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# Synchronizing chemistry, quantum mechanics and radioactivity in a revolutionary renewed atom model. Part 1: the elements where $Z$ is 1–10 (H, He, Li, Be, B, C, N, O, F, Ne)

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The alliance between the reigning quantum mechanical atom model and chemistry still is a difficult one when it comes to an adequate explanation for *e.g.* the covalent bond, inversion, chirality, or hydrogen bonds. Overruling Rutherford's extrapolation from gold to hydrogen, an atom model is described that provides improved answers to these phenomena while the hybridization principle and the covalent bond are re-defined by giving neutrons a much more prominent role than they have in the reigning quantum mechanical model. It is postulated that a neutron is not just there to assist the strong force in surpassing the repulsive coulombic forces between the protons in the nucleus, but the neutron is the modus operandi of molecular geometry, and as such plays a part in chemical reactivity, bond length and bond strength.

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## 1 Introduction

Based on the experience that an atom contains positive and negative charges, Thomson was the first to design a model of the atom (1904).<sup>1,2</sup> The positive charge formed a ball of even density, with the negatively charged electrons floating in the ball and forming regular geometric patterns by mutual repulsion. From the famous experiment (bombarding thin gold foils with alpha particles) performed by his students, Rutherford concluded in 1911 that Thomson's model required a serious adjustment: the complete positive charge and almost the entire mass of an atom are concentrated in a very small volume, the dense inner core of an atom, the nucleus.<sup>3</sup> This solar system model (electrons revolving in circular or elliptical orbits around the nucleus like planets around the sun) evolved *via* Bohr<sup>4</sup> and Schrodinger/Heisenberg<sup>5,6</sup> into the quantum mechanical atom model of today. This means a model with orbitals/probability clouds (areas within which an electron can be encountered) instead of orbits of an electron, and with neutrons plus protons bound together by the so-called strong force in the nucleus, accounting for 99.9% of the atom's mass. This strong force surpasses the Coulomb repulsion between the protons; if not, the nucleus of the atom converts to an energetically better situation by radioactive decay. In the latter case, the so-called weak nuclear force plays a role.

With respect to chemical aspects, the octet rule (1916) had been implemented as the closed shell principle, the "Aufbau

principle" had seen the light, and Pauling<sup>7</sup> had developed the hybridization concept ( $sp^3$  for single-bonded carbon,  $sp^2$  for double-bonded carbon,  $sp^1$  for triple-bonded carbon) as a proposition to account for the otherwise inexplicable fact that *e.g.*  $CH_4$  contains four equal CH-bonds. This hybridization concept also solved the issue of how a p-electron crosses a node and passes through the positively charged nucleus. A covalent bond became the result of overlap between two orbitals (two interfering waves, each with one electron) and two paired electrons, inversion (*e.g.* the  $NH_3$  molecule) and hydrogen bonds became the result of spontaneous tunneling.<sup>8,9</sup> Even empty orbitals could exhibit chemical reactivity such as the empty p-orbital of boron and alumina, and empty d-orbitals in case of octet rule disobeying compounds like  $H_3PO_4$ ,  $H_2SO_4$  or  $HClO_4$ . The octet rule disobeying  $HNO_3$  remained a nuisance, because nitrogen's quantum number  $n = 2$  forbids the presence of d-orbitals; only a Lewis structure remained descriptive for this compound.<sup>10</sup>

At around the time Ogilvie questioned the whole orbital concept,<sup>11</sup> we added an extra dimension to Pauling's geometric s-electron hybridization parameter. Organic fluorine chemistry is rather unusual and numerous dichotomies exist.<sup>12</sup> Some of these are accounted for by hypotheses like 'double-bond no-bond resonance'<sup>13</sup> or 'large repulsion integrals in the carbon-fluorine region'.<sup>14</sup> In an attempt to improve on this, we launched the concept of the s-orbital density deficiency of the F-atom as the driving force of its chemical behavior.<sup>15–17</sup> This concept was based on the quantum mechanical fact that lone pairs require more than their s-share in the  $sp^3$ -hybridization process.<sup>18</sup> Since F possesses three lone pairs, we postulated (1) that the F-atom is urgently in need for additional s-orbital

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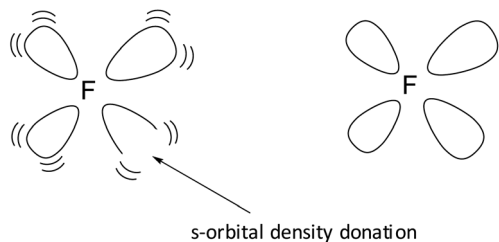


Fig. 1 Principle of s-orbital density deficiency and s-orbital density donation.

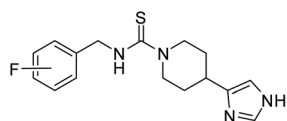
density *via* its bonding orbital, to release this tension (see Fig. 1), and (2) that the hydrogen atom and the carbon atom are the perfect s-orbital density donors for the F-atom.

According to this concept, the F-atom in  $F_2$  is the most s-orbital density deficient, leading to a weak F-F bond and extreme reactivity; in  $CH_3COOF$  this situation is slightly better and therefore it reacts less vigorously. Over and above that, although being the most electronegative element in the periodic system, when present as fluoride in water, the F-atom immediately shares its extra electron to form HF in exchange for s-orbital density, whereas fluoride is a strong nucleophile in the absence of  $H_2O$ . The concept also made clear why in organic chemistry the F-atom prefers to be bound to  $sp^3$ -carbon over  $sp^2$ -carbon: the  $sp^2$ -carbon atom had to use a great deal of its s-orbital density to construct the double bond and, therefore, its s-orbital density donor ability towards fluorine is diminished.

Later on, we reported that in a series of mono-substituted benzyl analogues of thioperamide, the aromatic F-derivatives showed, in contrast to computer predictions, a factor 10 less *in vitro* activity than its H, Cl, Br, and I counterparts (Fig. 2).<sup>19</sup>

We postulated that the aromatic ring of the fluor derivative was not flat anymore,<sup>20</sup> because F had forced the  $sp^2$ -carbon of the aromatic ring to re-hybridize into a  $sp^3$ -like carbon, leading to a Dewar benzene-like structure with reduced affinity for the receptor. In addition, we argued that also for fluorobenzene itself the literature data<sup>21</sup> (*ipso* angle increase and apparent bond shortening plus angle decrease for  $C_2$  and  $C_3$ ) strongly point to a non-flat configuration (Fig. 3 and 4).

The last decennia we have tried to find an adequate explanation for the re-hybridization phenomenon. We gradually came to the inevitable conclusion that the reigning atom model



R	pA <sub>2</sub> (±SEM)
H	7.32 (0.16)
2-F	6.04 (0.14)
3-F	6.44 (0.13)
4-F	6.25 (0.14)

Fig. 2 Fluorobenzyl thioperamide derivative, remarkably deviating a factor 10.

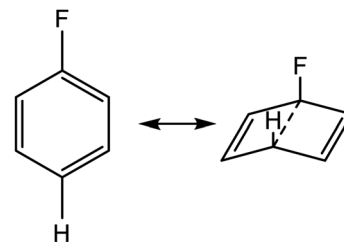
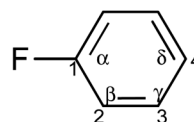


Fig. 3 Fluorobenzene transforming into fluor Dewar benzene.



	Bond length (Å)	Angle	
$C_1 - F$	1.356	$\alpha$	123.4°
$C_1 - C_2$	1.387	$\beta$	118.0°
$C_2 - C_3$	1.399	$\gamma$	120.2°
$C_3 - C_4$	1.401	$\delta$	120.2°

Fig. 4 Apparent bond shortening and angle changes when projected in flat fluorobenzene (angles and bond lengths are from <sup>21</sup>).

needed adjustment, and hereto some serious 'out of the box thinking' was required. Besides finding a concrete answer to the fluorine problem, it would be an added bonus when at the same time this renewed atom model would also comprise an adequate solution for phenomena like inversion, chirality and hydrogen bonds, and the reason for stability and instability of an atom. In this paper we report our proposal for such an atom model adjustment. The renewed atom model is based on the key premise that Rutherford's extrapolation of the findings for the heavy gold atom ( $Z = 79$ ) to the lighter atoms, is not correct.

## 2 The new model

### 2.1 Central thesis and definitions

In this part 1 paper we discuss our proposition for the atom configuration of the elements with  $Z = 1-10$ . We will just stick to the level of protons and neutrons held together by the strong force *via* quarks. Production and decay of their radioactive isotopes are used as confirmation of the proposed atom structure.

The new model will be discussed along the following lines:

**2.1.1 Central thesis.** (1) The nucleus of atoms with low  $Z$  is not a dense, concentrated bunch of neutrons and protons in some inner core, but a flexible constellation of neutrons and protons that can rock, stretch and bend (Fig. 5).

(2) This flexible constellation of neutrons and protons is strictly organized. Two protons are always separated from each other by a neutron; two neutrons are always separated from each other by a proton.

(3) In each constellation a neutron can bind to three protons at most, a proton can bind to three neutrons at most, because each have three strong force related quarks.





Fig. 5 (Left) Rocking, stretching and bending of the  ${}^4_2\text{He}$ -atom. (Right) In the  ${}^4_2\text{He}$ -unit, the anchor protons together form the anchor proton side and will be drawn on the low side throughout the paper; the anchor neutrons together form the anchor neutron side and are always drawn on top.

(4) In the strictly organized constellation of neutrons and protons each electron remains revolving in a probability cloud around its proton.

(5) A “square” proton or “square” neutron can be part of the strictly organized constellation of neutrons and protons. A square proton is defined as a proton that carries an electron that is too low in energy to chemically bind to another atom and therefore needs to become activated by a neutron (hybridization); a square neutron is defined as a neutron that is too low in energy to activate a square proton or to take part in hybridization.

**2.1.2 Building block and subunits.** For the elements Li ( $Z = 3$ ) through Ne ( $Z = 10$ ) the basic building block is a  ${}^4_2\text{He}$ -unit. Throughout the paper, the two neutrons of the  ${}^4_2\text{He}$ -unit will be called the anchor neutron side and will be drawn on top; the two protons of the  ${}^4_2\text{He}$ -unit will be called the anchor proton side and will be drawn on the low side (Fig. 5). Subunits at the anchor neutron side will bear the subscript N, subunits at the anchor proton side subscript P.

Nomenclature used for the subunits at the basic building block:

(a)  $P_N$  is a proton at the anchor neutron side of the basic building block;  $N_P$  is a neutron at the anchor proton side;

(b)  $D_N$  is a subunit consisting of a neutron and a proton at the anchor neutron side;  $D_P$  is the same subunit at the anchor proton side;

(c)  $T_P$  is a subunit consisting of two neutrons and a proton at the anchor proton side; a  $T_N$  subunit is only present in extremely short-living radioisotopes.

(d)  ${}^3_2\text{He}_N$ ,  ${}^4_2\text{He}_N$ ,  ${}^4_2\text{He}_P$  and  ${}^5_2\text{He}_P$  are subunits consisting of two protons and one, two or three neutrons, respectively, at the anchor (N or P) sides, and correspond chemically with a lone pair and quantum mechanically with a filled subshell;  ${}^3_2\text{He}_P$  and  ${}^5_2\text{He}_N$  are only present in extremely short-living radioisotopes.

(e) The \* in subunits  $D_N^*$ ,  $T_P^*$ ,  ${}^4_2\text{He}_N^*$  and  ${}^5_2\text{He}_P^*$  indicate that they bear a square neutron;  $P_N$  and  ${}^3_2\text{He}_N$  nearly always bear a square proton.

(f) A covalent bond implies formation of a “chemical” helium-unit between a  $P_N$ ,  $D_N$ ,  $D_P$  or  $T_P$  subunit of one atom and one of the subunits of the other atom.

(g) In the figures, the neutrons are depicted yellow, the protons blue; square neutrons are depicted as yellow stars, square protons as blue stars; in unstable atoms, neutrons are depicted pink, protons red. For the sake of clarity, in atoms  $Z =$

5 and higher, the anchor neutrons of the basic building  ${}^4_2\text{He}$ -block are depicted white, the anchor protons dark grey.

**2.1.3 Radioisotopes, production and decay.** – Production and decay of radioactive isotopes are used as confirmation. To this end, all isotopes and radioisotopes are written as  ${}^A_Z\text{X}$  wherein mass number  $A$  represents the number of protons plus neutrons, atomic number  $Z$  the number of protons, and X the element.

– A nuclear reaction is denoted as  $X(a, b)Y$  wherein X is the target element, a is the incoming particle, b is the outgoing particle and Y the newborn isotope; as a consequence of the impact, radioisotopes produced in a cyclotron or neutron generator do not contain square protons or square neutrons.

– Because in the new model every proton is separated by a neutron and *visa versa* (thesis 2, *vide supra*), the newborn proton formed after  $\beta^-$ -decay requires a shift within the constellation of the atom (away from the proton to which the disintegrated neutron was attached). The newborn neutron formed after  $\beta^+$ -decay needs a likewise transfer (away from the neutron to which the disintegrated proton was attached).

– An isomeric transition (IT) is a transfer of a neutron within the constellation of the atom to an energetically more favorable position (often temporarily better).

– Electron capture (EC) implies a transfer of the newborn neutron away from the neutron to which the proton was attached before capturing its electron.

Most of the production routes and decay modes can be found in the book Radionuclide Transformations.<sup>22</sup> Because individual referring to physicists involved in accurate determination of half-lives and isotope abundancies would make the reference list extremely long, we would like to thank them warmly here.

## 2.2 The new model at work: the carbon atom ( $Z = 6$ )

In organic chemistry, atom  ${}^{12}_6\text{C}$  can be regarded as the central atom of the hybridization principle. Therefore, as a first illustration of the new atom model the constellation of  ${}^{12}_6\text{C}$  is described (Fig. 6).

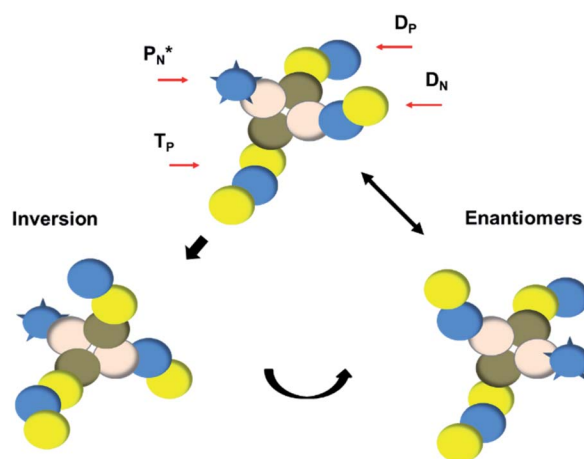


Fig. 6 Constellation of carbon atom  ${}^{12}_6\text{C}$  with  ${}^4_2\text{He}$  as building block and four different subunits:  $P_N^*$  and  $D_N$  at the anchor neutron side,  $D_P$  and  $T_P$  at the anchor proton side. Inversion and subsequent stereo isomerism of the C-atom when the C-atom bears four different chemical groups.



The  $^4_2\text{He}$ -building block contains as subunits at the anchor neutron side a  $\text{P}_\text{N}^*$  and a  $\text{D}_\text{N}$ , at the anchor proton side a  $\text{D}_\text{P}$  and a  $\text{T}_\text{P}$ . The anchor  $^4_2\text{He}$ -unit can flip, leading to chemical inversion in so-called  $\text{S}_\text{N}2$  reactions. The atom exhibits stereo isomerism in case four different chemical groups are bound to the atom: the inverted constellation is the enantiomer of the non-inverted one (Fig. 6).

**2.2.1 Molecules of carbon with hydrogen and carbon.**  $\text{D}_\text{N}$  and  $\text{T}_\text{P}$  are the neutron donors for the hybridization. The atom can hybridize in two ways (Fig. 6): the first mode is  $\text{P}_\text{N}^*$  with  $\text{T}_\text{P}$  and  $\text{D}_\text{N}$  with  $\text{D}_\text{P}$ . This represents the common symmetrical  $\text{sp}^3$ -hybridization and is present in the tetrahedral compound  $\text{CH}_4$  (and covers at the same time the observed subtle difference in bond strength of the four C–H bonds of the  $\text{CH}_4$  molecule<sup>23</sup>). The second mode of hybridization is  $\text{P}_\text{N}^*$  with  $\text{D}_\text{N}$  and  $\text{T}_\text{P}$  with  $\text{D}_\text{P}$ . In this hybridization mode, the distance between the anchor protons is slightly larger and is present in *e.g.* staggered carbon–carbon chains with the hybridized  $\text{P}_\text{N}^*/\text{D}_\text{N}$  bearing the hydrogen atoms.

Multiple bonds formed in the new model are intrinsically the concretization of the banana or bent bonds, whose description had already been shown to be energetically superior to the symmetry-restricted  $\sigma$ ,  $\pi$  bond representation of Hückel.<sup>24–27</sup>

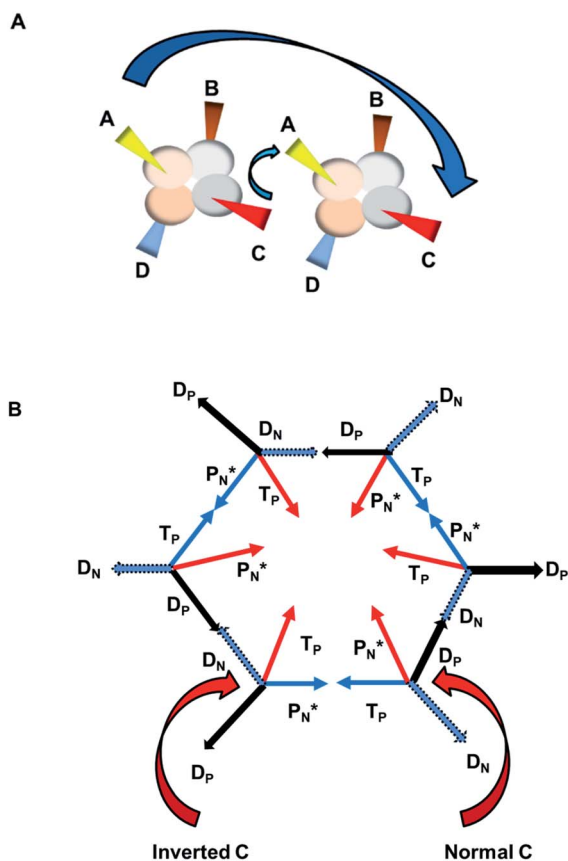


Fig. 7 (a) Principle of symmetrical double bond (AC–CA) formation between two non-inverted (“normal”) carbon atoms which leaves the remaining subunits B, D in cissoid conformation; (b) combining alternatingly three “normal” with three “inverted” carbon atoms via a  $\text{D}_\text{N}-\text{D}_\text{P}$  bond and a symmetrical  $\text{P}_\text{N}^*-\text{T}_\text{P}$  double bond creates the resonance structure of benzene.

The subunits ( $\text{P}_\text{N}$ ,  $\text{D}_\text{N}$ ,  $\text{T}_\text{P}$ ,  $\text{D}_\text{P}$ ) can form several double and triple bonds combinations, dependent on the history of the sample and the chemical group R. One may, however, expect the most energetically balanced, symmetrical molecule to be formed, especially at higher temperatures. In that case, the favorite combinations in double bonds, therefore, will be (1)  $\text{D}_\text{P}$  with  $\text{T}_\text{P}$ , and  $\text{T}_\text{P}$  with  $\text{D}_\text{P}$ , (2)  $\text{P}_\text{N}^*$  with  $\text{T}_\text{P}$ , and  $\text{T}_\text{P}$  with  $\text{P}_\text{N}^*$  or (3)  $\text{D}_\text{P}$  with  $\text{D}_\text{N}$ , and  $\text{D}_\text{N}$  with  $\text{D}_\text{P}$ . Option (1) will be the case in *e.g.* ethylene ( $\text{C}_2\text{H}_4$ ) with the hydrogen atoms at the hybridized ( $\text{P}_\text{N}^* + \text{D}_\text{N}$ ). Allenes provide an elegant example of option (2) and (3) in this respect, because in allenes the central carbon atom possesses both favorite symmetrical combinations, giving rise to the well-known two-bladed propeller geometry.<sup>28</sup>

The favorite combination in triple bonds will be  $\text{D}_\text{P}$  with  $\text{T}_\text{P}$ ,  $\text{T}_\text{P}$  with  $\text{D}_\text{P}$ , and  $\text{D}_\text{N}$  with  $\text{D}_\text{N}$  wherein the neutron of  $\text{T}_\text{P}$  is hybridized with  $\text{P}_\text{N}^*$ . In *e.g.* acetylene ( $\text{C}_2\text{H}_2$ ) this  $\text{P}_\text{N}^*$  bears the hydrogen atom. Molecule  $\text{N}_2$  also possesses this triple bond combination (*vide infra*, paragraph 2.4).

The structure of benzene is an intriguing one in the new model. As shown in Fig. 7A, when a symmetrical double bond is created between A and C of two ‘normal’ carbon atoms, B and D end up in a *cis*-position. So formation of the symmetrical double bond  $\text{P}_\text{N}^*$  with  $\text{T}_\text{P}$  and  $\text{T}_\text{P}$  with  $\text{P}_\text{N}^*$ , leads to a *cis*-position of the  $\text{D}_\text{P}$ 's (and *cis*-position for the  $\text{D}_\text{N}$ 's). The same symmetrical double bond, but with one of the carbon atoms inverted, leads to a *trans*-position of the  $\text{D}_\text{P}$ 's. By combining alternatingly three “normal” and three “inverted” carbon atoms in the way shown in Fig. 7B, for benzene a fascinating structure is obtained wherein a double bond between  $\text{P}_\text{N}^*$  and  $\text{T}_\text{P}$  can be formed to the left and to the right. Or in other words, a resonance system is created that answers the famous Kekulé benzene-structure problem from 1865.<sup>29,30</sup> Other examples of  $\text{P}_\text{N}^*-\text{T}_\text{P}$  resonance, namely between C and O, will be dealt with in paragraph 2.4.

**2.2.2 Carbon isotopes.** Compared with  $^{12}_6\text{C}$ , atom  $^{13}_6\text{C}$  bears a  $\text{D}_\text{N}^*$  instead of a  $\text{P}_\text{N}^*$ . This constellation of a carbon atom appears to be stable also, but the abundance of  $^{13}_6\text{C}$  is not high (1.1% abundance) (Fig. 8).

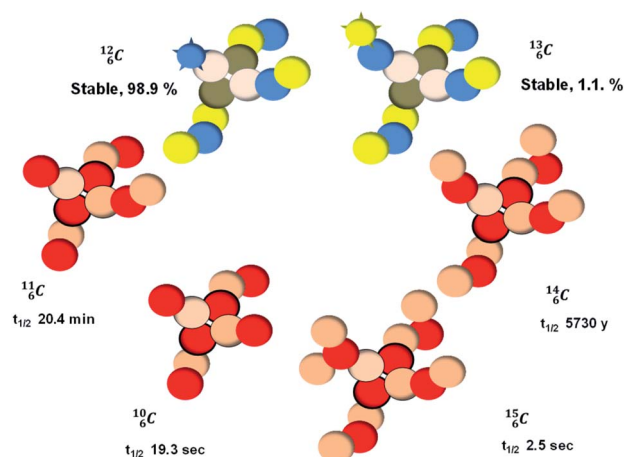


Fig. 8 Constellation of the main isotopes of carbon ( $1s^2 2s^2 2p^2$ ) in the new model.





The well-known long-living carbon isotope  $^{14}\text{C}$  ( $t_{1/2}$  of 5730 y, decays to  $^{14}\text{N}$ ) bears two  $\text{D}_\text{N}$ 's and two  $\text{T}_\text{P}$ 's. In the  $^{15}\text{C}$  atom there is no obvious place for the additional neutron: an exotic  $\text{T}_\text{N}$  is formed, and this isotope decays immediately ( $t_{1/2}$  2.5 s, decays to  $^{15}\text{N}$ ). Radioisotope  $^{11}\text{C}$  ( $t_{1/2}$  20.4 min, decays to  $^{11}\text{B}$ ) bears, compared to  $^{12}\text{C}$ , a  $\text{D}_\text{P}$  instead of a  $\text{T}_\text{P}$ , while in radioisotope  $^{10}\text{C}$  ( $t_{1/2}$  19.3 s, decays to  $^{10}\text{B}$ ) also the neutron at the  $\text{D}_\text{N}$  is missing (Fig. 8). From the latter constellation, it can be concluded that  $^{10}\text{C}$  is the last carbon isotope that can chemically react as carbon. For the radioisotopes  $^9\text{C}$  and  $^8\text{C}$  there is no obvious place for the proton, and these radioisotopes are therefore extremely fast deteriorating nuclei, ending up as  $\alpha$ -particles, mostly *via* proton loss.

In the new atom model, the weak nuclear force is transformed into a stability rule for each anchor side. The carbon isotopes  $^{12}\text{C}$  and  $^{13}\text{C}$  allow the deriving of these stability rules. The summarized subunits at the anchor proton side of the carbon isotopes  $^{12}\text{C}$  and  $^{13}\text{C}$  give  $n = 3, p = 2$ , with  $n$  for neutron and  $p$  for proton. When  $n = 2, p = 2$  ( $^{10}\text{C}, ^{11}\text{C}$ ) or  $n = 4, p = 2$  ( $^{14}\text{C}, ^{15}\text{C}$ ), the atom is instable. So our new model indicates that in order to be stable, the summarized number of neutrons at the anchor proton side should exceed that of protons by exactly one *i.e.* should follow the stability rule  $n = p + 1$ . Applying the same approach for the anchor neutron side, and counting a square neutron or proton for  $\frac{1}{2}$ , the stability rule for  $^{12}\text{C}$  and  $^{13}\text{C}$  appears to be  $n = p - \frac{1}{2}$ , namely  $n = 1, p = 1\frac{1}{2}$  for  $^{12}\text{C}$  and  $n = 1\frac{1}{2}, p = 2$  for  $^{13}\text{C}$ . Because radioisotopes produced in a cyclotron or neutron generator do not contain square protons or square neutrons (*vide supra* 1.1), the four carbon radioisotopes  $^{10}\text{C}, ^{11}\text{C}, ^{14}\text{C}$  and  $^{15}\text{C}$  deviate from the anchor neutron stability rule as well. In the new atom model, conversion will, therefore, take place until the new-born constellations comply to both rules.

### 2.3 The elements $Z = 1-6$

For an insight in how we arrived at the  $^{12}\text{C}$  atom constellation, and for a demonstration of the general applicability of the stability rules, first a short overview of the atom configuration of the elements with  $Z = 1-6$  in the new model.

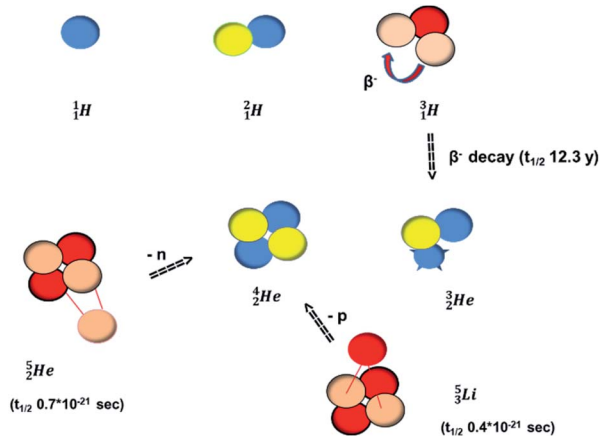


Fig. 9 Constellation of the main isotopes of hydrogen ( $1s$ ), helium ( $1s^2$ ) and  $^3\text{Li}$  in the new model, including transfer of the newborn proton during decay in case of  $^3\text{H}$  (red lines represent artificial distance, drawn for the sake of clarity; curved arrow indicates conversion plus shift).

**2.3.1 The  $1s$  and  $1s^2$ -elements H and He ( $Z = 1$  and  $Z = 2$ ).** The simplest of nuclei to demonstrate the transfer of a newborn proton after conversion of a neutron into a proton is the  $\beta^-$ -emitting radioisotope  $^3\text{H}$  ( $t_{1/2}$  12.3 y), also called tritium, and its daughter  $^3\text{He}$  (Fig. 9).

At the same time, the  $^3\text{He}$ -atom can be taken as the prototype of an atom that bears a square proton (Fig. 9). Because of this square proton, the  $^3\text{He}$ -atom is stable and in fact it is the only stable atom in the periodic system with more protons than neutrons. Its abundance is only  $1.34 \times 10^{-4}\%$ , so most probably originating solely from the decay of cosmic-produced  $^3\text{H}$ . With the noble gas  $^4\text{He}$ , a unit consisting of two neutrons and two protons alternatingly linked with each other, the first row ends. When adding an additional neutron at the anchor proton side, forming  $^5\text{He}$ , the neutron is immediately emitted ( $t_{1/2}$   $0.7 \times 10^{-21}$  s).

**2.3.2 The  $1s^2 2s$ - and  $1s^2 2s^2$ -elements Li and Be ( $Z = 3$  and  $Z = 4$ ).** With  $^4\text{He}$  as building block, it appears that the addition of a proton as the only subunit is not accepted (Fig. 9): from the thus assembled  $^5\text{Li}$  the proton is immediately emitted ( $t_{1/2}$   $0.4 \times 10^{-21}$  s). Adding a proton to the anchor neutron side requires compensation in the form of a neutron at the anchor proton side. What is more, the latter new neutron as well as the new proton are shared to evenly divide the burden of the new situation. With this shared neutron between the anchor protons, two stable isotopes of lithium exist:  $^6\text{Li}$  (abundance 7.6%) bearing a shared  $\text{P}_\text{N}^*$  at the anchor neutron side, and  $^7\text{Li}$  (abundance 92.4%) bearing a shared  $\text{D}_\text{N}^*$  at the anchor neutron side (Fig. 10 and 11).

Introduction of a neutron at each anchor proton is too much: when the anchor proton side of  $^6\text{Li}$  is hit by a neutron the composite atom breaks down into  $^3\text{H}$  and an  $\alpha$ -particle (a  $^4\text{He}$ -unit),<sup>31</sup> whereas with the  $(n, \gamma)$  reaction on  $^7\text{Li}$ , giving  $^8\text{Li}$ , a radioisotope with a  $t_{1/2}$  of 0.8 s is produced.<sup>32</sup>

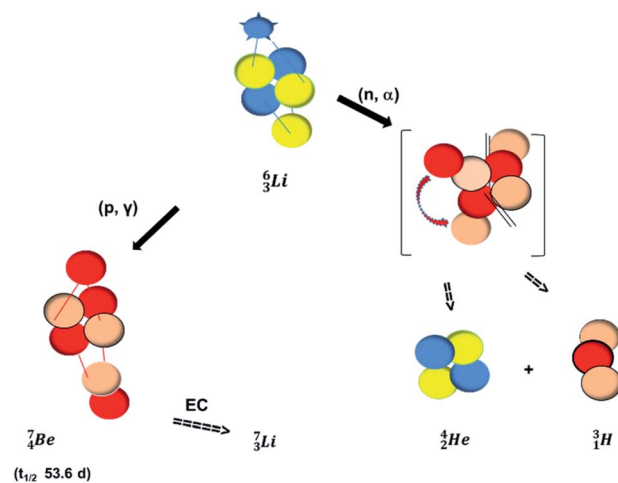


Fig. 10 Constellation of  $^6\text{Li}$  ( $1s^2 2s$ ) in the new model, including the decomposition of  $^6\text{Li}$  upon bombardment by neutrons and an illustrative production route to  $^7\text{Be}$  (red and blue lines represent artificial distance drawn for the sake of clarity, curved red pucker arrow indicates recombination, double black lines represent breakage).





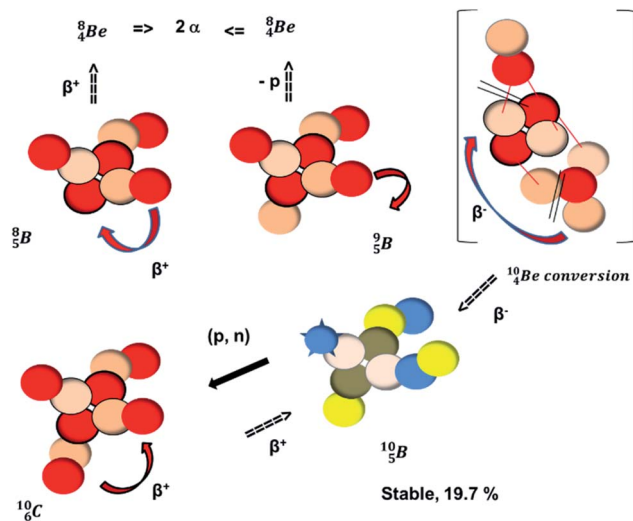


Fig. 13 Constellation of stable  $^{10}\text{B}$  ( $1s^22s^22p$ ) and of radioactive  $^8\text{B}$  and  $^9\text{B}$  in the new model, including conversions and some illustrative production routes.

deuteron part of the  $\alpha$ -particle is turned aside without interaction with the nucleus.

**2.3.3 The  $2s^22p$ - and  $2s^22p^2$ -elements B and C ( $Z = 5$  and  $Z = 6$ ).** The element boron is the second element whose constellation deviates from the Aufbau principle. Over and above that, the isotopes  $^{10}\text{B}$  and  $^{11}\text{B}$  are the first stable atoms that contain four separated subunits: both atoms bear a  $\text{D}_\text{N}$ , an  $\text{N}_\text{P}$  and a  $\text{D}_\text{P}$ , whereas  $^{10}\text{B}$  bears as the fourth a  $\text{P}_\text{N}^*$ ,  $^{11}\text{B}$  a  $\text{D}_\text{N}^*$  (Fig. 13 and 14). Consequently, the chemical versatility is increased. At the anchor proton side, the  $\text{D}_\text{P}$  can combine with the  $\text{N}_\text{P}$  and form a (formal) plus situation analogous to the one at the anchor proton side of  $^4\text{Be}$ . In combination with the  $\text{D}_\text{N}$  and the  $\text{P}_\text{N}^*$  ( $^{10}\text{B}$ ) or  $\text{D}_\text{N}^*$  ( $^{11}\text{B}$ ) at the anchor neutron side, this leads to the typical trigonal planar molecular geometry of boron compounds. Furthermore, the sole  $\text{N}_\text{P}$  represents the empty orbital of boron that exhibits chemical reactivity.  $\text{N}_\text{P}$  is capable of binding neutron-deficient ligands like

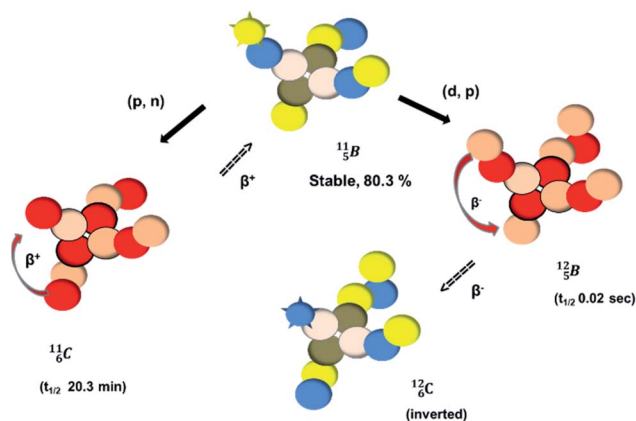


Fig. 14 Constellation of stable  $^{11}\text{B}$  ( $1s^22s^22p$ ) and of radioactive  $^{12}\text{B}$  in the new model, including conversions and two illustrative production routes.

water (as  $\text{BF}_3 \cdot \text{H}_2\text{O}$ ) or  $\text{F}^-$  (as  $\text{BF}_4^-$ ) with tetrahedral-like molecular geometry (see also paragraph 2.5).

Upon bombardment of  $^{10}\text{B}$  with protons, a (p, n) reaction gives the short living  $^{10}\text{C}$  ( $t_{1/2}$  19.5 s).<sup>39</sup> This  $^{10}\text{C}$  converts back to  $^{10}\text{B}$  via  $\beta^+$ -decay, which means that the  $^{10}\text{B}$  atom is formed as daughter isotope from  $^{10}\text{C}$  as well as from  $^{10}\text{B}$ . In case of  $^{10}\text{Be}$ , the neutron of the shared  $\text{T}_\text{P}$  at the anchor proton side converts into a square proton at the anchor neutron side, while during this process the shared  $\text{T}_\text{P}$  and shared  $\text{D}_\text{N}$  break open (Fig. 13). In case of  $^{10}\text{C}$ , one of the  $\text{D}_\text{P}$  protons converts into a neutron ( $\beta^+$ -decay) and forms a  $\text{D}_\text{N}$  with one of the  $\text{P}_\text{N}$ 's.

Upon bombardment of  $^{11}\text{B}$  with protons, a (p, n) reaction gives radioisotope  $^{11}\text{C}$  (Fig. 14).<sup>40</sup> This carbon radioisotope converts back to  $^{11}\text{B}$  via  $\beta^+$ -decay. Radioisotopes  $^8\text{B}$ ,  $^9\text{B}$  and  $^{12}\text{B}$  are very instable isotopes:  $^8\text{B}$  ( $\beta^+$ -decay) and  $^9\text{B}$  (proton emission) end up via  $^8\text{Be}$  as  $\alpha$ -particles, while  $^{12}\text{B}$  decays to  $^{12}\text{C}$  with a  $t_{1/2}$  of 0.02 s. The short half-life of radioisotope  $^{12}\text{B}$ , that is produced by a (d, p) reaction on  $^{11}\text{B}$ ,<sup>41</sup> confirms that two full  $\text{D}_\text{N}$ 's at the anchor neutron side together with the fact that the anchor proton side bears three neutrons versus one proton, give rise to severe instability.

Both stable boron isotopes  $^{10}\text{B}$  and  $^{11}\text{B}$  fit with the stability rules, with their  $n = 2, p = 1$  at the anchor proton side, and its  $n = 1, p = 1\frac{1}{2}$  and its  $n = 1\frac{1}{2}, p = 2$  at the anchor neutron side, respectively.

## 2.4 Nitrogen ( $Z = 7$ ), oxygen ( $Z = 8$ ) and their lone pairs

**2.4.1 Nitrogen.** With the atoms nitrogen (N) and oxygen (O) we now arrive at the lone pair principle of the new model. It appears that the  $^{14}\text{N}$  atom at the anchor neutron side possesses as lone pair a  $^3\text{He}$ -unit with a square proton (Fig. 15). Nitrogen is the first atom, since Li, that follows the Aufbau principle again ( $1s^22s^22p^3$ ). Fig. 15 also shows the constellation of the stable  $^{15}\text{N}$  (0.4% abundance), of the instable  $^{16}\text{N}$  ( $t_{1/2}$  7.1 s, decays to  $^{16}\text{O}$ ) and of the instable  $^{13}\text{N}$  ( $t_{1/2}$  9.96 min, decays to  $^{13}\text{C}$ ). The  $^{16}\text{N}$  isotope is produced by a (n,  $\gamma$ ) or (d, p) on  $^{15}\text{N}$ ,<sup>42,43</sup> and by a (n, p) on  $^{16}\text{O}$ .<sup>44</sup> These impacts give insight in the

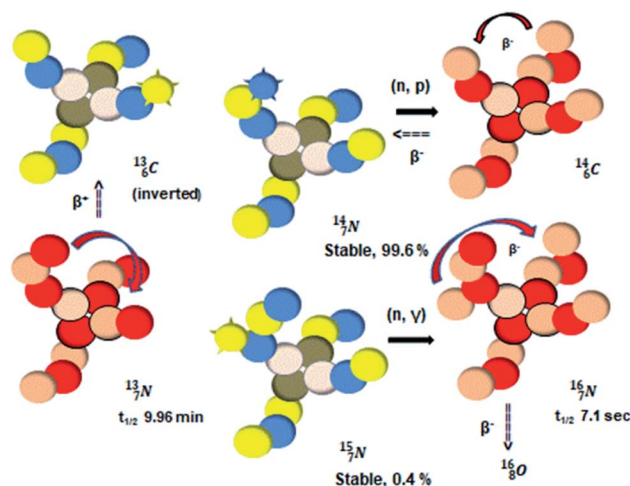


Fig. 15 Constellation of the main isotopes of nitrogen ( $1s^22s^22p^3$ ) in the new model, including conversions.





position of the second lone pair in the constellation of oxygen (see Fig. 18 in the next paragraph). Atoms  $^{14}\text{N}$  and  $^{15}\text{N}$  both have  $n = 3$ ,  $p = 2$  at the anchor proton side, just like  $^{12}\text{C}$  and  $^{13}\text{C}$ . At the anchor neutron side it is  $n = 2$ ,  $p = 2\frac{1}{2}$  for  $^{14}\text{N}$ , for  $^{15}\text{N}$  it is  $n = 2\frac{1}{2}$ ,  $p = 3$ . So both constellations obey the derived stability rules.

Radioactive  $^{13}\text{N}$  is produced in a cyclotron in various ways (Fig. 16). It is therefore an effectual isotope to demonstrate the consistency of the adjusted atom model in the field of isotope production.

The  $^{13}\text{N}$  atom is produced *via* a ( $\alpha$ , n) on  $^{10}\text{B}$ ,  $^{45-47}$  a (d, n) or (p,  $\gamma$ ) on  $^{12}\text{C}$ ,  $^{41b, 48-50}$  a (p, n) on  $^{13}\text{C}$ ,  $^{51}$  a (p, d) on  $^{14}\text{N}$   $^{52}$  and a (p,  $\alpha$ ) on  $^{16}\text{O}$   $^{51}$  (Fig. 16). In all cases, the impact takes place at the  $\text{D}_\text{N}$ -unit (for  $^{10}\text{B}$  the impact takes place at the  $\text{D}_\text{N}$ -unit and the  $\text{N}_\text{P}$ -unit in the way described for the  $\alpha$ -bombardment of  $^9\text{Be}$ , producing  $^{12}\text{C}$ ). The  $\text{D}_\text{N}$  is converted into a  $^3\text{He}_\text{N}$ -unit containing a full energy proton (not a square one), which leads to a fast decay ( $n = 1$ ,  $p = 3$  at the anchor neutron side). After proton impact on  $^{13}\text{C}$ ,  $^{14}\text{N}$  and  $^{16}\text{O}$ , the rule “last in, first out” is followed: for  $^{13}\text{C}$  the square neutron of the  $\text{D}_\text{N}^*$  is thrown out, for  $^{14}\text{N}$  the  $\text{D}^*$ -fragment from the  $^3\text{He}_\text{N}$ -unit, while for  $^{16}\text{O}$  the thrown-out  $\alpha$ -particle consists of the deuteron-parts from the  $^4\text{He}_\text{P}$ - and  $^3\text{He}_\text{N}$ -unit (see next paragraph for the configuration of  $^{16}\text{O}$ ). In the case of  $^{12}\text{C}$  as target material, the combined (d, n) and (p,  $\gamma$ ) bombardment,  $^{48, 49}$  both producing the same  $^{13}\text{N}$ , indicate that the proton of the incoming deuteron is built in and its neutron is turned aside without interaction with the nucleus. Notably, for  $^{10}\text{B}$  and  $^{12}\text{C}$  an additional consequence of the impact at  $\text{D}_\text{N}$  is the activation of  $\text{P}_\text{N}$  into a full energy proton.

The  $^{14}\text{C}$  atom, either produced in a neutron generator or in the cosmos, comes from a (n, p) reaction on  $^{14}\text{N}$  (Fig. 15).  $^{53}$  The neutron is incorporated onto the  $\text{D}_\text{P}$  of the  $^{14}\text{N}$ -atom, while throwing out the square proton of the  $^3\text{He}_\text{N}$ -unit, whereas  $^{14}\text{C}$  decays back to  $^{14}\text{N}$  by converting the neutron of the newborn  $\text{T}_\text{P}$  into a square proton at the  $\text{D}_\text{N}$ , forming the  $^3\text{He}_\text{N}$ -unit.

Lastly, atom  $^{11}\text{C}$  is, in addition to a (p, n) reaction on  $^{11}\text{B}$ , also produced *via* a (p,  $\alpha$ ) reaction on  $^{14}\text{N}$ .  $^{54}$  This (p,  $\alpha$ ) on  $^{14}\text{N}$  giving

$^{11}\text{C}$ , implies the impact of the proton at the  $\text{T}_\text{P}$  of the  $^{14}\text{N}$  atom. The thrown-out  $\alpha$ -particle consists of the deuteron parts from the  $^3\text{He}_\text{N}$ - and the  $\text{T}_\text{P}$ -unit. Thereby these two carbon isotope productions also follow the rule “last in, first out”.

**2.4.2 Molecules of nitrogen with hydrogen and carbon.** In  $\text{NH}_3$  (gas), the  $^3\text{He}_\text{N}$ -unit is a chemically quietened lone pair by hybridization with  $\text{T}_\text{P}$ , while  $\text{D}_\text{N}$  and  $\text{D}_\text{P}$  are hybridized as in the  $\text{CH}_4$ -molecule. These hybridized couples can easily flip, leading to the well-known pyramidal inversion of  $\text{NH}_3$ . In the new model no spontaneous tunneling of hydrogen atoms is required.  $^{55, 56}$  Notably, in  $\text{N}_2$ , the  $^3\text{He}_\text{N}$ -unit is also chemically quietened *via* hybridization with  $\text{T}_\text{P}$ , and the triple bond of the  $\text{N}_2$ -molecule consists of two mutual  $\text{D}_\text{P}$ - $\text{T}_\text{P}$  bonds plus a  $\text{D}_\text{N}$ - $\text{D}_\text{N}$  bond. In  $\text{NH}_4^+$ ,  $\text{T}_\text{P}$  is hybridized with  $\text{D}_\text{P}$ . At the anchor neutron side, the square proton of the  $^3\text{He}_\text{N}$ -unit is hybridized with the neutron of  $\text{D}_\text{N}$ , forming a symmetrical bridgehead at the anchor neutron side.

The full-energy proton of the  $^3\text{He}_\text{N}$ -unit forms the fourth NH-bond (Fig. 17A), whereas the square proton has turned over its electron to this latter hydrogen atom. Notably, the oxygen atom (see next paragraph) can even force both protons of the  $^3\text{He}_\text{N}$ -unit into covalent bond formation, demonstrating the versatility of the  $^3\text{He}_\text{N}$ -unit.

In combination with carbon, the intriguing existence of *Z* and *E* (formerly called *syn* and *anti*) isomers for N-alkyl substituted imines ( $\text{R}^1\text{R}^2\text{C}=\text{NR}^3$ ) provides a telling example.  $^{57-59}$  The stereo-isomerism originates from the fact that the double bond between carbon and nitrogen is a symmetrical one (carbon- $\text{D}_\text{P}$  with nitrogen- $\text{D}_\text{N}$ , carbon- $\text{D}_\text{N}$  with nitrogen- $\text{D}_\text{P}$ ), but with either a “normal” or an “inverted” nitrogen atom (Fig. 6 and 7A).

**2.4.3 Oxygen.** In Fig. 18, the constellation is depicted of the stable oxygen isotopes  $^{16}\text{O}$  (abundance 99.76%),  $^{17}\text{O}$  (abundance

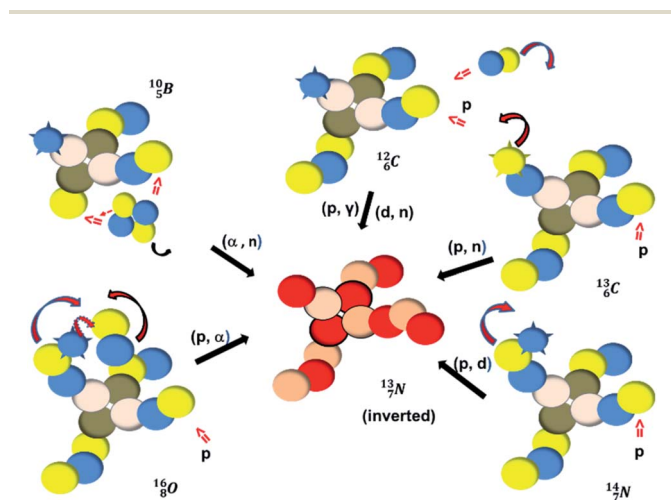


Fig. 16 Illustration of the consistency in production routes in the new model illustrated by production of  $^{13}\text{N}$  (red arrows indicate the point of impact).

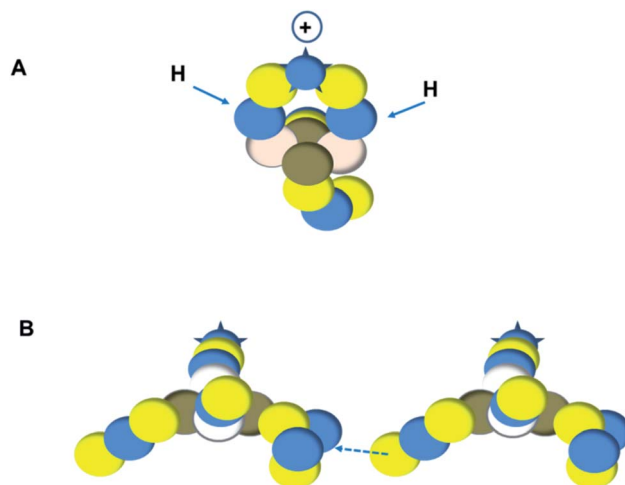


Fig. 17 Special lone pairs of nitrogen and oxygen: (A) formation of a bridgehead between the  $^3\text{He}_\text{N}$ -lone pair and the  $\text{D}_\text{N}$  of the nitrogen or oxygen atom, giving rise to the distorted tetrahedral  $\text{NH}_4^+$  or  $\text{H}_3\text{O}^+$  molecule (hydrogens at the anchor proton side are not shown); (B) the formation of a “hydrogen bond” *via* a neutron link between the oxygen- $\text{T}_\text{P}$  of a  $\text{H}_2\text{O}$  molecule and the neutron-deficient  $^4\text{He}_\text{P}$ -lone pair of the oxygen atom of a neighboring  $\text{H}_2\text{O}$  molecule (dashed blue arrow means formation of hydrogen bond).





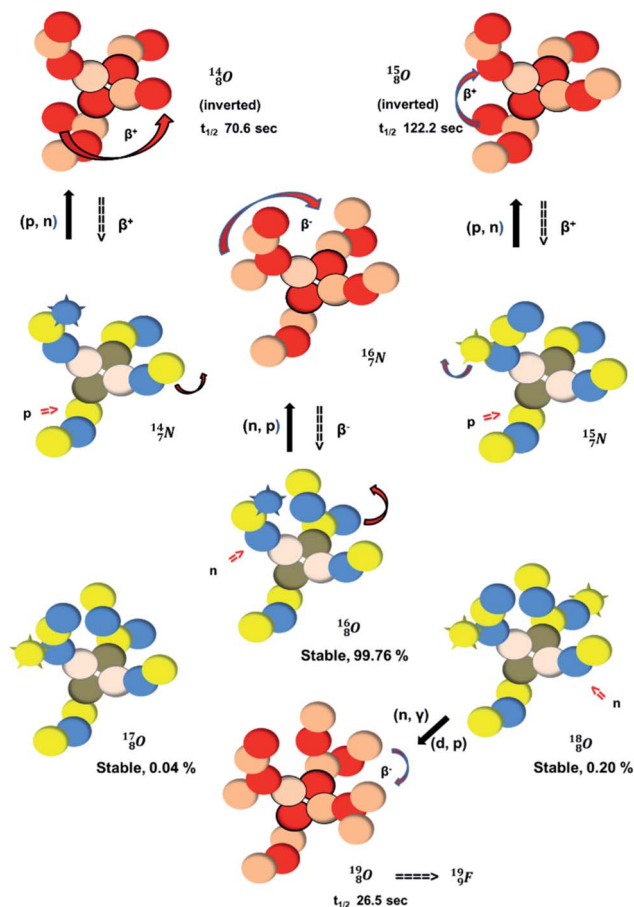


Fig. 18 Constellation of the main isotopes of oxygen ( $1s^2 2s^2 2p^4$ ) in the new model, including production and conversion of the instable ones.

0.04%) and  $^{18}\text{O}$  (abundance 0.2%), together with that of the instable oxygen isotopes  $^{14}\text{O}$  ( $t_{1/2}$  70.6 s),  $^{15}\text{O}$  ( $t_{1/2}$  122.2 s) and  $^{19}\text{O}$  ( $t_{1/2}$  26.5 s).

The main oxygen isotope  $^{16}\text{O}$  bears at the anchor neutron side the same  $\text{D}_\text{N}$  and the same versatile  ${}^3\text{He}_\text{N}^*$ -unit as described above for  $^{14}\text{N}$ , so  $n = 2$ ,  $p = 2\frac{1}{2}$ . It differs, however, from  $^{14}\text{N}$  by bearing a  ${}^4\text{He}_\text{P}$ -unit at the anchor proton side instead of a  $\text{D}_\text{P}$ . This  ${}^4\text{He}_\text{P}$  lone pair possesses an intriguing property, it is slightly neutron-deficient and is not closed yet ("open" lone pair). The  ${}^4\text{He}_\text{P}$ -unit is chemically closed upon interaction with an additional neutron, but not necessarily a neutron from its own constellation. The water molecule forms a beautiful illustration of this latter aspect (*vide infra*). Notably, one of the protons of this  ${}^4\text{He}_\text{P}$ -unit is thrown out in the (n, p) reaction on  $^{16}\text{O}$ , producing  $^{16}\text{N}$  (see Fig. 18).

With regard to other nuclear aspects,  $^{16}\text{O}$  and  $^{17}\text{O}$  bear with  $n = 4$ ,  $p = 3$  at the anchor proton side exactly one neutron more than the number of protons, obeying the stability rule. Atom  $^{17}\text{O}$  possesses the same anchor neutron subunits as  $^{15}\text{N}$ . Atom  $^{18}\text{O}$  is as neutron-saturated as  $^{14}\text{C}$  and  $^{10}\text{Be}$  are. The latter radioisotopes slowly convert a neutron into a proton, yielding  $^{14}\text{N}$  and  $^{10}\text{B}$ , respectively. In case of the  $^{18}\text{O}$  isotope, however, conversion

of a neutron into a proton yielding  $^{18}\text{F}$ , does not occur. In fact, it is the other way around: radioactive  $^{18}\text{F}$  decays to  $^{18}\text{O}$ . In  $^{18}\text{O}$  its tenth neutron appears to remain as a square neutron in the  ${}^4\text{He}_\text{P}$ -lone pair, as  ${}^5\text{He}_\text{P}^*$ -unit. With that,  $^{18}\text{O}$  is the first example of an isotope that is stable, despite its  $n = 4\frac{1}{2}$ ,  $p = 3$  at the anchor proton side *i.e.* the first isotope that follows a special anchor proton side stability rule, namely  $n = p + 1\frac{1}{2}$ .

For the  $^{19}\text{O}$  atom, produced either by a (n,  $\gamma$ ) or (d, p) reaction on  $^{18}\text{O}$ ,<sup>60,61</sup> or a (n, p) on  $^{19}\text{F}$ ,<sup>62</sup> there is, like  $^{15}\text{C}$ , no obvious place for the additional neutron, so again an exotic  $\text{T}_\text{N}$  is formed. This  $^{19}\text{O}$  isotope quickly decays ( $t_{1/2}$  26.5 s) to  $^{19}\text{F}$  *via* conversion of the neutron of the  ${}^5\text{He}_\text{P}$ -unit into a proton onto this  $\text{T}_\text{N}$ . Isotope  $^{15}\text{O}$  is produced *via* a (p, n) reaction on enriched  $^{15}\text{N}$ .<sup>63</sup> The proton impact takes place at the  $\text{T}_\text{P}$  while the square neutron of the  ${}^4\text{He}_\text{N}^*$ -unit is thrown out (so again last in, first out). Its short half live ( $t_{1/2}$  122.2 s, converts back to  $^{15}\text{N}$  *via*  $\beta^+$ -decay) demonstrates that a  $n = 3$ ,  $p = 3$  at the anchor proton side is an unacceptable situation. Atom  $^{14}\text{O}$  ( $t_{1/2}$  70.6 s) is the last atom configuration that may chemically act like oxygen and decays to  $^{14}\text{N}$ . Atoms  $^{13}\text{O}$  and  $^{12}\text{O}$  are extremely unstable, these decay to  $^{13}\text{C}$  or  $^{12}\text{C}$ , and  $^{11}\text{B}$  or  $^{10}\text{B}$ , respectively, *via*  $\beta^+$  and/or proton emission.

**2.4.4 Molecules of oxygen with hydrogen (O with H).** In  $\text{H}_2\text{O}$ , the  $\text{T}_\text{P}$  and  $\text{D}_\text{N}$  of the oxygen atom bear the hydrogen atom. In alkaline solutions, the  $\text{OH}^-$ -group has lost its hydrogen atom at the  $\text{T}_\text{P}$ . In acidic solutions, producing the  $\text{H}_3\text{O}^+$ -molecule, the square proton of the oxygen –  ${}^3\text{He}_\text{N}^*$ -unit is hybridized with the neutron of the oxygen- $\text{D}_\text{N}$ , forming a symmetrical bridgehead at the anchor neutron side as in  $\text{NH}_4^+$ . The full-energy proton of the oxygen –  ${}^3\text{He}_\text{N}^*$ -unit has formed the third OH-bond (Fig. 17A).

As a gas, the oxygen atom in  $\text{H}_2\text{O}$  is hybridized *via*  $\text{T}_\text{P}$  with the  ${}^3\text{He}_\text{N}^*$ -unit and  $\text{D}_\text{N}$  with the  ${}^4\text{He}_\text{P}$ -unit. As such, the  $\text{H}_2\text{O}$  molecule perfectly fits with the four different energy levels (2 OH-peaks, 2 lone pair peaks) observed in the photo-electronic spectra of  $\text{H}_2\text{O}$  ("no rabbit ears on the water").<sup>64</sup>

As a liquid,  $\text{H}_2\text{O}$  is a temperature-dependent mixture of the gas-phase hybridized form and a hybridized form in which the  ${}^3\text{He}_\text{N}^*$ -unit is linked with  $\text{D}_\text{N}$ , and in which the  $\text{T}_\text{P}$  is not linked intra-atomic with the  ${}^4\text{He}_\text{P}$ -unit, but with the  ${}^4\text{He}_\text{P}$ -unit of a neighboring water molecule (Fig. 17B). Such an energetically favorable closure of the  ${}^4\text{He}_\text{P}$ -unit by a neighboring neutron is the basis for hydrogen bonds, hydrates, and *e.g.* crystal water.

As a solid (around zero degrees and lower), the predominant form of  $\text{H}_2\text{O}$  will be the fully de-hybridized one, *i.e.* neutron ("hydrogen") bonds between  $\text{T}_\text{P}$  and the  ${}^4\text{He}_\text{P}$ -unit or  ${}^3\text{He}_\text{N}^*$ -unit of a neighboring water molecule, and neutron bonds between  $\text{D}_\text{N}$  and the  ${}^3\text{He}_\text{N}^*$ -unit or  ${}^4\text{He}_\text{P}$ -unit of a neighboring water molecule. This fully de-hybridized form of the water molecule corresponds with expansion, which means a change in volume and, therefore, a change in density. Dissolved cations, but also the  $^{17}\text{O}$  isotope with a square neutron at the  ${}^3\text{He}_\text{N}^*$ -unit and the  $^{18}\text{O}$  isotope with an additional square neutron at the  ${}^4\text{He}_\text{P}$ -unit (see Fig. 18) will of course disrupt this hydrogen bond network, and might well be part of the reason behind the geometric variation in hexagonal-shaped snowflakes.



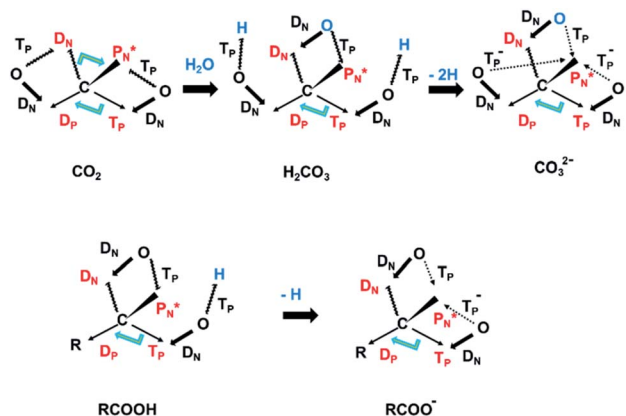


Fig. 19 Some illustrative carbon–oxygen combinations in the new model: (a)  $\text{CO}_2$ ; (b)  $\text{H}_2\text{CO}_3$  and resonance in  $\text{CO}_3^{2-}$ ; (c)  $\text{RCOOH}$  and resonance in  $\text{RCOO}^-$  (blue hooked arrow indicates hybridization).

**2.4.5 Molecules of oxygen with carbon (O with C).** From the various combinations of oxygen with carbon, Fig. 19 gives a few typical examples.

In carbon dioxide ( $\text{CO}_2$ ), the  $\text{D}_\text{N}$  of each oxygen atom is bound to the hybridized carbon ( $\text{T}_\text{P} + \text{D}_\text{P}$ ), the  $\text{T}_\text{P}$  of each oxygen atom is bound to the hybridized carbon ( $\text{P}_\text{N}^* + \text{D}_\text{N}$ ). Upon dissolving of  $\text{CO}_2$  in water, carbonic acid ( $\text{H}_2\text{CO}_3$ ) is formed. In this process, the two oxygen  $\text{T}_\text{P}$ 's become detached from the carbon ( $\text{P}_\text{N}^* + \text{D}_\text{N}$ ), forming two OH-groups, while the oxygen of the incoming  $\text{H}_2\text{O}$  molecule becomes bound with its  $\text{T}_\text{P}$  to the carbon  $\text{P}_\text{N}^*$  and with its  $\text{D}_\text{N}$  to the carbon  $\text{D}_\text{N}$ .

In ketones, aldehydes and carboxylic acids the double-bonded oxygen atom is bound in the same way to carbon's  $\text{P}_\text{N}^*$  and  $\text{D}_\text{N}$ , whereas the anchor proton side of that C-atom is hybridized into the ( $\text{T}_\text{P} + \text{D}_\text{P}$ ) form. Keto–enol tautomerism and chemical attack on ketones take place at  $\text{P}_\text{N}^*$  whereby the oxygen- $\text{T}_\text{P}$  of the double-bonded oxygen becomes OH or  $\text{O}^-$ . In carboxylic acids ( $\text{RCOOH}$ ), the OH-group is bound with its oxygen- $\text{D}_\text{N}$  to the hybridized carbon ( $\text{T}_\text{P} + \text{D}_\text{P}$ ). The oxygen- $\text{T}_\text{P}$  of this OH-group loses its hydrogen relatively easily because the oxygen- $\text{T}_\text{P}^-$  can form a resonance system with the versatile oxygen- $\text{T}_\text{P}$  plus carbon –  $\text{P}_\text{N}^*$  combination of the double-bonded oxygen. Finally, in phenols the OH-group is bound with its oxygen- $\text{D}_\text{N}$  to a  $\text{D}_\text{N}$  of the benzene ring, after which the oxygen- $\text{T}_\text{P}^-$  becomes part of the resonance system in alkaline solutions.

**2.4.6 Molecules of oxygen with nitrogen (O with N).** The colorless gas nitric oxide (NO) is a free radical compound disobeying the octet rule. It dimerizes only upon condensing to a liquid ( $-152^\circ\text{C}$ ), but the association of the presumed N-radicals is weak and reversible and the N–N distance in crystalline NO ( $-164^\circ\text{C}$ ) is reported to be nearly twice the NO distance.<sup>65,66</sup> In the new model, NO is a symmetrically balanced molecule containing a triple bond between oxygen and nitrogen with the oxygen atom containing the unpaired electron (Fig. 20).

The oxygen –  $\frac{3}{2}\text{He}^*$ -unit has formed a bridgehead with its  $\text{D}_\text{N}$ . The square proton of the  $\frac{3}{2}\text{He}_\text{N}^*$ -unit has kept its non-activated low-energy electron, whereas the remaining  $\text{D}_\text{N}$  of the  $\frac{3}{2}\text{He}_\text{N}^*$ -unit together with the  $\text{D}_\text{N}$  form two bonds with the

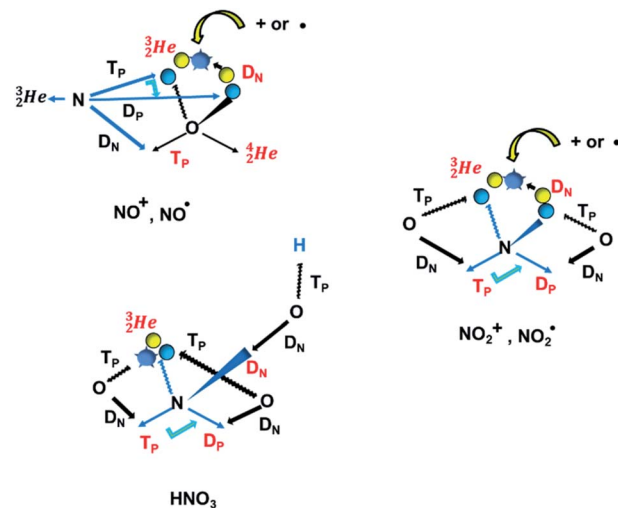


Fig. 20 Some illustrative nitrogen–oxygen combinations in the new model: (a)  $\text{NO}^+/\text{NO}^\bullet$ ; (b)  $\text{NO}_2^+/\text{NO}_2^\bullet$ ; (c)  $\text{HNO}_3$ .

hybridized nitrogen-( $\text{T}_\text{P} + \text{D}_\text{P}$ ). The third bond is formed between the oxygen- $\text{T}_\text{P}$  and the nitrogen- $\text{D}_\text{N}$ . In the compound  $\text{NO}^+$  the square  $\frac{3}{2}\text{He}_\text{N}^*$ -proton has lost its electron.

In  $\text{NO}_2^\bullet$  and  $\text{NO}_2^+$ ,<sup>67</sup> the nitrogen atom is the central atom with a bridge-headed ( $\frac{3}{2}\text{He}_\text{N}^* + \text{D}_\text{N}$ )-unit and the square proton of the  $\frac{3}{2}\text{He}_\text{N}^*$ -unit keeping its non-activated low energy electron or not. Each oxygen- $\text{T}_\text{P}$  is bound to the  $\text{D}_\text{N}$ 's of the bridge-headed ( $\frac{3}{2}\text{He}_\text{N}^* + \text{D}_\text{N}$ )-unit, each oxygen- $\text{D}_\text{N}$  is bound to the hybridized nitrogen-( $\text{T}_\text{P} + \text{D}_\text{P}$ ).

A final illustrative example is the acid  $\text{HNO}_3$ . This acid is a well-known octet rule disobeying compound (formally  $\text{N}^{5+}$  surrounded by 10 electrons) for which a Lewis structure has been developed. In the new atom model, the two double bonded oxygen atoms are bound with their  $\text{D}_\text{N}$  to the hybridized nitrogen-( $\text{T}_\text{P} + \text{D}_\text{P}$ ) of the nitrogen atom and with their  $\text{T}_\text{P}$  to the protons of the  $\frac{3}{2}\text{He}_\text{N}^*$ -unit. The oxygen of the OH-group bears an H-atom at its  $\text{T}_\text{P}$ , and is bound with its  $\text{D}_\text{N}$  to the nitrogen- $\text{D}_\text{N}$  (Fig. 20).

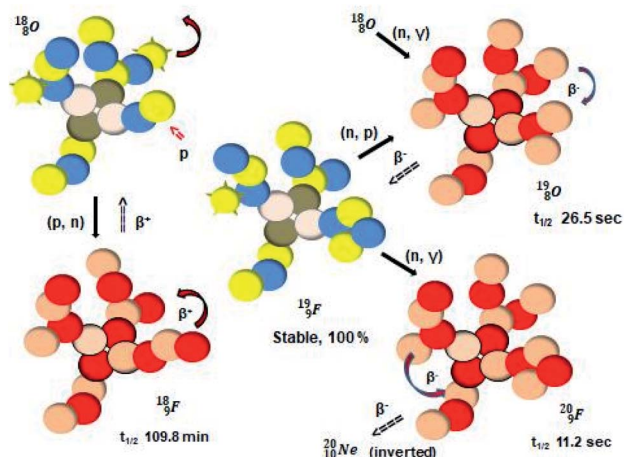


Fig. 21 Constellation of the main isotopes of fluorine ( $1s^2 2s^2 2p^5$ ) in the new model, including illustrative conversions.



## 2.5 Fluorine ( $Z = 9$ ), neon ( $Z = 10$ ) and their lone pairs

**2.5.1 Fluorine.** The fluorine atom  $^{19}\text{F}$  (100% abundance) possesses an open  $^4_2\text{He}_\text{N}^*$ -unit and a closed  $^4_2\text{He}_\text{N}$ -unit at the anchor neutron side, and, like  $^{16}\text{O}$ , a  $\text{T}_\text{P}$  and an open neutron-deficient  $^4_2\text{He}_\text{P}$ -unit at the anchor proton side (Fig. 21).

Closure of the latter unit by a neighboring neutron from an  $\text{H}_2\text{O}$  or  $\text{HF}$  molecule gives rise to a hydrogen bond. With its  $n = 4$ ,  $p = 3$  at the anchor proton side and  $n = 3\frac{1}{2}$ ,  $p = 4$  at the anchor neutron side,  $^{19}\text{F}$  follows the stability rules.

Radioisotope  $^{18}\text{F}$  ( $t_{1/2}$  110 min.), a widely known component of PET-chemistry, lacks the square neutron in the  $^4_2\text{He}_\text{N}^*$ -unit at the anchor neutron side. It is produced by a (p, n) reaction on  $^{18}\text{O}$ :  $^{68}$  the proton impact takes place at the  $\text{D}_\text{N}$ , forming a  $^3_2\text{He}_\text{N}$ -unit, and throws out the square neutron of the  $^5_2\text{He}_\text{P}^*$ -unit (last in, first out);  $^{18}\text{F}$  decays *via*  $\beta^+$ -emission back to  $^{18}\text{O}$  (Fig. 21). Notably,  $^{18\text{m}}\text{F}$  ( $t_{1/2}$  162 nanoseconds, decay to  $^{18}\text{F}^{69}$ ) is the result of the impact at  $\text{D}_\text{N}$  and throwing out the square neutron of the  $^4_2\text{He}_\text{N}^*$ -unit, giving two  $^3_2\text{He}_\text{N}$ -units with full energy protons; the IT to  $^{18}\text{F}$  implies the fast shift of a neutron from the  $^5_2\text{He}_\text{P}^*$ -unit to this very neutron-deficient anchor neutron side as a temporarily better situation. Radioisotope  $^{20}\text{F}$ , produced by a (n,  $\gamma$ ) reaction on  $^{19}\text{F}^{70}$  appears to be very unstable ( $t_{1/2}$  11 s) with its  $n = 4$ ,  $p = 4$  at the anchor neutron side and its  $n = 5$ ,  $p = 3$  at the anchor proton side, and decays quickly to  $^{20}\text{Ne}$ . Atom  $^{17}\text{F}$  ( $t_{1/2}$  65 s, produced by a (d, n) reaction on  $^{16}\text{O}^{71}$ ), bears two  $^3_2\text{He}_\text{N}$ -units and decays to  $^{17}\text{O}$  *via*  $\beta^+$ -emission (conversion of a proton from one of the  $^3_2\text{He}_\text{N}$ -units into a square neutron onto the other  $^3_2\text{He}_\text{N}$ -unit);  $^{16}\text{F}$  and lower are proton emitters.

**2.5.2 Neon.** With the noble gas neon, the quantum mechanical  $2s^2, 2p^6$ -series ends. Its main isotope  $^{20}\text{Ne}$  (abundance 90.48%) possesses at the anchor proton side a closed  $^4_2\text{He}_\text{P}$ -unit and a  $^5_2\text{He}_\text{P}$ -unit, at the anchor neutron side a  $^3_2\text{He}_\text{N}^*$ -unit and a closed  $^4_2\text{He}_\text{N}$ -unit. The  $^5_2\text{He}$ - and  $^3_2\text{He}$ -units are hybridized, and so are both  $^4_2\text{He}$ -units (Fig. 22).

Fig. 22 also shows the constellation of the stable isotopes  $^{21}\text{Ne}$  (0.27% abundance) and  $^{22}\text{Ne}$  (abundance 9.25%), and of the unstable  $^{19}\text{Ne}$  ( $t_{1/2}$  17.3 s). In the  $^{21}\text{Ne}$  atom, the  $^3_2\text{He}_\text{N}^*$ -unit

has become a  $^4_2\text{He}_\text{N}^*$ -unit with a square neutron like in  $^{19}\text{F}$ . The  $^{22}\text{Ne}$  atom bears two  $^5_2\text{He}_\text{P}$ -units (one with a square neutron) at the anchor proton side, and two  $^4_2\text{He}_\text{N}$ -units at the anchor neutron side (one with a square neutron). Neon isotopes  $^{20}\text{Ne}$ ,  $^{21}\text{Ne}$  both fit with the stability rules, with their  $n = 5$ ,  $p = 4$  at the anchor proton side and their  $n = 3$ ,  $p = 3\frac{1}{2}$  and  $n = 3\frac{1}{2}$ ,  $p = 4$ , respectively, at the anchor neutron side. The  $^{22}\text{Ne}$  atom is stable with  $n = 5\frac{1}{2}$ ,  $p = 4$  at the anchor proton side, and is, therefore, the second isotope that follows the special  $n = p + 1\frac{1}{2}$  anchor proton side stability rule. As was the case with  $^{18}\text{O}$ , the extra neutron appears to remain as a square neutron in the  $^4_2\text{He}_\text{P}$  lone pair, as  $^5_2\text{He}_\text{P}^*$ -unit, because conversion of a neutron into a proton yielding  $^{22}\text{Na}$ , does not occur. Again it is the other way around: radioactive  $^{22}\text{Na}$  decays to  $^{22}\text{Ne}$ .

In the short-living radioisotope  $^{19}\text{Ne}$ , the  $^5_2\text{He}_\text{P}$ -unit at the anchor proton side is replaced by a  $^4_2\text{He}_\text{P}$ -unit. During its production *via* a (p, n) reaction on  $^{19}\text{F}$ ,  $^{72}$  proton impact takes place at the  $\text{T}_\text{P}$  of  $^{19}\text{F}$  while the square neutron of the  $^4_2\text{He}_\text{N}^*$ -unit is thrown out. Atom  $^{19}\text{Ne}$  decays back to  $^{19}\text{F}$  *via* conversion of a proton from one of the  $^4_2\text{He}_\text{P}$ -units into a square neutron onto the  $^3_2\text{He}_\text{N}$ -unit ( $\beta^+$ -emission). Radioisotope  $^{18}\text{Ne}$  ( $t_{1/2}$  1.7 s) bears two  $^4_2\text{He}_\text{P}$ -units at the anchor proton side, and two  $^3_2\text{He}_\text{N}$ -units at the anchor neutron side. It decays as a first step to unstable  $^{18}\text{F}$  by conversion of a proton of one of the  $^4_2\text{He}_\text{P}$ -units below into a neutron at one of the  $^3_2\text{He}_\text{N}$ -units above. The short-living radioisotopes  $^{23}\text{Ne}$  ( $t_{1/2}$  37.1 s), and  $^{24}\text{Ne}$  ( $t_{1/2}$  3.38 min) at the right side of  $^{22}\text{Ne}$  will be dealt with in a forthcoming paper.

So in the new model also the last two elements of the  $2s^2, 2p^6$ -series, fluorine and neon, follow the remarkable regularity and consistency with respect to the stability or instability of the atoms. All stable isotopes  $Z = 3$ –10 appear to follow a strict  $n = p - \frac{1}{2}$  pattern at the anchor neutron side, and a  $n = p + 1$  pattern at the anchor proton side; only for  $^{18}\text{O}$  and  $^{22}\text{Ne}$  the pattern is  $n = p + 1\frac{1}{2}$ . Any deviation from these patterns leads to conversion. Another regularity is that the EC-decay of radioisotope  $^7\text{Be}$  as well as the  $\beta^+$ -decay of the nuclear medicine PET-isotopes  $^{11}\text{C}$ ,  $^{13}\text{N}$ ,  $^{15}\text{O}$  and  $^{18}\text{F}$  and of radioisotopes  $^{17}\text{F}$ ,  $^{19}\text{Ne}$  all imply conversion of a full energy proton into a square neutron. Even for  $^{10}\text{C}$  and  $^{14}\text{O}$  this is the case, although they seem to look like an exception: the newborn square neutron, temporarily bound as a square neutron to both  $\text{P}_\text{N}$ 's at the anchor neutron side, exchanges energy with the neighboring proton, leaving a  $\text{P}_\text{N}^*$  or  $^3_2\text{He}_\text{N}^*$ , respectively, behind under formation of a  $\text{D}_\text{N}$ .

**2.5.3 Poor fluorine atom.** The molecule  $\text{F}_2$  is extremely reactive with high heat release, and its bond strength is rather substandard ( $33 \text{ kcal mole}^{-1}$ ). $^{73}$  Taking  $^{20}\text{Ne}$ ,  $^{21}\text{Ne}$  and  $^{22}\text{Ne}$  as model, it can be derived that covalent bond formation strives in average for a chemical “ $^4_2\text{He}$  to  $^5_2\text{He}$ -unit” formation at the anchor proton side, and a chemical “ $^3_2\text{He}$  to  $^4_2\text{He}$ -unit” formation at the neutron anchor side. From the fact that F possesses a  $\text{T}_\text{P}$  as chemical binding unit, it follows that in case of the  $\text{F}_2$  molecule a  $\text{T}_\text{P}$  with a  $\text{T}_\text{P}$  is a very poor bond-proposition, because it would lead to a chemical “ $^6_2\text{He}$ -unit” as covalent bond. To avoid formation of an unfavorable chemical  $^6_2\text{He}$ -unit as covalent bond, the  $\text{T}_\text{P}$  of the F atom is compelled to hybridize with its  $^4_2\text{He}_\text{P}$ -unit. This forces the anchor protons a little closer to each other (and so the anchor neutrons a little further away from

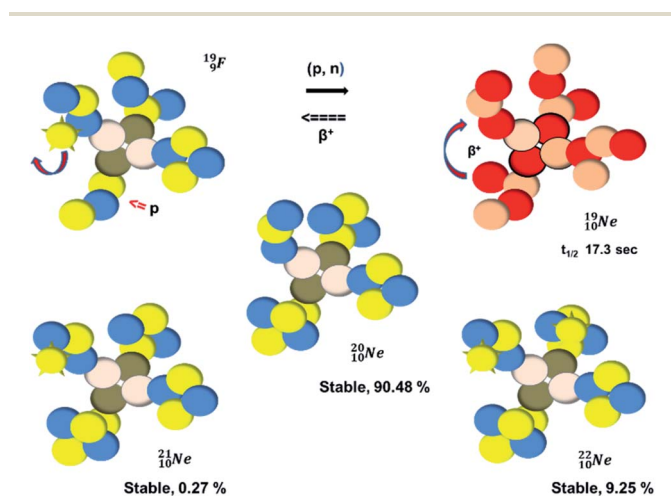


Fig. 22 Constellation of the main isotopes of neon ( $1s^2 2s^2 2p^6$ ) in the new model, including one illustrative conversion.





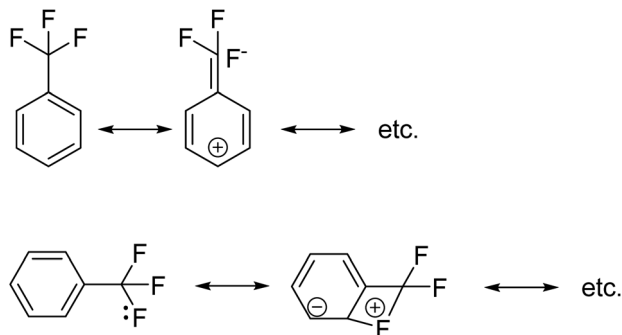


Fig. 23  $\text{CF}_3\text{-C}_6\text{H}_5$  in its double-bond no-bond resonance hypothesis (positive hyperconjugation hypothesis) and in its negative hyperconjugation hypothesis.

each other) creating an energetically disadvantageous tension. The high heat release upon reaction therefore originates from restoring the “normal” distance between the anchor protons and anchor neutrons. For the  $\text{O}_2$  molecule this bonding aspect is less problematic. The  $\text{O}_2$  molecule contains a solid bond between both  $\text{D}_\text{N}$ 's and a more fragile bond between both  $\text{T}_\text{P}$ 's, the neutrons of which are hybridized with their  ${}^3\text{He}_\text{N}^*$ -units, so no “ ${}^6\text{He}$ -ish” covalent bond, and therefore  $\text{O}_2$  reacts less extreme. The same holds for hydrogen peroxide ( $\text{H}_2\text{O}_2$ ) and its  $\text{T}_\text{P}\text{-T}_\text{P}$  bond. In acetyl hypofluorite ( $\text{CH}_3\text{COOF}$ ), the F-atom is bound to the  $\text{T}_\text{P}$  of the oxygen atom which is hybridized with its  ${}^3\text{He}_\text{N}^*$ -unit, and therefore this F-atom reacts less vigorous than in  $\text{F}_2$  (approximately as vigorous as  $\text{H}_2\text{O}_2$ ).

Upon reaction with the carbon atom, the fact that the  $\text{T}_\text{P}$  of fluorine strongly prefers covalent “ ${}^2\text{He}$ ”-bond formation leads to subtle conflicts. Upon bond formation with the  $\text{D}_\text{P}$  of carbon, the hybridized neutron (from  $\text{D}_\text{N}$  or  $\text{T}_\text{P}$ ) has to be pushed aside. This forced re-hybridization will have its effect on the carbon skeleton. At the anchor neutron side of the carbon atom, bond formation with  $\text{D}_\text{N}$  seems fine for the  $\text{T}_\text{P}$  of F, but a “ ${}^2\text{He}$ ”-bond is too much for the carbon- $\text{D}_\text{N}$ . The compromise will be a sort of “ ${}^4.5\text{He}$ ”-bond with the hybridized ( $\text{P}_\text{N} + \text{D}_\text{N}$ )-units. Bond formation with hybridized  $\text{P}_\text{N}$  will in case of a mono-fluorinated aliphatic compound suffer from easy elimination of HF in a process that resembles the keto-enol tautomerism for a carbonyl group. Finally, in the  $\text{CF}_3$ -group (one F at the  $\text{D}_\text{P}$  and two F's at the hybridized  $\text{P}_\text{N} + \text{D}_\text{N}$ ), the  $\text{T}_\text{P}$  of the carbon atom has become fully isolated and therefore exhibits more or less the same chemical behavior as the  $\text{T}_\text{P}$  of F, which explains *e.g.* the chemistry of the  $\text{CF}_3$ -group in trifluorotoluene ( $\text{CF}_3\text{-C}_6\text{H}_5$ ): in  $\text{CF}_3\text{-C}_6\text{H}_5$ , the isolated  $\text{T}_\text{P}$  of the carbon atom of the  $\text{CF}_3$ -group, bound at the  $\text{D}_\text{P}$  of the benzene ring, forces the benzene ring to re-hybridize, while the open neutron-deficient  ${}^4\text{He}_\text{P}$ -unit of the fluorine atoms of the  $\text{CF}_3$ -group interacts with the  $\text{D}_\text{N}$ -neutron of the neighboring carbon atoms of the benzene ring (the *ortho* positions). Notably, this explanation according to the new atom model, compiles in an elegant way the ‘double-bond no-bond’ resonance hypothesis, and the hypothesis wherein one of the three F-atoms of the  $\text{CF}_3$ -group has formed a bond with one of the carbon atoms at the *ortho*-position of the benzene ring (so with  $\text{F}^+$  formation) (Fig. 23).<sup>74,75</sup>

### 3 Concluding remarks

This paper describes a revolutionary adjustment of the reigning quantum mechanical atom model for the elements with  $Z = 1\text{--}10$ . The new atom model is based on the premise that in elements with low  $Z$  the mass is not concentrated for 99.9% in a very small dense positive inner core. In the adjusted model, which comprised a  ${}^4\text{He}$ -unit as backbone with various subunits ( $\text{P}_\text{N}$ ,  $\text{D}_\text{N}$ ,  $\text{D}_\text{P}$ ,  $\text{T}_\text{P}$ ,  ${}^3\text{He}_\text{N}$ ,  ${}^4\text{He}_\text{N}$ ,  ${}^4\text{He}_\text{P}$  and  ${}^5\text{He}_\text{P}$ ), the neutron has been given a much more prominent role than it has in the reigning quantum mechanical model. It is not just there to assist the strong force to surpass the repulsive coulombic forces between the protons in the nucleus, but the neutron is the modus operandi of the hybridization principle, molecular geometry and hydrogen bonds, and as such plays a part in chemical reactivity, bond length and bond strength, as shown for  $\text{F}_2$ . Moreover, the neutron plays an important role in the subtle change in the hybridization in the atom constellations of the molecule upon phase transition, as displayed for the boiling  $\text{H}_2\text{O}$  molecule.

The atom constellations arising from this new model not only provide an answer to the re-hybridizing power of fluorine, our primary objective. They also appear to be perfectly in accordance with the linear molecular geometry of beryllium, the trigonal planar molecular geometry of boron, and the tetrahedral molecular geometry of carbon, nitrogen and oxygen (including the special lone pairs of the latter two). In addition, the derived atom constellations follow a consistent pattern with respect to the stability of isotopes, the produced radioisotopes thereof, and the respective decay modes of the latter.

Other key topics are the new sound basis for covalent bond formation (formation of a “chemical” He-unit between a  $\text{P}_\text{N}$ ,  $\text{D}_\text{N}$ ,  $\text{D}_\text{P}$  or  $\text{T}_\text{P}$ -subunit with one of the subunits of the other atom), and the re-definition of the hydrogen bond (neutron bond between the  $\text{T}_\text{P}$ -subunit of the atom and the neutron-deficient  ${}^4\text{He}_\text{P}$ -unit or  ${}^3\text{He}_\text{N}^*$ -unit of a neighboring molecule). Furthermore, the new model offers an improved answer to phenomena like the hybridization principle, inversion, chirality, resonance and the secret behind the chemical reactivity of the empty orbital of boron.

In a forthcoming “Part II” we will investigate whether the adjusted model still holds for the slightly heavier elements  $Z = 11\text{--}20$ , and if so, what the configurations of the atoms Na ( $Z = 11$ ) through Ca ( $Z = 20$ ) look like in the new approach. And, as a further matter, whether the new model can provide a genuine solution for the occurrence of multiple valencies of the elements P, S, and Cl, with special attention to the well-known “octet-rule violating” compounds  $\text{H}_3\text{PO}_4$ ,  $\text{H}_2\text{SO}_4$  and  $\text{HClO}_4$ .

### Conflicts of interest

Prof. Dr A. D. Windhorst is editor-in-chief of Nuclear Medicine & Biology.

### Note added after first publication

This article replaces the version published on 19th August 2021, which contained multiple formatting errors.





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