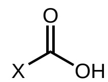
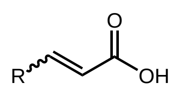
INORGANIC ACIDS

Substrate	pKa H_2O	(DMSO)
H_2O	15.7	(32)
H_3O^+	-1.7	
H_2S	7.00	
HBr	-9.00	(0.9)
HCl	-8.0	(1.8)
HF	3.17	(15)
HOCl	7.5	
$HClO_4$	-10	
HCN	9.4	(12.9)
HN_3	4.72	(7.9)
HSCN	4.00	
H_2SO_3	1.9, 7.21	
H_2SO_4	-3.0, 1.99	
H_3PO_4	2.12, 7.21, 12.32	
HNO_3	-1.3	
HNO_2	3.29	
H_2CrO_4	-0.98, 6.50	
CH_3SO_3H	-2.6	(1.6)
CF_3SO_3H	-14	(0.3)
NH_4Cl	9.24	
$B(OH)_3$	9.23	
HOOH	11.6	

CARBOXYLIC ACIDS



Substrate	pKa H_2O	(DMSO)
X= CH_3	4.76	(12.3)
CH_2NO_2	1.68	
CH_2F	2.66	
CH_2Cl	2.86	
CH_2Br	2.86	
CH_2I	3.12	
$CHCl_2$	1.29	
CCl_3	0.65	
CF_3	-0.25	
H	3.77	
HO	3.6, 10.3	
C_6H_5	4.2	(11.1)
o-$O_2NC_6H_4$	2.17	
m-$O_2NC_6H_4$	2.45	
p-$O_2NC_6H_4$	3.44	
o-ClC_6H_4	2.94	
m-ClC_6H_4	3.83	
p-ClC_6H_4	3.99	
o-$(CH_3)_3N^+C_6H_4$	1.37	
p-$(CH_3)_3N^+C_6H_4$	3.43	
p-$OMeC_6H_4$	4.47	

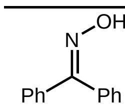
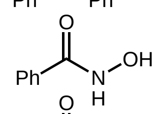
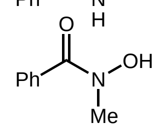


Substrate	pKa H_2O	(DMSO)
R= H	4.25	
trans-CO_2H	3.02, 4.38	
cis-CO_2H	1.92, 6.23	

ALCOHOLS

Substrate	pKa H_2O	(DMSO)
HOH	15.7	(31.2)
MeOH	15.54	(27.9)
i-PrOH	16.5	(29.3)
t-BuOH	17	(29.4)
c-hex_3COH	24	
CF_3CH_2OH	12.5	(23.5)
$(CF_3)_2CHOH$		(17.9)
C_6H_5OH	9.95	(18.0)
m-$O_2NC_6H_4OH$	8.35	
p-$O_2NC_6H_4OH$	7.14	(10.8)
p-$OMeC_6H_4OH$	10.20	(19.1)
2-napthol		(17.1)

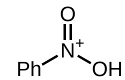
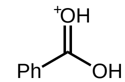
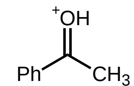
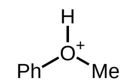
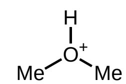
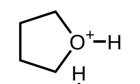
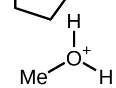
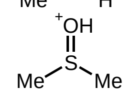
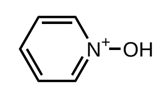
OXIMES & HYDROXAMIC ACIDS

Substrate	pKa H_2O	(DMSO)
	11.3	(20.1)
	8.88 (NH)	(13.7)
		(18.5)

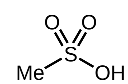
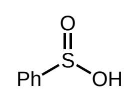
PEROXIDES

Substrate	pKa H_2O	(DMSO)
MeOOH	11.5	
CH_3CO_3H	8.2	

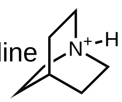
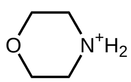
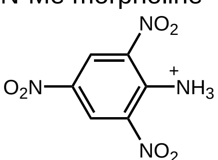
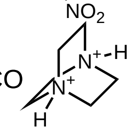
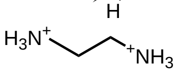
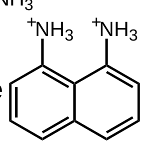
PROTONATED SPECIES

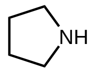
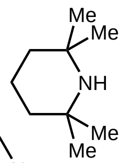
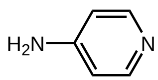
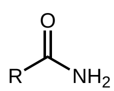
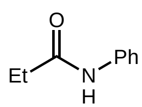
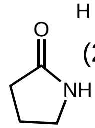
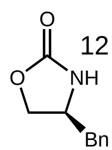
Substrate	pKa H_2O	(DMSO)
	-12.4	
	-7.8	
	-6.2	
	-6.5	
	-3.8	
	-2.05	
	-2.2	
	-1.8	
	0.79	

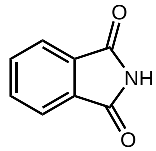
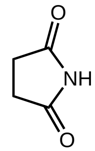
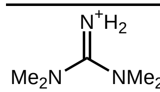
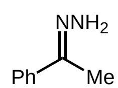
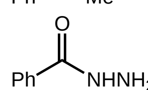
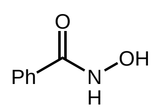
SULFINIC & SULFONIC ACIDS

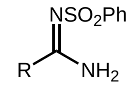
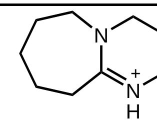
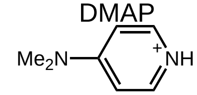
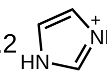
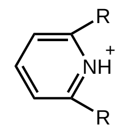
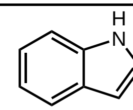
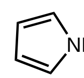
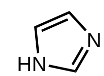
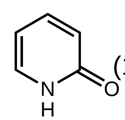
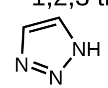
Substrate	pKa H_2O	(DMSO)
	-2.6	
	2.1	

*Values <0 for H_2O and DMSO, and values >14 for water and >35 for DMSO were extrapolated using various methods.

Substrate	pKa H_2O	(DMSO)
PROTONATED NITROGEN		
N^+H_4	9.2	(10.5)
EtN^+H_3	10.6	
i-$Pr_2N^+H_2$	11.05	
Et_3N^+H	10.75	(9.00)
PhN^+H_3	4.6	(3.6)
$PhN^+(Me)_2H$	5.20	(2.50)
$Ph_2N^+H_2$	0.78	
2-napthal-N^+H_3	4.16	
$H_2NN^+H_3$	8.12	
HON^+H_3	5.96	
Quinuclidine 	11.0	(9.80)
Morpholine 	8.36	
N-Me morpholine	7.38	
	-9.3	
DABCO 	2.97, 8.82	(2.97, 8.93)
	6.90, 9.95	
Proton Sponge 	-9.0, 12.0	(--, 7.50)
$PhCN^+H$	-10	

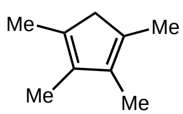
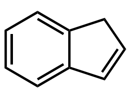
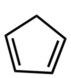
Substrate	pKa H_2O	(DMSO)
AMINES		
HN_3	4.7	(7.9)
NH_3	38	(41)
i-Pr_2NH	(36 THF))	
TMS_2NH	26(THF)	(30)
$PhNH_2$		(30.6)
Ph_2NH		(25.0)
$NCNH_2$		(16.9)
		(44)
TMP 		(37)
		(26.5)
AMIDES & CARBAMATES		
		
R= H		(23.5)
CH_3	15.1	(25.5)
Ph		(23.3)
CF_3		(17.2)
NH_2 (urea)		(26.9)
OEt		(24.8)
		(21.6)
		(24.1)
	12	(20.5)

Substrate	pKa H_2O	(DMSO)
IMIDES		
	8.30	
		(14.7)
Ac_2NH		(17.9)
SULFONAMIDE		
$MeSO_2NH_2$		(17.5)
$PhSO_2NH_2$		(16.1)
$CF_3SO_2NH_2$	6.3	(9.7)
$MeSO_2NHPh$		(12.9)
GUANIDINIUM, HYRDAZONES,- IDES, & -INES		
		(13.6)
		(21.6)
		(18.9)
$PhSO_2NHNH_2$		(17.2)
PhNHNHPh		(26.1)
HYDROXAMIC ACID		
	8.88 (NH)	(13.7)

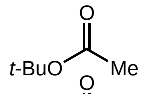
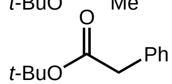
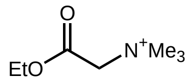
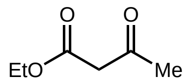
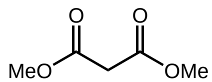
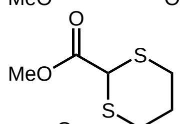
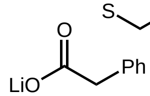
Substrate	pKa H_2O	(DMSO)
AMIDINES		
		
R= Me		(17.3)
Ph		(15.0)
PROTONATED HETEROCYCLES		
DBU 	(12) (estimate)	
DMAP 	9.2	
	6.95	
		
R= H (PPTS)	5.21	(3.4)
t-Bu	4.95	(0.90)
Me	6.75	(4.46)
Cl, H	0.72	
HETEROCYCLES		
		(20.95)
		(23.0)
		(18.6)
		(17.0)
1,2,3 triazole 		(13.9)

*Values <0 for H_2O and DMSO, and values >14 for water and >35 for DMSO were extrapolated using various methods.

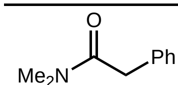
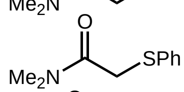
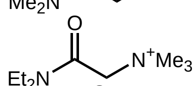
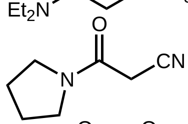
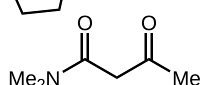
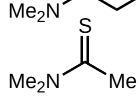
HYDROCARBONS

Substrate	pKa H_2O	(DMSO)
$(Me)_3CH$	53	
$(Me)_2CH_2$	51	
$CH_2=CH_2$	50	
CH_4	48	(56)
	46	
$CH_2=CHCH_3$	43	(44)
PhH	43	
$PhCH_3$	41	(43)
Ph_2CH_2	33.5	(32.2)
Ph_3CH	31.5	(30.6)
HCCH	24	
PhCCH	23	(28.8)
$XC_6H_4CH_3$		
X= *p*-CN		(30.8)
p-NO_2		(20.4)
p-COPh		(26.9)
		(26.1)
	20	(20.1)
	15	(18.0)
H_2	~36	

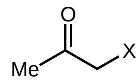
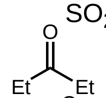
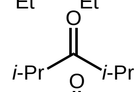
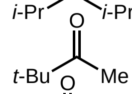
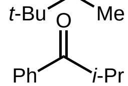
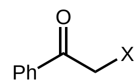
ESTERS

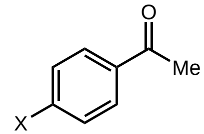
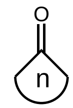
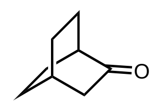
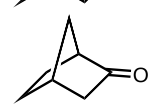
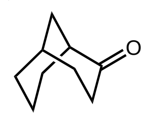
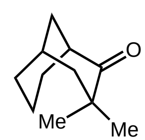
Substrate	pKa H_2O	(DMSO)
	24.5	(30.3)
		(23.6)
		(20.0)
	11	(14.2)
	13	(15.7)
		(20.9)
		[30.2 (THF)]

AMIDES

Substrate	pKa H_2O	(DMSO)
		(26.6)
		(25.9)
		(24.9)
		(17.2)
		(18.2)
		(25.7)

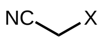
KETONES

Substrate	pKa H_2O	(DMSO)
		
X= H		(26.5)
Ph		(19.8)
SPh		(18.7)
$COCH_3$	9	(13.3)
SO_2Ph		(15.1)
	19-20	(27.1)
		(28.3)
		(27.7)
		(26.3)
		
X= H		(24.7)
CH_3		(24.4)
Ph		(17.7)
$COCH_3$		(12.7)
COPh		(13.3)
CO_2Et		(22.7)
CN		(10.2)
F		(21.6)
OMe		(22.85)
OPh		(21.1)
SPh		(16.9)
SePh		(18.6)
NPh_2		(20.3)
N^+Me_3		(14.6)
NO_2		(7.7)
SO_2Ph		(11.4)

Substrate	pKa H_2O	(DMSO)
		
X= H		(24.7)
OMe		(25.7)
NMe_2		(27.5)
Br		(23.8)
CN		(22.0)
		
n= 4		(25.1)
5		(25.8)
6		(26.4)
7		(27.7)
8		(27.4)
		(28.1)
		(29.0)
		(25.5)
		(32.4)

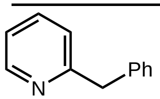
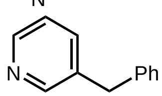
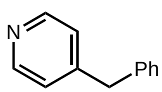
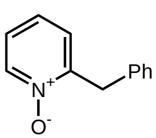
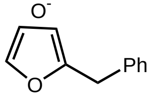
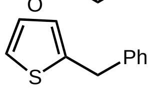
*Values <0 for H_2O and DMSO, and values >14 for water and >35 for DMSO were extrapolated using various methods.

NITRILES

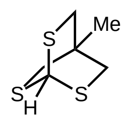
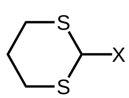


Substrate	pKa H_2O	(DMSO)
X= H		(31.3)
CH_3		(32.5)
Ph		(21.9)
COPh		(10.2)
$CONR_2$		(17.1)
CO_2Et		(13.1)
CN	11	(11.1)
OPh		(28.1)
N^+Me_3		(20.6)
SPh		(20.8)
SO_2Ph		(12.0)

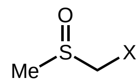
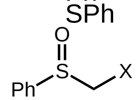
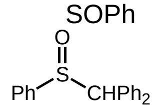
HETERO-AROMATICS

Substrate	pKa H_2O	(DMSO)
		(28.2)
		(30.1)
		(26.7)
		(25.2)
		(30.2)
		(30.0)

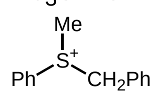
SULFIDES

Substrate	pKa H_2O	(DMSO)
$PhSCH_2X$		
X= Ph		(30.8)
CN		(20.8)
$COCH_3$		(18.7)
COPh		(16.9)
NO_2		(11.8)
SPh		(30.8)
SO_2Ph		(20.3)
SO_2CF_3		(11.0)
$POPh_2$		(24.9)
$MeSCH_2SO_2Ph$		(23.4)
$PhSCHPh_2$		(26.7)
$(PhS)_3CH$		(22.8)
$(PrS)_3CH$		(31.3)
		(30.5)
$(PhS)_2CHPh$		(23.0)
		
X= Ph		(30.7)
CO_2Me		(20.8)
CN		(19.1)
$RSCH_2CN$		
R= Me		(24.3)
Et		(24.0)
i-Pr		(23.6)
t-Bu		(22.9)
$PhSCH=CHCH_2SPh$		(26.3)
BuSH	10-11	(17.0)
PhSH	≈7	(10.3)

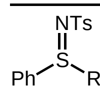
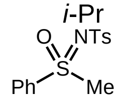
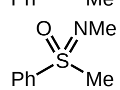
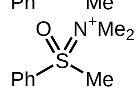
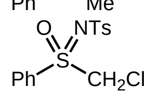
SULFOXIDES

Substrate	pKa H_2O	(DMSO)
		
X= H		(35.1)
Ph		(29.0)
SPh		(29.0)
		
X= H		(33)
Ph		(27.2)
SOPh		(18.2)
		(24.5)

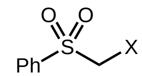
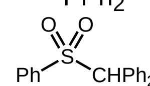
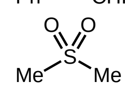
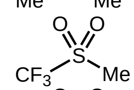
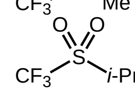
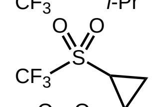
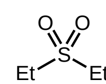
SULFONIUM

Substrate	pKa H_2O	(DMSO)
$Me_3S^+=O$		(18.2)
		(16.3)

SULFIMIDES & SULFOXIMINES

Substrate	pKa H_2O	(DMSO)
		
R= Me		(27.6)
i-Pr		(30.7)
		(24.5)
		(33)
		(14.4)
		(20.7)

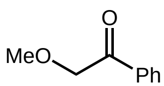
SULFONES

Substrate	pKa H_2O	(DMSO)
		
X= H		(29.0)
CH_3		(31.0)
t-Bu		(31.2)
Ph		(23.4)
$CH=CH_2$		(22.5)
CH=CHPh		(20.2)
CCH		(22.1)
CCPh		(17.8)
COPh		(11.4)
COMe		(12.5)
OPh		(27.9)
N^+Me_3		(19.4)
CN		(12.0)
NO_2		(7.1)
SMe		(23.5)
SPh		(20.5)
SO_2Ph		(12.2)
PPh_2		(20.2)
		(22.3)
		(31.1)
		(18.8)
		(21.8)
		(26.6)
		(32.8)
$(PhSO_2)_2CH_2Me$		(14.3)

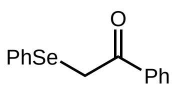
*Values <0 for H_2O and DMSO, and values >14 for water and >35 for DMSO were extrapolated using various methods.

pKa's of CH bonds at Heteroatom Substituted Carbon & References

ETHERS

Substrate	pKa H_2O	(DMSO)
CH_3OPh		(49)
$MeOCH_2SO_2Ph$		(30.7)
$PhOCH_2SO_2Ph$		(27.9)
$PhOCH_2CN$		(28.1)
		(21.1)

SELENIDES

Substrate	pKa H_2O	(DMSO)
		(18.6)
$PhSeCHPh_2$		(27.5)
$(PhSe)_2CH_2$		(31.3)
$PhSeCH_2Ph$		(31.0)
$PhSeCH=CHCH_2SePh$		(27.2)

AMMONIUM

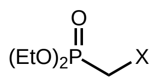
$Me_3N^+CH_2X$

Substrate	pKa H_2O	(DMSO)
X= CN		(20.6)
SO_2Ph		(19.4)
COPh		(14.6)
CO_2Et		(20.6)
$CONEt_2$		(24.9)

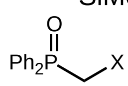
PHOSPHONIUM

Substrate	pKa H_2O	(DMSO)
P^+H_4	-14	
MeP^+H_3	2.7	
Et_3P^+H	9.1	
$Ph_3P^+CH_3$		(22.4)
Ph_3P^+*i*-Pr		(21.2)
$Ph_3P^+CH_2COPh$		(6.2)
$Ph_3P^+CH_2CN$		(7.0)

PHOSPONATES & PHOSPHINE OXIDES



Substrate	pKa H_2O	(DMSO)
X= Ph		(27.6)
CN		(16.4)
CO_2Et		(18.6)
Cl		(26.2)
$SiMe_3$		(28.8)



Substrate	pKa H_2O	(DMSO)
X= SPh		(24.9)
CN		(16.9)

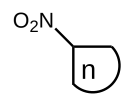
PHOSPHINES

Substrate	pKa H_2O	(DMSO)
$Ph_2PCH_2PPh_2$		(29.9)
$Ph_2PCH_2SO_2Ph$		(20.3)

NITRO

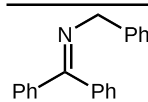
RNO_2

Substrate	pKa H_2O	(DMSO)
R= CH_3	≈10	(17.2)
CH_2Me		(16.7)
$CHMe_2$		(16.9)
CH_2Ph		(12.2)
CH_2Bn		(16.2)
CH_2SPh		(11.8)
CH_2SO_2Ph		(7.1)
CH_2COPh		(7.7)



Substrate	pKa H_2O	(DMSO)
n= 3		(26.9)
4		(17.8)
5		(16.0)
6		(17.9)
7		(15.8)

IMINES

Substrate	pKa H_2O	(DMSO)
		(24.3)

Oxime ethers are ~ 10 pka units less acidic than their ketone counterparts Streitwieser, JOC 1991, 56, 1989

REFERENCES

DMSO:

JACS 97, 7007 (1975)
JACS 97, 7160 (1975)
JACS 97, 442 (1975)
JACS 105, 6188 (1983)
JOC 41, 1883 (1976)
JOC 41, 1885 (1976)
JOC 41, 2786 (1976)
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*Values <0 for H_2O and DMSO, and values >14 for water and >35 for DMSO were extrapolated using various methods.