Steps Towards Complex Matter : Self-Organization by Design and by Selection

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Supramolecular chemistry is actively exploring systems undergoing self-organization, i.e. systems capable of spontaneously generating well-defined functional supramolecular architectures by self-assembly from their components, on the basis of the molecular information stored in the covalent framework of the components and read out at the supramolecular level through specific interactional algorithms, thus behaving as programmed chemical systems.

Supramolecular chemistry is intrinsically a dynamic chemistry in view of the lability of the interactions connecting the molecular components of a supramolecular entity and the resulting ability of supramolecular species to exchange their constituents. The same holds for molecular chemistry when the molecular entity contains covalent bonds that may form and break reversibility, so as to allow a continuous change in constitution by reorganization and exchange of building blocks. These features define a Constitutional Dynamic Chemistry (CDC) on both the molecular and supramolecular levels.

CDC is expressed in particular in Dynamic Combinatorial Chemistry (DCC). Whereas combinatorial chemistry is based on extensive libraries of prefabricated molecules, DCC implements the reversible connection of sets of basic components to give access to virtual combinatorial libraries (VCLs), whose constituents comprise all possible combinations that may potentially be generated. The constituent(s) actually expressed/selected among all those accessible is(are) expected to be that(those) presenting the strongest interaction with a given target, that is, the highest receptor/substrate molecular recognition. The overall process is thus instructed (target-driven), combinatorial, and dynamic. It bypasses the need to actually synthesize the constituents of a combinatorial library by letting the target perform the assembly of the optimal partner.

CDC introduces a paradigm shift with respect to constitutionally static chemistry. The latter relies on design for the generation of a target entity, whereas CDC takes advantage of dynamic diversity to allow variation and selection. The implementation of selection in chemistry introduces a fundamental change in outlook. Whereas self-organization by design strives to achieve full control over the output molecular or supramolecular entity by explicit programming, self-organization by selection operates on dynamic constitutional diversity in response to either internal or external factors to achieve adaptation in a darwinistic fashion.

The merging of the features: - information and programmability, - dynamics and reversibility, -constitution and structural diversity, points towards the emergence of adaptive and evolutive chemistry. Chemistry thus plays a major role in the progressive elaboration of a science of informed, organized, evolutive matter, a science of complex matter.

References

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