## Abstract Submitted for the MAR99 Meeting of The American Physical Society

Sorting Category: 11.9.3 (Theoretical)

Simple lower bound on the time of photoisomerization of retinal. EUGENE TSIPER, University of Rochester — I suggest a simple mechanistic argument that provides a time estimate for retinal photoisomerization. Retinal molecule plays key role in photobiology by working as a nature-created photodetector in vision. Its light-induced photoisomerization is a first step in a long chain of events that lead from the absorption of a single photon to the utilization its energy in a biological function [G. Wald, *Science* **162**, 230 (1968)]. The photoisomerization of retinal is believed to be complete in only 100–200 fs, making it one of the fastest known photoreactions [Q. Wang, R.W. Shoenlein, L.A. Peteanu, R.A. Mathies, and C.V. Shank, *Science* **266**, 422 (1994)]. My estimate is based on the comparison of the kinetic energy of nuclei necessary to achieve such a fast reaction rate to the energy  $\hbar\omega$  supplied by the photon. Calculation of the reduced momentum of inertia of a system in a model of classical nuclei give the minimum kinetic energy about 16 times larger than  $\hbar\omega \approx 2.5$  eV. The paradox can be resolved by assuming that (i) only a short portion of the molecule is affected by the structural change, however leading to an increase in the elastic energy for the rest of the molecule, or (ii) that the first stage of the reaction is, in fact, not isomerization. The last possibility is in line with recent ab-initio calculations [M. Garavelli, P. Celani, F. Bernardi, M.A. Robb, and M.J. Olivucci, J. Am. Chem. Phys. 119, 6891 (1997)], and experimental findings [L. Song and M.A. El-Sayed J. Am. Chem. Soc. 120, 8889 (1998)]. (http://feynman.chem.rochester.edu/ $\sim$ rr)

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