

MODELLING STRUCTURED DOMAINS USING DESCRIPTION GRAPHS AND LOGIC PROGRAMMING

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OUTLINE

1 MOTIVATION

2 DGLPs, IMPLEMENTATION AND OVERVIEW

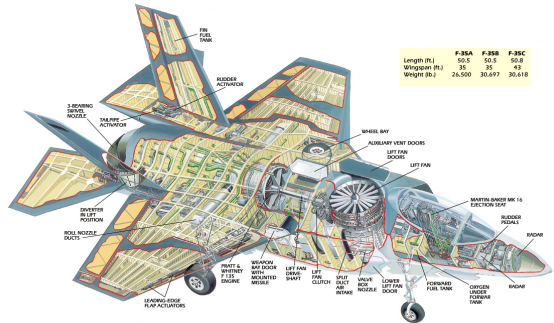
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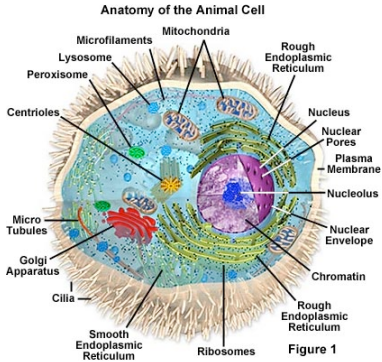


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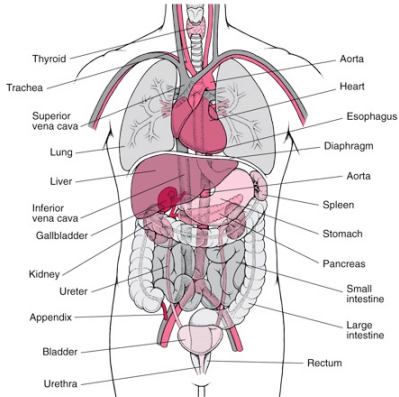
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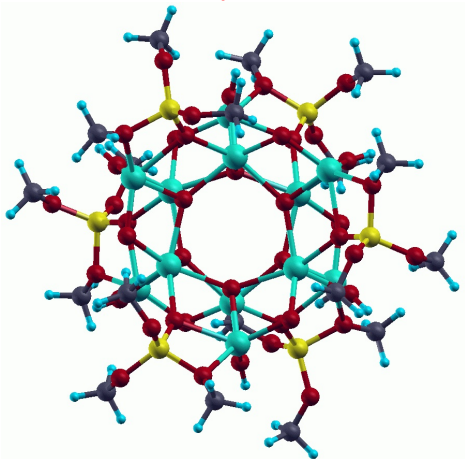
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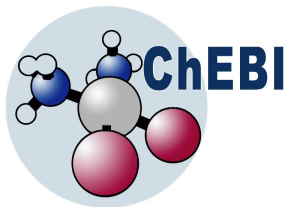
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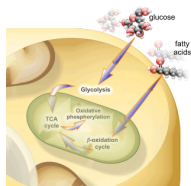
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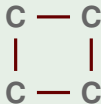
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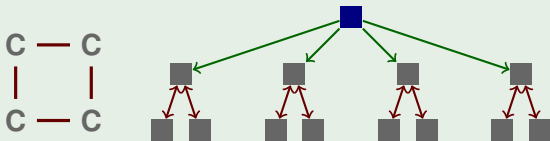


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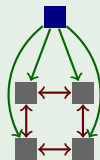
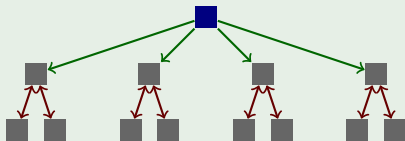
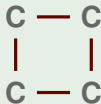


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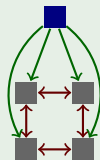
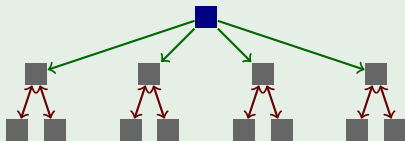
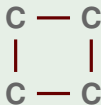


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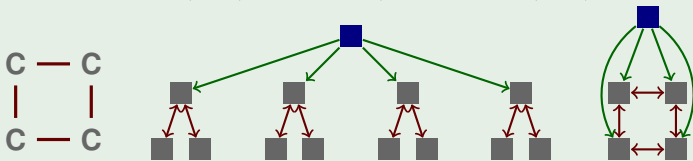
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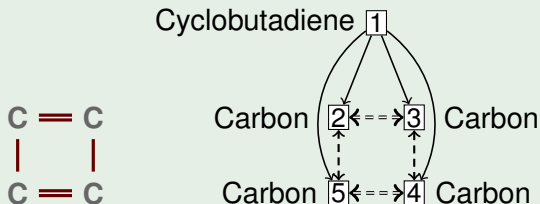
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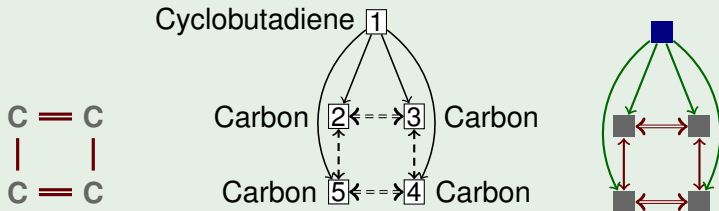
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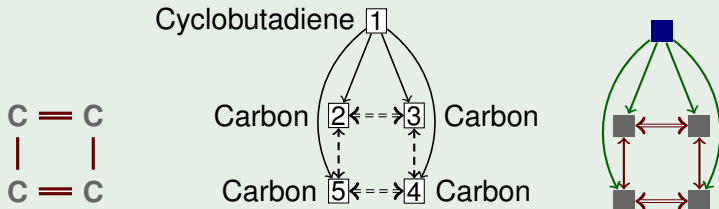
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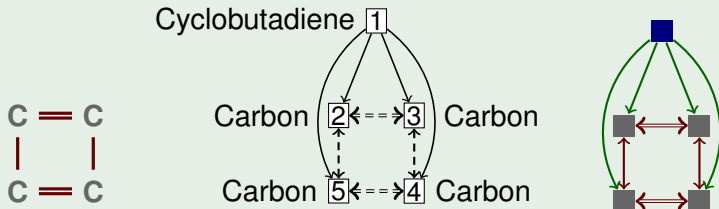


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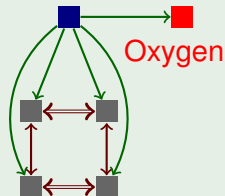
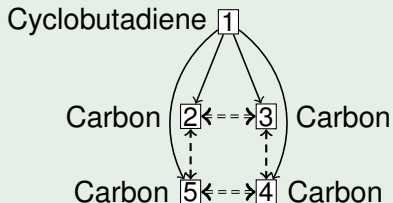
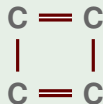


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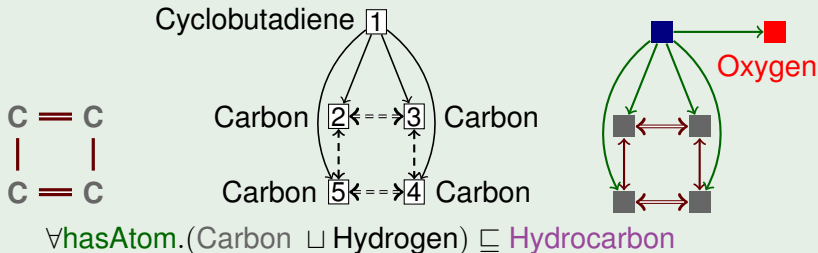
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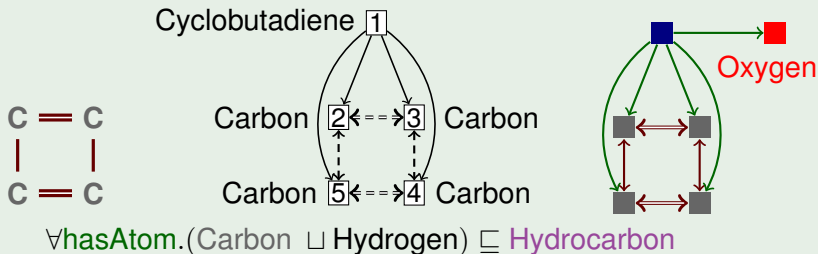
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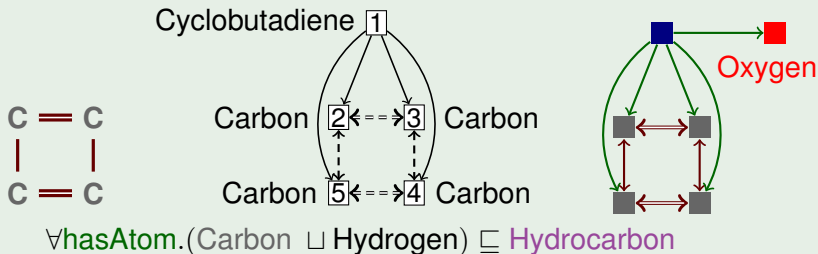


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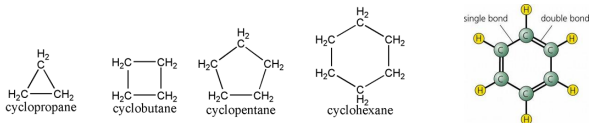
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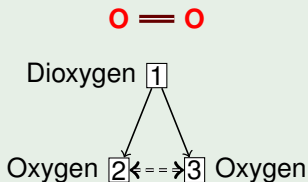
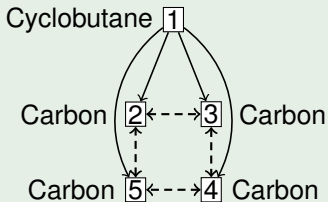
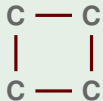
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$\text{Cyclobutane}(c_1), \text{Dinitrogen}(c_2), \dots$

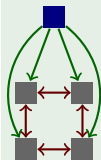
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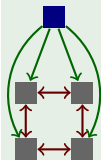
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Cyclobutane(x) $\rightarrow G_{cb}(x, f_1(x), f_2(x), f_3(x), f_4(x))$

$G_{cb}(x, y_1, y_2, y_3, y_4) \rightarrow$ **Cyclobutane**(x) \wedge
Carbon(y_1) \wedge Carbon(y_2) \wedge
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CLASSIFYING OBJECTS

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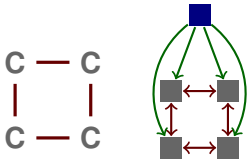
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EXAMPLE

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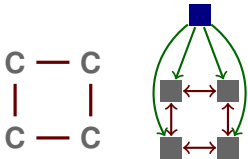


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- Is cyclobutane a hydrocarbon? ✓

CLASSIFYING OBJECTS

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$$\begin{aligned} & \text{Molecule}(x) \wedge \bigwedge_{1 \leq i \leq 4} \text{HasAtom}(x, y_i) \wedge \bigwedge_{1 \leq i \leq 3} \text{Bond}(y_i, y_{i+1}) \wedge \\ & \text{Bond}(y_4, y_1) \bigwedge_{1 \leq i < j \leq 4} \text{not } y_i = y_j \\ & \rightarrow \text{MoleculeWith4MemberedRing}(x) \end{aligned}$$

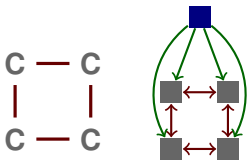
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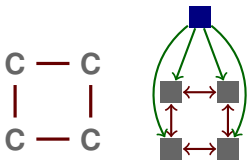
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- Does **cyclobutane** contain a **four-membered ring**? ✓

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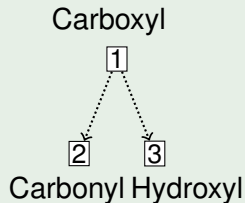
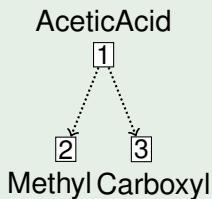
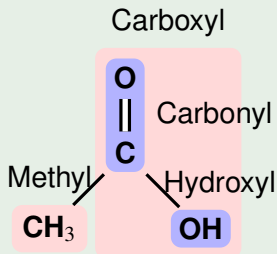
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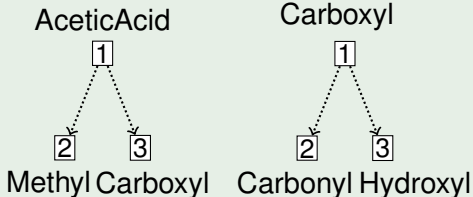
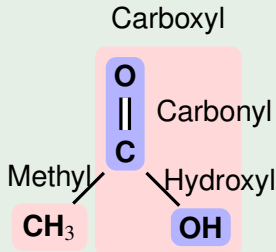
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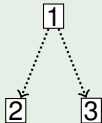
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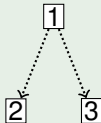
EXAMPLE

AceticAcid



Methyl Carboxyl

Carboxyl



Carbonyl Hydroxyl

AceticAcid \prec Carboxyl

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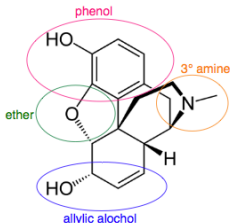
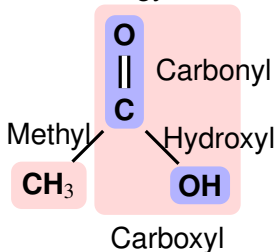
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