Chemical Programming: Models, Concepts, and Designs

Joshua Weinstein

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1 Introduction

Chemical Programming is a paradigm of programming that is modeled after the mechanics of chemical reactions. This style focuses on utilizing the features of chemical components, such as atoms, elements, compounds and reactions. The intention of this programming paradigm is to allow the functionality and mechanisms in chemical processes to be applied to computational values. Chemical computation permits highly customizable abstraction over traditional types like booleans, integers, and strings.

Purely modeling chemical reactions is not the goal, rather defining and modeling the components of chemistry to make them useful in programming. Computer science and chemistry are well defined, yet very different fields. The fashions and organizations of chemical reactions provide unique interfaces for program design. However, moles, molecular orbitals, and energy levels are not fruitful or applicable to abstract program designs, or a programming paradigm. Another goal in this book is to illustrate models and definitions such that components of chemicals can exist more fruitfully as a programming construct.

Traditionally, programming languages use typed values or data, such as integers, booleans, or characters. These are commonly referred to as *primitive* types. Such a type is normally the most basic level of abstraction in a programming language. They cannot be further decomposed into simpler types. The higher level abstractions such as functions or classes are composed of primitive types, which allows the creation of *user-defined* types. Similarly, elements, the most basic *type* of matter, exists in it's smallest form as an atom, which compose molecules and more sophisticated compounds.

Some fundamentals in chemistry are rather limiting when judged in a computational perspective. Reactions usually require an activation energy, E_a, in order to being and transition from reactants to products. This energy arises from a combination of heat, pressure, acidity, and other environment factors.

$$A, B \longrightarrow AB \tag{1}$$