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COMMENT/REPLY

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Comment on "Excess Enthalpies of Binary and Ternary Mixtures Containing Dibutyl Ether, Cyclohexane, and 1-Butanol at 298.15 K"

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I refer to the article "Excess Enthalpies of Binary and Ternary Mixtures Containing Dibutyl Ether, Cyclohexane, and 1-Butanol at 298.15 K" by Aguilar et al. in *J. Chem. Eng. Data*, **2009**, *54*, 1672−1679 and Corrections in *J. Chem. Eng. Data*, **2009**, *54*, 2341−2342.

I used the Redlich−Kister eq 1 with constants given in Table 4 of the original paper, to calculate the excess enthalpy of a binary (H^E). I found that eq 1 is incorrect. It should read as below.

$$H^E = x(1-x)\cdot\left[\sum_{i=0}^{n} A_i(2x-1)^i\right] \quad (1)$$

With the use of the above eq 1 and the constants given in Table 4, the values of H^E_{12}, H^E_{13}, and H^E_{23} match with values listed in Tables 3 (original paper) and 5 (correction).

For the calculation of H^E_{123}, I used eqs 6 and 8 with constants, given in Table 6 (correction). Values so calculated did not match with values, given in Table 5 (correction). I therefore used the following equation for the calculation of H^E_{123}.

$$H^E_{123} = (x_1 + x_2)H^E_{12} + (x_2 + x_3)H^E_{23} + (x_1 + x_3)H^E_{13} \pm x_1x_2x_3\Delta H^E_{123} \quad (6)$$

In the above eq 6, if the excess enthalpy of the ternary system (H^E_{123}) is endothermic, the last term will have negative sign and vice versa. I used the above eq 6 and calculated H^E_{123} for the following two compositions in Table 1.

Table 1

			calculated H^E for binary				calculated	reported
			H^E_{12}	H^E_{23}	H^E_{13}			
x_1	x_2	x_3	J·mol^{-1}			ΔH^E_{123}	H^E_{123} using above eq 6	H^E_{123} in corrected Table 5
0.06	0.6996	0.24	111.2	602.2	444.1	9621.9	686.9	690.7
0.16	0.6002	0.2398	220.4	619.1	764.3	9473.1	774.7	803.8

I found that calculated values of H^E_{123} match well with those reported in the corrected Table 5.

I did not check the other four correlations for calculating excess enthalpies of binaries (H^E). Also I did not check the calculations of ΔH^E_{123} with eq 7.

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