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Quasi-Groups and the Configuration Space of Symmetry-Constrained Motions

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In this work, the set of all possible positions and orientations of a large molecule within the crystallographic asymmetric unit is equated to the coset space of the continuous group of proper rigid-body motions modulo the chiral space group of the macromolecular crystal. Since every chiral space group is a co-compact subgroup in the full group of rigid-body motions (which is a six-dimensional Lie group), the resulting coset space is a compact 6D manifold. However, since none of the crystallographic groups are normal in the full group of rigid-body motions, this coset space is not a group. However, it can be endowed with an operation that satisfies all of the group axioms except for associativity, thereby giving it the structure of a quasi-group. The quasi-group properties of such spaces are explored in this work as an example of generalized symmetry. The mathematical formulation presented here, which builds on the author's prior work cited below, is relevant to both the Molecular Replacement (MR) method in biomolecular crystallography, and in the design of new engineered crystals.

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