Towards functorial chemistry

Completeness and universality for reaction representation

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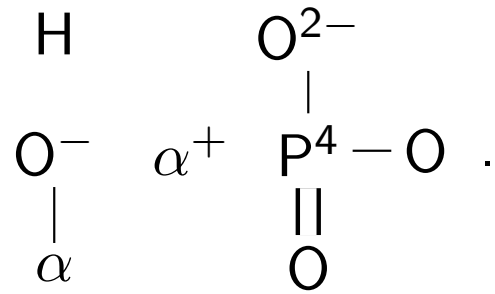
UCL

Birmingham Theory Seminar
15 March 2024

Outline

Chemical graphs and morphisms

Molecular entities are represented by labelled graphs:



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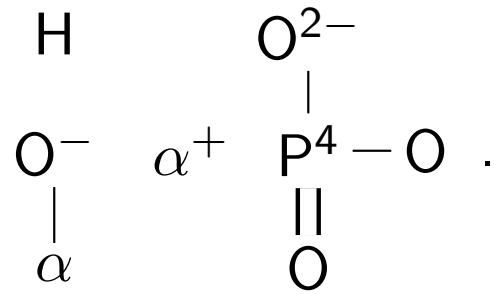
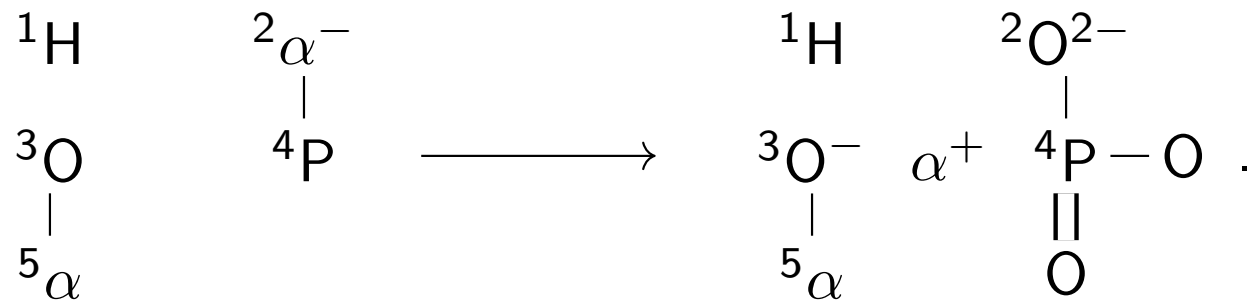
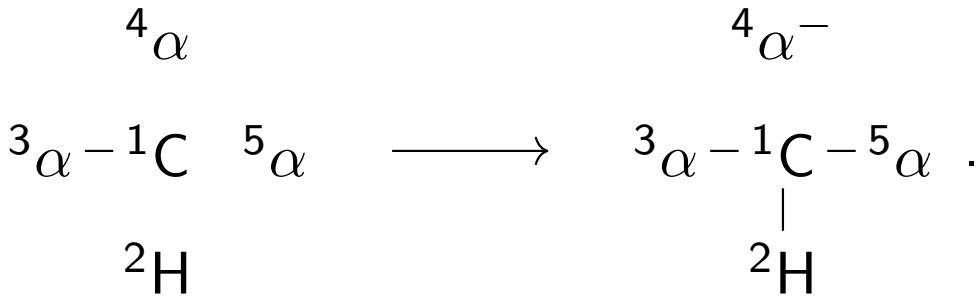


A morphism is a “matter non-decreasing” function:



Vertex embeddings and matchings

- A *vertex embedding* is a bijective morphism which preserves the atom labels:



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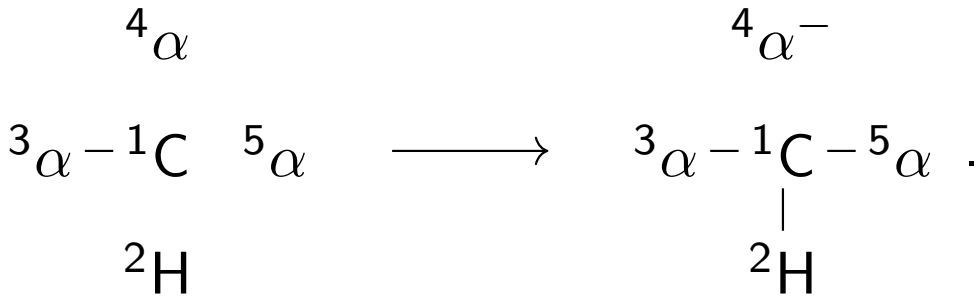
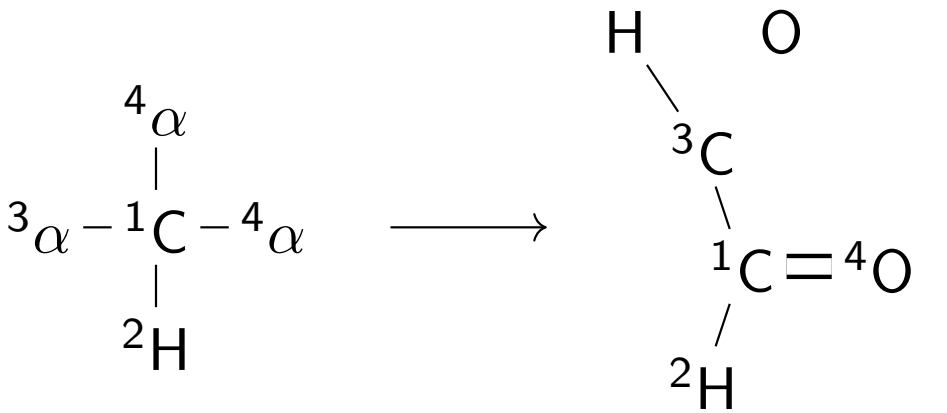


- A *matching* is a morphism which strictly preserves the charge and the number of bonds:



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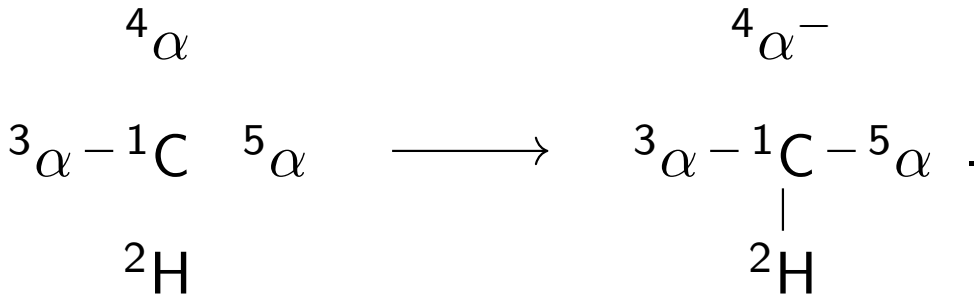

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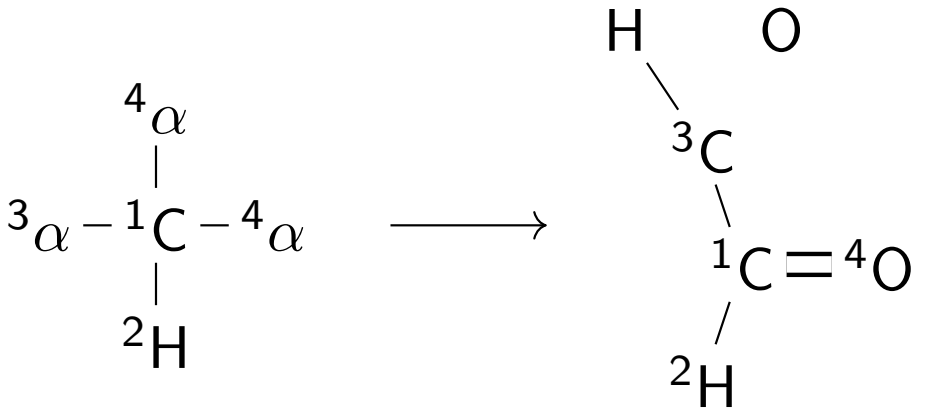
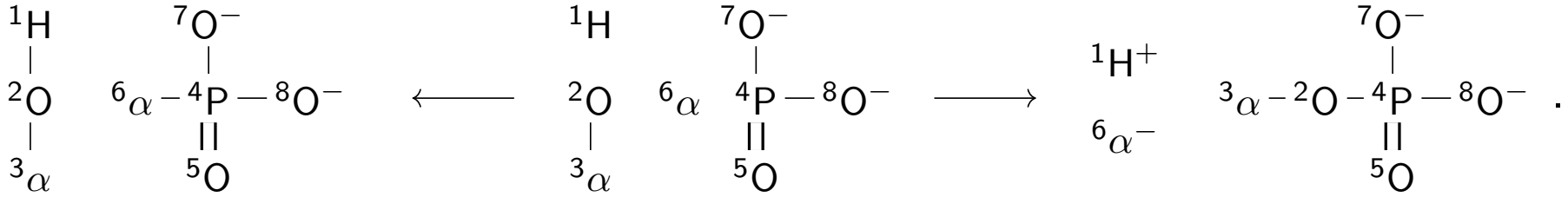


Theorem

The category of chemical graphs is $(\mathcal{E}, \mathcal{M})$*-adhesive.*

Reaction schemes

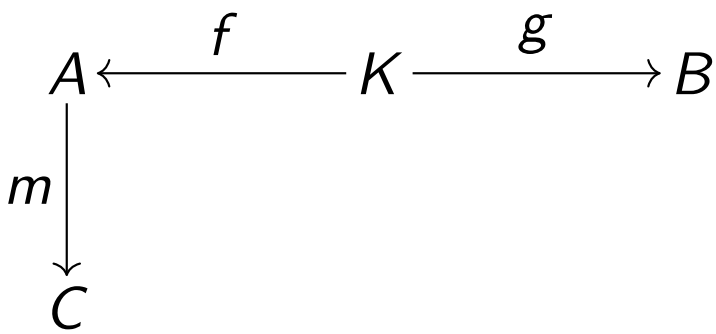
A *reaction scheme* is a terminal span of vertex embeddings whose boundary graphs have the same net charge and are valence complete:

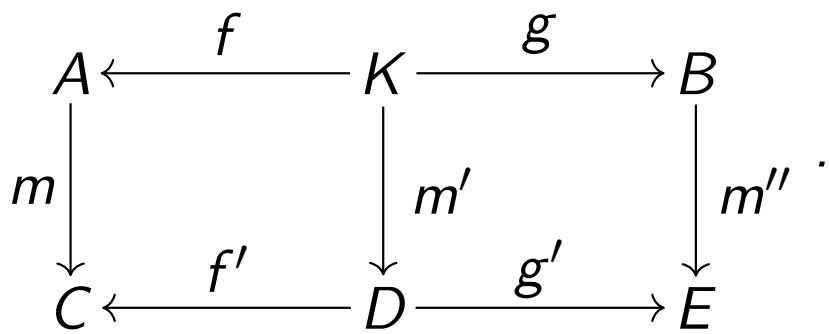


Reaction schemes

Proposition

The diagram below left, where the top span is a reaction scheme and $m \in \mathcal{M}$, can be uniquely completed to the one on the right, with $f', g' \in \mathcal{E}$ and $m', m'' \in \mathcal{M}$

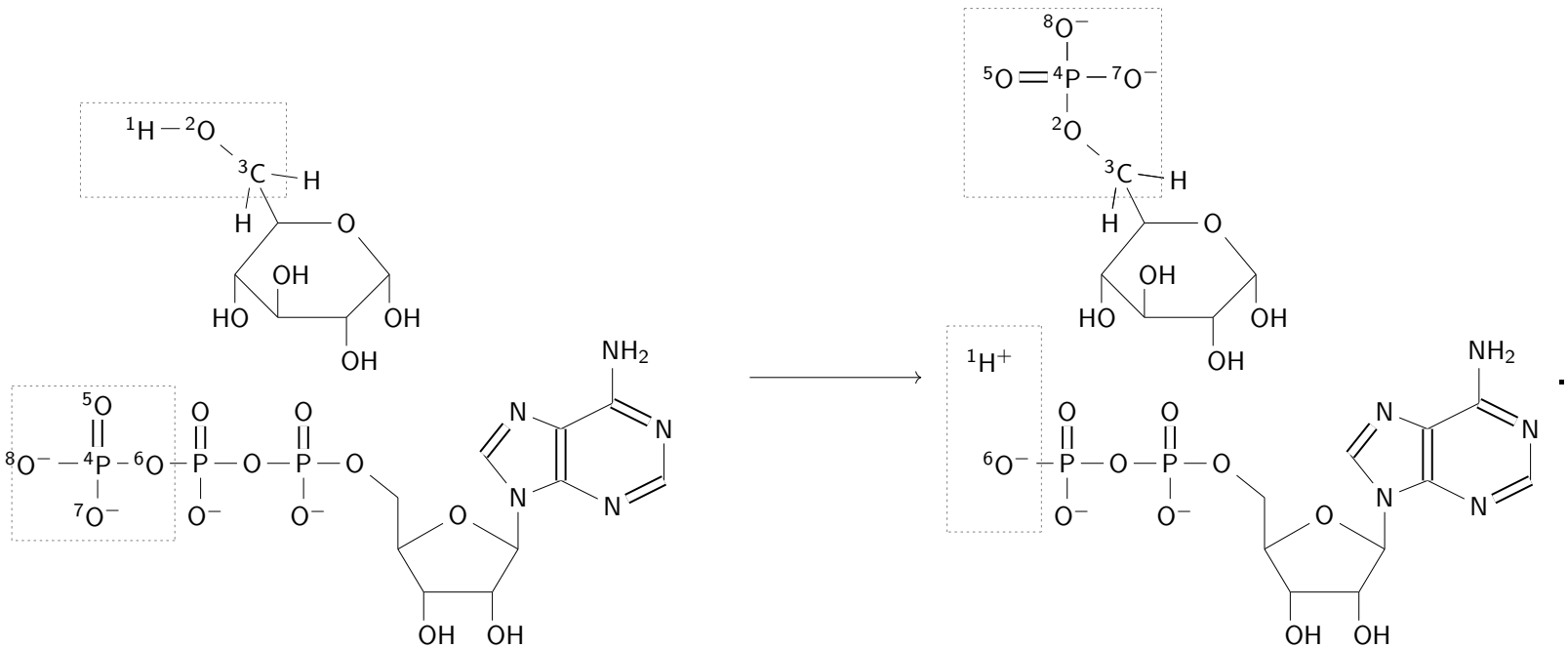




Moreover, if C is valence complete, then so is E.

Reactions

A *reaction* between valence complete chemical graphs is a partial bijection such that the domain and the image have the same net charge, atom labels are preserved and boundary vertices are mapped to boundary vertices:



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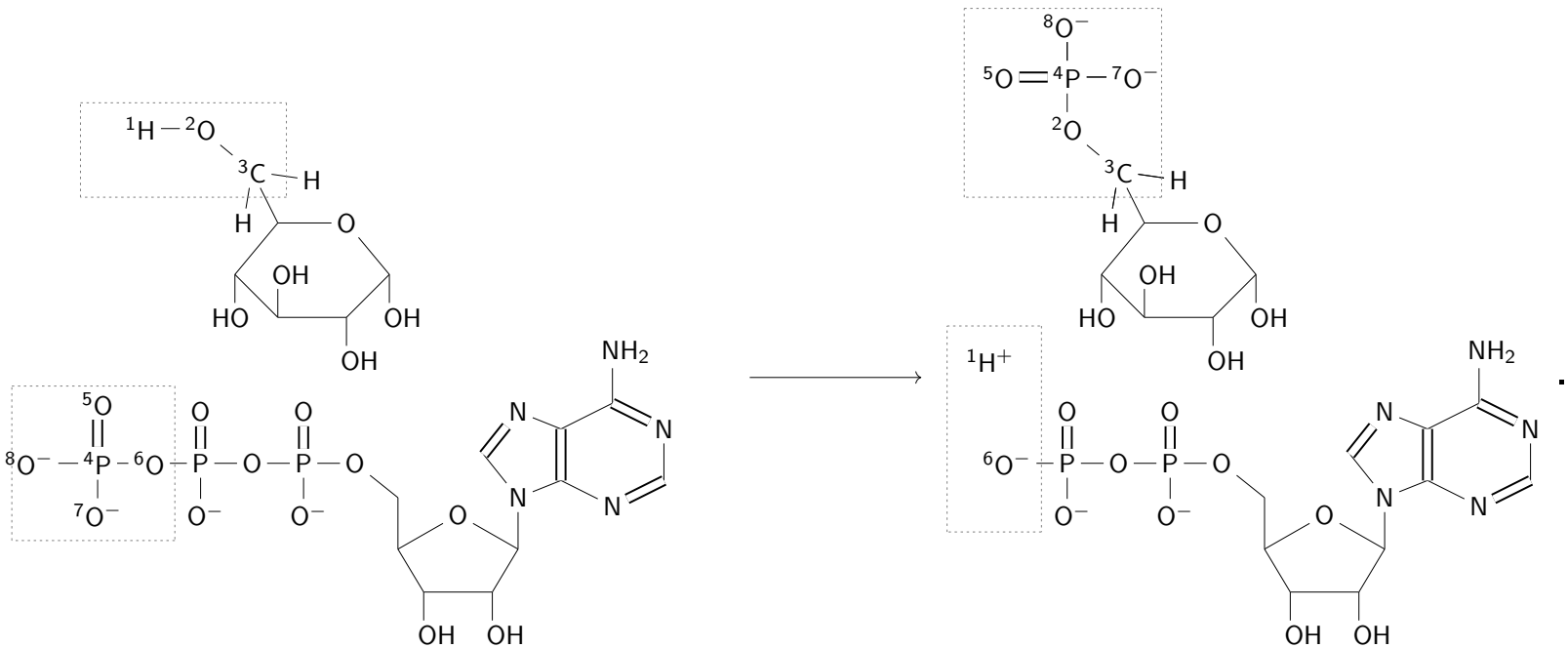

We denote the category of reactions by **React**.

Retrosynthetic analysis

(1) Start with the target molecule(s)

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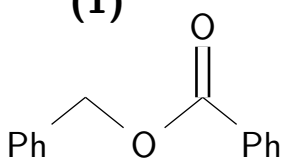

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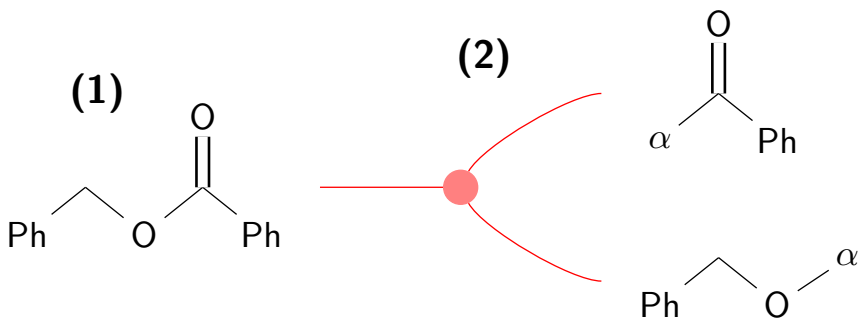
(1) Start with the target molecule(s)

(2) Cut the target along some bond, creating *synthons*



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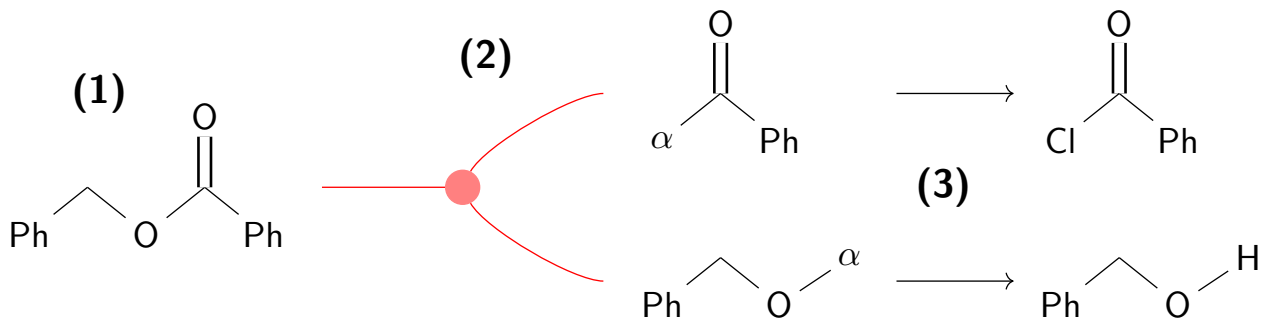

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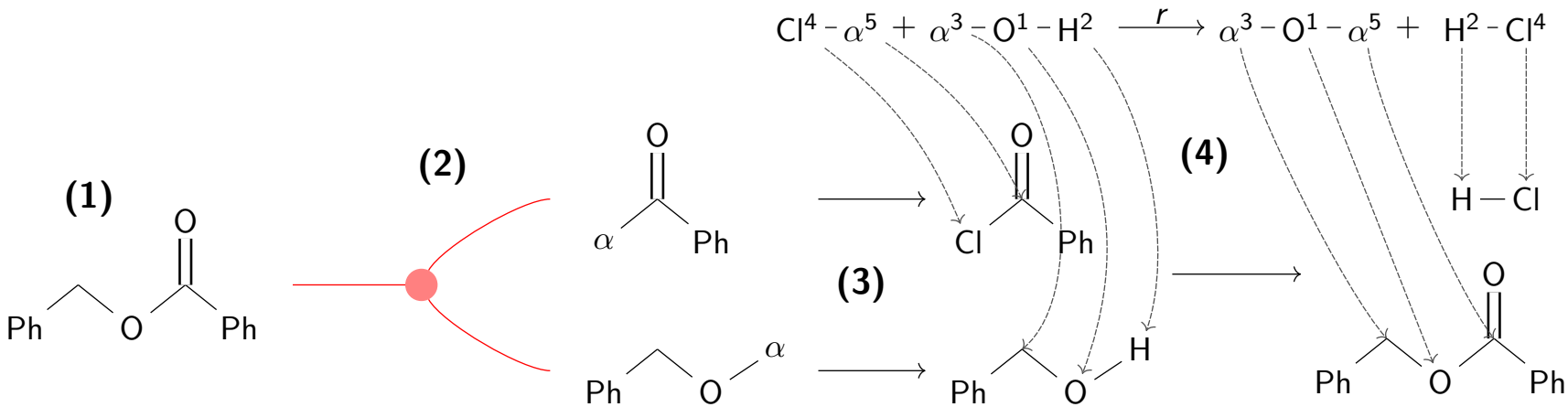

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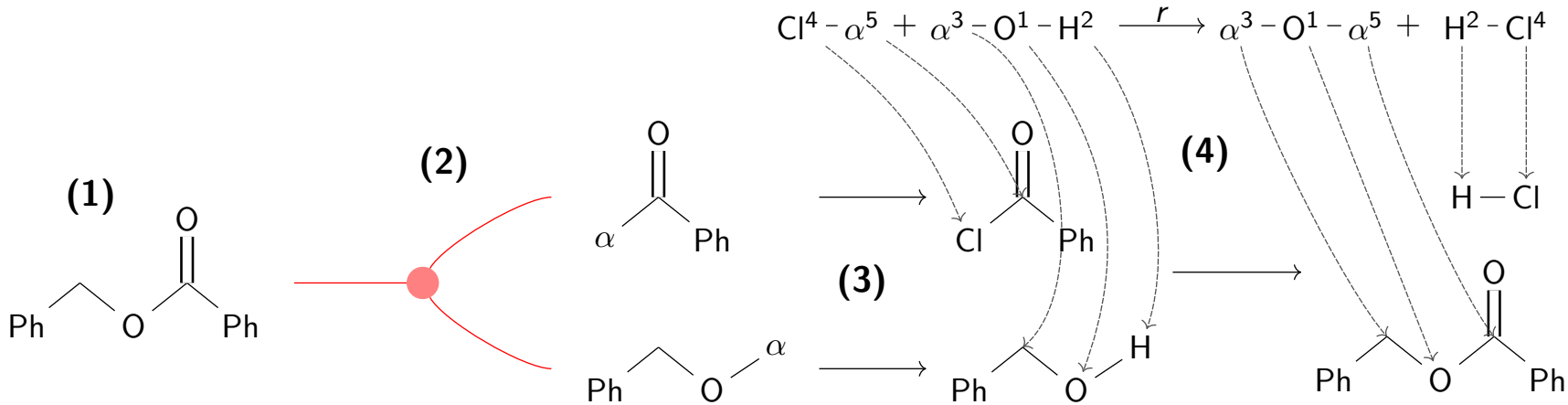
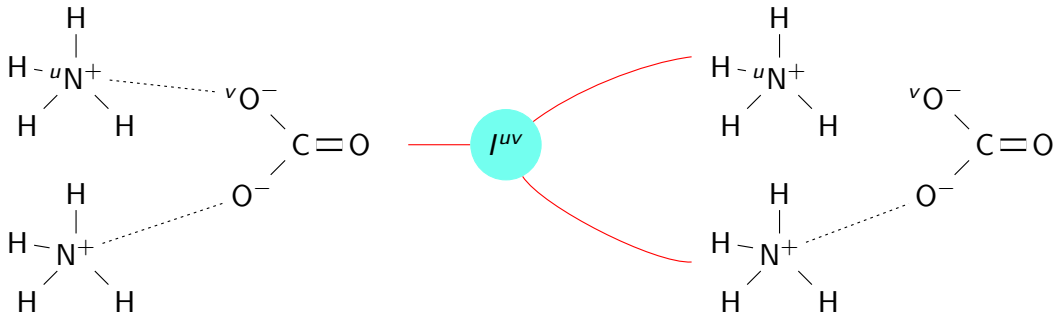
(5) Check whether the synthetic equivalents are known molecules: if yes, terminate, if no, return to **(1)** taking them as the target



Disconnection rules

Motto: Chemical reactions are movements of electrons



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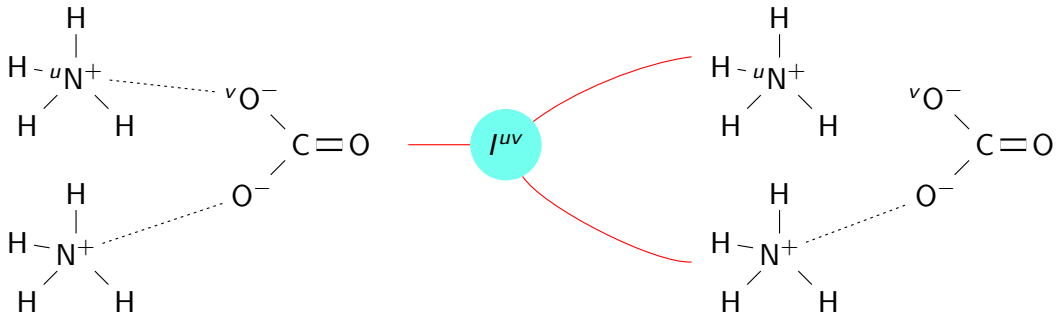

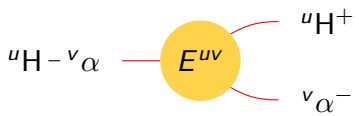

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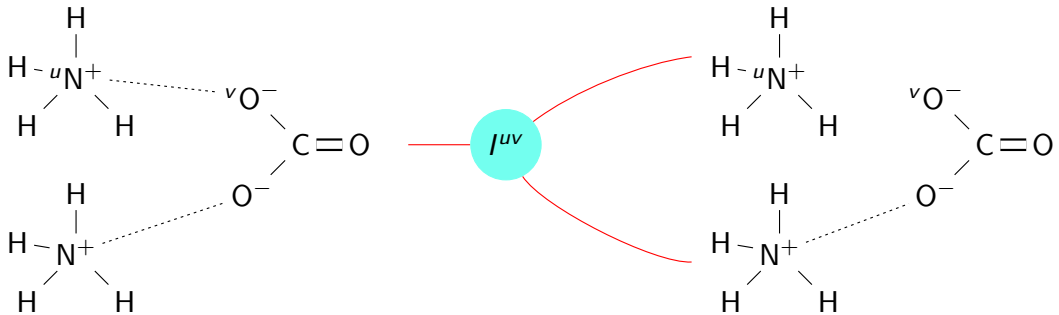

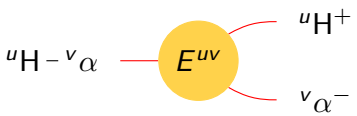

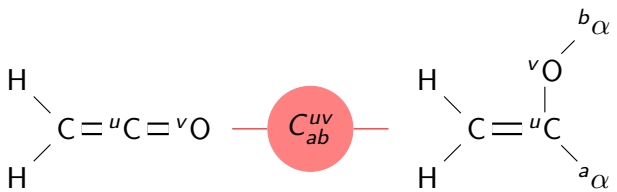

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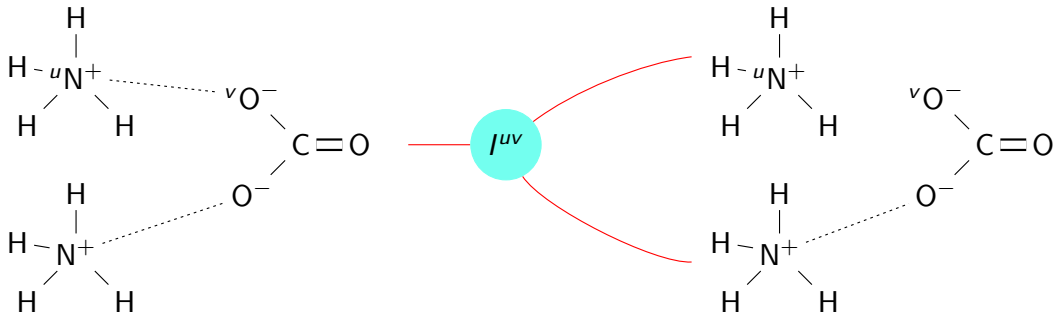

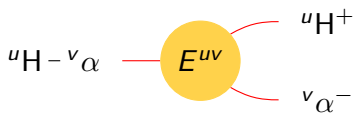

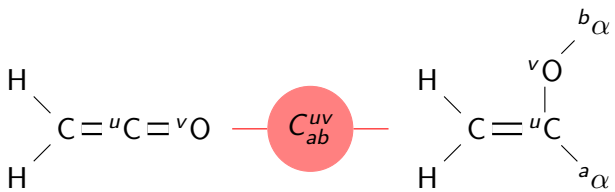

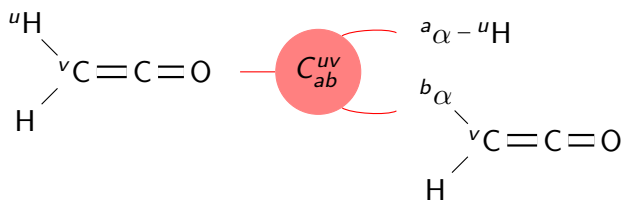

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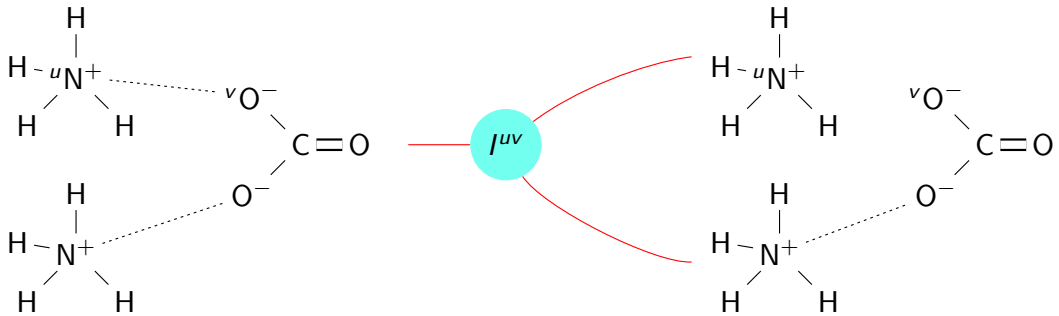

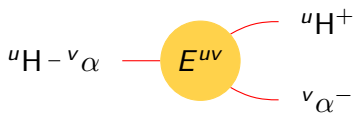

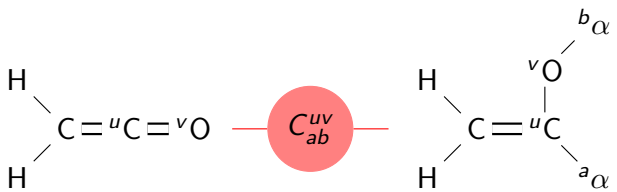

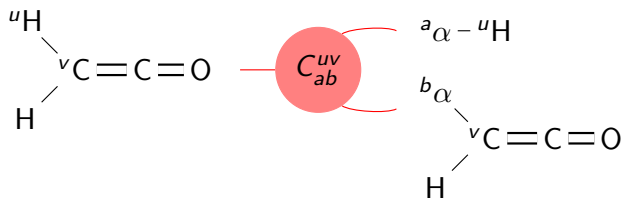

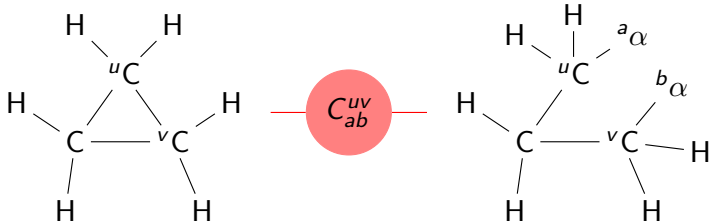

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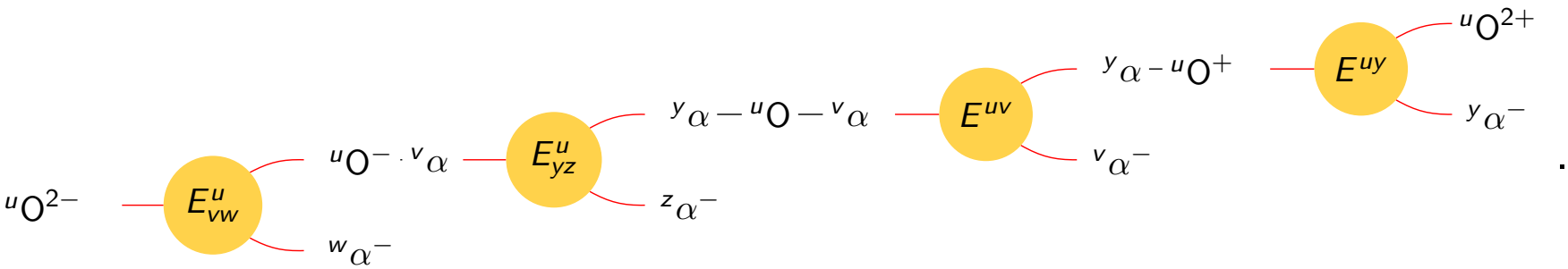

$\{u\} \longrightarrow \{u, y, z\}$

$\{u, v\} \longrightarrow \{u, v\}$

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Disconnection category

We define the set of terms with types as follows

- $\mathrm{id} : A \to A$,
- if $u \in \mathtt{Chem}(A)$, let $S^u : A \to A$,
- if $v \notin V_A \setminus \{u\}$, let $R^{u \mapsto v} : A \to A(u \mapsto v)$,
- $d^{uv}_{ab} : A \to d^{uv}_{ab}(A)$ and $\bar{d}^{uv}_{ab} : d^{uv}_{ab}(A) \to A$,
- if $\mathtt{t} : A \to B$ and $\mathtt{s} : B \to C$, then $\mathtt{t}; \mathtt{s} : A \to C$,
- if $\mathtt{t} : A \to B$ and $\mathtt{s} : C \to D$, then $\mathtt{t} + \mathtt{s} : A + C \to B + D$.

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The *disconnection category* **Disc** has valence complete chemical graphs as objects, and the terms (up to some equations) as morphisms.

From disconnections to reactions

Define the translation $R : \mathbf{Disc} \to \mathbf{React}$ by

- $R(E^u_{ab}) := (\{u\}, \{u, a, b\})$,
- $R(E^{uv}) := (\{u, v\}, \{u, v\})$,
- $R(I^{uv}) := (\{u\}, \{u\})$,
- $R(C^{uv}_{ab}) := (\{u\}, \{u, a, b\})$,
- $R(\mathrm{id}_A) := (\varnothing, \varnothing)$,
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Proposition (Soundness)

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The composite functor

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Corollary (Universality)

Given a reaction $r : A \to B$, there is a sequence of (dis)connection rules $d : A \to B'$ such that $B \simeq B'$.

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- What about reactions that are not valence complete?
- Incorporate chirality into the model
- Implement the algorithm that turns reactions into disconnection rules in normal form

References

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Thank you for your attention!