Improved Numerical Generalization of the Bethe-Weizsäcker Mass Formula for Prediction the Isotope Nuclear Mass, the Mass Excess Including of Artificial Elements 119 and 120

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Abstract: George Gamow’s liquid drop model of the nucleus can account for most of the terms in the formula and gives rough estimates for the values of the coefficients. Its semi-numerical equation was first formulated in 1935 by Weizsäcker and in 1936 Bethe [1, 2], and although refinements have been made to the coefficients over the years, the structure of the formula remains the same today. Their formula gives a good approximation for atomic masses and several other effects, but does not explain the appearance of magic numbers of protons and neutrons, and the extra binding-energy and measure of stability that are associated with these numbers of nucleons. Mavrodiev and Deliyergiyev [3] formalized the nuclear mass problem in the inverse problem framework. This approach allowed them to infer the underlying model parameters from experimental observation, rather than to predict the observations from the model parameters. They formulated the inverse problem for the numerically generalized semi-empirical mass formula of Bethe and von Weizsäcker going step-by-step through the AME2012 [4] nuclear database. The resulting parameterization described the measured nuclear masses of 2564 isotopes with a maximal deviation of less than 2.6 MeV, starting from the number of protons and number of neutrons equal to 1. The unknown functions in the generalized mass formula was discovered in a step-by-step way using the modified procedure realized in the algorithms developed by Aleksandrov [5-7] to solve nonlinear systems of equations via the Gauss-Newton method. In the presented herein article we describe a further development of the obtained by [3] formula by including additional factors,- magic numbers of protons, neutrons and electrons. This inclusion is based the well-known experimental data on the chemically induced polarization of nuclei and the effect of such this polarization on the rate of isotope decay. It allowed taking into account resonant interaction of the spins of nuclei and electron shells. As a result the maximal deviation from the measured nuclear masses of less than 1.9 MeV was reached. This improvement allowed prediction of the nuclear characteristics of the artificial elements 119 and 120.  

Keywords: Bethe-Weizsäcker Mass Formula, Magic Numbers, Binding Energy, Wigner Term, Inverse Problem, Electrons-Nucleus Interaction, Chemical Polarization, Isotopes  

1. Introduction  
In the last few years there has appeared new experimental data which demonstrated the dramatic change of decay rate due to the ionization of an atom and due to the resonant interaction between the electron shells and the nuclei [8-14]. For example, a strong dependence of the nuclear decay rate on ionization was shown for the 229 Th 90, 226 Rn 88, 152 Eu 63, 154 Eu 63 isotopes and the 178 mHf 72, 99 mTc 43 isomers. Testing the effectiveness of accounting for the
interaction of nuclei and the electron shell for accuracy of a well-known formula expands our understanding of the structure of atoms and the possible contribution of nucleus interaction to the formation of compounds and biological structures. Deepening our understanding of the nature of the interaction of nuclear and chemical processes can be very important both in solving the problem of radioactive waste and in solving a number of problems in biology and medicine [15].

Following are the steps involved in the generalization of the BW mass formula.

2. Bethe-Weizsäcker Mass Formula Digital Generalization

2.1. Original Bethe-Weizsäcker Mass Formula [1, 2]

Let A be the total number of nucleons, Z the number of protons, and N the number of neutrons, so that A = Z + N. The mass of an atomic nucleus will be

\[ m = Z m_p + N m_n - \frac{E_B}{c^2} \]

where \( m_p \) and \( m_n \) are the rest mass of proton and neutron, respectively, and \( E_B \) is the binding energy of the nucleus. The semi-empirical mass formula states that the binding energy \( E_B \) per nucleon will take the following form:

\[ BE = \text{Vol} - \text{Sur} - \text{Cha} - \text{Sym} + \text{Wig}. \]

In this paper we use the connections between atomic masses, nuclear masses, and mass excess as follows:

\[ \text{AtMass} = Z m_p + N m_n - \text{Be} \quad (1) \]

\[ \text{NuclMass} = \text{AtMass} - (mE E + Ael E^2 + Bel E^5) \quad (2) \]

\[ \text{MassExc} = \text{AtMass} - \text{Au} \quad (3) \]

where \( m_n = 939.565301 \), \( m_p = 938.2719982 \), \( ME = 0.510998902 \), \( 1u = 931.494028 \text{ MeV}/c^2 \) (2006, CODATA) correspondingly with fit parameters

\[ \text{Ael} = 1.44381 \times 10^{-5}, \text{Bel} = 1.554680 \times 10^{-12} \]

where \( E \) is the number of electrons in a shell.

2.2. Hypothesis for Digital Generalization of Bethe-Weizsäcker Mass Formula with the Influence of Magic Numbers [3, 16-20]

Here \( E \) is defined as

\[ E = \text{Even number of electrons in a shell}. \]

Eight electron magic numbers (2, 10, 18, 36, 54, 86, 118, 140) - from the periodic Mendeleev table of elements.

The method of discovering the explicit form of the functions \( \text{Vol}(Z, N, a), \text{Sur}(Z, N, a), \text{Cha}(A, Z, a), \text{Sym}(Z, N, a), \text{Wig}(Z, N, a), \text{SVol}(N, Z, E), K_M N(Z, N, a) \), \( P_1(Z, N, a), P_2(Z, N, a), P_3(Z, N, a), P_4(Z, N, a) \) and the calculated values of a set of unknown digital parameters is described in papers [3, 5-7, 16-20] using the 3 overdetermined algebraic system of the equality of experimental values of equations (1, 2, 3) and their model, calculated from equation (4). The number of the experimental data from the data base [21, 22] is \( M = 2536 \).

2.4. About the Choice of Arguments for Solving the Inverse Problem

Concerning the possibilities of REGN code, it is very convenient to choose the arguments which are linearly independent as well as with a variation near to zero. In our case we chose the arguments as follow:

\[ V_1 = \frac{Z}{A} \quad V_2 = \frac{N}{A} \quad V_3 = \frac{V_1}{12} \quad V_3 = \frac{V_1}{N} \quad V_4 = \frac{N}{A} \quad V_5 = V_42 \quad V_6 = V_43 \quad V_7 = \frac{N-Z}{A} \quad V_8 = V_72 \quad V_9 = V_73, \]
V_{10} = \frac{Z}{N+1}, \quad V_{11} = V_{102}, \quad V_{12} = V_{103}, \quad V_{13} = \frac{1}{\ln(A+1)}, \quad V_{14} = \frac{Z-Z_0}{Z+Z_0}, \quad V_{15} = \frac{N-N_0}{N+N_0}, \quad V_{16} = \frac{E-E_0}{E+E_0} \\
V_{17} = V_{142}, \quad V_{18} = V_{152}, \quad V_{19} = V_{162}, \quad V_{20} = \frac{1}{A} \text{ if } A \text{ is even, and } \frac{1}{A} \text{ if } A \text{ is odd}, \\
V_{21} = \frac{1}{Z+1} \text{ and } V_{22} = \frac{1}{N+1} \text{ correspondingly.}

3. The Explicit Form of Unknown Functions

These forms are as follows:

\[ Vol(Z,N,a,i) = \exp (a_1 + \text{CorPow}(a,N,isp)) + \text{CorS}(a,N,N_0+6), \]
\[ Sur(Z,N,a,i) = \exp (a_2 + \text{CorPow}(a,N,isp+nPow)) + \text{CorS}(a,N,N_0+12), \]
\[ Cha(Z,N,a,i) = \exp (a_3 + \text{CorPow}(a,N,isp+2\ nPow)) + \text{CorS}(a,N,N_0+18), \]
\[ Sym(Z,N,a,i) = \exp (a_4 + \text{CorPow}(a,N,isp+3\ nPow)) + \text{CorS}(a,N,N_0+24), \]
\[ Wig(Z,N,a,i) = \exp (a_5 + \text{CorPow}(a,N,isp+4\ nPow)) + \text{CorS}(a,N,N_0+30), \]

\[ SVol(Z,N,a,i) = a_{50+6} (\exp (a_6 + \text{CorPow}(a,N,isp+5\ nPow)) + \text{CorS}(a,N,N_0+36)) V_{19}, \]
\[ P_1(Z,N,a,i) = \exp (a_7 + \text{CorPow}(a,N,isp+6\ nPow)) + \text{CorS}(a,N,N_0+42), \]
\[ P_2(Z,N,a,i) = \exp (a_8 + \text{CorPow}(a,N,isp+7\ nPow)) + \text{CorS}(a,N,N_0+48), \]
\[ P_3(Z,N,a,i) = \exp (a_9 + \text{CorPow}(a,N,isp+8\ nPow)) + \text{CorS}(a,N,N_0+54), \]
\[ P_4(Z,N,a,i) = \exp (a_{10} + \text{CorPow}(a,N,isp+9\ nPow)) + \text{CorS}(a,N,N_0+60), \]
\[ P_5(Z,N,a,i) = \exp (a_{11} + \text{CorPow}(a,N,isp+10\ nPow)) + \text{CorS}(a,N,N_0+66), \]

Where:

\[ \text{CorPow}(a,N,i) = \exp (-\sum_{B<C} B^2 + \sum_{B<C} B + \sum_{B<C} B^2 + \sum_{B<C} B^2 + \sum_{B<C} B^2 + \sum_{B<C} B^2), \]

\[ \text{CorS}(a,N,i) = \exp (-\sum_{B<C} B^2 + \sum_{B<C} B + \sum_{B<C} B^2 + \sum_{B<C} B^2 + \sum_{B<C} B^2 + \sum_{B<C} B^2). \]

And

\[ K_{MN}(Z,Z_0,WZ,N,N_0,WN,a,i) = K(Z,Z_0,WZ,N,N_0,WN,a,isp + 11\ nPow)(1 + a_{N_0+5} v_3), \]

Where:

\[ K(Z,Z_0,WZ,N,N_0,WN,a,isp + 11\ nPow) = BZ(Z,Z_0,WZ,a,isp + 11\ nPow)(1 + \exp (-a_{N_0+1} v_1)^2 + a_{N_0+3} v_2), \]
\[ + BN(N,N_0,WN,a,isp + 11\ nPow)(1 + \exp (-a_{N_0+2} v_2)^2 + a_{N_0+4} v_4). \]

\[ BZ(Z,Z_0,WZ,N,N_0,WN,a,i) = Az(Z,Z_0,N,N_0,a,i) \exp (-\frac{(Z-Z_0)^2}{g_0(Z,Z_0,WZ,N,N_0,a,i)})/((Z-Z_0)^2 + Gz(Z,Z_0,WZ,N,N_0,a,i)), \]
\[ BN(Z,Z_0,WZ,N,N_0,WN,a,i) = An(Z,Z_0,WZ,N,N_0,a,i) \exp (-\frac{(N-N_0)^2}{g_0(Z,Z_0,WZ,N,N_0,a,i)})/(N-N_0)^2 + Gn(Z,Z_0,N,N_0,WN,a,i)), \]
\[ Az(Z,Z_0,N,N_0,a,i) = \text{CorAmp}(a,n,i), \quad An(Z,Z_0,N,N_0,a,i) = \text{CorAmp}(a,n,i + nBWA), \]
\[ Gz(Z,Z_0,WZ,N,N_0,a,i) = WZ + \text{CorAmp}(a,n,i + 2\ nBWA), \]
\[ Gn(Z,Z_0,N,N_0,WN,a,i) = WZ + \text{CorAmp}(a,n,i + 3\ nBWA), \]
\[ \text{CorAmp}(a,n,i) = \exp (a_{i+20} \sum_{j=1}^{19} a_{i+j} v_j^2), \]

Where the values of integer numbers are as follows:

iStr = 6, iPow = 5, iSP = iStr + iPow, nPow = 19, nBWA = 20, nBW = 4, nBWA = 20, MnZ = 10, MnN = 11, Dop = 72, N0 = iSP(1 +
nPow) + nBW, \( N = N_0 + D_{op} + 2 M_{nZ} + 2 M_{nN} \).

\( Z_0 \) is the nearest of a set of proton magic numbers: 2, 8, 14, 20, 28, 50, 82, 98, 108, 124,

\( N_0 \) is the nearest of a set of neutron magic numbers: 2, 8, 14, 20, 28, 50, 82, 124, 152, 184, 202.
The values of magic numbers \( Z_0, N_0 \) as well as the boundaries between them \( W_N, W_N, \) (half sum of consequently magic numbers) are the result of a fit procedure.

4. Description of Data

The following figures are a description of the data calculated.
Figure 7. The behaviour of atomic masses residuals.

Figure 8. Gauss fit of atomic masses residuals (w = 0.740 +/- 0.027 MeV).

Table 1. Illustrates the quality of description for Binding Energy, Nuclear Mass, Mass Excess and Atomic Masses as function of Z, N and A.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>N total</th>
<th>Mean</th>
<th>SD</th>
<th>Variance</th>
<th>RMS</th>
<th>MAD</th>
<th>Minimum</th>
<th>Median</th>
<th>Maximum</th>
</tr>
</thead>
<tbody>
<tr>
<td>Residual Binding energy</td>
<td>2536</td>
<td>-2.54E-05</td>
<td>0.00688</td>
<td>4.74E-05</td>
<td>0.008</td>
<td>0.00369</td>
<td>-0.06291</td>
<td>3.49E-06</td>
<td>0.06791</td>
</tr>
<tr>
<td>Residual Nuclear mass</td>
<td>2536</td>
<td>-1.03E-05</td>
<td>0.41962</td>
<td>0.17608</td>
<td>0.46</td>
<td>0.3207</td>
<td>-1.94926</td>
<td>-0.0023</td>
<td>1.47267</td>
</tr>
<tr>
<td>Residual Mass excess</td>
<td>2536</td>
<td>0.0179</td>
<td>0.41965</td>
<td>0.1761</td>
<td>0.46</td>
<td>0.32069</td>
<td>-1.94846</td>
<td>-0.0014</td>
<td>1.47305</td>
</tr>
<tr>
<td>Residual Atomic mass</td>
<td>2536</td>
<td>-1.04E-05</td>
<td>0.41962</td>
<td>0.17608</td>
<td>0.46</td>
<td>0.3207</td>
<td>-1.94926</td>
<td>-0.0023</td>
<td>1.47267</td>
</tr>
</tbody>
</table>

Where the abbreviations are as follows: SD = Standard Deviation, RMS = Root Mean Square and MAD = Mean Absolute Deviation.

Table 2. Comparison experimental and calculated data of the elements, which have a residual energy greater than module 1.5 MeV.

<table>
<thead>
<tr>
<th>El Name</th>
<th>A</th>
<th>Z</th>
<th>N</th>
<th>Be</th>
<th>ResBe</th>
<th>AtMass</th>
<th>ResAtMass</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ca</td>
<td>53</td>
<td>20</td>
<td>33</td>
<td>8.33</td>
<td>3.69E-02</td>
<td>49339.795</td>
<td>-1.96</td>
</tr>
<tr>
<td>Pb</td>
<td>208</td>
<td>82</td>
<td>126</td>
<td>7.87</td>
<td>9.04E-03</td>
<td>193729.006</td>
<td>-1.89</td>
</tr>
<tr>
<td>Sn</td>
<td>132</td>
<td>50</td>
<td>82</td>
<td>8.35</td>
<td>1.23E-02</td>
<td>122980.663</td>
<td>-1.63</td>
</tr>
<tr>
<td>Nh</td>
<td>278</td>
<td>113</td>
<td>165</td>
<td>7.18</td>
<td>5.74E-03</td>
<td>259114.241</td>
<td>-1.52</td>
</tr>
<tr>
<td>No</td>
<td>259</td>
<td>102</td>
<td>157</td>
<td>7.40</td>
<td>5.80E-03</td>
<td>241351.028</td>
<td>-1.51</td>
</tr>
</tbody>
</table>

Where the abbreviations are as follows: Be – Experimental Binding energy; ResBe – Difference of the calculated and experimental binding energy; AtMas – Experimental Atomic Mass; ResAtMass= Difference of the calculated and experimental atomic mass.

5. Proton and Neutron Drip Lines and Predictions

The definition of two proton and two neutron drip lines as a boundary of existing nuclear matter is as follow:

\[(Z+N) \text{Be}(Z,N,a) > (Z+N-2) \text{Be}(Z-2,N,a), \text{ for protons} \]  

and

\[(Z+N) \text{Be}(Z,N,a) > (Z+N-2) \text{Be}(Z,N-2,a), \text{ for neutrons} \]
Figure 9. Two proton and neutron drip lines.

Figure 10. Asymptotic of two proton and neutron drip lines: Z = 134, N = 206.

Figure 11. The comparison of our model with the $^{60}$Ca$_{20}$ RIKEN experiment [23] (PHYSICAL REVIEW LETTERS 121, 022501 (2018)).

Table 3. Presents the Atomic Masses and Nuclear Binding Energies [MeV] for comparison with the data for discovered isotopes from the $^{60}$Ca$_{20}$ RIKEN experiment [23].

<table>
<thead>
<tr>
<th>No</th>
<th>El. Name</th>
<th>A</th>
<th>Z</th>
<th>N</th>
<th>AtMass</th>
<th>NBe</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Sc</td>
<td>62</td>
<td>21</td>
<td>41</td>
<td>57755.72</td>
<td>480.90</td>
</tr>
<tr>
<td>2</td>
<td>Sc</td>
<td>61</td>
<td>21</td>
<td>40</td>
<td>56818.95</td>
<td>478.11</td>
</tr>
<tr>
<td>3</td>
<td>Sc</td>
<td>60</td>
<td>21</td>
<td>39</td>
<td>55884.56</td>
<td>472.93</td>
</tr>
<tr>
<td>4</td>
<td>Sc</td>
<td>59</td>
<td>21</td>
<td>38</td>
<td>54944.07</td>
<td>473.85</td>
</tr>
<tr>
<td>5</td>
<td>Sc</td>
<td>58</td>
<td>21</td>
<td>37</td>
<td>54010.17</td>
<td>468.19</td>
</tr>
<tr>
<td>6</td>
<td>Sc</td>
<td>57</td>
<td>21</td>
<td>36</td>
<td>53072.85</td>
<td>465.95</td>
</tr>
<tr>
<td>7</td>
<td>Sc</td>
<td>56</td>
<td>21</td>
<td>35</td>
<td>52138.51</td>
<td>460.72</td>
</tr>
<tr>
<td>8</td>
<td>Sc</td>
<td>55</td>
<td>21</td>
<td>34</td>
<td>51201.14</td>
<td>458.53</td>
</tr>
<tr>
<td>9</td>
<td>Sc</td>
<td>54</td>
<td>21</td>
<td>33</td>
<td>50267.14</td>
<td>452.96</td>
</tr>
<tr>
<td>10</td>
<td>Sc</td>
<td>53</td>
<td>21</td>
<td>32</td>
<td>49330.48</td>
<td>450.05</td>
</tr>
<tr>
<td>11</td>
<td>Sc</td>
<td>52</td>
<td>21</td>
<td>31</td>
<td>48397.49</td>
<td>443.48</td>
</tr>
<tr>
<td>12</td>
<td>Ca</td>
<td>60</td>
<td>20</td>
<td>40</td>
<td>55893.50</td>
<td>464.77</td>
</tr>
<tr>
<td>13</td>
<td>Ca</td>
<td>59</td>
<td>20</td>
<td>39</td>
<td>54958.81</td>
<td>459.89</td>
</tr>
<tr>
<td>14</td>
<td>Ca</td>
<td>58</td>
<td>20</td>
<td>38</td>
<td>54018.65</td>
<td>460.50</td>
</tr>
<tr>
<td>15</td>
<td>Ca</td>
<td>57</td>
<td>20</td>
<td>37</td>
<td>53085.43</td>
<td>454.15</td>
</tr>
<tr>
<td>16</td>
<td>Ca</td>
<td>56</td>
<td>20</td>
<td>36</td>
<td>52148.37</td>
<td>451.64</td>
</tr>
<tr>
<td>17</td>
<td>Ca</td>
<td>55</td>
<td>20</td>
<td>35</td>
<td>51213.94</td>
<td>446.50</td>
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<tr>
<td>18</td>
<td>Ca</td>
<td>54</td>
<td>20</td>
<td>34</td>
<td>50276.19</td>
<td>444.72</td>
</tr>
<tr>
<td>19</td>
<td>Ca</td>
<td>53</td>
<td>20</td>
<td>33</td>
<td>49341.74</td>
<td>439.57</td>
</tr>
<tr>
<td>20</td>
<td>Ca</td>
<td>52</td>
<td>20</td>
<td>32</td>
<td>48404.40</td>
<td>437.35</td>
</tr>
<tr>
<td>21</td>
<td>Ca</td>
<td>51</td>
<td>20</td>
<td>31</td>
<td>47470.86</td>
<td>431.32</td>
</tr>
<tr>
<td>22</td>
<td>K</td>
<td>59</td>
<td>19</td>
<td>40</td>
<td>54966.48</td>
<td>453.01</td>
</tr>
<tr>
<td>23</td>
<td>K</td>
<td>57</td>
<td>19</td>
<td>38</td>
<td>53095.12</td>
<td>445.24</td>
</tr>
</tbody>
</table>
In the following figure (Figure 12) we present the ZN coordinates, limited from the drip lines.
Figure 12. The ZN coordinates for which we will present the values of the Nuclear Binding Energy and Atomic Mass [MeV].

Figure 13. The values of Predicted Nuclear Binding Energies and Atomic Masses [MeV], Z in the interval 98-110 and N in the interval 154-167.

Figure 14. The values of Predicted Nuclear Binding Energies and Atomic Masses [MeV], Z in the interval 102-120 and N in the interval 168-184.
Figure 15. The values of Predicted Nuclear Binding Energies and Atomic Masses [MeV] Z in the interval 120-133 and N in the interval 185-205.

Figure 16. Illustration of the linear behavior of atomic masses in the Z, N plane, discovered in the Fig. 13-15, for all the elements in the Mendeleev table.
The linear independence of the used arguments and value of nonlinear equations has been obtained with the help of the Lubomir Aleksandrov’s auto-regularization method of the Gauss-Newton type for ill-posed problems.

The impact of the electron shell was determined as a nonmonotonic parabolic function which is equal to zero at the magic number of electrons (E = Em).

The result of the calculations allowed improved accuracy of nuclei mass estimation from 3.5 MeV of the original formula.
and 2.2MeV [17] to 1.8 MeV using an improved numerical generalization of the Bethe-Weizsäcker Mass Formula.

The development of this work may include a calculation of the full and kinetic energy of decay as well as an estimation of nuclei lifetime.

7. Conclusion

The generalization of the Bethe –Weizsäcker formulae was approached by insertion of additional terms estimating the influence of proton, neutron and electron magic numbers on the nuclear mass and binding energy. This approach allows the describing of atomic masses starting from 2H1 to 294Og118 with RMS=0.46 MeV and with residuals of less than or equal to 1.9 MeV.

For only five elements the residuals are greater than 1.5 MeV.

The resulting agreement with the experimental data permits us to calculate realistic two proton and neutron drip lines with an asymptotic point at Z=132, N=212.

There is an accordance of received model of nuclear and atomic masses with RICKEN experiment for creating of new 20Ca20 Isotopes [20].

The prediction for the masses of 295Og118 (118?177), 296Og118 (118?178), 119?176, 120?176 and some their isotopes are presented.

The like linear dependences discovered in Z, N plane for all elements in Mendeleev table are illustrated.

Recent published [3, 8-14, 16-20] and presented herein results allow the suggestion that the resonant interaction of the electron shell and the nuclei causes the existence of the magic numbers.

The existence of proton and neutron magic numbers is a result of the unknown strong nuclear interactions in the effective field of electron shell. Probably, the electron shell field effects the nucleon run length [24], nuclei volume, rate of decay, and difference of the nuclei shape from a sphere. Thus, the nuclei interaction with the electron shell may switch on/off the strong interaction between neutrons and protons.

The other possible mechanism of such resonant interaction is inner oscillations of the protons and neutrons, which were proposed by M. Gryzinski (1959) [24] and N. Chetaev (1931-1962) [25]. The conjugated oscillations of the neutrons and protons may lead to Hopf (Poincaré-Andronov-Hopf) bifurcations in three-dimensional nuclear structures. Such bifurcations may correspond to periodic solutions and low frequency oscillations providing a breaking of nuclei symmetry and its interaction with electrons shells or decay.

The neutron and proton pair’s spin (Gryzinski) interactions as proton oscillations are possible through nuclei - electrons resonance. The resonance and/or coherence may form an electronic bridge with resonant interactions between the nuclei of the atoms of most biological molecules, including H, C, N, P, etc. The totality of these molecules is the basis of the biosphere.


