

## Erratum to: Thermodynamic Prediction of Glycine Polymerization as a Function of Temperature and pH Consistent with Experimentally Obtained Results

Norio Kitadai<sup>1</sup>

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### Erratum to: J Mol Evol (2014) 78:171–187 DOI 10.1007/s00239-014-9616-1

In Table 1 on page 174, the values of the standard molal entropy ( $S^\circ$ ) at 25 °C and 1 bar for GlyGly<sup>-</sup>, and those of the standard molal heat capacity ( $C_p^\circ$ ) at 25 °C and 1 bar for GlyGly<sup>+</sup> and GlyGly<sup>-</sup> are incorrect. The correct values are 49.72, 55.9 and 15.5, respectively. The errors of the  $C_p^\circ$  values originated from the use of unit (J mol<sup>-1</sup> K<sup>-1</sup>) instead of (cal mol<sup>-1</sup> K<sup>-1</sup>). The error of the  $S^\circ$  value originated from mistyping. The corrected Table 1 is given here.

In Eq. 39 on page 185, the positive sign in the term  $\left(\frac{1}{T+\Theta}\right)$  must be changed to the negative sign. The corrected Eq. 39 is written below.

$$\begin{aligned} \Delta G^\circ = & \Delta G_f^\circ - S_{P_r, T_r}^\circ (T - T_r) - c_1 \left[ T \ln \left( \frac{T}{T_r} \right) - T + T_r \right] \\ & - c_2 \left\{ \left[ \left( \frac{1}{T - \Theta} \right) - \left( \frac{1}{T_r - \Theta} \right) \right] \left( \frac{\Theta - T}{\Theta} \right) \right\} \\ & + c_2 \left\{ \frac{T}{\Theta^2} \ln \left[ \frac{T_r (T - \Theta)}{T (T_r - \Theta)} \right] \right\} + a_1 (P - P_r) \\ & + a_2 \ln \left( \frac{\Psi + P}{\Psi + P_r} \right) \\ & + \left( \frac{1}{T - \Theta} \right) \left[ a_3 (P - P_r) + a_4 \ln \left( \frac{\Psi + P}{\Psi + P_r} \right) \right] \\ & + \omega \left( \frac{1}{\epsilon} - 1 \right) - \omega_{P_r, T_r} \left[ Y_{P_r, T_r} (T_r - T) + \frac{1}{\epsilon_{P_r, T_r}} - 1 \right] \end{aligned} \quad (39)$$

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✉ Norio Kitadai  
nkitadai@elsi.jp

<sup>1</sup> Earth–Life Science Institute, Tokyo Institute of Technology, 2-12-1-IE-1 Ookayama, Meguro-ku, Tokyo 152-8550, Japan

**Table 1** Standard molal thermodynamic data at 25 °C and 1 bar and revised HKF equation of state parameters for Gly, GlyGly, GlyGlyGly, and DKP in their zwitterionic and ionization states

Species	$\Delta_f G^{\circ a}$	$\Delta_f H^{\circ a}$	$S_{Pr, Tr}^{\circ b}$	$C_p^{\circ b}$	$V^{\circ c}$	$a_1^d \times 10$	$a_2^e \times 10^{-2}$	$a_3^f$	$a_4^g \times 10^{-4}$	$c_1^b$	$c_2^g \times 10^{-4}$	$\omega^e \times 10^{-5}$
Gly <sup>±</sup>	-88.62	-122.83	37.89	9.3 <sup>h</sup>	43.2 <sup>h</sup>	11.30 <sup>h</sup>	0.71 <sup>h</sup>	3.99 <sup>h</sup>	-3.04 <sup>h</sup>	28.5 <sup>h</sup>	-8.40 <sup>h</sup>	0.23 <sup>h</sup>
Gly <sup>+</sup>	-91.82 <sup>i</sup>	-123.79 <sup>i</sup>	45.44 <sup>i</sup>	39.7	49.9	15.57	-8.26	-6.62	0.47	39.5	-1.21	-0.33
Gly <sup>-</sup>	-75.27 <sup>i</sup>	-112.27 <sup>i</sup>	28.57 <sup>i</sup>	-0.8	45.7	9.74	3.54	20.07	-4.73	21.6	-7.92	0.69
GlyGly <sup>±</sup>	-117.00	-175.69	52.75	28.0	77.4	17.66	6.71	50.07	-15.91	69.3	-17.71	0.59
GlyGly <sup>+</sup>	-121.28 <sup>i</sup>	-175.72 <sup>i</sup>	67.03 <sup>i</sup>	55.9	84.7	22.05	-8.00	-22.99	5.69	34.1	-0.10	-2.46
GlyGly <sup>-</sup>	-105.72 <sup>i</sup>	-165.32 <sup>i</sup>	49.72 <sup>i</sup>	15.5	80.4	16.22	3.80	3.69	0.48	16.2	-6.81	-1.44
GlyGlyGly <sup>±</sup>	-144.74	-226.97	70.73	44.2 <sup>h</sup>	112.1 <sup>h</sup>	24.14	6.97	33.69	-10.69	63.9 <sup>h</sup>	-16.60 <sup>h</sup>	-1.54 <sup>h</sup>
GlyGlyGly <sup>+</sup>	-149.13 <sup>i</sup>	-227.17 <sup>i</sup>	84.80 <sup>i</sup>	72.2	119.4	28.52	-7.74	-39.37	10.91	28.7	1.01	-4.59
GlyGlyGly <sup>-</sup>	-133.70 <sup>i</sup>	-217.00 <sup>i</sup>	67.14 <sup>i</sup>	31.7	115.1	22.69	4.06	-12.69	5.70	10.8	-5.70	-3.57
DKP	-57.44 <sup>j</sup>	-99.30 <sup>j</sup>	53.50 <sup>j</sup>	34.4	76.8	16.84	3.27	10.94	-5.14	28.5	-7.44	-2.30
[Gly]	-3.75	-3.62	15.91	11.3	9.6	1.83	2.57	1.22	-1.27	6.9	2.20	0.00
[PBB]	-24.11	-47.67	3.01	-4.5 <sup>h</sup>	26.3 <sup>h</sup>	8.10 <sup>h</sup>	-3.75 <sup>h</sup>	-6.73 <sup>h</sup>	1.13 <sup>h</sup>	11.2 <sup>h</sup>	-7.50 <sup>h</sup>	0.05 <sup>h</sup>

Data and parameters for the side chain group of Gly ([Gly]) and the peptide backbone ([PBB]) are also listed

<sup>a</sup> kcal mol<sup>-1</sup>

<sup>b</sup> cal mol<sup>-1</sup> K<sup>-1</sup>

<sup>c</sup> cm<sup>3</sup> mol<sup>-1</sup>

<sup>d</sup> cal mol<sup>-1</sup> bar<sup>-1</sup>

<sup>e</sup> cal mol<sup>-1</sup>

<sup>f</sup> cal K mol<sup>-1</sup> bar<sup>-1</sup>

<sup>g</sup> cal K mol<sup>-1</sup>

<sup>h</sup> Dick et al. (2006)

<sup>i</sup> Goldberg et al. (2002)

<sup>j</sup> Shock (1992a)