

Equilibrium pKa Table (DMSO Solvent and Reference)

Ketones

X = H	26.5 ⁵²
Ph	19.8 ⁵⁸
OMe	24.6 ²⁷
SPh	18.7
COCH ₃	13.3
S(O)Ph	15.1
SO ₂ Ph	12.5 ⁵⁸
⁺ NMe ₃	16.3 ⁴⁴
⁺ Py	11.8 ⁴⁴

Ar = Ph	24.7 ¹
2-Py	23.6
4-Py	21.8
2-Furyl	23.9
2-Thienyl	24.0

X = H	24.7 ⁵²
Me	24.4 ⁵⁸
Ph	17.7 ⁵⁸
COMe	14.2 ⁵⁸
COPh	13.4 ⁴²
C≡N	10.2 ⁶
F	21.7 ⁵²
OPh	21.1 ³⁴
OMe	22.9 ³⁴
NPh ₂	20.3
NMe ₂	23.6 ⁵⁷
⁺ NMe ₃	14.6 ⁶
⁺ Py	10.7 ⁴⁴
NO ₂	7.7 ⁶
SPh	17.1 ³⁵
SO ₂ Ph	11.4 ⁶
SePh	18.6 ⁵

X = H	24.7 ¹
p-Me	25.2
p-Ph	24.5
p-OMe	25.7 ⁵⁰
m-OMe	24.5 ⁵⁰
p-NMe ₂	27.5 ⁵⁰
m-NMe ₂	25.3 ⁵⁰
p-F	24.5 ⁵⁰
m-F	23.5 ⁵⁰
p-Cl	23.8 ⁵⁰
m-Cl	23.2 ⁵⁰
p-Br	23.8 ⁵⁰
p-SPh	23.8 ⁵⁰
p-S(O)Ph	23.2
p-SO ₂ Ph	22.1 ⁵⁰
m-SO ₂ Ph	23.0 ⁵⁰
p-C≡N	22.0 ⁵⁰
p-CF ₃	22.7 ⁵⁰
m-CF ₃	22.8 ⁵⁰

Ketones

	18.7 ⁵⁸
	19.4 ⁵⁸
	18.8 ⁵⁸

	n	
	3	28.2
	4	24.9
	5	25.8
	6	26.7 ⁵⁸
	7	27.7
	8	27.4

	n	
	4	26.2
	5	25.8 ⁵¹
	6	26.4 ⁵¹
	7	27.8
	8	27.4
	10	26.7
	12	26.9

	24.8 ⁵⁹
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	25.8
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	16.9 ⁵¹
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	24.7
--	------

	29.0
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	28.1
--	------

	25.5
--	------

	32.4
--	------

	10.1 ⁵³
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Ketones

	27.1 ¹
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	27.7 ⁵⁸
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	26.3 ⁵⁸
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	28.2 ⁵⁸
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β-Diketones

X = H	13.3 ⁴²
Me	15.1 ⁴²
Et	15.3 ⁴³
Ac	8.6 ⁴³

	13.4 ⁴²
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	14.2 ⁵⁸
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X = H	11.2 ⁴²
Me	11.3 ⁴³
Ac	9.8 ⁴³

	10.3 ⁵⁹
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	18.2 ⁴²
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	14.2 ⁵²
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Lactones

	13.5 ⁵¹
--	--------------------

	10.7 ⁵¹
--	--------------------

	25.2 ⁵⁹
--	--------------------

	23.3 ⁵⁹
--	--------------------

	24.5 ⁵⁹
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Esters

X = H	29.5 ⁴⁴

⁺ NMe ₃	20.0 ⁴⁴
⁺ Py	14.1 ⁴⁴
Ph	22.7 ¹⁸
CN	13.1 ¹⁸
(MeO) SPh	21.4 ⁵²
SO ₂ CF ₃	6.4 ⁶¹
NO ₂	9.1 ⁶¹

	30.3
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	23.6 ¹⁸
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	16.9 ⁵¹
--	--------------------

	18.7 ⁵¹
--	--------------------

	16.9 ⁵¹
--	--------------------

	19.5 ³⁸
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	14.2 ⁵⁸
--	--------------------

	20.9
--	------

	11.5 ⁵⁹
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Malonate Esters

X = H	16.4 ⁴²

⁺ NMe ₃	11.8 ⁴⁴
⁺ Py	5.6 ⁴⁴

X = H	15.9 ⁴³

Me	18.0 ⁴³
Et	18.5 ⁴³
CO ₂ Me	10.8 ⁴³
CF ₃	10.8

X = H	7.3 ⁴³

Me	7.4 ⁴³
Et	7.6 ⁴³

Equilibrium pKa Table (DMSO Solvent and Reference)

Amides (C-H)

	(35)
	24.9 ⁴⁴
	26.6 ¹⁸
	25.9 ¹⁸
	24.9 ¹⁸
	18.2 ⁵¹
	17.2 ¹⁸
	25.7 ⁵¹
	21.3 ⁵¹
	18.5 ⁵¹
	10.0 ⁵¹
	13.5 ⁵¹

Amides (NH)

	R = H	23.5 ¹³
	Me	25.5 ¹³
	CH ₂ OPh	23.0 ²⁷
	CH ₂ OMe	23.9 ²⁷
	CH ₂ SPh	23.0 ²⁷
	CH ₂ F	22.3 ²⁷
	CH ₂ NH ₂	24.7
	CH ₂ NMe ₃ ⁺	15.3 ²⁷
	Ph	23.3 ⁴¹
	3-Py	22.0 ²⁷
	4-Py	21.6 ²⁷
	2-Fu	22.5
	CF ₃	17.2 ⁵²
	OEt	24.2 ⁵¹
	NH ₂	26.9
	R = Me	21.5 ⁴¹
	Ph	18.8 ⁴¹
	CH ₂ F	18.2
	CH ₂ OMe	19.4
	CH ₂ SPh	19.0
	CF ₃	12.6
	N≡C-NH ₂	17.0 ⁵⁷
	Me	25.9 ⁵⁷
	Me	18.5 ⁴¹
	X = O	23.3
	X = S	16.9 ⁴¹
	3,5-(CF ₃) ₂ Ph	16.9 ⁴¹
	X = O	24.2 ⁵¹
	X = S	13.3
		18.5 ⁵¹
		10.0 ⁵¹
		14.7
		15.0 ⁴⁸

Amides (NH)

	20.7 ⁵¹
	26.6 ⁵¹
	25.4
	X = O 17.0
	X = S 13.3
	X = O 14.8
	X = S 11.9
	X = H 14.1
	X = F 12.7

Carbamates (NH)

	24.2 ⁵¹
	20.8 ⁵¹

Nitro

	O ₂ N-CH ₂ -X	X = H	17.2 ¹
		Me	16.7 ¹
		Et	17.0
		Ph	12.2 ⁹
		SPh	11.8 ¹⁰
		SO ₂ Ph	7.1 ⁶
		COPh	7.7 ⁶
		CH=CH ₂	11.3

	16.9 ²	
	n = 3	26.9 ¹²
	4	17.8 ¹²
	5	16.0 ¹²
	6	17.9 ¹²
	7	15.8 ¹²

Acetylenes

	28.8 ^{1,23}
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Nitriles

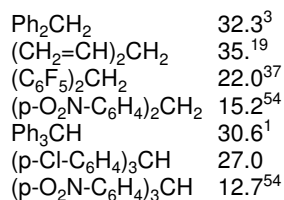
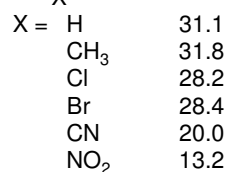
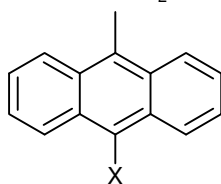
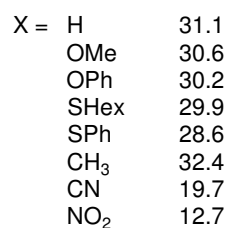
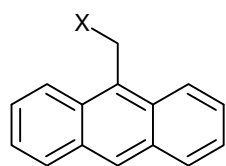
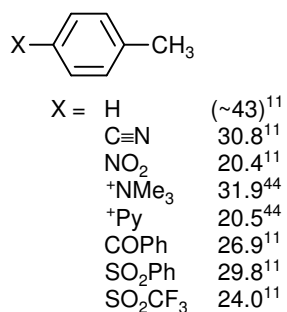
	X = H	31.3 ¹
	Me	32.5 ⁵
	Ph	21.9 ⁹
	C ₆ F ₅	15.8 ³⁷
	2-Furyl	21.4
	1-Naphthyl	20.9 ⁶⁰
	2-Naphthyl	20.7 ⁶⁰
	9-Anthryl	19.8 ⁶⁰
	COPh	10.2 ⁶
		17.2 ¹⁸
	CO ₂ Et	13.1 ¹⁸
	C≡N	11.1 ¹
	OPh	28.1 ⁵
	+NMe ₃	20.6 ⁶
	+Py	16.5 ⁴⁴
	SPh	20.8 ⁵
	SMe	24.3 ³⁶
	SO ₂ Ph	12.0 ⁶
	X = H	21.9 ^{9,60}
	p-Me	22.9 ⁶⁰
	Me ₃	24.6
	p-Ph	20.8 ⁶⁰
	p-Bz	16.0 ⁶⁰
	p-NMe ₂	24.6 ⁶⁰
	p-OMe	23.8 ⁶⁰
	m-OMe	21.6 ⁶⁰
	p-F	22.2 ^{37,60}
	m-F	20.0 ^{37,60}
	o-F	20.4 ³⁷
	p-Cl	20.5 ⁶⁰
	m-Cl	19.5 ⁶⁰
	m-Br	19.4 ⁶⁰
	p-CN	16.0 ⁶⁰
	m-CN	18.7 ⁶⁰
	p-NO ₂	12.3 ⁶⁰
	m-NO ₂	18.1 ⁶⁰
	m-CF ₃	19.2 ⁶⁰
	p-SPh	19.6 ⁶⁰
	m-SPh	20.4 ⁶⁰
	p-SO ₂ Ph	15.8 ⁶⁰
	m-SO ₂ Ph	18.5 ⁶⁰
	(NC) ₂ CHCH ₃	12.4 ¹³
	N≡CCHPh ₂	17.5 ^{9,60}
	N≡CCH(C ₆ F ₅) ₂	8.0 ³⁷
	N≡C-FI	8.3 ¹
	PhCH(Me)CN	23.0 ⁶⁰

Malononitriles

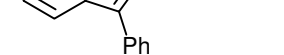
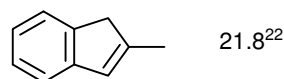
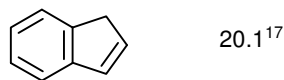
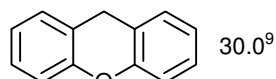
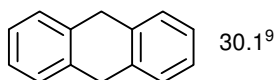
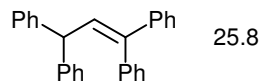
	R = H	11.1 ¹
	Me	12.4 ¹³
	Ph	4.2
	pClC ₆ H ₄	3.1
	pMeOC ₆ H ₄	5.6
	tBu	13.2
	NH ₂	13.7 ³⁴
	NMe ₂	

Equilibrium pKa Table (DMSO Solvent and Reference)

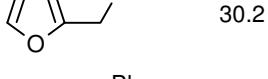
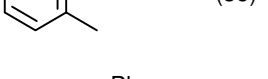
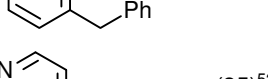
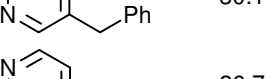
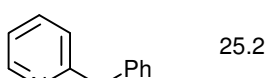
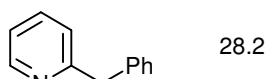
Hydrocarbons



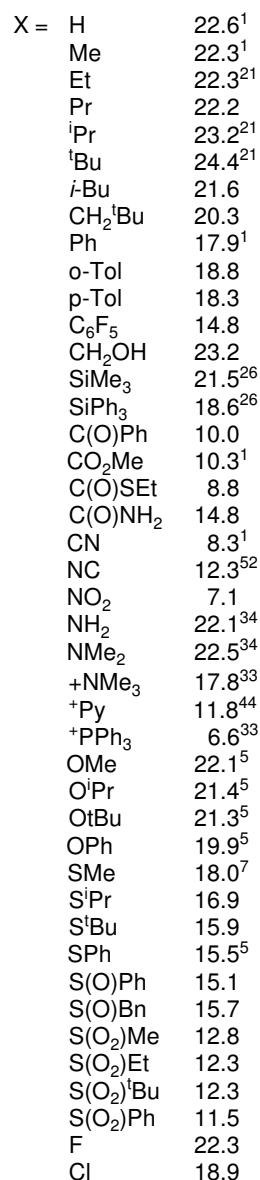
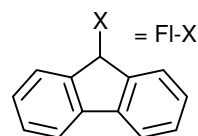
Hydrocarbons



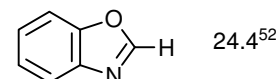
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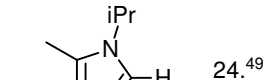
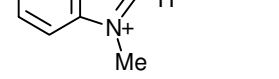
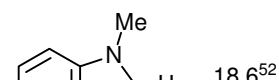
Fluorenes



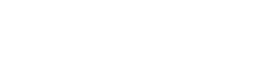
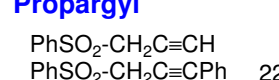
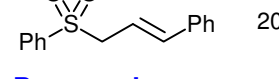
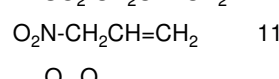
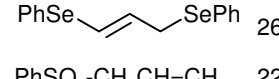
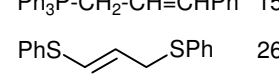
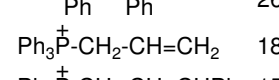
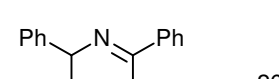
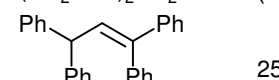
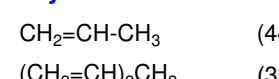
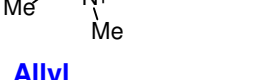
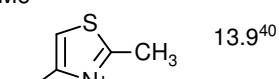
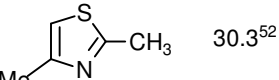
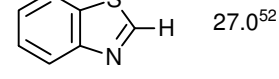
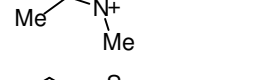
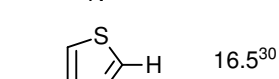
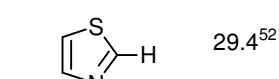
Oxazole



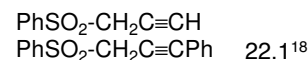
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Thiazole



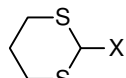
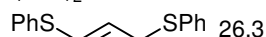
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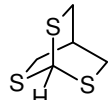
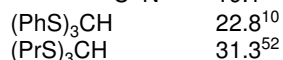
Equilibrium pKa Table (DMSO Solvent and Reference)

Sulfides

MeS-CH ₃	(45) ⁵²
PhS-CH ₂ -X	
X = H	(42) ⁵²
Ph	30.8 ¹⁰
C≡N	20.8 ⁵
COMe	18.7 ¹⁰
COPh	17.1 ³⁵
NO ₂	11.8 ¹⁰
⁺ NMe ₃	28.0 ⁴⁴
⁺ Py	17.7 ⁴⁴
SPh	30.8 ³
SO ₂ Ph	20.5 ⁵
SO ₂ CF ₃	11.0 ¹⁰
POPh ₂	24.9
MeS-CH ₂ -SO ₂ Ph	23.4 ⁵
MeS-FI	18.0 ⁷
PhS-FI	15.5 ⁵
MeS-CH ₂ -CN	24.3 ²¹
<i>t</i> -BuS-CH ₂ -CN	22.9 ²¹
PhSCHPh ₂	26.7 ¹⁰
(PhS) ₂ CHPh	23.0 ¹⁰

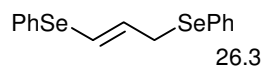


X = H	(39) ²³
Ph	30.7 ¹⁰
PhPh	29.0 ²³
CO ₂ Me	20.8 ²³
C≡N	19.1 ²³

30.5¹⁰

Selenides

Ph-CH ₂ -SePh	18.6 ⁵
PhSeCHPh ₂	27.5
(PhSe) ₂ CH ₂	31.3
PhSeCH ₂ Ph	31.0
(PhSe) ₂ CHPh	16.2 ⁵²



Sulfoxides

Ph-S(=O)-CH ₂ -X	
X = H	33.1 ⁵
Ph	27.2
SOPh	18.2
Me-S(=O)-CH ₂ -X	
X = H	35.1 ¹
SMe	29.0
Ph	29.0 ¹
Ph-S(=O)-CHPh ₂	24.6

Sulfimides

Ph-S(=N-Ts)-Me	27.6
Ph-S(=N-SO ₂ Ph)-Me	30.7

Sulfonium Salts

Me ₃ S ⁺ =O	18.2
Ph-S ⁺ (Me)-CH ₂ -Ph	16.3
Me-S ⁺ (Me)-CH ₂ -Ph	17.8 ³²
FI-S ⁺ Me ₂	6.5 ³²

Sulfoximides (C-H)

Ph-S(=O)-NMe	33.0 ¹⁵
Ph-S(=O)-N-Ts	
CH ₂ -X	
X = H	24.5 ¹⁵
Cl	20.7
Ph-S(=O)-CH(SiMe ₃) ₂	19.1 ²⁶
Ph-S(=O)-NSO ₂ Ph	28.5
Ph-S(=O)-NSO ₂ Ph	28.7
Ph-S(=O)-N ⁺ Me ₂	14.4 ¹⁵

Sulfonates

Me-S(=O) ₂ -OPh	25.2
PhCH ₂ -S(=O) ₂ -OPh	19.9 ⁵³
PhCH ₂ -S(=O) ₂ -SPh	19.1
PhCH ₂ -S(=O) ₂ -F	16.9

Sulfonamides (C-H)

Ph-N(S(=O) ₂)-CH ₂ Ph	24.1 ⁵³
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Sulfones

Ph-S(=O) ₂ -X	
X = H	29.0 ¹
Me	31.0 ⁵
<i>t</i> -Bu	31.2 ⁵
Ph	23.4 ¹
α-Naphth	22.5
β-Naphth	22.3 ¹
2-Py	20.5
3-Py	21.6
4-Py	18.6
CH=CH ₂	22.5
CH=CHPh	20.2 ⁵¹
C≡CH	
C≡CPh	22.1 ¹⁸
COMe	12.5 ⁵
COPh	11.4 ⁵
C≡N	12.0 ⁵
OPh	27.9 ⁵
OMe	30.7 ⁵
⁺ NMe ₃	19.4 ⁵
NO ₂	7.1 ⁵
SMe	23.4 ⁵
SPh	20.5 ⁵
SO ₂ Ph	12.2 ⁶
PPh ₂	20.2 ³
SiMe ₃	26.1 ²⁶
SiPh ₃	21.3 ²⁶
F	28.5 ⁵²
Cl	23.8 ⁵²

Ph-SO ₂ - <i>i</i> -Pr	32.1
Ph-S(=O) ₂ -Cyclopropyl	31.8
Me-S(=O) ₂ -Me	31.1 ⁵²
Et-S(=O) ₂ -Et	32.8 ⁹

Sulfones

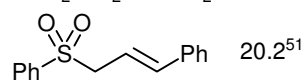
X-S(=O) ₂ -CH ₂ Ph	
X = Me	25.4 ⁵⁵
<i>t</i> -Bu	24.9 ²¹
NMePh	24.1 ⁵³
CH ₂ Ph	23.9 ⁵²
CF ₃	14.6 ⁵²

CF ₃ -SO ₂ -CH ₃	18.8 ²
CF ₃ -SO ₂ -Et	20.4
CF ₃ -SO ₂ - <i>i</i> -Pr	21.8 ²

CF ₃ -S(=O)-Cyclopropyl	26.6 ²
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(CF ₃ -SO ₂) ₂ CH ₂	2.1 ⁵²
Ph-SO ₂ -CHPh ₂	22.3 ⁹
(PhSO ₂) ₂ CHMe	14.3 ¹⁰
PhSO ₂ CH(SiMe ₃) ₂	20.4 ²⁶

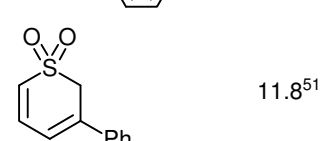
PhSO ₂ -CH ₂ CH=CH ₂	22.5 ⁵²
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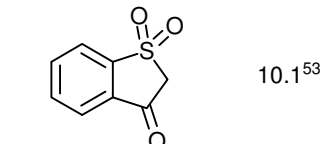
PhSO ₂ -CH ₂ C≡CH	
PhSO ₂ -CH ₂ C≡CPh	22.1 ¹⁸

PhSO ₂ -C ₆ H ₄ -CH ₃	29.8
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CF ₃ SO ₂ -C ₆ H ₄ -CH ₃	24.1
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(MeSO ₂) ₂ CH ₂	15.0 ²¹
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Equilibrium pKa Table (DMSO Solvent and Reference)

Halides

Ph-SO ₂ -CH ₂ -X	
X = H	29.0 ¹
F	28.5 ⁵²
Cl	23.8
	20.7
	16.9
	26.2
	20.2 ⁵²

Silanes (C-H)

X = H	29.0 ¹
SiMe ₃	26.1 ²⁶
SiPh ₃	21.3 ²⁶
	28.7 ⁵²
PhSO ₂ CH(SiMe ₃) ₂	20.4 ²⁶
	19.1 ²⁶
X = H	22.6 ¹
Me	22.3 ¹
SiMe ₃	21.5 ²⁶
SiEt ₃	21.4 ²⁶
SiPh ₃	18.6 ²⁶

Germanes (Ge-H)

Ph ₃ Ge-H	23.1 ⁶³
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Ethers

PhO-CH ₃	(49) ⁵²
MeO-CH ₂ COPh	22.9 ⁵
PhO-CH ₂ COPh	21.1 ⁵
MeO-CH ₂ SO ₂ Ph	30.7 ⁵
PhO-CH ₂ SO ₂ Ph	27.9 ⁵
PhO-CH ₂ C≡N	28.1 ⁵
X = H	22.6 ²¹
Ph	17.9 ⁵²
MeO	22.1 ⁵
iPrO	21.4 ⁵
tBuO	21.3 ⁵
PhO	19.9 ⁵

X = H	31.1
OMe	30.6
OPh	30.2

Phosphines

Ph ₂ P-CH ₂ -PPh ₂	29.9 ³
Ph ₂ P-CH ₂ -SO ₂ Ph	20.2 ³

Phosphonium (As) Salts

Ph ₃ P ⁺ -CH ₂ -X	
X = H	22.4 ³³
Ph	17.4 ³³
p-C ₆ H ₄ -CN	13.0 ²⁹
p-C ₆ H ₄ -NO ₂	11.0 ²⁹
p-C ₆ H ₄ -OEt	18.8 ²⁹
SPh	14.9 ³³
CO ₂ Et	8.5 ³³
COMe	7.1 ³³
CHO	6.1 ³³
CN	6.9 ³³
COPh	6.0 ³³
Ph ₃ P ⁺ -CHMeCO ₂ Et	9.3 ³³
Ph ₃ P ⁺ -Pr- <i>i</i>	21.2
Ph ₃ P ⁺ -CH ₂ -C ₆ H ₄ CN	13.0 ²⁹
Ph ₃ As ⁺ -CH ₂ -C ₆ H ₄ CN	17.0 ²⁹
Ph ₃ P ⁺ -CH ₂ -CH=CH ₂	18.5 ²⁹
Ph ₃ P ⁺ -CH ₂ -CH=CHPh	15.6 ²⁹
Ph ₃ P ⁺ -Fl	6.6 ³³

Phosphonates

X = Ph	27.6
C≡N	16.4
CO ₂ Et	18.6
Cl	26.2
SiMe ₃	28.7 ⁵²
X = Cl	26.2
R = H	23.2
Me	24.9
Ph	18.3

Phosphine Oxides

X = SPh	24.9
C≡N	16.9
	16.3
	19.3

Equilibrium pKa Table (DMSO Solvent and Reference)

Amines (CH)

	20.3 ⁵²
	X = F-I-X
X = H	22.6 ⁵²
NMe ₂	22.5 ³⁶
NEt ₂	21.4 ³⁶
NiPr ₂	22.5 ³⁶

Amines (NH)

NH ₃	(41) ¹⁹
	(44) ¹⁹
	X = H
m-CH ₃	30.6 ^{11,54}
p-Ac	31.0 ^{11,54}
p-Bz	25.3 ⁵⁴
p-F	24.4 ⁵⁴
p-F	30.7 ⁵⁴
o-F	28.7 ⁵⁴
o-Cl	27.6 ⁵⁴
m-Cl	28.5 ⁵⁴
p-Cl	29.4 ⁵⁴
m-Br	28.4 ⁵⁴
p-Br	29.1 ⁵⁴
m-OMe	30.5 ⁵⁴
p-C≡N	25.3 ¹¹
m-C≡N	27.5 ¹¹
p-PhCO	24.4 ¹¹
p-PhS	28.2 ⁵⁴
p-PhSO ₂	24.9 ^{11,54}
p-MeSO ₂	25.6 ⁵⁴
p-CF ₃ SO ₂	21.8 ⁵⁴
p-CF ₃	27.0 ⁵⁴
m-CF ₃	28.2 ⁵⁴
p-NO ₂	20.9 ^{11,54}

	27.7 ⁵⁴
	28.5
	26.5 ⁵⁴
N≡C-NH ₂	17.0 ¹⁹
Ph ₂ NH	25.0 ¹⁶

Ammonium Salts (NH)

NH ₄ ⁺	10.5 ⁵²
BuNH ₃ ⁺	11.1 ⁶⁴
PhNH ₃ ⁺	3.8 ⁶⁴
	R = H 2.4
	OMe 3.6
	Me 3.0
Et ₃ N ⁺ -H	9.0 ^{47,64}
BnNH ₃ ⁺	10.2 ⁶⁴
BnMe ₂ N ⁺ -H	7.6 ⁴⁷
Bn ₃ N ⁺ -H	3.7 ⁴⁶
	11.1 ⁶⁴
	9.8 ⁴⁵
	8.9 ^{45,64}
	10.9 ⁶⁴
	9.2 ⁶⁴
	7.5 ⁴⁵
	3.4 ⁵²
	4.1

Imides (NH)

	R = H 13.1 ⁴⁸
	R = Ph 9.9 ⁴⁸
	11.0 ⁴⁸
	R = H 15.1 ⁴⁸
	R = Me 15.0 ⁴⁸
	14.7

Ammonium Salts (CH)

Me ₃ N ⁺ -CH ₂ -X	(42) ^{33,44}
X = H	19.4 ⁵
SO ₂ Ph	20.6 ⁵
C≡N	16.3 ³³
COMe	14.6 ⁵
COPh	20.0 ³³
CO ₂ Et	24.9 ¹⁸
CONEt ₂	15.3 ²⁷
CONEt ₂	31.9 ³³
SPh	28.0 ³³
1-Py ⁺ -CH ₂ -X	X = C≡N 16.5 ⁴⁴
	COMe 11.8 ⁴⁴
	COPh 10.7 ⁴⁴
	CO ₂ Et 14.1 ⁴⁴
	CONEt ₂ 24.9 ¹⁸
	Ph 20.5 ⁴⁴
	SPh 17.7 ⁴⁴
Me ₃ N ⁺ -FI	17.8 ³³
Py ⁺ -FI	11.8 ⁴⁴

Isocyanide

PhCH ₂ N=C	27.4 ⁵²
	12.3 ⁵²

Imines (CH)

	14.4
	26.5
	24.3 ⁵²
	22.1

Imines (NH)

	31.0 ⁴¹
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Pyrrole, Indole (N-H)

	23.0 ¹⁹
	21.0 ¹⁹
	19.9 ¹⁹

Azoles (NH)

	18.6 ⁵²
	19.8 ⁵²
	14.8 ⁵²
	13.9 ⁵²
	8.2 ⁵²
	16.4 ⁵²
	15.3

Oximes (OH)

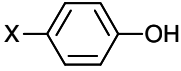
	20.2 ³¹
	17.0 ³¹
	28.5 ³¹
	25.2 ³¹
	20.1 ³¹
	14.9 ³¹

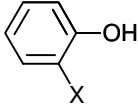
Equilibrium pKa Table (DMSO Solvent and Reference)

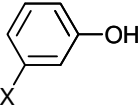
Alcohols (OH)

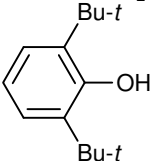
HOH	31.4 ²⁴
MeOH	29.0 ²⁴
EtOH	29.8 ²⁴
<i>i</i> -PrOH	30.3 ²⁴
<i>t</i> -BuOH	32.2 ²⁴
CF ₃ CH ₂ OH	23.5 ⁵²
(CF ₃) ₂ CHOH	17.9
(CF ₃) ₃ COH	10.7 ⁵²

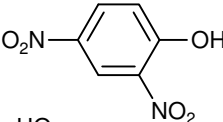
Phenols (OH)

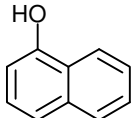
	
X = H	18.0 ²⁵
Me	18.9 ²⁵
OMe	19.1
OAc	14.1
NMe ₂	19.8
NO ₂	10.8
CF ₃	15.3
Cl	16.7 ²⁵
F	18.0
NMe ₃ ⁺	14.7
SO ₂ Me	13.6
CN	13.2

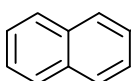
	
F	15.6
OMe	17.8
Ac	14.8
CN	12.1
NH ₂	18.2

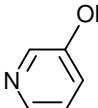
	
X = Cl	15.8 ²⁵
F	15.8 ²⁵
CN	14.8 ²⁵
NO ₂	14.4 ²⁵

	16.8
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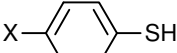
	5.1
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	16.2
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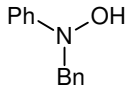
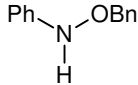
	17.2
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	15.7
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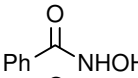
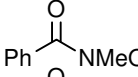
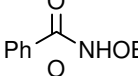
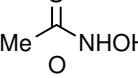
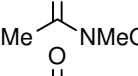
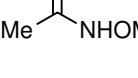
Thiols (SH)

	
X = H	10.3 ²⁰
OMe	11.2 ²⁰
Br	9.0 ²⁰
NO ₂	5.5 ²⁰
<i>t</i> -BuSH	17.9
<i>n</i> -BuSH	17.0
MeO ₂ CCH ₂ -SH	12.9
PhCH ₂ -SH	15.3
PhC(O)-SH	5.2 ⁶²
Ph-SeH	7.1 ⁶²

Hydroxylamine (NH, OH)

	23.9
	23.5
PhNHOH	24.2

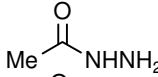
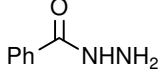
Hydroxamic Acid (NH, OH)

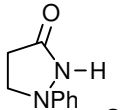
	13.7 ²⁷
	18.0 ²⁷
	14.4 ²⁷
	16.0 ²⁷
	19.6 ²⁷
	17.1 ²⁷

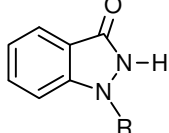
Inorganic Acids

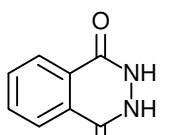
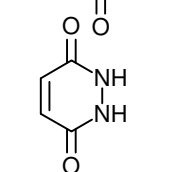
HCN	12.9 ⁵²
HN ₃	7.9 ⁵²
HF	15. ⁵²
HCl	1.8 ⁵²
HBr	0.9 ⁵²
NH ₄ ⁺	10.5 ⁵²
HOH	31.4 ²⁴
HON=O	7.5 ⁵²
NH ₃	(41) ¹⁹
H ₂ N-CN	16.9 ⁵²

Hydrazide (NH)

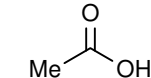
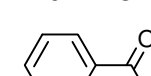
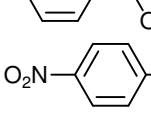
	21.8 ⁵²
	18.9 ⁵²
PhSO ₂ -NHNH ₂	17.1 ⁵²
PhSO ₂ -NHNMe ₂	15.8 ⁵²
Me(C=O)-NHNH ₂	21.8 ²⁷
Ac-NHNH-Ac	16.7 ⁵⁶
Ph(C=O)-NHNMe ₂	19.7
Ph(C=O)-NHNH ₂	18.9 ²⁷
Ph(C=O)-NHNMe ₂	19.7 ²⁷
3-Py(C=O)-NHNH ₂	17.5 ²⁷
EtO ₂ C-NHNH ₂	22.2 ⁵⁶
O=C(NHNH ₂) ₂	23.3 ⁵⁷
S=C(NHNH ₂) ₂	16.6 ⁵⁷

	15.3 ⁵⁶
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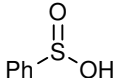
	
R=H	14.9 ⁵⁶
R=Ph	15.2 ⁵⁶

	12.7 ⁵⁶
	13.2 ⁵⁶

Carboxylic Acids (OH)

	12.6 ³⁹
	11.1 ⁴²
	9.1

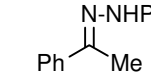
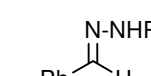
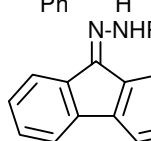
Sulfinic Acids (OH)

	7.1
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Sulfonic Acids (OH)

Me-SO ₂ -OH	1.6 ³⁹
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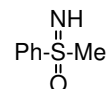
Hydrazone (NH)

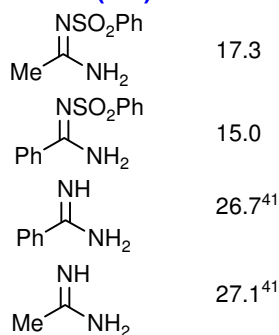
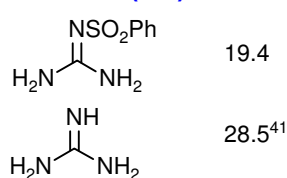
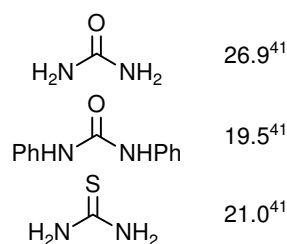
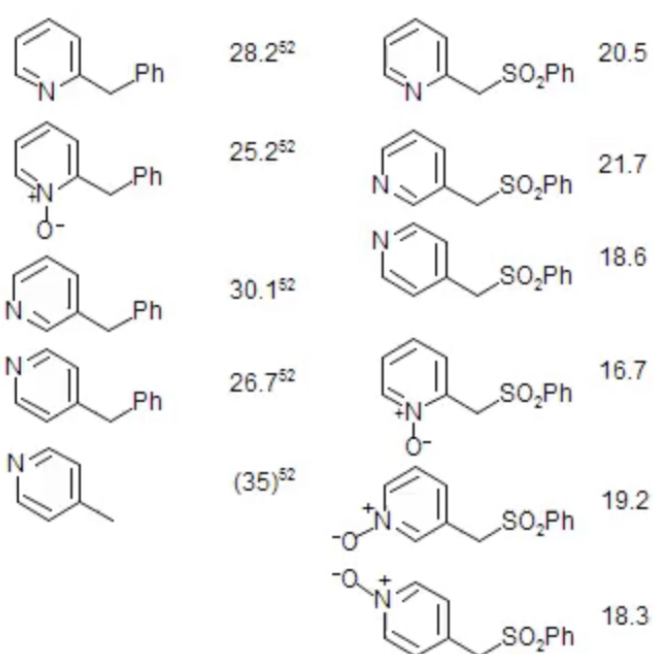
	21.6
	21.1
	14.9

Hydrazine (NH)

Ph-NHNH-Ph	26.2 ⁵⁶
Ph-NHNH ₂	28.8 ⁵⁶
Ph-NHNPh ₂	24.5 ⁵⁶
2,4-(NO ₂) ₂ PhNHNPh ₂	12.1 ⁵⁶
4-CF ₃ PhNHNH ₂	25.7 ⁵⁶
4-NC-PhNHNH ₂	25.1 ⁵⁶

Sulfonamide (NH)

Me-SO ₂ -NH ₂	17.5 ³⁹
CF ₃ -SO ₂ -NH ₂	9.7 ³⁹
Ph-SO ₂ -NH ₂	16.1 ²⁷
Ph-SO ₂ -NHOH	15.4 ⁵⁷
Me-SO ₂ -NHPh	12.9
Ph-SO ₂ -NHNH ₂	17.1 ²⁷
Ph-SO ₂ -NHNMe ₂	15.8 ⁵⁷
	24.3

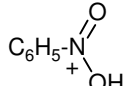
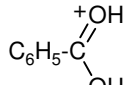
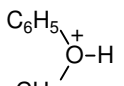
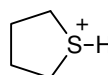
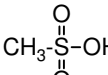


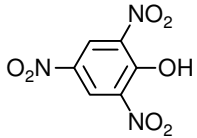
Amidine (NH)**Guanidine (NH)****Ureas (NH)****Pyridyl****Equilibrium pKa Table (DMSO Solvent and Reference)****References (Bordwell et al.)**

- J. Am. Chem. Soc.* **1975**, 97, 7006.
 - J. Am. Chem. Soc.* **1975**, 97, 7160.
 - J. Am. Chem. Soc.* **1975**, 97, 442.
 - J. Am. Chem. Soc.* **1967**, 89, 2752.
 - J. Org. Chem.* **1976**, 41, 1885.
 - J. Org. Chem.* **1976**, 41, 1883.
 - J. Org. Chem.* **1976**, 41, 2786.
 - J. Org. Chem.* **1976**, 41, 2508.
 - J. Org. Chem.* **1977**, 42, 321.
 - J. Org. Chem.* **1977**, 42, 326.
 - J. Org. Chem.* **1977**, 42, 1817.
 - J. Org. Chem.* **1978**, 43, 3113.
 - J. Org. Chem.* **1978**, 43, 3095.
 - J. Org. Chem.* **1978**, 43, 1764.
 - J. Org. Chem.* **1980**, 45, 3884.
 - J. Org. Chem.* **1980**, 45, 3305.
 - J. Org. Chem.* **1980**, 45, 3325.
 - J. Org. Chem.* **1981**, 46, 4327.
 - J. Org. Chem.* **1981**, 46, 632.
 - J. Org. Chem.* **1982**, 47, 3224.
 - J. Org. Chem.* **1982**, 47, 2504.
 - J. Am. Chem. Soc.* **1983**, 105, 6188.
 - J. Am. Chem. Soc.* **1986**, 108, 7310.
 - J. Org. Chem.* **1980**, 45, 3295.
 - J. Org. Chem.* **1984**, 49, 1424.
 - J. Am. Chem. Soc.* **1995**, 117, 602.
 - J. Org. Chem.* **1995**, 55, 3330.
 - J. Am. Chem. Soc.* **1996**, 118, 8777.
 - J. Org. Chem.* **1996**, 61, 4103.
 - J. Am. Chem. Soc.* **1991**, 113, 985.
 - J. Org. Chem.* **1992**, 57, 3019.
 - J. Org. Chem.* **1998**, 63, 7574.
 - J. Am. Chem. Soc.* **1994**, 116, 968.
 - J. Am. Chem. Soc.* **1989**, 111, 7558.
 - J. Am. Chem. Soc.* **1992**, 114, 7623.
 - J. Am. Chem. Soc.* **1994**, 116, 973.
 - J. Org. Chem.* **1988**, 53, 780.
 - J. Am. Chem. Soc.* **1988**, 110, 8520.
 - J. Org. Chem.* **1976**, 41, 2507.
 - J. Am. Chem. Soc.* **1990**, 112, 792.
 - J. Am. Chem. Soc.* **1991**, 113, 8398.
 - J. Org. Chem.* **1980**, 45, 3299.
 - Arnett *J. Am. Chem. Soc.* **1984**, 106, 6759.
 - J. Org. Chem.* **1993**, 58, 3061.
 - Benoit *Can. J. Chem.* **1987**, 65, 996.
 - Kreevoy *J. Phys. Chem.* **1977**, 81, 1924.
 - Kolthoff *J. Am. Chem. Soc.* **1968**, 90, 23.
 - Bausch *J. Org. Chem.* **1990**, 55, 5806.
 - Alder *Chem. Commun.* **1995**, 1267.
 - J. Org. Chem.* **1978**, 43, 1763.
 - J. Org. Chem.* **1991**, 56, 4218.
 - Acc. Chem. Res.* **1988**, 21, 456, 463.
 - J. Org. Chem.* **1991**, 56, 4448.
 - J. Am. Chem. Soc.* **1988**, 110, 2964.
 - J. Am. Chem. Soc.* **1974**, 76, 1214.
 - J. Am. Chem. Soc.* **1997**, 119, 9125.
 - J. Org. Chem.* **1990**, 55, 3337.
 - Can. J. Chem.* **1990**, 68, 1714.
 - Arnett *J. Am. Chem. Soc.* **19874**, 109, 809.
 - J. Phys. Org. Chem.* **1988**, 1, 209.
 - Terrier *J. Org. Chem.* **2003**, 68, 6566.
 - Courtet-Coupez *Bull. Soc. Chim. Fr.* **1969**, 1033.
 - Curtis *J. Am. Chem. Soc.* **1969**, 91, 6011.
 - Crampton *J. Chem. Res. (S)* **1997**, 22.
- All others are F. G. Bordwell, private communication. For a review, see: F. G. Bordwell *Acc. Chem. Res.* **1988**, 21, 456, 463.

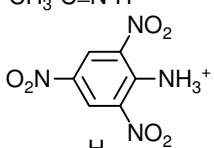
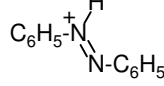
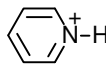
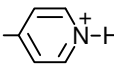
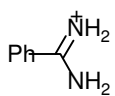
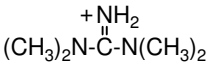
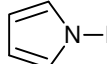
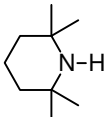
Equilibrium pKa Table (H₂O Solvent and Reference)

Values outside the boxes were determined by approximate methods.

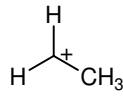
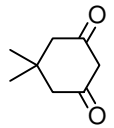
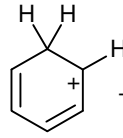
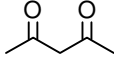
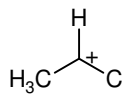
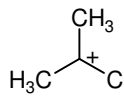
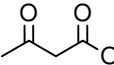
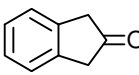
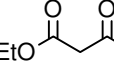

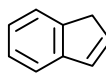


Oxygen Acids

CF ₃ SO ₃ H	
	-12.4
	-7.8
	-6.5
(CH ₃) ₂ S ⁺ -H	-5.4
	-4.4
(CH ₃) ₂ O ⁺ -H	-3.8
	-2.6
CH ₃ -OH ₂ ⁺	-2.2
	-2.1
(CH ₃) ₂ S=OH ⁺	-1.8
	-1.4
CF ₃ -CO ₂ H	-0.3
	0.3
(CH ₃) ₂ Se=OH ⁺	2.6
C ₆ H ₅ -CO ₂ H	4.2
CH ₃ CO ₂ H	4.8
HOCO ₂ H	6.3
C ₆ H ₅ -SH	6.5
CH ₂ =C(Ph)OH	8.0 ²
C ₆ H ₅ -OH	10.0
HCO ₃ ⁻	10.3
RS-H	10.5
CH ₂ =CHOH	10.5
CH ₂ =C(CH ₃)OH	10.9
HOOH	11.7
H ₂ O	14.0 ¹⁰
CH ₃ -OH	16
(CH ₃) ₃ C-OH	20

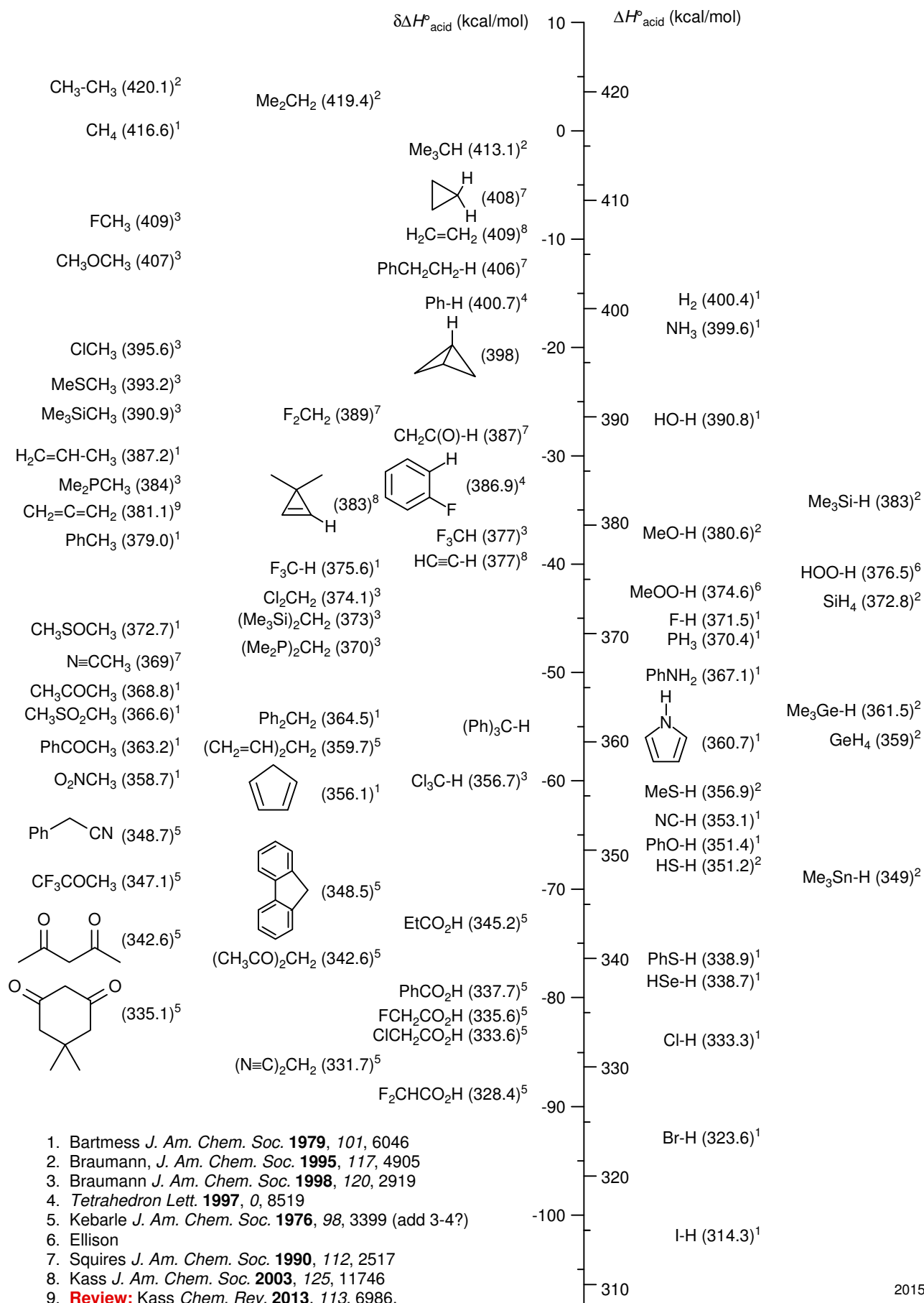
Nitrogen Acids

P ⁺ H ₄	-14.
C ₆ H ₅ -C≡N ⁺ -H	-10.5
CH ₃ -C≡N ⁺ -H	-10.
	-9.3
	-2.9
(C ₆ H ₅) ₂ NH ⁺	0.8
CH ₃ -P ⁺ H ₃	2.7
C ₆ H ₅ -NH ⁺ ₃	4.6
	5.2
N≡C-CH ₂ CH ₂ -NH ⁺ ₃	7.9
(CH ₃ CH ₂) ₃ P ⁺ -H	9.1
H ₂ N- 	9.2
NH ₄ ⁺	9.2
N≡N ⁺ -H	10.0
CH ₃ CH ₂ NH ⁺ ₃	10.6
(CH ₃ CH ₂) ₂ NH ⁺ ₂	11.0
(CH ₃ CH ₂) ₃ NH ⁺	10.8
O=N-H	11.5
	11.2 ⁴
	13.6
	15.
C ₆ H ₅ -NH ₂	28.
((CH ₃) ₃ Si) ₂ N-H	30.
(i-C ₃ H ₇) ₂ N-H	36.
	37.
Halogen Acids	
H-I	-5.2
H-Br	-4.7
H-Cl	-2.2
H-F	3.2

Carbon Acids

(O ₂ N) ₂ CH ₂	3.6		-24.8
	5.2		-24.3
	9.0 ³		-18.5
N≡C-H	9.1		-12.5
CH ₃ N ⁺ ≡N	10.0 ¹		
O ₂ N-CH ₃	10.2		
	10.7		
(CF ₃) ₃ CH	11.		
(NC) ₂ CH ₂	11.2		
	12.2 ⁶		
	12.9		
	15.		
CH ₃ -C(=O)-H	16.7		
CH ₃ -C(=O)-Ph	18.3		
CH ₃ -C(=O)-CH ₃	19.3		
	20		
C ₆ H ₅ -CH ₂ -C≡N	21		
C ₆ H ₅ -C≡C-H	23		
CH ₃ CO ₂ Et	24		
H-C≡C-H	24		
CH ₃ -C≡N	25		
	29		
CF ₃ -H	32		
CH ₃ -S(=O) ₂ -CH ₃	33		
(C ₆ H ₅) ₃ C-H	32		
CH ₃ -S(=O)-CH ₃	33		
C ₆ H ₅ -CH ₃	41		
	44		
CH ₃ CH ₃	50		

Gas Phase Acidities



1. Bartmess *J. Am. Chem. Soc.* **1979**, *101*, 6046
2. Braumann, *J. Am. Chem. Soc.* **1995**, *117*, 4905
3. Braumann *J. Am. Chem. Soc.* **1998**, *120*, 2919
4. *Tetrahedron Lett.* **1997**, *0*, 8519
5. Kebarle *J. Am. Chem. Soc.* **1976**, *98*, 3399 (add 3-4?)
6. Ellison
7. Squires *J. Am. Chem. Soc.* **1990**, *112*, 2517
8. Kass *J. Am. Chem. Soc.* **2003**, *125*, 11746
9. **Review:** Kass *Chem. Rev.* **2013**, *113*, 6986.
10. Meister *Helv. Chim. Acta* **2014**, *97*, 1.