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CHEMISTRY DATA BOOKLET

August 2001

To be used in the teaching and examination of
Diploma Programme chemistry

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Chemistry Data Booklet
August 2001

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International Baccalaureate Organization
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4. Names of the First 103 Elements

Element	Symbol	Atomic Number	Element	Symbol	Atomic Number
actinium	Ac	89	mercury	Hg	80
aluminium	Al	13	molybdenum	Mo	42
americium	Am	95	neodymium	Nd	60
antimony	Sb	51	neon	Ne	10
argon	Ar	18	neptunium	Np	93
arsenic	As	33	nickel	Ni	28
astatine	At	85	niobium	Nb	41
barium	Ba	56	nitrogen	N	7
berkelium	Bk	97	nobelium	No	102
beryllium	Be	4	osmium	Os	76
bismuth	Bi	83	oxygen	O	8
boron	B	5	palladium	Pd	46
bromine	Br	35	phosphorus	P	15
cadmium	Cd	48	platinum	Pt	78
caesium	Cs	55	plutonium	Pu	94
calcium	Ca	20	polonium	Po	84
californium	Cf	98	potassium	K	19
carbon	C	6	praseodymium	Pr	59
cerium	Ce	58	promethium	Pm	61
chlorine	Cl	17	protactinium	Pa	91
chromium	Cr	24	radium	Ra	88
cobalt	Co	27	radon	Rn	86
copper	Cu	29	rhenium	Re	75
curium	Cm	96	rhodium	Rh	45
dysprosium	Dy	66	rubidium	Rb	37
einsteinium	Es	99	ruthenium	Ru	44
erbium	Er	68	samarium	Sm	62
europium	Eu	63	scandium	Sc	21
fermium	Fm	100	selenium	Se	34
fluorine	F	9	silicon	Si	14
francium	Fr	87	silver	Ag	47
gadolinium	Gd	64	sodium	Na	11
gallium	Ga	31	strontium	Sr	38
germanium	Ge	32	sulfur	S	16
gold	Au	79	tantalum	Ta	73
hafnium	Hf	72	technetium	Tc	43
helium	He	2	tellurium	Te	52
holmium	Ho	67	terbium	Tb	65
hydrogen	H	1	thallium	Tl	81
indium	In	49	thorium	Th	90
iodine	I	53	thulium	Tm	69
iridium	Ir	77	tin	Sn	50
iron	Fe	26	titanium	Ti	22
krypton	Kr	36	tungsten	W	74
lanthanum	La	57	uranium	U	92
lawrencium	Lr	103	vanadium	V	23
lead	Pb	82	xenon	Xe	54
lithium	Li	3	ytterbium	Yb	70
lutetium	Lu	71	yttrium	Y	39
magnesium	Mg	12	zinc	Zn	30
manganese	Mn	25	zirconium	Zr	40
mendelevium	Md	101			

7. First Ionization Energy, Electron Affinity and Electronegativity of the Elements

1310 -72		First ionization energy / kJ mol^{-1} Electron affinity / kJ mol^{-1} Element Electronegativity																2370
H																		He
519 -52	900											799 -29	1090 -120	1400 -3	1310 -142 ($\text{O}^- +844$)	1680 -348	2080	
Li	Be											B	C	N	O	F	Ne	
1.0	1.5											2.0	2.5	3.0	3.5	4.0		
494 -71	736											577 -47	786 -180	1060 -70	1000 -200 ($\text{S}^- +532$)	1260 -364	1520	
Na	Mg											Al	Si	P	S	Cl	Ar	
0.9	1.2											1.5	1.8	2.1	2.5	3.0		
418	590	632	661	648	653	716	762	757	736	745	908	577	762	966	941	1140 -342	1350	
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr	
0.8	1.0	1.3	1.5	1.6	1.6	1.5	1.8	1.8	1.8	1.9	1.6	1.6	1.8	2.0	2.4	2.8		
402	548	636	669	653	694	699	724	745	803	732	866	556	707	833	870	1010 -314	1170	
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe	
0.8	1.0	1.2	1.4	1.6	1.8	1.9	2.2	2.2	2.2	1.9	1.7	1.7	1.8	1.9	2.1	2.5		
376	502	540	531	760	770	762	841	887	866	891	1010	590	716	703	812	920	1040	
Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn	
0.7	0.9	1.1	1.3	1.5	1.7	1.9	2.2	2.2	2.2	2.4	1.9	1.8	1.8	1.9	2.0	2.2		
381	510	669																
Fr	Ra	Ac																

0.7	0.9	1.1
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8. Atomic and Ionic Radii of the Elements

30																					
H																	He				
154 (1-)																					
152	112															88	77	70	66	58	
Li	Be															B	C	N	O	F	Ne
68 (1+)	30 (2+)															16 (3+)	260 (4-)	171 (3-)	146 (2-)	133 (1-)	
186	160															143	117	110	104	99	
Na	Mg															Al	Si	P	S	Cl	Ar
98 (1+)	65 (2+)															45 (3+)	42 (4+) 271 (4-)	212 (3-)	190 (2-)	181 (1-)	
231	197	160	146	131	125	129	126	125	124	128	133	141	122	121	117	114					
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr				
133 (1+)	94 (2+)	81 (3+)	90 (2+) 68 (4+)	88 (2+) 59 (5+)	63 (3+)	80 (2+) 60 (4+)	76 (2+) 64 (3+)	74 (2+) 63 (3+)	72 (2+)	96 (1+) 69 (2+)	74 (2+)	62 (3+)	53 (4+) 272 (4-)	222 (3-)	202 (2-)	196 (1-)					
244	215	180	157	141	136	135	133	134	138	144	149	166	162	141	137	133					
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe				
148 (1+)	110 (2+)	93 (3+)	80 (4+)	70 (5+)	68 (4+)		65 (4+)	86 (2+)		126 (1+)	97 (2+)	81 (3+)	112 (2+) 71 (4+)	245 (3-)	222 (2-)	219 (1-)					
262	217	188	157	143	137	137	134	135	138	144	152	171	175	170	140	140					
Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn				
167 (1+)	34 (2+)	115 (3+)	81 (4+)	73 (5+)	68 (4+)		67 (4+)	66 (4+)		137 (1+) 85 (3+)	127 (1+) 110 (2+)	95 (3+)	120 (2+) 84 (4+)	120 (3+)							
270	220	200																			
Fr	Ra																				

Atomic radius/ 10^{-12} m	Element
	Ionic radius/ 10^{-12} m

		Ac
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9. Covalent Bond Lengths

Bond	Bond length /nm	Bond	Bond length /nm
H-H	0.074	C-H	0.109
C-C	0.154	Si-H	0.146
C=C	0.134	N-H	0.101
C≡C	0.120	P-H	0.142
C-C (in benzene)	0.139	O-H	0.096
Si-Si	0.235	S-H	0.135
N-N	0.146	F-H	0.092
N=N	0.120	Cl-H	0.128
N≡N	0.110	Br-H	0.141
P-P (P ₄)	0.221	I-H	0.160
O-O	0.148		
O=O	0.121	C-O	0.143
S-S (S ₈)	0.207	C=O	0.122
S=S	0.188	C-O (in phenol)	0.136
F-F	0.142	C-N	0.147
Cl-Cl	0.199	C=N	0.127
Br-Br	0.228	C≡N	0.116
I-I	0.267	C-N (in phenylamine)	0.135
		C-F	0.138
		C-Cl	0.177
		C-Cl (in chlorobenzene)	0.169
		C-Br	0.193
		C-I	0.214
		Si-O	0.150

10. Average Bond Enthalpies at 298 K

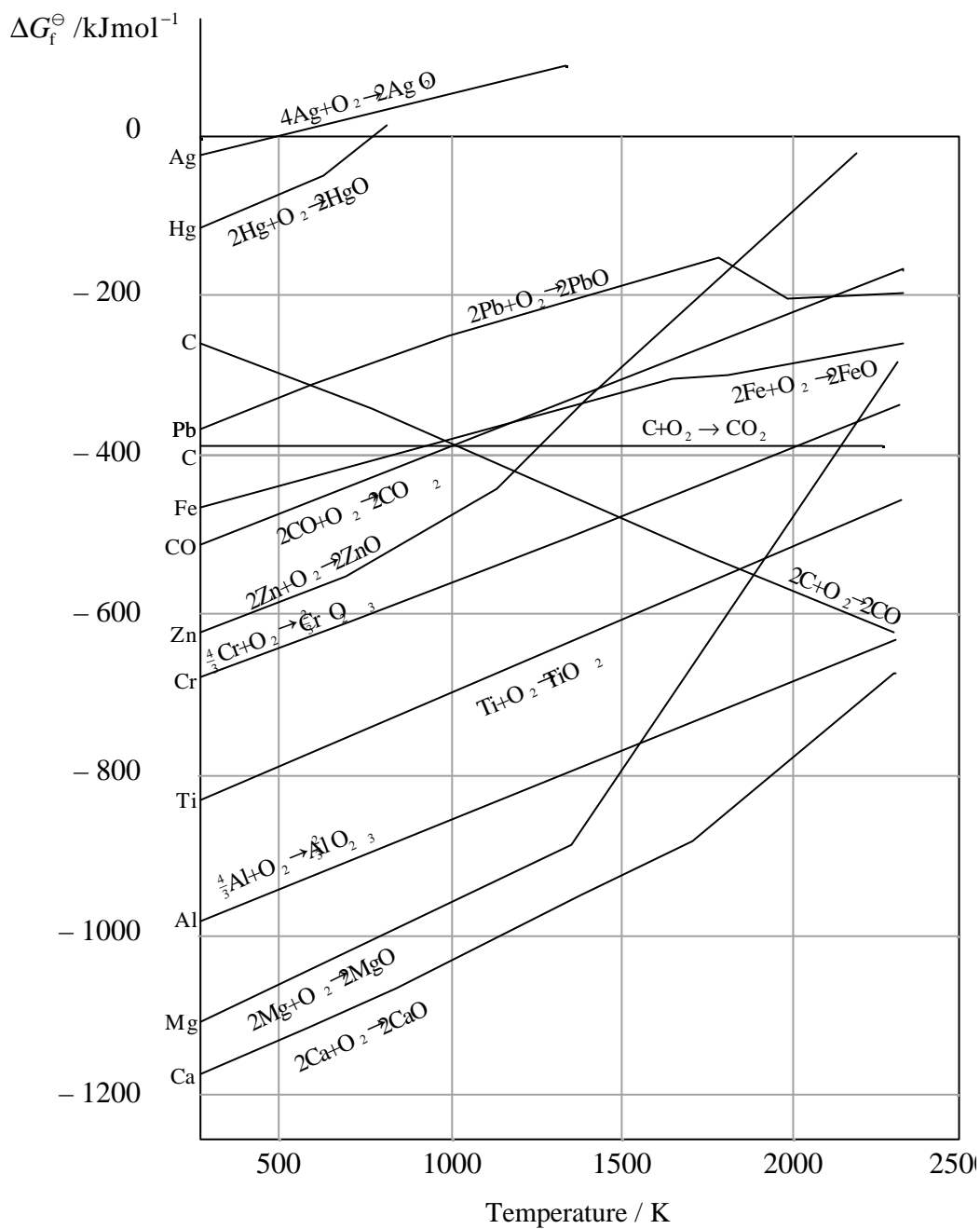
Bond	DH / kJ mol ⁻¹	Bond	DH / kJ mol ⁻¹
H-H	436	C-H	412
D-D	442	Si-H	318
C-C	348	N-H	388
C=C	612	P-H	322
C≡C	837	O-H	463
C-C (benzene)	518	S-H	338
Si-Si	226	F-H	562
Ge-Ge	188	Cl-H	431
Sn-Sn	151	Br-H	366
N-N	163	I-H	299
N=N	409		
N≡N	944	C-O	360
P-P	172	C=O	743
O-O	146	C-N	305
O=O	496	C=N	613
S-S	264	C≡N	890
F-F	158	C-F	484
Cl-Cl	242	C-Cl	338
Br-Br	193	C-Br	276
I-I	151	C-I	238
		Si-O	374

11. Organic Compounds—Thermodynamic Data

Substance	Formula	State	$DH_f^\ominus / \text{kJ mol}^{-1}$	$DG_f^\ominus / \text{kJ mol}^{-1}$	$S^\ominus / \text{J K}^{-1} \text{mol}^{-1}$
methane	CH ₄	g	-75	-51	186
ethane	C ₂ H ₆	g	-85	-33	230
propane	C ₃ H ₈	g	-104	-24	270
butane	C ₄ H ₁₀	g	-125	-16	310
pentane	C ₅ H ₁₂	g	-146	-8	348
hexane	C ₆ H ₁₄	g	-167	0	387
ethene	C ₂ H ₄	g	52	68	219
propene	C ₃ H ₆	g	20	63	267
but-1-ene	C ₄ H ₈	g	1	72	307
<i>cis</i> -but-2-ene	C ₄ H ₈	g	-6	67	301
<i>trans</i> -but-2-ene	C ₄ H ₈	g	-10	64	296
ethyne	C ₂ H ₂	g	227	209	201
propyne	C ₃ H ₄	g	185	194	248
buta-1,3-diene	C ₄ H ₆	g	112	152	279
cyclohexane	C ₆ H ₁₂	l	-156	27	204
benzene	C ₆ H ₆	g	83	130	269
benzene	C ₆ H ₆	l	49	125	173
methylbenzene	C ₆ H ₅ CH ₃	g	50	122	320
ethylbenzene	C ₆ H ₅ CH ₂ CH ₃	g	30	131	360
phenylethene	C ₆ H ₅ CHCH ₂	g	148	214	345
chloromethane	CH ₃ Cl	g	-82	-59	234
dichloromethane	CH ₂ Cl ₂	l	-117	-63	179
trichloromethane	CHCl ₃	l	-132	-72	203
bromomethane	CH ₃ Br	g	-36	-26	246
tribromomethane	CHBr ₃	l	-20	3	222
iodomethane	CH ₃ I	l	-8	20	163
triiodomethane	CHI ₃	s	141		
chloroethane	C ₂ H ₅ Cl	g	-105	-53	276
bromoethane	C ₂ H ₅ Br	l	-85		
iodoethane	C ₂ H ₅ I	l	-31		
chloroethene	C ₂ H ₃ Cl	g	31	52	264
1,2-dichloroethane	CH ₂ ClCH ₂ Cl	l	-166	-80	208
chlorobenzene	C ₆ H ₅ Cl	g	52	99	314
methanol	CH ₃ OH	g	-201	-162	238
methanol	CH ₃ OH	l	-239	-166	127
ethanol	C ₂ H ₅ OH	g	-235	-169	282
ethanol	C ₂ H ₅ OH	l	-278	-175	161
phenol	C ₆ H ₅ OH	s	-163	-51	146
methanal	HCHO	g	-116	-110	219
ethanal	CH ₃ CHO	g	-166	-134	266
propanone	(CH ₃) ₂ CO	g	-216	-152	295
methanoic acid	HCOOH	l	-409	-346	129
ethanoic acid	CH ₃ COOH	l	-487	-392	160
benzoic acid	C ₆ H ₅ COOH	s	-385	-245	167
ethyl ethanoate	CH ₃ COOC ₂ H ₅	l	-481		
ethanamide	CH ₃ CONH ₂	s	-320		
methylamine	CH ₃ NH ₂	g	-28	28	242
ethylamine	C ₂ H ₅ NH ₂	g	-49	37	285
urea	CO(NH ₂) ₂	s	-333	-47	105

12. Ellingham Diagram

Standard Gibbs free energy changes of formation, ΔG_f^\ominus , for oxides given per mole of oxygen gas as a function of temperature.



13. Enthalpies of Combustion

The values of the molar enthalpy of combustion (ΔH_c^\ominus) in the following table refer to a temperature of 298 K and a pressure of 1.01×10^5 Pa (1 atm).

Substance	Formula	State	$(\Delta H_c^\ominus) / \text{kJ mol}^{-1}$	Substance	Formula	State	$\Delta H_c^\ominus / \text{kJ mol}^{-1}$
hydrogen	H ₂	g	-286	propan-1-ol	C ₃ H ₇ OH	l	-2010
sulfur	S	s	-297	butan-1-ol	C ₄ H ₉ OH	l	-2673
carbon (graphite)	C	s	-394	phenylmethanol	C ₆ H ₅ CH ₂ OH	l	-4056
carbon (diamond)	C	s	-395	cyclohexanol	C ₆ H ₁₁ OH	s	-3727
carbon monoxide	CO	s	-283	phenol	C ₆ H ₅ OH		-3064
methane	CH ₄	g	-890	ethoxyethane	(C ₂ H ₅) ₂ O	l	-2727
ethane	C ₂ H ₆	g	-1560	methanal	HCHO	g	-561
propane	C ₃ H ₈	g	-2220	ethanal	CH ₃ CHO	l	-1167
butane	C ₄ H ₁₀	g	-2877	benzaldehyde	C ₆ H ₅ CHO	l	-3520
pentane	C ₅ H ₁₂	g	-3509	propanone	(CH ₃) ₂ CO	l	-1786
hexane	C ₆ H ₁₄	l	-4194	pentan-3-one	(C ₂ H ₅) ₂ CO	l	-3078
octane	C ₈ H ₁₈	l	-5512	phenylethanone	CH ₃ COC ₆ H ₅	s	-4138
cyclohexane	C ₆ H ₁₂	l	-3924	diphenylmethanone	(C ₆ H ₅) ₂ CO	s	-6512
ethene	C ₂ H ₄	l	-1409	methanoic acid	HCOOH	l	-263
buta-1,3-diene	C ₄ H ₆	g	-2542	ethanoic acid	CH ₃ COOH	l	-876
ethyne	C ₂ H ₂	g	-1299	benzoic acid	C ₆ H ₅ COOH	s	-3227
benzene	C ₆ H ₆	g	-3273	ethanedioic acid	(COOH) ₂	s	-246
methylbenzene	C ₆ H ₅ CH ₃	l	-3909	ethyl ethanoate	CH ₃ COOC ₂ H ₅	l	-2246
naphthalene	C ₁₀ H ₈	l	-5157	ethanamide	⁵	s	-1182
anthracene	C ₁₄ H ₁₀	s	-7114	benzamide	CH ₃ CONH ₂	s	-3546
chloroethane	C ₂ H ₅ Cl	s	-1325	methylamine	C ₆ H ₅ CONH ₂	g	-1072
bromoethane	C ₂ H ₅ Br	g	-1425	ethylamine	CH ₃ NH ₂	g	-1709
iodoethane	C ₂ H ₅ I	g	-1490	phenylamine	C ₆ H ₅ NH ₂	l	-3397
(chloromethyl)benzene	C ₆ H ₅ CH ₂ Cl	l	-3709	nitrobenzene	C ₆ H ₅ NH ₂	l	-3094
trichloromethane	CHCl ₃	l	-373	urea	C ₆ H ₅ NO ₂	s	-634
methanol	CH ₃ OH	l	-715	glucose	CO(NH ₂) ₂	s	-2816
ethanol	C ₂ H ₅ OH	l	-1371	sucrose	C ₆ H ₁₂ O ₆	s	-5644
					C ₁₂ H ₂₂ O ₁₁		

14. Lattice Enthalpies at 298 K (Experimental and Theoretical Values)

The lattice enthalpy ($\Delta H_{\text{lattice}}^{\ominus}$) values given relate to the endothermic process in $\text{MX(s)} \rightarrow \text{M}^+(\text{g}) + \text{X}^-(\text{g})$ which the gaseous ions of a crystal are separated to an infinite distance from each other.

Experimental Values

The data in these two tables are experimental values obtained by means of a suitable Born-Haber cycle.

Alkali metal halides	$\Delta H_{\text{lattice}}^{\ominus} / \text{kJ mol}^{-1}$			
	F	Cl	Br	I
Li	1022	846	800	744
Na	902	771	733	684
K	801	701	670	629
Rb	767	675	647	609
Cs	716	645	619	585

Other substances	$\Delta H_{\text{lattice}}^{\ominus} / \text{kJ mol}^{-1}$	Other substances	$\Delta H_{\text{lattice}}^{\ominus} / \text{kJ mol}^{-1}$
CaF ₂	2602	MgS	3238
BeCl ₂	3006	CaS	2966
MgCl ₂	2493	SrS	2779
CaCl ₂	2237	BaS	2643
SrCl ₂	2112	CuCl	976
BaCl ₂	2018	AgF	955
MgO	3889	AgCl	905
CaO	3513	AgBr	890
SrO	3310	AgI	876
BaO	3152	NH ₄ Cl	640

Theoretical Values

These two tables contain lattice enthalpies calculated from electrostatic principles on the basis of a purely ionic model for the crystal.

Alkali metal halides	$\Delta H_{\text{lattice}}^{\ominus} / \text{kJ mol}^{-1}$			
	F	Cl	Br	I
Li	1004	833	787	728
Na	891	766	732	686
K	795	690	665	632
Rb	761	674	644	607
Cs	728	636	611	582

Other substances	$\Delta H_{\text{lattice}}^{\ominus} / \text{kJ mol}^{-1}$	Other substances	$\Delta H_{\text{lattice}}^{\ominus} / \text{kJ mol}^{-1}$
CaF ₂	2611	AgF	870
MgO	3929	AgCl	770
CaO	3477	AgBr	758
SrO	3205	AgI	736
BaO	3042		

15. Standard Electrode Potentials

Oxidized species	\rightleftharpoons	Reduced species	E^\ominus / V
$\text{Li}^+(\text{aq}) + \text{e}^-$	\rightleftharpoons	$\text{Li}(\text{s})$	-3.03
$\text{K}^+(\text{aq}) + \text{e}^-$	\rightleftharpoons	$\text{K}(\text{s})$	-2.92
$\text{Ca}^{2+}(\text{aq}) + 2\text{e}^-$	\rightleftharpoons	$\text{Ca}(\text{s})$	-2.87
$\text{Na}^+(\text{aq}) + \text{e}^-$	\rightleftharpoons	$\text{Na}(\text{s})$	-2.71
$\text{Mg}^{2+}(\text{aq}) + 2\text{e}^-$	\rightleftharpoons	$\text{Mg}(\text{s})$	-2.36
$\text{Al}^{3+}(\text{aq}) + 3\text{e}^-$	\rightleftharpoons	$\text{Al}(\text{s})$	-1.66
$\text{Mn}^{2+}(\text{aq}) + 2\text{e}^-$	\rightleftharpoons	$\text{Mn}(\text{s})$	-1.18
$\text{H}_2\text{O}(\text{l}) + \text{e}^-$	\rightleftharpoons	$\frac{1}{2}\text{H}_2(\text{g}) + \text{OH}^-(\text{aq})$	-0.83
$\text{Zn}^{2+}(\text{aq}) + 2\text{e}^-$	\rightleftharpoons	$\text{Zn}(\text{s})$	-0.76
$\text{Fe}^{2+}(\text{aq}) + 2\text{e}^-$	\rightleftharpoons	$\text{Fe}(\text{s})$	-0.44
$\text{Ni}^{2+}(\text{aq}) + 2\text{e}^-$	\rightleftharpoons	$\text{Ni}(\text{s})$	-0.23
$\text{Sn}^{2+}(\text{aq}) + 2\text{e}^-$	\rightleftharpoons	$\text{Sn}(\text{s})$	-0.14
$\text{Pb}^{2+}(\text{aq}) + 2\text{e}^-$	\rightleftharpoons	$\text{Pb}(\text{s})$	-0.13
$\text{H}^+(\text{aq}) + \text{e}^-$	\rightleftharpoons	$\frac{1}{2}\text{H}_2(\text{g})$	0.00
$\text{Cu}^{2+}(\text{aq}) + \text{e}^-$	\rightleftharpoons	$\text{Cu}^+(\text{s})$	+0.15
$\text{SO}_4^{2-}(\text{aq}) + 4\text{H}^+(\text{aq}) + 2\text{e}^-$	\rightleftharpoons	$\text{H}_2\text{SO}_3(\text{aq}) + \text{H}_2\text{O}(\text{l})$	+0.17
$\text{Cu}^{2+}(\text{aq}) + 2\text{e}^-$	\rightleftharpoons	$\text{Cu}(\text{s})$	+0.34
$\frac{1}{2}\text{O}_2(\text{g}) + \text{H}_2\text{O}(\text{l}) + 2\text{e}^-$	\rightleftharpoons	$2\text{OH}^-(\text{aq})$	+0.40
$\text{Cu}^+(\text{aq}) + \text{e}^-$	\rightleftharpoons	$\text{Cu}(\text{s})$	+0.52
$\frac{1}{2}\text{I}_2(\text{s}) + \text{e}^-$	\rightleftharpoons	$\text{I}^-(\text{aq})$	+0.54
$\text{Fe}^{3+}(\text{aq}) + \text{e}^-$	\rightleftharpoons	$\text{Fe}^{2+}(\text{aq})$	+0.77
$\text{Ag}^+(\text{aq}) + \text{e}^-$	\rightleftharpoons	$\text{Ag}(\text{s})$	+0.80
$\frac{1}{2}\text{Br}_2(\text{l}) + \text{e}^-$	\rightleftharpoons	$\text{Br}^-(\text{aq})$	+1.09
$\frac{1}{2}\text{O}_2(\text{g}) + 2\text{H}^+(\text{aq}) + 2\text{e}^-$	\rightleftharpoons	$\text{H}_2\text{O}(\text{l})$	+1.23
$\text{Cr}_2\text{O}_7^{2-}(\text{aq}) + 14\text{H}^+(\text{aq}) + 6\text{e}^-$	\rightleftharpoons	$2\text{Cr}^{3+}(\text{aq}) + 7\text{H}_2\text{O}(\text{l})$	+1.33
$\frac{1}{2}\text{Cl}_2(\text{g}) + \text{e}^-$	\rightleftharpoons	$\text{Cl}^-(\text{aq})$	+1.36
$\text{MnO}_4^-(\text{aq}) + 8\text{H}^+(\text{aq}) + 5\text{e}^-$	\rightleftharpoons	$\text{Mn}^{2+}(\text{aq}) + 4\text{H}_2\text{O}(\text{l})$	+1.51
$\text{F}_2(\text{g}) + \text{e}^-$	\rightleftharpoons	$\text{F}^-(\text{aq})$	+2.87

16. Strengths of Organic Acids and Bases

The acid strengths in the following tables are given in terms of pK_a values, where $pK_a = -\log_{10} K_a$. The dissociation constant, K_a , values are for aqueous solutions at 298 K. Base strengths are given in terms of pK_b values.

Carboxylic Acids

Name	Formula	pK_a
methanoic	HCOOH	3.75
ethanoic	CH ₃ COOH	4.76
propanoic	CH ₃ CH ₂ COOH	4.87
butanoic	CH ₃ (CH ₂) ₂ COOH	4.82
2-methylpropanoic	(CH ₃) ₂ CHCOOH	4.85
pentanoic	CH ₃ (CH ₂) ₃ COOH	4.86
2,2-dimethylpropanoic	(CH ₃) ₃ CCOOH	5.05
benzoic	C ₆ H ₅ COOH	4.20
phenylethanoic	C ₆ H ₅ CH ₂ COOH	4.31

Halogenated Carboxylic Acids

Name	Formula	pK_a
chloroethanoic	CH ₂ ClCOOH	2.86
dichloroethanoic	CHCl ₂ COOH	1.29
trichloroethanoic	CCl ₃ COOH	0.65
fluoroethanoic	CH ₂ FCOOH	2.66
bromoethanoic	CH ₂ BrCOOH	2.90
iodoethanoic	CH ₂ ICOOH	3.17

Phenols

Name	Formula	pK_a
phenol	C ₆ H ₅ OH	10.00
2-nitrophenol	O ₂ NC ₆ H ₄ OH	7.21
3-nitrophenol	O ₂ NC ₆ H ₄ OH	8.35
4-nitrophenol	O ₂ NC ₆ H ₄ OH	7.15
2,4-dinitrophenol	(O ₂ N) ₂ C ₆ H ₃ OH	4.01
2,4,6-trinitrophenol	(O ₂ N) ₃ C ₆ H ₂ OH	0.42

Alcohols

Name	Formula	pK_a
methanol	CH ₃ OH	15.5
ethanol	C ₂ H ₅ OH	16 (approximately)

Amines

Name	Formula	p <i>K</i> _b
ammonia	NH ₃	4.75
methylamine	CH ₃ NH ₂	3.36
ethylamine	CH ₃ CH ₂ NH ₂	3.27
dimethylamine	(CH ₃) ₂ NH	3.28
trimethylamine	(CH ₃) ₃ N	4.20
diethylamine	(C ₂ H ₅) ₂ NH	3.07
triethylamine	(C ₂ H ₅) ₃ N	3.36
phenylamine	C ₆ H ₅ NH ₂	9.38

17. Acid–base Indicators

			Colour change	
Indicator	p <i>K</i> _a	pH range	Acid	Alkali
methyl orange	3.7	3.1–4.4	red	yellow
bromophenol blue	4.0	3.0–4.6	yellow	blue
bromocresol green	4.7	3.8–5.4	yellow	blue
methyl red	5.1	4.2–6.3	red	yellow
bromothymol blue	7.0	6.0–7.6	yellow	blue
phenol red	7.9	6.8–8.4	yellow	red
phenolphthalein	9.3	8.3–10.0	colourless	red

18. Infrared Data

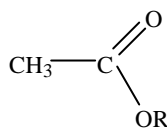
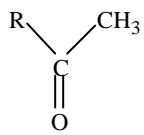
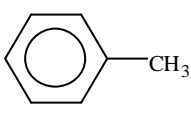
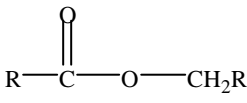
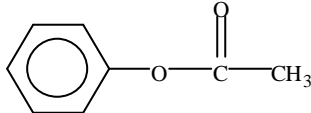
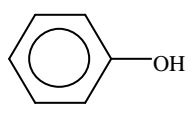
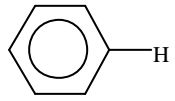
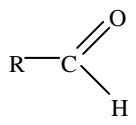
Characteristic ranges for infrared absorption due to stretching vibrations in organic molecules.

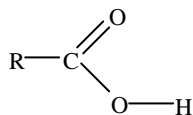
Bond	Organic molecules	Wavenumber / cm^{-1}
C–Cl	halogenoalkanes	700 to 800
C–O	alcohols, ethers, esters	1000 to 1300
C=C	alkenes	1610 to 1680
C=O	aldehydes, ketones, acids, esters	1680 to 1750
C≡C	alkynes	2070 to 2250
O–H	“hydrogen bonded” in acids	2500 to 3300
C–H	alkanes, alkenes, arenes	2840 to 3095
O–H	“hydrogen bonded” in alcohols, phenols	3230 to 3550
N–H	primary amines	3350 to 3500

19. ¹H NMR Data

Typical proton chemical shift values (δ) relative to TMS = 0.

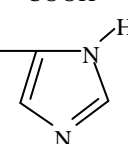
(These values can vary slightly in different solvents.)

Type of proton	Chemical shift/ppm
$R-CH_3$	0.9
$R-CH_2-R$	1.3
R_3CH	2
	2.0
	2.1
	2.3
$R-C\equiv C-H$	2.6
$R-CH_2-Hal$	3.2–3.7
$R-O-CH_3$	3.8
	4.1
	4.0–4.2
$R-O-H$	0.5–6.5 (can vary considerably under different conditions)
$RHC=CH_2$	4.9–5.9
	7
	7.3
	9.7



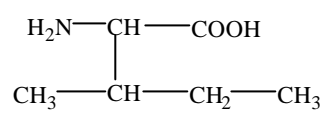
11.5

20. 2-amino Acids

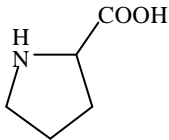
Common name	Symbol	Structural formula	pH of isoelectric point
alanine	Ala	$\begin{array}{c} \text{H}_2\text{N}-\text{CH}-\text{COOH} \\ \\ \text{CH}_3 \end{array}$	6.0
arginine	Arg	$\begin{array}{c} \text{H}_2\text{N}-\text{CH}-\text{COOH} \\ \\ \text{CH}_2-\text{CH}_2-\text{CH}_2-\text{NH}-\text{C}-\text{NH}_2 \\ \parallel \\ \text{NH} \end{array}$	10.8
asparagine	Asn	$\begin{array}{c} \text{H}_2\text{N}-\text{CH}-\text{COOH} \\ \\ \text{CH}_2-\text{C}-\text{NH}_2 \\ \parallel \\ \text{O} \end{array}$	5.4
aspartic acid	Asp	$\begin{array}{c} \text{H}_2\text{N}-\text{CH}-\text{COOH} \\ \\ \text{CH}_2-\text{COOH} \end{array}$	2.8
cysteine	Cys	$\begin{array}{c} \text{H}_2\text{N}-\text{CH}-\text{COOH} \\ \\ \text{CH}_2-\text{SH} \end{array}$	5.1
glutamine	Gln	$\begin{array}{c} \text{H}_2\text{N}-\text{CH}-\text{COOH} \\ \\ \text{CH}_2-\text{CH}_2-\text{C}-\text{NH}_2 \\ \parallel \\ \text{O} \end{array}$	5.7
glutamic acid	Glu	$\begin{array}{c} \text{H}_2\text{N}-\text{CH}-\text{COOH} \\ \\ \text{CH}_2-\text{CH}_2-\text{COOH} \end{array}$	3.2
glycine	Gly	$\text{H}_2\text{N}-\text{CH}_2-\text{COOH}$	6.0
histidine	His	$\begin{array}{c} \text{H}_2\text{N}-\text{CH}-\text{COOH} \\ \\ \text{CH}_2-\text{C}_4\text{H}_3\text{N}_2 \end{array}$ 	7.6

isoleucine

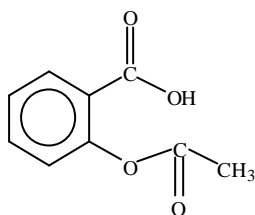
Ile



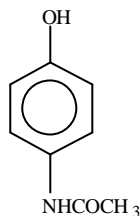
6.0

Common name	Symbol	Structural formula	pH of isoelectric point
leucine	Leu	$ \begin{array}{c} \text{H}_2\text{N}-\text{CH}-\text{COOH} \\ \\ \text{CH}_2 \\ \\ \text{CH}_3-\text{CH}-\text{CH}_3 \end{array} $	6.0
lysine	Lys	$ \begin{array}{c} \text{H}_2\text{N}-\text{CH}-\text{COOH} \\ \\ \text{CH}_2-\text{CH}_2-\text{CH}_2-\text{CH}_2-\text{NH}_2 \end{array} $	9.7
methionine	Met	$ \begin{array}{c} \text{H}_2\text{N}-\text{CH}-\text{COOH} \\ \\ \text{CH}_2-\text{CH}_2-\text{S}-\text{CH}_3 \end{array} $	5.7
phenylalanine	Phe	$ \begin{array}{c} \text{H}_2\text{N}-\text{CH}-\text{COOH} \\ \\ \text{CH}_2-\text{C}_6\text{H}_5 \end{array} $	5.5
proline	Pro		6.3
serine	Ser	$ \begin{array}{c} \text{H}_2\text{N}-\text{CH}-\text{COOH} \\ \\ \text{CH}_2-\text{OH} \end{array} $	5.7
threonine	Thr	$ \begin{array}{c} \text{H}_2\text{N}-\text{CH}-\text{COOH} \\ \\ \text{CH}_3-\text{CH}-\text{OH} \end{array} $	5.6
tryptophan	Trp	$ \begin{array}{c} \text{H}_2\text{N}-\text{CH}-\text{COOH} \\ \\ \text{CH}_2-\text{C}_8\text{H}_6\text{N}_2 \end{array} $	5.9
tyrosine	Tyr	$ \begin{array}{c} \text{H}_2\text{N}-\text{CH}-\text{COOH} \\ \\ \text{CH}_2-\text{C}_6\text{H}_4-\text{OH} \end{array} $	5.7
valine	Val	$ \begin{array}{c} \text{H}_2\text{N}-\text{CH}-\text{COOH} \\ \\ \text{CH}_3-\text{CH}-\text{CH}_3 \end{array} $	6.0

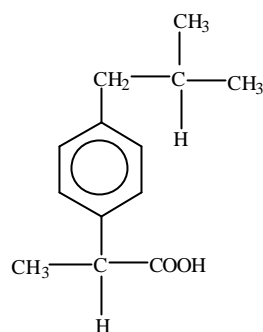
21. Structural Formulas of Some Important Medicines and Drugs



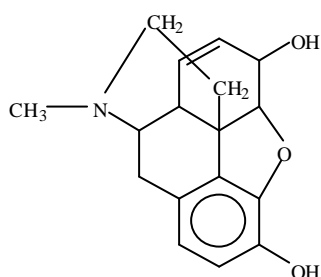
aspirin



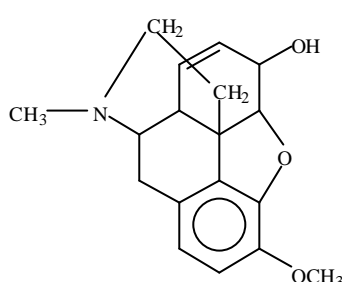
paracetamol (acetaminophen)



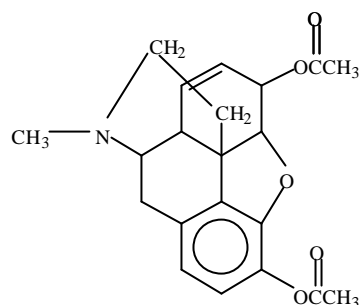
ibuprofen



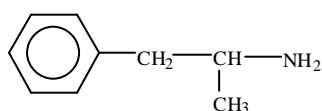
morphine



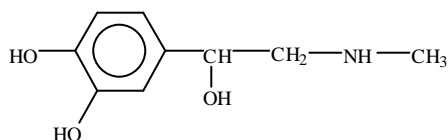
codeine



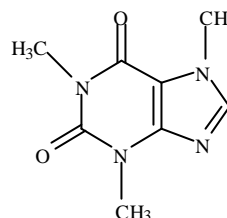
heroin



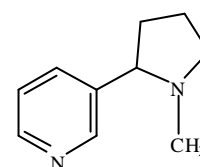
amphetamine



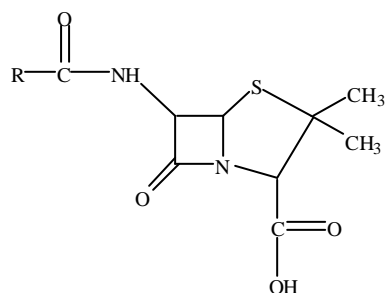
adrenaline



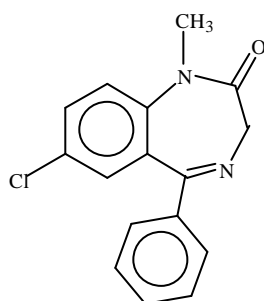
caffeine



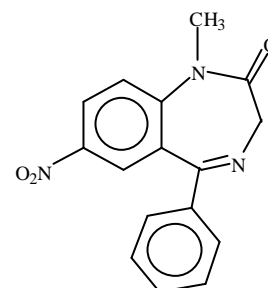
nicotine



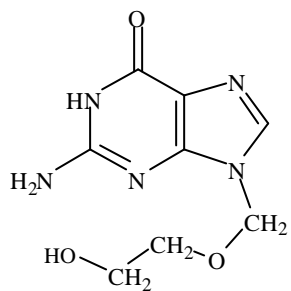
penicillin



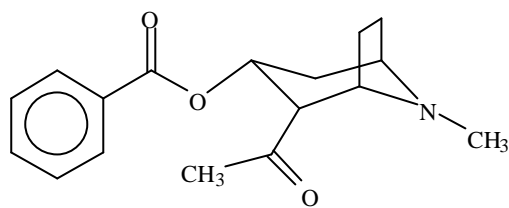
diazepam (valium®)



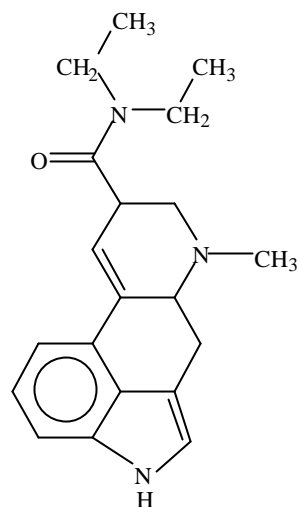
nitrazepam (mogadon®)



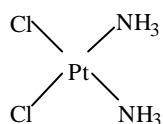
acyclovir



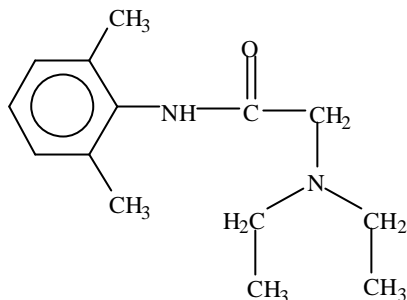
cocaine



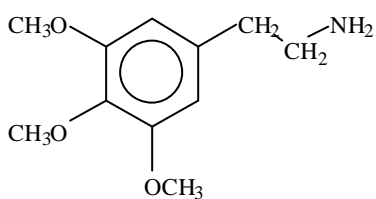
(LSD)



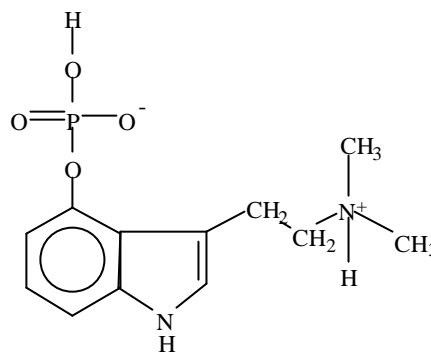
cisplatin



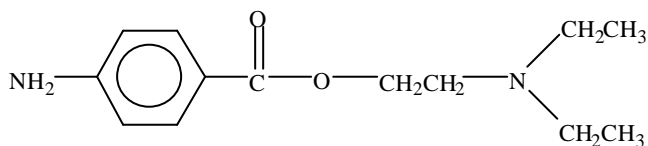
Lidocaine



mescaline

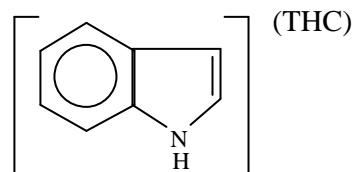
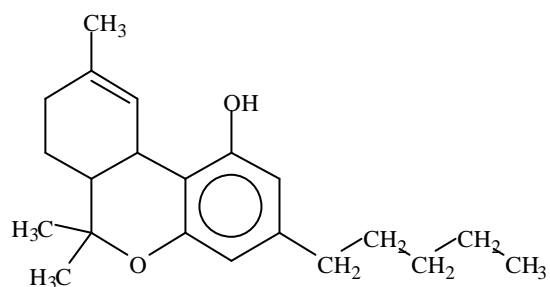
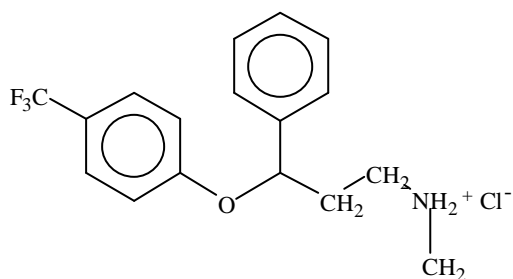


psilocybin



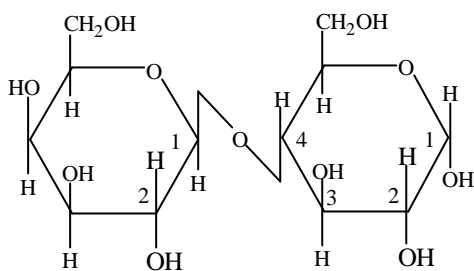
fluoxetine hydrochloride (prozac®)

fluoxetine hydrochloride (prozac®)

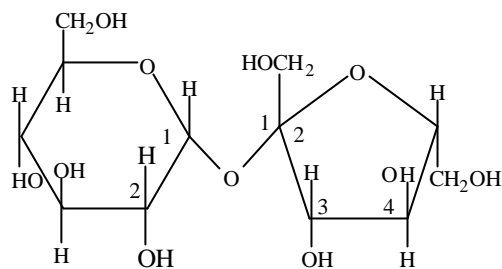


indole

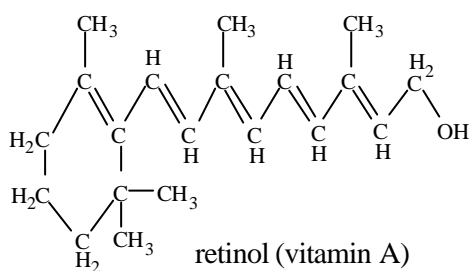
22. Structural Formulas of Some Important Biological Molecules



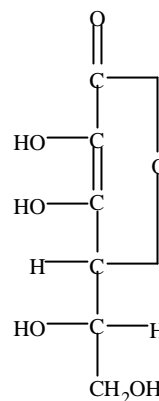
lactose



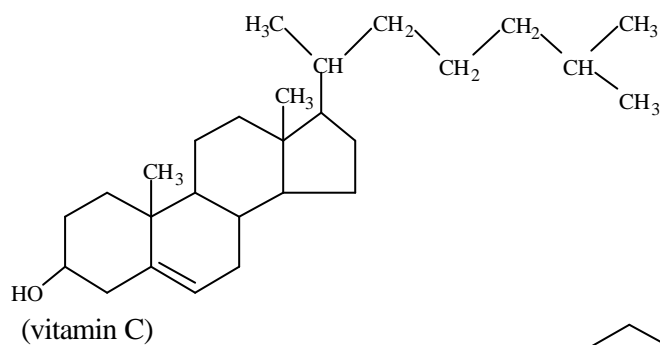
sucrose



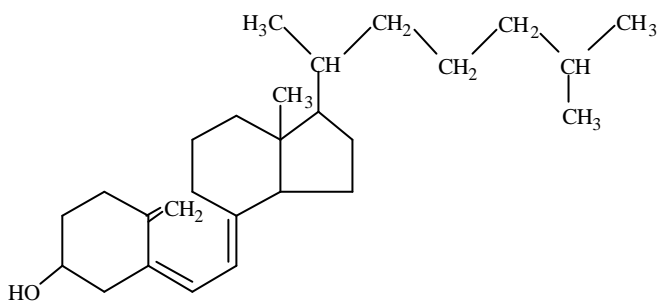
retinol (vitamin A)



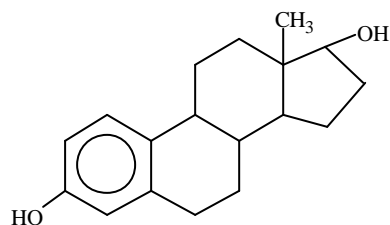
ascorbic acid



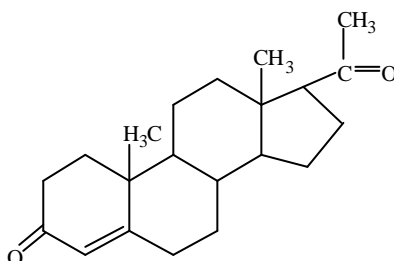
cholesterol



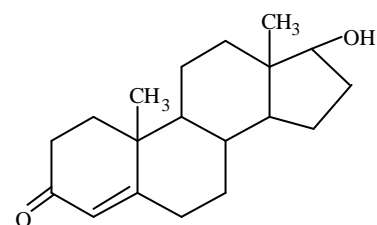
vitamin D



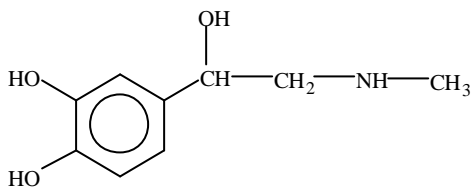
oestradiol



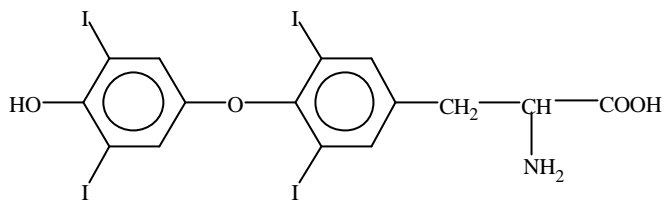
progesterone



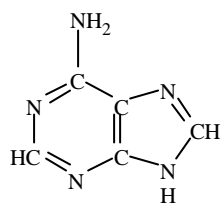
testosterone



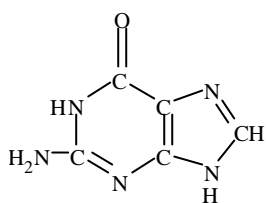
adrenaline



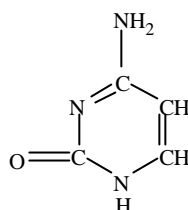
thyroxine



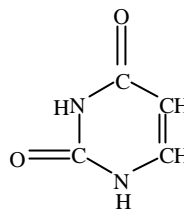
adenine



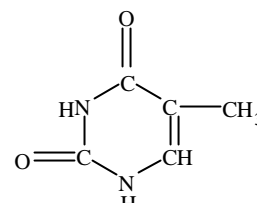
guanine



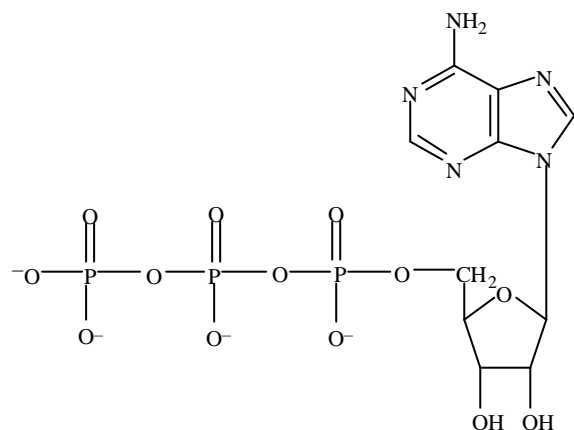
cytosine



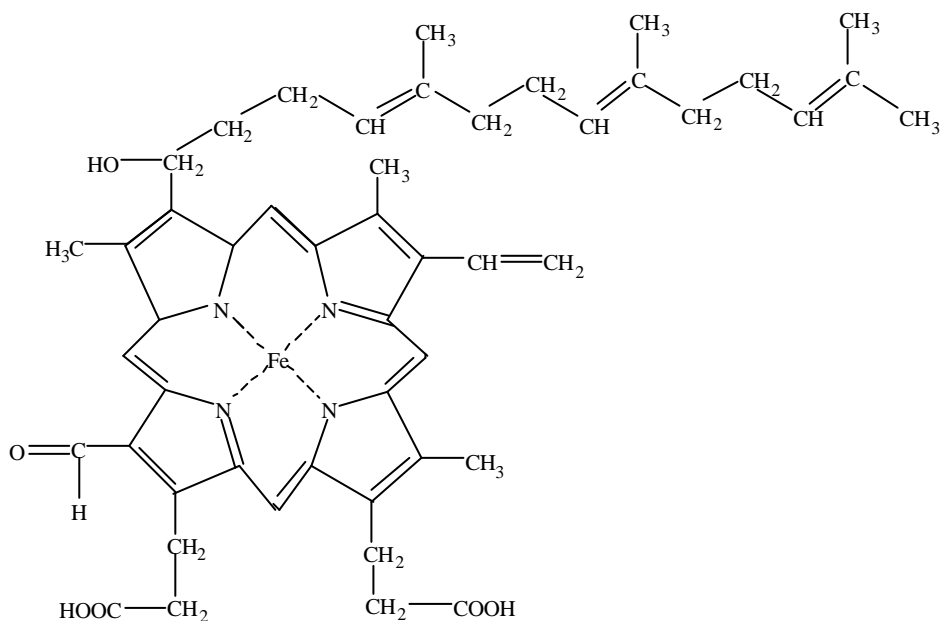
uracil



thymine



adenosine triphosphate (ATP)



The haem group from cytochrome oxidase