Molecular Photonics
Exercise **4**

1. a. Draw a diagram that illustrates the possible pathways for a charge separation process (electron and hole transfer).

   b. In vacuum there is a large dependence of k_{ET} over distance. What will happen when 1) the donor and acceptor are in a solvent, 2) there is a saturated hydrocarbon bridge between them?

2. a. Explain what was the general idea behind Markus theory.

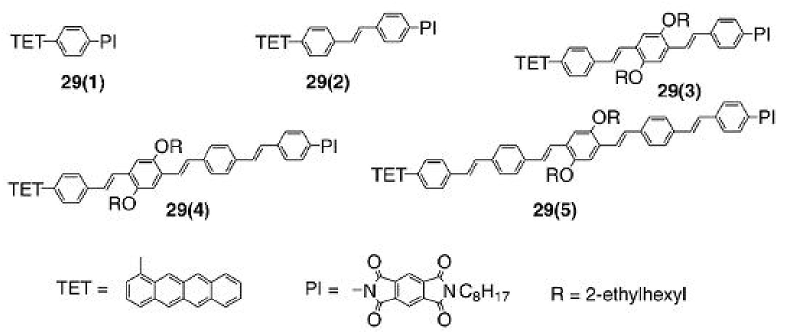
   b. Draw schematically the four general predicted situations; state for each one the relation between ΔG_{cs} and λ.

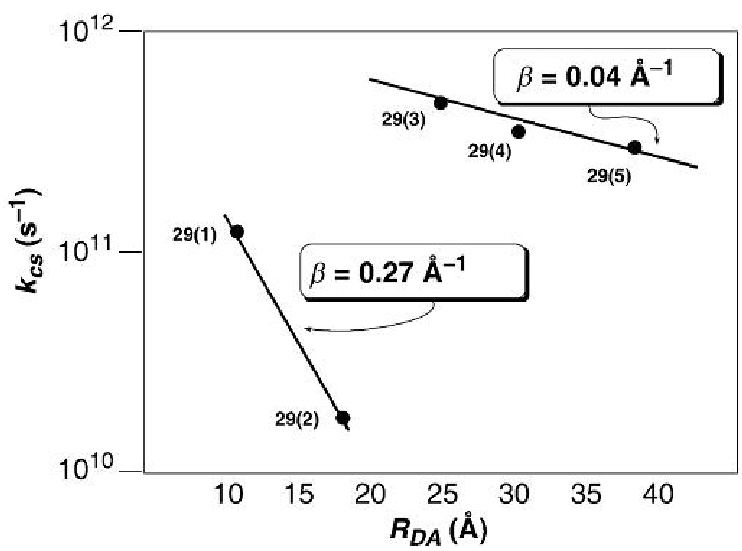
   c. Explain what does λ represent and how it affects the rates of the process.

   d. Write down Marcus-Hush equation. What is V_{el} and how it is related to k_{ET} and to the distance between the donor the acceptor?

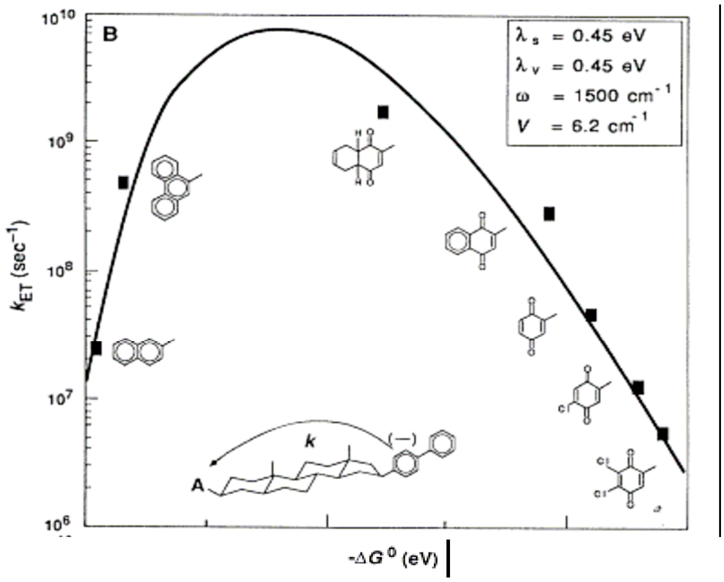
3. a. What are the differences between a superbridge (superexchange regime) and a molecular wire? Explain and draw schemes if needed.

   b. The graph below describes the charge separation rate of molecules 29(1-5). Explain the observed rate trends in the graph.

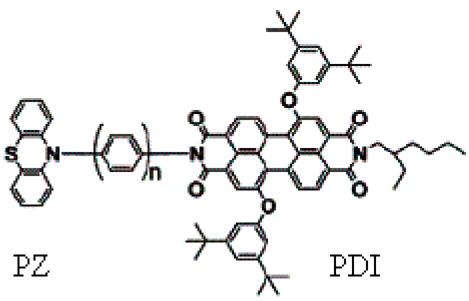


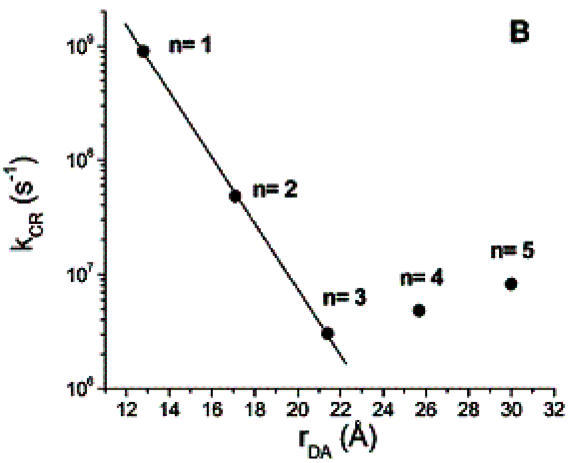


4. The dependence of the electron transfer rate on the driving force is given below for a series of compounds in butyl ether (acceptor, A, is varied). Why is the maximum observed? How would the reorganization energy change if more polar solvent would be used?



5. See below the structure of the donor-bridge-acceptor family of molecules. Photoinduced electron transfer (PET) takes place in all of these molecules.
   b. Estimate, using Rehm-Weller equation the upper limit for the thermodynamic driving force of PET (Perylene diimide (PDI) 0-0 emission is at 565 nm, PDI one-electron reduction potential is -0.6 V, one electron oxidation potential > 2.0 V, one electron oxidation potential of phenothiazine (PZ) is 0.6 V)
   c. The rate of charge (k_{CR}) recombination as a function of distance between donor and acceptor is given. Explain the observed behavior.





For questions please contact Dr. Haim Weissman:
E-mail: haim.weissman at weizmann.ac.il; Tel.: 2628