Table D-1 (in the appendix). Calculations based on the UNIQUAC equation are more involved compared to other methods but the method is appealing because it works well with many nonideal systems. The calculation of the activity coefficients and of the *Pxy* graph are demonstrated in the example below.

Example 12.10: Calculation of *Pxy* Graph from UNIQUAC

Use the UNIQUAC equation to calculate the *Pxy* graph of ethanol(1)/acetonitrile(2) at 45 °C. The interaction parameters are

$$a_{12} = 294.5 \text{ K}, \quad a_{21} = -41.3 \text{ K}.$$

Solution Ethanol consists of three subgroups, CH_3, CH_2, and OH. Acetonitrile consists of a single group, CH_3CN. The parameters of these subgroups from Table D-1 in the appendix are

Subgroup	k	$R^{(k)}$	$Q^{(k)}$
CH_3	1	0.9011	0.848
CH_2	2	0.6744	0.540
OH	14	1.0000	1.200
CH_3CN	40	1.8701	1.724

The parameters of ethanol are

$$r_1 = (1)(0.9011) + (1)(0.6744) + (1)(1.000) = 2.5755,$$
$$q_1 = (1)(0.848) + (1)(0.540) + (1)(1.200) = 2.588,$$

and for acetonitrile,

$$r_2 = (1)(1.8701) = 1.8701,$$
$$q_2 = (1)(1.724) = 1.724.$$

A sample calculation is shown at $x_1 = 0.8$:

$$\Phi_1 = \frac{(0.8)(2.5755)}{(0.8)(2.5755) + (0.2)(1.8701)} = 0.846362,$$
$$\Phi_2 = \frac{(0.2)(1.8701)}{(0.8)(2.5755) + (0.2)(1.8701)} = 0.153638,$$
$$\theta_1 = \frac{(0.8)(2.588)}{(0.8)(2.588) + (0.2)(1.724)} = 0.857237,$$
$$\theta_2 = \frac{(0.2)(1.724)}{(0.8)(2.588) + (0.2)(1.724)} = 0.142763,$$