

2006, Volume 45

Nicholas E. Grossoehme, Shreeram Akilesh, Mary Lou Guerinot, and Dean E. Wilcox*: Metal-Binding Thermodynamics of the Histidine-Rich Sequence from the Metal-Transport Protein IRT1 of *Arabidopsis thaliana*.

Page 8505. In the preparation of ref 20, we have recently assessed the analysis of ITC data when coupled equilibria are involved and determined the accurate method to obtain free energies from experimental stability constants. Because eq 1 is not appropriate for this analysis, certain ΔG^0 values in Tables 2 and 3, including those for buffer protonation, need to be corrected. This leads to modified values in Table 4 (corrected version below) and minor adjustments to the plots of these values in Figures 8 and 9, as well as a new value of $\Delta\Delta S^0 = -26$ cal mol⁻¹ K⁻¹ on page 8507. While these new values do not alter the original conclusions based on these data, they are quantitatively more correct.

Table 4. Summary of pH- and Buffer-Independent Thermodynamic Values for Metal-Ion Binding to IRT1pep Determined from Data Collected at 298 K and pH 7.25 (values in parentheses indicate error)

metal	$\log K$	ΔG^0 (kcal/mol) a	ΔH^0 (kcal/mol)	ΔS^0 (cal mol ⁻¹ K ⁻¹) ^b
Mn ²⁺	1.3 (48)	$-1.72 (36)^{c}$	$-2(28)^{c}$	-1.76 (31)
Fe^{2+}	3.10 (0.04)	-4.22(0.38)	-6.49(0.73)	-7.6(2.8)
Co^{2+}	3.95 (0.04)	-5.39(0.46)	-10.39(0.66)	-16.76(2.7)
	$3.92(0.06)^d$	-5.34(0.68)		
Ni^{2+}	6.47 (0.04)	-8.83(0.76)	-15.89(1.71)	-23.7(6.3)
	$6.59 (0.03)^d$	-8.99(0.33)		
Cu^{2+}	9.13 (0.04)	-12.47(1.17)	-16.76(2.13)	-14.4(8.2)
Zn^{2+}	5.23 (0.05)	-7.14(0.84)	$-5.87 (0.88)^e$	4.19 (4.1)
	$5.37 (0.04)^d$	-7.33(0.66)		
Cd^{2+}	4.27 (0.07)	-5.83(0.67)	-9.71(0.80)	-13.0(3.5)
	$4.08(0.03)^d$	-5.57(0.33)		
Fe^{3+}	20.67 (0.01) ^f	-28.19(0.48)	$1.29 (1.00)^f$	98.9 (3.7)

 a $\Delta G^0=-RT$ ln K. b $\Delta S^0=-(\Delta G^0-\Delta H^0)/T.$ c From estimated values (see text). d From data collected at pH 8.22 with a 100 mM Tris buffer. e See ref 30. f From data collected at pH 6.45.

IC061652C

10.1021/ic061652c Published on Web 09/16/2006