October 9, 2024

Series 4: Menchutkin's reaction

1 Analysis of the design

In organic chemistry, the Menchutkin's reaction converts a tertiary amine into a quaternary ammonium salt. The reaction scheme is given in Fig.1.

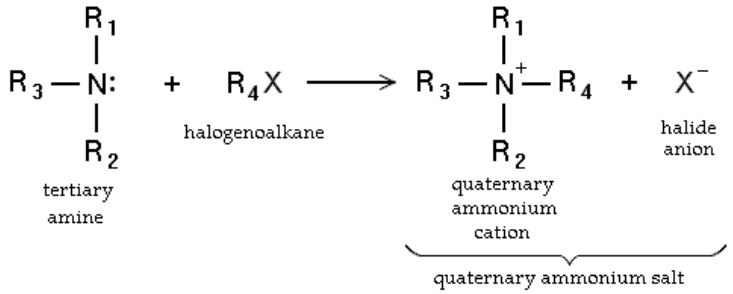

Figure 1: Menchutkin's reaction

The table 1 gives the values of the coefficients of induction σ_F and resonance σ_R of 19 amines that can be used for the reaction. (The same data is also available in the file *Date_Exercises_Doe.xlsx* in Moodle). We are interested in making a model of the reaction rate as a function of these two parameters. For linear, linear with interactions and quadratic models:

1. Visualize measurement points using a *scatterplot*,
2. Compute the dispersion matrices for the three models,
3. Calculate variance inflation factors,
4. Draw the variance function,
5. Analyze the quality of the different models that could be identified using the 19 experiments,
6. Determine the 5,10 and 15 most interesting experiments to identify a linear model with interactions, compare with the situations of 19 experiments using the dispersion matrix (trace and determinant), VIF, variance function or d information (we will focus on minimum and maximum).

Table 1: Coefficients of inductions σ_F, resonance σ_R of 19 amines and the reaction rate K during the experiment

Run	Amines	σ_F	σ_R	K
1	H	0	0	4390
2	t-C_4H_9	0	-0.07	4180
3	i-C_3H_7	0	-0.07	4060
4	C_2H_5	0	-0.07	3950
5	CH_3	0	-0.08	3850
6	CH_2OH	0.14	-0.06	3510
7	C_6H_5	0.1	-0.22	3350
8	CH=CH_2	0.06	-0.15	3260
9	NH_2	0.14	-0.52	2600
10	$NHCH_3$	0.12	-0.58	2520
11	$N(CH_3)_2$	0.1	-0.64	2250
12	OH	0.3	-0.38	2110
13	$CO_2C_2H_5$	0.31	0	2020
14	OCH_3	0.28	-0.42	1700
15	Br	0.45	-0.15	1290
16	Cl	0.45	-0.17	1230
17	F	0.44	-0.25	1060
18	CN	0.6	0	1000
19	NO_2	0.65	0	660