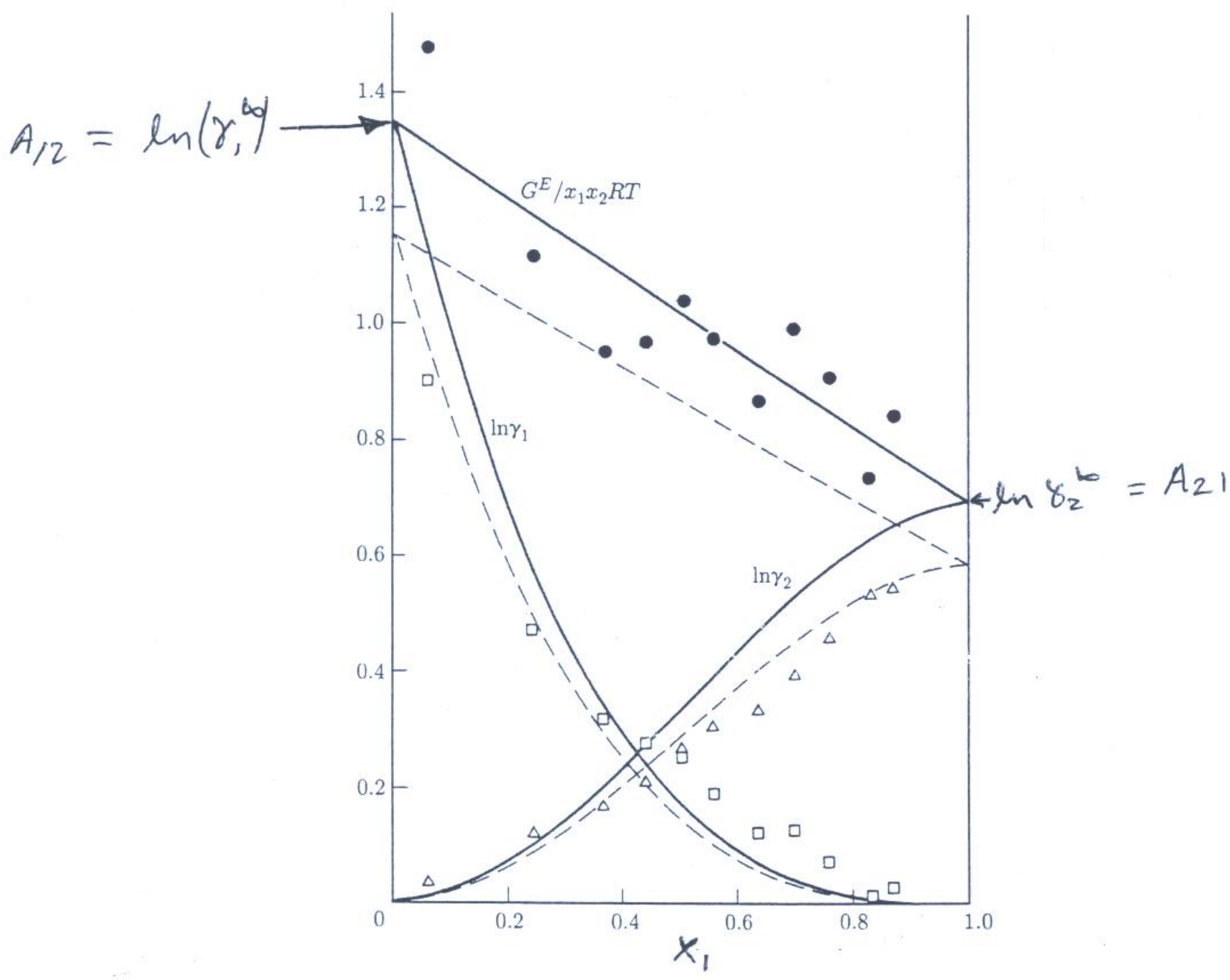
Example 12.1 Reduce the VLE data set for diethyl ketone(1)/n-hexane(2) at 65°C reported by Maripuri and Ratcliff,[6] and given in the first three columns of Table 12.4.

Table 12.4: VLE Data for diethyl ketone(1)/n-hexane(2) at 65°C

P/kPa	x_1	y_1	$\ln\gamma_1^*$	$\ln\gamma_2^*$	$\left(\frac{G^E}{x_1x_2RT}\right)^*$
90.15(P_2^{sat})	0.000	0.000		0.000	
91.78	0.063	0.049	0.901	0.033	1.481
88.01	0.248	0.131	0.472	0.121	1.114
81.67	0.372	0.182	0.321	0.166	0.955
78.89	0.443	0.215	0.278	0.210	0.972
76.82	0.508	0.248	0.257	0.264	1.043
73.39	0.561	0.268	0.190	0.306	0.977
66.45	0.640	0.316	0.123	0.337	0.869
62.95	0.702	0.368	0.129	0.393	0.993
57.70	0.763	0.412	0.072	0.462	0.909
50.16	0.834	0.490	0.016	0.536	0.740
45.70	0.874	0.570	0.027	0.548	0.844
29.00(P_1^{sat})	1.000	1.000	0.000		



To reduce the experimental data we fit it to Margules equation:

$$\frac{G^E}{RT\,x_1 x_2} = A_{21}\,x_1 + A_{12}\,x_2$$

$$\lim_{x_1 \to 1}\left(\frac{G^E}{RT\,x_1 x_2}\right) = A_{21} = 0.7 \quad \text{(see figure)}$$

$$\lim_{x_1 \to 0}\left(\frac{G^E}{RT\,x_1 x_2}\right) = A_{12} = 1.35 \quad (\text{"} \quad)$$

$$\Rightarrow \frac{G^E}{RT\,x_1 x_2} = 0.7\,x_1 + 1.35\,x_2$$

and using eq. 12.10

$$\ln(\gamma_1) = x_2^2\left[1.35 + 2\,(0.70 - 1.35)\,x_1\right]$$

$$\ln(\gamma_2) = x_1^2\left[0.70 + 2\,(1.35 - 0.70)\,x_2\right]$$