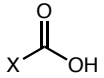
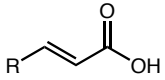
INORGANIC ACIDS

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	

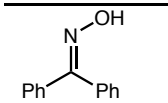


R= H	4.25	
trans-CO_2H	3.02, 4.38	
cis-CO_2H	1.92, 6.23	

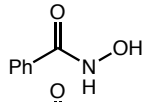
ALCOHOLS

HOH	15.7	(31.2)
MeOH	15.5	(27.9)
i-PrOH	16.5	(29.3)
t-BuOH	17.0	(29.4)
c-hex_3COH	24.0	
CF_3CH_2OH	12.5	(23.5)
$(CF_3)_2CHOH$	9.3	(18.2)
C_6H_5OH	9.95	(18.0)
m-$O_2NC_6H_4OH$	8.4	
p-$O_2NC_6H_4OH$	7.1	(10.8)
p-$OMeC_6H_4OH$	10.2	(19.1)
2-napthol		(17.1)

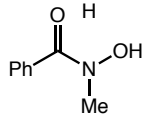
OXIMES & HYDROXAMIC ACIDS



11.3	(20.1)



8.88 (NH)	(13.7)

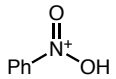


	(18.5)

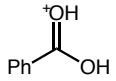
PEROXIDES

MeOOH	11.5
CH_3CO_3H	8.2

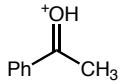
PROTONATED SPECIES



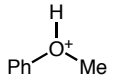
-12.4



-7.8



-6.2



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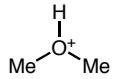
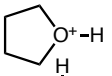
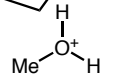


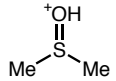
-3.8



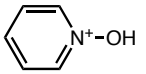
-2.05



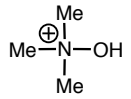
-2.2



-1.8

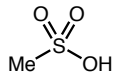


0.79	(+1.63)

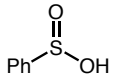


	(+5.55)

SULFINIC & SULFONIC ACIDS



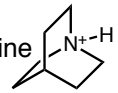
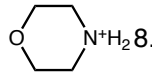
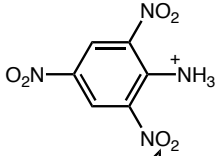
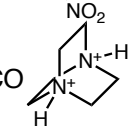
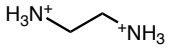
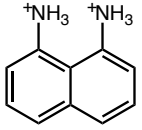
-2.6

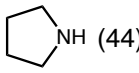
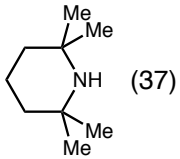
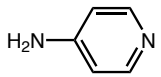
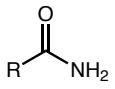
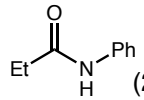
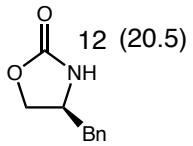
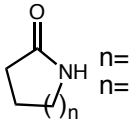
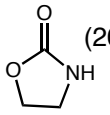
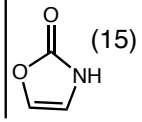
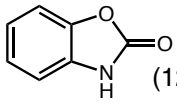


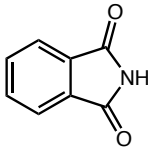
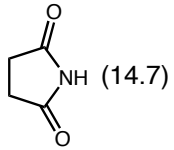
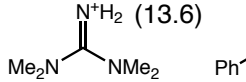
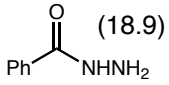
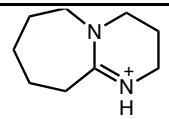
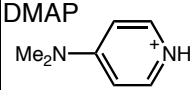
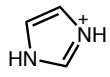
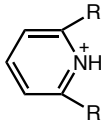
2.1

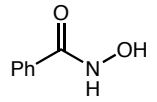
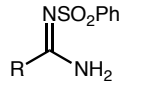
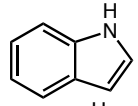
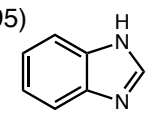
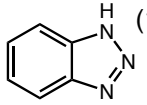
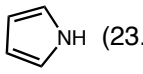
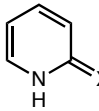
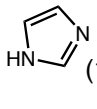
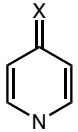
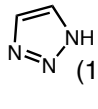
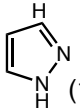
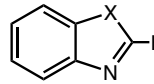
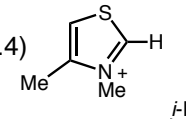
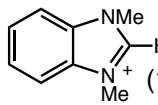
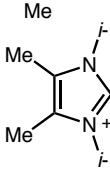
*Values <0 for H_2O and DMSO, and values >14 for water and >35 for DMSO were extrapolated using various methods.

For a comprehensive compilation of Bordwell pKa data see: **http://www.chem.wisc.edu/areas/reich/pkatable/index.htm**

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	

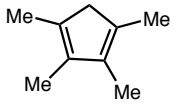
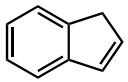
Substrate	pKa H_2O	(DMSO)
AMINES		
HN_3	4.7	(7.9)
NH_3	38	(41)
i-Pr_2NH	(36 THF))	
TMS_2NH	26(THF)	(30)
$PhNH_2$ (30.6)		
Ph_2NH (25.0)		
$NCNH_2$ (16.9)		
	(44)	
	(37)	
	(26.5)	
AMIDES & CARBAMATES		
	R= H	(23.5)
	CH_3 15.1	(25.5)
	Ph	(23.3)
	CF_3	(17.2)
	(urea) NH_2	(26.9)
	OEt	(24.8)
	(21.6)	
	12 (20.5)	
	n= 1 (24.1) n= 2 (26.4)	
	(20.8)	
	(15)	
	(12.1)	

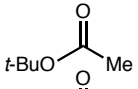
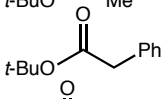
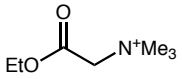
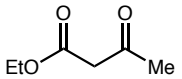
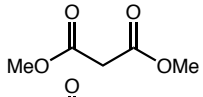
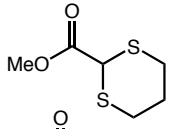
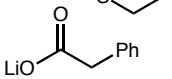
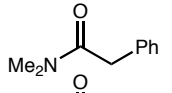
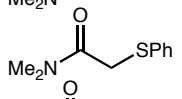
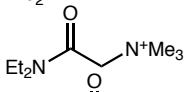
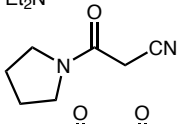
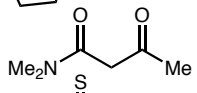
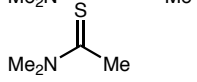
Substrate	pKa H_2O	(DMSO)
IMIDES		
	8.30	
		(14.7)
Ac_2NH		(17.9)
SULFONAMIDE		
RSO_2NH_2	R = Me	(17.5)
	Ph	(16.1)
	CF_3 6.3	(9.7)
$MeSO_2NHPh$		(12.9)
GUANIDINIUM, HYRDAZONES,- IDES, & -INES		
	N^+H_2 (13.6)	NNH_2 (21.6)
	(18.9)	
$PhSO_2NHNH_2$		(17.2)
PhNHNHPh		(26.1)
PROTONATED HETEROCYCLES		
DBU 	(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

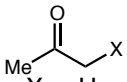
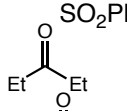
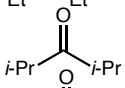
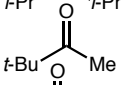
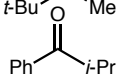
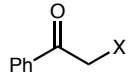
Substrate	pKa H_2O	(DMSO)
HYDROXAMIC ACID & AMIDINES		
	8.88 (NH)	(13.7)
	R= Me	(17.3)
	Ph	(15.0)
HETEROCYCLES		
	(20.95)	
	(16.4)	
	(11.9)	
	(23.0)	
	X= O (24) X= S (13.3)	
	(18.6)	
	X= O (14.8) X= S (11.8)	
	(13.9)	
	(19.8)	
	X= O (24.4) X= S (27.0)	
	(29.4)	
	(16.5)	
	(18.4)	
	(24)	

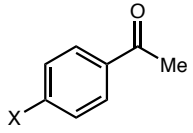
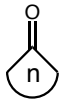
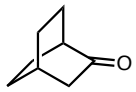
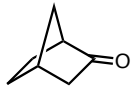
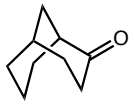
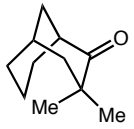
*Values <0 for H_2O and DMSO, and values >14 for water and >35 for DMSO were extrapolated using various methods.

For a comprehensive compilation of Bordwell pKa data see: **http://www.chem.wisc.edu/areas/reich/pkatable/index.htm**

Substrate	pKa H_2O	(DMSO)
HYDROCARBONS		
$(Me)_3CH$	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	

Substrate	pKa H_2O	(DMSO)
ESTERS		
	24.5	(30.3)
		(23.6)
		(20.0)
	11	(14.2)
	13	(15.7)
		(20.9)
		[30.2 (THF)]
AMIDES		
		(26.6)
		(25.9)
		(24.9)
		(17.2)
		(18.2)
		(25.7)

Substrate	pKa H_2O	(DMSO)
KETONES		
		
X= H		(26.5)
Ph		(19.8)
SPh		(18.7)
$COCH_3$	9	(13.3)
SO_2Ph		(12.5)
	19-20	(27.1)
		(28.3)
		(27.7)
		(26.3)
		
X= H		(24.7)
CH_3		(24.4)
Ph		(17.7)
$COCH_3$		(14.2)
COPh		(13.3)
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)

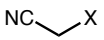
Substrate	pKa H_2O	(DMSO)
		
X= H		(24.7)
OMe		(25.7)
NMe_2		(27.5)
Br		(23.8)
CN		(22.0)
		
n= 4		(25.1)
5		(25.8)
6		(26.4)
7		(27.7)
8		(27.4)
		(28.1)
		(29.0)
		(25.5)
		(32.4)

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

For a comprehensive compilation of Bordwell pKa data see: **http://www.chem.wisc.edu/areas/reich/pkatable/index.htm**

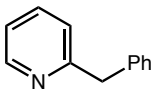
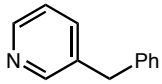
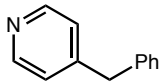
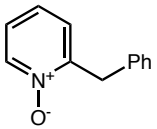
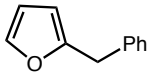
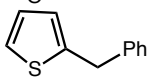
pKa's of CH bonds at Nitrile, Heteroaromatic, and Sulfur Substituted Carbon

NITRILES



X=	Substrate	pKa H_2O	(DMSO)
	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)

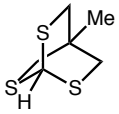
HETERO-AROMATICS

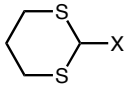
Substrate	pKa H_2O	(DMSO)
		(28.2)
		(30.1)
		(26.7)
		(25.2)
		(30.2)
		(30.0)

SULFIDES

$PhSCH_2X$

X=	Substrate	pKa H_2O	(DMSO)
	Ph		(30.8)
	CN		(20.8)
	$COCH_3$		(18.7)
	COPh		(16.9)
	NO_2		(11.8)
	SPh		(30.8)
	SO_2Ph		(20.5)
	SO_2CF_3		(11.0)
	$POPh_2$		(24.9)

Substrate	pKa H_2O	(DMSO)
$MeSCH_2SO_2Ph$		(23.4)
$PhSCHPh_2$		(26.7)
$(PhS)_3CH$		(22.8)
$(PrS)_3CH$		(31.3)
		(30.5)
$(PhS)_2CHPh$		(23.0)



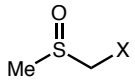
X=	Substrate	pKa H_2O	(DMSO)
	Ph		(30.7)
	CO_2Me		(20.8)
	CN		(19.1)

Substrate	pKa H_2O	(DMSO)
$RSCH_2CN$		

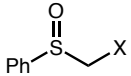
R=	Substrate	pKa H_2O	(DMSO)
	Me		(24.3)
	Et		(24.0)
	i-Pr		(23.6)
	t-Bu		(22.9)

Substrate	pKa H_2O	(DMSO)
$PhSCH=CHCH_2SPh$		(26.3)
BuSH	10-11	(17.0)
PhSH	≈7	(10.3)

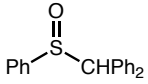
SULFOXIDES



X=	Substrate	pKa H_2O	(DMSO)
	H		(35.1)
	Ph		(29.0)
	SPh		(29.0)

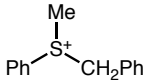


X=	Substrate	pKa H_2O	(DMSO)
	H		(33)
	Ph		(27.2)
	SOPh		(18.2)

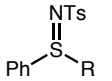


Substrate	pKa H_2O	(DMSO)
$Ph(CHPh_2)SO$		(24.5)

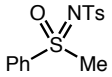
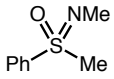
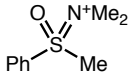
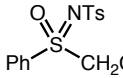
SULFONIUM

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

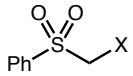
SULFIMIDES & SULFOXIMINES



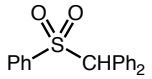
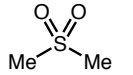
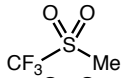
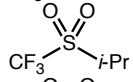
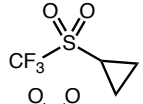
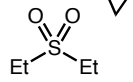
R=	Substrate	pKa H_2O	(DMSO)
	Me		(27.6)
	i-Pr		(30.7)

Substrate	pKa H_2O	(DMSO)
		(24.5)
		(33)
		(14.4)
		(20.7)

SULFONES

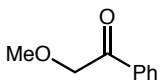
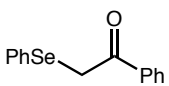


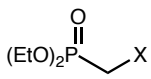
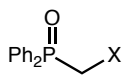
X=	Substrate	pKa H_2O	(DMSO)
	H		(29.0)
	CH_3		(31.0)
	t-Bu		(31.2)
	Ph		(23.4)
	$CH=CH_2$		(22.5)
	CH=CHPh		(20.2)
	CCH		(22.1)
	CCPh		(17.8)
	COPh		(11.4)
	COMe		(12.5)
	OPh		(27.9)
	N^+Me_3		(19.4)
	CN		(12.0)
	NO_2		(7.1)
	SMe		(23.5)
	SPh		(20.5)
	SO_2Ph		(12.2)
	PPh_2		(20.2)

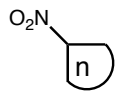
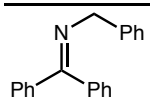
Substrate	pKa H_2O	(DMSO)
		(22.3)
		(31.1)
		(18.8)
		(21.8)
		(26.6)
		(32.8)
$(PhSO_2)_2CH_2Me$		(14.3)

*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

Substrate	pKa H_2O	(DMSO)
ETHERS		
CH_3OPh		(49)
$MeOCH_2SO_2Ph$		(30.7)
$PhOCH_2SO_2Ph$		(27.9)
$PhOCH_2CN$		(28.1)
		(22.85)
SELENIDES		
		(18.6)
$PhSeCHPh_2$		(27.5)
$(PhSe)_2CH_2$		(31.3)
$PhSeCH_2Ph$		(31.0)
$PhSeCH{=}CHCH_2SePh$		(27.2)
AMMONIUM		
$Me_3N^+CH_2X$		
X= CN		(20.6)
SO_2Ph		(19.4)
COPh		(14.6)
CO_2Et		(20.0)
$CONEt_2$		(24.9)

Substrate	pKa H_2O	(DMSO)
PHOSPHONIUM		
P^+H_4		-14
MeP^+H_3		2.7
Et_3P^+H		9.1
$Ph_3P^+CH_3$		(22.4)
$Ph_3P^+i\text{-}Pr$		(21.2)
$Ph_3P^+CH_2COPh$		(6.2)
$Ph_3P^+CH_2CN$		(7.0)
PHOSPONATES & PHOSPHINE OXIDES		
		
X= Ph		(27.6)
CN		(16.4)
CO_2Et		(18.6)
Cl		(26.2)
$SiMe_3$		(28.8)
		
X= SPh		(24.9)
CN		(16.9)
PHOSPHINES		
$Ph_2PCH_2PPh_2$		(29.9)
$Ph_2PCH_2SO_2Ph$		(20.2)

Substrate	pKa H_2O	(DMSO)
NITRO		
RNO_2		
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)
		
n= 3		(26.9)
4		(17.8)
5		(16.0)
6		(17.9)
7		(15.8)
IMINES		
		(24.3)

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

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JOC 41, 2508 (1976)
JOC 42, 1817 (1977)
JOC 42, 321 (1977)
JOC 42, 326 (1977)
JOC 43, 3113 (1978)
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JOC 43, 1764 (1978)
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JOC 45, 3305 (1980)
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Acc. Chem. Res. 21, 456 (1988)
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J. March (1985)
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THF:
JACS 110, 5705 (1988)

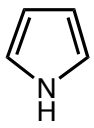
See cited website below for additional data

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

For a comprehensive compilation of Brodwell pKa data see: **http://www.chem.wisc.edu/areas/reich/pkatable/index.htm**

DMSO Acidities of Common Heterocycles

Bordwell, ACR, **1988**, *21*, 456
Bordwell http://www.chem.wisc.edu/areas/reich/pkatable/index.htm



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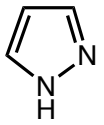

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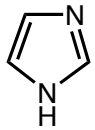

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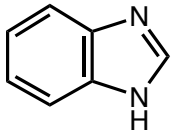

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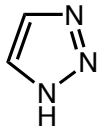

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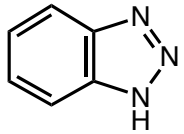

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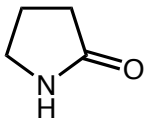

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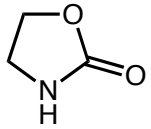

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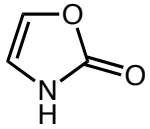

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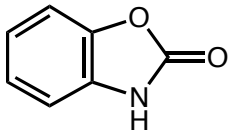

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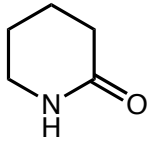

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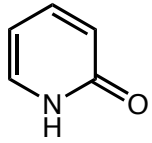

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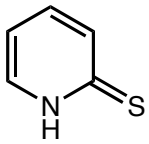

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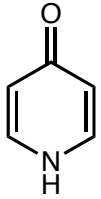

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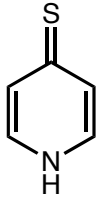

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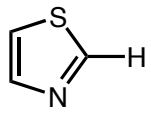

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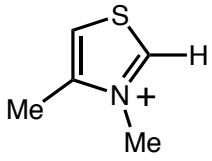

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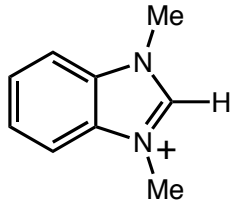

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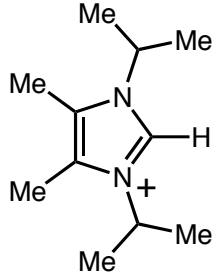

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