

Title: **The geometrowave potential quantified and unified properties in general chemistry**

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To date, size-dependent properties for atoms, ions, clusters, molecules, nanoparticles (or NPs) haven't been quantitatively predicted, differentiated, and unified, leaving many questions long-unanswered in chemistry. This work has introduced a geometrowave-number ($\tilde{\nu}_{GW}$) and GW-potential (μ_{GW}) to quantitatively predict, compare, and unify these particles' size-dependent properties. Such geometry-quantized chemical properties quantify the energy (or spontaneity) in self-assemble bonding, macromolecules' folding–unfolding, surface defects' reactivity, ions' GW-electronegativity, and NPs' redox change.

If predicting 64 Au-NPs (each 2-nm large) spontaneous self-assembly to an 8-nm NP, directly (*Route-A*) or stepwise (*Route B* + *Route C*) (**Fig. 1a**), each route's Gibbs free energy change¹ $\Delta G < 0$, supposedly. In chemical thermodynamics, however, NP formation's enthalpy (ΔH_f), entropy (ΔS_f), and ΔG_f ($\approx \Delta H_f - T\Delta S_f$) are unquantified or undefined, leaving self-assemblies²⁻⁷ never predicted and compared quantitatively.

To tackle many such problems in the thermodynamics- and quantum mechanics

(QM)-based general chemistry, let's quantize the zero-dimensional (0D), 1D-, 2D- and 3D-particles' Surface Area-to-Volume (SA/V) ratio (see the **Extended Data Table S1**) into a geometrowave-number ($\tilde{\nu}_{GW}$) with a unit of (length^{-1}). Thus, at $T = 298.15$ ($^{\circ}\text{K}$) and 1 (atm), the GW-potential $\mu_{f\text{GW}}^{\circ} = hc \cdot \tilde{\nu}_{GW}$, where the c = speed of light, h = Planck constant, and $hc \approx 1.24$ ($\text{keV} \cdot \text{nm}$). Therefore,

$$\begin{aligned}\Delta\mu_{f\text{GW(Route-A)}}^{\circ} &= \mu_{f\text{GW(8nm-NP)}}^{\circ} - 64\mu_{f\text{GW(2nm-NPs)}}^{\circ} \\ &= \{6/8 - 64(6/2)\}hc = -237.2 \text{ (keV)},\end{aligned}$$

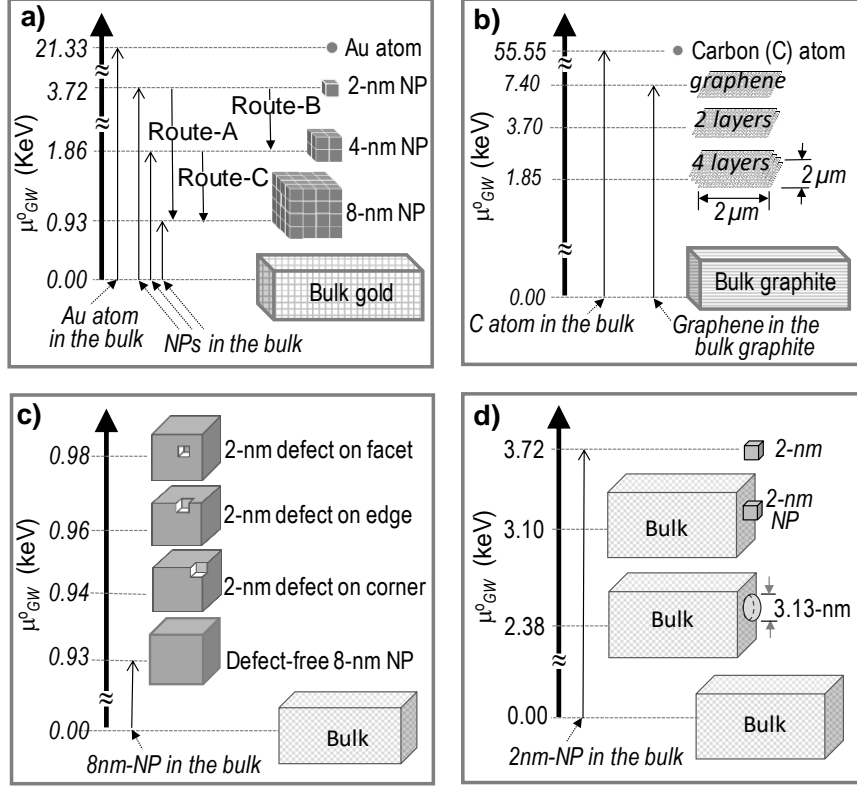


Fig. 1. The μ°_{GW} values. For the Au-NPs self-assembly (a), the graphene-layers (b), a 2-nm surface-defects on an 8-nm NP (c), and a 2-nm NP's adsorption and sintering on a large surface (d).

$$\Delta\mu^\circ_{fGW(\text{Route-B})} = 8\mu^\circ_{fGW(4\text{nm-NPs})} - 64\mu^\circ_{fGW(2\text{nm-NPs})}$$

$$= \{8(6/4) - 64(6/2)\}\hbar c = -223.2 \text{ (keV)},$$

$$\Delta\mu^\circ_{fGW(\text{Route-C})} = \mu^\circ_{fGW(8\text{nm-NP})} - 8\mu^\circ_{fGW(4\text{nm-NPs})}$$

$$= \{6/8 - 8(6/4)\}\hbar c = -14.0 \text{ (keV)}, \text{ and}$$

$$\Delta\mu^\circ_{fGW(\text{Route-A})} = \Delta\mu^\circ_{fGW(\text{Route-B})} + \Delta\mu^\circ_{fGW(\text{Route-C})},$$

confirming the $\Delta\mu^\circ_{fGW}$ as a state function.

Accordingly, a NP's μ°_{fGW} reduction in the hierarchical self-assembly bonding

(see the **Extended Data Table S2a**) is quantifiable:

$$\Delta\mu^\circ_{fGW(2\text{nm-NP in } 8\text{nm-NP})} = \Delta\mu^\circ_{fGW(\text{Route-A})}/64 = -3.71$$

$$\text{(keV)} = -(99.73\% \cdot \mu^\circ_{fGW(2\text{nm-NP})}),$$

$$\Delta\mu^\circ_{fGW(2\text{nm-NP in } 4\text{nm-NP})} = \Delta\mu^\circ_{fGW(\text{Route-B})}/64 = -3.49$$

$$\text{(keV)} = -(96.16\% \cdot \mu^\circ_{fGW(2\text{nm-NP})}),$$

$$\Delta\Delta\mu^\circ_{fGW(4\text{nm-NP in } 8\text{nm-NP})} = \Delta\mu^\circ_{fGW(\text{Route-C})}/8 = -1.75$$

$$\text{(keV)} = -(94.09\% \cdot \mu^\circ_{fGW(4\text{nm-NP})}).$$

These equations indicate smaller NPs' inter-bonding stronger than larger NPs', matching a stronger bonding between smaller atoms. Every NP's $\mu_{f\text{GW}}^0$ loses nearly 100% in the bulk, since the $\tilde{V}_{\text{GW}(\text{bulk})}^0 = 0$ i.e. $\mu_{f\text{GW}(\text{bulk})}^0 = 0$. This hierarchical bonding, driven by minimizing smaller particles higher $\mu_{f\text{GW}}^0$ and generalizable to all self-assemblies²⁻⁷, can complement with the electron-centered Chemical Bonding⁸ Theory.

If assuming the $\Delta H_{f\text{GW}}^0 \ll \Delta \mu_{f\text{GW}}^0$ in the self-assembly, then the $\Delta S_{f\text{GW}(\text{environment})}^0 = -\Delta H_{f\text{GW}}^0/T \approx 0$, and $\Delta S_{f\text{GW}}^0 \approx -\Delta \mu_{f\text{GW}}^0/T > 0$. This helps predict quantitatively the $S_{f\text{GW}}^0$ to complement with Boltzmann entropy-based thermodynamics.

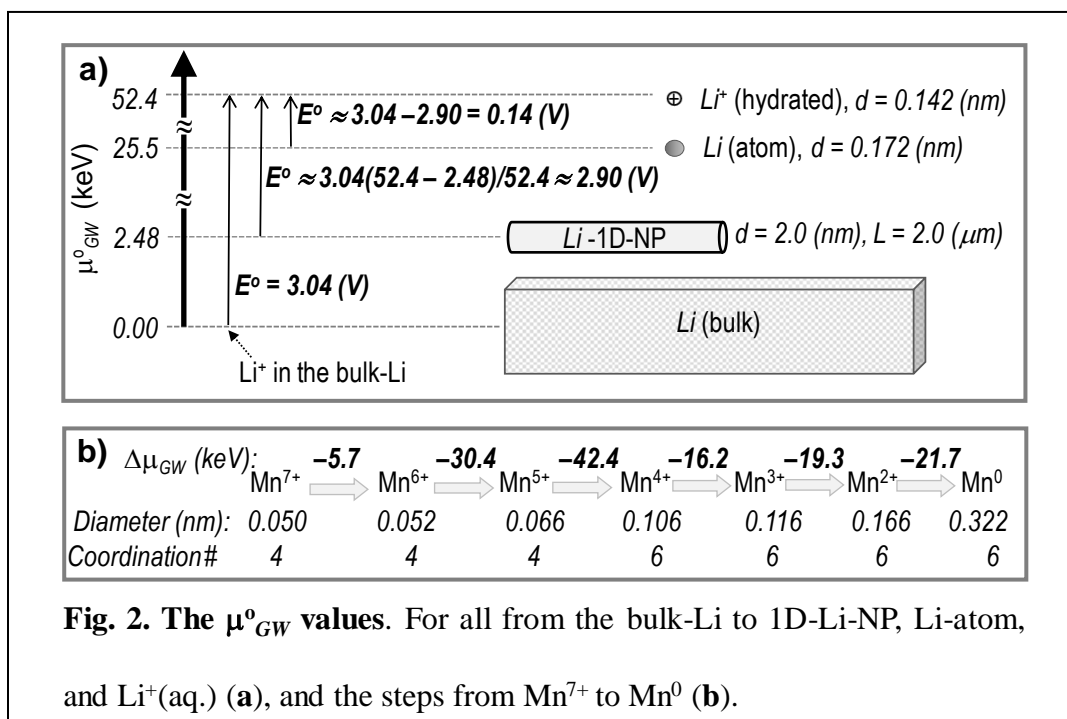
If folding a 150-nm long 1D-polyethylene (PE) to an 8-nm NP (or backward unfolding), since the $d_{(\text{ethylene})} \approx 0.390 \text{ (nm)}$ ⁹, the $\Delta \mu_{f\text{GW}(\text{Folding})}^0 = \mu_{f\text{GW}(\text{0D-PE-NP})}^0 - \mu_{f\text{GW}(\text{1D-PE-oligomer})}^0 \approx (6/8)hc - (4/0.390)hc = -11.78 \text{ (keV)} = -$

$\Delta \mu_{f\text{GW}(\text{Unfolding})}^0$. This can help generalize a thinner 1D-NP's greater $\mu_{f\text{GW}}^0$ for quantifying macromolecules inter-bonding (see the **Extended Data Tables S1 & S2a**).

For a mole of 8-nm NPs at $T = 298$ (°K), the $\mu_{\text{mf}\text{GW}(8\text{nm-AuNP})}^0 = 0.93 \text{ (keV/NP)} \times (6.023 \times 10^{23}) \text{ (NP/mole)} \times (1.60 \times 10^{-19}) \text{ (kJ/keV)} \approx 8.96 \times 10^4 \text{ (kJ/mole)}$. Accordingly, the $S_{\text{mf}\text{GW}(8\text{nm-AuNP})}^0 = -\mu_{\text{mf}\text{GW}(8\text{nm-AuNP})}^0/298 \approx -3.01 \times 10^5 \text{ (J/K}\cdot\text{mole)}$.

Given the $\Delta \mu_{f\text{GW}(\text{bulk graphite})}^0 = 0$ and $d_{(\text{C-atom})} \approx 0.134 \text{ (nm)}$ ¹⁰, the $\mu_{f\text{GW}}^0$ (see the **Extended Data Table S2b**) helps characterize large graphenes of different layers ($\sim 0.335 \text{ nm/layer}$) (**Fig. 1b**). The **Fig. 1b** can help quantify all thinner 2D-materials' higher $\mu_{f\text{GW}}^0$ generally.

On an 8nm-NP, the $\mu_{f\text{GW}}^0$ values of 2.0 nm-large surface vacancy defects (see the **Extended Data Table S2c**) are facet-defect's > edge-defect's > corner-defect's (**Fig. 1c**).

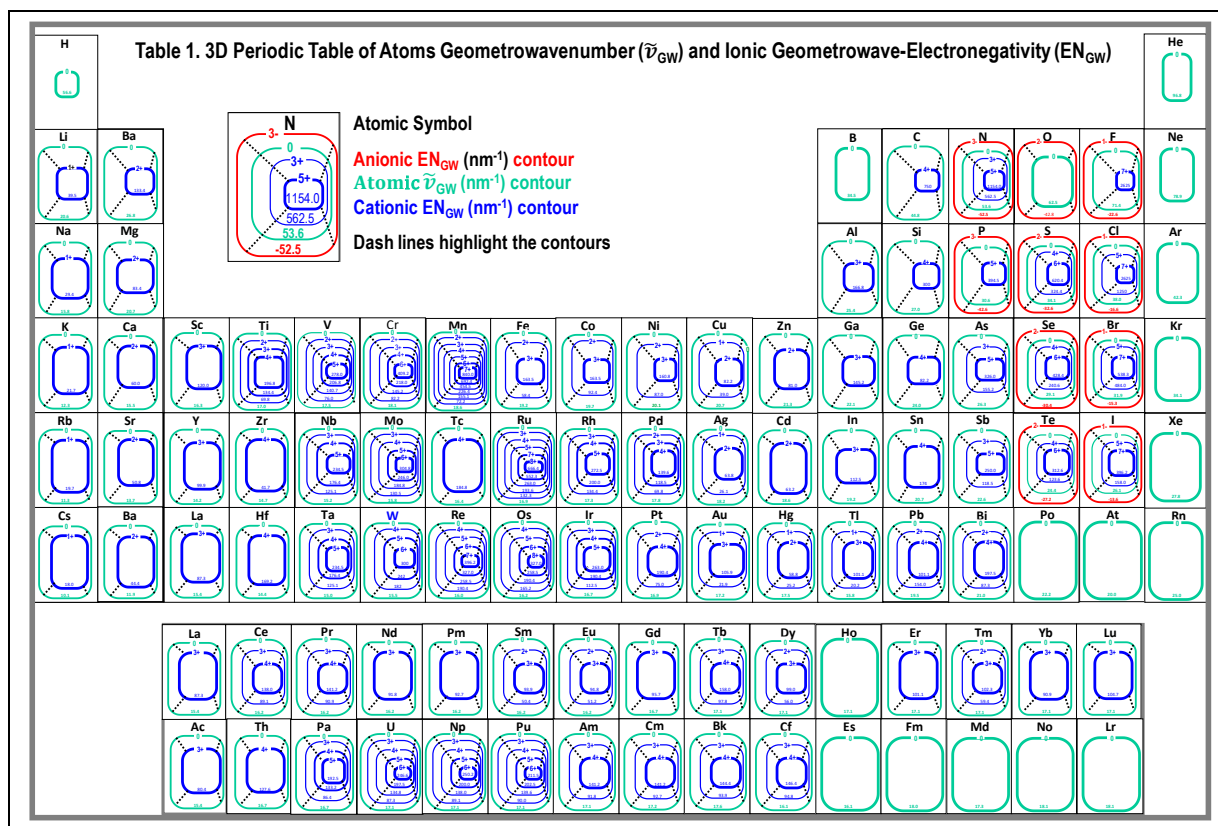


This helps generalize smaller defects' higher reactivity in the same order, to help study e.g. zeolites pores, proteins pockets and channels, and semiconductor surface vacancy defects.

On a bulk flat surface, the 2.0 nm-sized NP's spontaneous adsorption and "sintering" (see the **Extended Data Table S2d**) are each quantitatively characterizable (**Fig. 1d**). This can help quantitatively predict the μ°_{fQGD} in Surface Chemistry and Catalytic Chemistry, generally.

In Li-ion batteries¹¹⁻¹³, the electrochemically hard-to-measuring¹⁴

reduction potential from a $\text{Li}^+(\text{aq.})$ ¹⁵ to a 2- μm -long, 2-nm-thick Li-1D-NP electrode (**Fig. 2a**) is estimable (see the **Extended Data Table S2e**), i.e. $E^\circ_{(\text{cation-to-NP})} = E^\circ_{(\text{cation-to-bulk})} \cdot (\mu^\circ_{\text{fGW}(\text{cation})} - \mu^\circ_{\text{fGW}(\text{NP})}) / \mu^\circ_{\text{fGW}(\text{cation})} \approx -2.90$ (V). This can help quantify the $\Delta\mu^\circ_{\text{fGW}}$ (**Fig. 2b**) between NPs, atoms, and ions (see the **Extended Data Tables S2f, S3 & S4**) for expanding the electrochemistry, redox chemistry, and Lewis acid-base chemistry, using ions' GW-electronegativity ($\text{EN}_{\text{GW}} = (6/d) \times \pm(\text{ion's charge})$) (**Table 1**). Thus, the $\text{EN}_{\text{GW}} = -(\text{GW-electropositivity, or } \text{EP}_{\text{GW}})$,



for quantifying all ions' Lewis acidity (or basicity) in their compounding effectively using their EN_{GW} values.

The **Extended Data Table S1** supports a new nomenclature, " $\tilde{\nu}_{GW}$ -(point-group)-composition", for characterizing NPs-bonded countless compounds. For example, an 1.5-nm PbS-0D-NP can be thus-labeled as (6/1.5)-(R₃)-PbS, a 10-nm 0D-ZnSe-NP as (6/10)-(R₃)-ZnSe, their 1:1 compound as (6/1.5)-(R₃)-PbS•(6/10)-(R₃)-ZnSe, the 1.5-nm PbS-0D-NPs' linear

100mer as 1D-{(6/1.5)-(D_{∞d})-PbS}₁₀₀, and a 2-nm 0D-ZnO-NP's compound with a kinesin as (6/3)-(R₃)-ZnO-NP•kinesin, respectively.

In conclusion, the thermodynamics- and QM-complemented $\mu_f^o_{GW}$ has enabled consistently unifying and quantitatively predicting and comparing the particles' $\mu_f^o_{GW}$ -quantized properties including their hierarchical self-assembly bonding, redox activity, folding–unfolding, acidity and/or basicity, surface defects reactivity, etc.

Atoms' and monoatomic ions' EN_{GW} values could help develop new basics for (see in **Extended Data Table S3**), potentially overhauling modern chemistry¹⁶, which generalizable to the particles and oligomers, should be discussed separately.^{17,18}

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EXTENDED DATA.

I. Extended Data Tables S1–S4.





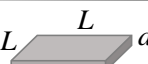



II. References.

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I. Extended Data Tables.

1). Extended Data¹ TableS1:

| Table S1. Simple-Shape Particles' $\tilde{\nu}_{GW}$ and Point Group (Symmetry) | | | | | |
|---|---|------------------------|-----------------|--|----------------|
| | Shape | Surface-Area (SA) | Volume (V) | $\tilde{\nu}_{GW}(= SA/V)$ | Point Group |
| 0D |  d | πd^2 | $\pi d^3/6$ | $(6/d)^*$ | R_3 |
| 1D |  L d | $4dL + 2d^2$ | $d^2 L$ | $(4/d + 2/L)^{**}$ or $(4/d)^{**}$ if $d \ll L$ | D_{4d} |
| |  L d | $\pi d^2/2 + \pi dL$ | $\pi d^2 L/4$ | $(4/d + 2/L)^{**}$ or $(4/d)^{**}$ if $d \ll L$ | $D_{\infty d}$ |
| 2D |  D d | $\pi D^2/2 + \pi dD$ | $d\pi D^2/4$ | $2/d + 4/D;$ or $2/d$ if $d \ll D$ | $D_{\infty d}$ |
| |  L L d | $2(dL + dL + L^2)$ | dL^2 | $2/d + 2/L + 2/L;$ or $2/d$ if $d \ll L$ | D_{4d} |
| 3D |  d | $6d^2$ | d^3 | $(6/d)^*$ | O_h |
| |  d | $2 \times 3^{1/2} d^2$ | $2^{1/2} d^3/3$ | $3 \times 6^{1/2}/d$ | O_h |
| |  d | $1.732d^2$ | $0.118d^3$ | $14.678/d$ | T_d |

*The spherical and cubic particles share the same $\tilde{\nu}_{GW}$ formula;
**The two 1D-particles share the same $\tilde{\nu}_{GW}$ formula.

2). Extended Data Table S2:

Table S2. Calculations of the μ_{GW}^0

a) $\mu_{GW}^0(\text{Au-atom}) = (17.2)hc = 21.33 \text{ (keV)},$
 $\mu_{GW}^0(2\text{nm-AuNP}) = (6/2)hc = 3.72 \text{ (keV)},$
 $\mu_{GW}^0(4\text{nm-AuNP}) = (6/4)hc = 1.86 \text{ (keV)},$
 $\mu_{GW}^0(8\text{nm-AuNP}) = (6/8)hc = 0.93 \text{ (keV)}.$

b) $\mu_{GW}^0(\text{C-atom}) = (44.8)hc = 55.55 \text{ (keV)},$
 $\mu_{GW}^0(1\text{-layer graphene}) = hc\{2/(1 \times 0.335)\} = 7.40,$
 $\mu_{GW}^0(2\text{-layer graphene}) = hc\{2/(2 \times 0.335)\} = 3.70 \text{ (keV)},$
 $\mu_{GW}^0(4\text{-layer graphene}) = hc\{2/(4 \times 0.335)\} = 1.85 \text{ (keV)}.$

c) $\mu_{GW}^0(\text{facet-defect}) = hc\{(SA/V)_{(2\text{-nm defect on } 8\text{-nm NP})}\} = hc\{(4 \times 2^2 + 6 \times 8^2)/(8^3 - 2^3)\} = hc\{(4 \times 2^2 + 384)/504\} = 0.98 \text{ (keV)},$
 $\mu_{GW}^0(\text{edge-defect}) = hc\{(2 \times 2^2 + 384)/504\} = 0.96 \text{ (keV)},$
 $\mu_{GW}^0(\text{corner-defect}) = hc\{384/504 - 17.2\} = 0.94 \text{ (keV)}.$

d) $\mu_{GW}^0(2\text{nm-NP-on-large flat surface}) = hc\{(5 \times 2^2)/8\} = 3.10 \text{ (keV)},$
 $\mu_{GW}^0(\text{hemisphere-on-large flat surface}) = hc\{(\pi d^2)/(\pi d^3/6)\} \approx hc(6/d) = hc(6/3.13) = 2.38 \text{ (keV)}.$

e) $\mu_{GW}^0(\text{Li (I) hydrated cation}) = hc(SA/V)_{\text{hydrated-Li-(I)-cation}} = hc(6/0.142) = 52.4 \text{ (keV)},$
 $\mu_{GW}^0(\text{Li atom}) = hc(SA/V)_{\text{Li-atom}} = hc(20.6) = 25.5 \text{ (keV)},$
 $\mu_{GW}^0(\text{Li-1D-NP}) \approx hc(4/d) = hc(4/2) = 2.48 \text{ (keV)}.$

f) $\mu_{GW}^0(\text{Mn(VII)}) = hc(6/0.050) = 148.8 \text{ (keV)},$
 $\mu_{GW}^0(\text{Mn(VI)}) = hc(6/0.052) = 143.1 \text{ (keV)},$
 $\mu_{GW}^0(\text{Mn(V)}) = hc(6/0.066) = 112.7 \text{ (keV)},$
 $\mu_{GW}^0(\text{Mn(IV)}) = hc(6/0.106) = 70.3 \text{ (keV)},$
 $\mu_{GW}^0(\text{Mn(III)}) = hc(6/0.116) = 64.1 \text{ (keV)},$
 $\mu_{GW}^0(\text{Mn(II)}) = hc(6/0.166) = 44.8 \text{ (keV)},$
 $\mu_{GW}^0(\text{Mn(0)}) = hc(6/0.322) = 23.1 \text{ (keV)}$

3. Extended Data Table S3:

| Table S3. Periodicities of Atoms \tilde{V}_{GW} | | | | | | | | | | | | | | | | | |
|---|-----------------------------|-----------------------------|-----------------------------|--|-----------------------------|-----------------------------|-----------------------------|-----------------------------|-----------------------------|-----------------------------|-----------------------------|-----------------------------|-----------------------------|-----------------------------|-----------------------------|-----------------------------|-----------------------------|
| H 0.106 56.6 2.20 | | | | | | | | | | | | | | | | | He 0.062 96.8 |
| | | La 0.390 15.4 1.10 | | Atomic Symbol Atomic diameter* (unit: (nm)) \tilde{V}_{GW} (unit: nm ⁻¹) Pauling's EN** | | | | | | | | | | | | | |
| Li 0.234 20.6 0.98 | Be 0.224 26.8 1.57 | | | | | | | | | | | B 0.174 34.5 2.04 | C 0.134 44.8 2.55 | N 0.112 53.6 3.04 | O 0.096 62.5 3.44 | F 0.084 71.4 3.98 | Ne 0.076 78.9 |
| Na 0.380 15.8 0.93 | Mg 0.290 20.7 1.31 | | | | | | | | | | | Al 0.236 25.4 1.61 | Si 0.222 27.0 1.90 | P 0.196 30.6 2.19 | S 0.176 34.1 2.58 | Cl 0.158 38.0 3.16 | Ar 0.142 42.3 |
| K 0.486 12.3 0.82 | Ca 0.388 15.5 1.00 | Sc 0.368 16.3 1.36 | Ti 0.352 17.0 1.54 | V 0.342 17.5 1.63 | Cr 0.332 18.1 1.66 | Mn 0.322 18.6 1.55 | Fe 0.312 19.2 1.83 | Co 0.304 19.7 1.88 | Ni 0.298 20.1 1.91 | Cu 0.290 20.7 1.90 | Zn 0.282 21.3 1.65 | Ga 0.272 22.1 1.81 | Ge 0.250 24.0 2.01 | As 0.228 26.3 2.18 | Se 0.206 29.1 2.55 | Br 0.188 31.9 2.96 | Kr 0.176 34.1 |
| Rb 0.530 11.3 0.82 | Sr 0.438 13.7 0.95 | Y 0.424 14.2 1.22 | Zr 0.412 14.7 1.33 | Nb 0.396 15.2 1.6 | Mo 0.380 15.8 2.16 | Tc 0.366 16.4 2.10 | Ru 0.356 16.9 2.2 | Rh 0.346 17.3 2.28 | Pd 0.338 17.8 2.20 | Ag 0.330 18.2 1.93 | Cd 0.322 18.6 1.69 | In 0.312 19.2 1.78 | Sn 0.290 20.7 1.96 | Sb 0.266 22.6 2.05 | Te 0.246 24.4 2.1 | I 0.230 26.1 2.66 | Xe 0.216 27.8 2.60 |
| Cs 0.596 10.1 0.79 | Ba 0.506 11.9 0.89 | La 0.390 15.4 1.10 | Hf 0.416 14.4 1.3 | Ta 0.400 15.0 1.5 | W 0.386 15.5 1.7 | Re 0.376 16.0 1.9 | Os 0.370 16.7 2.2 | Ir 0.360 17.2 2.2 | Pt 0.354 17.5 2.2 | Au 0.348 17.9 2.4 | Hg 0.342 18.1 1.9 | Tl 0.312 19.5 1.8 | Pb 0.308 20.0 1.8 | Bi 0.286 21.0 1.9 | Po 0.270 22.2 2.0 | At 0.300 23.0 2.2 | Rn 0.240 25.0 |
| | | La 0.390 15.4 1.10 | Ce 0.370 16.2 1.12 | Pr 0.370 16.2 1.13 | Nd 0.370 16.2 1.1 | Pm 0.370 16.2 1.17 | Sm 0.370 16.2 1.17 | Eu 0.370 16.2 1.20 | Gd 0.360 16.7 1.20 | Tb 0.350 17.1 1.20 | Dy 0.350 17.1 1.22 | Ho 0.350 17.1 1.23 | Er 0.350 17.1 1.24 | Tm 0.350 17.1 1.25 | Yb 0.350 17.1 1.25 | Lu 0.350 17.1 1.0 | |
| | | Ac 0.390 15.4 1.1 | Th 0.360 16.7 1.3 | Pa 0.360 16.7 1.5 | U 0.350 17.1 1.7 | Np 0.350 17.1 1.3 | Pu 0.350 17.1 1.3 | Am 0.350 17.1 1.7 | Cm 0.348 17.2 1.7 | Bk 0.340 17.6 1.6 | Cf 0.372 16.1 1.6 | Es 0.372 16.1 1.6 | Fm 0.334 18.0 1.8 | Md 0.346 17.3 1.7 | No 0.332 18.1 1.8 | Lr 0.322 18.1 1.8 | |

2,3

Table S4. Monoatomic ions' EN_{GW} values

| ions | C.N. ^a | r (nm) | 6/d (nm ⁻¹) | EN _{SW} (nm ⁻¹) ^{**} | ions | C.N. | r (nm) | 6/d (nm ⁻¹) | EN _{SW} | ions | C.N. | r (nm) | 6/d (nm ⁻¹) | EN _{SW} | ions | C.N. | r (nm) | 6/d (nm ⁻¹) | EN _{SW} |
|------------------|-------------------|--------|-------------------------|--|------------------|------|--------|-------------------------|------------------|------------------|------|--------|-------------------------|------------------|------------------|------|--------|-------------------------|------------------|
| F ⁻ | 6 | 0.133 | 22.6 | -22.6 | BK ⁺⁴ | 6 | 0.083 | 36.1 | 144.4 | Cu ⁺¹ | 2 | 0.046 | 65.2 | 65.2 | Ir ⁺³ | 6 | 0.068 | 44.1 | 132.3 |
| Cl ⁻ | 6 | 0.181 | 16.6 | -16.6 | | 8 | 0.093 | 32.3 | 129.2 | | 4 | 0.060 | 50.0 | 50.0 | Ir ⁺⁴ | 6 | 0.063 | 47.6 | 190.4 |
| Br ⁻ | 6 | 0.196 | 15.3 | -15.3 | Br ⁺⁵ | 3 | 0.031 | 96.8 | 484 | | 6 | 0.077 | 39.0 | 39.0 | Ir ⁺⁵ | 6 | 0.057 | 52.6 | 263 |
| I ⁻ | 6 | 0.220 | 13.6 | -13.6 | Br ⁺⁷ | 4 | 0.025 | 120 | 840 | Cu ⁺² | 4 | 0.057 | 52.6 | 105.2 | K ⁺¹ | 4 | 0.137 | 21.9 | 21.9 |
| OH ⁻ | 4 | 0.135 | 22.2 | -22.2 | | 6 | 0.039 | 76.9 | 538.3 | | 6 | 0.073 | 41.1 | 82.2 | | 6 | 0.138 | 21.7 | 21.7 |
| | 6 | 0.137 | 21.9 | -21.9 | C ⁺⁴ | 4 | 0.015 | 200 | 800 | Dy ⁺² | 6 | 0.107 | 28.0 | 56.0 | | 8 | 0.151 | 19.9 | 19.9 |
| O ⁻² | 2 | 0.121 | 24.8 | -49.6 | | 6 | 0.016 | 187.5 | 750 | | 8 | 0.119 | 25.2 | 50.4 | | 12 | 0.164 | 18.3 | 18.3 |
| | 6 | 0.140 | 21.4 | -42.8 | Ca ⁺² | 6 | 0.100 | 30.0 | 60.0 | Dy ⁺³ | 6 | 0.091 | 33.0 | 99.0 | La ⁺³ | 6 | 0.103 | 29.1 | 87.3 |
| | 8 | 0.142 | 21.1 | -42.2 | | 8 | 0.112 | 26.8 | 53.6 | | 8 | 0.103 | 29.1 | 87.3 | | 8 | 0.116 | 25.9 | 77.7 |
| S ⁻² | 6 | 0.184 | 16.3 | -32.6 | | 10 | 0.123 | 24.4 | 48.8 | Er ⁺³ | 6 | 0.089 | 33.7 | 101.1 | | 10 | 0.127 | 23.6 | 708 |
| Se ⁻² | 6 | 0.198 | 15.2 | -30.4 | | 12 | 0.134 | 22.4 | 44.8 | | 8 | 0.100 | 30.0 | 90.0 | | 12 | 0.136 | 22.1 | 66.3 |
| Te ⁻² | 6 | 0.221 | 13.6 | -27.2 | Cd ⁺² | 4 | 0.078 | 38.5 | 77.0 | Eu ⁺² | 6 | 0.117 | 25.6 | 51.2 | Li ⁺¹ | 4 | 0.059 | 50.8 | 50.8 |
| N ⁻³ | 6 | 0.171 | 17.5 | -52.5 | | 6 | 0.095 | 31.6 | 63.2 | | 8 | 0.125 | 24.0 | 48.0 | | 6 | 0.076 | 39.5 | 39.5 |
| P ⁻³ | 6 | 0.212 | 14.2 | -42.6 | | 8 | 0.110 | 27.3 | 54.6 | | 10 | 0.135 | 22.2 | 44.4 | | 8 | 0.092 | 32.6 | 32.6 |
| | | | | | | 12 | 0.131 | 22.9 | 45.8 | Eu ⁺³ | 6 | 0.095 | 31.6 | 94.8 | Lu ⁺³ | 6 | 0.086 | 34.9 | 104.7 |
| Ac ⁺³ | 6 | 0.112 | 26.8 | 80.4 | Ce ⁺³ | 6 | 0.101 | 29.7 | 89.1 | | 8 | 0.107 | 21.1 | 63.3 | | 8 | 0.097 | 30.9 | 92.7 |
| Ag ⁺¹ | 4 | 0.100 | 30.0 | 30.0 | | 8 | 0.114 | 26.3 | 78.9 | F ⁺⁷ | 6 | 0.008 | 375 | 2625 | Mg ⁺² | 4 | 0.057 | 52.6 | 105.2 |
| | 6 | 0.115 | 26.1 | 26.1 | | 10 | 0.125 | 24.0 | 72.0 | Fe ⁺² | 4 | 0.063 | 47.6 | 95.2 | | 6 | 0.072 | 41.7 | 83.4 |
| | 8 | 0.128 | 23.4 | 23.4 | | 12 | 0.134 | 22.4 | 67.2 | | 6 | 0.061 | 49.2 | 58.4 | | 8 | 0.089 | 33.7 | 67.4 |
| Ag ⁺² | 4 | 0.079 | 38.0 | 76.0 | Ce ⁺⁴ | 6 | 0.087 | 34.5 | 138 | | 8 | 0.092 | 32.6 | 65.2 | Mn ⁺² | 4 | 0.066 | 45.5 | 91.0 |
| | 6 | 0.094 | 31.9 | 63.8 | | 8 | 0.097 | 30.9 | 123.6 | Fe ⁺³ | 4 | 0.049 | 61.2 | 183.6 | | 6 | 0.083 | 36.1 | 72.2 |
| Al ⁺³ | 4 | 0.039 | 76.9 | 230.7 | | 10 | 0.107 | 28.0 | 112 | | 6 | 0.055 | 54.5 | 163.5 | | 8 | 0.096 | 31.3 | 62.6 |
| | 5 | 0.048 | 62.5 | 187.5 | | 12 | 0.114 | 26.3 | 105.2 | | 8 | 0.078 | 38.5 | 115.5 | Mn ⁺³ | 6 | 0.058 | 51.7 | 155.1 |
| | 6 | 0.054 | 55.6 | 166.8 | Cf ⁺³ | 6 | 0.095 | 31.6 | 94.8 | Ga ⁺³ | 4 | 0.047 | 63.8 | 191.4 | Mn ⁺⁴ | 4 | 0.039 | 76.9 | 307.6 |
| Am ⁺³ | 6 | 0.098 | 30.6 | 91.8 | Cf ⁺⁴ | 6 | 0.082 | 36.6 | 146.4 | | 6 | 0.062 | 48.4 | 145.2 | | 6 | 0.053 | 56.6 | 226.4 |
| | 8 | 0.109 | 27.5 | 82.5 | | 8 | 0.092 | 32.6 | 130.4 | Gd ⁺³ | 6 | 0.094 | 31.9 | 95.7 | Mn ⁺⁵ | 4 | 0.033 | 90.9 | 454.5 |
| Am ⁺⁴ | 6 | 0.085 | 35.3 | 141.2 | Cf ⁺⁵ | 3 | 0.012 | 250 | 1250 | | 8 | 0.105 | 28.6 | 85.8 | Mn ⁺⁶ | 4 | 0.026 | 115.4 | 692.4 |
| | 8 | 0.095 | 31.6 | 126.4 | Cf ⁺⁷ | 4 | 0.008 | 375 | 2625 | Ge ⁺² | 6 | 0.073 | 41.1 | 82.2 | Mn ⁺⁷ | 4 | 0.025 | 120 | 840 |
| As ⁺³ | 6 | 0.058 | 51.7 | 155.2 | Cm ⁺³ | 6 | 0.097 | 30.9 | 92.7 | Ge ⁺⁴ | 4 | 0.039 | 76.9 | 307.6 | Mo ⁺³ | 6 | 0.069 | 43.5 | 130.5 |
| As ⁺⁵ | 4 | 0.034 | 88.2 | 441 | Cm ⁺⁴ | 6 | 0.085 | 35.3 | 141.2 | | 6 | 0.053 | 56.6 | 226.4 | Mo ⁺⁴ | 6 | 0.065 | 46.2 | 184.8 |
| | 6 | 0.046 | 65.2 | 326 | | 8 | 0.095 | 31.6 | 126.4 | Hf ⁺⁴ | 4 | 0.058 | 51.7 | 206.8 | Mo ⁺⁵ | 4 | 0.046 | 65.2 | 326 |
| Au ⁺¹ | 6 | 0.137 | 21.9 | 21.9 | Co ⁺² | 4 | 0.056 | 53.6 | 107.2 | | 6 | 0.071 | 42.3 | 169.2 | | 6 | 0.061 | 49.2 | 246 |
| Au ⁺³ | 4 | 0.064 | 46.9 | 140.7 | | 6 | 0.065 | 46.2 | 92.4 | | 8 | 0.083 | 36.1 | 144.4 | Mo ⁺⁶ | 4 | 0.041 | 73.2 | 439.2 |
| | 6 | 0.085 | 35.3 | 105.9 | | 8 | 0.090 | 33.3 | 66.6 | Hg ⁺¹ | 6 | 0.119 | 25.2 | 25.2 | | 6 | 0.059 | 50.8 | 304.8 |
| Ba ⁺² | 6 | 0.135 | 22.2 | 44.4 | Co ⁺³ | 6 | 0.055 | 54.5 | 163.5 | Hg ⁺² | 2 | 0.069 | 43.5 | 87.0 | | 7 | 0.073 | 41.1 | 246.6 |
| | 8 | 0.142 | 21.1 | 42.2 | Cr ⁺² | 6 | 0.073 | 41.1 | 82.2 | | 4 | 0.096 | 31.3 | 62.6 | N ⁺³ | 6 | 0.016 | 187.5 | 562.5 |
| | 12 | 0.161 | 18.6 | 37.2 | Cr ⁺³ | 6 | 0.062 | 48.4 | 145.2 | | 6 | 0.102 | 29.4 | 58.8 | N ⁺⁵ | 6 | 0.013 | 230.8 | 1154 |
| Be ⁺² | 4 | 0.027 | 111.1 | 222.2 | Cr ⁺⁴ | 4 | 0.041 | 73.2 | 292.8 | | 8 | 0.114 | 26.3 | 52.6 | Na ⁺¹ | 4 | 0.099 | 30.3 | 30.3 |
| | 6 | 0.045 | 66.7 | 133.4 | | 6 | 0.055 | 54.5 | 218 | I ⁺⁵ | 3 | 0.044 | 68.2 | 341 | | 6 | 0.102 | 29.4 | 29.4 |
| Bi ⁺³ | 5 | 0.096 | 31.3 | 93.9 | Cr ⁺⁶ | 4 | 0.026 | 115.4 | 692.4 | | 6 | 0.095 | 31.6 | 158 | | 8 | 0.118 | 25.4 | 25.4 |
| | 6 | 0.103 | 29.1 | 87.3 | | 6 | 0.044 | 68.2 | 409.2 | I ⁺⁷ | 4 | 0.042 | 71.4 | 499.8 | | 9 | 0.124 | 24.2 | 24.2 |
| | 8 | 0.117 | 25.6 | 76.8 | Cs ⁺¹ | 6 | 0.167 | 18.0 | 18.0 | | 6 | 0.053 | 56.6 | 396.2 | | 12 | 0.13 | 23.1 | 23.1 |
| Bi ⁺⁵ | 6 | 0.076 | 39.5 | 197.5 | | 8 | 0.174 | 17.2 | 17.2 | In ⁺³ | 4 | 0.062 | 48.4 | 145.2 | Nb ⁺³ | 6 | 0.072 | 41.7 | 125.1 |
| Bk ⁺³ | 6 | 0.096 | 31.3 | 93.9 | | 10 | 0.181 | 16.6 | 16.6 | | 6 | 0.080 | 37.5 | 112.5 | | 8 | 0.079 | 38.0 | 114 |
| | | | | | | 12 | 0.188 | 16.0 | 16.0 | | | | | | | | | | |

*CN: Coordination Number, and CN = 6 for most cases in the **Table 1**

****EN_{GW} unit: (nm⁻¹)**

4). Extended Data Table S4 (continued):

| Ions | C.N. | r (nm) | 6/d (nm ⁻¹) | EN _{GW} | Ions | C.N. | r (nm) | 6/d (nm ⁻¹) | EN _{GW} | Ions | C.N. | r (nm) | 6/d (nm ⁻¹) | EN _{GW} | Ions | C.N. | r (nm) | 6/d (nm ⁻¹) | EN _{GW} |
|------------------|------|--------|-------------------------|------------------|------------------|------|--------|-------------------------|------------------|------------------|------|--------|-------------------------|------------------|------------------|------|--------|-------------------------|------------------|
| Nb ¹⁴ | 6 | 0.068 | 44.1 | 177.6 | Pr ¹⁴ | 6 | 0.085 | 35.3 | 141.2 | Sm ¹² | 6 | 0.119 | 25.2 | 50.4 | Tm ¹² | 6 | 0.101 | 29.7 | 59.4 |
| Nb ¹⁵ | 4 | 0.048 | 62.5 | 312.5 | | 8 | 0.096 | 31.3 | 125.2 | | 8 | 0.127 | 23.6 | 47.2 | | 7 | 0.109 | 27.5 | 55.0 |
| | 6 | 0.064 | 46.9 | 234.5 | Pt ¹² | 4 | 0.060 | 50.0 | 100 | Sm ¹³ | 6 | 0.096 | 31.3 | 93.9 | Tm ¹³ | 6 | 0.088 | 34.1 | 102.3 |
| | 8 | 0.074 | 40.5 | 202.5 | | 6 | 0.080 | 37.5 | 75.0 | | 8 | 0.108 | 27.8 | 83.4 | | 8 | 0.099 | 30.3 | 90.9 |
| Nd ¹³ | 6 | 0.098 | 30.6 | 91.8 | Pt ¹⁴ | 6 | 0.063 | 47.6 | 190.4 | | 12 | 0.124 | 24.2 | 72.6 | U ¹³ | 6 | 0.103 | 29.1 | 87.3 |
| | 8 | 0.112 | 26.8 | 80.4 | Pu ¹³ | 6 | 0.100 | 30.0 | 90.0 | Sn ¹⁴ | 4 | 0.055 | 54.5 | 218 | U ¹⁴ | 6 | 0.089 | 33.7 | 134.8 |
| | 9 | 0.116 | 25.9 | 77.7 | Pu ¹⁴ | 6 | 0.086 | 34.9 | 139.6 | | 6 | 0.069 | 43.5 | 174 | | 8 | 0.100 | 30.0 | 120 |
| | 12 | 0.127 | 23.6 | 70.8 | Pu ¹⁵ | 6 | 0.074 | 40.5 | 202.5 | | 8 | 0.081 | 37.0 | 148 | | 12 | 0.117 | 25.6 | 102.4 |
| Ni ¹² | 4 | 0.049 | 61.2 | 122.4 | Pu ¹⁶ | 6 | 0.071 | 42.3 | 211.5 | Sr ¹² | 6 | 0.118 | 25.4 | 50.8 | U ¹⁵ | 6 | 0.076 | 39.5 | 197.5 |
| | 6 | 0.069 | 43.5 | 87.0 | Rb ¹¹ | 6 | 0.152 | 19.7 | 19.7 | | 8 | 0.126 | 23.8 | 47.6 | U ¹⁶ | 2 | 0.045 | 66.7 | 400.2 |
| Ni ¹³ | 6 | 0.056 | 53.6 | 160.8 | | 8 | 0.161 | 18.6 | 18.6 | | 10 | 0.136 | 22.1 | 44.2 | | 4 | 0.052 | 57.7 | 346.2 |
| Np ¹³ | 6 | 0.101 | 29.7 | 89.1 | | 10 | 0.166 | 18.1 | 18.1 | | 12 | 0.144 | 20.8 | 41.6 | | 6 | 0.073 | 41.1 | 246.6 |
| Np ¹⁴ | 6 | 0.087 | 34.5 | 138 | | 12 | 0.172 | 17.4 | 17.4 | Ta ¹³ | 6 | 0.072 | 41.7 | 125.1 | | 8 | 0.086 | 34.9 | 209.4 |
| Np ¹⁵ | 6 | 0.075 | 40.0 | 200 | Re ¹⁴ | 6 | 0.063 | 47.6 | 190.4 | Ta ¹⁴ | 6 | 0.068 | 44.1 | 176.4 | V ¹² | 6 | 0.079 | 38.0 | 76.0 |
| Np ¹⁶ | 6 | 0.072 | 41.7 | 250.2 | Re ¹⁵ | 6 | 0.058 | 51.7 | 258.5 | Ta ¹⁵ | 6 | 0.064 | 46.9 | 234.5 | V ¹³ | 6 | 0.064 | 46.9 | 140.7 |
| Os ¹⁴ | 6 | 0.063 | 47.6 | 190.4 | Re ¹⁶ | 6 | 0.055 | 54.5 | 327 | Tb ¹³ | 6 | 0.092 | 32.6 | 97.8 | V ¹⁴ | 5 | 0.053 | 56.6 | 226.4 |
| Os ¹⁵ | 6 | 0.058 | 51.7 | 258.5 | Re ¹⁷ | 4 | 0.038 | 78.9 | 552.3 | | 8 | 0.104 | 28.8 | 86.4 | | 6 | 0.058 | 51.7 | 206.8 |
| Os ¹⁶ | 6 | 0.055 | 54.5 | 327 | | 6 | 0.053 | 56.6 | 396.2 | Tb ¹⁴ | 6 | 0.076 | 39.5 | 158 | | 8 | 0.072 | 41.7 | 166.8 |
| Os ¹⁸ | 6 | 0.039 | 76.9 | 615.2 | Rh ¹³ | 6 | 0.067 | 44.8 | 134.4 | | 8 | 0.088 | 34.1 | 136.4 | V ¹⁵ | 4 | 0.036 | 83.3 | 416.5 |
| P ¹⁵ | 4 | 0.017 | 176.5 | 882.5 | Rh ¹⁴ | 6 | 0.060 | 50.0 | 200 | Tc ¹⁴ | 6 | 0.065 | 46.2 | 184.8 | | 5 | 0.046 | 65.2 | 326 |
| | 6 | 0.038 | 78.9 | 394.5 | Rh ¹⁵ | 6 | 0.055 | 54.5 | 272.5 | Te ¹⁴ | 4 | 0.066 | 45.5 | 182 | | 6 | 0.054 | 55.6 | 278 |
| Pa ¹³ | 6 | 0.104 | 28.8 | 86.4 | Ru ¹³ | 6 | 0.068 | 44.1 | 132.3 | | 6 | 0.097 | 30.9 | 123.6 | W ¹⁴ | 6 | 0.066 | 45.5 | 182 |
| Pa ¹⁴ | 6 | 0.090 | 33.3 | 133.2 | Ru ¹⁴ | 6 | 0.062 | 48.4 | 193.6 | Te ¹⁶ | 4 | 0.043 | 69.8 | 418.8 | W ¹⁵ | 6 | 0.062 | 48.4 | 242 |
| Pa ¹⁵ | 6 | 0.078 | 38.5 | 192.5 | Ru ¹⁵ | 6 | 0.057 | 52.6 | 263 | | 6 | 0.056 | 53.6 | 321.6 | W ¹⁶ | 4 | 0.042 | 71.4 | 428.4 |
| Pb ¹² | 6 | 0.119 | 25.2 | 50.4 | Ru ¹⁷ | 4 | 0.038 | 78.9 | 552.3 | Th ¹⁴ | 6 | 0.094 | 31.9 | 127.6 | | 5 | 0.051 | 58.8 | 352.8 |
| | 8 | 0.129 | 23.3 | 46.6 | Ru ¹⁸ | 4 | 0.036 | 83.3 | 670.4 | | 8 | 0.105 | 28.6 | 114.4 | | 6 | 0.060 | 50.0 | 300 |
| | 10 | 0.140 | 21.4 | 42.8 | S ¹⁴ | 6 | 0.037 | 81.1 | 324.4 | | 10 | 0.113 | 26.5 | 106 | Y ¹³ | 6 | 0.090 | 33.3 | 99.9 |
| | 12 | 0.149 | 20.1 | 40.2 | S ¹⁶ | 4 | 0.012 | 250 | 1500 | | 12 | 0.121 | 24.8 | 99.2 | | 8 | 0.102 | 29.4 | 88.2 |
| Pb ¹⁴ | 4 | 0.065 | 46.2 | 184.8 | | 6 | 0.029 | 103.4 | 620.4 | Ti ¹² | 6 | 0.086 | 34.9 | 69.8 | | 9 | 0.108 | 27.8 | 83.4 |
| | 6 | 0.078 | 38.5 | 154 | Sb ¹³ | 4 | 0.076 | 39.5 | 118.5 | Ti ¹³ | 6 | 0.067 | 44.8 | 134.4 | Yb ¹² | 6 | 0.102 | 29.4 | 58.8 |
| | 8 | 0.094 | 31.9 | 127.6 | | 6 | 0.076 | 39.5 | 118.5 | Ti ¹⁴ | 4 | 0.042 | 71.4 | 285.6 | | 8 | 0.114 | 26.3 | 52.6 |
| Pd ¹² | 4 | 0.064 | 46.9 | 93.8 | Sb ¹⁵ | 6 | 0.060 | 50.0 | 250 | | 6 | 0.061 | 49.2 | 196.8 | Yb ¹³ | 8 | 0.099 | 30.3 | 90.9 |
| | 6 | 0.086 | 34.9 | 69.8 | Sc ¹³ | 6 | 0.075 | 40.0 | 120 | | 8 | 0.074 | 40.5 | 162 | | 9 | 0.104 | 28.8 | 86.4 |
| Pd ¹³ | 6 | 0.076 | 39.5 | 118.5 | | 8 | 0.087 | 34.5 | 103.5 | Th ¹¹ | 6 | 0.150 | 20.0 | 20.2 | Zn ¹² | 4 | 0.060 | 50.0 | 100 |
| Pd ¹⁴ | 6 | 0.062 | 48.4 | 193.6 | Se ¹⁴ | 6 | 0.050 | 60.0 | 240 | | 8 | 0.159 | 18.9 | 18.9 | | 6 | 0.074 | 40.5 | 81.0 |
| Pm ¹³ | 6 | 0.097 | 30.9 | 92.7 | Se ¹⁶ | 4 | 0.028 | 107.1 | 642.6 | | 12 | 0.170 | 17.6 | 17.6 | | 8 | 0.090 | 33.3 | 66.6 |
| | 8 | 0.109 | 27.5 | 82.5 | | 6 | 0.042 | 71.4 | 428.4 | Ti ¹³ | 4 | 0.075 | 40.0 | 120 | Zr ¹⁴ | 4 | 0.059 | 50.8 | 203.2 |
| Pr ¹³ | 6 | 0.099 | 30.3 | 90.9 | Si ¹⁴ | 4 | 0.026 | 115.4 | 461.6 | | 6 | 0.089 | 33.7 | 101.1 | | 6 | 0.072 | 41.7 | 166.8 |
| | 8 | 0.113 | 26.5 | 79.5 | | 6 | 0.040 | 75.0 | 300 | | 8 | 0.098 | 30.6 | 91.8 | | 8 | 0.084 | 35.7 | 142.8 |
| | | | | | | | | | | | | | | | | 9 | 0.089 | 33.7 | 134.8 |

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