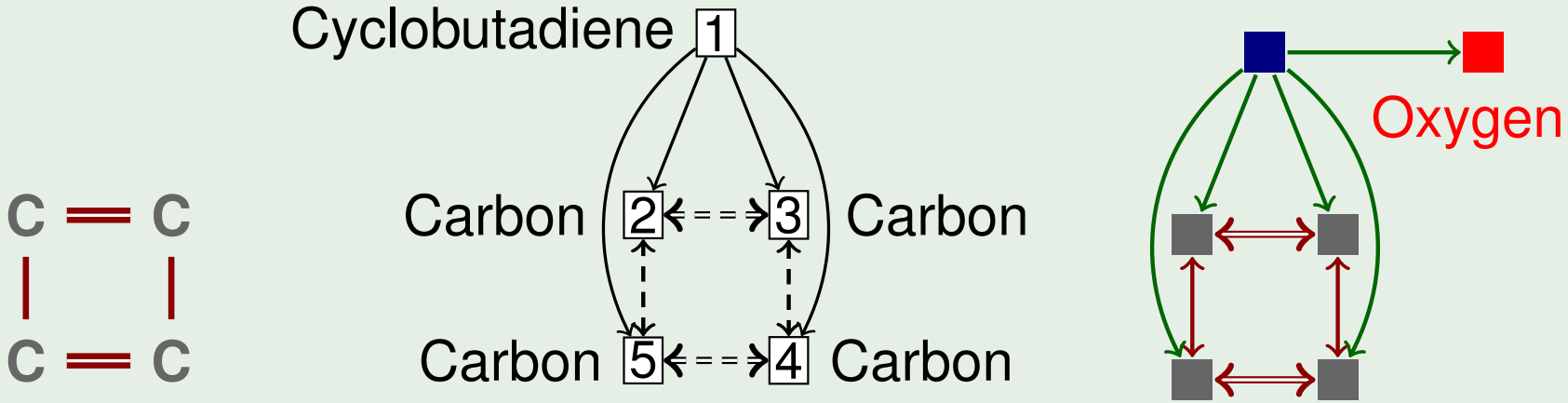

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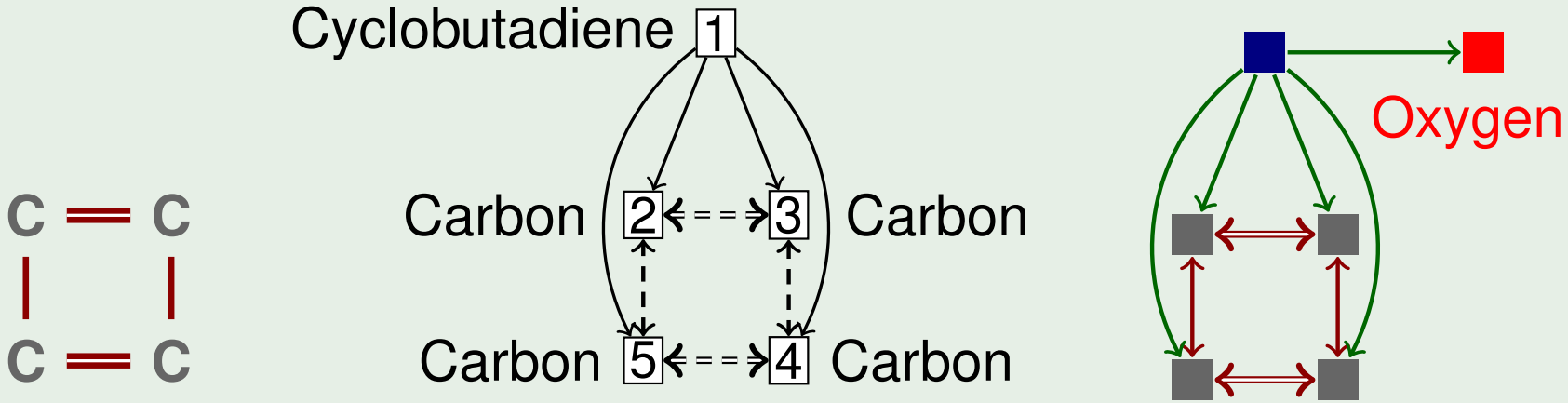

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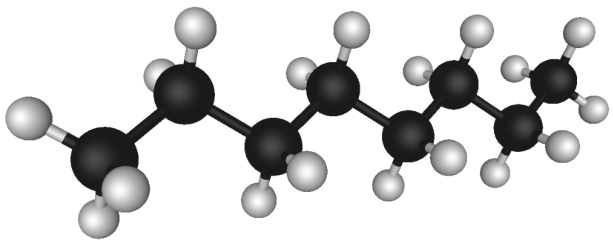

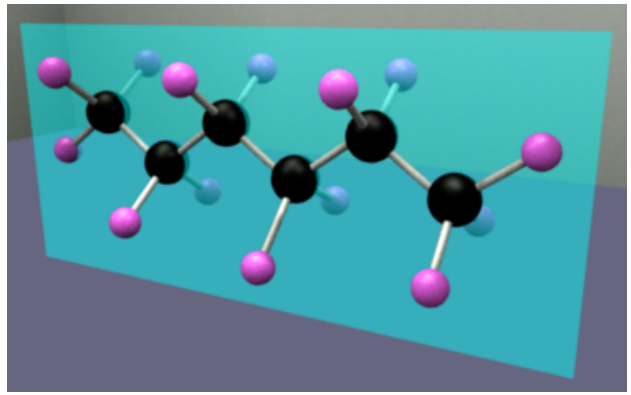

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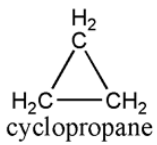

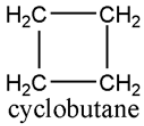

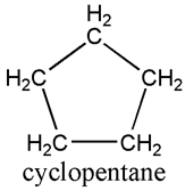

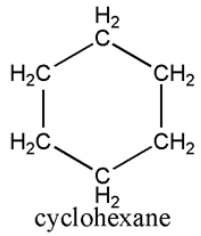

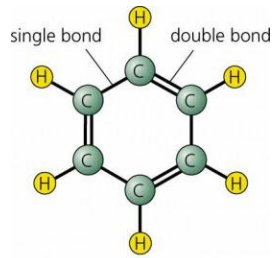

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Results Overview

- Key idea:
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- Prototypical implementation of a logic-based chemical classification software

Outline

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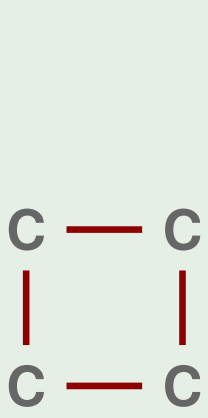

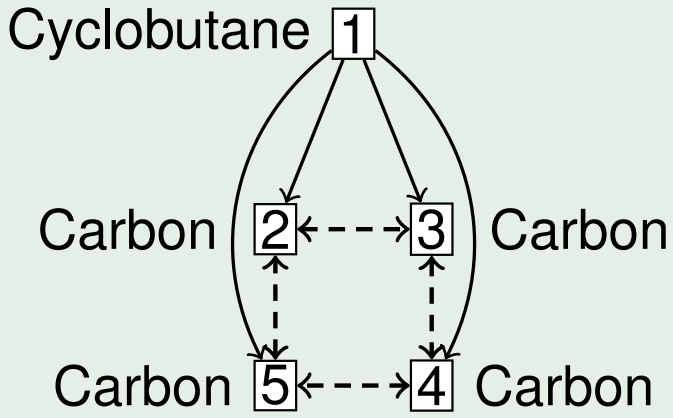

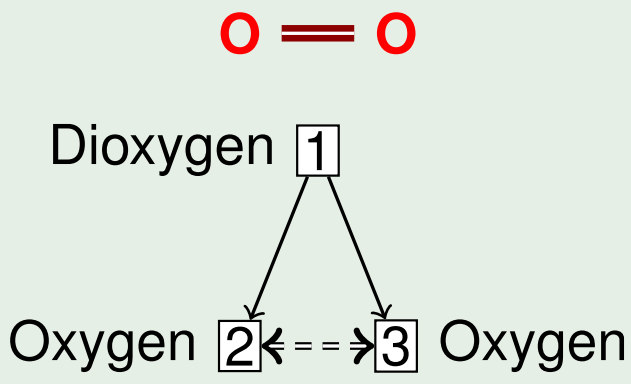

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Example

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

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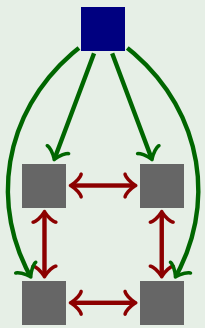

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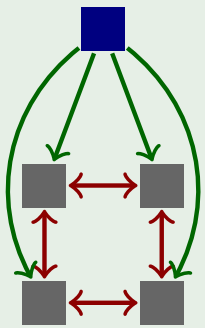

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\text{Cyclobutane}(x) \quad & \rightarrow G_{cb}(x, f_1(x), f_2(x), f_3(x), f_4(x)) \\
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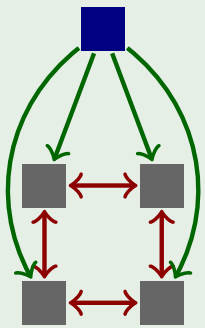

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- Function symbols allow for schema-level reasoning

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Example

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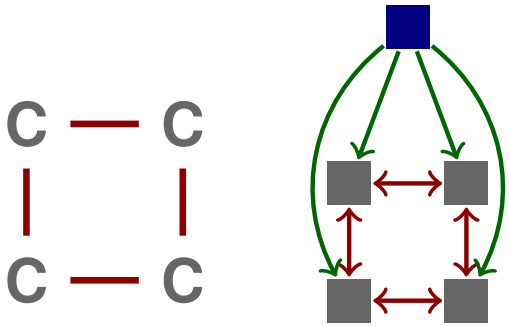

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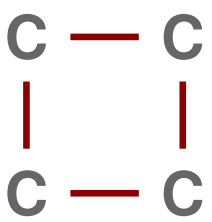

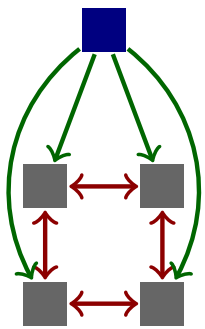

- Is cyclobutane a hydrocarbon? ✓

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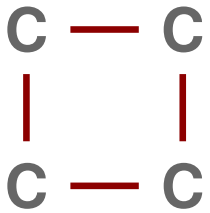

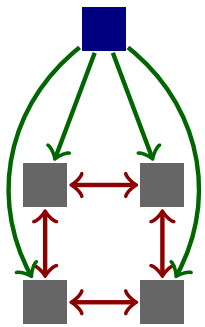

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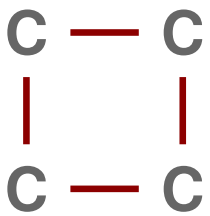

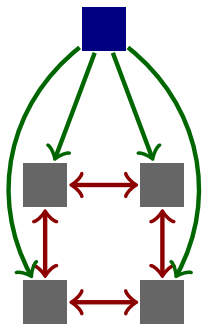

- Does cyclobutane contain a four-membered ring? ✓

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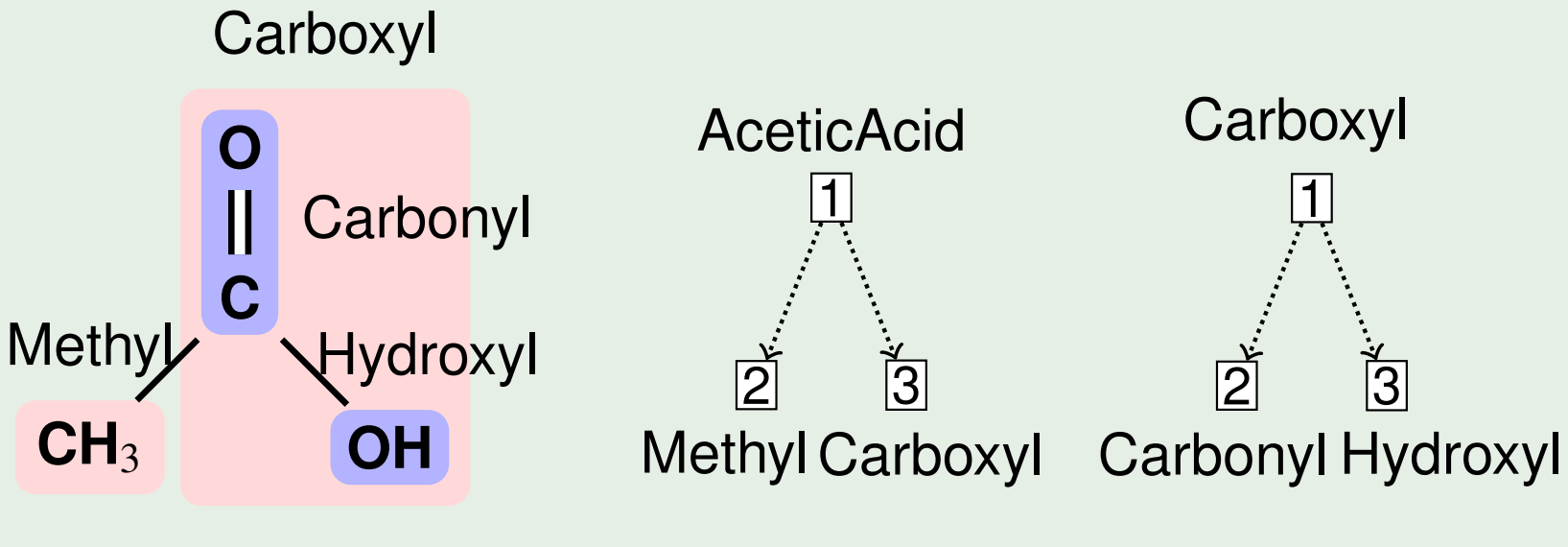

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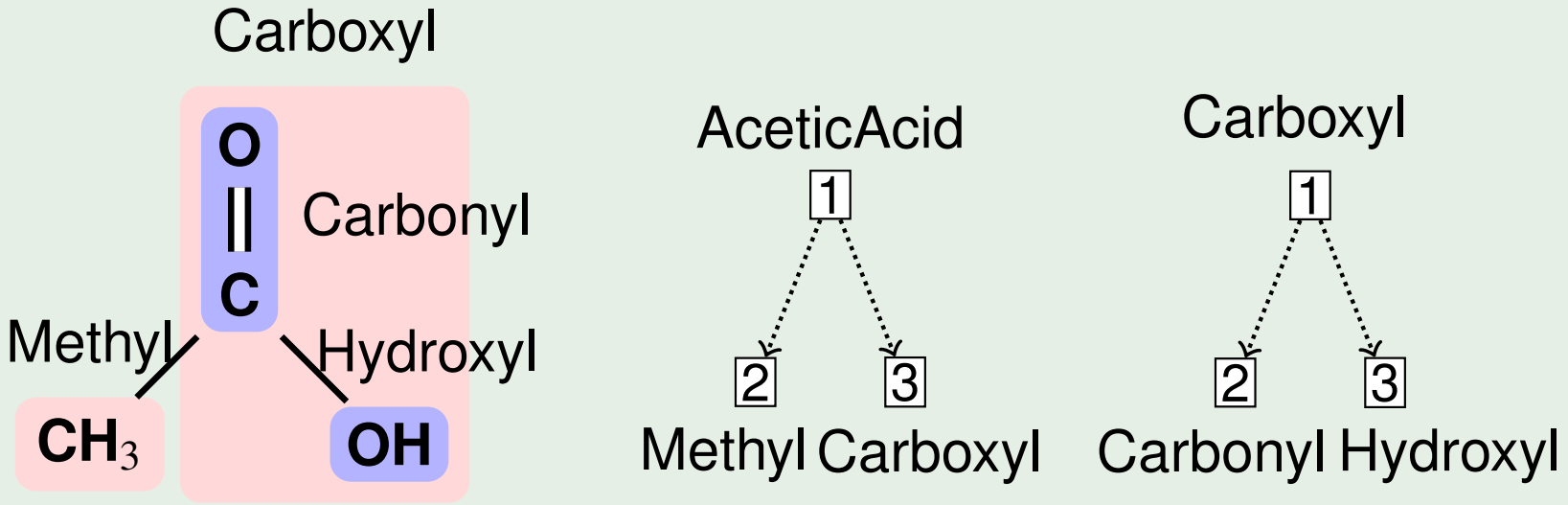

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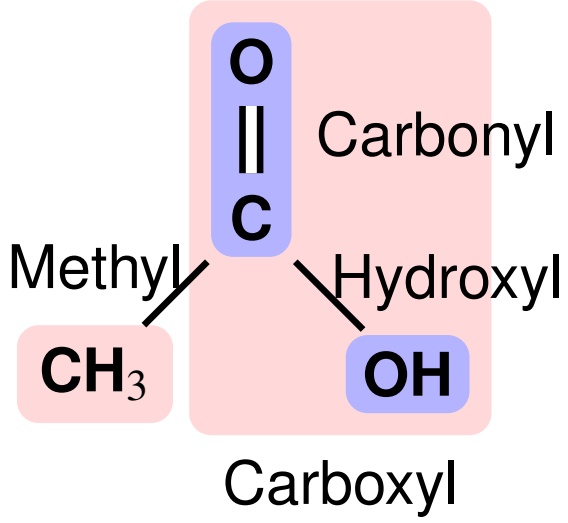

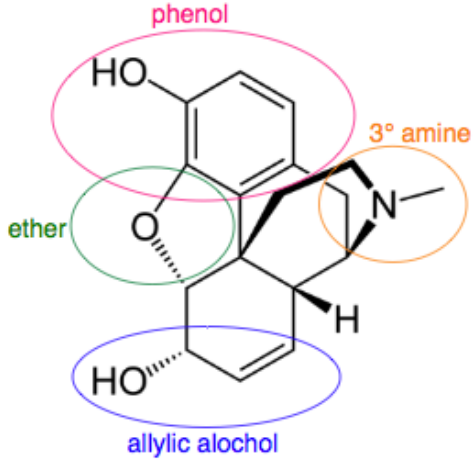

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- Thank you for listening. Questions?