

Noderīga informācija

"Bonding the World with Chemistry"

49. Starptautiskā ķīmijas olimpiāde

NakhonPathom, Taizeme



Konstantes un formulas

Avogadro skaitlis, $N_A = 6.0221 \times 10^{23} \text{ mol}^{-1}$

Bolcmaņa konstante, $k_B = 1.3807 \times 10^{-23} \text{ J K}^{-1}$

Universālā gāzu konstante, $R = 8.3145 \text{ J K}^{-1} \text{ mol}^{-1} = 0.08205 \text{ atm L K}^{-1} \text{ mol}^{-1}$

Gaismas ātrums, $c = 2.9979 \times 10^8 \text{ m s}^{-1}$

Planka konstante, $h = 6.6261 \times 10^{-34} \text{ J s}$

Faradeja konstante, $F = 9.64853399 \times 10^4 \text{ C}$

Elektrona masa, $m_e = 9.10938215 \times 10^{-31} \text{ kg}$

Spiediens standartstākļos, $P = 1 \text{ bar} = 10^5 \text{ Pa}$

Atmosfēras spiediens, $P_{\text{atm}} = 1.01325 \times 10^5 \text{ Pa} = 760 \text{ mmHg} = 760 \text{ torr}$

Nule Celsija skalā, 273.15 K

1 picometrs (pm) = 10^{-12} m ; $1 \text{ \AA} = 10^{-10} \text{ m}$; 1 nanometrs (nm) = 10^{-9} m

1 eV = $1.6 \times 10^{-19} \text{ J}$

1 amu = $1.66053904 \times 10^{-27} \text{ kg}$

Izdālas gāzes stāvokļa vienādojums: $PV = nRT$

Entalpija: $H = U + PV$

Gibbsa enerģija: $G = H - TS$ $\Delta G = \Delta G^\circ + RT \ln Q$

$$\Delta G^\circ = -RT \ln K = -nFE_{\text{cell}}^\circ$$

Entropijas izmaiņa: $\Delta S = \frac{q_{\text{rev}}}{T}$, where q_{rev} is heat for the reversible process

$$\Delta S = nR \ln \frac{V_2}{V_1} \text{ (for isothermal expansion of an ideal gas)}$$

Nernsta vienādojums: $E = E^\circ + \frac{RT}{nF} \ln \frac{C_{\text{ox}}}{C_{\text{red}}}$

$$E = E^\circ - \frac{RT}{nF} \ln Q$$

Fotona enerģija: $E = \frac{hc}{\lambda}$ Lamberta-Bēra likums: $A = \log \frac{I_0}{I} = \epsilon b C$

Integrētie ātruma vienādojumi kinētikā:

Nultās pakāpes $[A] = [A]_0 - kt$ Pirmās pakāpes $\ln [A] = \ln [A]_0 - kt$

Otrās pakāpes $\frac{1}{[A]} = \frac{1}{[A]_0} + kt$

Arrēniusa vienādojums

$$k = Ae^{-E_a/RT}, \text{ kur } A - \text{Arrēniusa konstante (faktors)}$$

Kīmisko elementu periodiskā tabula

18																	
8A																	
2																	
He 4.003																	
10																	
Ne 20.18																	
18																	
Ar 39.95																	
36																	
Kr 83.80																	
54																	
Xe 131.3																	
86																	
Rn (222)																	
118																	
Og (294)																	
1																	
1A																	
1																	
H 1.008																	
2																	
2A																	
4																	
Be 9.012																	
12																	
Mg 24.31																	
20																	
Ca 40.08																	
38																	
Sr 87.62																	
56																	
Ba 137.3																	
88																	
Ra (226)																	
3																	
3B																	
21																	
Sc 44.96																	
39																	
Y 88.91																	
57																	
La 138.9																	
89																	
Ac (227)																	
4																	
4B																	
22																	
Ti 47.88																	
40																	
Zr 91.22																	
72																	
Hf 178.5																	
80																	
Rf (261)																	
5																	
5B																	
23																	
V 50.94																	
41																	
Nb 92.91																	
73																	
Ta 180.9																	
81																	
Re 186.2																	
87																	
Os 190.2																	
105																	
Db (262)																	
6																	
6B																	
24																	
Cr 52.00																	
42																	
Mo 95.95																	
74																	
W 183.8																	
82																	
Sg (263)																	
7																	
7B																	
25																	
Mn 54.94																	
43																	
Tc (98)																	
75																	
Re 186.2																	
83																	
Ir 192.2																	
107																	
Bh (262)																	
8																	
8B																	
26																	
Fe 55.85																	
44																	
Ru 101.1																	
76																	
Os 190.2																	
108																	
Hs (265)																	
9																	
9B																	
27																	
Co 58.93																	
45																	
Rh 102.9																	
77																	
Ir 192.2																	
109																	
Mt (266)																	
10																	
10B																	
28																	
Ni 58.69																	
46																	
Pd 106.4																	
78																	
Pt 195.1																	
110																	
Ds (281)																	
11																	
11B																	
29																	
Cu 63.55																	
47																	
Ag 107.9																	
79																	
Au 197.0																	
111																	
Rg (272)																	
12																	
12B																	
30																	
Zn 65.39																	
48																	
Cd 112.4																	
80																	
Hg 200.6																	
112																	
Cn (285)																	
13																	
3A																	
5																	
B 10.81																	
13																	
Al 26.98																	
31																	
Ga 69.72																	
49																	
In 114.8																	
81																	
Tl 204.4																	
113																	
Nh (286)																	
6																	
6A																	
6																	
C 12.01																	
14																	
Si 28.09																	
32																	
Ge 72.61																	
50																	
Sn 118.7																	
82																	
Pb 207.2																	
114																	
Fl (289)																	
7																	
7A																	
7																	
N 14.01																	
15																	
P 30.97																	
33																	
As 74.92																	
51																	
Sb 121.8																	
83																	
Bi 209.0																	
115																	
Mc (289)																	
8																	
8A																	
8																	
O 16.00																	
16																	
S 32.07																	
34																	
Se 78.97																	
52																	
Te 127.6																	
84																	
Po (209)																	
116																	
Lv (293)																	
9																	
9A																	
9																	
F 19.00																	
17																	
Cl 35.45																	
35																	
Br 79.90																	
53																	
I 126.9																	
85																	
At (210)																	
117																	
Ts (294)																	
70																	
70																	
Yb 173.0																	
71																	
Lu 175.0																	
102																	
No (259)																	
101																	
Md (258)																	
100																	
Fm (257)																	
99																	
Es (252)																	
98																	
Cf (251)																	
97																	
Bk (247)																	
96																	
Cm (247)																	
95																	
Am (243)																	
94																	
Pu (244)																	
93																	
Np (237)																	
92																	
U 238.0																	
91																	
Pa 231.0																	
90																	
Th 232.0																	
89																	
Pr 140.1																	
59																	
Pr 140.1																	
60																	
Nd 144.2																	
61																	
Pm (145)																	
62																	
Sm 150.4																	
63																	
Eu 152.0																	
64																	
Gd 157.3																	
65																	
Tb 158.9																	
66																	
Dy 162.5																	
67																	
Ho 164.9																	
68																	
Er 167.3																	
69																	
Tm 168.9																	
70																	
Yb 173.0																	
71																	
Lu 175.0																	

Raksturīgās ^1H NMR ķīmiskās nobīdes

Ūdeņraža veids (R=Alkyl, Ar=Aryl)	Ķīmiskā nobīde (ppm)	Ūdeņraža veids (R=Alkyl, Ar=Aryl)	Ķīmiskā nobīde (ppm)
$(\text{CH}_3)_4\text{Si}$	0 (pēc definīcijas)		
RCH_3	0.9	$\text{RCH}=\text{O}$	9.5-10.1
RCH_2R	1.2-1.4	RCOOH'	10-13
R_3CH	1.4-1.7	RCOCH_3	2.1-2.3
RCH_2I	3.2-3.3	RCOCH_2R	2.2-2.6
RCH_2Br	3.4-3.5	RCOOCH_3	3.7-3.9
RCH_2Cl	3.6-3.8	RCOOCH_2R	4.1-4.7
RCH_2F	4.4-4.5	$\text{R}_2\text{C}=\text{CRCHR}_2$	1.6-2.6
RCH_2NH_2	2.3-2.9	$\text{R}_2\text{C}=\text{CH}_2$	4.6-5.0
RCH_2OH	3.4-4.0	$\text{R}_2\text{C}=\text{CHR}$	5.0-5.7
RCH_2OR	3.3-4.0	$\text{RC}\equiv\text{CH}$	2.0-3.0
$\text{RCH}_2\text{CH}_2\text{OR}$	1.5-1.6	ArCH_3	2.2-2.5
R_2NH	0.5-5.0	ArCH_2R	2.3-2.8
ROH	0.5-6.0	ArH	6.5-8.5

Raksturīgās ^{13}C NMR ķīmiskās nobīdes

Oglekļa veids (R=Alkyl, Ar=Aryl)	Ķīmiskā nobīde (ppm)	Oglekļa veids (R=Alkyl, Ar=Aryl)	Ķīmiskā nobīde (ppm)
RCH_3	10-25	$\text{RC}(\text{triplebond})\text{CR}$	65-85
RCH_2R	20-35	$\text{RCH}=\text{CHR}$	120-140
R_3CH	25-35	ArylC	120-140
RCH_2COR	35-50	RCOOR	160-180
RCH_2Br	25-35	RCONR_2 (amide)	165-180
RCH_2Cl	40-45	RCOOH	175-185
RCH_2NH_2	30-65	RCHO	190-205
RCH_2OH	60-70	RCOR	200-215
RCH_2OR	65-70		

Adapted from RSC E-learning website.

Raksturīgās IR absorbcijas joslas

Raksturīgās organisko savienojumu funkcionālo grupu IR absorbcijas frekvences			
Funkcionālā grupa	Svārstību veids	Raksturīgās absorbcijas joslas (cm ⁻¹)	Intensitāte
Alcohol			
O-H	(stretch, H-bonded)	3200-3600	strong, broad
O-H	(stretch, free)	3500-3700	strong, sharp
C-O	(stretch)	1050-1150	Strong
Alkane			
C-H	stretch	2850-3000	Strong
-C-H	bending	1350-1480	Variable
Alkene			
=C-H	stretch	3010-3100	Medium
=C-H	bending	675-1000	Strong
C=C	stretch	1620-1680	Variable
Alkyl Halide			
C-F	stretch	1000-1400	Strong
C-Cl	stretch	600-800	Strong
C-Br	stretch	500-600	Strong
C-I	stretch	500	Strong
Alkyne			
C-H	stretch	3300	strong, sharp
-C≡C-	stretch	2100-2260	variable, not present in symmetrical alkynes
Amine			
N-H	stretch	3300-3500	medium (primary amines have two bands; secondary have one band, often very weak)
C-N	stretch	1080-1360	medium-weak
N-H	bending	1600	Medium
Aromatic			
C-H	stretch	3000-3100	Medium
C=C	stretch	1400-1600	medium-weak, multiple bands
Analysis of C-H out-of-plane bending can often distinguish substitution patterns			
Carbonyl			
C=O	stretch	1670-1820	Strong
(conjugation moves absorptions to lower wave numbers)			
Ether			
C-O	stretch	1000-1300 (1070-1150)	Strong
Nitrile			
CN	Stretch	2210-2260	Medium
Nitro			
N-O	stretch	1515-1560 & 1345-1385	strong, two bands

Karbonilgrupu (C=O) saturošo savienojumu IR absorbcijas frekvences [angļu val. IR Absorption Frequencies of Functional Groups Containing a Carbonyl (C=O)]			
Funkcionālā grupa	Svārstību veids	Raksturīgās absorbcijas joslas (cm⁻¹)	Intensitāte
Carbonyl			
C=O	stretch	1670-1820	Strong
(conjugation moves absorptions to lower wave numbers)			
Acid			
C=O	stretch	1700-1725	Strong
O-H	stretch	2500-3300	strong, very broad
C-O	stretch	1210-1320	Strong
Aldehyde			
C=O	stretch	1740-1720	Strong
=C-H	stretch	2820-2850 & 2720-2750	medium, two peaks
Amide			
C=O	stretch	1640-1690	Strong
N-H	stretch	3100-3500	unsubstituted have two bands
N-H	bending	1550-1640	
Anhydride			
C=O	stretch	1800-1830 & 1740-1775	two bands
Ester			
C=O	stretch	1735-1750	Strong
C-O	stretch	1000-1300	two bands or more
Ketone			
acyclic	stretch	1705-1725	Strong
cyclic	stretch	3-membered - 1850 4-membered - 1780 5-membered - 1745 6-membered - 1715 7-membered - 1705	Strong
α,β-unsaturated	stretch	1665-1685	Strong
aryl ketone	stretch	1680-1700	Strong

Data from <http://www2.ups.edu/faculty/hanson/Spectroscopy/IR/IRfrequencies.html>