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Step by Step Water Molecule Contraction and Extension

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Abstract: *Respecting zero water molecule enthalpy of transformation and double-surface geometry the water molecule deposited energy being equal the water splitting energy 2.46 eV is calculated.*

Keywords: *Orbital energy and orbit length, double-surface geometry, zero enthalpy of transformation, water molecule contraction and extension, energy transmitter and receiver, deposited and raised energy, water splitting energy*

1. Preface

Previously one proposed the contraction[1] and the extension[2] of gaseous water molecule with the help of an exchange of the orbital energies between the bound Hydrogen and non-bound Oxygen electrons in the water molecule. In the present paper the concept is upgraded with limitations proposed to be inherent to the participants – the transmitter and the receiver –of the energy exchange. Briefly, since all the transmitted energy cannot be received, the difference should be deposited first and then raised in the reverse process.

2. The Outer Water Molecule Electrons

Let us recall again the outer electron structure of water molecule [1], [2]. It consists of four non-bound Oxygen electrons creating the negative pole as well as two bound Hydrogen electrons and two bound Oxygen electrons enabling the positive pole of the molecule as presented in Figure1[1], [2]:

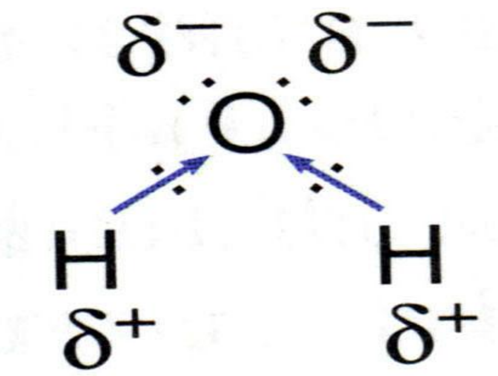

Figure1. *The outer water molecule electrons*

3. The Initial Orbital Energies and Orbit Lengths

The initial orbital energy of Oxygen non-bound electron is proposed to be that one in the ground state of Oxygen atom and the initial orbital energy of Hydrogen bound electron is deduced from the water molecule geometry in the gas state[1], [2]:

$$E_{O\ non-bound}^{initial} = -15{,}147\ 218\ eV. \tag{1}$$

$$E_{H\ bound}^{initial} = -19.023\ 237\ eV. \tag{2}$$

The orbital energies and orbit lengths are in inverse proportion[1], [2]:

$$E\ x\ s = Ry\ x\ \alpha^{-1}. \tag{3}$$

Where $Ry = 13.605\ 693\ 009$ eV and $\alpha^{-1} = 137.035\ 999\ 139\ \lambda_e$.

So the initial orbit length for the non-bound Oxygen electron as well as for bound Hydrogen electron is given:

$$s_{O\ non-bound}^{initial} = 123.089\ 912\ \lambda_e . \quad (4)$$

$$s_{H\ bound}^{initial} = 98.010\ 120\ \lambda_e . \quad (5)$$

4. THE ZERO ENTHALPY OF TRANSFORMATION

At the zero enthalpy of transformation the sum of interacting orbital energies conserves[1], [2].In the case of non-bound Oxygen electron and bound Hydrogen electron interaction we have:

$$2(E_{O\ non-bound}^{initial} - E_{O\ non-bound}^{changed}) = (E_{H\ bound}^{changed} - E_{H\ bound}^{initial}). \quad (6)$$

Factor 2 means that two non-bound Oxygen electrons interact with one bound Hydrogen electron.

And applying (3) the next relation for the orbit lengths belonging to the energies (6) is given:

$$2\left(\frac{1}{s_{O\ non-bound}^{initial}} - \frac{1}{s_{O\ non-bound}^{changed}}\right) = \left(\frac{1}{s_{H\ bound}^{changed}} - \frac{1}{s_{H\ bound}^{initial}}\right). \quad (7)$$

It can be examined that the interacting orbital energies (and consequently the concerned orbit lengths) are in inverse proportion. Lower the orbital energy and shorter the orbit length of the transmitter means higher the orbital energy and longer the orbit length of the receiver. And of course vice versa. Find also, that orbital energies are signed negative and the highest yields zero.

5. THE STABLE ELECTRON ORBIT

Respecting double-surface geometry a stable electron circulation on the orbit is enabled satisfying the next formula for the orbit length expressed in the wavelengths of the electron:

$$s(n) = n\left(2 - \frac{1}{\sqrt{1+\frac{\pi^2}{n^2}}}\right), \qquad n \in \mathbb{N}. \quad (8)$$

Here n is the elliptic length and in the same time the number of the orbit. For instance, the initial orbit length for the non-bound Oxygen electron and bound Hydrogen electron should be the next:

$$s_{O\ non-bound}^{conceptual\ \ initial} = s(123) = 123.040 \quad (9)$$

$$s_{H\ bound}^{conceptual\ \ initial} = s(98) = 98.050 \dots . \quad (10)$$

The given values are comparable to that (4), (5) from section 3.

6. THE WATER MOLECULE CONTRACTION

The water molecule contraction takes place when the bound Hydrogen electron is a transmitter of the orbital energy[1]. Let us propose that the energy transmitting electron should gradually step down to the shorter orbits than 98, i.e. n < 98. The descent to non-adjacent orbit is not allowed. Consequently the non-bound Oxygen electron as an energy receiver should gradually step up to the longer orbits than 123, i.e. n > 123. Since the temporary received energy put the energy receiving electron on the unstable orbit $m \notin \mathbb{N}$ (8) the surplus of received energy should be somehow deposited. Its value is given taking into account the next relation:

$$E_{deposited} = Ry\ x\ \alpha^{-1}\left(\frac{1}{s(n \in \mathbb{N})} - \frac{1}{s(m \notin \mathbb{N})}\right) \quad for\ m - n < 1\ on\ the\ interval\ \ 123 < n < 18743 \quad (11)$$

The data for the whole finite step by step contraction are collected in Table1. The whole deposited energy is then step by step raised up in the inverse process from the final 34th bound Hydrogen orbit back to the initial 98th one.

Table1. *Deposited energy at expected 64-fold step by step water molecule contraction from Hydrogen 98th to 34th orbit accompanied by non-bound Oxygen orbit elongation from 123th to 18743th orbit.*

	Transmitter	Temporary Receiver	Final Receiver	Deposited Energy		Transmitter	Temporary Receiver	Final Receiver	Deposited Energy
n^{th} step	H-orbit length (λ_e)	O-orbit length(λ_e)	O-orbit length(λ_e)	Inner wave (eV)	n^{th} step	H-orbit length (λ_e)	O-orbit length(λ_e)	O-orbit length(λ_e)	Inner wave (eV)
0	98,05032	123,0401	123,0401	0	33	65,07579	150,6232	150,0329	0,0487
1	97,05083	123,8403	123,0401	0,0979	34	64,07697	152,7781	152,0325	0,0599
2	96,05136	123,8571	123,0401	0,1000	35	63,07818	154,9430	154,0320	0,0712
3	95,05190	123,8744	123,0401	0,1021	36	62,07944	157,1183	157,0314	0,0066
4	94,05245	123,8922	123,0401	0,1042	37	61,08074	160,3473	160,0308	0,0230
5	93,05302	123,9106	123,0401	0,1065	38	60,08208	163,5929	163,0303	0,0393
6	92,05359	123,9297	123,0401	0,1088	39	59,08346	166,8565	166,0297	0,0556
7	91,05418	123,9493	123,0401	0,1112	40	58,08490	170,1394	170,0290	0,0071
8	90,05478	123,9696	123,0401	0,1136	41	57,08638	174,4963	174,0284	0,0287
9	89,05540	123,9906	123,0401	0,1161	42	56,08791	178,8822	178,0277	0,0500
10	88,05602	124,0124	123,0401	0,1188	43	55,08950	183,2999	183,0270	0,0152
11	**87,05667**	**124,0349**	**123,0401**	**0,1215**	44	54,09115	188,8161	188,0262	0,0415
12	86,05732	124,0581	124,0398	0,0022	45	53,09286	194,3785	194,0254	0,0175
13	85,05800	125,0990	125,0395	0,0071	46	52,09464	201,0653	201,0245	0,0019
14	84,05869	126,1417	126,0391	0,0120	47	51,09649	208,8980	208,0237	0,0375
15	83,05939	127,1863	127,0388	0,0170	48	50,09840	216,8165	216,0228	0,0316
16	82,06011	128,2330	128,0385	0,0221	49	49,10040	225,9233	225,0219	0,0331
17	81,06085	129,2819	129,0382	0,0272	50	48,10248	236,2529	236,0209	0,0078
18	80,06161	130,3330	130,0379	0,0325	51	47,10465	248,9592	248,0199	0,0284
19	79,06239	131,3865	131,0377	0,0378	52	46,10690	263,0031	262,0188	0,0266
20	78,06319	132,4425	132,0374	0,0432	53	45,10926	279,5885	279,0177	0,0136
21	77,06401	133,5012	133,0371	0,0487	54	44,11173	299,9989	299,0165	0,0204
22	76,06485	134,5628	134,0368	0,0544	55	43,11431	324,457	324,0152	0,0078
23	75,06571	135,6273	135,0365	0,0601	56	42,11700	355,6613	355,0139	0,0096
24	74,06660	136,6951	136,0363	0,0660	57	41,11983	395,4291	395,0125	0,0050
25	73,06751	137,7662	137,0360	0,0721	58	40,12280	448,5500	448,0110	0,0050
26	72,06844	138,8409	138,0357	0,0783	59	39,12592	522,3084	522,0095	0,0020
27	71,06940	139,9194	139,0355	0,0847	60	38,12920	632,2643	632,0078	0,0012
28	70,07039	141,0019	140,0352	0,0913	61	37,13266	812,7891	812,0061	0,0022
29	69,07141	142,0887	142,0347	0,0050	62	36,13630	1162,450	1162.000	0,0006
30	68,07245	144,2106	144,0343	0,0158	63	35,14015	2135,177	2135,021	6E-05
31	67,07353	146,3400	146,0338	0,0267	64	34,14422	18743,79	18743.00	4E-06
32	66,07464	148,4773	148,0333	0,0377					$\sum 2.7413\ eV$

7. THE WATER MOLECULE EXTENSION

The water molecule extension takes place when the non-bound Oxygen electron is a transmitter of orbital energy[2]. Let us propose that the energy transmitting electron should gradually step down to the shorter orbits than 123, i.e. n < 123.The descent to non-adjacent orbit is not allowed. Consequently the bound Hydrogen electron as an energy receiver should gradually step up to the longer orbits than 98, i.e. n > 98. Since the temporary received energy put the energy receiving electron on the unstable orbit $m \notin \mathbb{N}$ (8) the surplus of received energy should be somehow deposited. Its value is given taking into account the next relation:

$$E_{deposited} = Ry\ x\ \alpha^{-1}\left(\frac{1}{s(n \in \mathbb{N})} - \frac{1}{s(m \notin \mathbb{N})}\right) \quad for\ m - n < 1\ on\ the\ interval\ \ 98 < n < 3939. \qquad (12)$$

The data for the whole finite step by step extension are collected in Table 2. The whole deposited energy is then step by step raised up in the inverse process from the final 73thnon-bound Oxygen orbit back to the initial 123th one.

Table2. *Deposited energy expected at 50-fold step by step water molecule extension from Hydrogen 98^{th} to 3939^{th} orbit caused by non-bound Oxygen orbit shortening from 123^{th} to 73^{th} orbit*

	Transmitter	Temporary Receiver	Final Receiver	Deposited Energy		Transmitter	Temporary Receiver	Final Receiver	Deposited Energy
n^{th} step	O-orbit length (λ_e)	H-orbit length(λ_e)	H-orbit length(λ_e)	Inner wave (eV)	n^{th} step	O-orbit length (λ_e)	H-orbit length(λ_e)	H-orbit length(λ_e)	Inner wave (eV)
0	123,0401	98,05032	98,05032	0	26	97,05083	146,4029	146,0338	0,0322
1	122,0404	99,34732	99,04981	0,0564	27	96,05136	150,7547	150,0329	0,0595
2	121,0408	100,3957	100,0493	0,0643	28	95,05190	155,1287	155,0318	0,0075
3	120,0411	101,4459	101,0488	0,0722	29	94,05245	160,5988	160,0308	0,0412
4	119,0414	102,4979	102,0483	0,0801	30	93,05302	166,1019	166,0297	0,0049
5	118,0418	103,5519	103,0479	0,0881	31	92,05359	172,7215	172,0287	0,0435
6	117,0422	104,6078	104,0474	0,0960	32	91,05418	179,3878	179,0276	0,0209
7	116,0425	105,6658	105,0470	0,1039	33	90,05478	187,1968	187,0264	0,0091
8	115,0429	106,7259	106,0465	0,1119	34	89,05540	196,1703	196,0252	0,0070
9	114,0433	107,7884	107,0461	0,1199	35	88,05602	206,3343	206,0240	0,0136
10	113,0436	108,8531	108,0457	0,1280	36	87,05667	217,7190	217,0227	0,0275
11	112,0440	109,9203	109,0452	0,1361	37	86,05732	230,3600	230,0215	0,0119
12	**111,0444**	**110,9900**	**110,0448**	**0,1443**	38	85,05800	245,4364	245,0201	0,0129
13	110,0448	112,0624	112,0440	0,0027	39	84,05869	263,0358	263,0188	0,0005
14	109,0452	114,1753	114,0433	0,0189	40	83,05939	284,4339	284,0174	0,0096
15	108,0457	116,2937	116,0425	0,0347	41	82,06011	309,8191	309,0160	0,0156
16	107,0461	118,4177	118,0418	0,0501	42	81,06085	340,6420	340,0145	0,0101
17	106,0465	120,5477	120,0411	0,0653	43	80,06161	379,7788	379,0130	0,0099
18	105,0470	122,6840	122,0404	0,0801	44	79,06239	430,5306	430,0115	0,0052
19	104,0474	124,8267	124,0398	0,0948	45	78,06319	499,5687	499,0099	0,0042
20	103,0479	126,9764	126,0391	0,1092	46	77,06401	598,1627	598,0083	0,0008
21	102,0483	129,1332	129,0382	0,0106	47	76,06485	751,1366	751,0066	0,0004
22	101,0488	132,3490	132,0374	0,0332	48	75,06571	1018,769	1018,005	0,0014
23	100,0493	135,5770	135,0365	0,0550	49	74,06660	1605,366	1605,003	0,0003
24	99,04981	138,8179	138,0357	0,0761	50	73,06751	3939,654	3939,001	8E-05
25	98,05032	142,0723	142,0347	0,0035					$\sum 2.1854eV$

8. RESULTS AND CONCLUSIONS

Both deposited energies at the water molecule contraction and extension being collected in Table1 and Table2, respectively, are also represented in Figure2.

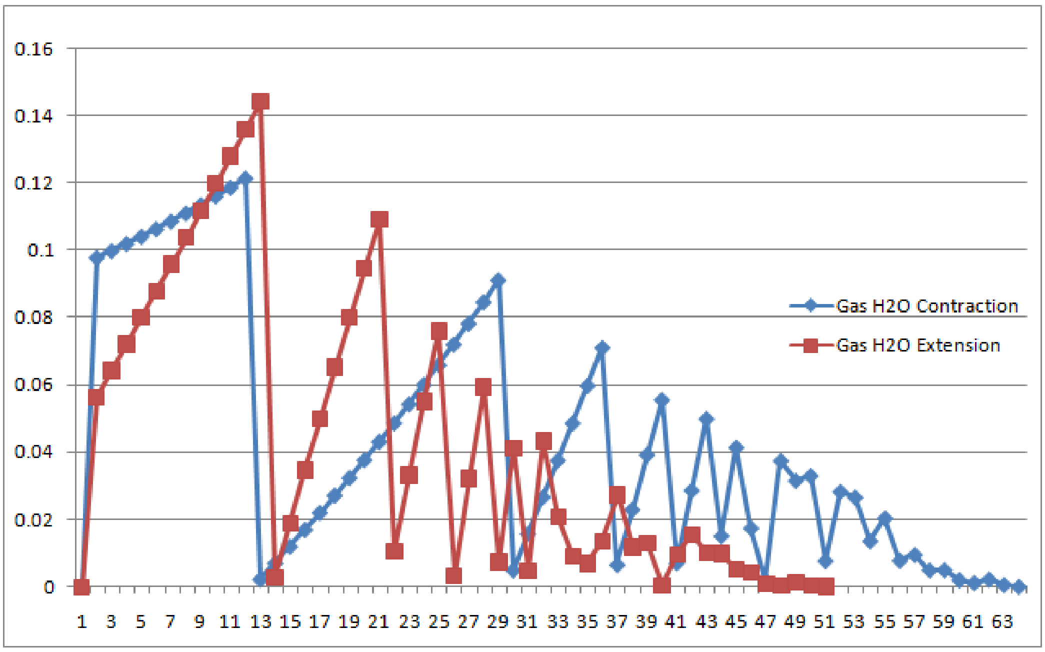

Figure2. *Deposited energy (expressed in eV) expected at the water molecule contraction and extension*

We can see that more energy is deposited in the contraction than in extension process since:

$$E_{contraction}^{whole} = 2.7413\ eV > E_{extension}^{whole} = 2.1854\ eV. \quad (13)$$

Although the greatest single deposited energy is found amongst the extension process quanta as follows:

$$E_{contraxion}^{maximal\ \ single} = 0.1443\ eV > E_{extension}^{\text{maximal}\ \ single} = 0.1215\ eV. \quad (14)$$

The average value of both in principle equally probable whole deposited energies is interesting. Thus:

$$E_{average}^{whole} = \frac{E_{cont\,raction}^{whole} + E_{extension}^{whole}}{2} = 2.4634\ eV. \quad (15)$$

Encouraging indeed, since the given value equals the water splitting energy to hydrogen and oxygen known from Chemical references[3]:

$$E_{average}^{whole} = E_{splitting}^{H2O} = 2.46\ eV. \quad (16)$$

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Thanks God for Life and Water again

DEDICATION

This fragment is dedicated to the Water itself and Pharmacy as an art of Living

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