## Abstract Submitted for the 4CF15 Meeting of The American Physical Society

Temperature Effect on Intramolecular Electron Transfer MORTEZA MOGHIMI WASKASI, GERDENIS KODIS, Department of Chemistry Biochemistry, Arizona State University, DMITRY MATYUSHOV, Department of Physics and Department of Chemistry Biochemistry, Arizona State University, MATYUSHOV GROUP COLLABORATION, EFRC COLLABORATION — A deeper understanding of the electron transfer process in Porphyrin-Fullerene (P-C60) dyad can be helpful in the development of chemical systems with high efficiency in the conversion of light to electricity. The rate of charge recombination in the P-C60 dyad can be described in the frame of the Marcus approach. Based on this approach, the kinetics of electron transfer depend on (i) driving force, (ii) reorganization energy, (iii) electronic coupling, and (iv) temperature. The temperature dependence can be complicated since reorganization energy and free energy are functions of temperature through the polarization of the solvent. The density functional theory is employed to obtain charge and optimized structures of ground, excited and charge separated states of the dyad. The free energy and reorganization energy at various temperatures are calculated using SolvMol code in 2-mTHF, and THF solvents. We found a good agreement between the temperature dependence of the recombination rate in experimental and computational approaches. It has a very pronounced bell shape and provides a critical test of the theory. The appropriate choice of solvent and temperature can provide a powerful tool for tuning the dynamics of electron transfer.

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