

Composite pK_a Chart

COMPOSITE pK_a CHART

The Acidic H is in Boldface¹

Oxygen acids

pK_a Acid

Base

	FSO ₃ H	FSO ₃ [⊖]
-12	RNO ₂ H [⊖]	RNO ₂
-10	HClO ₄	ClO ₄ [⊖]
	H ₂ SO ₄	HSO ₄ [⊖]
-9		
-8		
-7		
-6.5	ArSO ₃ H	ArSO ₃ [⊖]
-6	CH ₃ SO ₃ H	CH ₃ SO ₃ [⊖]
-6.5		
-6.4	ArOH ₂ [⊖]	ArOH
-6		
-6		ArO [⊖]
-3.5		RO [⊖]
-2.4	CH ₃ CH ₂ OH ₂ [⊖]	CH ₃ CH ₂ OH
-1.7	H ₃ O [⊖]	H ₂ O
-1.5		
-1.5	(CH ₃) ₂ S=OH [⊖]	(CH ₃) ₂ S=O
-1.4	HNO ₃	NO ₃ [⊖]
-0.5		
0.5	CF ₃ -C(=O)OH	CF ₃ -C(=O)O [⊖]
0.7		
1.5	Ph-S(=O) ₂ OH	Ph-S(=O) ₂ O [⊖]
1.7	O ₂ N-CH ₂ -C(=O)OH	O ₂ N-CH ₂ -C(=O)O [⊖]
1.8	(CH ₃) ₃ NCH ₂ -C(=O)OH	(CH ₃) ₃ NCH ₂ -C(=O)O [⊖]
2.0	HSO ₄ [⊖]	SO ₄ ²⁻







2.2	H ₃ PO ₄	H ₂ PO ₄ [⊖]
2.4		
2.5	N≡C-CH ₂ -C(=O)OH	N≡C-CH ₂ -C(=O)O [⊖]
2.5		
2.9	Cl-CH ₂ -C(=O)OH	Cl-CH ₂ -C(=O)O [⊖]
3.1	CF ₃ CH ₂ -C(=O)OH	CF ₃ CH ₂ -C(=O)O [⊖]
3.3	HO-N=O	NO [⊖]
3.4	O ₂ N-C ₆ H ₄ -C(=O)OH	O ₂ N-C ₆ H ₄ -C(=O)O [⊖]
3.6	CH ₃ -C(=O)-CH ₂ -C(=O)OH	CH ₃ -C(=O)-CH ₂ -C(=O)O [⊖]
3.6	CH ₃ OCH ₂ -C(=O)OH	CH ₃ OCH ₂ -C(=O)O [⊖]
4.2		
4.5	CH ₃ O-C ₆ H ₄ -C(=O)OH	CH ₃ O-C ₆ H ₄ -C(=O)O [⊖]
4.6	(CH ₃) ₃ N [⊖] -OH	(CH ₃) ₃ N [⊖] -O [⊖]
4.8	CH ₃ -C(=O)OH	CH ₃ -C(=O)O [⊖]
6.4	H ₂ CO ₃	HCO ₃ [⊖]
7.2	H ₂ PO ₄ [⊖]	HPO ₄ ²⁻
7.2	O ₂ N-C ₆ H ₄ -OH	O ₂ N-C ₆ H ₄ -O [⊖]
10.0		
10.2	CH ₃ O-C ₆ H ₄ -OH	CH ₃ O-C ₆ H ₄ -O [⊖]
10.3	HCO ₃ [⊖]	CO ₃ ²⁻
11.6	HO-OH	O [⊖]
12.2	(CH ₃) ₂ C=N-OH	(CH ₃) ₂ C=N-O [⊖]
12.4	HPO ₄ ²⁻	PO ₄ ³⁻
12.4	CF ₃ CH ₂ OH	CF ₃ CH ₂ O [⊖]
13.3	HOCH ₂ OH	HOCH ₂ O [⊖]
14.2	HOCH ₂ CH ₂ OH	HOCH ₂ CH ₂ O [⊖]
15.5	CH ₃ OH	CH ₃ O [⊖]
15.7	H ₂ O	O [⊖]
16	CH ₃ CH ₂ OH	CH ₃ CH ₂ O [⊖]
18	(CH ₃) ₂ CHOH	(CH ₃) ₂ CHO [⊖]

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Nitrogen acids

pK _a	Acid	Base
-10	$\text{RC}\equiv\text{N}^{\ominus}$	$\text{RC}\equiv\text{N}:$
-5	$\text{Ar}_3\text{N}^{\ominus}$	Ar_3N
1	$\text{Ar}_2\text{N}^{\ominus}$	Ar_2NH
1.0	$\text{O}_2\text{N}-\text{C}_6\text{H}_4-\text{NH}_3^{\oplus}$	$\text{O}_2\text{N}-\text{C}_6\text{H}_4-\text{NH}_2$
4.6	$\text{C}_6\text{H}_5\text{NH}_3^{\oplus}$	$\text{C}_6\text{H}_5\text{NH}_2$
5.2	$\text{C}_6\text{H}_5\text{N}^{\oplus}\text{H}$	$\text{C}_6\text{H}_5\text{N}:$
5.4	$\text{CH}_3\text{O}-\text{C}_6\text{H}_4-\text{NH}_3^{\oplus}$	$\text{CH}_3\text{O}-\text{C}_6\text{H}_4-\text{NH}_2$
5.8	$\text{H}_2\text{N}-\text{NH}_3^{\oplus}$	$\text{H}_2\text{N}-\text{NH}_2$
7.0	$\text{HN}=\text{N}-\text{NH}_3^{\oplus}$	$\text{HN}=\text{N}-\text{NH}_2$
7.9	$\text{H}_2\text{N}-\text{NH}_3^{\oplus}$	$\text{H}_2\text{N}-\text{NH}_2$
9.3	<i>anilinium</i>	
8.5	$\text{PhSO}_2\text{NH}_3^{\oplus}$	PhSO_2NH_2
9.2	NH_4^{\oplus}	NH_3
9.3	$\text{C}_6\text{H}_5\text{CH}_2\text{NH}_3^{\oplus}$	$\text{C}_6\text{H}_5\text{CH}_2\text{NH}_2$
5.8	$\text{HOCH}_2\text{NH}_3^{\oplus}$	HOCH_2NH_2
9.6	<i>DMAP</i>	<i>DMAP</i>
9.6	$(\text{CH}_2\text{C}(\text{O})\text{NH})_2$	$(\text{CH}_2\text{C}(\text{O})\text{N})_2$
9.8	$\text{EtO}-\text{C}(\text{O})-\text{CH}_2\text{NH}_3^{\oplus}$	$\text{EtO}-\text{C}(\text{O})-\text{CH}_2\text{NH}_2$
10.6	EtNH_3^{\oplus}	EtNH_2
10.7	$\text{Et}_3\text{N}^{\oplus}\text{H}$	Et_3N
11	$\text{Et}_2\text{N}^{\oplus}\text{H}_2$	Et_2NH
11.6	<i>DBU</i>	<i>DBU</i>
13.6	$(\text{H}_2\text{N})_2\text{C}=\text{NH}_3^{\oplus}$	$(\text{H}_2\text{N})_2\text{C}=\text{NH}_2$
17	$\text{R}-\text{C}(\text{O})-\text{NH}_3^{\oplus}$	$\text{R}-\text{C}(\text{O})-\text{NH}_2$
25.8	$((\text{CH}_3)_3\text{Si})_2\text{NH}_3^{\oplus}$	$((\text{CH}_3)_3\text{Si})_2\text{NH}_2$
27	PhNH_3^{\oplus}	PhNH_2
35	NH_3	NH_2
36	$\text{Et}_2\text{N}^{\oplus}\text{H}$	Et_2N

Carbon acids

pK _a	Acid	Base
-5	$\text{HC}(\text{CN})_3$	$\text{C}^{\ominus}(\text{CN})_3$
3.6	$\text{H}_2\text{C}(\text{NO}_2)_2$	$\text{H}_2\text{C}^{\ominus}(\text{NO}_2)_2$
5	$\text{H}_2\text{C}(\text{C}(\text{O})\text{H})_2$	$\text{H}_2\text{C}^{\ominus}(\text{C}(\text{O})\text{H})_2$
9	$\text{H}_2\text{C}(\text{C}(\text{O})\text{CH}_3)_2$	$\text{H}_2\text{C}^{\ominus}(\text{C}(\text{O})\text{CH}_3)_2$
9	$\text{N}\equiv\text{C}-\text{CH}_2-\text{C}(\text{O})\text{CH}_3$	$\text{N}\equiv\text{C}-\text{CH}^{\ominus}-\text{C}(\text{O})\text{CH}_3$
9.2	$\text{HC}\equiv\text{N}$	$\text{C}^{\ominus}\equiv\text{N}$
10		
10.2	$\text{H}_3\text{C}-\text{NO}_2$	$\text{H}_2\text{C}^{\ominus}-\text{NO}_2$
10.7	$\text{CH}_3-\text{C}(\text{O})-\text{CH}_2-\text{C}(\text{O})\text{OEt}$	$\text{CH}_3-\text{C}^{\ominus}(\text{O})-\text{CH}-\text{C}(\text{O})\text{OEt}$
11.2	$\text{H}_2\text{C}(\text{C}\equiv\text{N})_2$	$\text{H}_2\text{C}^{\ominus}(\text{C}\equiv\text{N})_2$
12.5	$\text{H}_2\text{C}(\text{SO}_2\text{CH}_3)_2$	$\text{H}_2\text{C}^{\ominus}(\text{SO}_2\text{CH}_3)_2$
13	$\text{H}_2\text{C}(\text{C}(\text{O})\text{OEt})_2$	$\text{H}_2\text{C}^{\ominus}(\text{C}(\text{O})\text{OEt})_2$
13.5	$\text{H}_3\text{C}-\text{C}(\text{O})-\text{O}-\text{C}(\text{O})\text{CH}_3$	$\text{H}_2\text{C}^{\ominus}-\text{C}(\text{O})-\text{O}-\text{C}(\text{O})\text{CH}_3$
13.6	HCCl_3	$\text{C}^{\ominus}\text{Cl}_3$
-14	$\text{H}_3\text{C}-\text{C}(\text{O})\text{SR}$	$\text{H}_2\text{C}^{\ominus}-\text{C}(\text{O})\text{SR}$
15.9	$\text{H}_3\text{C}-\text{C}(\text{O})-\text{CH}_2\text{Ph}$	$\text{H}_3\text{C}-\text{C}^{\ominus}(\text{O})-\text{CHPh}$
16		
16	$\text{H}_3\text{C}-\text{C}(\text{O})-\text{CH}_2\text{Cl}$	$\text{H}_3\text{C}-\text{C}^{\ominus}(\text{O})-\text{CHCl}$
-16	$\text{H}_3\text{C}-\text{C}(\text{O})\text{Cl}$	$\text{H}_2\text{C}^{\ominus}-\text{C}(\text{O})\text{Cl}$
16.7	$\text{H}_3\text{C}-\text{C}(\text{O})\text{H}$	$\text{H}_2\text{C}^{\ominus}-\text{C}(\text{O})\text{H}$
19.2	$\text{H}_3\text{C}-\text{C}(\text{O})\text{CH}_3$	$\text{H}_2\text{C}^{\ominus}-\text{C}(\text{O})\text{CH}_3$
23	$\text{H}_3\text{C}-\text{SO}_2\text{CH}_3$	$\text{H}_2\text{C}^{\ominus}-\text{SO}_2\text{CH}_3$
24	$\text{H}_3\text{C}-\text{C}(\text{O})\text{OR}$	$\text{H}_2\text{C}^{\ominus}-\text{C}(\text{O})\text{OR}$
25	$\text{H}_3\text{C}-\text{C}\equiv\text{N}$	$\text{H}_2\text{C}^{\ominus}-\text{C}\equiv\text{N}$
25	$\text{HC}\equiv\text{CH}$	$\text{C}^{\ominus}\equiv\text{CH}$
-28	$\text{H}_3\text{C}-\text{C}(\text{O})\text{NR}_2$	$\text{H}_2\text{C}^{\ominus}-\text{C}(\text{O})\text{NR}_2$
31.1		
31.5	$\text{Ph}_3\text{C}-\text{H}$	$\text{Ph}_3\text{C}^{\ominus}$

Carbon acids (continued)

pK_a	Acid	Base
33.5	Ph_2CH_2	$\text{Ph}_2\overset{\ominus}{\text{C}}\text{H}$
35	$\text{H}_3\text{C}-\overset{\ominus}{\text{C}}(\text{O})-\text{CH}_3$	$\text{H}_2\overset{\ominus}{\text{C}}-\overset{\ominus}{\text{C}}(\text{O})-\text{CH}_3$
35	$\text{H}_3\text{C}-\overset{\ominus}{\text{P}}\text{Ph}_3$	$\text{H}_2\overset{\ominus}{\text{C}}-\overset{\ominus}{\text{P}}\text{Ph}_3$
41	$\text{H}_3\text{C}-\text{Ph}$	$\text{H}_2\overset{\ominus}{\text{C}}-\text{Ph}$
43	$\text{H}_3\text{C}-\text{HC}=\text{CH}_2$	$\text{H}_2\overset{\ominus}{\text{C}}-\text{HC}=\text{CH}_2$
43	HPh	αPh
44	$\text{H}_2\text{C}=\text{CH}_2$	$\overset{\ominus}{\text{C}}\text{H}=\text{CH}_2$
48	CH_4	αCH_3
50	$\text{H}_3\text{C}-\text{CH}_3$	$\text{H}_2\overset{\ominus}{\text{C}}-\text{CH}_3$
51	$\text{H}_2\text{C}(\text{CH}_3)_2$	$\overset{\ominus}{\text{C}}\text{H}(\text{CH}_3)_2$
>52	$\text{HC}(\text{CH}_3)_3$	$\alpha\text{C}(\text{CH}_3)_3$

Miscellaneous acids

pK_a	Acid	Base
-10	HI	I^-
-9	HBr	Br^-
-7	HCl	Cl^-
-7	$\text{R}\overset{\ominus}{\text{S}}\text{H}_2$	RSH
-5.3	$\text{R}_2\overset{\ominus}{\text{S}}\text{H}$	R_2S
2.7	$\text{Ph}_3\overset{\ominus}{\text{P}}\text{H}$	$\text{Ph}_3\text{P:}$
3.2	HF	F^-
3.3	$\text{CH}_3-\overset{\ominus}{\text{C}}(\text{O})-\text{SH}$	$\text{CH}_3-\overset{\ominus}{\text{C}}(\text{O})-\overset{\ominus}{\text{S}}\text{H}$
3.9	H_2Se	HS^-
6.5	$\text{Ph}\overset{\ominus}{\text{S}}\text{H}$	$\text{Ph}\overset{\ominus}{\text{S}}$
7.0	$\text{H}_2\overset{\ominus}{\text{N}}$	$\text{H}\overset{\ominus}{\text{N}}$
8.7	$\text{Et}_3\overset{\ominus}{\text{P}}\text{H}$	$\text{Et}_3\text{P:}$
10.6	$\text{Et}\overset{\ominus}{\text{S}}\text{H}$	$\text{Et}\overset{\ominus}{\text{S}}$
35	H_2	H^-

Acid Strength

Strong acids have low pK_a 's

Base Strength

Strong bases have high pK_{abH} 's

Proton Transfer

Proton transfer reactions usually form the weaker base.

$$\log K_{eq} = pK_{abH} - pK_{aHA}$$

$$K_{eq} = 10^{(pK_{abH} - pK_{aHA})}$$

Simply take the pK_{abH} of the base and subtract from it the pK_a of the acid to get the exponent of the K_{eq} . If the K_{eq} is equal to or greater than approximately 10^{-8} (negative by 8 pK_a units), the proton transfer is within the useful range. If the proton transfer K_{eq} is greater than 10^{+7} , it can for all practical purposes be considered irreversible. Proton transfer is the first thing that happens in many common reactions.

The ΔpK_a Rule

The leaving group or anion produced should be no more than about 8 pK_a units more basic than the incoming nucleophile or base. Reactions tend to form the weaker base. No reaction has huge jumps upward in the pK_{abH} of its intermediates. The energy drops if the pK_{abH} drops significantly.

Hard and Soft Acids and Bases

The HSAB principle: Hard bases favor binding with hard acids; soft bases favor binding with soft acids.

When a pair of molecules collide, two attractive forces lead to reaction: the hard-hard attraction (opposite charges attracting each other), and the soft-soft attraction (the interaction of filled orbitals with empty orbitals).