

Thermodynamically Consistent Atomic Radii of Main Group Elements

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Abstract

Atomic radius is a fundamentally important quantity shaping multiple properties of atoms, molecules, and materials. Due to its fundamental importance, precise quantification and interpretation of atomic radii has been the subject of numerous studies for more than a century. It has resulted in a broad variety of estimations of atomic radii which so far have not been amenable to extensive verification by experiment. The present study follows our recent work demonstrating that electron iso-density surfaces, contoured at a certain cut-off density, accurately represent molecular surfaces determined via thermodynamic phase change data. Here we provide thermodynamically consistent estimates of atomic radii for the main group elements.

Atomic radii are fundamentally important quantities governing many properties of atoms such as electronegativity [1, 2], hardness [3], polarizability [4, 5], ionization potential [6, 7], and electrophilicity index [8, 9]. Precise quantification of atomic radii is crucial in numerous applications in physics and chemistry, including but not limited to theoretical studies of solvent effects via continuum solvation models [10-13], (supra-)molecular interactions [14-16], materials properties such as electrical conductivity [17], melting points [18], porosity [19] and magnetic behavior [20], strength of chemical bonds [21], non-covalent interactions [22-26], design of van der Waals (vdW) materials [27-30], and many other applications. Due to its fundamental importance, quantification of atomic radii has been a subject of numerous studies for more than a century, starting from the pioneering work of Meyer [31], followed by a wide variety of experimental [32-37] and theoretical approaches [38-47] developed in the past decades.

A review of the literature reveals a broad spread, and even some inconsistencies, among available estimations of atomic radii. For experimental methods, atomic radii are commonly determined via interatomic distances measured in the condensed phase. The radii estimated this way are therefore susceptible to be largely influenced by interatomic interactions, resulting in broad range of radii estimations heuristically classified as covalent, ionic, metallic, or vdW radii [48, 49]. Radii estimation from interatomic distances also commonly relies on the assumption of the additivity of

atomic radii and approximating the most probable value of each radius from a broad distribution of interatomic distances between a specific element and probe atom(s), which introduces some arbitrariness and uncertainty. The other sources of inaccuracy in conventional experimental methods are due to neglecting the dependence of atomic radii on the chemical environment [50-52], electron distribution anisotropy and bond polarity [33, 53], and crystallographic direction [54]. In contrast, theoretical methods do typically not suffer from such issues. Nevertheless, the uncertainty in experimental reference data has hindered a fair comparison and extensive verification of the theoretical approaches. Among available theoretical methods, the Bader method which considers the atomic radii as the distance to iso-density surfaces for a certain cut-off density is probably the most widely-accepted approach [55-58]. However, extensive and broad application of this method has long been hindered by the ambiguity in defining the most appropriate value of the cut-off density due to lack of experimental verification [59], as discussed above.

In our recent studies [59, 60], we shed light on the above-mentioned issues by exploiting a recent method allowing precise experimental evaluation of the surfaces of molecules via thermodynamic phase change data [11] and comparing them with iso-density surfaces evaluated for different cut-off densities. We demonstrated that for a large dataset of studied compounds, adopting a cut-off density of 0.0016 a.u., which is roughly at the mid-point of the values suggested by Bader (0.002 a.u.) [61] and Boyd (0.001 a.u.) [44], yields iso-density surfaces that almost perfectly match with the experimental estimates of molecular surfaces. As pointed out by Ashcroft and co-workers, outstanding advantages of this approach stems from linking atomic radii to electron density as an (in principle) experimentally observable quantity, and also because Pauli, exchange, or same-spin repulsions are mainly determined by electron density at the outermost regions of atoms [55]. Additionally, this approach also benefits from the possibility of highly precise estimation of electron density via modern quantum chemical methods, allowing to uniquely define atomic surfaces, taking into account atomic surface asymmetry and anisotropy, and being experimentally verified for a large dataset of compounds [59]. Therefore, in the present study we exploit this approach to provide an estimation of atomic radii for the main group elements. Because the employed value of the cut-off density (0.0016 a.u.) is obtained with reference to experimental thermodynamic phase change data, the atomic radii estimated by this approach are coined thermodynamically consistent.

To estimate atomic radii via electron iso-density surfaces, we computed electron densities of elements in the isolated state (isolated atoms) at coupled cluster CCSD(T) level of theory, which is conventionally considered to be the gold standard in quantum chemistry. We used the large Def2-QZVPPD quadruple-zeta basis set, which was previously shown by us to be highly accurate in reproduction of experimental estimations of molecular resurfaces [59]. Additionally, to study the importance of relativistic corrections which might be important for heavy elements, we also used the ANO-RCC basis set and the Douglas–Kroll–Hess second-order scalar relativistic Hamiltonian [62] which have been commonly used to evaluation of atomic radii [42, 55]. In comparison to single reference computations, the much more computationally demanding multireference methods are more robust, especially for open shell elements where multiple spin configurations might contribute to the expectation values of atomic properties. Nevertheless, for evaluation of electron density and radii approximation, less demanding single reference

computations, even at DFT level of theory, can closely reproduce the results obtained via multireference computations, as demonstrated by Rahm et al [55]. Therefore, in this study, we considered the Complete Active Space Self-Consistent Field (CASSCF) multireference computations only for the first 36 elements, to investigate the accuracy of various applied methods. To approximate atomic radii from electron density distributions, we spherically averaged the electron density for shells with 0.0001 Å radii intervals and took the mid-point of the shell with closest value to the required cut-off density as the atomic radius. All electronic structure computations were carried out in Orca 5.0.3. [63] and post-processed by Multiwfn software [64]. For all studied levels of theory, details of the estimated atomic radii based on different cut-off densities from 0.001 a.u. to 0.002 a.u. with 0.0001 a.u. intervals are provided as supplementary information. Our results show that the radii estimated with the Def2-QZVPPD basis set closely agree with those obtained with the ANO-RCC basis set and based on relativistic correction as well as via CASSCF, with average unsigned deviation of only 0.020 Å and 0.015 Å, respectively. Accordingly, for sake of consistency among elements and also with our previously reported results [59, 60], we report the atomic radii based on computations with the Def2-QZVPPD basis set. According to the results reported in Table 1, our estimated atomic radii are on average 6.8% smaller than those reported by Rahm et al., which are based on a cut-off density of 0.001 a.u. Furthermore, the atomic radii estimated from electron density distribution of isolated atoms are in good agreement with the values reported by us for H, C, N, O, and F elements in our previous study obtained from a different approach. In that work, we found the atomic radii of isolated elements via optimization and in a way that the radii of atoms in molecules evaluated through free and effective volumes reproduce most accurately the overall molecular surfaces [60]. Accordingly, for the effective volumes calculated via iterative Hirshfeld partitioning, we obtained atomic radii of 1.47, 1.87, 1.65, 1.49, and 2.06 Å for H, C, N, O, and F elements, respectively, which are in good agreement with results reported here.

Table 1- Comparison of different estimations of atomic radii (Å)

| | Present study | Bondi [34, 65] | Equilibrium vdW radius [41] | Rahm et al., [55] | Alvarez [32] | MM3 [26] | COSMO-RS [66] |
|-----------|---------------|----------------|-----------------------------|-------------------|--------------|----------|---------------|
| H | 1.41 | 1.20 | | 1.54 | 1.20 | 1.62 | 1.30 |
| He | 1.24 | 1.40 | | 1.34 | 1.43 | 1.53 | |
| Li | 1.90 | 1.81 | 2.63 | 2.20 | 2.12 | 2.55 | |
| Be | 2.03 | | 2.23 | 2.19 | 1.98 | 2.23 | |
| B | 1.92 | | 2.05 | 2.05 | 1.91 | 2.15 | |
| C | 1.79 | 1.70 | 1.96 | 1.90 | 1.77 | 2.04 | 2.00 |
| N | 1.67 | 1.55 | 1.79 | 1.79 | 1.66 | 1.93 | 1.83 |
| O | 1.59 | 1.52 | 1.71 | 1.71 | 1.50 | 1.82 | 1.72 |
| F | 1.52 | 1.47 | 1.65 | 1.63 | 1.46 | 1.71 | |
| Ne | 1.45 | 1.54 | | 1.56 | 1.58 | 1.60 | |
| Na | 1.88 | 2.27 | 2.77 | 2.25 | 2.50 | 2.70 | |
| Mg | 2.22 | 1.73 | 2.42 | 2.40 | 2.51 | 2.43 | |
| Al | 2.24 | | 2.40 | 2.39 | 2.25 | 2.36 | |
| Si | 2.19 | 2.10 | 2.26 | 2.32 | 2.19 | 2.29 | |
| P | 2.10 | 1.80 | 2.14 | 2.23 | 1.90 | 2.22 | |
| S | 2.02 | 1.80 | 2.06 | 2.14 | 1.89 | 2.15 | |

| | | | | | | | |
|-----------|------|------|------|------|------|------|------|
| Cl | 1.94 | 1.75 | 2.05 | 2.06 | 1.82 | 2.07 | 2.05 |
| Ar | 1.87 | 1.88 | | 1.97 | 1.83 | 1.99 | |
| K | 1.94 | 2.75 | 3.02 | 2.34 | 2.73 | 3.09 | |
| Ca | 2.45 | | 2.78 | 2.70 | 2.62 | 2.81 | |
| Sc | 2.42 | | 2.62 | 2.63 | 2.58 | 2.61 | |
| Ti | 2.38 | | 2.44 | 2.57 | 2.46 | 2.39 | |
| V | 2.34 | | 2.27 | 2.52 | 2.42 | 2.29 | |
| Cr | 2.12 | | 2.23 | 2.33 | 2.45 | 2.25 | |
| Mn | 2.27 | | 2.25 | 2.42 | 2.45 | 2.24 | |
| Fe | 2.23 | | 2.27 | 2.26 | 2.44 | 2.23 | |
| Co | 2.20 | | 2.25 | 2.22 | 2.40 | 2.23 | |
| Ni | 2.01 | 1.63 | 2.23 | 2.19 | 2.40 | 2.22 | |
| Cu | 1.99 | 1.40 | 2.27 | 2.17 | 2.38 | 2.26 | |
| Zn | 2.11 | 1.39 | 2.24 | 2.22 | 2.39 | 2.29 | |
| Ga | 2.20 | 1.87 | 2.41 | 2.33 | 2.32 | 2.46 | |
| Ge | 2.28 | | 2.32 | 2.34 | 2.29 | 2.44 | |
| As | 2.17 | 1.85 | 2.25 | 2.31 | 1.88 | 2.36 | |
| Se | 2.13 | 1.90 | 2.18 | 2.24 | 1.82 | 2.29 | |
| Br | 2.08 | 1.83 | 2.10 | 2.19 | 1.86 | 2.22 | |
| Kr | 2.01 | 2.02 | | 2.12 | 2.25 | 2.15 | |
| Rb | 2.05 | | 3.15 | 2.40 | 3.21 | 3.25 | |
| Sr | 2.52 | | 2.94 | 2.79 | 2.84 | 3.00 | |
| Y | 2.66 | | 2.71 | 2.74 | 2.75 | 2.71 | |
| Zr | 2.49 | | 2.57 | 2.68 | 2.52 | 2.54 | |
| Nb | 2.48 | | 2.46 | 2.51 | 2.56 | 2.43 | |
| Mo | 2.26 | | 2.39 | 2.44 | 2.45 | 2.39 | |
| Tc | 2.35 | | 2.37 | 2.41 | 2.44 | 2.36 | |
| Ru | 2.18 | | 2.37 | 2.37 | 2.46 | 2.34 | |
| Rh | 2.15 | | 2.32 | 2.33 | 2.44 | 2.34 | |
| Pd | 1.97 | | 2.35 | 2.15 | 2.15 | 2.37 | |
| Ag | 2.08 | | 2.37 | 2.25 | 2.53 | 2.43 | |
| Cd | 2.20 | | 2.37 | 2.38 | 2.49 | 2.50 | |
| In | 2.31 | 1.93 | 2.53 | 2.46 | 2.43 | 2.64 | |
| Sn | 2.35 | 2.17 | 2.46 | 2.48 | 2.42 | 2.59 | |
| Sb | 2.32 | | 2.41 | 2.46 | 2.47 | 2.52 | |
| Te | 2.30 | 2.06 | 2.36 | 2.42 | 1.99 | 2.44 | |
| I | 2.26 | 1.98 | 2.22 | 2.38 | 2.04 | 2.36 | |
| Xe | 2.21 | 2.16 | | 2.32 | 2.06 | 2.28 | |

For the challenging case of hydrogen atom for which large discrepancies of predicting atomic radius has been reported in several studies [33, 67, 68], our previously reported and current estimations seem quite consistent and are also in better agreement with those parameterized in the COSMO-RS solvation model and reported by Bondi and Alvarez, in comparison to other methods (Table 1). Accordingly, we propose a radius of 1.41 Å for hydrogen.

In summary, we provide quantum chemistry-based estimates of atomic radii for main group elements. The radii are computed as the distance to the nucleus of spherically averaged iso-density surfaces contoured at 0.0016 a.u. The radii obtained from this approach are grounded on experimental phase change thermodynamic data related to molecular surfaces, and are thus thermodynamically consistent.

References:

1. Ghosh, D.C., *A new scale of electronegativity based on absolute radii of atoms*. Journal of theoretical and computational chemistry, 2005. **4**(01): p. 21-33.
2. Allred, A.L. and E.G. Rochow, *A scale of electronegativity based on electrostatic force*. Journal of Inorganic and Nuclear Chemistry, 1958. **5**(4): p. 264-268.
3. Ghosh, D.C. and N. Islam, *Semiempirical evaluation of the global hardness of the atoms of 103 elements of the periodic table using the most probable radii as their size descriptors*. International Journal of Quantum Chemistry, 2010. **110**(6): p. 1206-1213.
4. Szarek, P. and W. Grochala, *Most probable distance between the nucleus and HOMO electron: the latent meaning of atomic radius from the product of chemical hardness and polarizability*. The Journal of Physical Chemistry A, 2014. **118**(44): p. 10281-10287.
5. Ayers, P.W., *The physical basis of the hard/soft acid/base principle*. Faraday Discussions, 2007. **135**: p. 161-190.
6. Bohórquez, H.J. and R.J. Boyd, *Is the size of an atom determined by its ionization energy?* Chemical Physics Letters, 2009. **480**(1-3): p. 127-131.
7. Tamura, S., *An empirical correlation between the atomic radius and the first ionization energy for elements*. Journal of materials science letters, 1996. **15**(19): p. 1678-1679.
8. Tandon, H., T. Chakraborty, and V. Suhag, *A new scale of the electrophilicity index invoking the force concept and its application in computing the internuclear bond distance*. Journal of Structural Chemistry, 2019. **60**: p. 1725-1734.
9. Islam, N. and D.C. Ghosh, *A new radial dependent electrostatic algorithm for the evaluation of the electrophilicity indices of the atoms*. International Journal of Quantum Chemistry, 2011. **111**(14): p. 3556-3564.
10. Alibakhshi, A. and B. Hartke, *Implicitly perturbed Hamiltonian as a class of versatile and general-purpose molecular representations for machine learning*. Nature Communications, 2022. **13**(1): p. 1245.
11. Alibakhshi, A. and B. Hartke, *Dependence of Vaporization Enthalpy on Molecular Surfaces and Temperature: Thermodynamically Effective Molecular Surfaces*. Physical Review Letters, 2022. **129**(20): p. 206001.
12. Alibakhshi, A. and B. Hartke, *Improved prediction of solvation free energies by machine-learning polarizable continuum solvation model*. Nature Communications, 2021. **12**(1): p. 1-7.
13. Ye, R., et al., *Variable van der waals radii derived from a hybrid gaussian charge distribution model for continuum-solvent electrostatic calculations*. Zeitschrift für Physikalische Chemie, 2016. **230**(5-7): p. 681-701.
14. Mandal, N., S.M. Pratik, and A. Datta, *Exploring Ultrashort Hydrogen–Hydrogen Nonbonded Contacts in Constrained Molecular Cavities*. The Journal of Physical Chemistry B, 2017. **121**(4): p. 825-834.
15. Weinhold, F. and R.A. Klein, *What is a hydrogen bond? Mutually consistent theoretical and experimental criteria for characterizing H-bonding interactions*. Molecular Physics, 2012. **110**(9-10): p. 565-579.

16. Mingos, D.M.P. and A.L. Rohl, *Size and shape characteristics of inorganic molecules and ions and their relevance to molecular packing problems*. Journal of the Chemical Society, Dalton Transactions, 1991(12): p. 3419-3425.
17. Fourmigué, M. and P. Batail, *Activation of hydrogen-and halogen-bonding interactions in tetrathiafulvalene-based crystalline molecular conductors*. Chemical reviews, 2004. **104**(11): p. 5379-5418.
18. Slovokhotov, Y.L., I.S. Neretin, and J.A. Howard, *Symmetry of van der Waals molecular shape and melting points of organic compounds*. New Journal of Chemistry, 2004. **28**(8): p. 967-979.
19. Evans, J.D., et al., *Computational identification of organic porous molecular crystals*. CrystEngComm, 2016. **18**(22): p. 4133-4141.
20. Novoa, J.J., *Using Computational Quantum Chemistry as a Tool to Understand the Structure of Molecular Crystals and the Nature of their Intermolecular Interactions*. 2017.
21. Chakraborty, T., K. Gazi, and D.C. Ghosh, *Computation of the atomic radii through the conjoint action of the effective nuclear charge and the ionization energy*. Molecular Physics, 2010. **108**(16): p. 2081-2092.
22. Hu, X., M.-O. Lenz-Himmer, and C. Baldauf, *Better force fields start with better data: A data set of cation dipeptide interactions*. Scientific Data, 2022. **9**(1): p. 327.
23. Visscher, K.M. and D.P. Geerke, *Deriving a polarizable force field for biomolecular building blocks with minimal empirical calibration*. The Journal of Physical Chemistry B, 2020. **124**(9): p. 1628-1636.
24. Murray, J.S. and P. Politzer, *Statistical analysis of the molecular surface electrostatic potential: an approach to describing noncovalent interactions in condensed phases*. Journal of Molecular Structure: THEOCHEM, 1998. **425**(1-2): p. 107-114.
25. Murray, J.S., et al., *Statistically-based interaction indices derived from molecular surface electrostatic potentials: a general interaction properties function (GIPF)*. Journal of Molecular Structure: THEOCHEM, 1994. **307**: p. 55-64.
26. Allinger, N.L., X. Zhou, and J. Bergsma, *Molecular mechanics parameters*. Journal of Molecular Structure: THEOCHEM, 1994. **312**(1): p. 69-83.
27. Nallasani, U.R., et al., *Structural and surface characterizations of 2D β -In₂Se₃/3D β -Ga₂O₃ heterostructures grown on c-Sapphire substrates by molecular beam epitaxy*. Scientific Reports, 2024. **14**(1): p. 5146.
28. Valadkhani, M., et al., *Curvature and van der Waals interface effects on thermal transport in carbon nanotube bundles*. Scientific Reports, 2022. **12**(1): p. 19531.
29. Liu, Y., et al., *Helical van der Waals crystals with discretized Eshelby twist*. Nature, 2019. **570**(7761): p. 358-362.
30. Liu, Y., Y. Huang, and X. Duan, *Van der Waals integration before and beyond two-dimensional materials*. Nature, 2019. **567**(7748): p. 323-333.
31. Meyer, L., *Die natur der chemischen elemente als function ihrer atomgewichte*. 1870.
32. Alvarez, S., *A cartography of the van der Waals territories*. Dalton Transactions, 2013. **42**(24): p. 8617-8636.
33. Batsanov, S.S., *Van der Waals radii of elements*. Inorganic materials, 2001. **37**(9): p. 871-885.
34. Bondi, A.v., *van der Waals volumes and radii*. The Journal of physical chemistry, 1964. **68**(3): p. 441-451.
35. Pauling, L., *The Nature of the Chemical Bond and the Structure of Molecules and Crystals: An Introduction to Modern Structural Chemistry*. 3d Ed. 1960: Cornell university press.
36. Biltz, W., *Raumchemie der festen Stoffe*. Berichte der deutschen chemischen Gesellschaft (A and B Series), 1935. **68**(7): p. A91-A108.
37. Bragg, W., *The arrangement of atoms in crystals*. Nature, 1921. **106**(2675): p. 725-725.

38. Mroz, A.M., et al., *An electric field-based approach for quantifying effective volumes and radii of chemically affected space*. Chemical Science, 2022. **13**(22): p. 6558-6566.
39. Tandon, H., et al., *Computation of absolute radii of 103 elements of the periodic table in terms of nucleophilicity index*. Journal of Mathematical Chemistry, 2020. **58**: p. 1025-1040.
40. Szarek, P., A. Chlebicki, and W. Grochala, *Atomic/ionic radius as mathematical limit of system energy evolution*. The Journal of Physical Chemistry A, 2019. **123**(3): p. 682-692.
41. Batsanov, S.S., *Thermodynamic determination of van der Waals radii of metals*. Journal of Molecular Structure, 2011. **990**(1-3): p. 63-66.
42. Mantina, M., et al., *Consistent van der Waals radii for the whole main group*. The Journal of Physical Chemistry A, 2009. **113**(19): p. 5806-5812.
43. Zunger, A. and M.L. Cohen, *First-principles nonlocal-pseudopotential approach in the density-functional formalism. II. Application to electronic and structural properties of solids*. Physical Review B, 1979. **20**(10): p. 4082.
44. Boyd, R., *Relative sizes of atoms.[Density contour, scaling]*. J. Plasma Phys.:(United Kingdom), 1977. **10**(12).
45. Slater, J.C., *Atomic radii in crystals*. The Journal of Chemical Physics, 1964. **41**(10): p. 3199-3204.
46. Clementi, E. and D.-L. Raimondi, *Atomic screening constants from SCF functions*. The Journal of Chemical Physics, 1963. **38**(11): p. 2686-2689.
47. Slater, J.C., *Atomic shielding constants*. Physical review, 1930. **36**(1): p. 57.
48. Yadav, P., et al., *A quest for the universal atomic radii*. Structural Chemistry, 2022: p. 1-6.
49. Politzer, P., P. Jin, and J.S. Murray, *Atomic polarizability, volume and ionization energy*. The Journal of chemical physics, 2002. **117**(18): p. 8197-8202.
50. del Valle, F.O. and M. Aguilar, *Solute-solvent interactions: Part 5. An extended polarizable continuum model including electrostatic and dispersion terms and electronic correlation in the solute*. Journal of Molecular Structure: THEOCHEM, 1993. **280**(1): p. 25-47.
51. del Valle, F.O. and M. Aguilar, *Correlation and solvation effects. IV. A systematic analysis of the influence of cavity size and shape on solvation properties in the polarizable continuum model with electron correlation*. Journal of Computational Chemistry, 1992. **13**(2): p. 115-134.
52. Miertuš, S., J. Bartoš, and M. Trebaticka, *Dependance of atomic radii and volumes on the electron distribution in solute molecule and on solute-solvent interaction*. Journal of molecular liquids, 1987. **33**(2-3): p. 139-156.
53. Bent, H.A., *Structural chemistry of donor-acceptor interactions*. Chemical Reviews, 1968. **68**(5): p. 587-648.
54. Harris, P.M., E. Mack Jr, and F. Blake, *The atomic arrangement in the crystal of orthorhombic iodine*. Journal of the American Chemical Society, 1928. **50**(6): p. 1583-1600.
55. Rahm, M., R. Hoffmann, and N. Ashcroft, *Atomic and ionic radii of elements 1–96*. Chemistry–A European Journal, 2016. **22**(41): p. 14625-14632.
56. Zhou, B., M. Agarwal, and C.F. Wong, *Variable atomic radii for continuum-solvent electrostatics calculation*. The Journal of chemical physics, 2008. **129**(1).
57. Foresman, J.B., et al., *Solvent effects. 5. Influence of cavity shape, truncation of electrostatics, and electron correlation on ab initio reaction field calculations*. The Journal of Physical Chemistry, 1996. **100**(40): p. 16098-16104.
58. Deb, B., R. Singh, and N. Sukumar, *A universal density criterion for correlating the radii and other properties of atoms and ions*. Journal of Molecular Structure: THEOCHEM, 1992. **259**: p. 121-139.
59. Alibakhshi, A. and L.V. Schäfer, *Reconciling Experiment with Quantum Chemical Calculations: Electron Iso-Density Surfaces Represent Atomic and Molecular Surfaces*. 2024.

60. Alibakhshi, A. and L.V. Schäfer, *Theoretical Evaluation of Radii of Atoms in Molecules and their Dependence on Atomic Partial Charge*. 2024.
61. Bader, R., W.H. Henneker, and P.E. Cade, *Molecular charge distributions and chemical binding*. The Journal of Chemical Physics, 1967. **46**(9): p. 3341-3363.
62. Douglas, M. and N.M. Kroll, *Quantum electrodynamical corrections to the fine structure of helium*. Annals of Physics, 1974. **82**(1): p. 89-155.
63. Neese, F., *The ORCA program system*. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2012. **2**(1): p. 73-78.
64. Lu, T. and F. Chen, *Multiwfn: A multifunctional wavefunction analyzer*. Journal of computational chemistry, 2012. **33**(5): p. 580-592.
65. Bondi, A., *Van der Waals volumes and radii of metals in covalent compounds*. The Journal of Physical Chemistry, 1966. **70**(9): p. 3006-3007.
66. Klamt, A., et al., *Refinement and parametrization of COSMO-RS*. The Journal of Physical Chemistry A, 1998. **102**(26): p. 5074-5085.
67. Cramer, C.J. and D.G. Truhlar, *A universal approach to solvation modeling*. Accounts of chemical research, 2008. **41**(6): p. 760-768.
68. Rowland, R.S. and R. Taylor, *Intermolecular nonbonded contact distances in organic crystal structures: Comparison with distances expected from van der Waals radii*. The Journal of Physical Chemistry, 1996. **100**(18): p. 7384-7391.