Comprehensive definition of valence as a quantity (Provisional Recommendation 2026)

Pavel Karen[1,*], Lidia Armelao[2], Ian S. Butler[3], Vladislav Tomišić[4], and Makoto Yamashita[5]

[1]University of Oslo, Norway; [2]National Research Council (CNR) and University of Padua, Italy; [3]Department of Chemistry, McGill University, Canada; [4]Department of Chemistry, Faculty of Science, University of Zagreb, Croatia; [5]Department of Chemistry, School of Science, Institute of Science Tokyo, Japan

*Corresponding author: pavel.karen@kjemi.uio.no

This report was prepared under the framework of IUPAC project 2018-030-2-200. *Task Group Chair*: Pavel Karen, *Task Group Members*: Lidia Armelao, Ian S. Butler, Vladislav Tomišić, and Makoto Yamashita.

Article note: Sponsoring bodies: The IUPAC Inorganic Chemistry Division II, Physical and Biophysical Chemistry Division I, the Organic and Biomolecular Chemistry Division III, the Committee on Chemistry Education (CCE); more details on p. 12.

Abstract: In one of many uses of the chemical term valence, it means a quantity that characterizes the bonding situation of an atom. Historically, the definition of the valence quantity has varied across different branches of chemistry. Based on our analysis of the use of this quantity, we recommend limiting the definitions to two contexts; the noun valence as the number of two-electron bonds associated with an atom, and the adjective *n*-valent for the oxidation state of a metal, which cover the past 70 years.

Keywords: bond order; bond valence; Lewis formula; valence; valence electrons

CONTENTS

1 Introduction

The term valence in general refers to the atom's ability to bond other atoms. It enters many chemistry concepts, as outlined in the 2025 IUPAC Technical Report[1] about the project. A survey prior this project revealed differing perceptions of valence values and helped formulate candidate definitions. Nine quantities behind eight alternative definitions were evaluated on 39 chemical entities of 48 bonding formulas, giving sensible values with mutual relationships. The actual usage was obtained from Google Scholar searches of "valen" for each compound and evaluated to imply the definition behind the stated value of the valence, the frequency of such use, and the chemistry field. Summarized preferences for the alternative definitions identified two main areas of use. Organic and physical chemists obtain valence as a count of two-electron bonds

at the atom. Inorganic chemists working with metallic elements use *n*-valent as an adjective for the oxidation state.

As a quantity, valence describes a specific bonded atom; it is a chemical dimensionless variable. It has a long history,[1] starting slowly between 1860 and 1890, exemplified by Kekulé[2,3], Meyer[4], Wichelhaus[5] in German (die Äquivalenz[2], die Valenz[3,4,5]), Hofmann[6] and Frankland[7] in English, as a stated or suggested synonym of the widely used "atomicity" as atom-fixing power toward a "standard" atom such as H or Cl. After Werner's theory of complexes[8] in 1890s, the central-atom valence gradually branched off into a primary valence as bonds to charged species to fulfill stoichiometry of a simple compound and secondary valence as bonds to independent molecules or independently stable substances (Werner's 1905 book[9]) as the bond donors. Between 1900 and 1920, the concept of electrons in inorganic redox chemistry necessitated valences of positive and negative values[10,11], while organic chemistry kept counting bonds[12]. In 1938, the introduction of standard redox potentials brought a change in terminology when Latimer[13] used the rarely adopted term oxidation state for the formal ionic states of the given element in the half-reaction pair to which the redox potential refers to. This caused a succession of the term ionic valence (or electrochemical valence) by the term oxidation state, which culminated around the London 11th International Congress of Pure and Applied Chemistry in 1947 where Linus Pauling presided over the Section II Physical Chemistry. In his 1948 paper[14], while keeping the organic valence untouched, Pauling saw the inorganic quantity valence as an adjective *n*-valent for the term oxidation number that lacks it, but only when the meaning is clear.

Analyses in the Technical Report[1] confirm these two main areas of the valence quantity in chemistry papers. The use is modest. Among textbooks, Organic Chemistry

by Wade[15] gives the value *n* of *n*-valent 17 times, compared with oxidation state that is given 4 times. Inorganic Chemistry by Housecroft and Sharpe[16] gives *n*-valent 3 times and oxidation state 578 times in quantitative context. Physical Chemistry by Atkins and De Paula[17] has *n*-valent 5 times and oxidation state 18 times.

The 1994 IUPAC Glossary of terms used in physical organic chemistry[18] defines valence as "the maximum number of *univalent* atoms (originally hydrogen or chlorine atoms) that may combine with an atom of the element under consideration, or with a fragment, or for which an atom of this element can be substituted". The Technical Report[1] shows that, for a properly chosen bonding segment of the given atom keeping its formal charge from the Lewis formula of all valence electrons, this definition yields a value identical to the count of two-electron bonds or their equivalents at that atom. The 2022 IUPAC Recommendation update of the Glossary[19] shortened the formulation to a "maximum number of single bonds that can be commonly formed by an atom or ion of the element under consideration" that involves a degree of opinion inconsistent with anything definitional.[1]

The different meaning of the valence quantity in organic chemistry and of the adjective *n*-valent in inorganic chemistry of metals is a disadvantage. Differing perceptions obscure communication. Yet some continuity with years of the current valence quantity use in chemistry papers is desirable. Besides covering the use, the definition must emphasize the need for clarity about the intended context.

2 The definition

The two widely used valence quantities that characterize a bonded atom originate in two different areas of chemistry, which may minimize ambiguity:

Valence (as a quantity)

- **In organic chemistry, valence of an atom is the sum of two-electron bonds and/or simple fractions of such bonds at the atom in the Lewis formula**.
- **In chemistry of metals, the adjective *n*-valent denotes the atom's oxidation state.**

Note 1. When stating the valence quantity, the intended meaning must be clear. If the adjective *n*-valent is used for oxidation state, it must be identified by naming oxidation state or using its notation[20] nearby, such as Cr^{II} or chromium(II).

Note 2. The algorithm behind the organic-chemistry valence count consists of drawing the full Lewis formula with all valence electrons and correct bond orders.

Note 3. The count of two-electron bonds yields the same value as the original IUPAC definition[18] applied to an atom in its actual bonding situation (a segment with its bonds and lone pairs) that keeps its formal charge in the Lewis formula.

Note 4. The oxidation state behind the term *n*-valent metal in a compound is often counted from fixed ionic charges and electroneutrality. IUPAC Recommendation[21] gives two algorithms to obtain it from a Lewis formula, one of which applies also to bond graphs of extended solids.

Note 5. In papers on chemistry of semimetals and non-metals, both connotations occur, yielding different values when: (a) an atom forms homonuclear bonds. (b) An atom bonds reversibly as an acceptor or donor to a molecular ligand. (c) When a Lewis acid-base adduct ion does not clearly reshuffle the electron density to ligands' ionic bonds (reshuffling to single-atom ligands is nearly complete; see Section 4.2 and 4.3).

Note 6. The organic chemistry definition suits reaction mechanisms described via electron pairs and electron affinity (electrophiles and nucleophiles), while the redox aspect is absent or irrelevant. For inorganic chemistry, redox reactions are one of its central pillars, hence the occasional adjective *n*-valent for the oxidation state.

Note 7. Two mathematically related quantities also characterize bonding in a full Lewis formula; formal charge[1] and the number of electrons an atom uses in bonds. The latter equals the number of atom's two-electron bonds plus its formal charge[1].

Example organic chemistry: C_2H_2 of tetravalent carbon.

Example metal chemistry: Hg_2Cl_2 of monovalent mercury, Hg^I.

Related terms: The term "bond valence" in solid-state chemistry corresponds to the bond order in molecular chemistry. Bond valence expresses the number of two-electron bond equivalents between two atoms, calculated from the bond length[22]. The sum of bond valences at an atom is called the bond-valence sum[22]. The Werner's primary and secondary valence[9] are also related terms (Ref. 20, p. 144). The former denotes ligands bonded by bonds sharing electrons, the latter by donated bonds.

3 A combined example

Dichromium tetraacetate combines organic and inorganic components in its paddlewheel molecule (Fig. 1). Speaking about it, organic chemists might mention the tetravalent carbon and divalent oxygen, inorganic chemists perhaps the blue solution of divalent chromium at the start of the synthesis. Organic chemists would avoid claiming valence 6 for chromium of oxidation state 2. Searches in Ref. 1 reveal five papers stating Cr divalent versus none stating Cr hexavalent in this acetate. On the opposite end, who would consider the valence of carbon atoms in acetic acid +3 and −3?

[1] Obtained on a Lewis formula of all valence electrons by bisecting bonds of that atom and counting its remaining ionic charge.

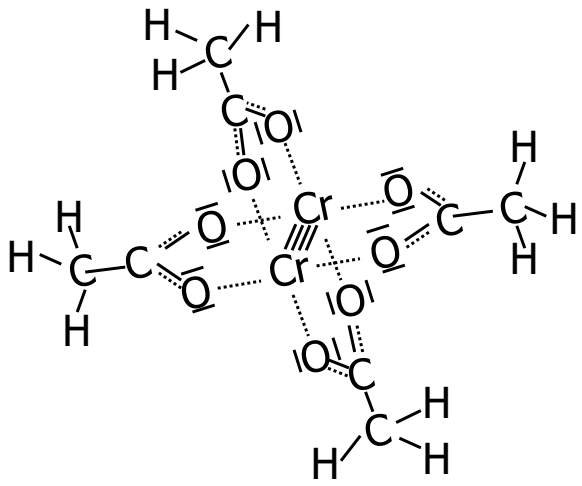

Fig. 1: Lewis formula of dichromium tetraacetate molecule. The solid dash is an electron pair; the dotted dash is its simple fraction, 1/2.

4 Discussion

4.1 Differing valences by the two definition approaches

Counting two-electron bonds in the Lewis formula |$\overline{\text{Cl}}$−Hg−Hg−$\overline{\text{Cl}}$| yields 2 for both Hg atoms of oxidation state 1. Of these two valence quantity alternatives, a search[1] reveals 24 papers stating Hg monovalent and 0 divalent in Hg_2Cl_2. Referring to mercury in Hg_2Cl_2 as monovalent is then reasonably clear for the reader, yet using a Hg^{I} nearby or naming dimercury(I) dichloride would still improve clarity.

Counting bonds in the Lewis formula H−C≡C−H yields valence 4 for its carbons of oxidation state −1. As expected, all papers stating the valence quantity in ethyne refer to its carbon as tetravalent.

Google Scholar literature searches in Ref. 1 reveal both contexts of valence for nonmetallic main-group elements. Outside the metal chemistry and organic chemistry, clarity thus becomes a problem. A heading “halides of divalent sulfur” for lecture about SX_2 halogenides might make the audience to expect also S_2X_2.

The two valence quantity definition approaches yield different values also when a metal atom accepts dative bonds from neutral molecules (ligands of the Werner's secondary-valence type[9]), such as in $Ni(CO)_4$ with 18-plet of electrons at Ni. The Ni of oxidation state 0 has four Ni−C bonds of 181.7 pm (1.817 Å)[2] at 198 K by single-crystal X-ray diffraction[23], a length that yields bond order 1.00 by the bond valence approach[24]. The bond length 112.7 pm (1.127 Å) in the CO ligand[23] yields bond order 2.05 that complies with the 8−*N* rule (Ref. 1, p. 181) for oxygen. Room-temperature bond lengths are available from gas electron-diffraction.[25] For the 183.8 pm (1.838 Å) distance Ni−C, the bond-valence approach[24] confirms the single bond, and the 114.1 pm (1.141 Å) in the CO ligand gives bond order 1.97. As the bond-valence approach is less precise for high bond orders, a mere comparison of bond lengths may be illustrative for the carbonyl. CO_2 has double bonds of 116.3 pm (1.163 Å)[26] and CO gas has 112.8 pm (1.128 Å)[27] for its bond order of ~2.6[28]. The 114.1 pm (1.141 Å) in $Ni(CO)_4$ then approaches the CO_2 value. Yet the "conventional" $Ni(CO)_4$ formula is drawn with C and O bonded by triple bond whose one pair is donated by O. Fig. 2 shows these two limiting Lewis formulas. On both, counting two-electron bonds yields valence 4 at Ni of oxidation state 0. A search[1] revealed 23 papers stating Ni zerovalent, 0 tetravalent.

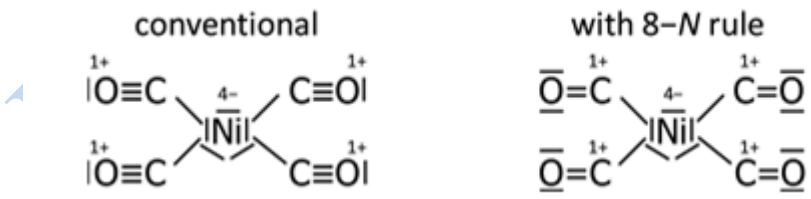

Fig. 2: Alternative Lewis formulas of tetracarbonylnickel with formal (hence not actual) charges.

[2] Bond-valence parameters for elements in Ref. 24 or their bonded pairs of given oxidation states in Ref. 24 refer to bond distances in units of Å.

For C and O, only the oxidation state remains the same on both formulas, C^{II} and O^{-II}. Whereas counting two-electron bonds yields C tetravalent on left and trivalent on right of Fig. 2, O is trivalent on left and divalent on right. The carbon–oxygen bonding reality in this carbonyl is a compromise between the octet rule and 8−*N* rule.

4.2 Equal valence by the two approaches

Note 5 of the valence definition implies that the organic-chemistry and metal-chemistry approaches yield the same valence value for relatively electropositive atoms that have no homonuclear bonds [3], accept no dative bonds from neutral permanent molecules, and appear with correct bond orders in Lewis formula. Clarifying examples of the latter condition are illustrated in the following.

Tetrafluoridoborate anion BF_4^- of 32 valence electrons is formed by a Lewis acid–base reaction. BF_3 accepts an electron pair from F^- in Fig. 3 left. Then it reshuffles the electron behind the formal charge −1 at the electropositive boron to the "ionic" bonds of four F atoms, thus keeping the 8−*N* rule (8−7 = 1) for the bond-order sum at each of them in Fig. 3 right. In that final formula, the two differing approaches to valence quantity yield equal values at the central atom B even though it's not a metal. The F valence then differs from its oxidation state by sign. See also Section 4.3.

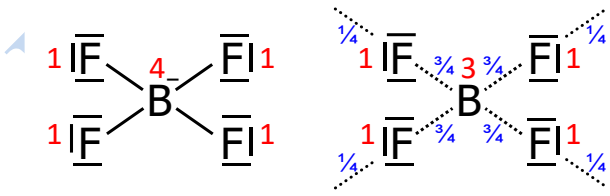

Fig. 3: Valence counts on Lewis formulas of compounds/ions formed from Lewis acid and base should refer to the completed reaction (on right), not merely to a first-step adduct (BF_3 + F^- on left). The formal charge (on left) is in black, bond orders (on right) are in blue, and valences in red.

[3] Unless their polarity is resolved to count the oxidation state as done at times in thiosulfate formula to obtain central S^{VI} and terminal S^{-II}.

The difluoridohydrogenate anion HF_2^- (Ref. 20, p. 114) of 16 valence electrons in Lewis formula · |F̄ · H · F̄| · has two one-electron bonds at F by the 8−*N* rule[1]. The central-atom bond length 112.9 pm (1.129 Å) in KHF_2[29] yields bond order 0.492 via Ref. 24, hence monovalent hydrogen by both valence-definition approaches.

A transition-metal example is the $KNiCl_3$ hexagonal perovskite with Ni-coordination octahedra sharing their opposite delta △ faces to form anionic chains[30]. Imagine two octahedra of that chain. Each of the three shared Cl ligands of one delta face bonds two Ni of bond-valence sum 2.07 (via Ref. 24) from six such bonds of bond valence 0.345. That means "divalent nickel" Ni^{II} of 6 idealized bond orders ⅓ inside the octahedron. Each Cl thus collects bond-valence sum of ⅔ from two Ni. Each K bonds 12 Cl by bonds of order 1/12. Each Cl bonds 4 K atoms and collects from them bond order 4/12 = 1/3 to sum with those 2/3 from Ni atoms to 1 for the Cl valence by counting two-electron bond equivalents.[4] A user counting three single bonds at Ni in $[NiCl_3]^-$ would not obtain correct valences. This might be another reason why the term *n*-valent in inorganic chemistry of metals refers to the oxidation state—the ionic approximation avoids such errors. Even in the plain summary formula $[NiCl_3]^-$, the directly seen Ni oxidation state +2 yields correct valences by the implied bond order 2/3 inside that anion and 1/3 from each of its Cl to K. The result complies with the 8−*N* rule on Cl. More examples of valences in extended solids are in Ref. 1, pp. 164–5.

[4] In contrast, transition-metal complexes with coordinated water, ammonia, or other molecular Lewis-basic ligands yield different valences by the organic- and metal-chemistry approaches. Only their ionic approximation gives the quantity value that already is covered by the term oxidation state and does not need to be called valence.

4.3 Cases of some ambiguity

Since the valence quantity aims to describe the actual bonding of the atom, it may be less suited for compounds of alternative Lewis formulas where averaging similar to the resonance-structure approach yields decimal values. The actual bonding may be a bonding compromise, as illustrated in the IUPAC Technical Report[1] on the CO molecule of competing octet- and 8−*N* rules.

Although the BF_4^- formula on the right of Fig. 3 is chemically better (the experimental B–F bond expands from BF_3 gas[31] to KBF_4 crystal[32]), the actual length increase is only about ⅔ of the prediction (by the "*B* = 0.37" formula[22]) for the bond-order decreasing from 1 to ¾. The B–F bond order in KBF_4 thus remains a bit higher than 3/4 due to a small remaining charge at B. The NH_4^+ of two alternative formulas in Ref. 1 gives a similar result: The N–D bond in ND_4NO_3[33] shows only about ½ of the expected increase from the length in ND_3[34]. Here, however, the main culprit is hydrogen bonds that in solid ND_3 expand the single bonds of the isolated molecule.

Another Lewis-formula uncertainty appears when bonding-electron counts in transition-metal clusters are approximated by neutral atom counting, where halogenide μ_2-bridges count with full 2 two-electron bonds to yield the actual and correct homonuclear-bond order of the metal cluster itself. Ambiguities are bound to appear for the valence quantity that is not an approximation or ionic extrapolation.

5 Concluding remarks

The count of two-electron bonds or their equivalents at an atom in the Lewis formula differs from the oxidation state if that atom forms homonuclear bonds (often organic) or has bonds donated by unchanging neutral molecules or by multiatomic anionic ligands (often inorganic). Counting two-electron bonds in organic-chemistry formulas

is straightforward, and so is the "inorganic" calculation of the oxidation state behind the adjective *n*-valent for metals and metalloids. The same quantity value by the two alternative definitions of valence is obtained when bond orders at the given atom in the Lewis formula sum to oxidation state, hence, formally, that atom must be more electropositive than its neighbors and must not carry formal charge. That can be fulfilled even for sp-central-atom anions, but only if their Lewis formula follows the 8−N rule[1] for the bond-order total at the electronegative terminal atoms forming "ionic" bonds included in the count. For d-metal complexes, the two alternative valence quantities often differ. The organic-chemistry valence quantity and the metal chemistry adjective *n*-valent for oxidation state then do not create a huge ambiguity (except perhaps for MOFs), but it still is important to clarify the meaning.

Two specialized quantities, introduced since 1975, also use the term valence. The older one is the mentioned bond valence[22] that means "bond order" in a crystal, expressed as the count of two-electron-bond equivalents calculated from the given bond length. The newer is the rarely used CBC (covalent bond classification) valence number[35,36] for the count of atom's electrons in bonds. Both terms are easy to verbalize by these explanatory words. More details and examples are reported in the Technical Report[1].

Membership of sponsoring bodies

Membership of the Inorganic Chemistry Division (II) for 2024–2025:

President: L. Armelao (Italy); **Vice President**: R. Macaluso (USA); **Secretary**: J.L. Colón (Puerto Rico); **Titular Members**: Y.F.H. Abdul Aziz (Malaysia), M.C. Gimeno (Spain), M. Hasegawa (Japan), P. Karen (Norway), A. Logsdail (UK), J. Meija (Canada), O. Metin (Turkey). **Associate Members**: A. Aukauloo (France), B. DeBruin

(Netherlands), M. Diop (Senegal), L. Krivosudský (Slovakia), A. Sanson (Italy), X. Zhu (China/Beijing); **National Representatives**: J.K. Bera (USA), S. Chantrapromma (Thailand), J.D.G. Correia (Portugal), M.A. Gruden-Pavlović (Serbia), R. Hocking (Australia), J. John (Czech Republic), S. Mathura (South Africa), V. Stilinović (Croatia), R. Stoyanova (Bulgaria), Y.-C. Tsai (China/Taipei).

Membership of the Physical and Biophysical Chemistry Division (I) for 2024–2025: **President**: F. Separovic (Australia); **Vice President**: J. Frey (UK); **Secretary**: J.L. Faria (Portugal); **Titular Members**: M. Fall (Senegal), H.N. Ghosh (India), R. Oriňáková (Slovakia), A. Rodger (Australia), T. Wallington (USA), M. Witko (Poland); **Associate Members**: K.F. Chong (Malaysia), T. Frankcombe (Australia), E. Kazuma (Japan), M. Rissanen (Finland), I. Schapiro (Israel), I. Voets (Netherlands); **National Representatives**: N. Bregović (Croatia), C. Contini (UK), K. Ghandi (Canada), E.V. Golubina (Russia), L. Liu (China/Beijing), P. Nelson (Jamaica), V. Parasuk (Thailand), I.A. Pasti (Serbia), B. Rangelov (Bulgaria), C.-L. Wang (China/Taipei).

Membership of the Organic and Biomolecular Chemistry (III) for 2024–2025: **President**: E. Uggerud (Norway); **Vice President**: A.M.P. Koskinen (Finland); **Secretary**: C. Nativi (Italy); **Titular Members**: M. Donnard (France), D. Margetić (Croatia), T.M. Pinho de Melo (Portugal), I.H. Williams (United Kingdom), M. Yamashita (Japan), Z. Zakaria (Malaysia); **Associate Members**: J.B. Harper (Australia), M. Hegazy (Egypt), M. Ludwig (Czech Republic), E. Dimitrova-Naydenova (Bulgaria), S.-S. Sun (China/Taipei), Zhen Xi (China/Beijing); **National Representatives**: M.S. Alam (Bangladesh), M. Donova (Russia), X.-Y. Hu

(China/Beijing), R. Jansen-van Vuuren (Slovenia), N.E. Nifantiev (Russia), I.M. Opsenica (Serbia), R. Orru (Netherlands), N.T. Patil (India), W. van Otterlo (South Africa), S. Wacharasindhu (Thailand).

Membership of the Committee on Chemistry Education (CCE) for 2024–2025:

Standing Committee Chair: M. Potgieter (South Africa); **Standing Committee Secretary**: F.M. Ho (Sweden); **Titular Members**: R.S. Cole (USA), U. Maitra (India), M. Mocerino (Australia), Antonella Rossi (Italy), T.-K. Soon (Malaysia), S. Wiedmer (Finland); **National Representatives**: M.A. Beckett (UK), S. Boniface (New Zealand), Y.-C. Cheng (China/Taipei), E. de Jesús Alcañiz (Spain), D.-S. Di Fuccia (Germany), S. Grecea (Netherlands), M. Guene (Senegal), R. Lucas (France), A. Lykknes (Norway), R. Mamlok-Naaman (Israel), G. Obuzor (Nigeria), R. Pandit (Nepal), M. Sözbilir (Turkey), A. Tafrova-Grigorova (Bulgaria), S. Tantayanon (Thailand), D. Trivic (Serbia), S. Uchinokura (Japan), B. Van Tiggelen (Belgium), R. Vladušić (Croatia), D. Zhilin (Russia), J. Zhou (China/Beijing); **Division Representatives**: J.L. Faria (D-I, Portugal), Y.F.H. Abdul Aziz (D-II, Malaysia), J.B. Harper (D-III, Australia), J. Merna (D-IV, Czech Republic), L.S. Vargas (D-IV, France), S. Wiedmer (D-V, Finland), R. Kallenborn (D-VI, Norway), V. Gubala (D-VII, GB), R.M. Hartshorn (D-VIII, New Zealand).

Acknowledgments: We thank Andrew Logsdail of IUPAC Division II for comments on our final version of the manuscript.

Research ethics: Not applicable.

Informed consent: Not applicable.

Author contributions: All authors have accepted responsibility for the entire content of this manuscript and approved its submission.

Use of Large Language Models, AI and Machine Learning Tools: Not used.

Conflict of interest: The authors state no conflict of interest.

Research funding: Authors are grateful for resources/facilities at home institutions.

Data availability: Not applicable.

References

1. Karen, P.; Armelao, L.; Butler, I. S.; Tomišić, V.; Yamashita, M. Toward a definition of valence as a quantity (IUPAC Technical Report). *Pure Appl. Chem*., **2025**, *97*, 149–187. https://doi.org/10.1515/pac-2023-0402
2. Kekulé, A. *Lehrbuch der Organischen Chemie oder der Chemie der Kohlenstoffverbindungen, Erster Band*; Verlag von Ferdinand Enke: Erlangen, 1861, pp. 108–115.
3. Kekulé, A. Ueber die Constitution des Mesitylens. *Zeitschrift für Chemie* **1867**, *10*, 215–219.
4. Meyer, L. *Die modernen Theorien der Chemie*; Verlag von Maruschke & Berendt: Breslau, 1864, p. 67.
5. Wichelhaus, H. Phosphor, ueber die Verbindungen desselben und die Valenz des Phosphoratoms. *Annalen der Chemie und Pharmacie, Supplement VI.* **1868**, 257–280.
6. Hofmann, A. W. *Introduction to Modern Chemistry Experimental and Theoretic*; Walton and Maberley: London, 1865, p. 169.
7. Frankland, E.; Japp, F. R. *Inorganic Chemistry*; Lea Brothers & Co.: Philadelphia, 1885, p. 78.
8. Werner, A. Beitrag zur Konstitution anorganischer Verbindungen. *Z. Anorg. Allgem. Chem*. **1893**, *3*, 267–330. https://doi.org/10.1002/zaac.18930030136
9. Werner, A. *Neuere Anschauungen auf dem Gebiete der Anorganischen Chemie*; Friedrich Vieweg und Sohn: Braunschweig, 1905, p. 58.
10. Abegg, R. Die Valenz und das periodische System. Versuch einer Theorie der Molekularverbindungen. *Z. Anorg. Allgem. Chem*. **1904**, *39*, 330–380. https://doi.org/10.1002/zaac.19040390125
11. Fry, H. S. The electronic conception of positive and negative valences. *J. Am. Chem. Soc*. **1915**, *37*, 2368–2373. https://doi.org/10.1021/ja02175a016
12. Bray, W. C.; Branch, G. E. K. Valence and tautomerism. *J. Am. Chem. Soc*. **1913**, *35*, 1440–1447. http://dx.doi.org/10.1021/ja02199a003
13. Latimer, W. M. *The oxidation states of the elements and their potentials in aqueous solutions*; Prentice Hall, Inc.: New York, NY, 1938.
14. Pauling, L. The modern theory of valency. *J. Chem. Soc. **1948***, 1461–1467. http://dx.doi.org/10.1039/JR9480001461
15. Wade Jr., L. G. *Organic Chemistry*, 6th ed.; Pearson Prentice Hall: Upper Saddle River, NJ, USA, 2006.
16. Housecroft, C. E.; Sharpe, A. *Inorganic Chemistry*, 3rd ed.; Pearson Education Ltd: Harlow, UK, 2008.
17. Atkins, P.; De Paula, J. *Atkins' Physical Chemistry*, 8th ed.; Oxford University Press: Oxford, UK 2006,
18. Muller, P. Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994). *Pure Appl. Chem*. **1994**, *66*, 1077–1184. http://dx.doi.org/10.1351/pac199466051077
19. Perrin, C. L.; Agranat, I.; Bagno, A.; Braslavsky, S. E.; Fernandes, P. A.; Gal, J.-F.; Lloyd-Jones, G. C.; Mayr, H.; Murdoch, J. R.; Nudelman, N. S.; Radom, L.; Rappoport, Z.; Ruasse, M.-F.; Siehl, H.-

U.; Takeuchi, Y.; Tidwell, T. T.; Uggerud, E.; Williams. I. H. Glossary of terms used in physical organic chemistry (IUPAC Recommendations 2021) *Pure Appl. Chem*. **2022**, *94*, 353–534. https://doi.org/10.1515/pac-2018-1010
20. Connelly, N. G.; Damhus, T.; Hartshorn, R. M.; Hutton, A. T. *Nomenclature of inorganic chemistry*, *IUPAC Recommendations 2005*, RSC Publishing, 2005. https://iupac.org/what-we-do/books/redbook/
21. Karen, P.; McArdle, P.; Takats, J. Comprehensive definition of oxidation state (IUPAC Recommendations 2016). *Pure Appl. Chem*. **2016**, *88*, 831–839. http://dx.doi.org/10.1515/pac-2015-1204
22. Brown, I. D.; Altermatt, D. Bond-valence parameters obtained from a systematic analysis of the Inorganic Crystal Structure Database. *Acta Crystallogr. Ser. B* **1985**, *41*, 244–247. https://doi.org/10.1107/S0108768185002063
23. Braga, D.; Grepioni, F.; Orpen, A. G. Nickel carbonyl [$Ni(CO)_4$] and iron carbonyl [$Fe(CO)_5$]: molecular structures in the solid state. *Organometallics* **1993**, *12*, 1481–1483. https://doi.org/10.1021/om00028a082
24. O'Keeffe, M.; Brese, N. E. Atom sizes and bond lengths in molecules and crystals. *J. Am. Chem. Soc*. **1991**, *113*, 3226–3229. https://doi.org/10.1021/ja00009a002
25. Hedberg, L.; Iijima, T.; Hedberg, K. Nickel tetracarbonyl, $Ni(CO)_4$. I. Molecular structure by gaseous electron diffraction. II. Refinement of quadratic force field. *J. Chem. Phys*. **1979**, *70*, 3224–3229. https://doi.org/10.1063/1.437911
26. Glockler, G. Carbon–oxygen bond energies and bond distances. *J. Phys. Chem*. **1958**, *62*, 1049–1054. https://doi.org/10.1021/j150567a006
27. Gilliam, O. R.; Johnson, C. M.; Gordy, W. Microwave spectroscopy in the region from two to three millimeters. *Phys. Rev*. **1950**, *78*, 140–144. https://doi.org/10.1103/PhysRev.78.140
28. Martinie, R. J.; Bultema, J. J.;Vander Wal, M. N.; Burkhart, B. J.; Vander Griend, D. A.; DeKock, R. L. Bond order and chemical properties of BF, CO, and N_2. *J. Chem. Educ*. **2011**, *88*, 1094–1097. https://dx.doi.org/10.1021/ed100758t
29. Peterson, S. W.; Levy, H. A. A single crystal neutron diffraction determination of the hydrogen position in potassium bifluoride. *J. Chem. Phys*. **1952**, *20*, 704–707. https://doi.org/10.1063/1.1700520
30. Visser, D.; Verschoor, G. C.; Iido, D. J. W. The structure of $KNiCl_3$ at room temperature. *Acta Crystallogr. Ser. B* **1980**, 36, 28–34 https://doi.org/10.1107/S0567740880002385
31. Kuchitsu, K.; Konaka. S. B–F bond distance of boron trifluoride determined by gas electron diffraction. *J. Chem. Phys*. **1966**, *45*, 4342–4347. https://doi.org/10.1063/1.1727494
32. Brunton, G. The crystal structure of KBF_4. *Acta Crystallogr. Ser. B* **1969**, *25*, 2161–2162. https://doi.org/10.1107/S0567740869005309
33. Ahtee, M.; Smolander, K. J.; Lucas, B. W.; Hewat, A. W. The structure of the low-temperature phase V of ammonium nitrate, ND_4NO_3. *Acta Crystallogr. Ser. C* **1983**, *39*, 651–655. https://doi.org/10.1107/S0108270183005806
34. Hewat, A. W.; Riekel. C. The crystal structure of deuteroammonia between 2 and 180 K by neutron powder profile refinement. *Acta Crystallogr. Ser. A* **1979**, *39*, 567–571. https://doi.org/10.1107/S0567739479001340
35. Parkin, G. Valence, oxidation number, and formal charge: Three related but fundamentally different concepts. *J. Chem. Educ.* **2006**, *83*, 791–799. https://doi.org/10.1021/ed083p791
36. Green, J. C.; Green, M. L. H.; Parkin. G. The occurrence and representation of three-centre two-electron bonds in covalent inorganic compounds. *Chem. Commun*. **2012**, *48*, 11481–11503. http://dx.doi.org/10.1039/C2CC35304K