Modelling Structured Domains With Logic

Despoina Magka, Boris Motik and Ian Horrocks

Department of Computer Science, University of Oxford

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Outline

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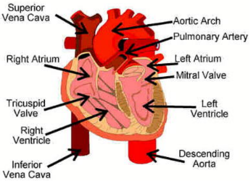

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- What are Description Logics?
  $\rightsquigarrow$ Decidable fragments of first-order logic with well-understood computational properties

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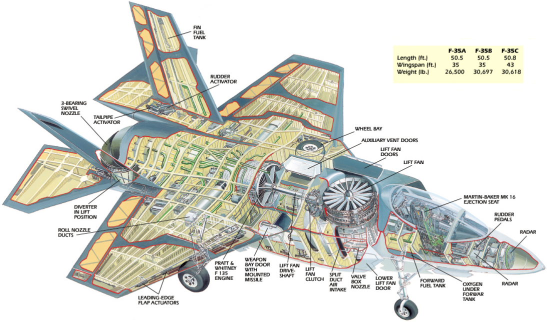

	F-35A	F-35B	F-35C
Length (ft.)	50.5	50.5	50.8
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Weight (lb.)	26,500	30,697	30,618

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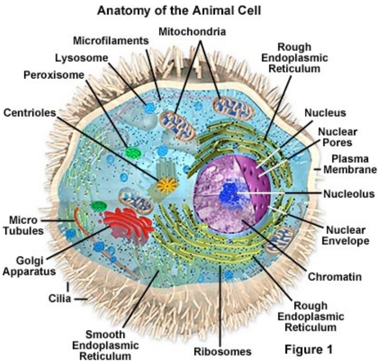

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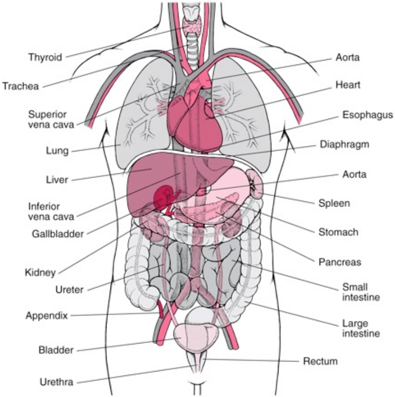

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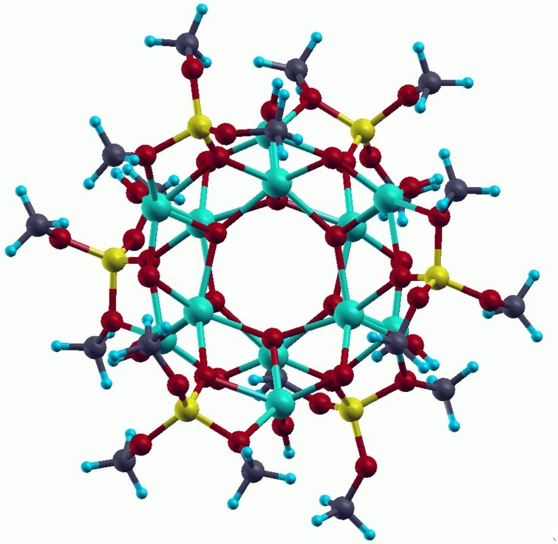

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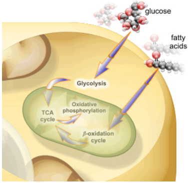

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$\text{Uncle} \sqsubseteq \text{Male} \sqcap \exists \text{hasSibling}.\exists \text{hasChild}.(\text{Human})$

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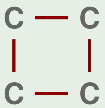

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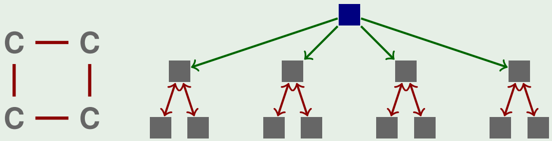

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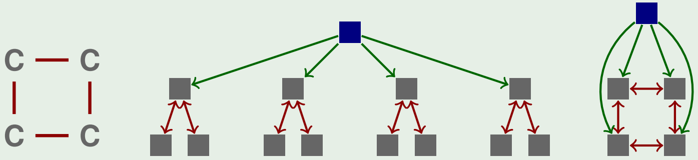

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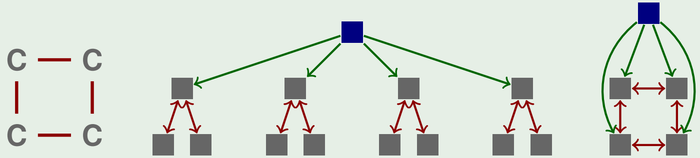

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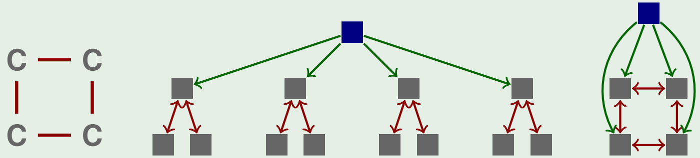

- OWL-based reasoning support
  - Does cyclobutane contain a four-membered ring? ✗
  - Does benzaldehyde contain a benzene ring? ✗

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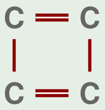

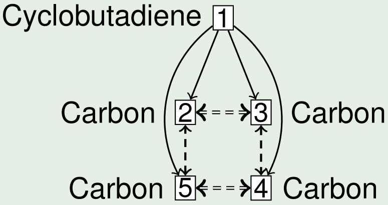

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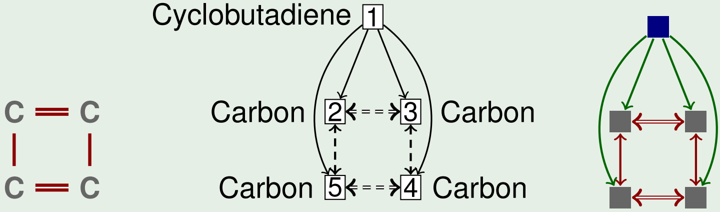

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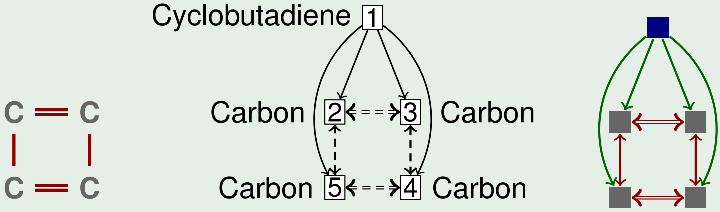

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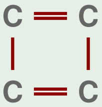

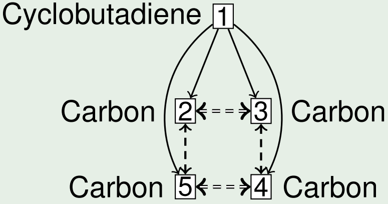

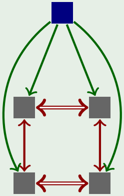

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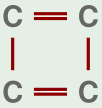

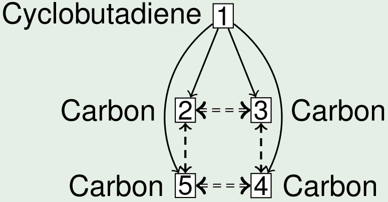

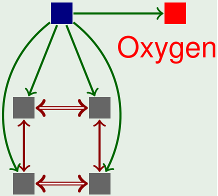

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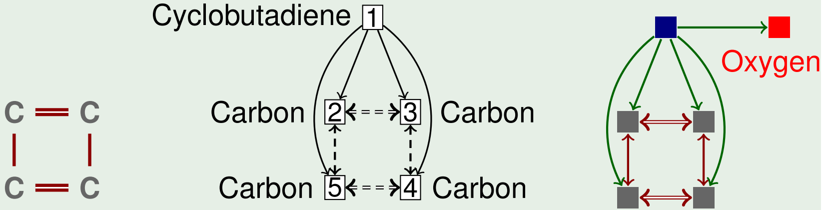

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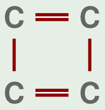

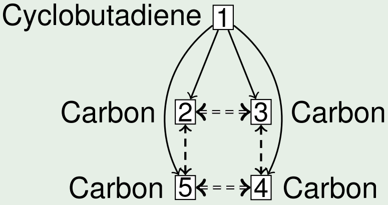

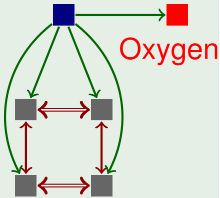

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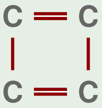

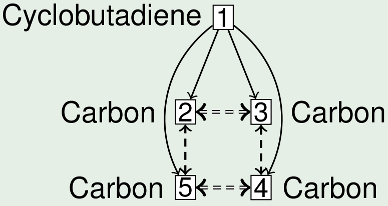

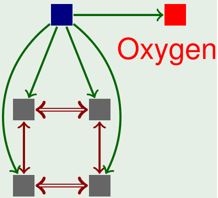

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  - Represent rings with adequate precision (no tree-model property)

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- Encouraging results of a preliminary evaluation

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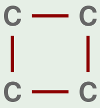

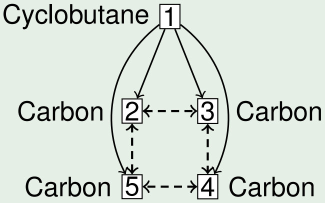

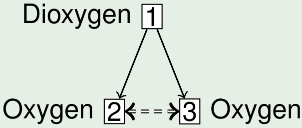

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$\mathrm{Cyclobutane}(c_1), \quad \mathrm{Dinitrogen}(c_2), \ldots$

Semantics of DGs

- Translate DGs into logic programs with function symbols

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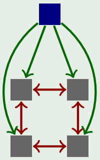

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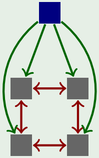

$$
\begin{aligned}
\mathrm{Cyclobutane}(x) &\rightarrow G_{cb}(x, f_1(x), f_2(x), f_3(x), f_4(x)) \\
G_{cb}(x, y_1, y_2, y_3, y_4) &\rightarrow \mathrm{Cyclobutane}(x) \wedge \\
&\quad \mathrm{Carbon}(y_1) \wedge \mathrm{Carbon}(y_2) \wedge \\
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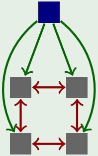

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- Function symbols allow for schema-level reasoning

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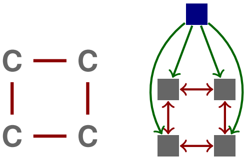

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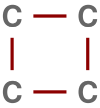

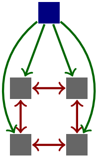

- Is cyclobutane a hydrocarbon? ✓

Classifying objects

Example

$$\mathsf{Molecule}(\mathsf{x}) \wedge \bigwedge_{1 \le \mathsf{i} \le 4} \mathsf{HasAtom}(\mathsf{x}, \mathsf{y_i}) \wedge \bigwedge_{1 \le \mathsf{i} \le 3} \mathsf{Bond}(\mathsf{y_i}, \mathsf{y_{i+1}}) \wedge$$

$$\mathsf{Bond}(\mathsf{y_4}, \mathsf{y_1}) \bigwedge_{1 \le i < j \le 4} \textbf{not } \mathsf{y_i} = \mathsf{y_j}$$

$$\rightarrow \mathsf{MoleculeWith4MemberedRing}(\mathsf{x})$$

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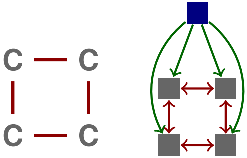

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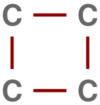

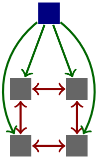

- Does cyclobutane contain a four-membered ring? ✓

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$$\begin{array}{lcl} A(x) & \rightarrow & G(x, f_1(x), f_2(x)) \\ G(x, y_1, y_2) & \rightarrow & A(y_1) \wedge A(y_2) \end{array}$$

$$\{A(a),\ G(a, f_1(a),\ f_2(a)),\ A(f_1(a)),\ A(f_2(a)),\ \ldots\}$$

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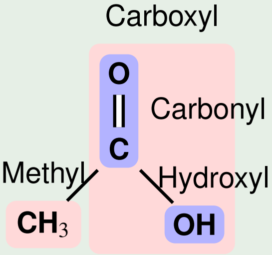

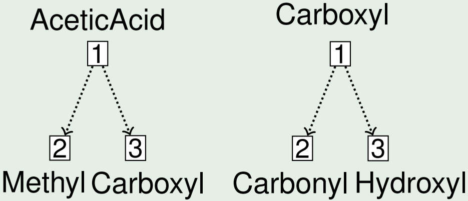

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Example

$$\begin{aligned}
\mathrm{AceticAcid}(x) &\rightarrow G_{AA}(x, f_1(x), f_2(x)) \\
G_{AA}(x_1, x_2, x_3) &\rightarrow \mathrm{AceticAcid}(x_1) \wedge \mathrm{Methyl}(x_2) \wedge \mathrm{Carboxyl}(x_3) \wedge \\
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\mathrm{Methyl}(x_2) \wedge \mathrm{Carboxyl}(x_3) &\wedge \mathrm{HasPart}(x_1, x_2) \wedge \mathrm{HasPart}(x_1, x_3) \\
&\rightarrow G_{AA}(x_1, x_2, x_3) \\
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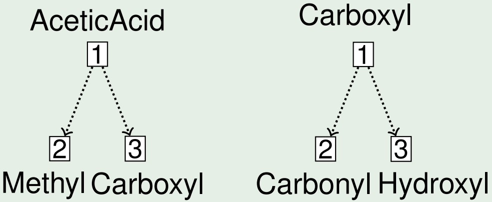

AceticAcid $\prec$ Carboxyl

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Example

$\mathrm{G}_{\mathrm{AA}}(\mathrm{x}_1, \mathrm{x}_2, \mathrm{x}_3) \wedge \mathrm{AceticAcid}(\mathrm{x}_2) \rightarrow \mathrm{Cycle}$

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- DGLP ontology with acetic acid is semantically acyclic ✓

Technical results

- Decidability for negation-free DGLP ontologies

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Outline

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No mol.	T_1	T_2	T_3	T_4	T_5	Total time
10	< 0.01	< 0.01	< 0.01	0.36	0.02	2.47
20	< 0.01	< 0.01	0.02	2.07	0.21	10.66
30	0.01	< 0.01	0.03	2.23	0.23	13.85
40	0.01	< 0.01	0.04	2.58	0.29	19.06
50	0.01	0.01	0.06	3.55	0.41	27.15
60	0.04	0.02	0.51	109.88	21.68	300.84
70	0.06	0.03	0.75	172.14	35.08	447.12

- T_1: hydrocarbons, T_2: inorganic molecules
- T_3: molecules with exactly two carbons
- T_4: molecules with a four-membered ring
- T_5: molecules with a benzene

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No mol.	T_1	T_2	T_3	T_4	T_5	Total time
10	< 0.01	< 0.01	< 0.01	0.36	0.02	2.47
20	< 0.01	< 0.01	0.02	2.07	0.21	10.66
30	0.01	< 0.01	0.03	2.23	0.23	13.85
40	0.01	< 0.01	0.04	2.58	0.29	19.06
50	0.01	0.01	0.06	3.55	0.41	27.15
60	0.04	0.02	0.51	109.88	21.68	300.84
70	0.06	0.03	0.75	172.14	35.08	447.12

- T_1: hydrocarbons, T_2: inorganic molecules
- T_3: molecules with exactly two carbons
- T_4: molecules with a four-membered ring
- T_5: molecules with a benzene

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- Thank you for listening. Questions?