

Comparisons Among Different Approaches Toward Atomic Radii

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Ameliorated polynomial relationships between a recently proposed set of atomic radii and other well known experimental and theoretical data are presented. These improved equations allow the discussion of several chemical bonding features in a more accurate way.

Keywords: Atomic radii, Solid-state density, Main block elements, d Transition metals

Even before Dalton raised the issue of the atom's existence, man has tried to answer the fundamental question: which is the atom size? As science evolved we have seen the difficulty answering this question and nowadays we have not achieved a unique and universally accepted response. From the last part of 19th century, when there were rather good estimations of Avogadro's number, it was known the order of magnitude of atomic size. Later on, several experimental procedures were designed to obtain more accurate results. For example, the incidence of X-rays on crystals has allowed to get very good interatomic distances. However, since there exist a large number of crystalline systems, it was soon recognized that an atom size depends on the environment surrounding the atom (Cruz-Garriz et al. 1986).

It is well known that the atom is not a rigid sphere, consequently its size changes depending upon the external forces acting on it. Besides, an atom has a variable number of external electrons taking part in the chemical bond/s according to its vicinal atoms. Thus, in order to discuss the atomic size issue it is necessary to identify the different milieus.

While the ionic model is the best way to describe the chemical bonding for a solid, the sizes of the involved chemical species are quantified as to their "ionic radius". If a covalent bond exists between two atoms, then a "covalent radius" can be determined from the bond length. For metallic atoms there is a characteristic "metallic radius" defined as the half distance between vicinal atoms within the metal bulk. Another typical definition of atomic radii is "Van der Waals radius" defined from the distances separating two vicinal atoms (noble gas atoms or those forming part of molecules bonded by this sort of interaction) where exist dispersion forces. Furthermore, assigning a single consistent set of atomic radii for transition elements becomes problematic due the various coordination patterns and spin states available for them. Besides, the preferred coordination state as well as the spin state often depends on the attached ligands.

This sketchy classification of atomic radii makes clear the relative content of the atomic radius concept so that it has leads to the analysis of several possibilities to surpass this situation in order to generalize it and to define a rather "universal" set of atomic radii which should be useful in any circumstance. It is therefore necessary to have a consistent and universally accepted approach to understand the periodic nature of atomic radii.

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In a recent paper Suresh and Koga (2001) presented a method which makes consistent carbon-based atomic radii suitable for all the main block elements and the *d* block transition elements. The authors found good linear correlations with other well known atomic radii values and a satisfactory expected density of the elements which show a good linear correlation with solid-state density of elements when they are metals, suggesting similarity in their atomic packing. In this work, we report a further analysis of such correlations, showing they can be ameliorated through the employment of higher-order polynomial relationships.

Atomic Radius

The first approach to obtain a universal atomic radii scale was proposed by Bragg in 1920 on the basis of crystallographic data taken from ionic, covalent and metallic solids. He tried to get a set of radius values capable of reproducing in the best possible way, the internuclear distances when considered in pairs. He obtained a good fitting to such additivity rule. Later on, Slater improved this approach and proposed an empirical set of atomic radii (R_{Slater}) via the comparison of 1,200 bond types in ionic, metallic, and covalent molecules and crystals. Although these propositions were very valuable as a first step to determine a universal definition, Bragg and Slater's radii present some drawbacks. In fact, they are somewhat minor than metallic radii so that they do not reproduce satisfactorily distances within the metal bulk. Since they do not consider the coordination number it can lead to considerable errors in some extreme cases.

Theoretical estimations are the sensible option in obtaining a satisfactory universal atomic radii. The three mains approaches are:

- a) The expected value of the distance between the nucleus and the valence electron/s.
- b) The distance value to the nucleus where the radial distribution function corresponding to the valence electron is a maximum.
- c) The distance value to the nucleus enclosing a given percentage of the valence electron/s charge.

Clementi et al (1967) determined a set of theoretical atomic radii (R_{CRR}) from minimal basis-set SCF wave functions for ground state atoms. Another quantity sometimes referred to as a good criterion of atomic size in molecules is the covalent radius (R_{covalent}), which is defined as half of the single bond length between two atoms of same kind (Sanderson, 1962; Sutton, 1965 and Porterfield, 1984). Alcock (1990) proposed a consistent approach to understand the periodic of atomic radii which is based on carbon-based radii.

His values are determined by subtracting the radius of carbon from C(sp³)-X distances (R_{Alcock}). More recently, Suresh and Koga (2001) have given a consistent approach toward atomic radii resorting to hybrid density functional calculations on methyl group substituted elemental hydrides of the form H₃C-EH_n as the C-E distance minus half of the C-C bond distance of ethane. E is any main block or *d* block transition element and *n* = 0, 1,2,3, or 4, depending on the position of E in the periodic table. These distances (R_A) give quite good linear correlations with different atomic radii such as experimental covalent radii, Slater's empirical set of atomic radii, and experimental carbon-based atomic radii particularly for the main block elements. Since such R_A data reproduces very well the corresponding mean single bond distances in molecules and provide the calculation of an expected density of the elements, it should be interesting to know whether the correlations with other current available atomic radii data can be improved through higher order fitting equations.

Methodology

Simple regression involving a single independent variable restricts regression analysis considerably. Many correlations need not be linear. In fact, a quadratic regression may result in a better description of the relationship than a simple model. Non-linear models may be fitted to data sets by the inclusion of functions of the independent variable in a linear regression model (Livingstone, 1995). Construction of linear regression models containing non-linear terms is most often prompted when the data is clearly not well fitted by a linear model, but where regularity in the data suggests that some other model will fit. In general, one should test single descriptor regression for quadratic dependence and, if warranted, for higher order polynomial relationships or other functional dependence (Randic et al.).

In this work we present results for linear, quadratic, and cubic correlations between R_A and atomic radii from other standard sources. The data were taken from Ref. 2 and the corresponding values are given in Tables 1 and 2 for main block elements and *d* block transition elements. The goodness of atomic radii values can be judged through solid-state density (Ds) data since this quantity is directly correlated with the atomic size. In fact, Ds is the mass of 1 m³ of the solid element at specified conditions. Because the volume enclosed by a sphere of radius R_A contains the atomic mass of an element, one can calculate the mass of 1 m³ of the element as its expected density, Ds', by assuming no free space in it. Ds and Ds' values are also inserted in Tables 1 and 2.

Table 1. Various atomic radii (in Å) and solid state density (Kg/m³) for main block elements.

Atom	R _A	R _{covalent}	R _{CCR}	R _{Slater}	R _{Alcock}	Ds'	Ds
H	0.327	0.37	0.53	0.25	0.299	11504	89.8
Li	1.219	1.34	1.67	1.45	-	1518	535
Be	0.911	0.90	1.12	1.05	1.060	4726	1848
B	0.793	0.82	0.87	0.85	0.830	8607	2530
C	0.766	0.77	0.67	0.70	0.767	10585	2267
N	0.699	0.75	0.56	0.65	0.702	16290	1250
O	0.658	0.73	0.48	0.60	0.659	22234	1429
F	0.633	0.71	0.42	0.50	0.619	29697	1710
Na	1.545	1.54	1.90	1.80	-	2473	968
Mg	1.333	1.30	1.45	1.50	-	4072	1738
Al	1.199	1.18	1.18	1.25	1.180	6205	2700
Si	1.123	1.11	1.11	1.10	1.090	7871	2330
P	1.110	1.06	0.98	1.00	1.088	8975	1823
S	1.071	1.02	0.88	1.00	1.052	10355	1960
Cl	1.039	0.99	0.79	1.00	1.023	12533	3210
K	1.978	1.96	2.43	2.20	-	2003	856
Ca	1.745	1.74	1.94	1.80	-	2993	1550
Zn	1.187	1.31	1.42	1.35	-	15500	7140
Ga	1.199	1.26	1.36	1.30	1.250	16039	5904
Ge	1.179	1.22	1.25	1.25	1.220	17569	5323
As	1.209	1.19	1.14	1.15	1.196	16819	5727
Se	1.201	1.16	1.03	1.15	1.203	18092	4819
Br	1.201	1.14	0.94	1.15	1.199	18285	3140
Rb	2.217	2.11	2.65	2.35	-	3111	1532
Sr	1.928	1.92	2.19	2.00	-	4848	2630
Cd	1.429	1.48	1.61	1.55	-	15275	8650
In	1.385	1.44	1.56	1.55	1.41	17122	7310
Sn	1.380	1.41	1.45	1.45	1.39	17918	7310
Sb	1.421	1.38	1.33	1.45	1.37	6836	6697
Te	1.400	1.35	1.23	1.4	1.391	18430	6240
I	1.397	1.33	1.15	1.4	1.395	18460	4660
Cs	2.442	2.25	2.98	2.6	-	3620	1879
Ba	2.149	1.98	2.53	2.15	-	5488	3510
Hg	1.465	1.49	1.71	1.5	-	25281	13590
Tl	1.531	1.48	1.56	1.9	-	22570	11850
Pb	1.434	1.47	1.54	1.8	-	27881	11340
Bi	1.496	1.46	1.43	1.6	-	24748	9780

The large deviations between Ds and Ds' is due to the fact that the latter is the density "assuming no free space" in the mass of 1 m³ of the element, while the former is the mass of 1 m³ of the solid element at specified conditions.

Linear, quadratic and cubic polynomial fitting equations between R_A versus R_{Slater}, R_{covalent}, R_{CCR},

R_{Alcock} and R_{Pauling}, and Ds' versus Ds were determined for elements cited in Tables 1 and 2 resorting to standard multilinear regression techniques [11]. Multilinear regression analysis was performed up to the third order since for higher order results do not change appreciably.

Table 2. Atomic radii (\AA) and solid state density (Kg/m^3) for d block transition elements.

Atom	R_A	R_{covalent}	R_{CCR}	R_{Slater}	R_{metallic}	Ds'	Ds
Sc	1.337	1.44	1.84	1.60	1.641	7453	2985
Ti	1.274	1.36	1.76	1.40	1.462	7932	4507
V	1.236	1.25	1.71	1.35	1.346	10707	6110
Cr	1.128	1.27	1.66	1.40	1.282	14367	7140
Mn	1.180	1.39	1.61	1.40	1.264	13242	7470
Fe	1.091	1.25	1.56	1.40	1.274	17064	7874
Co	1.089	1.26	1.52	1.35	1.252	19521	8900
Ni	1.077	1.21	1.49	1.35	1.246	18604	8908
Cu	1.146	1.38	1.45	1.35	1.278	16755	8920
Y	1.482	1.62	2.12	1.80	1.801	10822	4472
Zr	1.377	1.48	2.06	1.55	1.602	13847	6511
Nb	1.353	1.37	1.98	1.45	1.468	14858	8570
Mo	1.240	1.45	1.90	1.45	1.400	19933	10280
Tc	1.287	1.56	1.83	1.35	1.360	18395	11500
Ru	1.212	1.26	1.78	1.30	1.339	22478	12370
Rh	1.229	1.35	1.73	1.35	1.345	24362	12450
Pd	1.240	1.31	1.69	1.40	1.376	22152	12023
Ag	1.362	1.53	1.65	1.60	1.445	16934	10450
La	1.653	1.95	-	1.65	1.877	12185	6146
Hf	1.364	1.50	2.08	1.55	1.580	27910	13310
Ta	1.346	1.38	2.00	1.45	1.467	29426	16650
W	1.256	1.46	1.93	1.35	1.408	36742	19250
Re	1.258	1.59	1.88	1.35	1.375	36742	21020
Os	1.222	1.28	1.85	1.30	1.353	41311	22610
Ir	1.227	1.37	1.80	1.35	1.357	45279	22650
Pt	1.227	1.28	1.77	1.35	1.387	41848	21090
Au	1.273	1.44	1.74	1.35	1.442	37894	19300

Results and Discussion

In Tables 3 and 4 the data corresponding to the multilinear regression correlations between R_A and R_{covalent} , R_{Slater} and R_{Alcock} atomic radii and Ds' versus Ds are given for all the main block elements and the d block transition elements, respectively. In Tables 5 and 6 some representative results are given for illustrative purposes. Complete results can be requested to the corresponding author.

Analysis of statistical data for main block elements shows that even though one obtains some amelioration when resorting to higher-order regression equations, it is rather modest. The most significant improvement results for Ds calculations, where linear relationship has a regression coefficient equal to 0.6802 while the value for cubic equation is 0.7171.

The R_{CCR} fitting gives higher mean deviations since Clementi et al (1967) determined the set of atomic radii

Table 3. Coefficients and statistical parameters for correlations equations of different radii versus R_A of main block elements.

Correlation	Coefficients ¹				R2	S3
	a	b	c	d		
R_{covalent} vs R_A						
Linear5	0.1105	0.9097			0.9916	0.0543
Quadratic	0.0170	1.0594	-0.0536		0.9923	0.0526
Cubic	0.1722	0.6167	0.3080	-0.0873	0.9929	0.0513
R_{CRR} vs R_A						
Linear5	-0.3179	1.2976			0.9551	0.1839
Quadratic	0.0887	0.6470	0.2329		0.9618	0.1723
Cubic	0.4641	-0.4243	1.1082	-0.2115	0.9634	0.1713
R_{Slater} vs R_A						
Linear5	-0.1084	1.1314			0.9778	0.1107
Quadratic	-0.2738	1.3961	-0.0947		0.9793	0.1085
Cubic	-0.0966	0.8905	0.3183	-0.0998	0.9798	0.1089
R_{Alcock} vs R_A						
Linear5	0.0120	0.9927			0.9908	0.0415
Quadratic	-0.0956	1.2472	-0.1343		0.9917	0.0404
Cubic	-0.1547	1.4893	-0.4256	0.1072	0.9918	0.0414
Ds vs Ds' ⁴						
Linear	362.0072	0.2969			0.6802	2562.0383
Quadratic	1223.4416	0.3469	0.0		0.6810	2596.8928
Cubic	2991.7432	-0.6912	0.0001	0.0	0.7171	2508.6473

¹ $R_X = bR_A + c[R_A]^2 + d[R_A]^3 + a$; X = covalent, CRR, Slater, Alcock.²Regression coefficient.³Standard error of estimate.⁴Ds = $bDs' + c[Ds']^2 + d[Ds']^3 + a$.⁵Data reported in Ref.5.**Table 4.** Coefficients and statistical parameters for correlations equations of different radii versus R_A of *d* block transition elements.

Correlation	Coefficient ¹				R2	S3
	a	b	c	d		
R_{covalent} vs R_A						
Linear	0.0517	1.0711			0.8476	0.0845
Quadratic	2.1065	-2.0553	1.1765		0.8690	0.0805
Cubic	-7.7128	20.2748	-15.5704	4.1389	0.8744	0.0806
R_{CRR} vs R_A						
Linear	-0.1358	1.5354			0.8345	0.1017
Quadratic	-1.4583	3.6526	-0.8423		0.8366	0.1033
Cubic	-0.5297	1.4584	0.8759	-0.4460	0.8364	0.1056
R_{Slater} vs R_A						
Linear	0.483	0.7456			0.7607	0.0802
Quadratic	1.5125	-0.8186	1.5125		0.7707	0.0804
Cubic	39.2278	-86.5809	64.9037	-15.8939	0.9072	0.0542
R_{metallic} vs R_A						
Linear	-0.0942	1.1990			0.9389	0.0554
Quadratic	0.7826	-0.1349	0.5020		0.9424	0.0550
Cubic	17.4347	-37.9975	28.8934	-7.0156	0.9563	0.0491
Ds' vs Ds' ⁴						
Linear	-71.0362	0.5267			0.9868	979.4842
Quadratic	-1025.1558	0.6181	0.0		0.9873	980.1233
Cubic	229.3199	0.4220	0.0	0.0	0.9876	991.6225

1, 2, 3, 4: Same comments as in Table 3.

from minimal-basis-set SCF wave functions for ground-state atoms and it is well known that better quality basis sets must be employed to get satisfactory results.

The atomic radii predictions for *d* block transition elements show a somewhat different behavior regarding main block elements. In fact, calculations improved markedly for R_{covalent} vs R_A , R_{Slater} vs R_A , and R_{metallic} vs R_A relationships, while R_{CCR} vs R_A and Ds' vs Ds equations present moderate ameliorations. In

this last case we see the second-order and third-order contributions are null.

The average absolute deviations corresponding to the predicted radii of main block elements are low for R_{CCR} and R_{Slater} while they are rather large for R_{covalent} and R_{Alcock} . Regarding *d* block transition elements, only R_{CCR} predictions are rather large, while the remaining ones are quite close to the original values.

Table 5. Some predicted radii for main block elements derived from the multilinear regression equations.

Atom	R_{covalent}	R_{covalent}^1	R_{CCR}	R_{CCR}^2	R_{Alcock}	R_{Alcock}^1	R_{Slater}	R_{Slater}^2
H	0.37	0.40	0.53	0.33	0.299	0.291	0.25	0.17
Li	1.34	1.32	1.67	1.22	-	-	1.45	1.29
Be	0.90	0.92	1.12	0.87	1.060	0.930	1.05	0.92
B	0.82	0.81	0.87	0.75	0.830	0.812	0.85	0.77
C	0.77	0.79	0.67	0.72	0.767	0.785	0.70	0.74
N	0.75	0.72	0.56	0.65	0.702	0.715	0.65	0.66
O	0.73	0.69	0.48	0.62	0.659	0.672	0.60	0.60
F	0.71	0.66	0.42	0.59	0.619	0.645	0.50	0.57
Na	1.54	1.54	1.90	1.64	-	-	1.80	1.66
Mg	1.30	1.33	1.45	1.36	-	-	1.50	1.42
Al	1.18	1.20	1.18	1.20	1.180	1.204	1.25	1.26
Si	1.11	1.13	1.11	1.11	1.090	1.133	1.10	1.17
P	1.06	1.12	0.98	1.09	1.088	1.121	1.00	1.16
S	1.02	1.08	0.88	1.05	1.052	1.084	1.00	1.11
Cl	0.99	1.05	0.79	1.01	1.023	1.053	1.00	1.07
K	1.96	1.92	2.43	2.28	-	-	2.20	2.12
Ca	1.74	1.72	1.94	1.93	-	-	1.80	1.87
Zn	1.31	1.19	1.42	1.18	-	-	1.35	1.25
Ga	1.26	1.20	1.36	1.20	1.250	1.204	1.30	1.26
Ge	1.22	1.18	1.25	1.18	1.220	1.185	1.25	1.24
As	1.19	1.21	1.14	1.21	1.196	1.213	1.15	1.28
Se	1.16	1.21	1.03	1.20	1.203	1.206	1.15	1.27
Br	1.14	1.21	0.94	1.20	1.199	1.206	1.15	1.27
Rb	2.11	2.10	2.65	2.67	-	-	2.35	2.36
Sr	1.92	1.88	2.19	2.20	-	-	2	2
Cd	1.48	1.43	1.61	1.49	-	-	1.55	1.53
In	1.44	1.39	1.56	1.43	1.41	1.38	1.55	1.48
Sn	1.41	1.38	1.45	1.43	1.39	1.37	1.45	1.47
Sb	1.38	1.42	1.33	1.48	1.37	1.41	1.45	1.52
Te	1.35	1.40	1.23	1.45	1.391	1.390	1.40	1.50
I	1.33	1.40	1.15	1.45	1.395	1.388	1.40	1.49
Cs	2.25	2.24	2.98	3.06	-	-	2.6	2.6
Ba	1.98	2.05	2.53	2.55	-	-	2.15	2.29
Hg	1.49	1.46	1.71	1.53	-	-	1.5	1.6
Tl	1.48	1.52	1.56	1.63	-	-	1.9	1.6
Pb	1.47	1.43	1.54	1.50	-	-	1.8	1.5
Bi	1.46	1.49	1.43	1.58	-	-	1.6	1.6
Average absolute deviation	-	0.036	-	0.132	-	0.026	-	0.083

¹ Third-order regression equation.

² Second-order regression equation.

Table 6. Some predicted atomic radii (Å) for *d* block transition elements.

Atom	R_{covalent}	R_{covalent}^1	R_{CRR}	R_{CCR}^2	R_{Slater}	R_{Slater}^1	R_{metallic}	R_{metallic}^2
Sc	1.44	1.45	1.84	1.92	1.60	1.50	1.641	1.499
Ti	1.36	1.40	1.76	1.83	1.40	1.40	1.462	1.425
V	1.25	1.38	1.71	1.77	1.35	1.36	1.346	1.383
Cr	1.27	1.29	1.66	1.59	1.40	1.34	1.282	1.269
Mn	1.39	1.33	1.61	1.68	1.40	1.32	1.264	1.322
Fe	1.25	1.25	1.56	1.52	1.40	1.38	1.274	1.233
Co	1.26	1.25	1.52	1.52	1.35	1.39	1.252	1.231
Ni	1.21	1.23	1.49	1.50	1.35	1.41	1.246	1.220
Cu	1.38	1.30	1.45	1.62	1.35	1.32	1.278	1.287
Y	1.62	1.61	2.12	2.10	1.80	1.73	1.801	1.685
Zr	1.48	1.49	2.06	1.97	1.55	1.57	1.602	1.549
Nb	1.37	1.47	1.98	1.94	1.45	1.53	1.468	1.519
Mo	1.45	1.38	1.90	1.78	1.45	1.36	1.400	1.387
Tc	1.56	1.41	1.83	1.85	1.35	1.42	1.360	1.440
Ru	1.26	1.37	1.78	1.73	1.30	1.33	1.339	1.356
Rh	1.35	1.37	1.73	1.76	1.35	1.35	1.345	1.375
Pd	1.31	1.38	1.69	1.78	1.40	1.36	1.376	1.387
Ag	1.53	1.47	1.65	1.95	1.60	1.55	1.445	1.530
La	1.95	1.95	-	-	1.65	1.67	1.877	1.931
Hf	1.50	1.48	2.08	1.96	1.55	1.55	1.580	1.532
Ta	1.38	1.46	2.00	1.93	1.45	1.52	1.467	1.510
W	1.46	1.39	1.93	1.80	1.35	1.38	1.408	1.405
Re	1.59	1.39	1.88	1.80	1.35	1.38	1.375	1.407
Os	1.28	1.36	1.85	1.75	1.30	1.34	1.353	1.367
Ir	1.37	1.37	1.80	1.76	1.35	1.35	1.357	1.373
Pt	1.28	1.37	1.77	1.76	1.35	1.35	1.387	1.373
Au	1.44	1.40	1.74	1.83	1.35	1.40	1.442	1.424
Average absolute deviation	-	0.051	-	0.079	-	0.040	-	0.040

1 Third-order regression equation.

2 Second-order regression equation.

Table 7. Mean single bond length (*d*) in molecules corresponding to main block elements and the sum of bonded atom radii values (R_{sum}) given in A for a typical calculation.

Bond	<i>d</i>	R_{sum}^1	Bond	<i>d</i>	R_{sum}	Bond	<i>d</i>	R_{sum}
As-N	1.858	1.93	C-I	2.162	2.19	N-S	1.710	1.80
As-Cl	2.268	2.26	C-N	1.469	1.51	N-N	1.425	1.44
As-F	1.678	1.87	C-O	1.432	1.48	N-Si	1.748	1.85
As-C	1.963	2.00	C-S	1.809	1.87	N-O	1.463	1.41
As-O	1.710	1.90	C-Si	1.863	1.92	N-P	1.730	1.84
As-S	2.275	2.29	C-Te	2.158	2.19	O-P	1.689	1.81
As-As	2.459	2.42	C-P	1.855	1.91	O-S	1.645	1.77
B-B	1.701	1.62	C-Se	1.970	2.00	O-Te	2.133	2.09
B-Br	1.967	2.02	Cl-P	2.008	2.17	P-P	2.214	2.24
B-C	1.597	1.60	Cl-S	2.072	2.13	P-Si	2.264	2.25
B-P	1.806	1.93	Cl-Si	2.020	2.18	Zn-I	2.574	2.59
B-S	1.806	1.89	Cl-Te	2.520	2.45	Zn-Br	2.390	2.40
B-Cl	1.833	1.86	F-S	1.527	1.74	Zn-Cl	2.255	2.24
B-F	1.365	1.47	F-N	1.406	1.38	Cd-Br	2.611	2.64
B-N	1.549	1.53	F-P	1.579	1.78	Cd-Cl	2.499	2.48
B-O	1.468	1.50	F-Si	1.694	1.79	Cd-I	2.754	2.83
C-C	1.530	1.58	H-N	1.009	1.12	Hg-Br	2.539	2.67
C-Cl	1.793	1.84	H-O	0.967	1.09	Hg-Cl	2.423	2.51
C-F	1.399	1.45	I-I	2.917	2.80	Hg-I	2.702	2.86
C-H	1.092	1.19	I-Te	2.926	2.80	Hg-S	2.624	2.54

Average absolute deviation = 0.07

¹ R_{covalent} calculated from third order regression equation (third column Table 5).

Table 8. Mean single bond length (d) in molecules corresponding to transition metals and the sum of bonded atom radii values (R_{sum}) given in Å for a typical calculation.

Bond	d	R_{sum}	Bond	d	R_{sum}	Bond	d	R_{sum}
O-Ti	1.847	2.09	S-V	2.378	2.46	Cl-Co	2.254	2.30
O-V	1.917	2.07	S-Mn	2.328	2.41	Cl-Ni	2.217	2.28
O-Cr	1.816	1.98	S-Fe	2.271	2.33	Cl-Cu	2.179	2.35
O-Mn	1.914	2.02	S-Co	2.254	2.33	Cl-Zr	2.426	2.54
O-Fe	1.913	1.94	S-Ni	2.187	2.31	Cl-Nb	2.374	2.52
O-Co	1.899	1.94	S-Cu	2.292	2.38	Cl-Mo	2.398	2.43
O-Ni	1.848	1.92	S-Mo	2.401	2.46	Cl-Tc	2.323	2.46
O-Cu	1.899	1.99	S-Tc	2.302	2.49	Cl-Ru	2.409	2.42
O-Zr	1.924	2.18	S-Ru	2.238	2.45	Cl-Rh	2.369	2.42
O-Nb	1.869	2.16	S-Pd	2.351	2.46	Cl-Pd	2.326	2.43
O-Mo	1.911	2.07	S-Ag	2.493	2.55	Cl-Ta	2.383	2.51
O-Rh	2.035	2.06	S-Ir	2.382	2.45	Cl-W	2.390	2.44
O-Pd	2.016	2.07	S-Pt	2.320	2.45	Cl-Re	2.368	2.44
O-W	1.900	2.08	Cl-Ti	2.313	2.45	Cl-Os	2.357	2.41
O-Re	1.890	2.08	Cl-V	2.224	2.43	Cl-Ir	2.361	2.42
O-Os	1.914	2.05	Cl-Cr	2.309	2.34	Cl-Pt	2.323	2.42
O-Pt	2.028	2.06	Cl-Mn	2.346	2.38	Cl-Au	2.276	2.45
S-Ti	2.432	2.48	Cl-Fe	2.195	2.30	-	-	-

Average absolute deviation = 0.11

 $^1R_{\text{covalent}}$ calculated from third order regression equation (third columns in Table 5 and Table 6).

If atomic radii obtained from this calculation scheme are a reliable measure of the atomic size in molecules, the sum of any two radii values in Tables 5 and 6 must be close to the corresponding interatomic single bond distances in molecules. A test based on this criterion is performed by comparing the sum of any two radii values to the corresponding mean bond length, d (Orpen et al., 1994). Some representative values are given in Tables 7 and 8 for a total of 113 different mean bond distances in molecules.

A close inspection of results presented in Tables 7 and 8 show that d values showing absolute deviation from R_{sum} are relatively few and the agreement between experimental data and calculated bond distances is quite satisfactory. Similar results are obtained for other atomic radii and could be requested from the corresponding author.

Conclusions

New theoretical data for different types of atomic radii calculated on the basis of a new reliable scale for all the main group elements and the d block transition elements were obtained. The predicted radii are in a satisfactory

enough agreement with the experimentally determined data. The calculations of some typical bond distances on the basis of the predicted radii compare fairly well with experimental available data, which shows that the computed atomic radii make up a reliable measure of the atomic size in molecules. Equally satisfactory are the density of elements results when compared with the solid-state density of the elements.

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