

DONOR-ACCEPTOR TWO-ELECTRON TRANSFER REACTIONS: CONCERTED AND SEQUENTIAL PATHWAYS IN PROTEIN STRUCTURES

*E. G. Petrov, YE. V. Shevchenko,
V. I. Teslenko, V. May¹*

Bogolyubov Institute for Theoretical Physics,
Nat. Acad. Sci. of Ukraine
(14b, *Metrohichna Str., Kyiv 03143, Ukraine*),
¹Institut für Physik, Humboldt-Universität zu Berlin
(*Hausvogteiplatz, D-10117 Berlin, Germany*)

S u m m a r y

Nonadiabatic donor-acceptor (DA) two-electron transfer (TET) is described by a model where the intersite electronic transitions are assumed to proceed against the background of fast relaxations (a) within the electronic substates as well as (b) between those substates related to the same electronic state. It is shown that the DA TET appears as a single-exponential reaction between the initial and final electronic states, and the corresponding overall transfer rate can be represented as an additive contribution of the concerted and sequential electronic pathways. Two specific two-electron superexchange mechanisms of DA TET are proposed (the repeated and direct mechanisms), and the conditions of their realization are discussed in detail.

If the electronic substates are associated with protonated and deprotonated states, the used model allows one to derive the dependence of the overall transfer rate on the actual pH-value, and thus the pH-dependence of the proton-assisted TET can be explained.