Chemical Frustration in Dynamic Multilevel Systems

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ABSTRACT Dynamic multilevel systems constructed with sequential-communicating reactions are a poorly studied type of thermodynamic systems. Recent work of our group showed that multilevel sequential systems are history-dependent and nonconmutative, since different compositions can be attained when one cycle of reactions is carried out by affecting the order of activation. In this work, we show that compositional divergence observed in previous work is the result of trapping the composition in frustrated states placed on local minima of the energy landscape. These intermediary steps in the trajectory can be overcome by the system, when it approaches the global energy minimum of the energy landscape, as expected in usual thermodynamic systems. The behavior of the multilevel system depends on its underlying energy landscape and can be externally regulated by adjusting starting materials and reaction conditions.

Keywords: dynamic covalent chemistry; dynamic multilevel systems; frustration; energy landscapes

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