

## Popular science abstract

Nowadays, the radiation damage primary seen as pure negative effect such as cosmic rays in the outer space e.g. on the astronauts is also considered as the positive trigger in the post-radiational processes e.g. on the formation of the matter in the interstellar medium, which is of prime interests in the future cosmos exploration. Moreover, the irradiation can be used for pushing of the chemical reaction towards desired product and to control the formation and breaking of the given chemical bond (see Fig. 1).

Nobel prizes for development of "click chemistry" and organocatalysis have been already given, however, the reverse click reaction that will generate back the given substrates is unknown. Especially, its chemistry in the charged and excited states are very different from the typical synthetic conditions in the organic chemistry field.

The purpose is to understand the physical mechanisms of emission and ionization so as to make quantitative use of the cross-beam experimental set-up on these systems.

Our methodology will allow identifying the key processes responsible for the "de-click" observations and required for further novel experimental development. Building an extensive database of our theoretical findings will be performed starting with nitrogen based heterocycle - 1H-1,2,3-triazole. For the aforementioned molecule it will be an initial test for benchmarking the methodology with experimental cross-beam measurements and to determine the initial parameters for multiply charged triazoles and its further predictions for clusters of triazole derivatives. A detailed theoretical condition of the desired "de-click" chemistry i.e. given charge state, chemical substituents, excited state and energy deposition will be disentangled and delivered to the experimental cross-beam setups; experiments will undoubtedly determine the given mass over charge ratios of azide and alkyne proving the concept being possible.

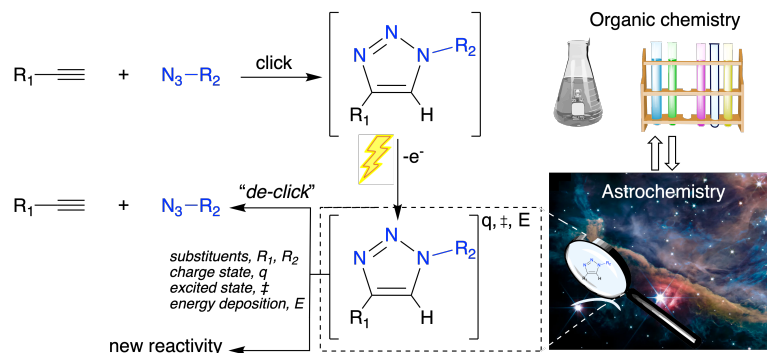


Figure 1: Scheme of the reversible click reaction for 1H-1,2,3-triazole derivative ( $R_1, R_2$ ) controlled by radiation source as a function of parent target state i.e. charge ( $q$ ), excited state ( $\ddagger$ ) and/or energy deposition ( $E$ ).

The attractiveness of this project lies both in the generalization of the theoretical approach to obtain an original tool for radiation damage induced investigation and in the open perspectives towards a number of catalytic applications. This work allows theoretical chemists to establish a link between laser and molecular physics community with applications in organic chemistry like e.g. photo-induced anion-binding organocatalysis.