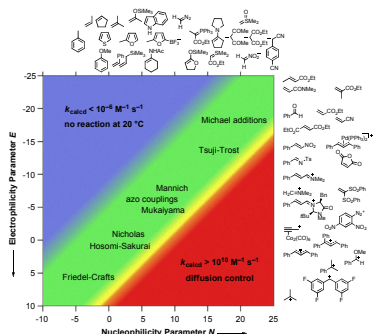


# Reactivity Scales



The reactivity posters show 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)

# Nucleophilicity $N/s_N$

In  $\text{CH}_2\text{Cl}_2$ , if not mentioned otherwise. Parentheses indicate estimated  $s_N$  parameters.

	-1.46/1.05		(-1.55/1.10)
	(-0.57/0.95)		-1.13/1.46
	-0.57/1.06		-0.31/0.99
	-0.13/1.21		0.06/0.71
	(0.25/1.00)		0.08/1.15
	0.65/1.17		0.58/0.91
	0.78/0.95		1.18/1.17
	0.84/1.06		(1.77/1.10)
	0.90/1.17		(1.98/1.10)
	1.11/0.98		2.30/1.06
	(1.20/0.90)		(2.60/1.00)
	1.68/1.00		2.65/0.72
	1.70/1.06		(3.09/1.00)
	1.95/0.98		3.58/0.70
	(2.60/1.00)		3.55/0.75
	2.82/0.89		(3.87/1.00)
	3.09/0.90		3.94/1.00
	4.17/0.83		3.99/0.73
	4.41/0.96		(4.46/1.15)
	4.67/0.81		5.07/0.91
	(4.74/1.15)		5.21/1.00
	(5.13/0.90)		5.41/0.91
	5.38/0.89		6.22/0.96
	5.46/0.89		6.22/0.96
	6.68/0.81		6.57/0.93
	6.78/0.95		(6.62/1.00)
	6.98/0.85		(6.77/1.00)
	7.48/0.89		8.23/0.81
	(7.69/0.76)		9.00/0.98
	9.63/0.57 (H2O)		9.81/0.81
	9.91/0.55 (H2O)		10.21/0.82
	10.36/0.70		10.38/0.87
	(10.50/0.73) (H2O)		10.38/0.87
	11.05/0.73 (H2O)		10.61/0.86
	11.44/0.68 (H2O)		10.61/0.86
	(11.70/0.67)		11.50/0.91
	12.29/0.75		12.56/0.70
	12.58/0.65		12.56/0.70
	12.79/0.77		12.56/0.70
	(12.90/0.67)		13.09/0.50 (H2O)
	13.19/0.56 (H2O)		13.58/0.52 (H2O)
	(13.70/0.67)		13.91/0.86 (DMSO)
	14.33/0.65		14.25/0.46 (H2O)
	15.29/0.70 (MeCN)		14.33/0.69 (H2O)
	15.44/0.64		15.57/0.58 (H2O)
	15.49/0.69		16.03/0.86 (DMSO)
	15.80/0.66		16.27/0.77 (DMSO)
	(15.90/0.67)		16.27/0.77 (DMSO)
	16.17/0.62		16.27/0.77 (DMSO)
	16.28/0.67 (MeCN)		16.27/0.77 (DMSO)
	18.39/0.64		17.64/0.73 (DMSO)
	18.42/0.65 (DMSO)		18.38/0.72 (DMSO)
	18.69/0.72 (DMSO)		18.82/0.69 (DMSO)
	19.20/0.69 (DMSO)		19.36/0.67 (DMSO)
	19.46/0.58 (DMSO)		19.50/0.55 (H2O)
	19.92/0.67 (DMSO)		20.22/0.65 (H2O)
	21.07/0.68 (DMSO)		20.72/0.58 (MeOH)

# How to read the scales:

The compounds are arranged in such a way that...

- nucleophiles and electrophiles located on similar levels combine with measurable rates ( $E + N = 0$  and  $k_{20^\circ\text{C}} = 1 \text{ M}^{-1} \text{ s}^{-1}$ ),
- nucleophiles at the top do not react with the electrophiles at the bottom, and
- nucleophiles at the bottom react with the electrophiles at the top with diffusion control.

# Electrophilicity $E$

	(8.02)		(7.96)
	7.52		6.70
	6.87		6.11
	6.23		6.04
	5.47		5.74
	5.20		5.01
	4.43		4.15
	3.63		3.20
	2.90		2.97
	2.11		2.89
	1.48		2.41
	0.61		2.16
	0.00		1.90
	-0.81		1.44
	-1.36		1.12
	-2.64		0.98
	-3.14		0.14
	-3.85		-0.25
	-4.72		-0.84
	-5.53		-0.97
	-5.89		-1.45
	-6.89		-1.60
	-7.02		-2.14
	-7.69		-2.57
	-8.22		-2.90
	-8.63		-3.49
	-8.76		-3.66
	-9.45		-4.67
	-10.04		-4.95
	-10.47/0.61 (H2O)		-5.06
	10.48/0.65 (H2O)		-5.17
	10.67/0.91		-5.77
	11.05/0.52 (H2O)		-5.91
	11.41/0.55 (H2O)		-6.19
	11.52/0.67 (DMSO)		-6.26
	11.63/0.95		-6.69
	12.15/0.65 (DMSO)		-7.15
	12.26/0.63 (H2O)		-7.37
	12.66/0.59 (H2O)		-7.76
	13.21/0.54		-8.37
	13.33/0.56 (H2O)		-8.54
	13.51/0.58		-8.84
	13.60/0.84 (MeCN)		-9.21
	14.30/0.67 (DMSO)		-9.27
	14.80/0.53 (H2O)		-9.42
	15.00/0.90 (DMSO)		-10.11
	15.40/0.55 (H2O)		-10.28
	15.62/0.54 (H2O)		-10.80
	16.03/0.66 (DMSO)		-11.16
	16.03/0.66 (DMSO)		-11.31
	16.27/0.70 (H2O)		-11.87
	16.33/0.56 (H2O)		-12.18
	16.56/0.67 (DMSO)		-12.29
	17.19/0.71 (DMSO)		-12.33
	17.20/0.72 (MeCN)		-12.76
	17.94/0.60 (DMSO)		-13.19
	18.08/0.50 (H2O)		-13.56
	18.13/0.44 (H2O)		-13.90
	18.80/0.70 (MeCN)		-14.10
	19.60/0.60 (DMSO)		-14.68
	20.33/0.64 (DMSO)		-14.91
	20.50/0.59 (DMSO)		-15.38
	20.54/0.60 (MeCN)		-15.71
	20.54/0.60 (MeCN)		-16.19
	20.54/0.60 (MeCN)		-16.36
	20.54/0.60 (MeCN)		-17.18
	20.54/0.60 (MeCN)		-17.29
	20.54/0.60 (MeCN)		-17.90
	20.54/0.60 (MeCN)		-18.06
	20.54/0.60 (MeCN)		-18.98
	20.54/0.60 (MeCN)		-19.49
	20.54/0.60 (MeCN)		-20.55

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Further reactivity parameters can be obtained at:  
<http://www.cup.lmu.de/oc/mayr/DBintro.html>