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Rotational Isomeric State Models in Macromolecular Systems

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Foreword

The Rotational Isomeric State (RIS) method has become a popular tool for the analysis of the conformational behavior of macromolecules when proper attention to the details of the chemical structure - constitution and configuration - of the unperturbed chain is required. It has been implemented in several commercial software packages and is simple enough that many researchers have coded their own programs to carry out the necessary computations. Several review articles and two books have been dedicated to this topic and it seemed as if there was no need for a further publication. The practitioner of the art of RIS calculations will quickly find out, however, that while it is one thing to be able to carry out the calculations and thereby obtain a wealth of information on the conformational behavior of a macromolecule, it is quite another matter to devine the parameters necessary for the calculations. And when he resorts to the literature, he finds it difficult to find the necessary publications since little standardization exists in the field and, once the appropriate sources are located, he will often be confused when more than one source is found that provides different, seemingly contradictory values and models. Even a researcher intimately familiar with the method and its foundation, is often faced with the task of finding RIS parameters from the literature for unfamiliar constitutions and configurations, a task that can prove formidable.

We set out, in consequence, to ease the task of finding and comparing RIS models and parameters in the literature. A review seemed to be the most appropriate method, but in the process of its compilation it became rapidly clear that a complete representation of the published work since Volkenstein´s first article on the subject in 1951 was not possible. Nevertheless we are confident that we were able to provide a sufficiently complete listing of the most relevant publications on fundamental aspects of RIS theory as well as a comprehensive overview of the published models available to the end of 1994. More than 680 models for structures of symmetric and asymmetric synthetic polymers, polysaccharides, polypeptides, polynucleotides, rigid chains, branched, comb, and star molecules, and others are compiled here.

We would like to thank many of the authors of the reviewed publications for patiently checking the accuracy and completeness of their contributions and hope for the understanding of those researchers whose work we have inadvertently overlooked.

December 1996

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