Structural analysis (CH-314)

Week 1

Definitions & Formulas

1. Atomic number (Z) – the number of protons in an atomic nucleus.
2. Neutron number (N) – the number of neutrons in an atomic nucleus.
3. Mass number (A) – total number of nucleons (protons and neutrons) in an atomic nucleus:
$$A = Z + N$$
4. Isotopes – atoms with nuclei of the same atomic number differing in the number of neutrons.
5. Mass units:
$$1\ a.m.u. = {}^{1}/_{12} \cdot m({}^{12}C) = 1.6605390666 \cdot 10^{-27} kg$$
$$1\ Da = 1\ u = 1\ a.m.u.$$
6. Isotopic mass – the exact mass of an isotope.
7. Isotopic abundance – the relative concentration of an isotope.
8. Nominal mass of an element - the integer mass of its most abundant isotope.
9. Monoisotopic mass of an element – the exact mass of its most abundant isotope.
10. Relative atomic mass (atomic weight) – the weighted average of the exact masses of the naturally occurring isotopes of an element:
$$A_r = \frac{\sum \alpha_i \cdot m_i}{\sum \alpha_i} = \sum \alpha_i \cdot m_i\,, \alpha_i - abundance\ of\ the\ i^{th}\ isotope$$
11. Nominal, monoisotopic, and average molecular mass (molecular weight) is the sum of the nominal, monoisotopic, and relative atomic masses, respectively, of the elements in its empirical formula:
$$m = \sum n_i \cdot m_i$$
12. Exact mass of an isotopic species is the sum of the isotopic masses of its constituent elements.
13. Isobars – species with the same nominal mass but different exact masses.
14. Isotopologues – species that differ only in their isotopic composition.
15. Isotopic distribution in case of a di-isotopic element:
$$\Pr(\mathrm{A} + \mathrm{k}) = \frac{n!}{k! \cdot (n-k)!} \cdot \alpha^{n-k} \cdot (1-\alpha)^{k}$$
16. Isotopic distribution in case of a poly-isotopic element:
$$\Pr(A + k_1 + k_2 + k_3 + \ldots) = \frac{n!}{k_1! \cdot k_2! \cdot k_3! \cdot \ldots} \cdot (\alpha_1)^{k_1} \cdot (\alpha_2)^{k_2} \cdot (\alpha_3)^{k_3} \cdot \ldots$$
17. Isotopic distribution in case of presence of several di- or poly-isotopic elements:
$$\Pr({}^{a1}A_{k1}{}^{a2}A_{k2} \ldots {}^{b1}B_{l1}{}^{b2}B_{l2} \ldots) = \Pr({}^{a1}A_{k1}{}^{a2}A_{k2} \ldots) \cdot \Pr({}^{b1}B_{l1}{}^{b2}B_{l2} \ldots)$$
18. Masses of an electron and of a proton:
$$m_e = 0.000549\ Da$$
$$m(H^+) = 1.007276\ Da$$

Natural Isotopes of Some Elements

Isotope	Abundance (%)	Mass (Da)
^{1}**H**	99.985	1.007825
^{2}**H**	0.015	2.014101
^{6}**Li**	7.5	6.01512
^{7}**Li**	92.5	7.016
^{12}**C**	98.89	12
^{13}**C**	1.11	13.00335
^{14}**N**	99.64	14.00307
^{15}**N**	0.36	15.00011
^{16}**O**	99.76	15.99491
^{17}**O**	0.04	16.99913
^{18}**O**	0.2	17.99916
^{19}**F**	100	18.99840
^{23}**Na**	100	22.98976

Isotope	Abundance (%)	Mass (Da)
^{28}**Si**	92.232	27.97693
^{29}**Si**	4.699	28.97649
^{30}**Si**	3.092	29.97377
^{31}**P**	100	30.97376
^{32}**S**	95.0	31.97207
^{33}**S**	0.76	32.97146
^{34}**S**	4.22	33.96786
^{36}**S**	0.014	35.96709
^{35}**Cl**	75.77	34.96885
^{37}**Cl**	24.23	36.96590
^{79}**Br**	50.69	78.91838
^{81}**Br**	49.31	80.91629
^{127}**I**	100	126.90447