A Concise Treatise on Converting Stellar Mass Fractions to Abundances to Molar Ratios

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Abstract

Understanding stellar composition is fundamental not only to our comprehension of the Galaxy, especially chemical evolution, but it can also shed light on the interior structure and mineralogy of exoplanets, which are formed from the same material as their host stars. Unfortunately, the underlying mathematics describing stellar mass fractions and stellar elemental abundances is difficult to parse, is fragmented across the literature, and contains vexing omissions that makes any calculation far from trivial, especially for nonexperts. In this treatise, we present a clear mathematical formalism and clarification of inherent assumptions and normalizations within stellar composition measurements, which facilitates the conversion from stellar mass fractions to elemental abundances to molar ratios, including error propagation. We also provide an example case study of HIP 544 to further illustrate the provided equations. Given the important chemical association between stars, as well as the interdisciplinary relationship between stars and their planets, it is vital that stellar mass fractions and abundance data be more transparent and accessible to people within different subfields and scientific disciplines.

Unified Astronomy Thesaurus concepts: High resolution spectroscopy (2096); Stellar abundances (1577); Planetary structure (1256); Meteorite composition (1037); Solar abundances (1474); Interdisciplinary astronomy (804)

1. Motivation

In the early universe, the only elements created in any notable amount were hydrogen, helium, and to a lesser extent lithium. With the formation of the first stars, where interior temperatures and pressures reached levels for nuclear fusion, the lighter elements combined to form heavier atoms (Arnett 1996 and references therein). This first generation of extremely massive stars, \( \sim 100 \, M_\odot \), ended their lives by exploding, sending out the newly created heavy elements (referred to as “metals” by astronomers) that diversified the chemical population of the universe. The next generation of stars was formed not only from the Big Bang H and He, but they also contained some of the heavy elements, which they continued to fuse during their lifetimes. It was through the cycles of multiple generations of stars that most of the elements in the periodic table were formed. Since stars and planets are created at the same time, from the same molecular birth cloud, the chemistry of planets is intrinsically linked to that of their host stars (e.g., Gonzalez 1997; Fischer & Valenti 2005; Meléndez et al. 2009; Ramirez et al. 2009; Mulders 2018).

The field of exoplanet science is inherently interdisciplinary. In most cases, nearly everything that we know about a given exoplanet is inferred from the way that it interacts with its host star. For example, understanding the way in which the planet gravitationally influences the star (e.g., via the radial-velocity technique) provides a means for the calculation of planetary mass (e.g., Wright 2018 and references therein). The planet radius may be determined by comparing the size of the planet to the host star during a transit observation (e.g., Kane et al. 2009; Deeg & Alonso 2018). Similarly, the composition of the exoplanet atmosphere can be determined from how the light of the host star is transmitted or absorbed as it passes through a planet’s exosphere, such as with JWST4 (Kreidberg 2018; Madhusudhan 2018 and references therein).

Smaller rocky planets are not directly resolvable from their host stars and they contribute a comparatively insignificant amount of light. Therefore, it is not currently possible to measure the interior structure or solid surface composition of rocky planets. However, the amount of various elements within the star, or elemental abundances, can be used as a logical 1:1 proxy when modeling the interior makeup and mineralogy of a small planet (e.g., Bond et al. 2010; Thiabaud et al. 2015; Hinkel & Unterborn 2018; Schulze et al. 2021).

Stars are made up of shells of nuclear fusion; these “burning” shells transport energy via convection or radiation. While interior shells are observationally opaque, it is from the outer layers of the star—or the photosphere—that light is observable (Arnett 1996 and references therein). It is therefore predominantly the photosphere that is measured when determining the stellar composition. Since the photosphere does not experience the temperatures and pressures required for burning, it is assumed to be similar in composition to the proto-solar cloud from which the star formed. However, there are a few processes that may impact the abundances over time: heavy elements in the photosphere will settle into the interior over the course of the star’s lifetime (or gigayears, e.g., Dotter et al. 2017), radioactive isotopes will decay, and nuclear processing may destroy fragile elements (Li, Be, and B) mixed from the stellar surface by convection. Elemental abundances are therefore indirectly measured by using realistic models of the physics within the stellar photosphere. High accuracy atomic and molecular line data, usually determined within a laboratory, are also necessary for identifying lines within the stellar spectrum.

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4 www.jwst.nasa.gov/
To take advantage of all of the ways in which stars and planets may interact, scientists from a variety of backgrounds need to be able to convert measurements and units across disciplines. Here, we peel back the stellar composition notation to clearly outline how stellar hydrogen ($X$), helium ($Y$), and the remaining heavier elements ($Z$), are defined by stellar theorists. We discuss how to convert from stellar $XYZ$ mass fractions to elemental abundance ratios to more geologically useful units, namely molar ratios. While there have been partial, piecemeal explanations of stellar composition in the literature (e.g., Hinkel et al. 2014; Roederer & Barklem 2018; Hinkel et al. 2020; Gebruers et al. 2021), there does not exist a clear breakdown of the notation and conversion making the compositional relationships between stars and also their planets more difficult to decipher. More importantly, this limits the tractability, reproducibility, and accessibility of stellar composition data for astrophysicists outside of the stellar abundance subfield and for scientists as a whole.

In this paper, we provide a rigorous mathematical explanation of the many ways in which stellar composition may be presented by either theorists or observers. In Section 2, we go over the deep-rooted formalism within stellar elemental abundances, outlining a clear mathematical notation while also providing alternatives found within the literature. In Section 3, we explain the definition of stellar mass fractions and the underlying assumptions associated with those terms. In Section 4, we show generally how to determine molar ratios from stellar abundances and demonstrate how to propagate errors. In Section 5, we illustrate the equations outlined in Section 3 and Section 4 by providing a step-by-step walkthrough of an example case study of HIP 544, including a table of calculated values for each step. In light of the solar normalization associated with the stellar abundance notation, in Section 6 we go over key aspects necessary for solar abundance determination and briefly describe the variations between popular measurements. Finally, in Section 7 we provide a discussion and go over major caveats when working with stellar composition, such as observing elements in different ionization states and the application of nonlocal thermodynamic equilibrium (NLTE) to stellar abundance prescriptions.

2. Mathematical Formalism

Most observed stellar elemental abundance values are reported in dex, or “decadic logarithmic unit” (Lodders 2019). Logarithmic scales (metrics) are useful for tracking observables that span large dynamic ranges and/or when observables are more naturally represented as ratios in linear units, which then become simple addition and subtraction of operations in log-space. The “decadic” of dex tells us that our log base is 10, and not the natural log often seen in other applications. Another common base-10 log unit commonly seen is the decibel (dB). While the dB scale is defined absolutely with $1 W = 0$ dB, the relative span of the units can be simply compared to dex as the change in $\Delta$1 dex = $\Delta$10 dB.

While we define dex as a unit on a base-10 log scale, we distinguish dex-abundance-notation as an additional formalism that includes absolute scaling (i.e., to hydrogen, as discussed in Section 2.1) and defines allowed operations on abundance values. However, the abundance literature rarely makes this disambiguation, leaving the reader to determine from context whether the unit or the abundance formalism is being discussed.

Dex-abundance-notation includes numerous expressions to indicate comparison, for example: brackets to indicate inherent solar normalization (see Section 2.3), e.g., $[Q/H]$ or $[Q/Fe]$. While this notation has historical precedent and utility to experts, the reported measurements are often difficult for those outside of the subfield to interpret, distinguish, or convert to other quantities. Here, we explain the underlying meaning and mathematical framework for stellar abundances.

To begin the formalism of dex-abundance-notation, we summarize variables and definitions. Abundance number fractions (not to be confused with more geologically driven molar ratios discussed in Section 4) have a scale that ranges $[0, 1]$, where 0 means this element is not present and 1 means that an object is composed entirely of that element, such that the sum of all number fractions within an object add to 1. The letter “$q$” is used to represent a number fraction for a generalized element and the letter “$h$” is used to represent the number fraction of hydrogen. Similarly, “fe” represents the number fraction of iron and is used as a specific example of a generalized element, other than $h$ and $q$, to demonstrate scaling by that element.

2.1. Scaling to Hydrogen

The logarithmic and relative scale of dex-abundance-notation offers a quick way to compare across elements and between stars. In the following section we demonstrate the process for going from number fractions for an element to the relative scale of dex-abundance-notation, which makes comparisons simple by using subtractions in log-space.

Astronomers define the abundance of an element starting from a ratio with respect to the number of hydrogen atoms fixed at a trillion (or $10^{12}$ per Payne 1925a, 1925b; Claas 1951). For a generic element $Q$, let $Q$ represent the number of atoms in a star per every $(10^{12})$ hydrogen atoms. Written in terms of number fractions, we have

$$Q = \frac{q}{h} \times 10^{12}. \quad (1)$$

For the element $Q$ we define the absolute stellar abundance, $A(Q)$, as

$$A(Q) \equiv \log_{10}(Q), \quad (2)$$

such that the two quantities are mathematically equivalent ($\equiv$) to each other. Combining Equations (1) and (2) for the case of $q = h$ shows that the absolute stellar abundance of hydrogen, represented by $H$, is

$$A(H) = \log_{10}(H) = \log_{10} \left( \frac{h}{h} \times 10^{12} \right) = \log_{10}(10^{12}) = 12. \quad (3)$$

Hydrogen is the dominant element for all stars; thus the upper bound for the absolute abundance of elements, $A(Q)$, in the dex-abundance-notation is 12 and is equal to the absolute abundance of hydrogen. There is no lower limit to the dex-abundance-notation and negative values are allowed. Although absolute abundances in dex-abundance-notation are, for the most part, positive. Written in a purely mathematical sense, the dex scale for absolute abundances can be any number in the
range \((-\infty, 12]\), however there are practical limits on the measurement of sufficiently rarefied elements.

Because hydrogen is the most prevalent element for all stars, we can formally state that the number fraction for \(h\) is nearly equal to 1, which we write as:

\[
h \approx 1. \tag{4}\]

Equation (4) leads to the simplification of Equation (1), namely

\[
Q \approx q \times 10^{12}. \tag{5}\]

With Equation (5), we are now prepared to write Equation (2) in terms of the number fraction, \(q\), and the definition of the absolute abundance of hydrogen in Equation (3) as

\[
A(Q) = \log_{10}(q \times 10^{12}) = \log_{10}(q) + 12 = \log_{10}(q) + A(H). \tag{6}\]

Note that Equation (6) contains a factor of \(10^{12}\) required to scale a number fraction of unity to an absolute stellar abundance 12, as is the case for hydrogen. In addition, because the logarithm of any number fraction value \(<1\) is negative, that means that any nonhydrogen \(A(Q)\) will be less than 12. To acknowledge that \(A(Q)\) is defined in terms of \(H\), dex-abundance-notation defines the absolute abundance with respect to hydrogen, \(Q/H\) as

\[
Q/H \equiv A(Q). \tag{7}\]

Classically, there are a number of reasons solar and stellar spectroscopists scale abundances to hydrogen. In terms of observations, stellar abundances are determined as a ratio between the element line opacity and the continuum opacity determined by \(H\) in the stellar photosphere. More broadly, hydrogen is the most abundant element within the universe, making up \(\sim 90\%\) of baryonic material by atom number or \(\sim 75\%\) by mass in the universe. Because the formation of most elements heavier than \(H\) and \(He\) has increased since the Big Bang (with the exception of \(Li, Be,\) and \(B\)), those elements compared as a ratio to hydrogen will show the rate of that element’s production in time.

With that in mind, it should be noted that geological and/or meteoritic abundances are historically scaled to \(10^{12}\) \(Si\) atoms, since it most abundant element by mole in Earth, and \(Si\) is an easy to measure positively charged ion in Earth’s crust (Goldschmidt 1937). Fortunately, it is possible to convert between the \(Si\)-scaled meteoritic (met) scale and the astronomical \(H\)-scaled (astro) scale using:

\[
A(Q) = A(Q_{\text{astro}}) = A(Q_{\text{met}}) + C. \tag{8}\]

The factor \(C\) is determined by taking the average ratio of astronomical abundance (per \(10^{12}\) \(H\) atoms) per meteoritic abundance (per \(10^{12}\) \(Si\) atoms) from elements that span a wide range of properties to account for the chemical and physical differences between solar and meteoritic data. We refer the reader to Lodders (2019) and Lodders et al. (2009, specifically their Section 3.4.5), who provide an excellent explanation of this calculation and walk-through example. Magg et al. (2022) also explain an important caveat that converting meteoritic abundances to the \(H\)-scale imbues two uncertainty terms: one that is with respect to each abundance measurement (uncorrelated) and another that is associated with the conversion itself (systematic). Overall, this comparison is currently only possible for the Sun and therefore varies depending on the solar abundance measurement. We discuss the most popular solar abundances in more detail in Section 6, where we provide the \(C\) factor for each data set, where possible.

### 2.2. Scaling to Iron or Other Elements

For the purposes of comparison, it can be useful to scale elemental abundances with respect to another element, often iron. For example, iron is created from multiple events (such as Type I and Type II supernovae) that occur on different time frames; thus scaling an element to iron enables a more direct understanding of the production site and rate for that element (e.g., Tinsley 1980; Timmes et al. 1995; Kobayashi & Nakasato 2011; Hinkel et al. 2014 and references therein). We have chosen iron in subsequent equations for clarity and consistency with the literature, but note that in the following subsection all nonhydrogen elements can be substituted for iron in the formalism.

For general element, \(Q\), and iron, \(Fe\), with absolute abundance measurement \(Q/H = A(Q)\) and \(Fe/H = A(Fe)\) respectively, we define the stellar abundance scaled to iron, \(Q/Fe\), as

\[
Q/Fe \equiv Q/H - Fe/H
= A(Q) - A(Fe)
= \log_{10}(q) + A(H) - \log_{10}(fe) - A(H)
= \log_{10}(q) - \log_{10}(fe)
= \log_{10}\left(\frac{q}{fe}\right). \tag{9}\]

Substitutions from Equation (7) and then Equation (6) show the stellar abundance scaled to iron in terms of the number fractions \(q\) and \(fe\). By noting that that total mass of the star is the same for both elements, we also relate to the number densities for \(Q\) and \(Fe\), which are \(n_q\) and \(n_{fe}\), respectively. As the notation suggests and the calculation confirms, values for \(Q/Fe\) are independent of the absolute scale with respect to \(H\).

### 2.3. Solar Normalization

After scaling with respect to hydrogen or any other element, observed stellar abundances, \(\ast\), are often compared with solar abundances, \(\odot\). In dex-abundance-notation, a solar normalization is denoted with [ ] (which may have been introduced by Helfer et al. 1959). We will first consider the case where both solar and stellar abundance values are themselves normalized in reference to hydrogen (i.e., an absolute elemental abundance). We define the solar normalized abundances, \([Q/H]\), as

\[
[Q/H] \equiv \frac{Q_{\ast}/H_{\ast}}{Q_{\odot}/H_{\odot}}
= A(Q_{\ast}) - A(Q_{\odot})
= \log_{10}(q_{\ast}) + A(H) - \log_{10}(q_{\odot}) - A(H)
= \log_{10}(q_{\ast}) - \log_{10}(q_{\odot})
= \log_{10}\left(\frac{q_{\ast}}{q_{\odot}}\right). \tag{10}\]


The relation to number fractions $q_\ast$ and $q_\circ$ is given by a substitution from Equation (6). As with scaling to hydrogen, solar normalization is also an intuitive subtraction operation in log-space. In this notation, stars that have stellar abundances that are the same as the Sun will have $[Q/H] = 0.0$ dex.

As with absolute abundances, for solar normalized data we may need to examine general element $Q$ with respect to another element. For example, with respect to iron, $[Q/Fe]$, it is defined as

$$[Q/Fe] = \log_{10} \left( \frac{q_\ast}{fe_\ast} - \frac{q_\circ}{fe_\circ} \right)$$

This substitution from Equation (9), shows how $[Q/Fe]$ relates to the stellar number fractions, $q_\ast$ and $fe_\ast$, and solar number fractions, $q_\circ$ and $fe_\circ$. Here, again, $[Q/Fe] = 0.0$ dex means that the abundance ratio is the same as that in the Sun. There are many literature sources that have determined solar abundances and may have observed different elements and/or reported varying measured values—due in large part to differing techniques (see Section 6). Calculations of solar abundance, $Q_\circ/Fe_\circ = \log_{10} \left( \frac{q_\circ}{fe_\circ} \right)$, requires that the solar number fractions $q_\circ$ and $fe_\circ$ come from the same literature source. It is therefore not recommended that different solar normalizations be mixed together, for example in order to achieve wider element coverage, since it will impart systematic shifts between solar abundance values across measurements.

In addition, it may be useful to alter the solar normalization of an abundance measurement in order to, for example, have varying measured values—due in large part to differing techniques (see Section 6). Calculations of solar abundance, $Q_\circ/Fe_\circ = \log_{10} \left( \frac{q_\circ}{fe_\circ} \right)$, requires that the solar number fractions $q_\circ$ and $fe_\circ$ come from the same literature source. It is therefore not recommended that different solar normalizations be mixed together, for example in order to achieve wider element coverage, since it will impart systematic shifts between solar abundance values across measurements.

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To express the same concepts that we have outlined and it is important to understand the alternative notations to promote mathematical comprehension.

For example, while we have defined the absolute abundance of an element in Equations (6) and (7) as $A(Q)$, it may also be equivalently presented in other literature sources as $\log \epsilon (Q)$, $\log (Q)$, or $\log (Q_{ref,\lambda})$, where the subscript in the latter example specifies the rest-frame, radial-velocity-corrected wavelength of the line used to calculate the abundance, or 6158 Å in this case (e.g., Bertran de Lis et al. 2015). In this notation, $[Q/H] \equiv \log \epsilon (Q) - \log \epsilon (Q)$, where the latter term is the absolute value of $Q$ within the Sun (e.g., Shan et al. 2021). We also note that, for these alternative notations, all of the logs are implicitly base 10.

Equation (6) defines the absolute amount of an element $Q$ as the number of $Q$ atoms per $10^{12}$ H atoms, which may also be given as $\log_{10} (N_{Q}/N_{H}) + 12$. Similarly, Equation (11) can then be expressed as $[Q/Fe] = \log_{10} (N_{Q}/N_{Fe}) - \log_{10} (N_{Q}/N_{Fe})$, as seen in, e.g., Roederer & Barklem (2018) or Danielski et al. (2022).

3. Mass Fractions

For those not steeped in stellar minutiae, it is important to point out that the total amount of elements heavier than H and He, or “metals”, varies in stars. For the solar neighborhood ($\sim500$ pc or $\sim1630$ lt-yr from the Sun), most of the stars have between 0.1 and 3 times the heavy element content of the Sun. There are trends in the ratios of different elements with respect to overall heavy element content that are rooted in how elements are produced by stars over the course of Galactic history. For example, the ratio of Mg to Fe tends to go down as the total heavy element content increases. There is also a scatter in addition to those overall trends, such that Fe/Si may vary somewhat at a given heavy element abundance.

Theoretical discussions of stellar evolution and stellar interiors most frequently treat abundances in terms of mass fraction, $X_Q$, or nucleon fraction, $Y_Q$, which is determined from the mass fraction divided by atomic mass (equivalent to a mole fraction of nucleons). The mass fraction is simply the fraction of the total mass of a given amount of material made up by a given isotope, $X_Q = \frac{N_Q}{M_Q}$, where $N_Q$ is the number of atoms of isotope Q, $M_Q$ is the mass of isotope Q, $\rho$ is the mass density of the material, and $A_Q$ is Avogadro’s number. The difference between mass fraction and nucleon fraction is subtle. If nuclear reactions take place, $\rho$ is not conserved, even if there is no mass flux or change in volume, since some of the rest-mass energy of the reactants will be converted into the binding energy of the products (or vice versa in weak interactions and reverse reactions). Nucleon fraction is defined as $X_Q = \frac{N_A \rho_A}{\rho}$, where $A_Q$ is the atomic mass number. The nucleon density, $\rho_A$, is defined as

$$\rho_A \equiv \frac{1}{N_A} \sum_i A_i N_i$$

where we sum over all elemental (or molecular) species, $i$, in a star. Using the nucleon fraction, as opposed to the mass fraction, is more accurate for nuclear network calculations, because it correctly preserves the total mass-energy density and results in a more accurate equation of state. Thus it is typically used for modeling, but in general the effects are small and should never be measurable in the context of observed stellar abundances. For example, the maximum possible difference in mass excess of one atom of $^4$He = $4.86 \times 10^{-28}$ g, or 0.7% of the rest mass of an atom of H. For simulating a particular star, assuming a 1:1 equivalence between mass and nucleon fraction when creating initial model conditions is sufficient. This is why using $X$ interchangeably to denote both mass and nucleon
fraction is standard practice. The sum of mass or nucleon fractions \( \Sigma X_i = 1 \). A related quantity is \( Y_Q = \frac{Y_0}{X_0} = \frac{N_0}{\rho N_0} \), the mass fraction divided by atomic weight in AMU, or the ratio of the number of nuclei to the total number of nucleons in the system. \( Y_Q \) does not sum to one by definition.

A similar and somewhat confusing astronomical notation is \( X, Y, Z \), where \( X \) is the mass fraction of hydrogen, \( Y \) is the mass fraction of He, and \( Z \) is the total mass fraction of all other elements, also known as the metallicity. The mass fraction is defined such that \( X + Y + Z = 1 \). This notation is most frequently used in stellar astrophysics theory, because the heavy element content of the star is the second-most dominant effect on the stellar evolution (after mass). Historical paucity of multi-element abundance determinations has made the total metallicity, \( Z \), the default parameter considered in stellar modeling. Though the evolutionary effects are dependent on the detailed composition, the quoted \( Z \) usually implies a specific assumed set of abundance ratios. The notation is also frequently used in work on stellar populations, where comparisons are made with stellar model grids calculated with fixed \( Z \) values and/or observational limitations preclude detailed composition measurements. The metallicity is frequently expressed in two sets of units: one is the direct mass fraction of metals, such that \( Z = 0.015 \) is a mass fraction of heavy elements of 1.5%; the second gives the metallicity relative to solar, i.e., \( Z = 0.1Z_Z \) is one-tenth solar metallicity. This distinction is important, as the latter carries the implicit assumption that the proportions of each isotope are the same as they are in the Sun (see Section 6, also Table 7 in Lodders 2019 for the XYZ mass fractions from different solar normalizations). In reality, the abundance ratios can vary substantially from solar, and there are infinite combinations that can result in the same \( Z \). Different abundance ratios summing to the same \( Z \) can have substantial effects on the stellar evolution through modification of the opacity of the stellar material and on the initial composition of a protoplanetary disk.

It is worth noting at this point that the term “metallicity” is used observationally in a fashion similar to \( Z \). In this case, \( [M/H] \) is the dex-abundance-notation equivalent, where \( M \) is the sum of all elements heavier than He and follows the same rules as the general case, \( [Q/H] \) defined above. It is possible to convert between \( [M/H] \) and \( Z \) as described below for individual elements with one important caution: since \( [M/H] \) is inherently a number fraction and \( Z \) a mass fraction, the same \( Z \) made up of different proportions of various elements will yield different \( [M/H] \). As a simple example, it would take many more O atoms to make up 1% of a star’s mass than it would Fe atoms, meaning O would have a higher number fraction than Fe for the same mass fraction. Therefore converting directly from \( [M/H] \) to \( Z \) or vice versa requires choosing an assumed set of elemental abundance ratios; converting element by element for as many species as are measured gives a more precise result. A final complication is that the overall metallicity and \( [Fe/H] \) are often used interchangeably. This is primarily a historical convenience, since up until the last roughly twenty years, most stars with abundance information only had measurements of \( [Fe/H] \). It was therefore necessary to adopt a set of abundance ratios to address any other elements. Most often it was assumed that all elements scaled the same, such that the scaling of Fe would give the scaling for the total metallicity. It has become clear, however, that abundance ratios can vary substantially between stars with the same \( [Fe/H] \), so \( [M/H] \) must be treated as a distinct quantity. Still, it is common to see references in the literature discuss a star’s “metallicity” when they are really only referring to the star’s iron content, \( [Fe/H] \).

The simplest conversion from mass fraction to an observationally reported unit of measurement is the absolute abundance (also called atom number) or \( A(Q) \), as defined in Equation (2). However, even this first step is not straightforward. It is best to begin with \( Y_Q = A(Q) - \log_{10}(f_{\text{tr}}) \), where the normalization to hydrogen is \( f_{\text{tr}} = \Sigma N_A A_i \), or the sum of atom number times atomic number for all species in a star. But complications enter into the normalization to \( A(H) = 12 \) (see Section 2.1). It is tempting to calculate \( Y_Q \) for a star with a given \( [Q/H] \) as simply \( Y_Q = [Q/H] + A(Q) - 12 \). Changing the amount of any heavy element, however, changes the relative number of hydrogen atoms and therefore the normalization. Ideally \( f_{\text{tr}} \) would be recalculated for each star by summing all of the absolute measured abundances, but this is rarely practical given how sporadically elements are measured within stars. Failing this, the common strategy is to assume some increase in total metallicity and assume a coproduction rate of He with the total metals, or \( Y/Z \), to get the new normalization. Estimates of the \( Y/Z \) production rate are scattered and come from a wide variety of sources, including eclipsing binaries, late-type field stars, and H II regions (Ribas et al. 2000; Jimenez et al. 2003; Casagrande et al. 2007; Izotov et al. 2007), with a median value of 2.1 from literature determinations. For a star with a metallicity difference from solar, we see that \( \Delta Z = Z_{\odot} - Z \) and therefore \( Y = Y_\odot + 2.1 \times \Delta Z \). It follows that \( X = 1 - Z - Y \), from which the normalization can be determined as above. The best compromise available in most cases is to sum the measured elements, which under ideal circumstances constitute most of \( Z \), and use the empirical \( Y/Z \) and an assumed scaling of unmeasured heavy elements with measured species to determine \( f_{\text{tr}} \). We provide a more tangible example of these calculations for HIP 544 in Section 5.

### 4. Stellar Abundances to Molar Ratios

It is often more useful for fields outside of astronomy to use the stellar elemental abundance information in the form of moles or molar ratios. Therefore, we must step out of log-space and also remove the solar comparison implicit in the dex-abundance-notation. To convert the original measurement of \( [Q/H]_\star \) to moles \( Q_\star \), we use:

\[
Q_\star = 10^{Q_\star},
\]

\[
= 10^{Q_\star/H_\star}, \quad \text{then from Equation (10)},
\]

\[
= 10^{(Q_\star/H_\star + Q_\star/H_\star)}
\]

\[
= 10^{(Q_\star/H_\star + Q_\star)}, \quad (14)
\]

where \( Q_\star \) is the solar value used to normalize \( Q \).

In addition, while comparing \( Q \) to \( H \) and \( Fe \) are common techniques in the stellar abundance subfield to understand the chemistry of a star in the context of Galactic chemical evolution or with respect to the composition of stellar populations, other ratios may also be informative. Therefore, we introduce \( R \) as the hydrogen normalized stellar abundance of another element, where \( [R/H]_\star \) is the solar normalized...
abundance within the star for the R element. Now we are able to
define \( Q/R \) as the molar ratio of \( Q \) and R elements in the
star, such that:

\[
\frac{Q_*/R_*}{10^{Q_*/10R_*}} = \frac{10^{Q_*/H_*}}{10^{R_*}} = \frac{10^{Q_*/H_*}}{10^{R_*}} + \frac{10^{Q_*/H_*}}{10^{R_*}} + \frac{10^{Q_*/H_*}}{10^{R_*}},
\]

where \( R_* \) is the solar value for the R element that was
specifically used in the original measurement of \([R/H]_*\). We
discuss the various solar normalizations standard in the stellar
abundance community and how they compare in Section 6.

4.1. Propagating Errors to Moles

To determine the appropriate error propagation, we start with
the uncertainty of any function of one variable \( x \), or \( f(x) = y \). From
Taylor (1997, their Equation (3.23)), given that \( x \) is measured with
uncertainty \( \delta x \), then the uncertainty in \( y \), called \( \delta y \), is given by:

\[
\delta y = \left| \frac{dy}{dx} \right| \delta x,
\]

where \( \left| \frac{dy}{dx} \right| \) is the absolute value of the derivative of \( f(x) = y \).
We note that \( \delta x \) is half the total uncertainty of \( x \) or the plus/
minus error of \( x \), and thus it is a value that is nonzero and
positive.

The way that errors are reported for stellar elemental
abundances will vary depending on the methodology and/or team
who determined the measurements. For example, errors may
be reported on a star-by-star basis, i.e., “the carbon abundance
for HIP 100 is \([C/H] = 0.11 \pm 0.06 \text{ dex} \)” or from Equation (16),
\( \delta x = 0.06 \text{ dex} \). Alternatively, a general error may be given
for an element across all stars, i.e., “we estimate a total uncertainty
in \([N/H] \) of 0.08 dex,” or \( 2 \delta x = 0.08 \text{ dex} \). In the latter case, it is
assumed that the error distribution is centered around the
measurement such that the total uncertainty is equal to plus/
minus half the total uncertainty, or \( \pm 0.04 \) in our example.
However, propagating errors in the dex-abundance-notation is not
fully applicable because it is inherently in log-space and
normalized such that the Sun \( \pm 0.0 \text{ dex} \).

For error propagation, we have to work in the linear space,
namely Equation (14). Since we need to calculate a derivative,
we start by redefining Equation (14) as a more general power
law: \( y = 10^{y+c} \), where \( y = Q_*/[Q/H]_* \), and a constant
c = \( Q_*/Q_* \). Now we can rewrite \( Q_*/[Q/H]_* \) in terms of the natural number
e, and the natural logarithm \( \ln() \):

\[
y = Q_*/[Q/H]_* = Q_*(x) = 10^{y+c} = 10^y \times 10^c
\]

\[
\implies \ln(y) = \ln(10^y) + \ln(10^c) = \ln(10^y) + c \ln(10)
\]

\[
\implies y = e^{\ln(10^y) + c \ln(10)}.
\]

From here we can calculate the derivative of the power law
as:

\[
\frac{dy}{dx} = d(e^{\ln(10^y) + c \ln(10)})
\]

\[
= (\ln(10)^y + c \ln(10))^2
\]

\[
= \ln(10)^y.
\]

Applying the results of Equations (17) and (18) to
Equation (16) we are able to express fractional uncertainty \( \delta y \),
i.e., dividing the \( \delta \) error by the measurement value, as a function of \( \delta x \):

\[
\delta y = \left| \frac{dy}{dx} \right| \delta x
\]

\[
= \ln(10)^y \delta x
\]

\[
\implies \delta y = \ln(10)^y \delta x
\]

\[
\frac{\delta Q_*}{|Q_*|} = \ln(10)^y \delta [Q/H]_*.
\]

Given the definition of \( \delta [Q/H]_* \), which is half the total
uncertainty, Equation (19) will provide a plus/minus fractional
or percentage error (see Step 6 of Section 5). We also see that
the errors are not affected by the choice of solar normalization,
since the solar terms are no longer part of the equation.
Meaning, if we say that we have \([Q/H] = 0.0 \pm 0.05 \text{ dex} \),
that is the same as saying \( A(Q) = 7.46 \pm 0.05 \). Therefore, the errors
would be the same for \([Q/H] \) and \( A(Q) \).

Taking this a step further, we propagate the errors for two
elements in dex-abundance-notation, namely Equation (15).
The standard method for propagating errors is to convert
the total uncertainty to fractional uncertainty for both elements in the numerator (num) and denominator (denom) and then add those fractional uncertainties in quadrature:

\[
\sqrt{(\delta_{\text{num}})^2 + (\delta_{\text{denom}})^2}, \text{ per Taylor (1997, their Equation (3.47))}
\]

We therefore add the error in quadrature in order to get the fractional error of the molar ratio \( Q/R \):

\[
\delta Q_*/R_* = \sqrt{\left( \frac{\delta Q_*}{Q_*} \right)^2 + \left( \frac{\delta R_*}{R_*} \right)^2}
\]

\[
= \sqrt{(\ln(10)^y \delta [Q/H]_* + (\ln(10)^y \delta [R/H]_*))^2}
\]

\[
= \ln(10)^y \delta [Q/H]_* + \delta [R/H]_*
\]

We note that while Equation (20) is nearly identical to Equation (6) presented in Hinkel & Unterborn (2018, since \( \ln(10) \approx 2.303 \)), the results from Equation (6) were treated as
full uncertainties in moles when in reality the equation calculates fractional or percentage errors. As a result, the error
calculated relies on Table 5 of Hinkel & Unterborn (2018) were
all overreported. Therefore, it is our intention that the detailed
walk-through presented here that resulted in Equation (20) will
supersede what was presented in Hinkel & Unterborn (2018).
To provide an example walk-through for many of the equations we have discussed, we will examine HIP 544 (HD 166), a G8V-type star with $T_{\text{eff}} = 5400 \pm 100$ K (Soubiran et al. 2016; Linsky et al. 2020). We use the abundance values reported in the Hypatia Catalog for our calculations (Hinkel et al. 2014), since the Hypatia Catalog is the largest database of stellar abundances for stars within the solar neighborhood, currently containing 80 elements within $\sim$10,000 stars as compiled from +230 literature sources. Note that these values are used merely for performing an example calculation; no endorsement of the measurement from any particular source is implied. We will convert the stellar abundances of HIP 544 to the mass fraction of heavy elements, or $Z$, noting in Steps 1 and 2 then examine how changes in the abundance of one element affects $Z$ (Step 2 Caveat). Next, we will take the individual stellar abundances and renormalize to a different solar normalization (Step 3), then convert the denominator of the stellar abundances to be with respect to Fe (Step 4). In Step 5 we convert some of the abundance ratios to molar ratios and then propagate the errors in Step 6. The results of these example calculations, where applicable, are given in Table 1.

Step 1: The most straightforward way to calculate the $Z$ mass fraction is to first convert from [Q/H] to $A(Q)_{\odot}$. Equation (10) provides the conversion from [Q/H] to $A(Q)_{\odot}$, assuming a particular solar composition relative to which [Q/H] is measured. The example abundance data, [Q/H], is shown in Column 2 of Table 1, which uses the Lodders et al. (2009) solar composition for normalization—listed in Column 3, where the conversion to $A(Q)_{\odot}$ is provided in Column 4.

Step 2: Calculating $Z$ requires summing the absolute atom number of all of the isotopes in order to correctly account for the normalization. To do this, we use Equation (13) to determine $f_H$, such that $\sum_i N_A \cdot f_H = \sum_i (A(Q)_{\odot})A_i$.

The majority of elements, both measured in the Sun and on the periodic table in general, are not measured in a typical stellar abundance survey. In the best case, the unmeasured elements are low abundance species that will not change $f_H$ significantly. For example, $A$(Li) = 3.33 in the Sun, meaning that omitting Li from the calculation of $f_H$ would change its value in the eighth significant digit. By contrast, omitting C, where $A$(C) = 8.39, renders $f_H$ incorrect in the third significant figure. Therefore the precision of the normalization of H depends on what fraction (by mass or atom number) of the total heavy elements are measured. Lacking a value for an abundant element like C, N, or O thereby introduces significant uncertainty into the $A(Q)$ of other elements. For a precision of 1 in $10^{-4}$, using elements with $A(Q) > 5$ in the Sun would generally be sufficient.

The star HIP 544 provides some examples of the difficulties when determining the accurate metallicity without assuming fixed scaling to solar abundances, due to missing element measurements. Since Maldonado et al. (2015) do not report [N/H], the value provided in Table 1 is from a different survey than the rest of the elements (which was normalized to the same solar abundance). Abundance determinations from different surveys frequently display systematic differences larger than the quoted errors, so values are not always interchangeable (Smiljanic et al. 2014; Hinkel et al. 2016). Since N is one of the most abundant elements, a measured value is still to be preferred to an arbitrary value, even if there may be some systematic difference between survey techniques, hence the use of Brewer et al. (2016). In addition, there is no observational determination of [Ne/H] since the only available Ne lines are chromospheric lines in the UV. But neon is too abundant to be
neglected. We have the option of simply using the solar value (see different measurements discussed in Section 6), looking for a star of similar composition with an [Ne/H] measurement, or assuming it was produced in similar proportions to elements at least partially coproduced in nucleosynthetic contexts. For illustrative purposes, we will use the last option, taking an intermediate value between [O/H] and [Mg/H] of [Ne/H] = 0.10 dex. The abundances derived from neutral and singly ionized Cr lines differed (see Section 7.1), both provided by Maldonado et al. (2015) and were within error bars, so we chose to use the median value of the two.

The biggest complication in calculating \( f_H \) is the change in He abundance. Helium is very rarely measured in stars, so we assume coproduction with metals, with \( \Delta Y = 2.1 \Delta Z \) as discussed in Section 3. Taking \( \sum \Delta Y = 10^{4(A(Q)_{\odot})} A_i \), the sum increases by 32% over solar. Using the Lodders et al. (2009) value for \( Z_\odot = 0.0154 \), we can estimate that \( \Delta Y = 2.1 (0.32 \times 0.0154) = 0.0104 \). Ideally, \( Y \) would be calculated iteratively with the renormalized values of \( Y \) for the heavier elements, using this value of \( Y \) as a starting point for the calculation. (Similarly for the lacking N value, one could scale N by a factor \( f_{2 \Delta Z} \) as we have done with He, since both are produced primarily in CNO cycle H burning. Analogous strategies can be used for other elements.)

For HIP 544, the resulting \( f_H \approx 12.187 \). For the Lodders et al. (2009) solar composition, \( f_H \approx 12.149 \). For each element, \( Y_\odot = A(Q) - \log_{10} f_{11} \), and mass fraction \( X_Q = Y_\odot \times A_Q \). Mass fraction \( X_Q \) is typically quoted in the literature instead of \( Y_\odot \), as it is more intuitive. Mass fractions \( X_Q \) are shown in Column 5 of Table 1. However, \( Y_\odot \) is inherently produced by the conversion and is useful for nucleosynthetic calculations, as discussed in Section 3. The \( Y_\odot \) values are shown in Column 6 as calculated from \( X_Q/A_Q \) using the atomic weights on the standard periodic table. The total metallicity of the star \( Z \approx 0.0184 \).

An additional item of note is that the values of \( A(Q)_{\odot} \) used in this example are the recommended primordial solar values of Lodders et al. (2009), not the present-day photospheric values (Section 6). Since HIP 544 is a young star, the measured abundances should reflect the bulk abundances of the star fairly close. Such is not the case for the average few-gigayear-old field star. The abundances of He and heavier elements in the photospheres of stars decrease relative to their total stellar abundance over time. Gravitational settling results in heavier elements sinking toward the core of a star. This is partly counteracted by radiative levitation, in which momentum of photons captured by atomic transitions drives atoms outwards. Both processes depend on atomic number \( Z \). The picture is further complicated by advective processes (e.g., convection, rotation, and internal waves) that transport material from one part of the star to another. The settling process takes place on long timescales, so the effect is minimal for massive stars or young low-mass stars. In the Sun, the present photospheric \( Z \) is \( \approx 10\% \) less than the bulk solar composition. For the purposes of stellar evolution calculations and inferences about the composition of protoplanetary building blocks, the bulk/primordial composition of the star is the relevant quantity. In order to derive primordial compositions from measurements, stellar models with adjusted initial compositions must be run iteratively until the predicted photospheric abundances match the observed values at the current stellar age.

Step 2 Caveat: In many cases, \( Z \) is assumed to scale with [Fe/H], which is often a necessary assumption because only the [Fe/H] abundance is known. But variations in the [Q/Fe], even on the level seen in the solar neighborhood, can have dramatic effects. To illustrate, we will use O as an example element (with a note that the process applies to all species) given the measured quantities [O/H] = 0.09 dex, \( A(O_{\odot}) = 8.73 \) dex, and \( A(O_{\odot}) = 8.82 \) dex. The primary effect on stellar evolution from changing metallicity is due to the change in opacity of stellar material as heavier elements with more electron transitions are added. Since O is the most abundant element after He, changing its abundance can have substantial evolutionary effects. Analysis using individual, self-consistent surveys to remove systematic scatter show that [O/Fe] at a given [Fe/H] can vary by more than a factor of 2 in either direction. To show the effect on \( Z \) from this level of variation, we recalculate the \( Z \) of HIP 544 with the abundance of O increased by a factor of 2, keeping other species the same and renormalizing to H. In this case, since \( \log_{10}(2) \approx 0.30 \), then \( A(O_{\odot}) = 9.12 \) dex. The new value gives \( f_H = 12.191, X_Q = 0.0154 \), and \( Z = 0.0260 \). This is a very substantial change in \( Z \) with only a tiny change in [Fe/H] (due to the change in the number of H atoms). A star with \( Z = 0.026 \) because of an enhancement in Fe, since Fe provides more opacity per gram than O. Planet formation would similarly be different for the two cases due to the difference in oxidation state and stoichiometry of mineral building blocks. Therefore using Z (or [Fe/H]) as a fundamental parameter without specifying the detailed composition is theoretically inadequate, even if often necessary. When given the option, it is always preferable to use the specific abundances measured within a star, especially those from a variety of nucleosynthetic origins.

Step 3: Instead of considering the heavy elements in bulk, we now walk through our HIP 544 example with respect to the individual elements to convert to a different solar normalization. The abundances provided in the Column 2 of Table 1 are normalized to the Lodders et al. (2009) solar measurement. Using Equation (12), we can renormalize the measurements with respect to the Grevesse et al. (2007) solar measurement, which is provided in Column 7. The renormalized [Q/H]_{G07} abundances are shown in Column 8.

Step 4: The second step of Equation (9) shows us how to compare \( Q \) to an element other than H and change the denominator, for example \( [Q/Fe] = [Q/H] - [Fe/H] \). We perform this operation on Column 8 of Table 1 in order to produce Column 9, [Q/Fe]_{G07}. We note that the [Fe/Fe] value was left blank.

Step 5: We switch now from the dex-abundance-notation to calculate molar ratios using Equation (15), where Mg is the comparison element, or R term. Continuing with the data that are normalized to Grevesse et al. (2007), we use Column 8 of Table 1 as [Q/H]_{G07} and Column 7 for \( A(Q)_{\odot} \), where [Mg/H] = 0.12 dex is \( [R/H]_{\odot} \) and \( A(Mg_{\odot}) = 7.53 \) dex is \( A(R)_{\odot} \). We calculate the molar ratios with respect to Mg in Column 10, \( Q/Mg_{G07} \), where the Mg/Mg entry was left blank. To show that the molar ratios are irrespective of solar normalization, we perform the same calculation again, but using Columns 2 and 3, respectively, where \( [R/H]_{\odot} = [Mg/H] = 0.11 \) dex and \( A(R_{\odot}) = A(Mg_{\odot}) = 7.54 \) dex. The Q/Mg molar ratios calculated from the Lodders et al. (2009) solar normalization are shown in Column 11, where we see that they are identical to the calculation from Grevesse et al. (2007) in Column 10.
Table 2
Equation Takeaway from the Section 5 HIP 544 Example

| Step | Description | Relevant Equations | Alternate Notations and Notes |
|------|-------------|--------------------|-------------------------------|
| 1    | Convert from [Q/H] to A(Q) using the solar composition | A(Q) ≡ absolute stellar abundance to H | log ε(Q), log(Q), log(Q), log(Q)/N(H)/N(H), 12 |
|      |             | [Q/H] ≡ Q_ρ /H_ρ - Q_ρ /H_ρ = A(Q)_ρ - A(Q)_ρ, normalized abundance to H | [Q/H] ≡ log ε(Q) - logε(Q) |
| 2    | Calculate the Z mass fraction | ρ_A = Σ_i A_i, nucleon density for species i, q ≡ number fraction, h ≈ 1, number fraction for hydrogen | X_q = Y_q × A_q, mass or nucleon fraction |
| 3    | Renormalize to different solar composition | [Q/H]_1 = [Q/H]_1 + A(Q)_ρ,1 - A(Q)_ρ,2 | There are dozens of solar abundance determinations |
| 4    | Change abundance ratio denominator | Q/Fe ≡ A(Q) - Fe/H, absolute normalized to Fe | [Q/Fe] ≡ log(N(Q)/N(Fe)) - log(N(Q)/N(Fe)) |
| 5    | Calculate molar ratios | Q_ρ /R_ρ = | log(10)δ[Q/H]_ρ*log10(Q/[H])_ρ | Determines fractional (percent) error. Using half of the total δ errors yields half (±) the total δQ/R error |
| 6    | Propagate errors to molar ratios | δQ/R = ln(10)δ[Q/H]_ρ + δ[R/H]_ρ | Due in part to the validation of solar abundances to meteoritic composition, which is not possible for any other star, the Sun is used as a comparison against which the elements within other stars in the Galaxy are compared. However, this comparison presumes that the Sun is a typical star with a composition that is similar to other G-type stars of similar age within the solar neighborhood. However, this assumption may not be entirely true given studies by, e.g., Meléndez et al. 2009, Ramírez et al. 2009, and Bedell et al. 2018, who found that the Sun is rich in volatile elements (which have a condensation temperature T_C < 900 K, such as C, N, and O) and deficient in refractory elements (T_C > 900 K, such as Na, P, and Si)—which may have been segregated into planets. In addition, it is also expected that because the solar abundances are so often measured they are also well measured, namely, that different solar abundance studies agree. Currently, the Hypatia Catalog (Hinkel et al. 2014) features ∼75 individual solar abundance determinations—from dedicated studies of the Sun, to line-by-line differential analyses, to those that determine their solar normalization by using the spectra of asteroids such as Ceres or Vesta. The variation among all of these different solar abundance measurements can be quite large. For example, the range across all Hypatia Catalog solar normalizations for two of the most commonly measured elements, Si and Fe, are ∆0.28 and ∆0.26 dex, respectively, in comparison to typical errors, which are ±0.05 and ±0.04 dex, respectively. So, it is important to the overall abundance study which solar normalization is employed (see Jofré et al. 2015; Hinkel et al. 2016 for a deeper explanation as to other possible discrepancies). In comparison, the range for Si, Fe, and most other elements between data sets that specifically focus on the composition of the Sun is much smaller. This is because solar abundance studies require a huge amount of effort and are a dedicated subfield within the stellar abundance community. Various teams often publish solar abundance determinations, only to... |

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6 In light of some of the topics/authors discussed here, we would like to acknowledge our support of a harassment-free research environment. We strongly believe in, and actively take steps to ensure, an open, inclusive community that allows researchers at any stage of their career and from all backgrounds to be welcome and supported.

...
make improvements on them a few years later. In an effort to inform nonexperts of the differences between standard solar normalizations so that they may determine which is best for their research application, we provide a brief overview of the most common solar abundance normalizations used within the literature (in chronological order):

Anders & Grevesse (1989): While not the first solar normalization ever published, this is one the oldest normalizations still in modern use. Its favor may be in part because the solar abundances were compiled from abundances found within CI-chondrites, the solar corona, and the solar photosphere—which were predominantly from Grevesse (1984) and Grevesse et al. (1984). For Equation (8), their $C = 1.554 \pm 0.020$.

Grevesse & Sauval (1998): This is an additional compilation of solar abundances, where the photospheric values were derived within Grevesse et al. (1996) and have notably larger uncertainties compared to the meteoritic data. While element abundances from the solar photosphere and meteorites all agree to within the (large) error, it was noted that “the solar photosphere is never at fault. Past errors have been shown to be due to errors in atomic or molecular data.” With that in mind, the continued use of Grevesse & Sauval (1998) may be attributed to more accurate line transition probabilities, which markedly reduced the differences between abundances from the Sun and CI-chondrites.

Lodders (2003): One of the most highly cited solar abundances in the last thirty-plus years, this solar abundance compilation not only provides a variety of photospheric abundances, but also compares the abundances from five different CI-chondrites and computes their weighted average compositions. The final recommended values for the solar normalization (their Table 1) carefully combines both the photospheric and meteoritic data. In addition, they provide the composition of the proto-Sun and early solar system, i.e., from $4.55 \times 10^9$ yr (Gya) ago. For Equation (8), their $C = 1.539 \pm 0.046$.

Asplund (2005): While the previous photospheric measurements of the Sun were determined using 1D hydrostatic models, this was the first comprehensive 3D hydrodynamic model of the solar atmosphere. As a result, it substantially changed the C and O photospheric abundances, which were considerably higher than those found in meteorites, and brought them into much better agreement. Unfortunately, the updated model also resulted in some issues with respect to other elements (namely, Na, Al, and Si) and created issues matching to helioseismology data and standard solar models that represent the evolution of the Sun.

Grevesse et al. (2007): This solar abundance measurement is an extension of the previous Grevesse & Sauval (1998) determination but using the 3D hydrodynamic model referenced in Asplund (2005). The authors noted, though, that the updated abundances were predominantly the result of updated atomic data and more a realistic treatment of nonlocal thermodynamic equilibrium (or NLTE, see Section 7.2), as opposed to the improved 3D model of the solar atmosphere. For example, they were better able to match helioseismology data. Interestingly, despite the fact that this solar abundance measurement is about fifteen years old, it has gained popularity as a solar normalization within the literature in the last five years or so.

Asplund et al. (2009): The abundances determined for the Sun in Asplund et al. (2009) are notably the most commonly used values for solar composition, easily making up $\sim 50\%$ of the solar normalizations for abundance measurements within the Hypatia Catalog. Improvements in the solar model as well as atomic and molecular data resulted in better agreement for the refractory elements between the solar photosphere and the CI-meteorites. Differences with helioseismology data and the standard solar model were also greatly improved.

Lodders et al. (2009): These solar abundances are an update from their earlier measurement where new data from meteorites, the solar photosphere, and theoretical models are included. Most notably, the photospheric solar abundances were improved and are distinctly lower compared to those of Lodders (2003). In addition, developments in instrumentation allowed for new trace elements to be measured within the CI-chondrites. Combined recommended solar abundances for the present day and at the beginning of the solar system (4.56 Gya) are provided. For Equation (8), their $C = 1.533 \pm 0.042$.

Lodders (2019): Provided here are updated solar abundance values, including from CI-chondrite data and an He estimate determined from helioseismology, as well as an extremely thorough review of solar elemental abundances. In addition, abundances determined from meteoritic compositions, CI-chondrites, the solar photosphere, and the solar corona/wind, overall solar system abundances, and mass fractions are compared among all major literature measurements to date, including references discussed here and more.

Asplund et al. (2021): A continued extension of previous solar abundance determinations from the same first author, there is a useful comparison between their different papers in their Table 1. The biggest change introduced in this paper is the greater accounting of full 3D NLTE dynamics (see Section 7.2) for a wide variety of elements. However, it was noted that the “modeling problem—a persistent discrepancy between helioseismology and solar interior models ... remains intact with our revised solar abundances.” See also Magg et al. (2022) for a thorough determination of NLTE solar abundances (i.e., C, N, O, Mg, Si, Ca, Fe, and Ni) using the most up-to-date atomic/molecular line data, NLTE model atoms, and varying solar model atmospheres.

7. Discussion and Additional Considerations

Relating the composition of the host star to the interior structure and mineralogy of a planet is a complicated task, involving a variety of physical and chemical processes. The endeavor is made more difficult by the need to bridge interdisciplinary fields and the realization that different scientific applications benefit from presenting data in a variety of ways. Stellar spectroscopists normalize data to universal quantities, such as H, while comparing the results to our nearest star. By contrast, geochemists, petrologists, and mineral physicists who study the interior chemistry, mineralogy, and phase equilibria of rocky planets normalize abundances to the most prevalent element in Earth’s crust, i.e., Si, and refer to abundances in terms of molar ratios or weight percent oxides.

It is equally important to create a common lexicon for interdisciplinary data notation, as well as to make the raw data products accessible from stellar abundance astronomers so that geochemists/geophysicists have the required context to understand complex exoplanet geochemical cycles. An excellent biologically driven example is phosphorus, which is fundamental to DNA, RNA, and ATP and therefore required to be on the planet’s surface in some significant amount, yet it has only been measured in $\sim 260$ stars (Hinkel et al. 2020; Maas et al. 2022). Therefore, in order to model the most influential planetary rocks and minerals, stellar spectroscopists should
focus their attention on measuring stellar elemental abundances that are necessary for building and modeling planet interiors: the “Major Elements” O, Mg, Al, Si, K, Ca, and Fe; the “Minor Elements” C, Na, P, S, and Ni; and key contributors to radioactive heat production (or their daughter products): ⁴⁰K, ²³²Th, and ²³⁵,²³⁸U (Hinkel & Unterborn 2018). To aid in further clarification of influential nuances within the stellar abundance field, we thought it necessary to discuss the standard practice of measuring lines from different ionization states (Section 7.1) and explain the use of stellar models that depart from LTE (Section 7.2).

7.1. Ionization States

It is easier to achieve a more robust abundance determination from a star’s spectrum when there are numerous elemental (or molecular) lines within the observed wavelength range. A variety of lines means an observer is more likely to identify strong lines that are free from blends, temperature sensitivity, Zeeman splitting, and other issues, which will yield consistent line-by-line results. While many lines may not always be available, spectroscopists will often examine neutral as well as ionized lines of a given element.

An element is ionized when it has either gained an electron and has a negative charge (anion) or lost an electron and has a positive charge (cation). In chemistry, when an element can form multiple cations, they are indicated by roman numerals, where Cu⁺⁺ is identified as Cu II. However, in the same way that astronomers have bogarted the definition of “metals,” they, too, have refashioned this notation such that a neutral Ti atom is signified as Ti I, while Ti II “means the singly ionized atom, i.e., the atom with one electron entirely removed” (Millikan & Bowen 1924) or Ti⁺. Similarly, though not as common, lines may also be doubly (e.g., Ti III) or triply (e.g., Ti IV) ionized. While potential confusion is understandable with this specific notation, especially to those from outside the field of astronomy, it is clear that historical precedent is at fault. Regardless of the notation, comparing the results from neutral and ionized lines can be informative. Many stellar abundance techniques vary the stellar parameters (T, log g, and [Fe/H]) within their models in order to compare the abundances from Fe I to Fe II lines (Jofré et al. 2015; Hinkel et al. 2016; Jofré et al. 2019). Iterations of the stellar parameters are continued until an ionization and excitation equilibrium is found within the star, or when the Fe I and II abundances yield the same result. And because it is expected that the neutral and ionized lines will yield similar abundances, many spectroscopists often use a combination of lines from different ionization states when determining the overall abundance of an element. It is for this reason that the Hypatia Catalog denotes an element as [X II]/[H] when it is computed only from singly ionized lines, whereas [X/H] could mean that it comes from neutral lines or a combination of neutral and ionized lines.

7.2. Nonlocal Thermodynamic Equilibrium (NLTE)

Many stellar models often assume local thermodynamic equilibrium (LTE) within the interior of the star, where small pockets are considered to be in a well-defined steady-state condition that is thermally isolated. However, these assumptions are not always applicable to the stellar atmosphere and may result in fluctuations in spectral line strengths and changes in overall line shape (Lodders 2019). Unfortunately, NLTE calculations require extensive lab data—such as NLTE atomic models and line transitions for every line of the element (Grevesse et al. 2007), as well as computationally expensive stellar atmosphere models to account for the additional physical processes.

While NLTE calculations may be difficult, they are important for resolving major abundance discrepancies. For example, the differences between abundances from the solar photosphere versus chondritic meteorites discussed in Section 6 were greatly reduced when accounting for NLTE corrections. Effects from NLTE may also result in an ionization imbalance (per Section 7.1), or when calculations using neutral and singly ionized lines result in markedly different elemental abundances that cannot be reconciled by varying stellar parameters (e.g., Allende Prieto et al. 2004 and references therein). Not only may departures from LTE impact metal-poor or evolved stars, but there are specific elements, such as Li and K, that require large (>0.4 dex) NLTE corrections to improve their overall accuracy (e.g., Lind et al. 2009 and Zhao et al. 2016, respectively).

Finally, we should note that, unlike measurements from different ionization states (Section 7.1), it is not recommended that abundances derived from LTE and NLTE calculations be combined (e.g., averaged) to determine an overall abundance for a single element. Namely, the physics underlying NLTE calculations is dissimilar enough to LTE that it makes the results separately comparable, but not equivalent. The best practice, therefore, is to treat LTE and NLTE abundance measurements as independent.

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