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Fock spaces for modeling macromolecular complexes

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Large macromolecular complexes play a fundamental role in how cells function. Here I describe a Fock space formalism for mathematically modeling these complexes. Specifically, this formalism allows ensembles of complexes to be defined in terms of elementary molecular "building blocks and "assembly rules. Such definitions avoid the massive redundancy inherent in standard representations, in which all possible complexes are manually enumerated. Methods for systematically computing ensembles of complexes from a list of components and interaction rules are described. I also show how this formalism readily accommodates coarse-graining. Finally, I introduce diagrammatic techniques that greatly facilitate the application of this formalism to both equilibrium and non-equilibrium biochemical systems.