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RIGID AND NON-RIGID ACHIRALITY

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In order to completely characterize a molecule it is useful to understand the symmetries of its molecular bond graph in 3-space. For many purposes the most important type of symmetry that a molecule can exhibit is mirror image symmetry. However, the question of whether a molecular graph is equivalent to its mirror image has different interpretations depending on what assumptions are made about the rigidity of the molecular structure. If there is a deformation of 3-space taking a molecular bond graph to its mirror image then the molecule is said to be *topologically achiral*. If a molecular graph can be embedded in 3-space in such a way that it can be rotated to its mirror image, then the molecule is said to be rigidly achiral. We use knot theory in $\mathbf{R}^3$ to produce hypothetical knotted molecular graphs which are topologically achiral but not rigidly achiral, this answers a question which was originally raised by a chemist.

A *molecular bond graph* is a graph in $\mathbf{R}^3$ which is a geometric model of the structure of a molecule, see [**Walb**] and [**Was**]. We will be working primarily with molecular bond graphs which consist only of a simple closed curve K in $\mathbf{R}^3$. Since we are addressing a question raised by chemists and are working in $\mathbf{R}^3$, we choose to use the term "achiral" from the chemical literature rather than using the corresponding mathematical term "amphicheiral" which is generally used for knots in S^3. It is not hard to show that K is topologically achiral if and only if there is an orientation reversing diffeomorphism of $\mathbf{R}^3$ leaving K setwise invariant. If K is rigidly achiral then there is some embedding of K in 3-space which can be rotated to its mirror image. This embedding is said to be a *symmetry presentation* for K. Let h be this rotation composed with a reflection so that $h(K) = K$. Since K is only supposed to be a model of reality we shall make the assumption that this rotation is through a rational angle. Hence h must be of finite order. On the other hand, any finite order diffeomorphism of $(\mathbf{R}^3, K)$ is conjugate to a rotation composed with a reflection. Thus K is rigidly achiral if and only if there is a finite order orientation reversing diffeomorphism of $(\mathbf{R}^3, K)$.

By giving K an orientation we can distinguish further between two types of topological achirality. If there is a diffeomorphism of $(\mathbf{R}^3, K)$ which reverses the orientations of both R^3 and K, then K is said to be *negative achiral*. Whereas, if there is a diffeomorphism of $\mathbf{R}^3$ and K which