Thesis Title A Knot-Theoretical Study of Molecular Chirality

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ABSTRACT

Knots, links and braids have been known and used since ancient times. As mathematical objects, however, they are rather difficult to deal with. Their definitions involve some subtle problems of placement and embedding of manifolds in abstract spaces, and their proper treatment needs a good background knowledge of geometry, topology and algebra. Only recently has knot theory been sufficiently developed to give effective methods and reasonably easy procedures for determining whether two knots (or links, or braids) are equivalent or not. For this purpose, the **Reidemeister moves** and various types of **knot polynomials** have been introduced. Some knot polynomials, such as the **Jones polynomial** with one variable, and the **HOMFLY polynomial** with two variables, can also express the **chirality** of a knot.

Molecular chirality is an important aspect of stereochemistry. The main objective of this thesis is to study molecular chirality from the standpoint of knot theory. The abstract **molecular knot** is generated by tying a piece of string around the molecular model in an appropriate manner. It has the chirality corresponding to that of the molecular model. In this study, it has been found that the molecular knot for a molecule with one chiral center is a trefoil. Those for molecules with two or more chiral centers are composite knots. For molecules

with a noncyclic sequence of chiral centers, the composite knot, is a sum of trefoils. The product rules of knot polynomials for composite knots can thus be used to express the chirality polynomials of these molecular knots. Molecules with cyclic arrangement of chiral centers, however, give more complicated molecular knots, with links and braids, and the associated polynomials involve non-integral powers.