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Hydrogen Covalent Bond Explained by Heracletean Dynamics

(From Physics to Chemistry)

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Abstract: *In this paper Hydrogen covalent bond of* $0.74\,x\,10^{-10} m$ *is explained respecting Heracletean dynamics.*

Keywords: *Electron orbital and radial probability in the Hydrogen ground state, Hydrogen covalent bond*

1. PREFACE

The subject of interest of this paper is with the help of the electron orbital and radial probability in the Hydrogen ground state to explain the Hydrogen covalent bond.

2. THE ELECTRON ORBITAL AND RADIAL PROBABILITY

Respecting Heracletean dynamics the probability of electron presence in the Hydrogen ground state orbit n (orbital probability $P_{orbital}\ (n)$) depends on the electron position radius Δr_nin that orbit[1]:

$$P_{orbital}\ (n) = \frac{\Delta r_n}{\sum_{n=1}^{n=274} \Delta r_n}. \tag{1}$$

The probability of electron presence at the average ground state radius $\bar{r}_n$of then^{th}Hydrogen ground state orbit (radial probability $P_{radial}\ (n)$) depends also on the orbit length $s$as well aselectron average speed $\bar{a}_n$on that orbit as follows:

$$P_{radial}\ (n) = \frac{\Delta r_n x \frac{\bar{a}_n}{s}}{\sum_{n=1}^{n=274} \Delta r_n x \frac{\bar{a}_n}{s}}. \tag{2}$$

The sum of all possible probabilities of the same kind is adjusted to unit:

$$\sum_{n=1}^{n=274} P_{orbital} = \sum_{n=1}^{n=274} P_{radial}\ (n) = 1\,, \qquad \mathrm{n} \in \mathbb{N}. \tag{3}$$

Orbital probabilities can be found in the reference article[1] and the radial probabilities are calculated applying the equations from the same address[1].

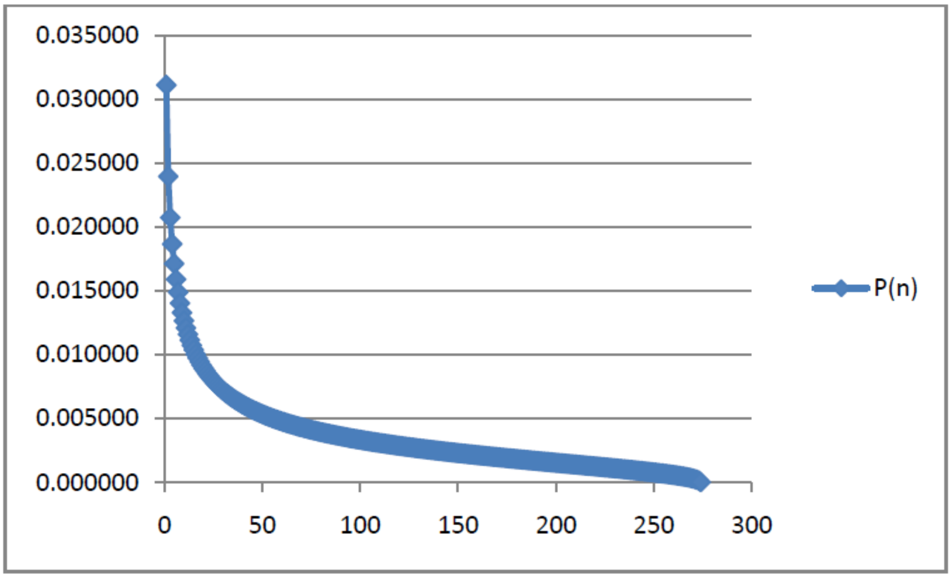
The radial probabilities are listed in $Table 1$.

Table1. *Electron Radial Probability* $P_{radial}\ (n)$*inHydrogen ground state*

n	$P_{radial}\ (n)$												
1	0,0311037	41	0,0060230	81	0,0039073	121	0,0028478	161	0,0021222	201	0,0015270	241	0,0009381
2	0,0239476	42	0,0059387	82	0,0038734	122	0,0028268	162	0,0021063	202	0,0015128	242	0,0009219
3	0,0207269	43	0,0058572	83	0,0038400	123	0,0028061	163	0,0020905	203	0,0014985	243	0,0009055
4	0,0186619	44	0,0057782	84	0,0038071	124	0,0027855	164	0,0020747	204	0,0014843	244	0,0008890
5	0,0171235	45	0,0057017	85	0,0037748	125	0,0027651	165	0,0020590	205	0,0014701	245	0,0008723
6	0,0158971	46	0,0056276	86	0,0037429	126	0,0027448	166	0,0020433	206	0,0014558	246	0,0008554
7	0,0148843	47	0,0055556	87	0,0037115	127	0,0027248	167	0,0020278	207	0,0014416	247	0,0008383
8	0,0140288	48	0,0054857	88	0,0036805	128	0,0027049	168	0,0020123	208	0,0014274	248	0,0008210
9	0,0132942	49	0,0054178	89	0,0036500	129	0,0026852	169	0,0019968	209	0,0014131	249	0,0008035
10	0,0126552	50	0,0053518	90	0,0036199	130	0,0026656	170	0,0019814	210	0,0013989	250	0,0007857
11	0,0120930	51	0,0052875	91	0,0035902	131	0,0026462	171	0,0019661	211	0,0013846	251	0,0007677
12	0,0115937	52	0,0052250	92	0,0035609	132	0,0026269	172	0,0019509	212	0,0013704	252	0,0007494

13	0,0111466	53	0,0051641	93	0,0035320	133	0,0026078	173	0,0019357	213	0,0013561	253	0,0007307
14	0,0107434	54	0,0051047	94	0,0035035	134	0,0025889	174	0,0019206	214	0,0013418	254	0,0007118
15	0,0103774	55	0,0050469	95	0,0034754	135	0,0025700	175	0,0019055	215	0,0013275	255	0,0006924
16	0,0100432	56	0,0049904	96	0,0034476	136	0,0025514	176	0,0018904	216	0,0013132	256	0,0006727
17	0,0097365	57	0,0049353	97	0,0034202	137	0,0025328	177	0,0018755	217	0,0012988	257	0,0006525
18	0,0094538	58	0,0048815	98	0,0033931	138	0,0025144	178	0,0018605	218	0,0012844	258	0,0006319
19	0,0091920	59	0,0048290	99	0,0033664	139	0,0024961	179	0,0018456	219	0,0012700	259	0,0006107
20	0,0089488	60	0,0047776	100	0,0033399	140	0,0024780	180	0,0018308	220	0,0012555	260	0,0005889
21	0,0087220	61	0,0047274	101	0,0033138	141	0,0024600	181	0,0018160	221	0,0012411	261	0,0005665
22	0,0085097	62	0,0046783	102	0,0032880	142	0,0024421	182	0,0018013	222	0,0012265	262	0,0005433
23	0,0083106	63	0,0046302	103	0,0032626	143	0,0024243	183	0,0017866	223	0,0012120	263	0,0005193
24	0,0081233	64	0,0045832	104	0,0032374	144	0,0024067	184	0,0017719	224	0,0011974	264	0,0004943
25	0,0079467	65	0,0045371	105	0,0032125	145	0,0023891	185	0,0017573	225	0,0011827	265	0,0004682
26	0,0077797	66	0,0044919	106	0,0031878	146	0,0023717	186	0,0017427	226	0,0011680	266	0,0004408
27	0,0076215	67	0,0044477	107	0,0031635	147	0,0023544	187	0,0017281	227	0,0011532	267	0,0004117
28	0,0074713	68	0,0044043	108	0,0031394	148	0,0023372	188	0,0017136	228	0,0011384	268	0,0003807
29	0,0073285	69	0,0043618	109	0,0031156	149	0,0023201	189	0,0016991	229	0,0011235	269	0,0003472
30	0,0071925	70	0,0043201	110	0,0030920	150	0,0023031	190	0,0016846	230	0,0011086	270	0,0003104
31	0,0070627	71	0,0042791	111	0,0030687	151	0,0022862	191	0,0016702	231	0,0010935	271	0,0002689
32	0,0069386	72	0,0042390	112	0,0030456	152	0,0022694	192	0,0016558	232	0,0010784	272	0,0002201
33	0,0068199	73	0,0041995	113	0,0030227	153	0,0022527	193	0,0016414	233	0,0010633	273	0,0001574
34	0,0067062	74	0,0041607	114	0,0030001	154	0,0022360	194	0,0016270	234	0,0010480	**274**	0,0000356
35	0,0065970	75	0,0041227	115	0,0029777	155	0,0022195	195	0,0016127	235	0,0010326		
36	0,0064921	76	0,0040852	116	0,0029555	156	0,0022031	196	0,0015984	236	0,0010171		
37	0,0063913	77	0,0040485	117	0,0029336	157	0,0021868	197	0,0015841	237	0,0010016		
38	0,0062942	78	0,0040123	118	0,0029118	158	0,0021705	198	0,0015698	238	0,0009859		
39	0,0062006	79	0,0039767	119	0,0028903	159	0,0021543	199	0,0015555	239	0,0009701		
40	0,0061103	80	0,0039417	120	0,0028689	160	0,0021383	200	0,0015412	240	0,0009542		

They are also figured in the $Graph$ 1:



Graph1. *Electron Radial Probability* P_{radial} (n)*in Hydrogen ground state*

3. The Hydrogen covalent bond

In covalent chemical bond[2] a pair of valence electrons is shared by two atoms. Such a bond enables a stable molecule if with the help of shared electrons a noble gas configuration is created for each atom.[2]Hydrogen gas forms the simplest covalent bond in the diatomic hydrogen molecule.[2]

$$H\cdot + \cdot H \rightarrow H \cdot\cdot H. \tag{4}$$

4. The Heracletean approach

The diatomic hydrogen molecule is consisted of equal atoms where one is arbitrary named "primary" possessing primary nucleus and electron. As well as the other one is then named "secondary" possessing secondary nucleus and electron. Primary electron is located at Bohr radius away from the primary nucleus and in the same time lies at the co-Bohr radius away from the secondary nucleus. And vice versa, the secondary electron is located approximately at Bohr radius away from secondary nucleus and lies at the co-Bohr radius away from primary nucleus. Neglecting the repulsion influence of equal charges the sum of Bohr radius and the co-Bohr radius equal the Hydrogen covalent bond.

5. Bohr radius

In the Hydrogen atom the electron survives approximately half of his presence beneath and approximately the other half beyond Bohr orbit. Indeed, following Heracletean dynamics[1] the electron cumulative orbital probabilities in the Hydrogen ground state confirm such a conclusion.

That is[1]:

$$\sum_{n=1}^{n=136} P_{orbital}\ (n) = 0.497436824 \approx 0.5. \tag{5}$$

$$\sum_{n=137}^{n=137} P_{orbital}\ (n) = 0.004645518. \tag{6}$$

$$\sum_{n=138}^{n=274} P_{orbital}\ (n) = 0.497917658 \approx 0.5. \tag{7}$$

The orbit $n = 137$ is Bohr orbit(6) having, of course, Bohr radius. More precise view shows that the cumulative outer position beyond Bohr orbit $(7)$is slightly more convenient than the cumulative inner position beneath Bohr orbit(5):

$$\frac{\sum_{n=138}^{n=274} P_{orbital}\ (n)}{\sum_{n=1}^{n=136} P_{orbital}\ (n)} = 1.0009666\ \ldots \tag{8}$$

Thus in the case of Hydrogen forming covalent bonds with other atoms Bohr radius (or its $1.00096666 \ldots -$multiple) should be taken into account as the primary contribution to the bond length.

6. The co-Bohr radius

The secondary contribution to the covalent bond length between Hydrogen atoms depends on the electron distance to the neighboring nucleus involved in the bond forming. This distance, named co-Bohr radius, mirrors the radial probability of the electron being found there. The electron survives approximately half of his presence beneath and approximately the other half beyond the co-Bohr radius. The concerned radius can be found with the help of the electron radial probabilities listed in Table 1.

That is:

$$\sum_{n=1}^{n=52} P_{radial}\ (n) = 0.497519887. \tag{9}$$

$$\sum_{53}^{53} P_{radial}\ (n) = 0.005164090. \tag{10}$$

$$\sum_{n=54}^{n=274} P_{radial}\ (n) = 0.497316023. \tag{11}$$

The orbit $n = 53$ is the co-Bohr orbit (10)having, of course, the co-Bohr radius. More precise view shows that the cumulative outer position beyond the co-Bohr radius (11) is slightly less convenient than the cumulative inner position beneath the co-Bohr radius(9):

$$\frac{\sum_{n=55}^{n=274} P_{orbital}\ (n)}{\sum_{n=1}^{n=53} P_{orbital}\ (n)} = 0.999590\ \ldots \tag{12}$$

Thus in the case of the Hydrogen atom forming covalent bond with other Hydrogenatom the co-Bohr radius (or its$0.999590\ldots-$multiple) should be taken into account as the secondary contribution to the bond length.

7. THE HYDROGEN COVALENT BOND LENGTH

Calculating the sum of Bohr and the co-Bohr radius the chemical covalent bond length of Hydrogen molecule is estimated:

$$bond\ length_{H_2} = R_{Bohr} + R_{co-Bohr}. \tag{13}$$

It can be expressed in the units of Bohr radius and calculated with the help of $53^{th}$and 137^{th} orbit lengthss_{53} ands_{137}, respectively[1]:

$$\frac{bond\ length_{H_2}}{R_{Bohr}} = 1 + \frac{R_{co-Bohr}}{R_{Bohr}} = 1 + \frac{s_{53}}{s_{137}}. \tag{14}$$

For $s_{53} = 53{,}092865[1]$ and $s_{137} = 137{,}036006[1]$we have:

$$\frac{bond\ length_{H_2}}{R_{Bohr}} = 1.387437. \tag{15}$$

For Bohr radius$R_{Bohr} = 0.52917721067\ x\ 10^{-10}m[3]$the next value of the Hydrogen covalent bond is given:

$$bond\ length_{H_2} = 0.7342\ x\ 10^{-10}m. \tag{16}$$

Taking into account the correction factors $(8), (12)$ only on the fourth decimal different result is given, i.e. $0.7344\ x\ 10^{-10}m$. Both results are in accordance with the value $0.7414\ x\ 10^{-10}m$ known from chemistry & physics books[4].

8. CONCLUSIONS

Heracletean dynamics explains Hydrogen covalent bond under the assumption that on the third decimal underestimated value$0.7344\ x\ 10^{-10}m$is a consequence of the unconsidered repulsion influence of equal charges involved in the bond forming.

ACKNOWLEDGEMENT

Gratitude to the electron message: "If we want to make bonds for better life we have to go there where is less convenient, too."

DEDICATION

This fragment is dedicated to the philosophical hint in the sixties:"Maybe we should go back to presocratics". And pharmaceutical teachings in the seventies: "Pharmacy is a link between many sciences."

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