Supplementary file

1. Introduction

This web supplement contains the transformation rules used for modelling polymerization and hydrolysis in the HCN chemistry. Additionally, several pathways from HCN to adenine are shown. The following chemical processes (and if necessary their reverse) were translated into graph-rewrite rules:

- amide hydrolysis,
- addition of nucleophiles (e.g., water, alcoholes, cyanide, ammonia) to the cyanide and imine funcional groups,
- hemiketal/ketal, hemiaminal/aminal formation,
- Schiff base formation,
- amide tautomerization, and
- all reactions from Oro's prebiotic adenine synthesis.

1.1. Transformation Rule Annotation

The general annotation of vertices in transformation rules is $\langle label \rangle, \langle id \rangle$. However, if a vertex changes label during transformation its label in K is on the form $\langle L\text{-}label \rangle \mid \langle R\text{-}label \rangle, \langle id \rangle$. The vertex labels follow the rules of SMILES strings, e.g., aromatic atoms in lower case and charges as a suffix of $-$ or $+$.

Parallel edges represent different chemical bond types, e.g., 2 and 3 parallel edges represents a double and triple bond respectively. Additionally, single edges annotated with a `:` (colon) represents "aromatic bonds", as in SMILES strings.

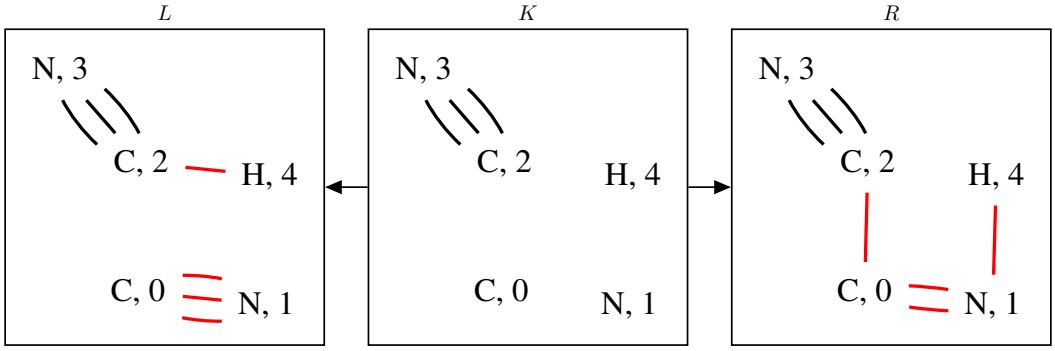
1.2. Pathway Annotation

In addition to the annotation described in the main paper, each molecule and reaction is annotated with a name. The names on reactions specify the transformation rule used. The molecule names are auto-generated identifiers in general, although core molecules have fixed chemical names.

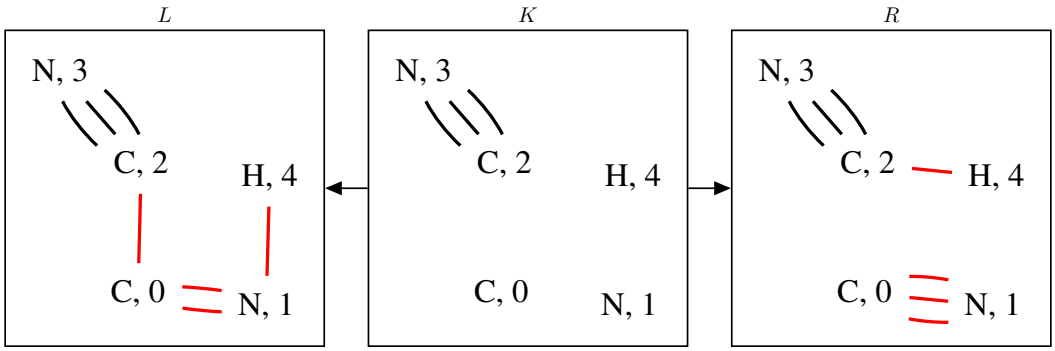
Note that all pathway figures have been automatically generated.

2. Polymerization Rules

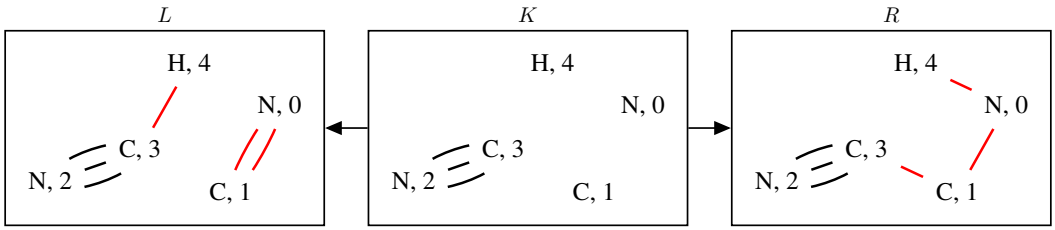
2.1. r_0, nu-add-hcn



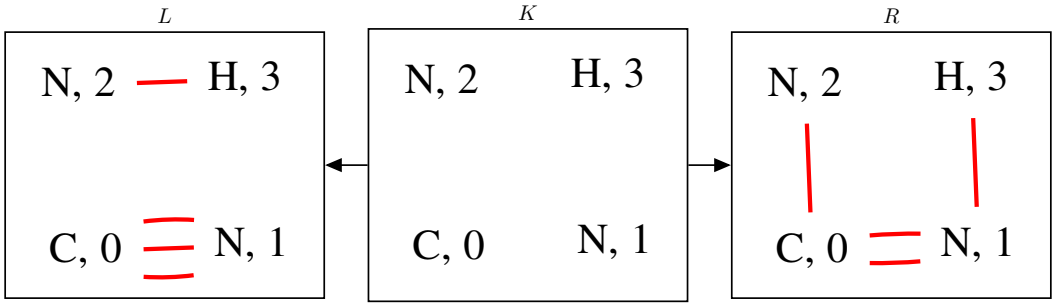
2.2. r_1, nu-add-hcn, reverse



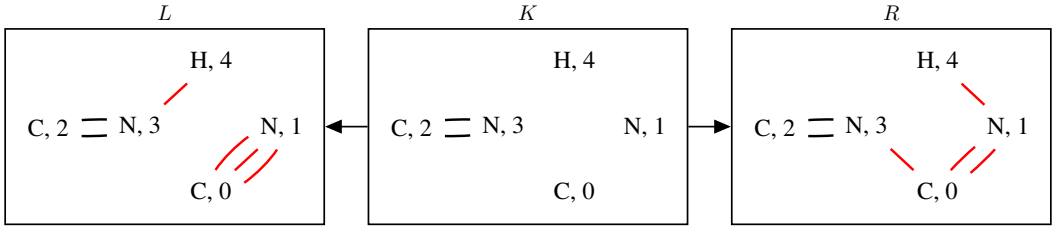
2.3. r_9, cn-to-imine



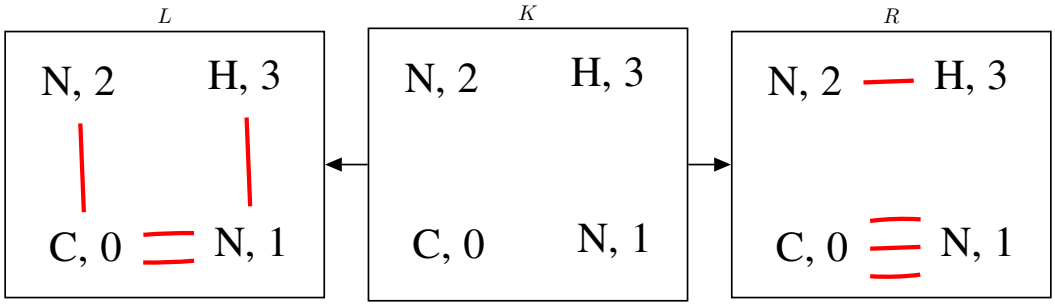
2.4. r_14, amine-to-cn



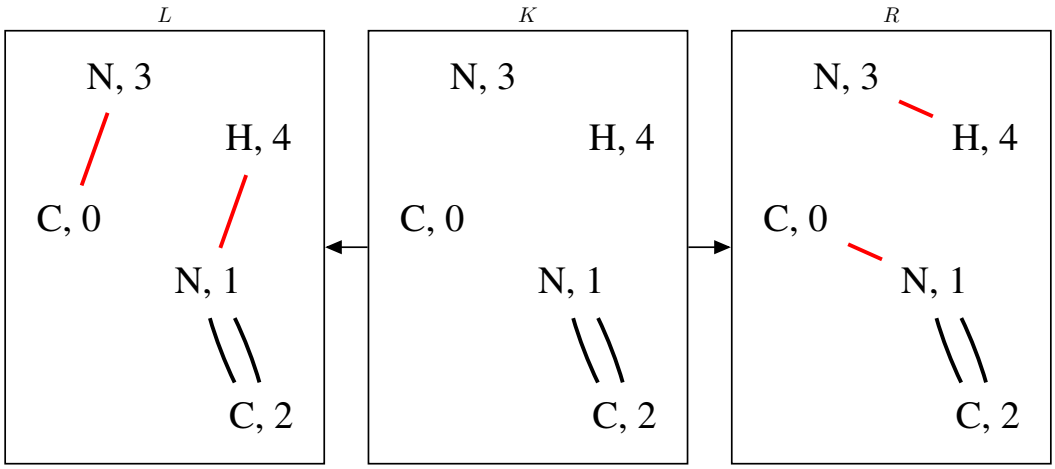
2.5. r_15, imine-to-cn



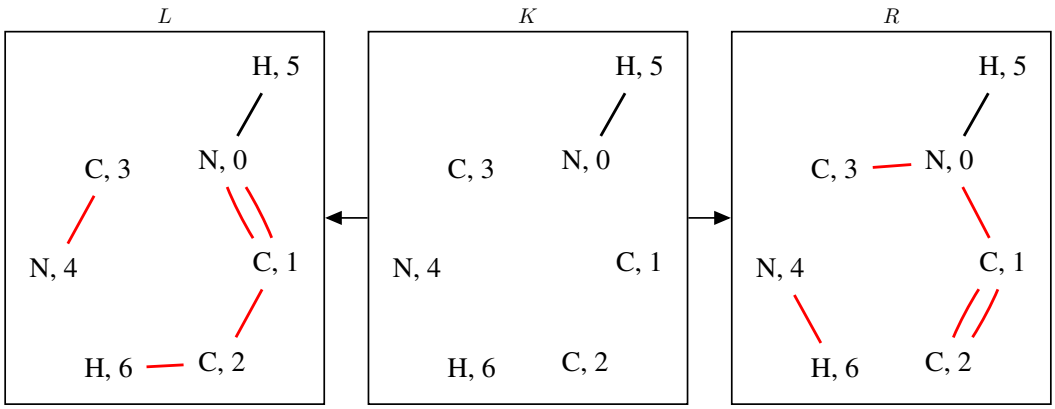
2.6. r_18, nu-add-amine, reverse



2.7. r_21, ring-imidazol

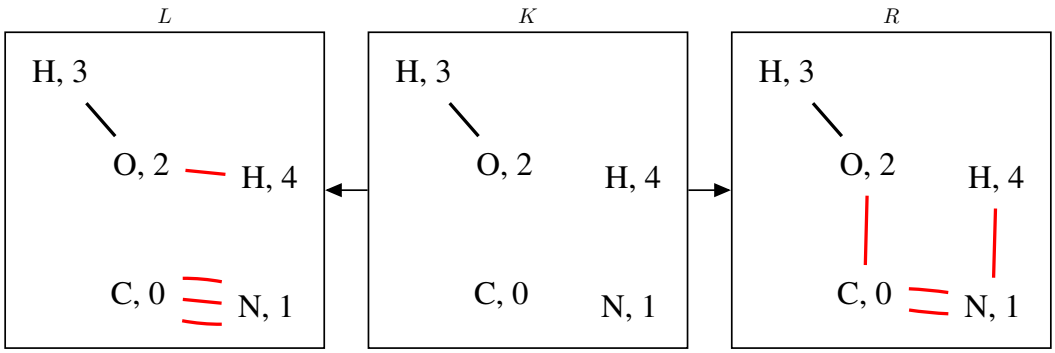


2.8. r_22, ring-imidazol2-diazine

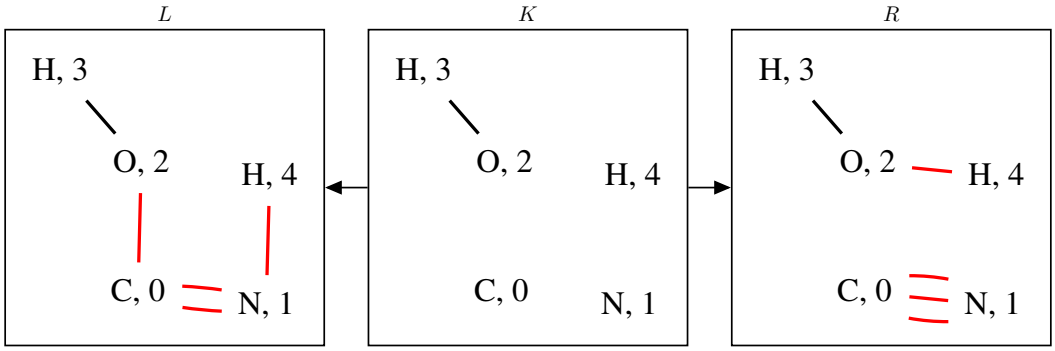


3. Hydrolysis Rules

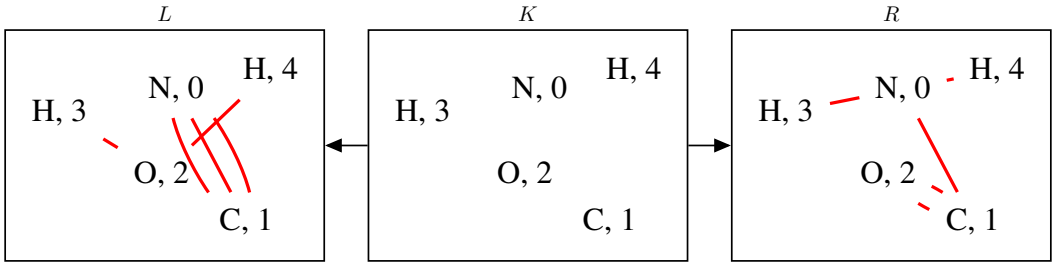
3.1. r_2, nu-add-h20



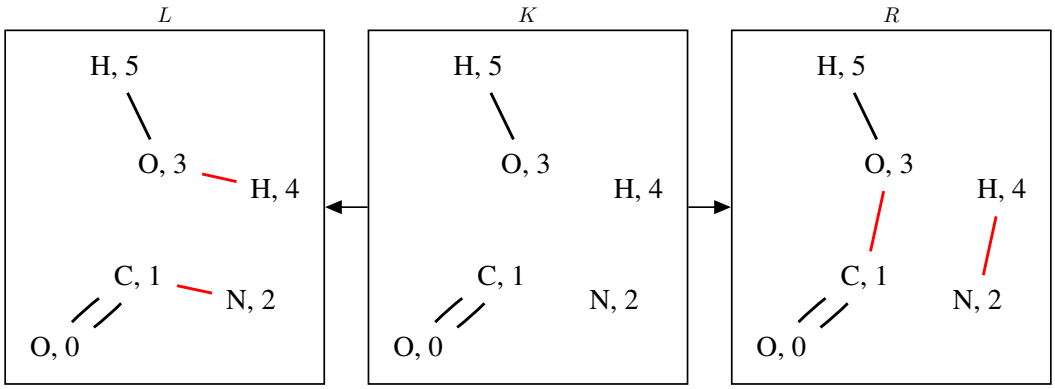
3.2. r_3, nu-add-h20, reverse



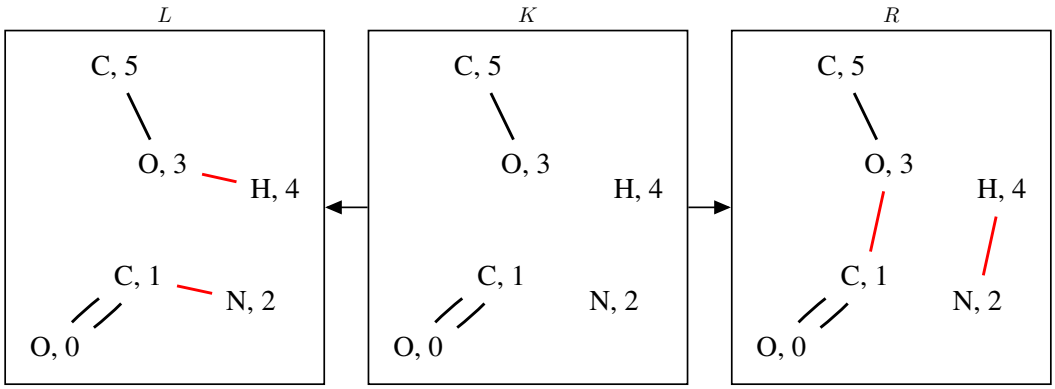
3.3. r_4, cn-to-amid



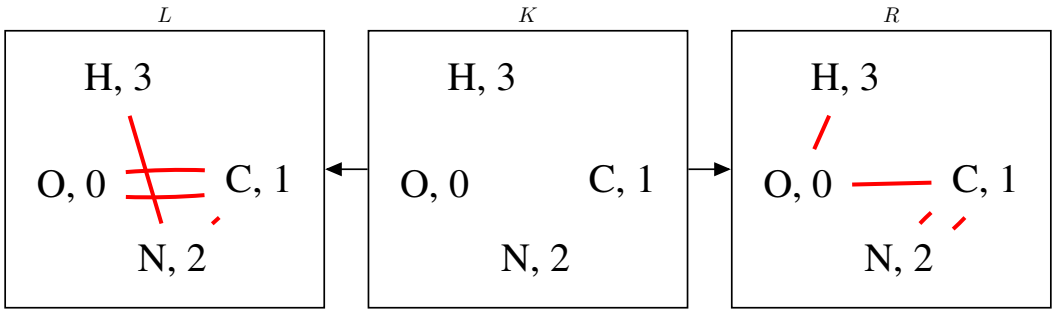
3.4. r_5, amid-to-acid-h20



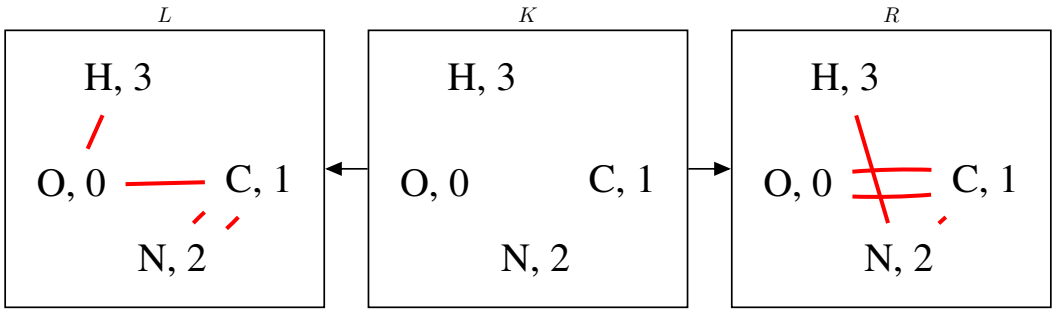
3.5. r_6, amid-to-acid-alc



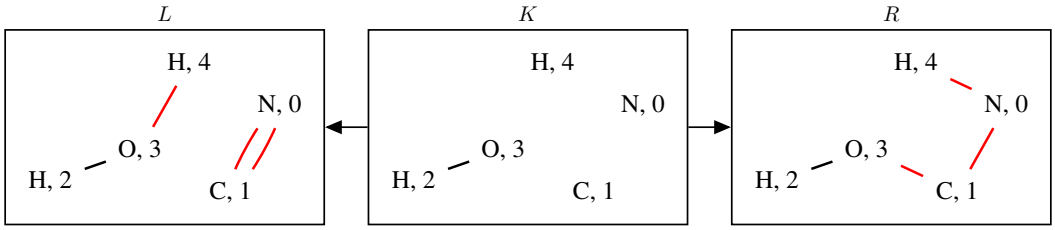
3.6. r_7, amid-to-imidic-acid



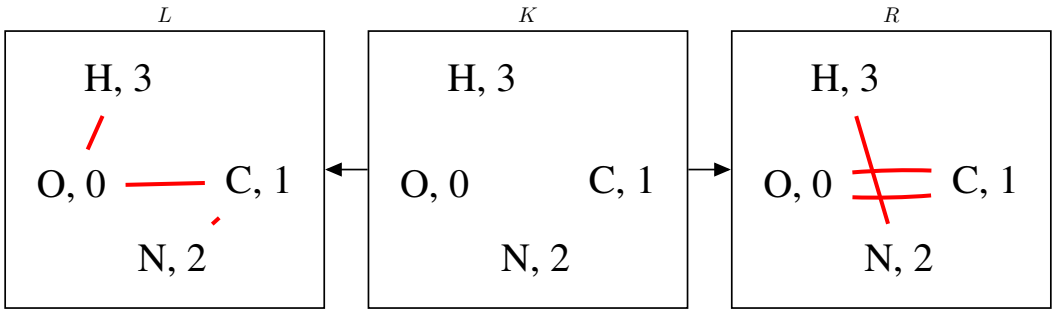
3.7. r_8, amid-to-imidic-acid, reverse



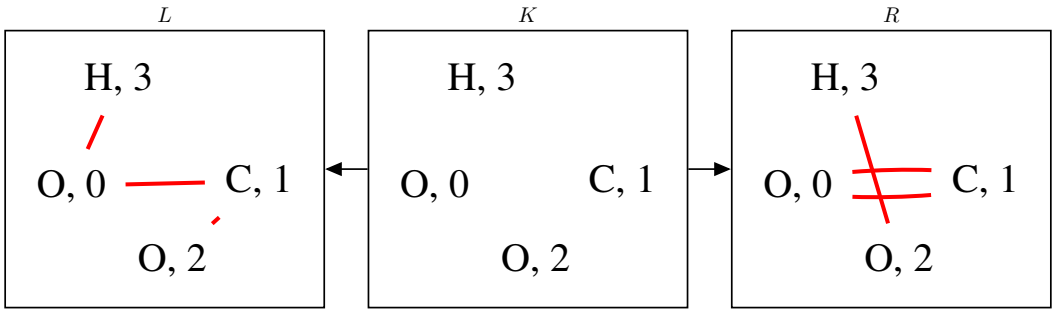
3.8. r_10, h20-to-imine



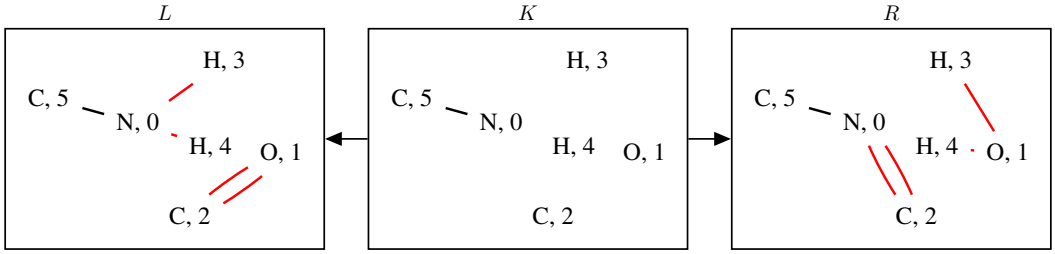
3.9. r_11, aminal



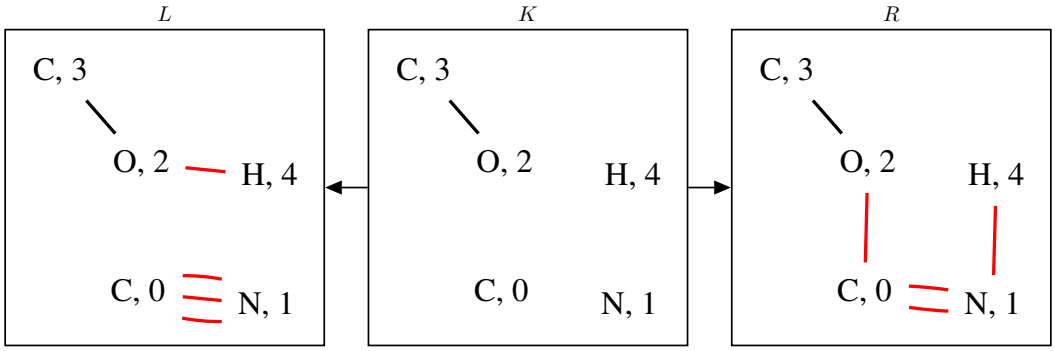
3.10. r_12, ketal



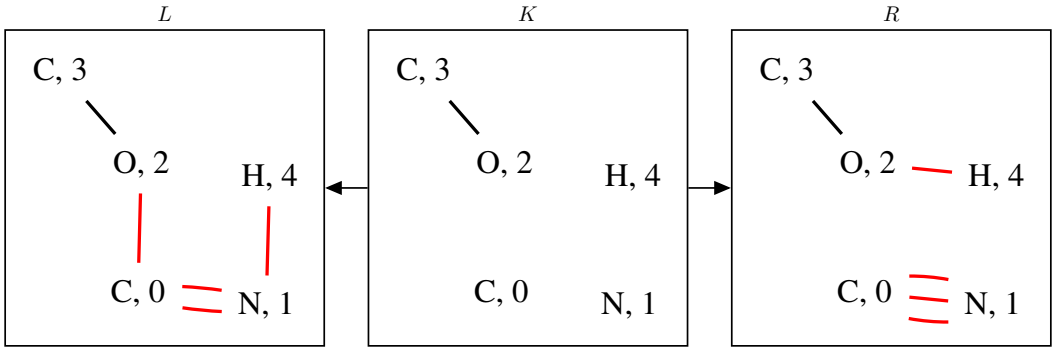
3.11. r_13, schiff ->



3.12. r_19, nu-add-alc

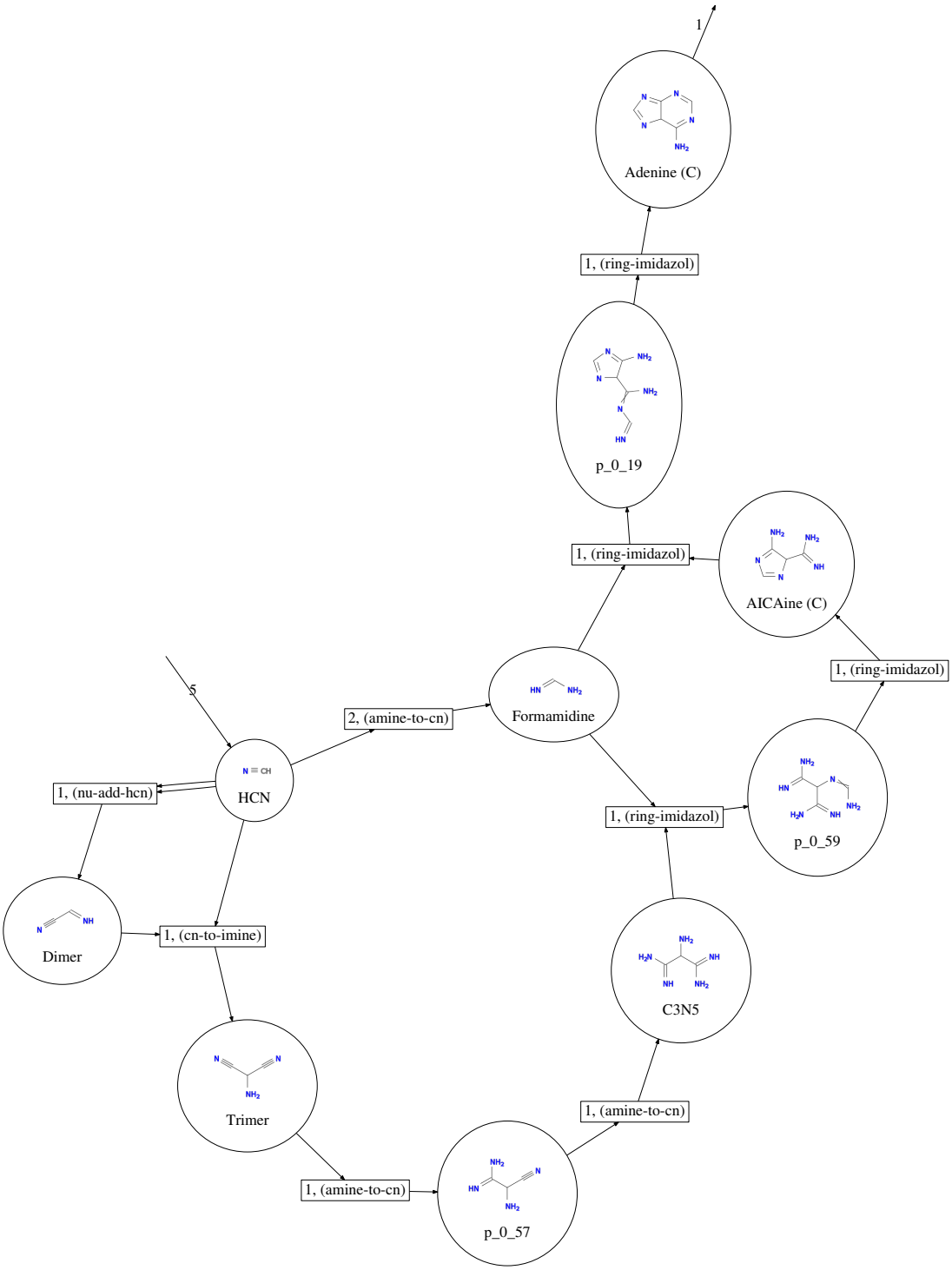


3.13. r_20, nu-add-alc-rev

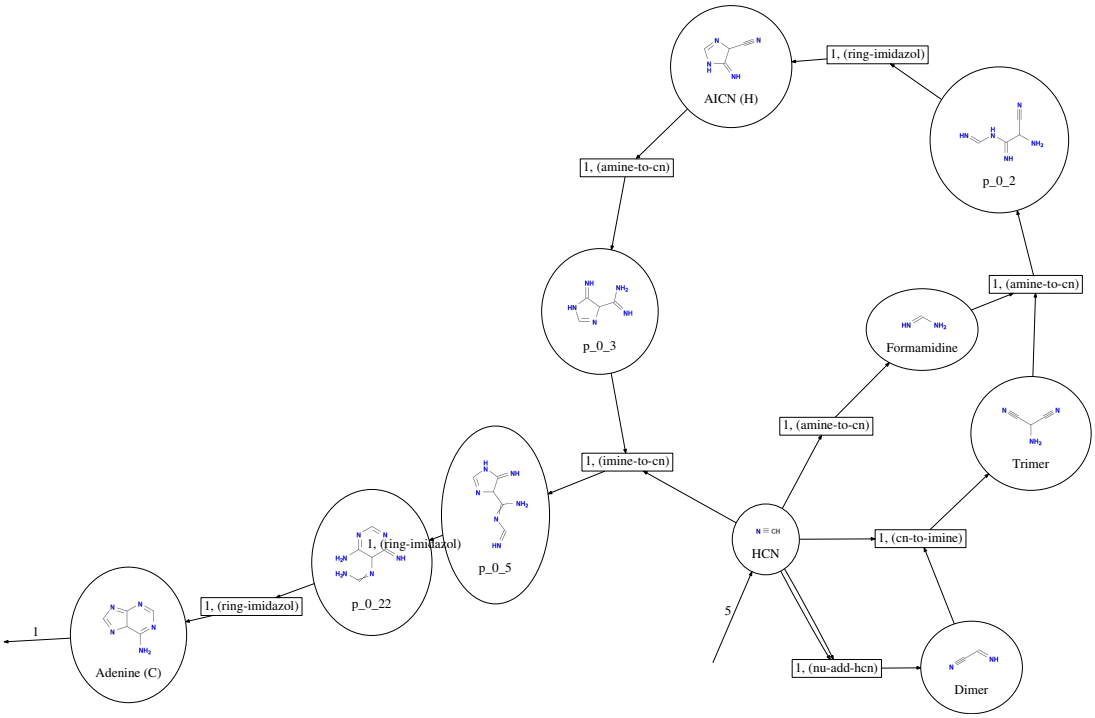


4. HCN to Adenine Pathways

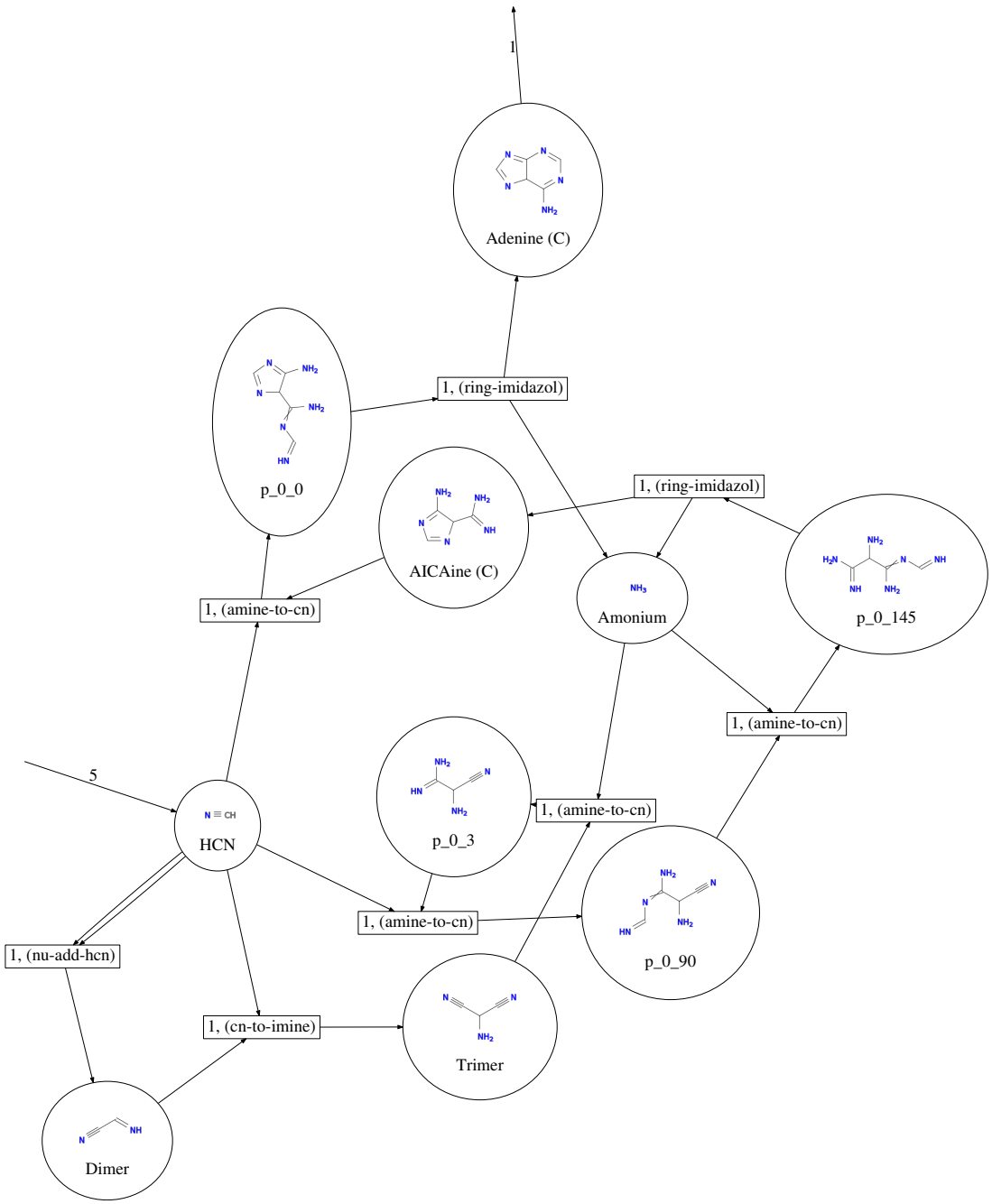
4.1. Oró



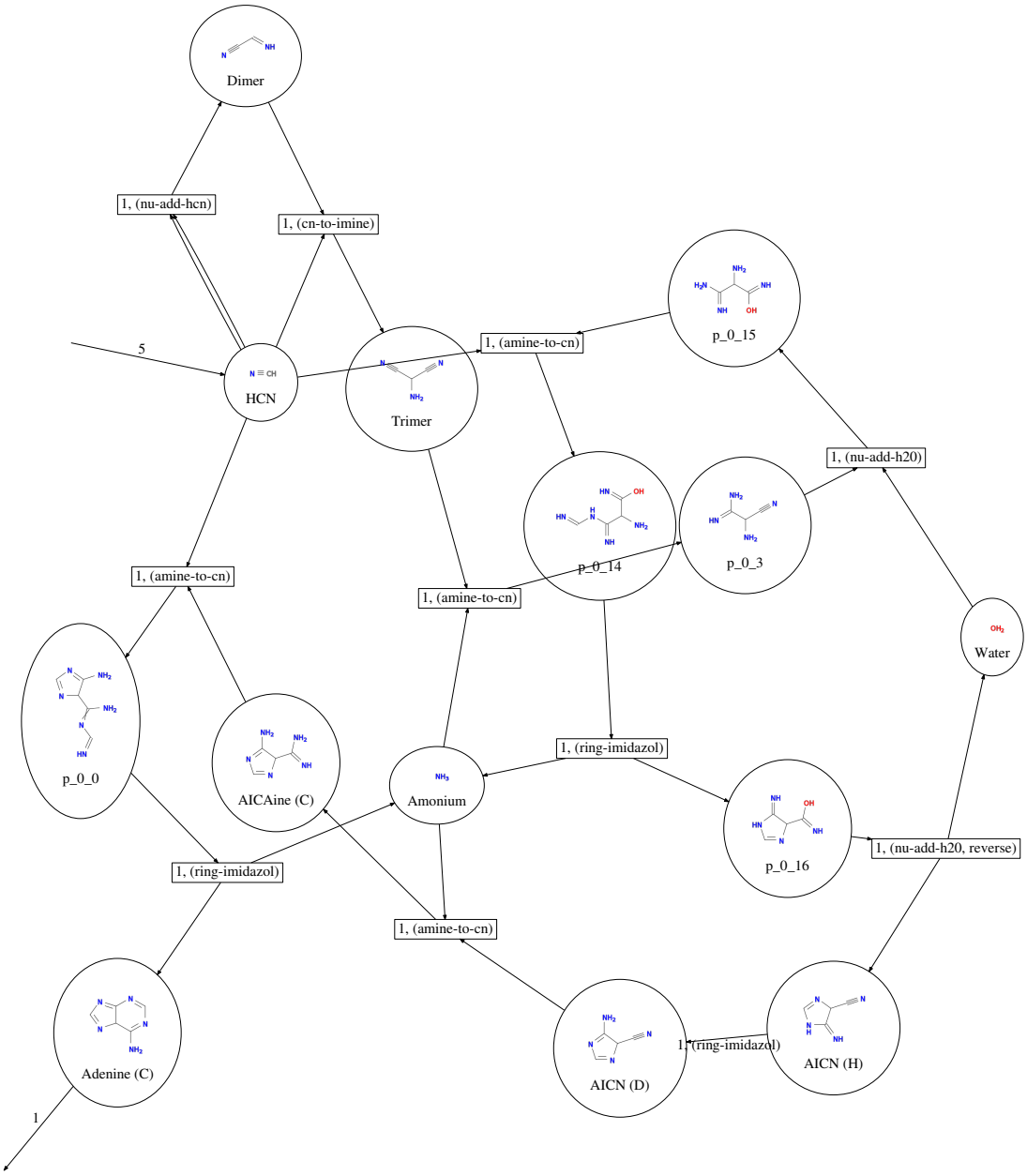
4.2. Without Oxygen 1



4.3. Without Oxygen 2



4.4. With Oxygen 1



4.5. With Oxygen 2