Given a CRS $\mathcal{Q} = (X, \mathcal{R}, C, F)$, a subset $\mathcal{R}'$ of $\mathcal{R}$ is a *RAF* for $\mathcal{Q}$ if $\mathcal{R}'$ is nonempty and satisfies the following two conditions.

- *Reflexively autocatalytic* (RA): each reaction $r \in \mathcal{R}'$ is catalysed by at least one molecule type that is either present in the food set or generated by another reaction in $\mathcal{R}'$.
- *Food-generated (F)*: for each reaction $r \in \mathcal{R}'$, the reactants of r are either present in the food set, or can be created from the food set F by using a series of reactions only from $\mathcal{R}'$.

In words, a RAF is a subset of reactions that is both self-sustaining (from the food set) and collectively autocatalytic. In forming a RAF from the food set, some reactions may initially need to proceed uncatalysed (so at a lower rate) but once formed every reaction in the RAF must be catalysed. A simple example of a RAF where this occurs is shown in Fig. 2.

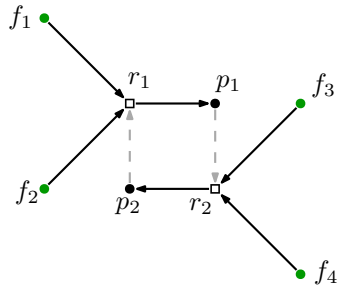

FIGURE 2. A simple RAF involving two reactions r_1, r_2 and a food set $F = \{f_1, f_2, f_3, f_4\}$, with catalysation arcs shown as dashed arrows. We can write this RAF by the pair of equations

$$r_1 : f_1 + f_2[p_2] \to p_1,$$
$$r_2 : f_3 + f_4[p_1] \to p_2.$$

where [*] denotes the that the reaction is catalysed by $*$. Note that r_1 or r_2 must first proceed uncatalysed, but once one reaction has occurred the system can then continue with both reactions catalysed (so this is a RAF and not a CAF, as described next).

2.1. **Further concepts for RAFs.** The *support* of a RAF $\mathcal{R}'$ is the set of molecule types that are either a reactant or a product of at least one reaction from $\mathcal{R}'$. The maxRAF may contain a proper subset of reactions that itself is an RAF for $\mathcal{Q}$ – we call such a subset a *subRAF* of the maxRAF (there may be no such subRAF, or many). An RAF $\mathcal{R}'$ is an *irreducible* RAF (or irrRAF) if contains no subRAF. In other words, removing any single reaction from $\mathcal{R}'$ gives a set of reactions that does not contain a RAF for $\mathcal{Q}$. We say that a reaction r from $\mathcal{R}'$ is *essential* if removing r from $\mathcal{R}'$) gives a set of reactions that does not contain a RAF for $\mathcal{Q}$. Thus a RAF $\mathcal{R}'$ is an irrRAF if and only if all its reactions are essential. A *co-RAF* is a subset of reactions that when combined with an RAF produces a larger RAF.

Given an RAF $\mathcal{R}'$ for $\mathcal{Q}$, the *closure* of $\mathcal{R}'$, denoted $\overline{\mathcal{R}'}$ is the (unique) minimal subset $\mathcal{R}''$ of $\mathcal{R}$ that contains $\mathcal{R}'$ and that satisfies the property that if $r \in \mathcal{R}$ has each its reactants and at least one catalyst is either in the food set or a product of a reaction from $\mathcal{R}''$ then r is in $\mathcal{R}''$. We say that a RAF $\mathcal{R}'$ is *closed* if it is equal to its closure (i.e. $\mathcal{R}' = \overline{\mathcal{R}'}$), and *closure-irreducible* if it is not equal to the closure of any subRAF. The maxRAF is always closed, and an irrRAF is closure-irreducible (but a closure-irreducible subRAF need not be an irrRAF).