

The interaction parameters between the subgroups are

	Interaction energy, $a_{mk}$			
	$k = 1$	$k = 2$	$k = 14$	$k = 40$
$m = 1$	0	0	986.5	597
$m = 2$	0	0	986.5	597
$m = 14$	156.4	156.4	0	6.712
$m = 40$	24.82	24.82	185.4	0

For example, the interaction between subgroup “CH<sub>3</sub>” ( $k = 1$ ) and subgroup “OH” ( $k = 14$ ) is  $a_{1,14} = 986.15$  K.

This is all that is required from the UNIFAC tables. Below we summarize the results for the various intermediate variables ( $i = 1$  refers to ethanol,  $i = 2$  refers to acetonitrile):

	$(i = 1)$	$(i = 2)$
$r$	2.5755	1.8701
$q$	2.588	1.724
$J$	1.32714	0.963651
$L$	1.42952	0.952276

make subscripts “mk”

The  $\tau_{mn}$  parameters are calculated as  $\exp(-a_{mn}/T)$ :

	$n = 1$	$n = 2$	$n = 14$	$n = 40$
$m = 1$	1	1	0.60687	0.9238
$m = 2$	1	1	0.60687	0.9238
$m = 14$	0.0428415	0.0428415	1	0.553193
$m = 40$	0.148609	0.148609	0.978794	1

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change “n” to “k”

transpose table: first row should become first column, etc.

All other parameters are summarized below:

$G_{ki}$		$s_{ki}$		$\theta_k$	$\eta_k$
$(i = 1)$	$(i = 2)$	$(i = 1)$	$(i = 2)$		
0.848	0	2.11624	1.59263	0.0848	1.64499
0.54	0	2.11624	1.59263	0.054	1.64499
1.2	0	1.25946	0.953705	0.12	0.98428
0.	1.724	1.38082	1.724	1.5516	1.68968

The combinatorial contributions are

$$\ln \gamma_1^C = -0.00925364, \quad \ln \gamma_2^C = -0.000066914,$$

and the residual contributions are

$$\ln \gamma_1^R = 0.7086, \quad \ln \gamma_2^R = 0.00920115.$$