Additions and Corrections

Diffusion-Controlled Association Rate of Cytochrome c and Cytochrome c Peroxidase in a Simple Electrostatic Model [*J. Am. Chem. Soc.* **1986**, *108*, 8162–8170]. SCOTT H. NORTHRUP,* JOHN C. L. REYNOLDS, CYNTHIA M. MILLER, KRISTI J. FORREST, and JEFFREY O. BOLES

The original paper contains errors resulting from the employment of translational and rotational diffusion coefficients which are a power of ten smaller than realistic values. This came about from a unit conversion involving the poise unit of viscosity. In Table III, the values for translational and rotational diffusion coefficients, D_T and D_R, respectively, should be multiplied by 10. This in no way affects the correctness of the simulations for β values, the diffusion-controlled bimolecular association probabilities reported in the original paper. However, when these β values are scaled into bimolecular rate constants in conventional units of M^{-1} s^{-1} for comparison with experiment, all the resulting reported rate constants are low by a factor of 10.

The only major conclusion change is that protein:protein interaction Model II (rather than Model I) now gives the best fit to experiment. Model II is, in fact, the one using the more correct hydrodynamic radii of the proteins, removing that troublesome feature of the original paper. Figure 4 should thus be replaced with the one presented here, in which all theoretical rate constants are increased by 1 log − 10 unit. The original Table V, which summarizes Model I results for various electrostatic treatments, can be corrected simply by multiplying the rate constants in the right-hand-most column by 10. Since Model II with corrected diffusion coefficients now most closely fits the experiment, we provide a corresponding Table V which summarizes results for simulation of Model II.

The conclusions in section IIIc regarding the influence of rotational torques are unchanged, since this influence depends on the *relative* time scales of encounter durations vs. rotational reorientation times. Table VI, which compares these various times, can be corrected by changing the time units from 10^6 ps to 10^5 ps. Although the various processes happen 10 times as fast, their relative times are the same.

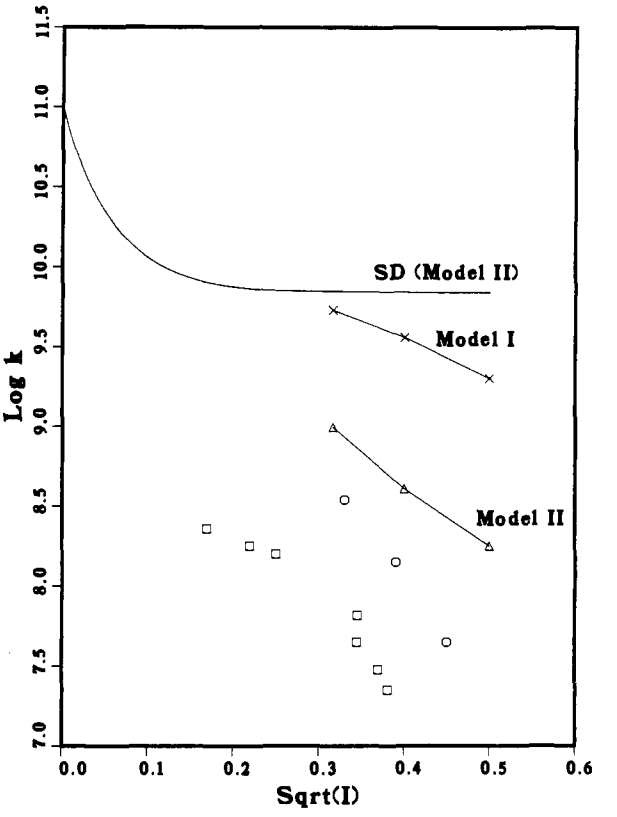

Figure 4. Brønsted–Bjerrum plot of log of the diffusion-controlled bimolecular rate constant for CYTC–CYP association vs. square root of ionic strength. Experimental results of Kang et al.[18] in chloride (○) and phosphate (□) buffers are compared with a primitive point-ion Smoluchowski–Debye (SD) treatment for isotropically reactive monopolar charged proteins (radii of Model II), and two Brownian-dynamics-simulated realistic monopole/dipole models (Model I and II differing in protein radii choice) with orientational constraints to reaction.

Table V. Diffusional Association Rate Constants for the CYP–CYTC Reaction Computed by BD Simulation Using Model II with Various Electrostatic Terms and Solvent Treatments

case						
cyp:cytc interaction[a]	solvent treatment	I	θ_{cyp}	θ_{cytc}	k^*(BD)	k(BD), M^{-1} s^{-1}
no charges			10	10	~0.0008	$\sim 5 \times 10^6$
M:M	DH	0.1	10	10	~0.0009	$\sim 6 \times 10^6$
MD:MD	DH	0.1	10	10	0.0045	3.1×10^7
MD:MD	DH with FIS	0.1	10	10	0.143	9.9×10^8
MD:MD	DH with FIS	0.16	10	10	0.059	4.1×10^8
MD:MD	DH with FIS	0.25	10	10	0.026	1.8×10^8

[a] M:M = monopole:monopole interaction only. MD:MD = monopole/dipole:monopole/dipole interaction. DH = for Debye–Hückel screening law treatment of ionic strength effects. FIS = for finite ion size correction in DH screening law.