

The direct determination of partial molar
volumes and reaction volumes in ultra-dilute
non-reactive and reactive multi-component
systems using a combined spectroscopic and
modified response surface model approach

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Table S1 Delta densities, $\rho - \rho^o$ (g cm⁻³) and volume difference Y (cm³ mole⁻¹) (eqn. (11) or (12)) of the solutes [Mo(CO)₆] (1) + [Mn₂(CO)₁₀] (2) + [Re₂(CO)₁₀] (3) dissolved in toluene (4) where x_i represents the mole fraction at T = 298.15 K and P = 0.1 MPa

Run	x_1	x_2	x_3	$\rho - \rho^{oa} / \text{g cm}^{-3}$	$Y / \text{cm}^3 \text{ mole}^{-1}$
I-1 ^b	0.000035	0.000000	0.000000	0.000039	0.0060
2	0.000035	0.000047	0.000000	0.000108	0.0185
3	0.000071	0.000046	0.000000	0.000145	0.0246
4	0.000071	0.000046	0.000011	0.000182	0.0279
5	0.000104	0.000045	0.000011	0.000218	0.0331
6	0.000138	0.000044	0.000010	0.000251	0.0388
7	0.000137	0.000056	0.000010	0.000268	0.0421
8	0.000135	0.000092	0.000010	0.000319	0.0508
9	0.000134	0.000092	0.000014	0.000331	0.0519
10	0.000132	0.000090	0.000047	0.000455	0.0602
11	0.000131	0.000090	0.000051	0.000468	0.0611
12	0.000129	0.000088	0.000083	0.000592	0.0686
II-1 ^b	0.000000	0.000036	0.000000	0.000054	0.0097
2	0.000000	0.000035	0.000046	0.000231	0.0223
3	0.000000	0.000071	0.000045	0.000282	0.0314
4	0.000010	0.000070	0.000045	0.000293	0.0328
5	0.000010	0.000104	0.000044	0.000343	0.0413
6	0.000010	0.000138	0.000044	0.000394	0.0496
7	0.000010	0.000137	0.000057	0.000444	0.0529

8	0.000010	0.000134	0.000093	0.000579	0.0622
9	0.000010	0.000134	0.000093	0.000579	0.0622
10	0.000047	0.000131	0.000091	0.000612	0.0670
11	0.000047	0.000131	0.000091	0.000612	0.0670
12	0.000082	0.000129	0.000090	0.000642	0.0719
III-1 ^b	0.000000	0.000000	0.000036	0.000138	0.0103
2	0.000046	0.000000	0.000035	0.000185	0.0178
3	0.000045	0.000000	0.000071	0.000322	0.0273
4	0.000044	0.000010	0.000070	0.000336	0.0298
5	0.000043	0.000010	0.000105	0.000469	0.0388
6	0.000042	0.000010	0.000138	0.000597	0.0477
7	0.000056	0.000010	0.000137	0.000609	0.0497
8	0.000093	0.000009	0.000134	0.000638	0.0553
9	0.000093	0.000010	0.000134	0.000638	0.0554
10	0.000091	0.000044	0.000132	0.000683	0.0632
11	0.000091	0.000047	0.000132	0.000686	0.0638
12	0.000089	0.000084	0.000129	0.000734	0.0722

^a Average value of pure toluene density, $\rho^0 = 0.862103 \text{ (gr.cm}^{-3}\text{)}$

^b Binary composition data

These compositions were pre-determined by the experimental design considerations for a semi-batch sequence