

# Theoretical Aspects of Ring-Chain Equilibria and Implications for Real Dynamic Libraries

Stefano Di Stefano

*Dipartimento di Chimica Università di Roma La Sapienza e IMC/CNR sezione sui Meccanismi di Reazione, P.zzale Aldo Moro 5, 00185 Roma. e-mail: stefano.distefano@uniroma1.it*

Macrocyclizations under thermodynamic control, also named ring-chain equilibria, have been fundamental processes in polymer chemistry. The first theoretical treatment related to such equilibria is due to two polymer chemists, Jacobson and Stockmayer, in the early fifties of the last century.<sup>1</sup> This theory was then enriched and repropounded in a form aimed at being more easily understandable by non-specialists.<sup>2</sup> The recent growing interest in Dynamic Combinatorial Chemistry (DCC),<sup>3</sup> calls for a deep and detailed knowledge for the theoretical and quantitative aspects of macrocyclization equilibria since most of the receptors involved in DCC are cyclic species. For example, in most of the studies published on DCC, the information related to the critical monomer concentration (CC) is completely neglected while it is necessary for a quantitative interpretation of the experimental results.<sup>4</sup> The accordance of the theory with the experimental results obtained for equilibrated systems of cyclic acetals<sup>5</sup> and olefines<sup>6</sup> will be illustrated in this talk.

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