7.54 In an effort to obtain maximum yield in a chemical reaction, the values of the following variables were chosen by the experimenter:

$$x_1 = \text{temperature (°C)}$$
$$x_2 = \text{concentration of a reagent (\%)}$$
$$x_3 = \text{time of reaction (hours)}$$

Two different response variables were observed:

$$y_1 = \text{percent of unchanged starting material}$$
$$y_2 = \text{percent converted to the desired product}$$

The data are listed in Table 7.4 (Box and Youle 1955, Andrews and Herzberg 1985, p. 188). Carry out the following for y_1:

(**a**) Find $\hat{\boldsymbol{\beta}}$ and s^2.

(**b**) Find an estimate of $\text{cov}(\hat{\boldsymbol{\beta}})$.

TABLE 7.4 Chemical Reaction Data

y_1	y_2	x_1	x_2	x_3
41.5	45.9	162	23	3
33.8	53.3	162	23	8
27.7	57.5	162	30	5
21.7	58.8	162	30	8
19.9	60.6	172	25	5
15.0	58.0	172	25	8
12.2	58.6	172	30	5
4.3	52.4	172	30	8
19.3	56.9	167	27.5	6.5
6.4	55.4	177	27.5	6.5
37.6	46.9	157	27.5	6.5
18.0	57.3	167	32.5	6.5
26.3	55.0	167	22.5	6.5
9.9	58.9	167	27.5	9.5
25.0	50.3	167	27.5	3.5
14.1	61.1	177	20	6.5
15.2	62.9	177	20	6.5
15.9	60.0	160	34	7.5
19.6	60.6	160	34	7.5

(**c**) Find R^2 and R_a^2.

(**d**) In order to find the maximum yield for y_1, a second-order model is of interest. Find $\hat{\boldsymbol{\beta}}$ and s^2 for the model $y_1 = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_4 x_1^2 + \beta_5 x_2^2 + \beta_6 x_3^2 + \beta_7 x_1 x_2 + \beta_8 x_1 x_3 + \beta_9 x_2 x_3 + \varepsilon$.

(**e**) Find R^2 and R_a^2 for the second-order model.