

Correction to “Solubility of 6-Chloropyridazin-3-amine in Different Solvents”

Xin-Xiang Cao,* Jin-Qiang Liu, Teng-Teng Lv, and Jing-Cai Yao

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In our previous paper “Solubility of 6-Chloropyridazin-3-amine in Different Solvents”, the values of the changes of Gibbs free energy in Table 5 were calculated incorrectly. As we

Table 5. Thermodynamic Functions of 6-Chloropyridazin-3-amine in Eight Solvents^a

solvent	ΔH_d	ΔS_d	T_{hm}/K	ΔG_d
	$KJ \cdot mol^{-1}$	$J \cdot mol^{-1} \cdot K^{-1}$		$KJ \cdot mol^{-1}$
methanol	24.56	36.09	315.19	13.19
ethanol	32.30	57.20	319.99	14.00
<i>n</i> -butanol	32.40	56.40	320.01	14.35
<i>N,N</i> -dimethylformamide	17.90	32.38	320.11	7.53
acetone	25.51	38.64	312.84	13.42
cyclohexanone	28.35	50.06	320.04	12.32
ethyl acetate	26.19	32.97	320.10	15.64
toluene	41.56	57.20	320.12	23.25

^aThe values of ΔG_d were calculated by the values of ΔH_d and ΔS_d at T_{hm} .

had pointed out in that article, the changes of Gibbs free energy are calculated at 278.15 K. However, in concept, the changes of Gibbs free energy should not be calculated at that temperature, as described below.

In solid–liquid equilibrium, the van’t Hoff equation can only be used in the case that the dissolution enthalpy and entropy are considered to be constant. Although the fusion enthalpy and entropy are replaced with dissolution enthalpy and entropy, respectively, to make the equation suitable for nonideal systems, the values of dissolution enthalpy and entropy are still considered to be constant in the experimental range. Of course, the changes of Gibbs free energy are calculated by the following:

$$\Delta G_d = \Delta H_d - T \Delta S_d \quad (1)$$

The temperature in eq 1 must be located in the experimental range of temperatures investigated. Once the dissolution enthalpy and entropy are considered to be constant, the change of Gibbs free energy seems to be a function of temperature over the experimental range investigated. However, the “constant” dissolution enthalpy and entropy are the average values in the experimental range, and thus, the change of Gibbs free energy is always calculated at the average temperature of the experimental data. In the literature, the mean harmonic temperature^{1,2} (T_{hm}) instead of average temperature³ is generally adopted to reduce the error propagation. The T_{hm} is calculated with eq 2:

$$T_{hm} = \frac{n}{\sum_{i=1}^n \frac{1}{T_i}} \quad (2)$$

Thus, the changes of Gibbs free energy are recalculated following eq 3:

$$\Delta G_d = \Delta H_d - T_{hm} \Delta S_d \quad (3)$$

Thus, 278.15 K was not the appropriate temperature to use to calculate the Gibbs free energy changes. The updated values of the changes of Gibbs free energy using T_{hm} are collected in an updated version of Table 5.

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