Key for Short Problem Set 6

We begin by completing the remaining entries in this table

experiment	b_0	b_a	b_b	b_c	b_{ab}	b_{ac}	b_{bc}	b_{abc}	rate (min^{-1})
1	+1	+1	−1	+1	−1	+1	−1	−1	6.69
2	+1	+1	+1	+1	+1	+1	+1	+1	11.71
3	+1	+1	+1	−1	+1	−1	−1	−1	14.79
4	+1	+1	−1	−1	−1	−1	+1	+1	8.05
5	+1	−1	−1	+1	+1	−1	−1	+1	6.33
6	+1	−1	+1	+1	−1	−1	+1	−1	11.11
7	+1	−1	+1	−1	−1	+1	−1	+1	14.08
8	+1	−1	−1	−1	+1	+1	+1	−1	7.59

and then using the table to organize our calculations, reporting, for now, exact values without regard to significant figures.

$$b_0 = \frac{6.69 + 11.71 + 14.79 + 8.05 + 6.33 + 11.11 + 14.08 + 7.59}{8} = 10.04375$$

$$b_a = \frac{6.69 + 11.71 + 14.79 + 8.05 - 6.33 - 11.11 - 14.08 - 7.59}{8} = 0.26625$$

$$b_b = \frac{-6.69 + 11.71 + 14.79 - 8.05 - 6.33 + 11.11 + 14.08 - 7.59}{8} = 2.87875$$

$$b_c = \frac{6.69 + 11.71 - 14.79 - 8.05 + 6.33 + 11.11 - 14.08 - 7.59}{8} = -1.08375$$

$$b_{ab} = \frac{-6.69 + 11.71 + 14.79 - 8.05 + 6.33 - 11.11 - 14.08 + 7.59}{8} = 0.06125$$

$$b_{ac} = \frac{6.69 + 11.71 - 14.79 - 8.05 - 6.33 - 11.11 + 14.08 + 7.59}{8} = -0.02625$$

$$b_{bc} = \frac{-6.69 + 11.71 - 14.79 + 8.05 - 6.33 + 11.11 - 14.08 + 7.59}{8} = -0.42875$$

$$b_{abc} = \frac{-6.69 + 11.71 - 14.79 + 8.05 + 6.33 - 11.11 + 14.08 - 7.59}{8} = -0.00125$$

Given that we have two decimal places for the rate, let's maintain three decimal places for each parameter and round any resulting calculations to two decimal places; thus, our model is

$$R = 10.044 + 0.266A^* + 2.879B^* - 1.084C^* + 0.61A^*B^* - 0.26A^*C^* - 0.429B^*C^* - 0.001A^*B^*C^*$$

To convert between coded and uncoded values, we note that

$$A = 37.5 + 2.5A^*$$

$$B = 13.9 + 13.4B^*$$

$$C = 5.6 - 0.8C*$$

Substituting in the desired values for A (36°C), for B (10.0 mM), and for C (5.0) gives $A^* = -0.600$, $B^* = -0.291$, and $C^* = 0.75$. Substitutin these into our model gives the rate as 8.35 min^{-1}.