



# PHOTOSYNTHESIS STRUCTURAL INTERACTION

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The application of methodology of spatial-energy interactions (P-parameter) to main stages of photosynthesis is given. Their energy characteristics are calculated. The values obtained correspond to the reference and experimental data.

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## Introduction

Photosynthesis is the process of converting electromagnetic energy of the sun rays into the energy of chemical bonds of vital organic substances.<sup>1</sup>

It is the only natural process through which the organic world obtains the reserve of free energy and which provides all bio-organisms with chemical energy. From the moment photosynthesis was discovered by Priestly, the researches passed several important stages. Further development of biophysicochemical aspects of synthesis till now resulted in its modern model and clarified the way of carbon during photosynthesis, concept of two photosystems, structure of reaction center etc.

The basis of photosynthesis, consecutive chain of redox reactions, during which electrons are transferred from donor-reducer to acceptor-oxidizer with the formation of reduced compounds (carbohydrates) and isolation of oxygen.

It is known that excitation energy for complex organic molecules of chlorophyll type lasts for  $10^{-8}$ - $10^{-9}$  sec and can be stored only for insignificant fractions of a second. But during photosynthesis the energy of absorbed light quantum is stored for a long period (from several minutes to millions of years). The energy is stored here in molecular as chemical bonds rich with energy in complex organic structures. Therefore, photosynthesis energy can be presented based on the analysis of changes in energies of chemical bonds of molecular structures in dynamics of all main types of photosynthesis. This is the aim to use the methodology of spatial-energy interactions (P-parameter) in this paper.

## Spatial-energy parameter (P-parameter)

Structural and interatomic interactions are sure to have electronic nature. Thus the registration of the extent to which electrons fill the atom valence states is the basis of the method of valence bonds in chemistry and is numerically expressed through coulomb electrostatic interaction.

Also important are exchange-promotional structural interactions that determine isomorphism, solubility of components in solid, liquid and molecular media.<sup>2</sup>

During the interactions of oppositely charged heterogeneous systems, the volume energy of interacting structures is compensated to a certain extent thus leading to the decrease in the resultant volume energy.

The analysis of different physical and chemical processes allows assuming that in many cases the principle of adding reciprocals of volume energies or kinetic parameters of interacting structures is executed e.g., ambipolar diffusion, total rate of topochemical reaction, change in the light velocity when transiting from vacuum into the given medium, resultant constant of chemical reaction rate (initial product – intermediary activated complex – final product).

Lagrange equation for relative movement of isolated system of two interacting material points with masses  $m_1$  and  $m_2$  in coordinate  $x$  can be presented as eqn. (1) where  $\Delta U_1$  and  $\Delta U_2$  are the potential energies of material points in elementary section of interactions and  $\Delta U$  is the resulting (mutual) potential energy of these interactions.

$$\frac{1}{\Delta U} \approx \frac{1}{\Delta U_1} + \frac{1}{\Delta U_2} \quad (1)$$

The atom system is formed from oppositely charged masses of nucleus and electrons. In this system energy characteristics of subsystems are the orbital energy of electrons ( $W_i$ ) and effective energy of nucleus that takes into consideration the screening effects.

Therefore, assuming that the resultant interaction energy of the system orbital-nucleus (responsible for interatomic interactions) can be calculated based on the principle of adding reciprocals of some initial energy components, we substantiate the introduction of P-parameter<sup>2</sup> as an averaged energy characteristic of valence orbitals in accordance with the following equations, where  $W_i$  is the bond energy of electrons,<sup>3</sup>  $r_i$  is the orbital radius of  $l$  orbital,<sup>4</sup>  $n_i$  is the number of electrons of the given orbital,  $Z^*$  and  $n^*$  are effective charge of nucleus and effective main quantum number<sup>5</sup> and  $R$  is the numerical characteristic of atom (bond).

$$\frac{1}{q^2/r_i} + \frac{1}{W_1 n_i} = \frac{1}{P_E} \quad (2)$$

$$P_E = \frac{P_0}{r_i} \quad (3)$$

$$P_E = \frac{P_0}{R} \quad (3a)$$

$$\frac{1}{P_0} = \frac{1}{q^2} + \frac{1}{(Wrn)_i} \quad (4)$$

$$q = \frac{Z^*}{n^*} \quad (5)$$

The  $P_0$  value will be called a spatial-energy parameter, and the  $P_E$  value is the effective  $P$  parameter. Effective  $P_E$  parameter has a physical sense of some averaged energy of valence electrons in atom and is measured in energy units, i.e. in electron-volts (eV).

The values of  $P_0$ - and  $P_E$ -parameters of some elements calculated based on eqns. (2-5) are given in Table 1.

Modifying the rules of adding reciprocals of energy characteristics of subsystems as applied to complex structures we can obtain<sup>6</sup> the equation for calculating  $P_C$ -parameters of complex structure where where  $N_1$  and  $N_2$  are the number of homogeneous atoms in subsystems.

$$\frac{1}{P_C} = \left( \frac{1}{NP_E} \right)_1 + \left( \frac{1}{NP_E} \right)_2 + \dots \quad (6)$$

The calculation results of some complex structures based on eqn. (6) are given in Table 2.

The calculations for 21 elements showed that the values of  $P_E$ -parameters are similar to corresponding values of total energy of valence electrons according to the statistic model of atom.

Simple dependence between  $P_E$ -parameter and electron density at the distance  $r_i$  can be obtained (according to the statistic model of atom) by eqn. (7), where  $A$  is a constant.

$$\beta_i^{2/3} = A \times \frac{P_0}{r_i} = AP_E \quad (7)$$

When the solution is formed in the places of atom-components contact, the unified electron density has to be established. The dissolving process is accompanied by the redistribution of this density between valence areas of both particles and transition of some electrons from external spheres to the neighboring ones.

It is obvious that if electron densities in free atom-components of the solution at the distances of orbital radius  $r_i$  are similar, the transition processes between boundary atoms of particles are minimal thus favoring the solution formation. Thus the task of evaluating the solubility in many cases comes to comparative evaluation of electron density of valence electrons in free atoms (on averaged orbitals) participating in the solution formation.

In this regard the maximum total solubility evaluated through the coefficient of structural interaction and isomorphism  $\alpha$  are determined by the state of minimal value that represent relative difference of effective energies of external orbital.

$$\alpha = \frac{P'_0/r'_i - P''_0/r''_i}{(P'_0/r'_i + P''_0/r''_i)/2} 100 \% \quad (8)$$

$$\alpha = \frac{P'_C - P''_C}{P'_C + P''_C} 200 \% \quad (9)$$

Multiple calculations and comparisons with the experiment allowed arranging the unified averaged figure-nomogram of degree of structural interaction and solubility ( $\rho$ ) dependence upon coefficient  $\alpha$ .<sup>2</sup>

The following spatial-energy principles defining the character of structural spatial-energy interactions were determined:

1. Complete (total-lot) isomorphic interaction takes place at relative difference of  $P$ -parameters of valence orbitals of interchanging atoms (within 4-6%).
2.  $P$ -parameter of the smallest value defines the orbital that is mainly responsible for isomorphism.
3. Qualitatively the isomorphism character is defined by geometrical similarity of orbital shapes responsible for isomorphism. At the same time, the more similar are the extensions, trajectories and inclination angles of such orbitals, the more perfect is isomorphism.

According to the degree of isomorphic similarity of interchanging structures they can be classified into three types (I, II, III) given for some cases in table 3.

## Photosynthesis - Initial stage

Magnesium atom, four-coordinated with nitrogen atoms, is included into chlorophyll in the central cavity of the whole structure. The porphinated chlorophyll ring is located in aqueous medium. Each central Mg atom forming chelate compound has two bonds by donor-acceptor mechanism and two covalent bonds. Two molecules of bacterio-chlorophyll are located close to each other (about 3 Å) and form competent-structure – dimer chlorophyll. In the dynamics of structural permutations all four bonds of each Mg atom become equivalent.<sup>7</sup> All this allows assuming that total effective  $P_E$ -parameter of Mg will be approximately two times greater than from  $2S^2$ -orbital ( $5.4867 \times 2 = 10.973$  eV).

In the first stage of photosynthesis in the system of PS-2 dimensional characteristics of hydrogen atom can change in structured water molecules under the radiation with energy  $h\nu$  from boron radius (0.529 Å) to atomic ("metal") i.e.. 0.46 Å, this corresponds to the obtaining of  $P_E$ -parameter equal 10.432 eV by hydrogen that is similar to  $P_E$ -parameter of 2 Mg.

It should be pointed out that general change in the scale of photosynthesis potentials PS-2 approximately equals 1.5 eV, and the difference between the data of  $P$ -parameters of hydrogen atoms equals 1.37 eV. The rest of hydrogen atoms with "boron"  $P_E$ -parameter equal to 9.0624 eV have similar values with  $P_E$ -parameters of  $2P^1$ -orbitals of nitrogen atoms surrounding magnesium

**Table 1.** P-parameters of atoms calculated via the bond energy of electrons

Atom	Valence electrons	W (eV)	$r_i$ (Å)	$q^2_0$ (eVÅ)	$P_0$ (eVÅ)	R (Å)	$P_0/R$ (eV)			
H	1S <sup>1</sup>	13.595	0.5295	14.394	4.7985	0.5295	9.0624			
						0.46	10.432			
	2P <sup>1</sup>	11.792	0.596	35.395	5.8680	0.28	17.137			
						R <sub>i</sub> =1.36	3.525			
						0.77	7.6208			
						0.69	8.5043			
2P <sup>2</sup>	11.792	0.596	35.395	10.061	0.77	13.066				
					0.69	14.581				
C	2P <sup>1</sup> <sub>r</sub>	19.201	0.620	37.240	4.4044	0.77	11.715			
	2P <sup>3</sup> <sub>r</sub>				13.213					
	2S <sup>1</sup>				9.0209					
	2S <sup>2</sup>				14.524					
	2S <sup>1</sup> +2P <sup>3</sup> <sub>r</sub>				22.234					
	2S <sup>1</sup> +2P <sup>1</sup> <sub>r</sub>				13.425					
	2S <sup>2</sup> +2P <sup>2</sup>				24.585					
	2P <sup>1</sup>				15.445					
N	2P <sup>2</sup>	17.195	0.4875	52.912	6.5916	0.70	9.4166			
	2P <sup>3</sup>				11.723	0.70	16.747			
	2P <sup>4</sup> <sub>r</sub>				15.830	0.70	22.614			
	2P <sup>5</sup> <sub>r</sub>				19.193	0.55	34.896			
	2S <sup>1</sup>				25.724	0.521	53.283	10.709	0.70	15.299
	2S <sup>2</sup>				25.724	0.521	53.283	17.833	0.70	25.476
	2S <sup>2</sup> +2P <sup>3</sup>				33.663	0.70	48.09			
	2P <sup>1</sup>				17.195	0.4135	71.383	4.663	0.66	9.7979
	2P <sup>1</sup>				17.195	0.4135	71.383	11.858	R <sub>i</sub> =1.36	4.755
	2P <sup>1</sup>								R <sub>i</sub> =1.40	4.6188
O	2P <sup>2</sup>	17.195	0.4135	71.383	20.338	0.66	8.7191			
	2P <sup>4</sup>					0.59	8.470			
	2S <sup>1</sup>					0.66	30.815			
	2S <sup>2</sup>					0.66	34.471			
	2S <sup>2</sup> +2P <sup>4</sup>					0.66	19.082			
	2S <sup>2</sup> +2P <sup>4</sup>					0.66	32.524			
Ca	4S <sup>1</sup>	5.3212	1.690	17.406	5.929	1.97	3.0096			
	4S <sup>2</sup>				8.8456	1.97	4.4902			
	4S <sup>2</sup>				11.901	0.808	48.108	6.0143	R <sup>2+</sup> =1.00	8.8456
	4S <sup>2</sup>								R <sup>2+</sup> =1.26	7.0203
	3P1				11.901	0.808	48.108	13.740	1.04	7.7061
	3P2				11.901	0.808	48.108	21.375	1.04	13.215
	3P4				11.904	0.808	48.108	13.659	1.04	20.553
S	3S1	23.933	0.723	64.852	22.565	1.04	13.134			
	3S2	23.933	0.723	64.852	43.940	1.04	42.250			
	3S2+3P4	10.963	0.909	61.803	8.5811	1.17	7.3343			
Se	4P1	10.963	0.909	61.803	8.5811	1.17	7.3343			
	4P2				15.070	1.17	12.880			
	4P2				15.070	1.6	9.4188			

	4P2				15.070	1.14	13.219
	4P4				24.213	1.17	20.710
	4P4					1.6	15.133
	4S1	22.787	0.775	85.678	14.642	1.17	12.515
	4S2				25.010	1.17	21.376
	4S2+4P4				49.214	1.17	42.066
	4S2+4P4				49.214	1.6	30.759
	3P1	10.659	0.9175	38.199	7.7864	1.10	7.0785
	3P1					R3=-1.86	P3=4.1862
P	3P3	10.659	0.9175	38.199	16.594	1.10	15.085
	3P3					R3=-1.86	8.9215
	3S2	18.951	0.803	50.922	19.050	1.10	17.318
	3S2+3P3				35.644	1.10	32.403
Mg	3S1	6.8859	1.279	17.501	5.8568	1.60	3.6618
	3S2				8.7787	1.60	5.4867
						R2+=1.02	8.6066
	4S1	6.7451	1.278	25.118	6.4180	1.30	4.9369
	4S2				10.223	1.30	7.8638
Mn	3d1	17.384	0.3885	177.33	6.5058	1.30	5.0043
	4S1+3d1				12.924	1.30	9.9414
	4S2+3d2				22.774	1.30	17.518
	4S2+3d5				38.590	1.30	29.684
Na	3S1	4.9552	1.713	10.058	4.6034	1.89	2.4357
						R+I=1.18	3.901
						R+I=0.98	4.6973
Cl	3P1	13.780	0.7235	59.849	8.5461	1.00	8.5461
						R-I=1.81	4.7216
	4S1	7.0256	1.227	26.572	6.5089	1.26	4.8325
Fe	3d1	17.603	0.364	199.95	6.2084		
	4S1+3d1				12.717	1.26	10.093
	4S2+3d1				16.664	1.26	13.226
	4S1	4.0130	2.612	10.993	4.8490	2.36	2.0547
K						R+I=1.45	3.344
	4S2(*)				7.2115	2.36	3.0557
						R+I=1.45	4.9734

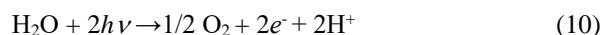
Other data are not less important. Initial value of  $P_E$ -parameter of  $2S^2$ -orbital of magnesium atom gives from  $P_E$ -parameter (Table 3) of radical (O-H)  $\alpha = 8.24\%$  and  $\rho \approx 77-82\%$ . This  $\rho$  value can increase to even 100% under the light action due to minor changes in dimensional characteristics of atoms-components. Absolute difference of these  $P$ -parameters equals 0.43 eV, thus corresponding to the changes in the scale of potentials during the synthesis of ATP.

Total spatial-energy action upon the bond H-O-H of magnesium and nitrogen atoms (Table 3) results in the possibility of breaking this bond with the isolation of free hydrogen and oxygen atoms.

This initial process finishes with the participation of manganese-containing system connected with proteins of reaction center PS-2. Structural reconstruction can take place in manganese cluster (two-nucleus or four-nucleus) under the action of radiation<sup>8,9</sup> from univalent state (4.9369 eV, this is similar to initial values of Mg  $P_E$ -parameter) to bivalent (9.9414 eV) and further to quadrivalent state (17.518 eV).

All this provides enzymatic action of Mn upon the bond H-O-H, both upon oxygen and hydrogen atoms, and hydroxyl group in general. This is confirmed by the approximate equality of  $P_E$ -parameters of bi- and quadrivalent Mn with  $P_E$ -

parameters of  $2P^1$  and  $2P^2$ -orbitals of oxygen atom (Table 3). Thus, all the above interactions and structural re-groupings induced with light result in the formation of oxidized chlorophyll based on the following reaction (eqn. 10),<sup>10</sup> with the isolation of two electrons and two protons. These electrons, broken off from the water, through the chain of "dark" reactions go further to PS-1 that utilizes them in the next photosynthesis stages to reduce  $NADP^+$  to NADPN that is carried out also with the help of proton transfer system.



For double bond of  $2P^1$ -orbital the carbon atom has a  $P_E$ -parameter (8.5043 eV) similar to  $P_E$ -parameter of hydrogen atom (Table 1). Therefore, one of the freed hydrogen atoms join the double bond C=C available in NADPN with the formation of single bond with carbon atom.<sup>9</sup>

### Phosphorylation

It is accepted<sup>7,11</sup> that directed transition of protons serves as energy source during phosphorylation. Between the numbers of transported protons and electrons certain stoichiometric relations are revealed. Thus, in the course of electron transfer

(along the whole transport system) ATP molecules are formed. Apparently, ATP phosphorylation energy can also be estimated through the system of electron transfer.

**Table 2.** Structural  $P_C$ -parameters calculated via the bond energy of electrons.

Radicals, fragments	$P_i^+$ (eV)	$P_i^-$ (eV)	$P_C$ (eV)	Orbitals
OH	17.967	10.432	6.5999	O ( $2P^2$ )
	9.7979	9.0624	4.7080	O ( $2P^1$ )
	9.7979	10.432	5.0525	O ( $2P^1$ )
	17.967	17.138	8.7712	O ( $2P^2$ )
H <sub>2</sub> O	2·9.0624	17.967	9.0226	O ( $2P^2$ )
	2·10.432	17.967	9.6537	O ( $2P^2$ )
	2·17.138	17.967	11.788	O ( $2P^2$ )
CH <sub>2</sub>	28.875	2·17.138	15.674	C ( $2S^12P^3_i$ )
	31.929	2·17.138	16.531	C ( $2S^22P^2$ )
	28.875	2·9.0624	11.125	C ( $2S^12P^3_i$ )
CH <sub>3</sub>	31.929	3·17.138	19.696	C ( $2S^22P^2$ )
	28.875	3·9.0624	14.003	C ( $2S^12P^3_i$ )
CH	28.875	17.138	10.755	C ( $2S^12P^3_i$ )
	31.929	9.0624	7.059	C ( $2S^22P^2$ )
	31.929	17.138	11.152	C ( $2S^22P^2$ )
H <sub>3</sub> O	3·17.138	17.967	13.314	O ( $2P^2$ )
C <sub>2</sub> H <sub>5</sub>	2·31.929	5·17.138	36.590	C ( $2S^22P^2$ )
CH <sub>2</sub>	31.929	2·9.0624	11.562	C ( $2S^22P^2$ )
CH <sub>3</sub>	28.875	3·17.138	18.491	C ( $2S^22P^3_i$ )
CH <sub>3</sub>	31.929	3·9.0624	14.684	C ( $2S^22P^2$ )
CH	28.875	10.432	7.6634	C ( $2S^22P^3_i$ )
CH	31.929	10.432	7.8630	C ( $2S^22P^2$ )
CO	31.929	20.048	12.315	C ( $2S^22P^2$ )
C=O	14.581	20.048	8.4416	C ( $2P^2$ )
C=O	17.435	20.048	9.3252	C ( $2S^12P^1_i$ )
C-O <sub>2</sub>	28.875	2·20.048	16.786	C ( $2S^12P^3_i$ )
C-O <sub>2</sub>	31.929	2·20.048	17.774	C ( $2S^22P^2$ )
CO-OH	12.315	8.7712	5.1226	C ( $2S^22P^2$ )
CH-OH	11.152	8.7712	4.9159	C ( $2S^22P^2$ )
CO-H	8.4416	9.0624	4.3705	C ( $2P^2$ )

In particular, electron transfer results in that phosphoric acid molecules present in ATP, NADP and NADPN contain oxygen atoms in the form of O<sup>-</sup>. Spatial-energy interactions (including isomorphous) are objectively expressed both at similar and opposite electrostatic charge of atoms-components. Such interactions can also take place between two heterogeneous atoms, if only their  $P_E$ -parameters are roughly equal, and geometric shapes of orbitals are similar or alike.

The radiation energy  $h\nu$  in PS-1 promotes, apparently, the changes in dimensional characteristics of phosphorous and oxygen atoms from covalent to anion ones. Therefore,  $P_0$ -parameters of free phosphorus and oxygen atoms are distributed at the distance of their anion radii 1.86 Å and 1.40 Å, respectively. This similarity of values of their  $P_E$ -parameters,  $\alpha = 5.19\%$  for  $2P^3$ -orbitals of phosphorous with  $2P^2$ -orbitals of oxygen (Table 3).

Such approximate equality of  $P_E$ -parameters and geometric similarity of shapes of orbitals of atoms-components shows that actual degree of their interaction  $\rho=100\%$ , thus providing the energy of formation of macroenergy bond P-O. Then bond energy of phosphorous and oxygen atoms from two different molecules of phosphoric acid necessary for structural formation during phosphorylation can be considered phosphorylation energy.

For double bond of  $2P^1$ -orbital the carbon atom has  $P_E$ -parameter – (8.5043 eV) – similar to  $P_E$ -parameter of hydrogen atom (Table 1). Therefore one of the freed hydrogen atoms join the double bond C=C available in NADPN with the formation of single bond with carbon atom.<sup>9</sup>

To calculate bond energies or energies of molecule reduction during photosynthesis (E) the technique previously tested<sup>6</sup> for 68 binary and more complicated compounds following the equation was applied, where N is the bond average repetition factor and K is the hybridization coefficient that usually equals the number of atom valence electrons registered.

$$\frac{1}{E} = \frac{1}{P_C} = \frac{1}{\left(P_E \frac{N}{K}\right)_1} + \frac{1}{\left(P_E \frac{N}{K}\right)_2} \quad (11)$$

The half of internuclear distance (for binary bond) of similar atoms or atomic, covalence or ionic radii (depending upon bond type) can be used as a dimensional characteristic of atoms.

The calculations involving anionic distances of atomic orbitals for P and O atoms were made,  $3P^1$  (phosphorous)- $2P^1$  (oxygen) and for  $3P^3$  (phosphorous)- $2P^2$  (oxygen). The values of E obtained appeared to be slightly greater than experimental and reference data (Table 4). But actual power physiological processes during photosynthesis have the efficiency below the theoretical, being in some cases about 83%.<sup>7</sup>



**Table 3.** Photosynthesis structural interactions

SEI types	I	II	II	II	II, III	II	I	II	I	
$\rho$ (mol%)	100	100	100	100	100	77-82	100	100	55-60	
$\alpha$ (%)	4.82	1.45	2.53	3.83	4.75	8.24	5.27	0.08	10.1	
2 comp.	$P_E, P_C, eV$	10.432	9.7979	17.967	9.0624	4.7080	5.0575	3.525	13.215	3.525
	Orbitals	1S <sup>1</sup>	2P <sup>1</sup>	2P <sup>2</sup>	1S <sup>1</sup>	2P <sup>1</sup> -2S <sup>1</sup>	2P <sup>2</sup> -1S <sup>1</sup>	1S <sup>1</sup>	2P <sup>2</sup>	1S <sup>1</sup>
1 comp.	$P_E, P_C, eV$	9.9414	9.9414	17.518	9.4166	4.3969	5.4867	3.344	13.226	3.901
	Orbitals	4S <sup>1</sup> 3d <sup>1</sup>	4S <sup>1</sup> 3d <sup>1</sup>	4S <sup>2</sup> 3d <sup>2</sup>	2P <sup>1</sup>	4S <sup>1</sup>	2S <sup>2</sup>	4S <sup>1</sup>	4S <sup>2</sup> 3d <sup>1</sup>	3S <sup>1</sup>
Atoms, molecules, radicals	Mn-H	Mn-O	Mn-O	N-H	Mn-OH	Mg-(O-H)	K <sup>+</sup> -H <sup>-</sup>	Fe-S	Na <sup>+</sup> -H <sup>-</sup>	

**Table 3.** contg.

SEI types	I	I	I	II	I	II	II, III	III	I	
$\rho$ (mol%)	100	60-65	100	100	100	90-95	100	100	100	
$\alpha$ (%)	5.19	9.83	5.16	5.79	3.01	7.51	2.21	1.53	5.05	
2 comp.	$P_E, P_C, eV$	8.9215*	4.1862*	9.0624	11.125	17.967	8.7712	9.0226	16.785	10.432
	Orbitals	3P <sup>3</sup>	3P <sup>1</sup>	1S <sup>1</sup>	2S <sup>1</sup> 2P <sup>3</sup> <sub>r-</sub> 1S <sup>1</sup>	2P <sup>2</sup>	2P <sup>2</sup> -1S <sup>1</sup>	1S <sup>1</sup> -2P <sup>2</sup>	2S <sup>1</sup> 2P <sup>3</sup> <sub>r-</sub> 2P <sup>2</sup>	1S <sup>1</sup>
1 comp.	$P_E, P_C, eV$	8.470*	4.6188*	8.6066	11.788	17.435	8.4416	9.3252	16.531	10.973
	Orbitals	2P <sup>2</sup>	2P <sup>1</sup>	3S <sup>2</sup>	1S <sup>1</sup> -2P <sup>2</sup>	2S <sup>1</sup> -2P <sup>1</sup>	2P <sup>2</sup> -2P <sup>2</sup>	2S <sup>1</sup> 2P <sup>1</sup> <sub>r-</sub> 2P <sup>2</sup>	2S <sup>2</sup> 2P <sup>2</sup> - 1S <sup>1</sup>	3S <sup>2</sup> (3S <sup>2</sup> )*
Atoms, molecules, radicals	O-P	O-P	Mg <sup>2+</sup> -H	H <sub>2</sub> O- CH <sub>2</sub>	C-O	CO-OH	CO-H <sub>2</sub> O	CH <sub>2</sub> -CO <sub>2</sub>	2Mg-H	

It is probable that electrostatic component of resulting interactions on anion-anion distances is registered in such a way. In fact, the calculated value  $0.83E$  practically corresponds to the experimental bond energy values during phosphorylation (first line in Table 4) and free energy for ATP in chloroplasts (second line in Table 4).

The calculations of bond energy based on the same technique but on covalence distances of atoms for free molecule  $P_{...}O$  (sesquialteral bond) and for molecule  $P=O$  in  $P_4O_{10}$  (double bond) are given in Table 4 for comparison. Sesquialteral bond was evaluated introducing the coefficient  $N=1.5$  using the average value of oxygen  $P_E$ -parameter for single and double bonds.

It is interesting to that calculations of  $E$  based on covalence distances correspond to experimental data without introducing the coefficient 0.83.

### Assimilation of CO<sub>2</sub>

Binding of CO<sub>2</sub> takes place in aqueous medium by the carboxylation reaction of ribulose-diphosphate (RuDP) with the formation of 3-phospho-glycerine acid (PGA). Water molecule and radical  $C=O$  at the distances of molecular interaction have quite similar values of  $P_E$ -parameters for forming the general structural grouping of dimeric composite type. Total  $P_E$ -parameter of water molecule and radical  $C=O$  nearly equals  $P_E$ -parameter of CO<sub>2</sub> and therefore the

molecules of CO<sub>2</sub> and H<sub>2</sub>O join RuDP with the formation of two radicals COOH<sub>B</sub> PGA. In ferment RuDP-carboxylase, Mg atoms and O<sup>-</sup> ions (5.4867 eV and 4.755 eV) play an active role, their  $P_E$ -parameters similar to  $P_E$ -parameter of radical COOH.

A great difference in the number of atoms of interacting structures proves that carboxylase can play only a fermentative role, "tuned" to obtain this final product (COOH).

The assimilations of CO<sub>2</sub> to form CH<sub>2</sub>O flows through a series of intermediate compounds and reactions (Calvin cycle). Let us show some results of calculations of total spatial-energy assimilation processes of CO<sub>2</sub>. When CO<sub>2</sub> is reduced to the level of its structural formation in CH<sub>2</sub>O, the chemical bonds are reconstructed on all stages of the cycle. Therefore, the additional activation energy from ATP and NADPN is required.

It is also obvious that power consumption should be rationally calculated taking into account the reconstruction processes of chemical bonds, i.e. via the values of bond energy for binary structures, and reduction energy for more complex molecules and radicals ( $E$ ).

Thus we calculated the value  $E$  based on equation (10) for several compounds and radicals during photosynthesis (Table 4). For radical  $-C=O$  the calculations were made in two possible variants of activity of valence orbitals of carbon atoms.

**Table 4.** Bond and reduction energies of molecules during photosynthesis (eV)

Notes	11	Phosphorylation	$\Delta G$ of ATP	Free PO molecule	In $P_4O_{10}$ molecule	Decomp. of one molecule				
$E$ by <sup>7,8,14</sup>	10	0.34-0.35	0.67-0.59	6.14	6.504	3.772	2.476	5.11	5.11	
Calculation	0.83E	9	0.33 0.34	0.64	—	—	—	—	—	—
	$E$	8	0.400 0.405	0.77	6.277 6.024 <6.15>	6.697	3.797	2.570	4.90	5.012
3 comp.	$N/K$	7	— —	—	— —	—	—	—	—	—
	$P_E$ , eV	6	— —	—	— —	—	—	—	—	—
2 comp.	$N/K$	5	1/6 1/6	1/6	1.5/6 1.5/6	2/2	1/1	1/6	1/1	2/4
	$P_E$ (eV)	4	4.6188 4.755	8.470	70.854 63.339	20.042	9.0624	17.967	9.7979	20.048
1 comp.	$N/K$	3	1/5 1/5	1/5	1.5/5	2/3	1/2	1/1	1/1	2/4
	$P_E$ (eV)	2	4.1862 4.1862	8.9215	32.403	15.085	13.066	2*9.0624	9.7979	20.048
Atoms, structures, orbitals	1	P-O 3P1-2P1	P-O 3P2-2P2	P...O 3S23P3- 2S22P4	P=O 3P3-2P2	C-H 2P2- 1S1	H2O 1S1-2S2	-O-O- 2P1- 2P1	O=O 2P2- 2P2	

**Table 4. contg.**

Notes	11	Reduction						Free energy of the formation of one mole	
$E$ by <sup>7,8,14</sup>	10	4.56		3.688	4.553	—	—	4.96-5.07	
Calculation	0.83E	9	—	—	—	—	4.390	—	
	$E$	8	4.717	8.8874	3.782	4.487	5.894 4.511	3.544	5.025
3 comp.	$N/K$	7	—	—	—	1/1	—	—	2/2
	$P_E$ , eV	6	—	—	—	9.0624	—	—	20.048
2 comp.	$N/K$	5	2/6	2/2	1/2	2/2	1/1 1/1	1/1	1/1
	$P_E$ , eV	4	2*20.04 8	20.048	17.967	20.048	17.137 9*062 4	5.894	2.90624
1 comp.	$N/K$	3	2/4	2/4	1/2	2/4	1/2 1/2	1/1	1.33/4
	$P_E$ , eV	2	14.581	31.929	13.066	31.929	17.967 17.967	8.8874	31.929
Atoms, structures, orbitals	1	CO <sub>2</sub> 2P <sup>2</sup> -2P <sup>2</sup>	=C=O 2S <sup>2</sup> 2P <sup>2</sup> -2P <sup>2</sup>	C-O 2P <sup>2</sup> -2P <sup>2</sup>	(C=O)-H (2S <sup>2</sup> 2P <sup>2</sup> -2P <sup>2</sup> )-1S <sup>1</sup>	-O-H 2P <sup>2</sup> - 1S <sup>1</sup>	CO- OH(2S <sup>2</sup> 2P <sup>2</sup> - 2P <sup>2</sup> )-(2P <sup>2</sup> - 1S <sup>1</sup> )	CH <sub>2</sub> O 2S <sup>2</sup> 2P <sup>2</sup> -1S <sup>1</sup> -2P <sup>2</sup>	

The agreement of calculated  $E$  values with reference data<sup>12,13</sup> was in the range of 5 % for all bonds of covalence type without introducing the coefficient of 0.83.

The main part of light energy is stored by a plant on the reduction stage to PGA. At the same time, 4.56 eV (per molecule) are spent<sup>12,13</sup>. Our calculations give the reduction energy of radical COH equal to 4.487 eV. Free energy for the formation of one mole of CH<sub>2</sub>O based on reference data<sup>7,12</sup> is 4.96-5.07 eV. The calculations following the method of  $P$ -parameter evaluate this energy as 5.025 eV.

In molecule O=C(H)-H the average repetition factor for carbon atom bond was taken as equal to  $(2+1+1)/3=1.33$ .

The values of bond energies (or the reduction energies) of structural subsystems for each stage,  $E_C$ , were calculated by using the accepted mode. It is known<sup>7</sup> that the cycle moving energy to PGA can be 1.06 eV due to three ATP molecules (per one CO<sub>2</sub> molecule), one ATP molecule is consumed in the cycle to PGA.

Following our data, the cycle moving energy ( $\Delta E_C$ ) equals the difference of  $E_C$  values for the corresponding stages:

$$1) \text{ stage CO}_2 - \text{FGAK: } \Delta E_C = 1.770 - 1.401 = 0.369 \text{ eV}$$

Phosphorylation energy of one ATP molecule = 0.34-0.35 eV

$$2) \text{ stage CO}_2 - \text{FGA: } \Delta E_C = 2.367 - 1.401 = 0.966 \text{ eV}$$

Phosphorylation energy of three ATP molecules =  $0.34 \times 3 = 1.02 \text{ eV}$

Thus  $P$ -parameter gives the satisfactory characteristics of energetics of the CO<sub>2</sub> assimilation cycle main stages. Photorespiration reaction is as if "competitive" to the CO<sub>2</sub> assimilation reaction. Also here it is possible to reveal similar values of  $P_E$ -parameters of interacting radicals C=O and HCOH with  $P_E$ -parameters of oxygen atoms. As in assimilation reaction the ferment RuDP-carboxylase "is tuned" for the formation of final product COOH. Other ferments can also participate in photosynthesis and photorespiration, for example, the substitution of Mg atoms for Fe atoms results in the formation of cytochromes, in which  $P_E$ -parameter of two-valence iron ( $P_E = 10.093 \text{ eV}$ ) is an active spatial-energy component of photosynthesis structural interactions. Therefore, iron-sulfur proteins – ferridoxins executing various transport functions connected with ATP synthesis are initial and secondary acceptors of electrons in the system PSI.

## Conclusion

In this approach, we have given the quantitative and semi-quantitative evaluation of spatial-energy interactions at main stages of complicated biophysical process of photosynthesis based on the utilization of initial atomic characteristics. The analysis of results after the application of  $P$ -parameter methodology shows that they correspond to reference data both in the direction and energetics of these processes.

## Abbreviations

- $m_1$  and  $m_2$  – masses of material points (kg);
- $\Delta U_1$  and  $\Delta U_2$  – potential energies of material points (J);
- $\Delta U$  – their resulting (mutual) potential energy of interaction (J);
- $Z^*$  – nucleus effective charge (Cl);
- $n^*$  – effective main quantum number;
- $W_i$  – bond energy of electrons on  $i$ -orbital (eV);
- $r_i$  – orbital radius of  $i$ -orbital (Å);
- $n_i$  – number of electrons on this orbital;
- $SEI$  – spatial-energy interactions;
- $P_0$  – spatial-energy parameter (eVÅ);
- $P_E$  – effective  $P$ -parameter (eV);
- $R$  – dimensional characteristic of atom or chemical bond (Å);
- $h\nu$  – light quantum energy (J, eV);
- $N_1, N_2, \dots$  – number of homogeneous atoms;
- $N$  – average repetition factor in the formula (10);
- $P_C$  – structural  $P$ -parameter of complex structure (eV);
- $\alpha$  – coefficient of structural interactions, isomorphism (%);
- $\rho$  – degree of structural interaction (%);
- PS – photosystem (PSI and PSII);
- ATP – adenosine triphosphate;
- RuDP – ribulose-diphosphate;
- PGA – 3 phosphoglyceric acid;
- NADP – nicotine-amide-adenine-dinucleotide-phosphate;
- PGA – phosphor-glycerin aldehyde;
- $E$  – energy of bond or molecule reduction (eV);
- $E_C$  – resulting energy of bond or reduction for radical groups (eV).

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