

Computer Chemistry: Exploring a Full Picture of Chemical Reactions

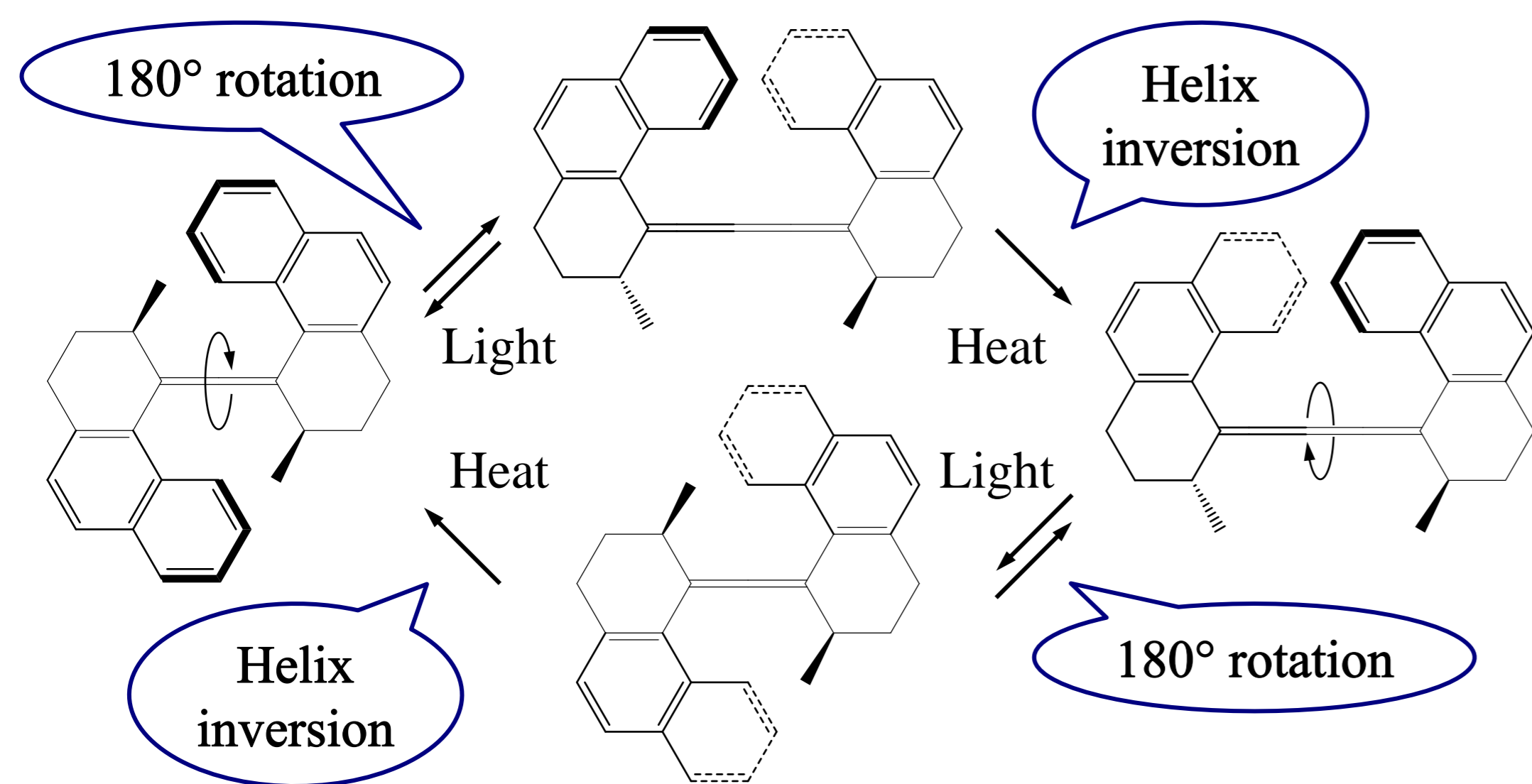
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Artificial molecular machines: Light-driven molecular motors

2016 Nobel Prize in Chemistry
“for the design and synthesis of molecular machines”

Light-driven molecular motors

Originally developed by the groups of B. Feringa (Nobel Prize winner) and N. Harada (Professor Emeritus at Tohoku University).

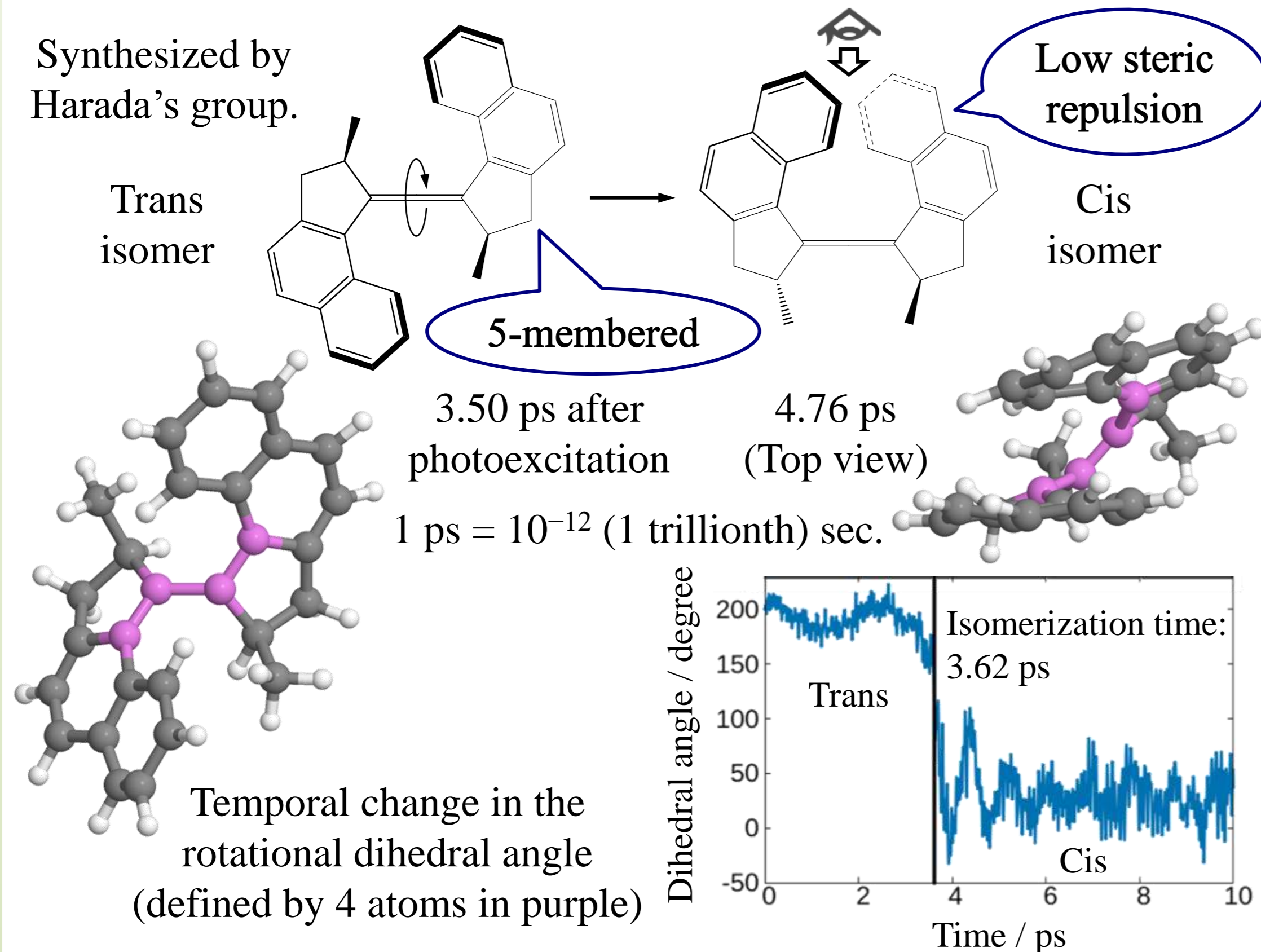


Detailed mechanism is unclear despite rising expectations of application.

Elucidate the initial rotational step (photoisomerization)!

Isomerization simulation of a novel molecular motor

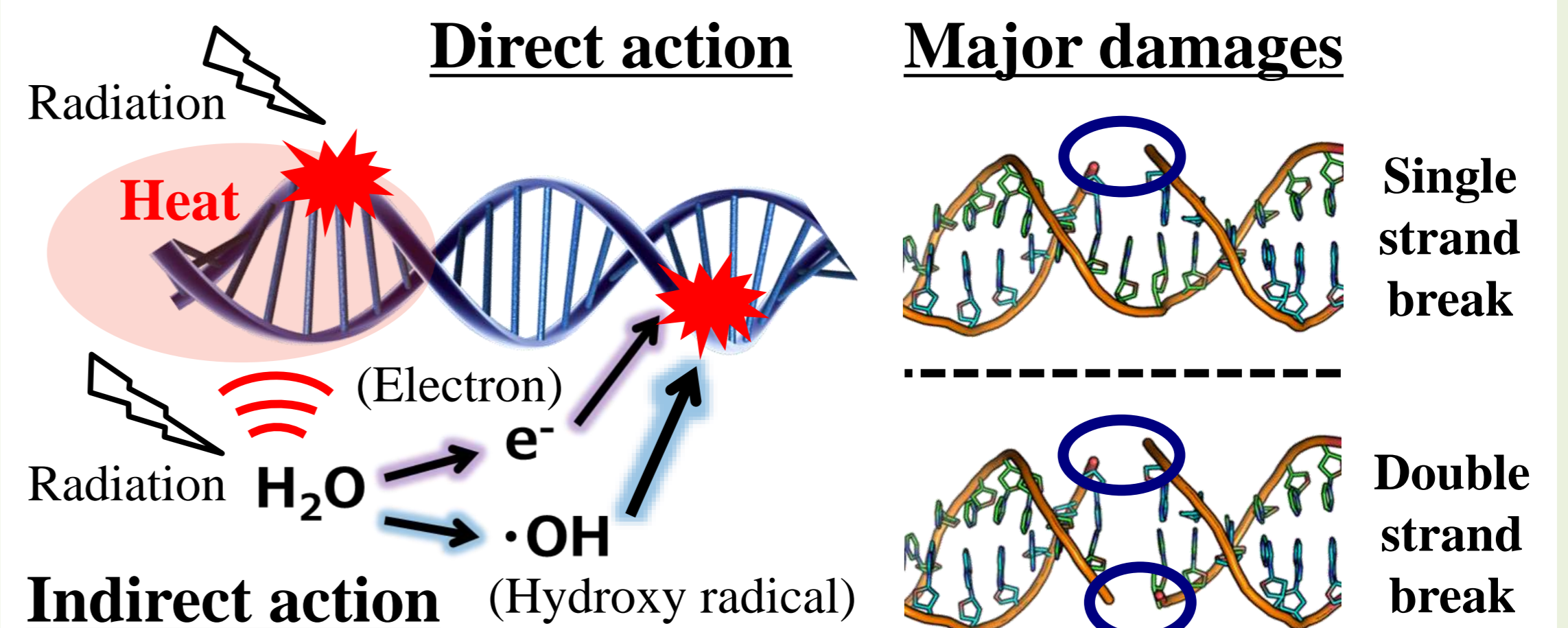
Synthesized by Harada's group.



Possibility of rapid isomerization pathways (on a ps scale)

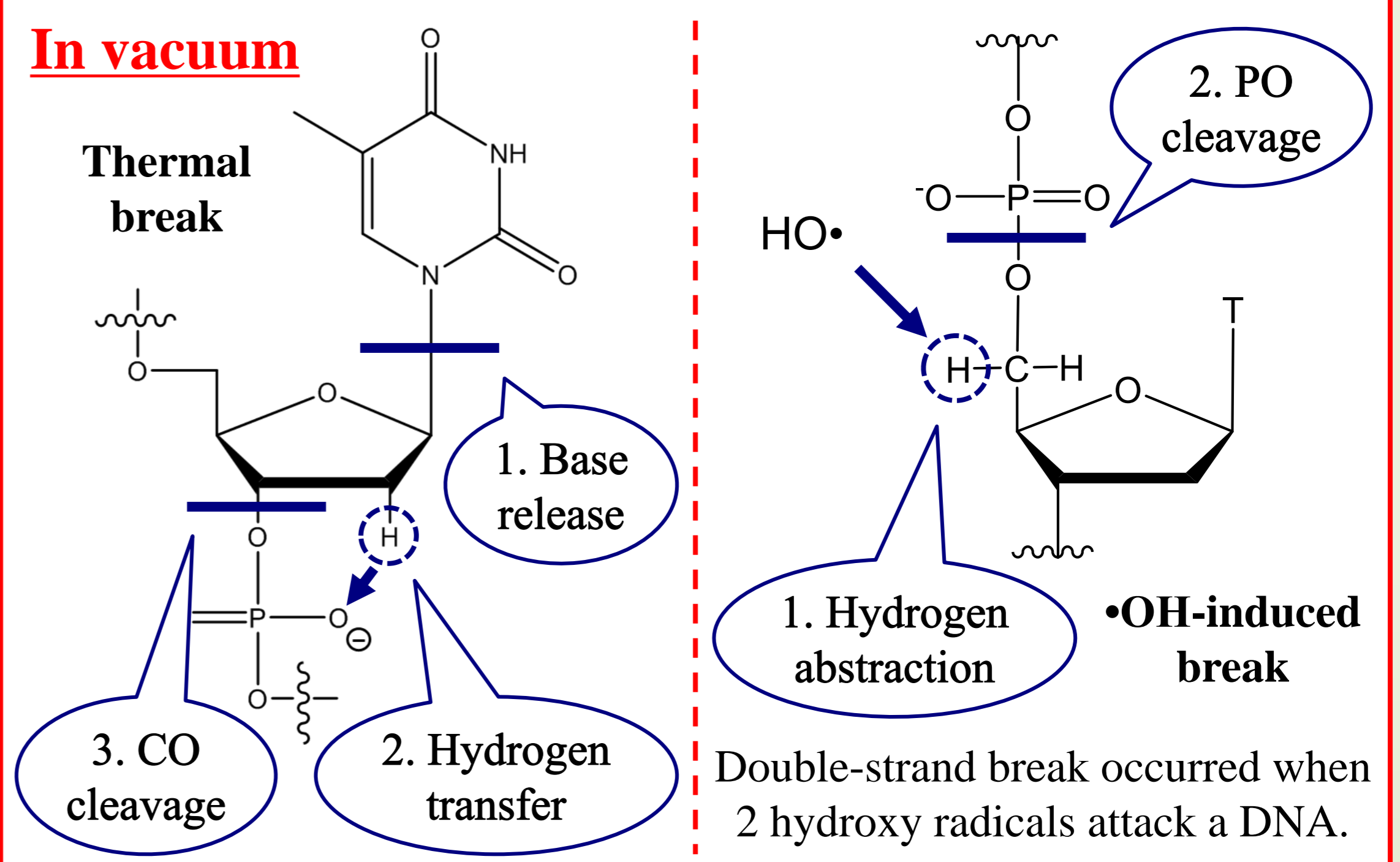
Radiation damage to living cells: Mechanism of DNA strand break

DNAs, which carry important genetic information, can be seriously damaged when exposed to radiation.

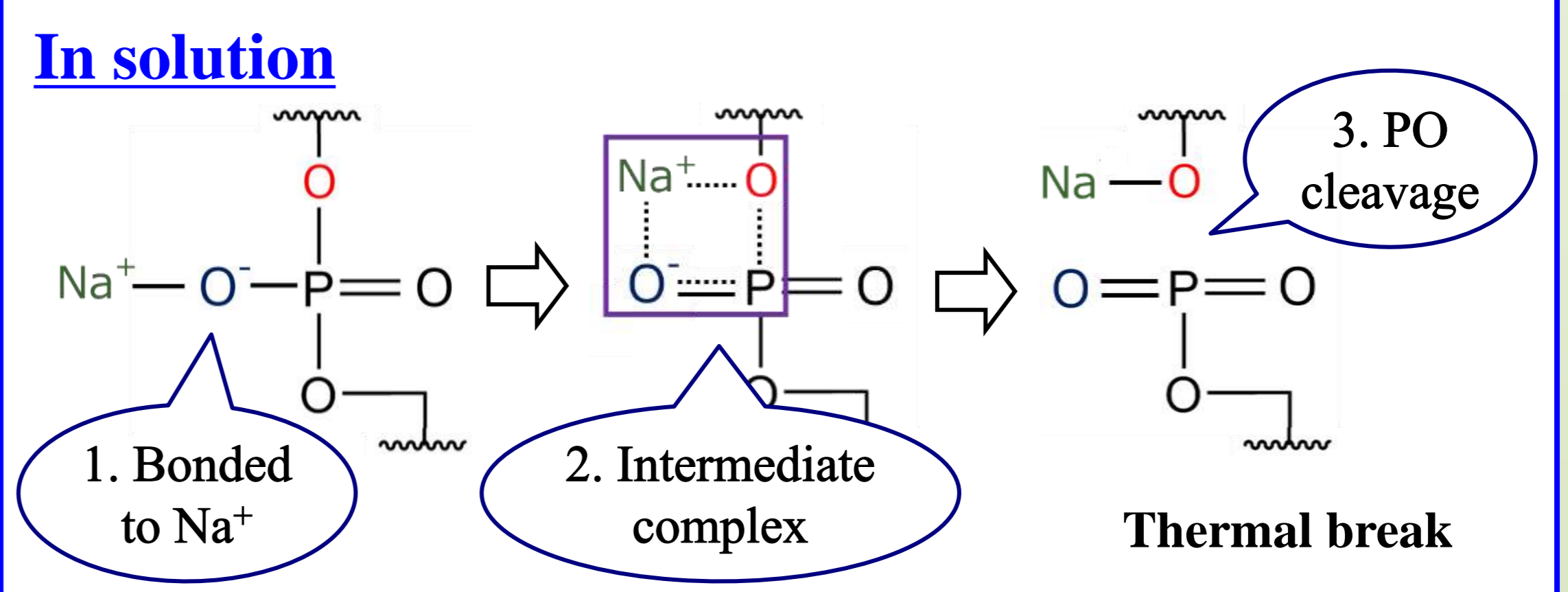


Simulate the dynamical process of DNA strand break!

In vacuum



In solution



The mechanism of DNA strand break depends on a damaging factor (heat/hydroxy radical) and environment.

Future prospects expected from progress in computers

Complete prediction of chemical reactions from beginning to end on a laboratory time scale
Discovery of novel reactions and molecular functions Design of laser pulses that maximize photochemical reaction yields

Promotion of nanotechnology and chemical biology by large-scale simulations
Development and application of light-driven molecular machines Evaluation of the stability and functionality of unknown DNAs

