cubic ellipsoid nuclear model: the correlation between the nuclear structure and the atomic covalent radius

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Abstract

This study analyzes the atomic covalent radius under the cubic nuclear model hypothesis, that the nuclear structure determines the atomic properties [1].

We find that the atomic covalent radius correlates with the relative distance of the corresponding valance proton from the nuclear center, meaning that the nuclear geometric shape is reflected by the atomic shape.

Our conclusions:

- The nuclear structure determines the atomic properties. •
- The nuclear geometry determines the atomic covalent radius. •
- The nuclear geometry possibly defines also the atomic shape. •

This might be a proof of the cubic nuclear model hypothesis.

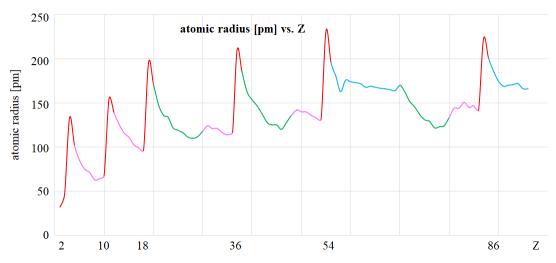
Remark: by "shell" we refer here to the electrons (or protons) of the elements of some row in the periodic table.

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Introduction

The following graph shows the experimental data of the atomic covalent single bond radius as a function of the atomic number [3].



atomic covalent radius vs. atomic number Z (Covalent single bond [<u>3</u>]). sub-orbitals: **S**, **P**, **D**, **F**.

The atomic covalent radius shows the following pattern:

- while moving from one row (period) of the periodic table to the next one, the size of the atom grows.
- along a row the size of the atom shrinks.

In this research we try to show how the nuclear geometric structure, according to the cubic ellipsoid model, determines the atomic covalent radius.

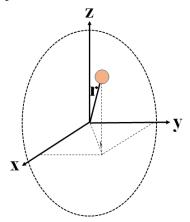
The research

Calculating the relative nuclear distance

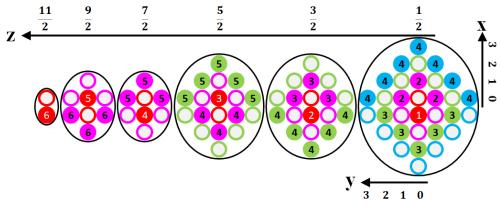
As a preparation we make two definitions:

- a valance proton: the one, that was last added to the current in-filling process suborbital.
- the relative nuclear distance: the relative geometric distances of the valance proton from the nuclear center.

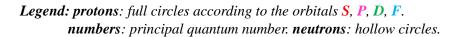
The following illustrations demonstrate the way the relative nuclear distance of the valance proton is calculated from the nuclear geometry via $r_{x,y,z} = \sqrt{x^2 + y^2 + z^2}$.



a proton in the nucleus



the *x*-*y* planes along the nuclear *z* axis (upper half only)



The protons in the illustration have a shift of 0.5 along the x-axis, but it is treated here, as if the S-proton has the x-y position (0, 0) and the rest follows in accordance; anyway this has only a small effect on the course of the graph and doesn't change the statements of this study.

We observe only nuclei with symmetric shape, meaning those with the following number of protons in the last sub-orbital:

- **s**: {2}
- **p**: {4, 6}
- $d: \{4, 8, 10\}$
- $f: \{4, 8, 12, 14\}$

this refers to the elements (till Z = 96):

- $s = \{He_2; Ca_{12}; He_2; Ca_{20}; Sr_{38}; Ba_{56}; Ra_{88}\}$
- $p = \{O_8, Ne_{10}; S_{16}, Ar_{18}; Se_{34}, Kr_{36}; Te_{52}, Xe_{54}; Po_{84}, Rn_{86}\}$
- $d = \{Cr_{24}, Ni_{28}, Zn_{30}; Mo_{42}, Pd_{46}, Pd_{48}; W_{74}, Pt_{78}, Hg_{80}\}$
- $f = \{Nd_{62}, Gd_{64}, Er_{68}, Yb_{70}; U_{92}, Cm_{96}\}$

with the relative coordinates:

- $s = \{x = 0; y = 0; z = \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \frac{7}{2}, \frac{9}{2}, \frac{11}{2}, \frac{13}{2}\}$ $p = \{x = 0, 1; y = 0, 1; z = \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \frac{7}{2}, \frac{9}{2}, \frac{11}{2}\}$ $d = \{x = 0, 1, 2; y = 0, 1, 2; z = \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \frac{7}{2}\}$ $f = \{x = 0, 1, 2, 3; y = 0, 1, 2, 3; z = \frac{1}{2}, \frac{3}{2}\}$

and the distance from the nuclear center, $r_{x,y,z} = \sqrt{x^2 + y^2 + z^2}$, is calculated by the following Excel table:

6.5	5.5	5.5	4.5	4.5		3.5	3.5	3.5	2.5	2.5	2.5	1.5	1.5	1.5	1.5			0.5	0.5	0.5	0.5	z
0	1	0	1	0	[2	1	0	2	1	0	3	2	1	0	ſ		3	2	1	0	у
															3.4	Ī	3.0				3.0	
								4.0			3.2			2.7	2.5	Ī	2.0			2.3	2.1	
	4	5.6		4.6			3.8	3.6		2.9	2.7		2.7	2.1	1.8	Ī	1.0		2.3	1.5	1.1	
6.5	5.6	5.5	4.6	4.5		4.0	3.6	3.5	3.2	2.7	2.5	3.4	2.5	1.8	1.5		0.0	3.0	2.1	1.1	0.5	

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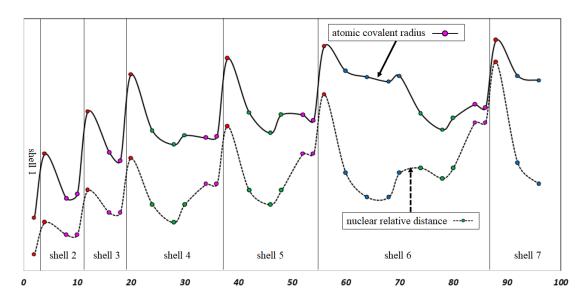
The table of the calculated values of the relative nuclear distance according to the orbitals S, P, D, F and the shells 1 to 7.

A comparison between the atomic covalent radius and the relative nuclear distance

The cubic ellipsoid model was first built in the search for a connection between the nuclear structure and the atomic properties. We now look for the behavior of the atomic covalent radius and compare it to the nuclear distance of the corresponding nuclear suborbital. For the elements with symmetric nuclei of the sub-orbitals (s, p, d, f as described in the previous section) in the atomic number of the range $Z \in [1, 96]$; two curves are observed and compared:

- The atomic covalent radius [3].
- The relative nuclear distance (taken from the table in the last paragraph).

The comparison between the two curves is of course done in relative values, since the two refer to different orders of magnitude.



The comparison between the atomic covalent radius and the relative nuclear distance. The curves have a different scale and the comparison is made in relative sizes.

We observe a seemingly correlation between the two curves, although the atomic curve is taken from the experimental data and the relative nuclear distance is a geometric property, measured according to the ellipsoid model.

This strengthens the hypothesis that the nuclear structure determines the atomic properties.

Discussion of the results and conclusions

We found a correlation between the nuclear geometric structure and the atomic covalent radius.

If we accept the assumption of the model, we can expect the atomic and nuclear shape to be correlated with each other; this correlation is therefore expected between the valence electron and the valance proton.

We emphasize that the covalent atomic radius is not necessarily the "furthest point" of the atom, but rather the point that matches the valence proton.

The van der Waals radius for instance, possibly refers to the "farthest position" on the surface of the atom.

This could mean also, that the angles of the chemical bonds between atoms are influenced by the nuclear structure.

We thus get one additional conclusion, that the atomic shape possibly correlates with the nuclear shape.

We summon our conclusions:

- The nuclear structure determines the atomic properties.
- The nuclear geometry determines the atomic covalent radius.
- The nuclear geometry possibly defines also the atomic shape and molecular geometry.

This might be a proof of the model assumption.

Sources and references

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- 3. Pekka Pyykkö, Michiko Atsumi (2009). "Molecular Double-Bond Covalent Radii for Elements Li–E112". <u>Chemistry: A European Journal 15 (46): 12770–12779</u>
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Appendix

The data of the atomic covalent radius and the relative nuclear distance

The following table includes the data that was used in this study of the atomic covalent radii (from [3]) and the calculated relative nuclear distances:

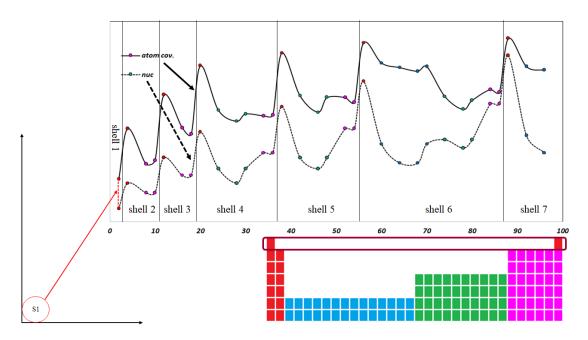
Z	element	atomic covalent radius	calculated relative nuclear distance
2	He	46	32
4	Be	102	60
8	0	63	32
10	Ne	67	36
12	Mg	139	69
16	S	103	53
18	Ar	96	46
20	Ca	171	73
24	Cr	122	64
28	Ni	110	68
30	Zn	118	60
34	Se	116	41
36	Kr	117	42
38	Sr	185	59
42	Мо	138	68
46	Pd	120	62
48	Cd	136	66
52	Те	136	34
54	Xe	131	29
56	Ba	196	42
60	Nd	174	89
64	Gd	169	105
68	Er	165	101
70	Yb	170	85
74	W	137	47
78	Pt	123	43
80	Hg	133	43
84	Ро	145	16
86	Rn	142	13
88	Ra	201	19
92	U	170	76
96	Cm	166	91

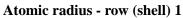
Remarks:

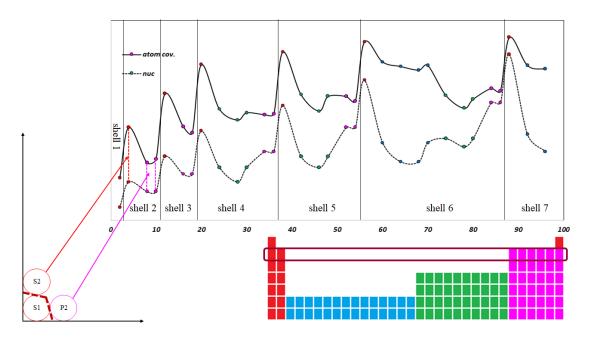
- The data for the covalent radius is available only till Z = 96, therefore not all elements are included in the table.
- The covalent radius is in $pm = 10^{-12}m$.
- The relative nuclear data is multiplied by a constant to appear in a similar size in the graph.

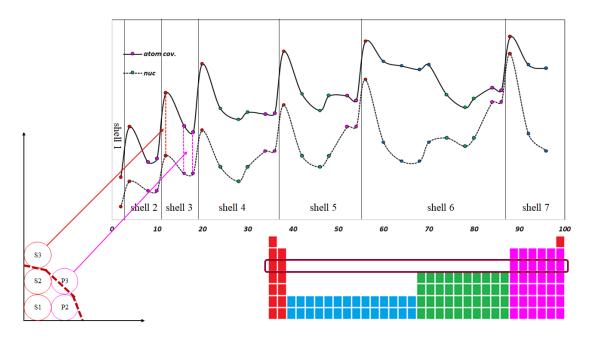
The graphs of the atomic covalent radius and the relative nuclear distance

The graphs show a comparison between the atomic covalent radius and the relative distance of the valance proton from the nuclear center.

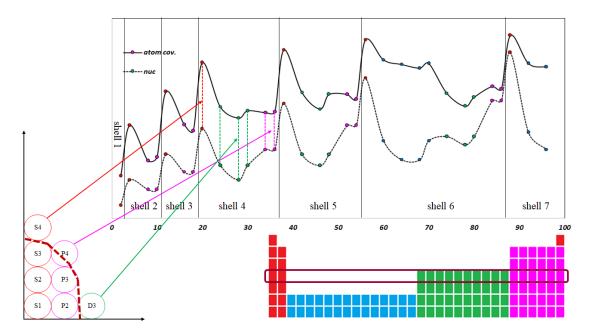








Atomic radius - row 4



Atomic radius - row 5

