



# Driving Force Analysis

Britest's **Driving Force Analysis (DFA)** tool is a qualitative model of the process for rigorous analysis of systems with competing rate processes. Together with experimental data, the DFA tool can be used to determine if the model is sufficiently well understood or quantified to explain known results at laboratory and plant scale – potentially identifying further areas for exploration and investigation.

*Influencing factors are listed as rows, including concentration of reagents*

*Desired reaction highlighted in green*

*One column for each rate process in the Transformation Map*

Driving Force	[R1] PhOOEt + PhMgBr → Ph <sub>2</sub> CO + EtOMgBr	[R2] Ph <sub>2</sub> CO + PhMgBr → Ph <sub>3</sub> COMgBr	[R3] PhMgBr + H <sub>2</sub> O → benzene + MgBrOH	[R4] PhMgBr + O <sub>2</sub> → PhOOMgBr	[R5] PhOOMgBr + PhMgBr → 2PhOMgBr
PHCOOEt	+				
PhMgBr	+	+	+	+	+
Ph <sub>2</sub> CO	P	+			
EtOMgBr	P				
Ph <sub>3</sub> COMgBr		P			
H <sub>2</sub> O			+		
benzene	+		P		
MgBrOH	++		P		
O <sub>2</sub>				+	
PhOOMgBr	P			P	+
PhOMgBr					P
Temp (rate)	+	++	+	+	+
Temp (eqm)					
Rate	Very fast	<[R1]	>[R1]	<[R1]	>[R4]
Heat (of reaction)	exo	exo	exo	exo?	exo?

*+ Drives reaction forwards (1<sup>st</sup> order)  
++ Drives reaction forwards (higher order)  
- Drives reaction backwards  
P Produced in reaction*

The table is populated by asking what would happen to the rate of the process being considered if the influencing factor was increased (e.g. impact of increase in concentration, temperature, etc). Question marks can be used to record unknown information, or in conjunction with other symbols where these represent an educated guess.

## Example Operating Strategies Analysis

Operating strategy	Possible process concept
Keep PhCOOEt concentration high to favour [R1]	Use fed batch with PhMgBr added to PhCOOEt in the reactor
Remove Ph <sub>2</sub> CO as it forms to avoid [R2]	Probably not possible
Exclude H <sub>2</sub> O to avoid [R3]	Dry solvent and process materials; take care to exclude moisture
Exclude O <sub>2</sub> to avoid [R4]	Use more thorough N <sub>2</sub> inerting than usual
Keep T down to suppress [R2]	Experimentation needed to identify appropriate T

*Not all strategies will be possible and some might be contradictory: select those with the most impact*

**Supporting organisations in gaining value  
from process understanding**