Computational study of the bivalent reaction of bispyrrolidine derivatives with dialdehydes

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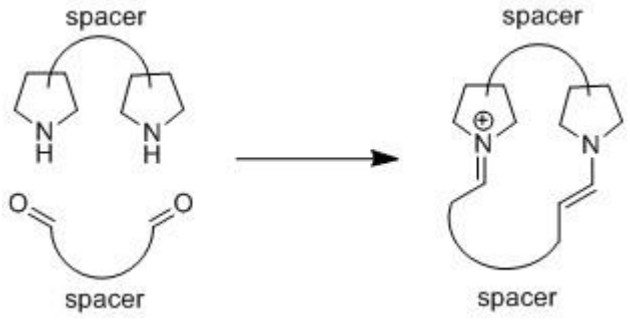

Abstract:

Computational electronic structure calculations should be performed for different bispyrrolidine derivatives and their reaction with dialdehydes. In a first step, the stability of different conformers of bispyrrolidine with different linkers will be investigated in vacuum and with different solvent models. The bivalent reaction of the bispyrrolidine with the dialdehyde with a rigid linker should be compared to a monovalent binding. The influence of different solvents should be investigated, both with implicit solvent models and explicit modeling of solvent molecules. In a second step, the effect of substituents, both on the bispyrrolidine and on the dialdehyde, on the binding strength will be analyzed. The methods used in this part of the projects are different density functionals including dispersion corrections and different solvent models. In the third part the project is extended to flexible linkers between the two aldehyde functions. To model the large configuration space of the reaction, next to first-principle calculations molecular dynamics simulations will be performed. The proposed project is in strong collaboration with the experimental working group of Prof. Mathias Christmann, who is synthesizing the compounds and analyzing the reaction.

Publication/s:

D. Mollenhauer, N. Gaston, E. Voloshina and B. Paulus: J. Phys. Chem. C 117, 4470 (2013)

F. R. Clemente and K. N. Houk: Angew. Chem. Int. Ed. 43, 5765 (2004)