# Complexation of Ferrocene Derivatives by the Cucurbit[7]uril Host – A Comparative Study of the Cucurbituril and Cyclodextrin Host Families

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## SUPPORTING INFORMATION

Complete Reference 16

M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, V. G. Zakrzewski, J. A. Montgomery, Jr., R. E. Stratmann, J. C. Burant, S. Dapprich, J. M. Millam, A. D. Daniels, K. N. Kudin, M. C. Strain, O. Farkas, J. Tomasi, V. Barone, M. Cossi, R. Cammi, B. Mennucci, C. Pomelli, C. Adamo, S. Clifford, J. Ochterski, G. A. Petersson, P. Y. Ayala, Q. Cui, K. Morokuma, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. Cioslowski, J. V. Ortiz, A. G. Baboul, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. Gomperts, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, C. Gonzalez, M. Challacombe, P. M. W. Gill, B. G. Johnson, W. Chen, M. W. Wong, J. L. Andres, M. Head-Gordon, E. S. Replogle and J. A. Pople, *Gaussian 98, Revision A.6*, Gaussian, Inc., Pittsburgh PA, 1998.

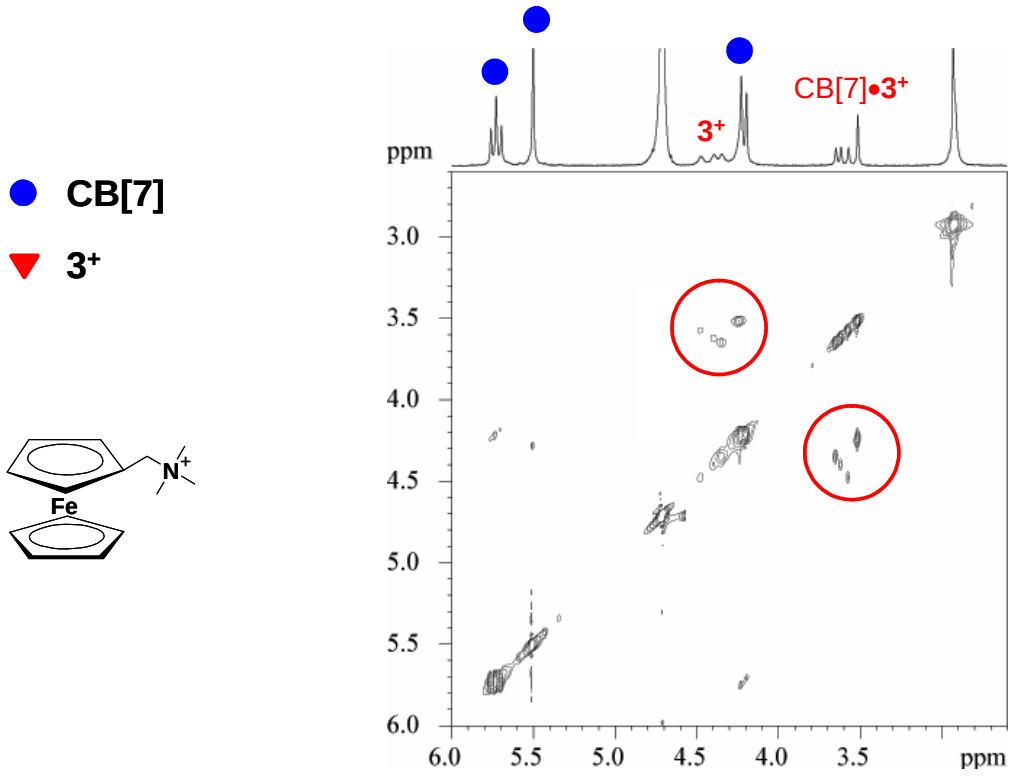


**Figure SI1.** 2D EXSY NMR spectrum of a mixture of the free guest $\mathbf{3}^+$ and the complex CB[7]•$\mathbf{3}^+$ in $D_2O$ at 298 K. The complex dissociation rate was estimated as ca. 2 $s^{-1}$.

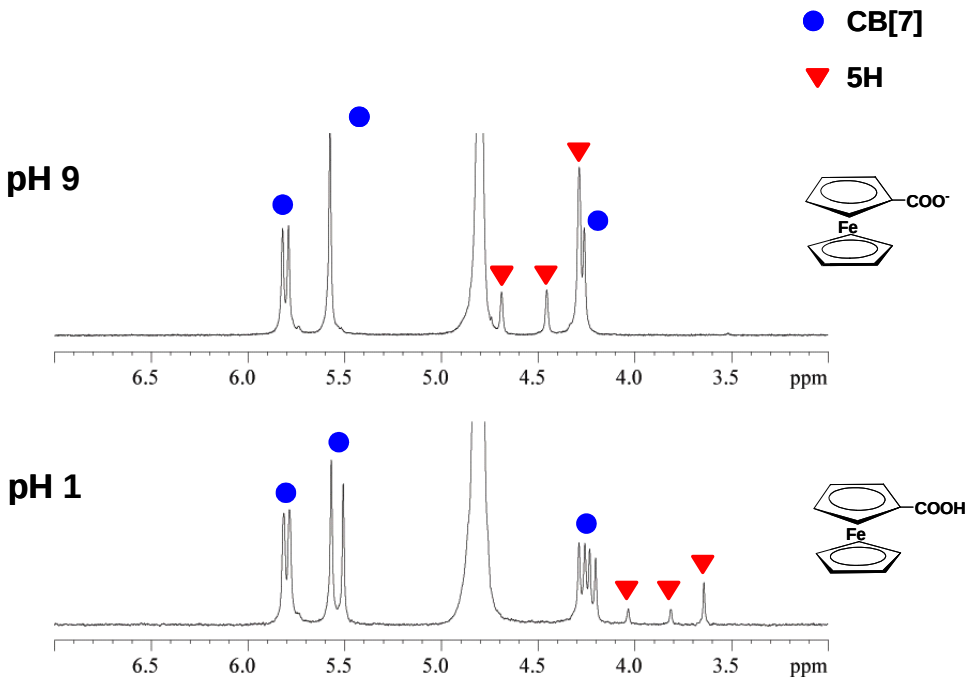


**Figure SI2**. $^1H$ NMR spectra of **5H** (bottom, pH 1) and $\mathbf{5}^-$ (top, pH 9) in the presence of excess CB[7] in $D_2O$ solution. Note that all the protons of **5H** are shifted upfield, as expected for CB[7] inclusion complexes.

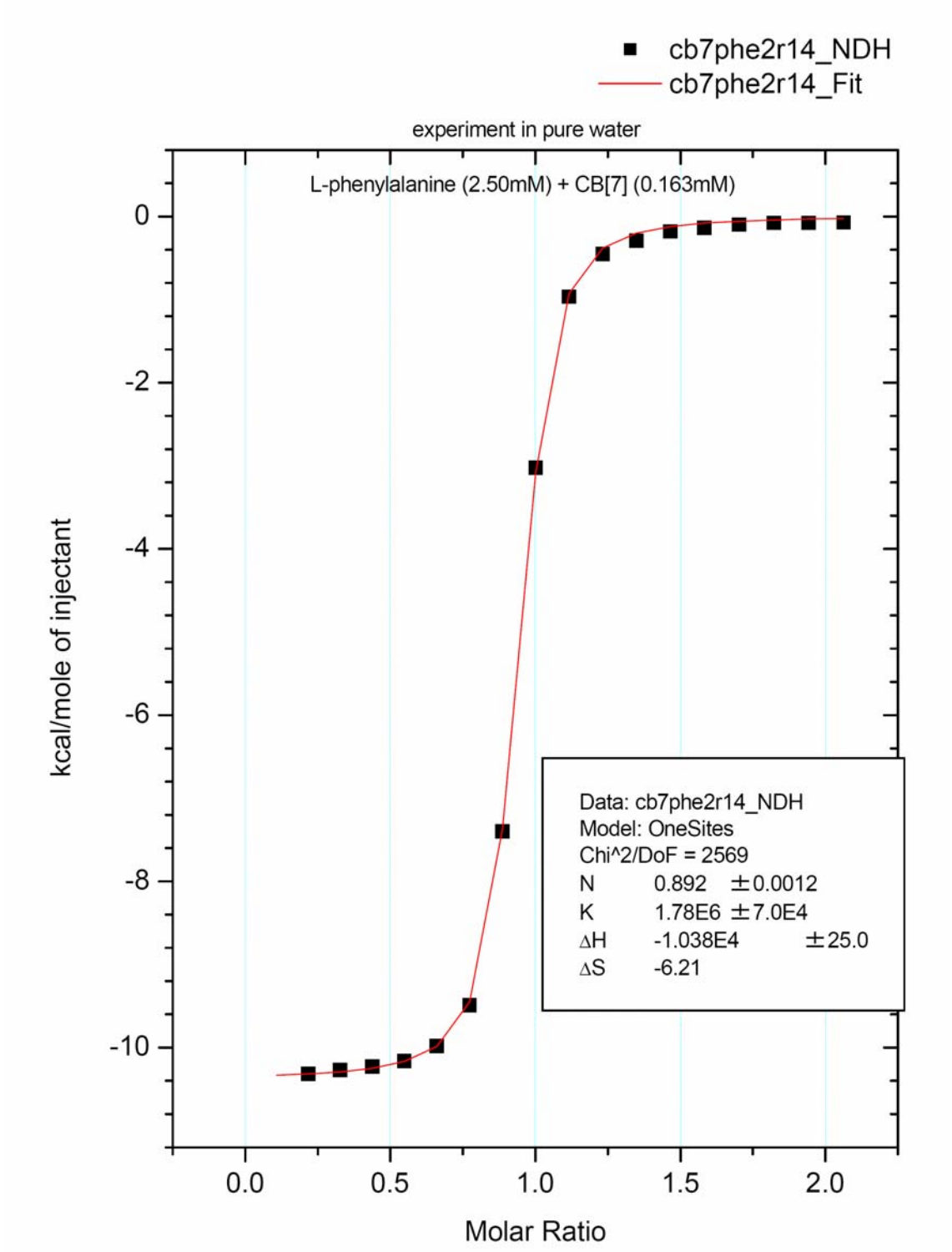


**Figure SI3.** Computer simulation of the ITC titration curve obtained by injecting an L-phenylalanine solution (2.50 mM in pure water; the volume of each injection: 10μL) to a CB[7] solution (0.163 mM in pure water) placed in the reaction cell of ITC instrument at 298.15K.

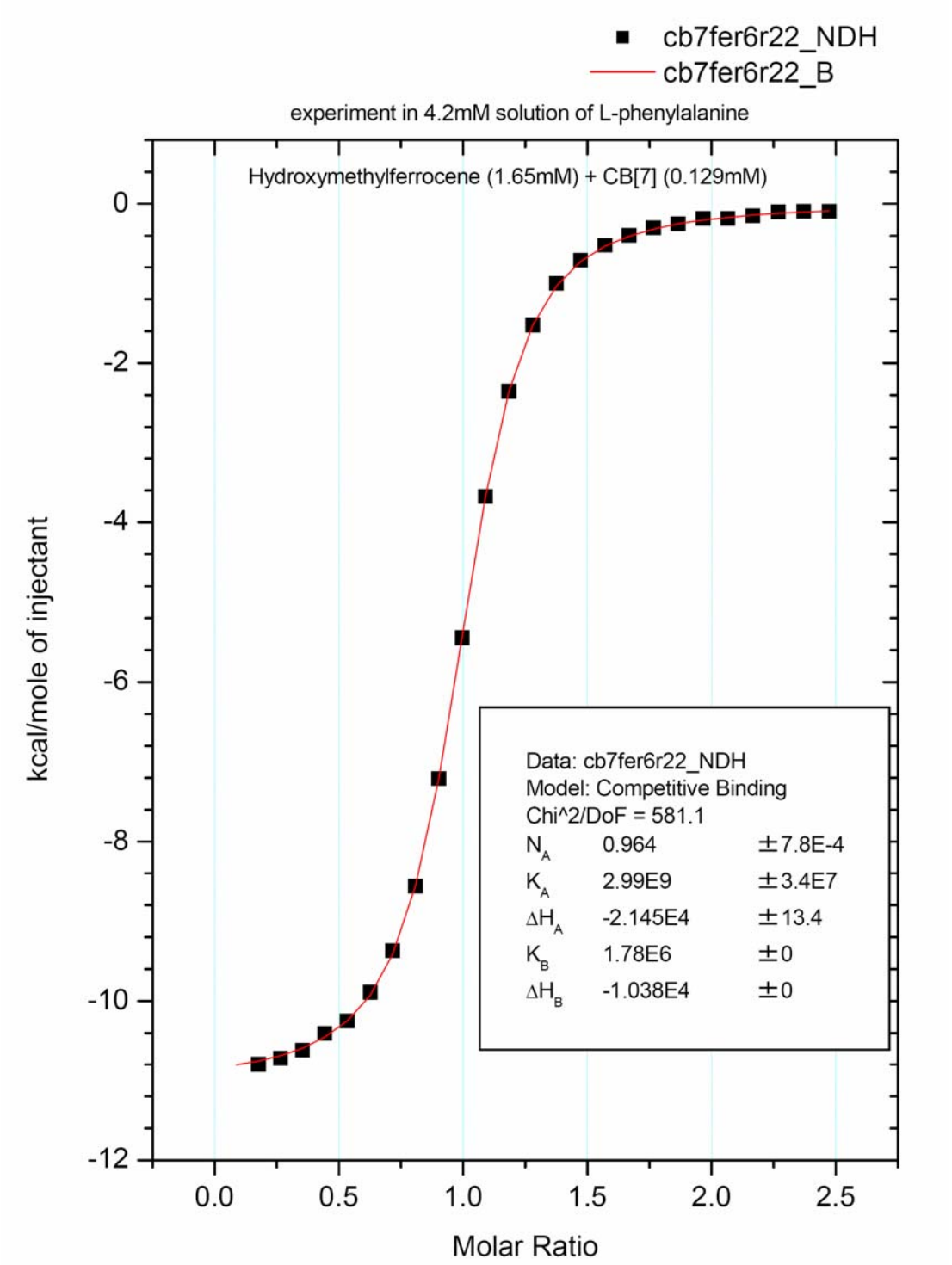


**Figure SI4.** Computer simulation of the competitive ITC titration experiment: the titration curve was obtained by injecting a hydroxymethylferrocene (**1**) solution (1.65mM in pure water; the volume of each injection: 10 μL) to a CB[7] solution (0.129 mM in pure water) containing 4.2 mM L-phenylalanine as a competitor at 298.15K. The association constant ($K_A$) and the reaction enthalpy ($\Delta H_A$) for **1** were calculated by fixing the $K_B$ and $\Delta H_B$ values for L-phenylalanine at those obtained in Figure SI3.