

Run	Symbol	Initial amount (in mols)			Temperature ( $\lambda$ , Kelvin)	Volume ( $V$ , litres)
		$A_0$	$D_0$	$E_0$		
1	$\mathbf{x}_1$	22.50	91.59	26.47	298.15	31.31
2	$\mathbf{x}_2$	45.00	91.59	26.47	298.15	32.56
3	$\mathbf{x}_3$	22.50	91.50	26.45	313.15	31.28
4	$\mathbf{x}_4$	45.00	91.50	26.45	313.15	32.53
5	$\mathbf{x}_5$	33.75	91.40	26.42	305.65	31.88
6	$\mathbf{x}_6$	33.75	91.40	26.42	305.65	31.88