Excess enthalpies of binary and ternary mixtures containing dibutyl ether (DBE), cyclohexane and 1-butanol at 298.15 K

Journal:	*Journal of Chemical & Engineering Data*
Manuscript ID:	je-2009-00560j
Manuscript Type:	Additions and Corrections
Date Submitted by the Author:	03-Jul-2009
Complete List of Authors:	Aguilar, Fernando; Universidad de Burgos, Electromechanical Engineering Alaoui, Fatima; Universidad de Burgos, Ingeniería Electromecánica Alonso-Tristán, Cristina; Universidad de Burgos, Electromechanical Engineering SEGOVIA, JOSÉ; UNIVERSITY OF VALLADOLID, INGENIERÍA ENERGÉTICA Y FLUIDOMECÁNICA Villamanan, Miguel; UNIVERSITY OF VALLADOLID, INGENIERÍA ENERGÉTICA Y FLUIDOMECÁNICA Montero, Eduardo; Universidad de Burgos, Ingeniería Electromecánica

Correction:

Excess enthalpies of binary and ternary mixtures containing dibutyl ether (DBE), cyclohexane and 1-butanol at 298.15 K. Fernando Aguilar, Fatima E.M. Alaoui, Cristina Alonso-Tristán, José J. Segovia, Miguel A. Villamañán, and Eduardo A. Montero. *J. Chem. Eng. Data* **2009,** *54*,, 1672-1679.

In the above publication we reported data of experimental excess molar enthalpies of the ternary system dibutyl ether DBE (1) + 1-butanol (2) + cyclohexane (3) at a temperature of 298.15 K. Regrettably, there was an error in the calculation of the experimental excess molar enthalpy of the ternary system H^E_{123} of Table 5 and, subsequently, in the fitted parameters shown in Table 6 and in the graphical representation of Figure 5. Corrected values are given in the revised tables and figure below. The new best fit of experimental data for the ternary system is obtained with eqs 6 and 7. The new root mean square deviation, rms ΔH^E, is of 12.4 J·mol^{-1}, and the maximum value of the absolute deviation, max$|\Delta H^E|$, is 25.6 J·mol^{-1}. The maximum experimental value of H^E is 928 J·mol^{-1}. These corrections do not affect the conclusions presented in the manuscript.

Table 5. Experimental excess molar enthalpies H^E_{2+13} at 298.15 K for the addition of cyclohexane to (DBE (1) + 1-butanol (3)) to form x_1 DBE + x_2 cyclohexane + (1-x_1-x_2) 1-butanol, and values of H^E_{123} calculated from eq. 5, using the smooth representation of H^E_{13} by Redlich-Kister equation with parameters given in Table 4.

x_2	H^E_{2+13}/J·mol^{-1}	H^E_{123}/ J·mol^{-1}	x_2	H^E_{2+13}/ J·mol^{-1}	H^E_{123}/ J·mol^{-1}
		x_1/x_3=0.2498	H^E_{13}/J·mol^{-1}=443.8		
0.9000	394.4	438.8	0.4004	475.1	741.2
0.8002	504.4	593.1	0.2998	387.6	698.4
0.6996	557.4	690.7	0.2003	277.7	632.7
0.6003	565.3	742.7	0.1001	144.2	543.7
0.5002	536.1	758.0			
		x_1/x_3=0.6669	H^E_{13}/J·mol^{-1}=764.2		
0.8999	350.8	427.3	0.4006	422.9	881.0
0.7997	446.5	599.6	0.3007	348.0	882.4
0.6998	491.2	720.6	0.2003	250.1	861.2
0.6002	498.3	803.8	0.0997	130.0	818.0
0.5002	473.6	855.6			
		x_1/x_3=1.4988	H^E_{13}/J·mol^{-1}=890.0		
0.9002	309.0	397.8	0.4001	369.5	903.4
0.8000	395.9	573.9	0.2998	303.5	926.6
0.6997	433.8	701.1	0.2005	216.8	928.4
0.5998	438.3	794.4	0.1001	112.8	913.7
0.4998	415.3	860.4			
		x_1/x_3=4.0531	H^E_{13}/J·mol^{-1}=773.3		
0.8998	256.9	334.4	0.4005	322.0	785.6
0.8006	342.6	496.8	0.2999	263.1	804.5
0.7002	380.0	611.8	0.1997	186.6	805.4
0.6003	383.8	692.8	0.0995	97.1	793.4
0.5009	363.7	749.7			

Table 6. Summary of the data reduction and prediction results obtained for the ternary system DBE (1) + cyclohexane (2) + 1-butanol (3) at 298.15 K.

CORRELATION[a]	ΔH^E_{123} (eq 7)	ΔH^E_{123} (eq 8)	NRTL	UNIQUAC
B_0	12036.1		-0.0721	-500.1
B_1	-32231.1	11944.0	0.8253	1204.5
B_2	-21829.8	13543.5	2.0214	2177.8
B_3	22371.7	-2370.0	0.6434	-628.3
B_4	-5113.5		2.7698	1815.1
B_5	81005.3		0.0487	-542.8
B_6	15579.8			
B_7	39001.6			
α_{12}			0.30	
α_{13}			0.30	
α_{23}			0.30	
rms ΔH^E/J·mol^{-1}	12.4	24.5	32.4	29.2
Max $\lvert\Delta H^E\rvert$/J·mol^{-1}	25.6	53.8	81.2	73.7
Max ($\lvert\Delta H^E\rvert/H^E$)	5.9 %	7.0 %	16.9 %	16.8 %
PREDICTION[a]			NRTL	UNIQUAC
B_0			-0.2065	-210.2
B_1			0.8622	467.4
B_2			2.3362	2160.1
B_3			0.6954	-629.7
B_4			1.9691	1960.8
B_5			0.0910	-588.4
α_{12}			0.30	
α_{13}			0.30	
α_{23}			0.30	
rms ΔH^E/J·mol^{-1}			59.1	76.3
Max $\lvert\Delta H^E\rvert$/J·mol^{-1}			131.2	144.1
Max ($\lvert\Delta H^E\rvert/H^E$)			38.9 %	39.8 %

[a] Equivalence between parameters: NRTL $B_0=\tau_{12}$; $B_1=\tau_{21}$; $B_2=\tau_{13}$; $B_3=\tau_{31}$; $B_4=\tau_{23}$; $B_5=\tau_{32}$; UNIQUAC $B_0=\Delta u_{12}$; $B_1=\Delta u_{21}$; $B_2=\Delta u_{13}$; $B_3=\Delta u_{31}$; $B_4=\Delta u_{23}$; $B_5=\Delta u_{32}$.

Figure Captions

Figure 5. Contours for constant values of H^{E}_{123} for DBE(1) + cyclohexane (2) + 1-butanol (3) at 298.15 K.

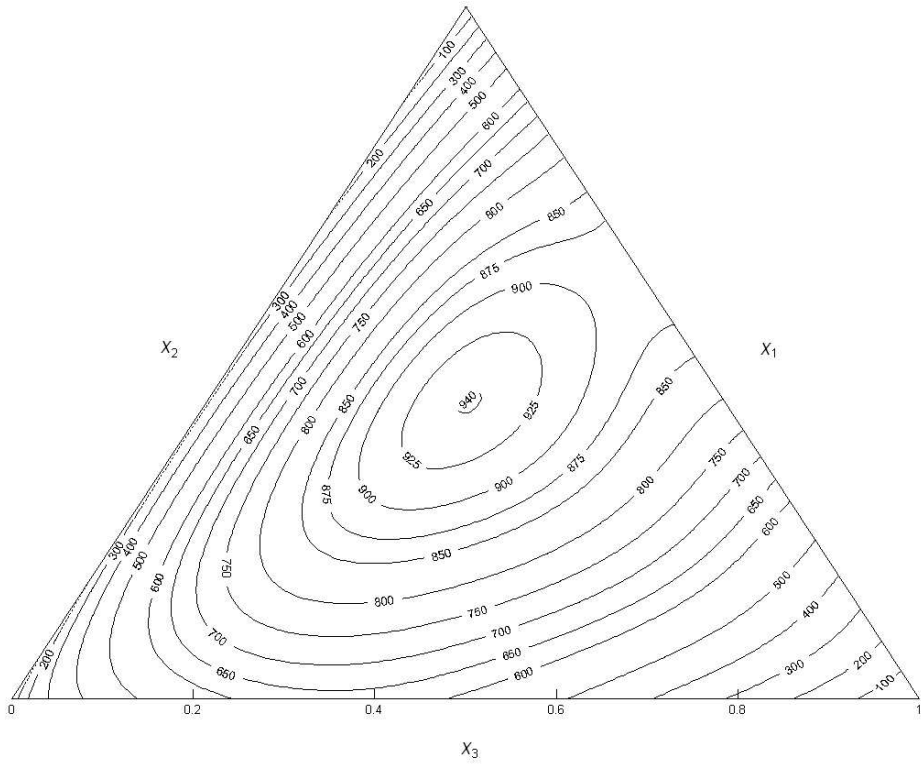

Figure 5. Contours for constant values of HE123 for DBE(1) + cyclohexane (2) + 1-butanol (3) at 298.15 K.
184x145mm (150 x 150 DPI)