

**Evidence for Partially Bound States in Cooperative Molecular Recognition Interfaces** [*J. Am. Chem. Soc.*, **2008**, *130*, 17718–17725] [*J. Am. Chem. Soc.* **2008**, *130*, 17718]. Elena Chekmeneva, Christopher A. Hunter,\* Martin J. Packer, and Simon M. Turega

Pages 17722–17723: Equations 3, 4, 6 and 8 relating to the analysis of the sequential binding equilibria are corrected below. The numerical values of the stepwise association constants and effective molarities reported in Tables 5 and 6 are corrected below. Qualitatively, the results are similar to those in the original publication, and the main conclusions are not affected. However, the overall association constant estimated for the doubly H-bonded complex in Table 6 is always larger than the value estimated for a singly H-bonded complex, even when the most populated state of the doubly H-bonded complex is the singly H-bonded species.

$$K_{\text{obs}} = K_0(1 + K_1) \quad (3)$$

$$K_{\text{obs}} = K_0(1 + K_1 + K_1K_2) \quad (4)$$

$$EM_1 = \frac{K_1}{4K_{\text{H}}} = \frac{K_{\text{obs}} - K_0}{4K_0K_{\text{H}}} \quad (6)$$

$$EM_2 = \frac{8K_2}{6K_{\text{H}}} = \frac{8(K_{\text{obs}} - K_0 - K_0K_1)}{6K_0K_1K_{\text{H}}} \quad (8)$$

**Table 5.** Effective Molarities,  $EM$  (M), Sequential Equilibrium Constants for H-Bond Interactions,  $K_1$  and  $K_2$  ( $\text{M}^{-1}$ ), in the Complexes Formed Between Porphyrin **3** and Ligands **4b** and **4d** at 298 K<sup>a</sup>

solvent	3·4b		3·4d	
	$K_1$	$EM_1$	$K_2$	$EM_2$
toluene	14	0.1	14	0.8
TCE	3	0.2	<i>b</i>	<i>b</i>
DCM	5	0.7	<i>b</i>	<i>b</i>
CHCl <sub>3</sub>	1	0.7	<i>b</i>	<i>b</i>
acetone	5	0.9	<i>b</i>	<i>b</i>

<sup>a</sup> Errors are  $EM_1 \pm 60\%$ ,  $K_1 \pm 40\%$ ,  $EM_2 \pm 80\%$  and  $K_2 \pm 60\%$ .

<sup>b</sup> The values of  $K_2$  are within experimental error of zero, and so the second H-bond does not confer a measurable additional stability on the complex.

**Table 6.** Estimated Overall Association Constants for Complexes Formed Between Porphyrin **3** and Ligand **4d** That Make Either One or Two H-bonds ( $\text{M}^{-1}$ ) and Populations of Partially Bound States Assuming  $EM_1 = EM_2 = 0.5$  M

solvent	singly H-bonded complex			doubly H-bonded complex			
	$K_{\text{est}}$	zero H-bonds (%)	one H-bond (%)	$K_{\text{est}}$	zero H-bonds (%)	one H-bond (%)	two H-bonds (%)
toluene	$4.2 \times 10^4$	1	99	$8.2 \times 10^5$	0	10	90
TCE	$2.7 \times 10^3$	8	92	$1.0 \times 10^4$	4	46	50
DCM	$5.3 \times 10^3$	13	87	$1.5 \times 10^4$	8	56	35
CHCl <sub>3</sub>	$1.5 \times 10^3$	35	65	$2.5 \times 10^3$	32	58	10
acetone	$4.3 \times 10^2$	16	84	$1.0 \times 10^3$	11	59	29

JA900730Z

10.1021/ja900730z

Published on Web 02/23/2009