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COMMENT/REPLY

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

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In response to the Comment sent by B. I. Bhatt related to "Excess Enthalpies of Binary and Ternary Mixtures Containing Dibutyl Ether, Cyclohexane, and 1-Butanol at 298.15 K" (*J. Chem. Eng. Data* **2009**, *54*, 1672−1679), which was our first article on the validation of the experimental technique and new data on H^E measurements, we can add the following clarifying comments.

With respect to the first statement that eq 1 is incorrect to calculate the excess enthalpy of binary systems with the constants given in Table 4 of the original paper, we agree with Mr. Bhatt that there is misleading information about the A_i coefficients. When eq 1 was introduced first to validate the experimental technique with literature references (Table 2), A_i coefficients started with i = 1, 2, etc.; then the same eq 1 was used to fit the new experimental binary data reported in Table 4, but we started with i = 0, 1, 2, etc. Obviously, the A_i parameters in eq 1 should be corrected to A^{i-1}.

The second statement is that, for the calculation of H^E_{123} with eqs 6 and 8 with the constants given in Table 6 (correction; see *J. Chem. Eng. Data* **2009**, *54*, 2341−2342), the calculated values did not match the experimental values given in Table 5 (corrected). Here we have to clarify that the form of eq 1 is correct for the calculation of binary systems ($x_1 + x_2 = 1$), where $(1 - x)^*$ is undoubtedly $x_2 = (1 - x_1)$. For ternary systems when calculating the terms H^E_{12}, H^E_{13}, and H^E_{23} in eq 6, with $x_1 + x_2 + x_3 = 1$, the calculation of, for example, H^E_{12}, refers to the x_1 and x_2 mole fractions of species 1 and 2 in the ternary mixture and not to x_1 and $(1 - x_1 = x_2 + x_3)$. Therefore, the following explicit form of eq 1 for the binary systems has been used to calculate eq 6:

$$H^E_{12} = x_1 \cdot x_2 \cdot \sum_{i=1}^{n} A_{i-1} \cdot (x_1 - x_2)^{i-1} \qquad (6)$$

Although the Redlich−Kister equation, eq 1, was used to validate the apparatus, eq 1 is not the only equation or model we have used to fit the new data of the binary systems, as commented in the Results and Discussion section of the original paper (*J. Chem. Eng. Data* **2009**, *54*, 1672−1679). In fact, when fitting the ternary data H^E_{123}, eq 6, the H^E_{13} representation by the Redlich−Kister equation is used (as it is used that for the calculation of eq 5). But for the H^E_{12} and H^E_{23} binary systems, the respective best fits (eqs 1 and 2) have been used, and the fitting parameters are those presented in Table 6 (correction; *J. Chem. Eng. Data* **2009**, *54*, 2341−2342). Even by using eq 1 for the fitting of H^E_{23}, the agreement is quite similar.

As an example we show our partial calculations with eqs 6 and 8, using the coefficients of Table 6 (correction), for the same mole fractions used by Mr. Bhatt in his letter, in Table 1.

Table 1

				calculated H^E for binary					
				H^E_{12}	H^E_{23}	H^E_{13}		calculated	reported
x_1/x_3	x_1	x_2	x_3	J·mol^{-1}			$x_1x_2x_3\Delta H^E_{123}$	H^E_{123} using eqs 6 and 8	H^E_{123} Table 5 (corrected)
0.250	0.0600	0.6996	0.2404	57.4	501.0	46.2	97.1	701.8	690.7
0.667	0.1600	0.6002	0.2398	119.0	361.9	127.3	218.11	826.39	803.84

The agreement between the calculated and the experimental data match well enough. The same procedure is followed with eqs 6 and 7. The results obtained are the ones reported in Table 6 (correction).

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