

Reactivity Scales

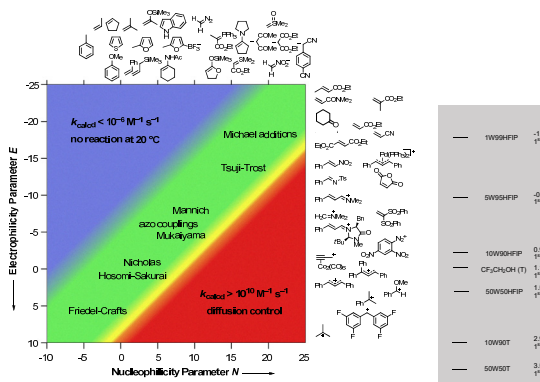
The reactivity poster shows a selection of the published reactivity parameters E , N , and S_N which allow the calculation of the rate constants for combination reactions of electrophiles with nucleophiles, with the following equation:

$$\log k_{20^\circ\text{C}} = S_N(N + E)$$

E = electrophilicity parameter
 N = nucleophilicity parameter
 S_N = nucleophile-specific sensitivity parameter (N and S_N are solvent-dependent; solvent is CH_2Cl_2 if not mentioned otherwise)

How to read the scales:

- Nucleophiles and electrophiles located on the same level ($E + N = 0$) combine with rate constants of $k = 1 \text{ M}^{-1} \text{ s}^{-1}$ at 20°C , corresponding to half-reaction times of 10 seconds for 0.1 M solutions.
- At 20°C electrophiles will generally not react with nucleophiles positioned more than 5 units higher.
- Electrophiles will generally undergo diffusion controlled (often unselective) reactions with nucleophiles positioned more than 9 units lower.

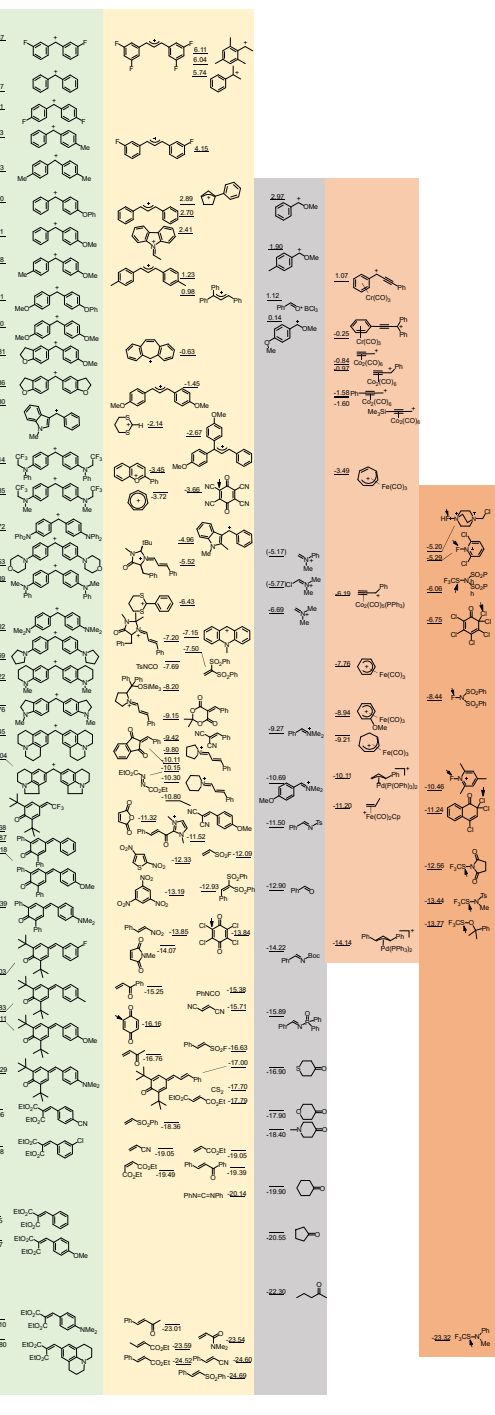


$\text{P}(\text{OPh})_3$	5.510.70	$\text{P}(\text{OMe})_3$	9.940.70 (91MAN)	$\text{P}(\text{OC}_2\text{H}_5)_3$	10.360.70	$\text{P}(\text{H}-\text{C}_6\text{H}_4)_3$	12.580.65	$\text{P}(\text{C}_6\text{H}_5)_3$	14.330.65	$\text{P}(\text{Me}-\text{C}_6\text{H}_4)_3$	15.440.68	$\text{P}(\text{Me}-\text{C}_6\text{H}_3)_3$	15.440.68	$\text{P}(\text{Me}-\text{C}_6\text{H}_2)_3$	15.440.68	$\text{P}(\text{Me}-\text{C}_6\text{H}_4)_3$	15.440.68	$\text{P}(\text{Me}-\text{C}_6\text{H}_3)_3$	15.440.68	$\text{P}(\text{Me}-\text{C}_6\text{H}_2)_3$	15.440.68
HO^-	15.190.62 (90SSAN)	HO^-	15.190.62 (90SSAN)	HO^-	15.190.62 (90SSAN)	HO^-	15.190.62 (90SSAN)	HO^-	15.190.62 (90SSAN)	HO^-	15.190.62 (90SSAN)	HO^-	15.190.62 (90SSAN)	HO^-	15.190.62 (90SSAN)	HO^-	15.190.62 (90SSAN)	HO^-	15.190.62 (90SSAN)	HO^-	15.190.62 (90SSAN)

I^-	-1.931.09 (1 st order)	Br^-	-2.860.80	Cl^-	-3.461.35	F^-	-4.611.11	O^{2-}	-5.510.70	S^{2-}	-6.411.10	HS^-	-7.310.21	HSO_4^-	-8.210.21	H_2PO_4^-	-9.110.21	H_2PO_3^-	-10.010.21	H_2PO_2^-	-10.910.21	$\text{H}_2\text{P}_2\text{O}_7^{4-}$	-11.810.21
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- A acetone
- AN acetonitrile
- E ethanol
- M methanol
- nPr n-propanol
- iPr isopropanol
- TFE trifluoroethanol
- W water

Nucleophiles

Further reactivity parameters are accessible at:
www.cup.lmu.de/oc/mayr/DBintro.html



Electrophiles

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www.cup.lmu.de/oc/mayr/MayrPoster.html