Open-ended versus bounded evolution: Mineral evolution as a case study

Robert M. Hazen [ID][a,*] and Michael L. Wong [ID][a,b]

[a]Earth and Planets Laboratory, Carnegie Institution for Science, 5251 Broad Branch Road NW, Washington, DC 20015, USA
[b]NASA Hubble Fellowship Program, Space Telescope Science Institute, Baltimore, MD 21218, USA
*To whom correspondence should be addressed: Email: rhazen@carnegiescience.edu
Edited By: Harry McSween

Abstract

To what extent are naturally evolving systems limited in their potential diversity (i.e. "bounded") versus unrestricted ("open-ended")? Minerals provide a quantitative model evolving system, with well-documented increases in mineral diversity through multiple stages of planetary evolution over billions of years. A recent framework that unifies behaviors of both biotic and abiotic evolving systems posits that all such systems are characterized by combinatorial richness subject to selection. In the case of minerals, combinatorial richness derives from the possible combinations of chemical elements coupled with permutations of their formulas' coefficients. Observed mineral species, which are selected for persistence through deep time, represent a miniscule fraction of all possible element configurations. Furthermore, this model predicts that as planetary systems evolve, stable minerals become an ever-smaller fraction of the "possibility space." A postulate is that "functional information," defined as the negative $\log_2$ of that fraction, must increase as a system evolves. We have tested this hypothesis for minerals by estimating the fraction of all possible chemical formulas observed from one stage of mineral evolution to the next, based on numbers of different essential elements and the maximum chemical formula complexity at each of nine chronological stages of mineral evolution. We find a monotonic increase in mineral functional information through these nine stages—a result consistent with the hypothesis. Furthermore, analysis of the chemical formulas of minerals demonstrates that the modern Earth may be approaching the maximum limit of functional information for natural mineral systems—a result demonstrating that mineral evolution is not open-ended.

Keywords: evolution, open-ended evolution, complex systems, functional information, mineral evolution

Significance Statement

The mineral kingdom is an example of a nonliving system that has systematically increased in diversity and complexity through Earth's 4.56-billion-year history. As such, mineral evolution provides a case study for a proposed model of evolving systems called the "law of increasing functional information"—the proposition that all evolving systems display increasing "functional information" as a consequence of selection. In the case of minerals, functional information is shown to increase monotonically through nine periods of Earth history. Furthermore, the information approaches an upper limit—a result that implies Earth's mineral evolution is "bounded," in contrast to some models of life's evolution as an unbounded or "open-ended" process.

Introduction

A key attribute of naturally evolving systems—i.e. systems that display sequential increases in diversity and patterning—is the extent to which they are "bounded," that is restricted in their potential diversity, versus "open-ended" and thus without such a limitation (1–5). An untested hypothesis is that some abiotic evolving systems (i.e. isotopes or minerals) are limited in the extent to which they can continue to complexify, whereas life and its byproducts (including technology) may be unrestricted in the degree to which they can become increasingly complex. This idea, which connects to other hypotheses in this domain, notably the predictions of Assembly Theory that abiotic processes cannot generate numerous identical copies of molecules of extreme complexity (6–8), has important implications regarding cosmic evolution and possible future evolutionary pathways.

Wong et al. (9) suggest that all evolving systems share three conceptually equivalent traits: (i) They form from numerous components (i.e. atoms, molecules, cells) that can be arranged in combinatorially large numbers of configurations; (ii) processes exist that generate large numbers of those configurations; and (iii) selection for one or more advantageous functions winnows the number of "surviving" configurations. Wong and colleagues further propose that functional information (10, 11) provides a metric for the increase in diversity, patterning, or "complexity" of such a

system. In brief, functional information (measured in bits), $I(E_x)$, is the negative $\log_2$ of the fraction of all possible configurations that achieves a degree of function, $F(E_x)$:

$$I(E_x) = -\log_2 [F(E_x)]. \qquad (1)$$

That fraction, $F(E_x)$, in most cases of interest is minute.

An important conclusion of Wong et al.'s study is a proposed law of evolving systems—the law of increasing functional information: "The functional information of a system will increase (i.e. the system will evolve) if many different configurations of the system are subjected to selection for one or more functions" [9]. In this formulation, evolution is viewed as a process of increasing information that is driven by selective pressures on a system of many interacting components. A key consequence is that selection for function causes an increase in system information—a temporally asymmetric arrow of increasing order that is not derivable from the second law of thermodynamics' increase in entropy.

Mineral evolution, which considers Earth's changing diversity and distribution of minerals at a planetary scale through deep time, provides an important quantitative test of these ideas. Mineralogical changes result from new mineral-forming environments as a consequence of emerging physical, chemical, and ultimately biological processes [12–15]. Mineral evolution can be modeled as a sequence of congruent stages, each of which expands the repertoire of mineral-forming mechanisms [14–17]. As such, the mineral kingdom represents a complex system that shares many characteristics with other evolving systems, both biotic and abiotic [18, 19].

It is important to note that functional information, as applied to minerals or other evolving systems, is conceptually different from calculations of chemical or structural complexity of minerals as introduced by Krivovichev [20–22]. In particular, the systematic increase in these measures of mineral complexity through geological time [23–25] does not imply a similar increase in functional information. The functional information of a system is context dependent and therefore not equivalent to the Kolmogorov information required to describe that system.

Mineral evolution and functional information

An important and potentially testable prediction of the Wong et al. framing of evolving systems is that any evolving system under continued selective pressure will display an increase in functional information. Rigorous calculations of functional information for many natural systems, especially living systems, are untenable at present. It is not possible in such instances to enumerate every possible configuration of molecules or cells, much less to determine the degree of function of each configuration. Furthermore, living systems display several concurrent levels of configurations: Elements form biomolecules; biomolecules form macromolecules; and macromolecules form subcellular structures, which in turn form cells, multicellular organisms, and ecosystems. However, in the case of minerals a semiquantitative evaluation of the changing functional information of suites of minerals at different stages of Earth's mineral evolution is possible. As such, minerals provide an important abiotic test of the law of increasing functional information.

The principal objective of this contribution was to estimate the functional information of nine different suites of minerals arranged chronologically, based on mineral cohorts that have been cataloged in the twelve parts of the "evolutionary system of mineralogy" [13, 15, 26–33]. These estimations rely on several

assumptions that underlie our calculations of the functional information of mineral systems:

1. The components of minerals are the mineral-forming elements, which can be combined in combinatorially large numbers of different configurations and ratios, as represented by their chemical formulas.
2. The "function" of an individual mineral species is stability (i.e. static persistence), which is the most basic function of an evolving system [9]. If a mineral survives long enough to be approved as a "species" by the International Mineralogical Association's (IMA's) Commission on New Minerals, Nomenclature, and Classification (CNMNC) [34–36], then it has achieved this most basic of functions. It is important to note that it is inherently more difficult for minerals from earlier stages of cosmic evolution to survive to present and be cataloged as mineral species. As Bermanec et al. [37] show, the evolution of mineral hardness reveals both changing parageneses and preservational bias. Due to preservational bias, the functional information that we estimate for earlier stages of mineral evolution is potentially too high. As we shall see, this observation supports our claim that the functional information of minerals has increased over geologic time.
3. At each stage of Earth's mineral evolution, the number of possible formula configurations is defined by the number of combinations of chemical elements multiplied by the number of permutations of the coefficients, as represented by the cumulative mineral inventory through that stage.
4. The functional information of the mineral system at each stage of mineral evolution is defined as the negative $\log_2$ of the fraction of all possible chemical configurations that are observed to occur cumulatively during that and prior stages.

Examples from nine sequential time periods spanning 4.56 billion years of Earth history serve to clarify these assumptions. In the following sections, "Part" refers to the published or in-preparation sequential parts of the 12-part evolutionary system of mineralogy [13, 15, 26–33].

Part I—The "ur-minerals" (> 4.6 Ga): The earliest minerals in the universe formed as high-temperature condensates in the expanding, cooling atmospheres of old stars. A comprehensive catalog of the stardust minerals, which appears in Part I of the evolutionary system of mineralogy, reveals 27 known mineral species (Table 1 in 26). These minerals are composed of 16 different chemical elements (Figure 1a in 26). Furthermore, the maximum number of elements in any one mineral is 4 [for example, in olivine; $(Mg, Fe)_2SiO_4$], while the maximum formula coefficient is 19 [in hibonite; $CaAl_{12}O_{19}$]. Determination of functional information therefore requires application of combinatorial and permutational mathematics in four steps:

1. Calculate the total number of combinations, C, of $k = 1$ to 4 different elements (out of $m = 16$ possibilities) with no element repeating. The general formula for the number of ways to select k different objects from a set of m objects is:

$$C(k, m) = m!/[(m - k)! \times k!]. \qquad (2)$$

A familiar example of this calculation is the number of possible five-card hands that can be drawn from a 52-card deck (the answer is 2.6×10^6; see, for example: https://www.calculatorsoup.com/calculators/discretemathematics/combinations.php, accessed 2024 March 4).

Table 1. Parameters related to the functional information of mineral systems for nine periods of Earth's mineral evolution.

Part	Age (Ga)	M	m	k	n	$C_{k,m}$	$C_{k-1,m}$	P'_k	P'_{k-1}	$(C \times P')_k$	$(C \times P')_{k-1}$	FI (bits)	Refs.
I	> 4.6	27	16	4	19	1,820	560	85,954	4,860	1.6×10^{8}	2.7×10^6	22.5	(26)
II	> 4.565	59	23	7	19	2.5×10^5	1.0×10^5	2.5×10^8	0.2×10^8	6.3×10^{13}	0.2×10^{13}	40.0	(27)
III	> 4.561	96	29	7	36	1.6×10^6	0.5×10^6	4.2×10^{10}	0.1×10^{10}	6.7×10^{16}	0.5×10^{15}	49.3	(28)
IV	> 4.560	141	34	8	36	1.8×10^7	5.4×10^6	1.2×10^{12}	4.2×10^{10}	2.2×10^{19}	2.3×10^{17}	57.2	(29)
V	> 4.550	296	42	8	71	1.2×10^8	2.7×10^7	4.3×10^{14}	6.7×10^{12}	5.2×10^{22}	1.8×10^{20}	67.3	(30)
VIA	> 4.370	442	48	10	72	6.5×10^9	1.7×10^9	1.9×10^{18}	3.1×10^{16}	1.2×10^{28}	5.3×10^{25}	84.5	(31)
VIB	> 4.0	883	61	11	72	4.2×10^{11}	9.0×10^{10}	1.2×10^{20}	1.9×10^{18}	5.0×10^{31}	5.3×10^{29}	95.5	(16, 31)
VII, VIII	> 2.5	3759	68	12	123	7.3×10^{12}	1.5×10^{12}	6.9×10^{24}	6.2×10^{22}	5.0×10^{37}	9.3×10^{34}	113.3	(32, 33)
IX to XII	0	9300	72	15	135	1.2×10^{15}	2.4×10^{14}	4.0×10^{31}	3.7×10^{29}	4.8×10^{46}	8.9×10^{43}	138.6	(13, 16, 38, 39)

Part, the part number of the evolutionary system of mineralogy; M, the cumulative number of different mineral species; m, the number of different essential chemical elements in mineral formulas; k, the maximum number of elements in a chemical formula; n, the maximum coefficient in a chemical formula; $C_{(k, m)}$, the number of combinations of k elements from a set of m elements (see Eq. 2); $C_{(k-1, m)}$, the number of combinations of $(k-1)$ elements from a set of m elements (see Eq. 2); $P'_{(k, n)}$, the number of permutations of k coefficients with a maximum coefficient of n (see Eqs. 3 and 4) (note that $P' \sim P$ for $k > 5$); $P'_{(k-1, n)}$, the number of permutations of $(k-1)$ coefficients with a maximum coefficient of n (see Eqs. 3 and 4); FI, the functional information (in bits), based on the fraction of all possible mineral formulas that are observed (see Eqs. 1 and 5).
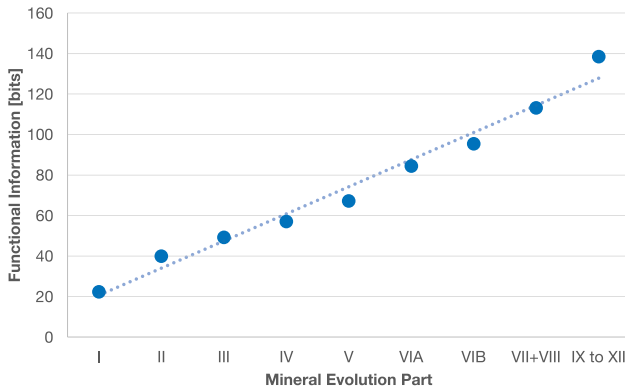
Fig. 1. A plot of functional information (in bits; see Table 1) versus the 12 sequential "Parts" of the evolutionary system of mineralogy reveals a significant monotonic increase in the functional information of evolving mineral systems through Earth's 4.56-billion-year history.

2. Calculate the number of permutations, P, of coefficients from 1 to 19 for combinations of 1 to 4 elements. Note that the general formula for the number of permutations of k objects from a set of n objects is:

$$P(k, n) = n!/(n-k)! \tag{3}$$

(see https://www.calculatorsoup.com/calculators/discrete mathematics/permutations.php, accessed 2024 March 4).

3. In the case of chemical formulas, an additional step may require consideration because of redundant combinations of coefficients with a common factor, which are therefore reduceable (i.e. the three-element formulas $X_2Y_4Z_6$ or $X_3Y_6Z_9$ are equivalent to XY_2Z_3). The corrected value of number of nonequivalent permutations, P', is a function of k:

$$P' \sim P \times \left\{ 1 - \sum_{2}^{n} [(1/k^n) \times (n/k^{n-1}) \times [(n-1)/k^{n-2}]] \right\}, \tag{4}$$

where values of n are restricted to prime numbers. Thus, for example, for any system of $k = 2$ elements, the total permutations of coefficients P are reduced by approximately $[1/4 + (1/9 \times 3/4) + (1/25 \times 3/4 \times 8/9) + \ldots] \times P \sim 0.36 \times P$. This sequence can be understood as follows: 1/4 of all coefficient pairs will be even–even and thus redundant. In addition, in 1/9 of all pairs both coefficients will be divisible by 3;

however, 1/4 of those pairs will have already been accounted in the even–even group; hence, $(1/9 \times 3/4)$ represents additional redundant coefficient pairs.

Similarly, for any system of three elements, the reduction from P to P' is $[1/8 + (1/27 \times 7/8) + (1/125 \times 7/8 \times 26/27) + \ldots] \times P \sim 0.164 \times P$. This factor decreases significantly to $\sim 0.076 \times P$, $\sim 0.035 \times P$, and $\sim 0.017 \times P$ for systems of $k = 4$, 5, and 6 elements, respectively. As we shall see, this correction becomes unnecessary (i.e. $P' \sim P$) for mineral systems with 7 or more elements in the chemical formula.

4. Finally, in the case of stellar minerals multiply $(C \times P')$ and sum for formulas with $k = 1$, 2, 3, and 4 different elements. Note that because of the exponential increase in combinations/permutations with k, we only calculate $(C \times P')$ for k_{max} and $(k_{max} - 1)$.

Applying these steps to the stellar minerals of Part I, for which $k_{max} = 4$, $m = 16$, and $n = 19$ (Table 1):

- For a single element, there are 16 different possible combinations; in each case, the coefficient is 1.
- For two different elements (from a population of 16), there are $[(16!)/(14! \times 2!)] = [(16^2 - 16)/2] = 120$ different element pairs. For each pair, the number of possible coefficient permutations of 1 to 19 is $[(19!)/(19-2)!] = 342$, of which 122 (35.7%) are reduceable by factoring. Therefore, there exist $120 \times 220 = 26,400$ possible chemical formulas with combinations of two elements (out of a population of 16 different elements) and permutations of coefficients from 1 to 19.
- For three different elements, $C = 560$, $P = 5,814$, and $P' \sim 5,814 \times 0.836 = 4,860$. Accordingly, there are $560 \times 4,860 = 2,721,600$ formula combinations of elements and permutations of coefficients for $k = 3$, $m = 16$, and $n = 19$.
- Finally, for $k = 4$ different elements: $C = 1,820$; $P = 93,024$; $P' = 93,024 \times 0.924 = 85,954$, and there are $1,820 \times 85,954 = 156,436,280$ possible formulas.

The total number of possible chemical formulas for $m = 16$ different elements, up to $k = 4$ elements in a formula, and with coefficients as large as $n = 19$ is thus ~159 million, compared to 27 known minerals. Therefore, we estimate the functional information, $I(E_x)$, for all Part I minerals to be:

$$I(E_x) = -\log_2 [27/1.59 \times 10^8] = 22.5 \text{ bits.} \tag{5}$$

Part II—Primary nebular condensates (> 4.565 Ga): The earliest stages of nebular condensation, as reviewed in Part II of the evolutionary system of mineralogy (27), saw a significant increase in both the number of mineral-forming elements and the diversity of mineral species. The 48 mineral species from Part II include the earliest of these condensates from calcium–aluminum-rich inclusions, ultra-refractory inclusions, and ameboid olivine aggregates, which are combined (and in part overlap) with Part I stellar minerals. These 48 minerals from Part II feature $m = 23$ different chemical elements (Figure 1c in 27), with as many as $k = 7$ different chemical elements in a formula, as in rhönite $\{Ca_2(Mg_4Fe^{3+}Ti^{4+})O_2[Si_3Al_3O_{18}]\}$, and coefficients up to $n = 19$ in hibonite.

Applying Eqs. 2, 3, and 4, we find that $C(7,23) = 245,157$; $C(6,23) = 100,947$; $P'(7,19) = 2.5 \times 10^8$; and $P'(6,19) = 0.2 \times 10^8$. Multiplying $C \times P'$ for $k = 7$ and 6 yields 6.3×10^{13} and 0.2×10^{13}, respectively. Note that 59 different mineral species appear in total in Parts I and II. The functional information of Earth's mineral systems at this earliest stage of Earth's mineral evolution is thus:

$$I(E_x) = -\log_2 [59/6.3 \times 10^{13}] = 40.0 \text{ bits.} \tag{6}$$

This value represents a significant increase in functional information for mineral systems between the prenebular stage of stellar minerals and the earliest stage of nebular condensation.

Part III—Primary chondrite minerals (> 4.561 Ga): The primary condensates of Part III (28) increase the total number of mineral species to 96, with formulas combining up to seven elements ($k_{max} = 7$) out of $m = 29$ different chemical elements. The maximum coefficient increases to $n = 36$, as found in sapphirine $\{(Mg, Fe)_4(Mg_3Al_9)O_4[Si_3Al_9O_{36}]\}$ (see Table 1). Therefore, applying Eqs. 2, 3, and 4, we find $\sim 6.8 \times 10^{16}$ potential chemical combinations and permutations, of which 96 are observed. The resulting functional information is:

$$I(E_x) = -\log_2 [96/6.8 \times 10^{16}] = 49.3 \text{ bits.} \tag{7}$$

Part IV—Primary achondrite minerals (>4.560 Ga): Planetesimal formation produced at least 94 primary igneous phases (29). These processes increased Earth's mineral inventory to 141 documented phases (all found in meteorites) that formed from $m = 34$ different chemical elements, with as many as eight elements [e.g. $k_{max} = 8$ in the formula of panethite $(Na, Ca, K)_{1-x}(Mg, Fe^{2+}, Mn^{2+})P^{5+}O_4$]. As in Part III, the largest coefficient is $n = 36$ in sapphirine. In this case, $C(8,34) = 1.8 \times 10^7$; $C(7,34) = 5.4 \times 10^6$; $P'(8,36) = 1.2 \times 10^{12}$; and $P'(7,36) = 4.2 \times 10^{10}$. Multiplying $C \times P'$ for $k = 8$ and 7 yields 2.2×10^{19} and 2.3×10^{17}, respectively. A total of 141 different mineral species appear cumulatively in Parts I through IV. The functional information of Earth's mineral systems including the earliest phases of planetesimal formation is thus:

$$I(E_x) = -\log_2 [141/2.2 \times 10^{19}] = 57.2 \text{ bits.} \tag{8}$$

Part V—Secondary achondrite minerals (>4.550 Ga): The formation of planetesimals was associated with the appearance of more than 200 secondary phases produced by thermal, aqueous, and shock alteration (30). These processes increased Earth's mineral inventory to 296 documented phases that form from $m = 42$ different chemical elements, with as many as $k_{max} = 8$ elements in several minerals and with coefficients as large as $n = 71$ in the formula of decagonite $(Al_{71}Ni_{24}Fe_5)$. The resulting functional information is:

$$I(E_x) = -\log_2 [296/5.2 \times 10^{22}] = 67.3 \text{ bits.} \tag{9}$$

Part VI—Earth's earliest Hadean crust (>4.370 Ga): Part VI of the evolutionary system of mineralogy proposes a list of 262 minerals that likely formed in near-surface environments during the earliest stages of Earth's accretion and cooling (31). Combined with almost 300 meteorite minerals described in Parts I through V, the total estimated mineral diversity was 442 species (Supplementary Table 1 in 31). Phases from this stage of mineral evolution feature $m = 48$ different elements, with as many as $k_{max} = 10$ elements in biotite $[K_2(Mg, Fe^{2+}, Fe^{3+}, Al, Ti)_6(Si, Al)_8O_{20}(OH, F)_4]$, and coefficients as large as $n = 72$ in stilbite $[NaCa_4(Si_{27}Al_9)O_{72}.28H_2O]$. The functional information is thus:

$$I(E_x) = -\log_2 [442/1.2 \times 10^{28}] = 84.5 \text{ bits.} \tag{10}$$

Part "VIB"—Earth's cumulative Hadean crust (>4.0 Ga): Hazen and Morrison (16) tabulated 57 different mineral formation processes (i.e. "paragenetic modes"), with assignments of one or more modes to each of 5,659 mineral species (the total number of IMA-CNMNC-approved species at that time). That survey thus expanded on the list of plausible Hadean minerals in Part VI by considering an additional 441 species that are estimated to have formed after ~ 4.4 Ga but prior to 4.0 Ga. These 883 species represent all minerals listed for paragenetic modes $p1$ through $p18$ (Supplementary Table 1 in 16). These minerals incorporate $m = 61$ different chemical elements, with $k_{max} = 11$ elements. As in Part VI, the maximum coefficient is $n = 72$. We therefore estimate the functional information for Earth's cumulative Hadean mineral repertoire (i.e. prior to 4 billion years) as:

$$I(E_x) = -\log_2 [883/5.0 \times 10^{31}] = 95.5 \text{ bits.} \tag{11}$$

Parts VII and VIII—Primary igneous and metamorphic minerals (>2.5 Ga): Parts VII and VIII of the evolutionary system of mineralogy enumerate 1,665 primary igneous (32) and 1,220 primary metamorphic (33) minerals, respectively. We combine these two parts because many of these minerals had to await the advent of plate tectonics, notably processes of burial, uplift, and orogenesis associated with subduction zones. Combined with all prior minerals, as well as secondary phases that likely formed prior to the Great Oxidation Event at ~ 2.5 Ga, we identify 3,759 mineral species that formed abiotically (Supplementary Table 1 in 16; paragenetic modes $p1$ through $p43$). These minerals incorporate $m = 68$ different chemical elements, with $k_{max} = 12$ [for example, in the mineral kentbrooksite, $(Na, La^{3+})_{15}(Ca, La^{3+})_6Mn^{2+}_3Zr^{4+}_3Nb^{5+}Si_{25}O_{73}(O, OH, H_2O)_3(F, Cl)_2$] and $n = 123$ [for example, in the mineral rogermitchellite, $Na_6(Sr, Na)_{12}Ba_2Zr^{4+}_{13}Si_{39}(B, Si)_6O_{123}(OH)_{12}.9H_2O$]. Application of Eqs. 2 and 3 yields:

$$I(E_x) = -\log_2 [3759/5.0 \times 10^{37}] = 113.3 \text{ bits.} \tag{12}$$

Parts IX to XII—Modern and future biotic Earth: What is the maximum possible functional information for Earth's evolving mineral system? Based on all known mineral formulas, including those for yet unpublished Parts IX to XII of the evolutionary system, it seems unlikely that k_{max} will exceed 15. Unless one counts rare earth elements separately, there are $m_{max} = 72$ mineral-forming elements in the periodic table (38). And, unless fractional coefficients are considered, a maximum coefficient much greater than the observed 131 seems unlikely. Applying Eqs. 2 and 3 for $m = 72$, $k = 15$, and $n = 135$: $C(15,72) = 1.2 \times 10^{15}$ and $P'(15,135) = 4.0 \times 10^{31}$, yielding $C \times P' = 4.8 \times 10^{46}$. The total number of mineral species on Earth, including those not yet discovered and described, has been calculated by Hystad et al. (39) using the Bayesian estimation to be approximately 9,300 species. Therefore, a rough

estimate of the maximum functional information of Earth's minerals is:

$$I(E_x) = -\log_2 [9300/4.8 \times 10^{46}] = 138.6 \text{ bits.} \qquad (13)$$

Caveats

The estimations of functional information presented above must be taken with important caveats related to the calculation of functional information, which depends on determining the number of possible configurations of a system. In the case of mineral systems, we have assumed that the number of configurations aligns closely with the number of possible chemical formulas, based on combinations and permutations of: (i) the number of participating chemical elements, m, in that cohort of minerals; (ii) the maximum number of elements in any one formula from those minerals, k; and (iii) the largest coefficient, n, from chemical formulas of minerals in that cohort. This approximation may be in error for at least three reasons.

First, we do not consider structural variations and polymorphs. It is well known that, for a given chemical formula, minerals can adopt multiple crystal structures. For example, there are seven approved structure types for SiO_2, while three or more polymorphs are known for Al_2SiO_5, $MgSiO_3$, Mg_2SiO_4, and native sulfur (see: https://rruff.info/ima, accessed 2024 March 4). Nevertheless, more than 90% of mineral chemical formulas are only associated with one structure type. Therefore, the additional consideration of structure type in estimations of functional information would result in inconsequential changes. For example, if we generously allow an average of two polymorphs for every Part VII/VIII mineral, effectively doubling the number of Part VII/VIII minerals, the functional information contained in Part VII/VIII minerals would only change from 113.3 to 112.3 bits. We conclude that inclusion of polytype information would have a minimal effect on our calculations.

A second concern regarding the validity of our estimations of functional information relates to solid solutions—the substitution of two or more chemical elements in a single structural site. The IMA is somewhat inconsistent in their application of rules for defining a mineral's formula. In most instances, an idealized end-member formula is used, such as forsterite (Mg_2SiO_4) or fayalite (Fe_2SiO_4), even though natural samples invariably have both Mg and Fe in solid solution represented by $[(Mg, Fe)_2SiO_4]$. However, in many other instances the official IMA formula explicitly acknowledges solid solution, as in the metamorphic mineral prismatine $[(Mg, Al, Fe)_6Al_4(Si, Al)_4(B, Si, Al)(O, OH, F)_{22}]$ or the rare igneous mineral ikranite $[(Na, H_3O)_{15}(Ca, Mn, REE)_6Fe_2^{3+}Zr_{3-}Si_{24}O_{66}(O, OH)_6Cl \cdot nH_2O]$. In such cases, the maximum number of elements in a structure, k_{max}, as well as the number of different essential elements in a cohort of minerals, m, may be inflated by including minor elements that would not necessarily be included in an idealized reduced formula. Nevertheless, by systematically employing the official IMA chemical formulas our calculations are both internally consistent and reproducible, while not significantly altering the overall trends in our calculations.

Thirdly, our treatment does not recognize the existence of fractional coefficients, which do occur in a small percentage of IMA-CNMNC-approved chemical formulas. Examples such as algodonite $[Cu_{1-x}As_x \ (x \approx 0.15)]$, chibaite $[SiO_2 \cdot n(CH_4, C_2H_6, C_3H_8, C_4H_{10}); \ (n_{max} = 3/17)]$, digenite $[Cu_{1.8}S]$, kidwellite $[NaFe_{9+x}^{3+}(PO_4)_6(OH)_{11} \cdot 3H_2O \ (x \approx 0.33)]$, and rathite $[Ag_2Pb_{12-x}Tl_{x/2}As_{18+x/2}S_{40}]$ may complicate the assignment of a maximum integral coefficient, n. In these instances, we employ the nearest integral value, because

in most cases the fractional coefficient results from a modest fraction of vacancies in a specific crystallographic site.

A closely related caveat is also needed. Minerals of the sartorite group feature complex combinations of (in some cases) incommensurate substructures that lead to formulas of extreme complexity, such as in dekatriasartorite $[TlPb_{58}As_{97}S_{204}]$, hendekasartorite $[Tl_2Pb_{48}As_{82}S_{172}]$, incomsartorite $[Tl_6Pb_{144}As_{246}S_{516}]$, and other similar examples. In each case, the coefficients in these formulas can be reduced to smaller integral values by recognizing that two simpler building blocks occur in combination.

Discussion

Despite the caveats noted above, a convincing conclusion of this study is that the functional information of mineral systems on Earth has increased monotonically through 4.56 billion years of planetary history. Over this time span, the number of mineral species increased dramatically, from 27 stellar minerals to 300 meteorite minerals in the first 5 million years (>4.56 Ga) to more than 800 species by the end of the Hadean Eon (4.0 Ga), an estimated almost 4,000 different minerals formed by abiotic processes prior to the Great Oxidation Event (~2.5 Ga), to more than 9,000 species on Earth today. One might conclude that the *fraction* of all possible mineral species that were generated steadily increased through time. In that case, functional information of mineral systems would have steadily decreased.

What we observe instead is a dramatic decrease in this fraction because of the rapidly increasing potential combinatorial richness of the mineral kingdom. An ever-greater number of different chemical elements led to the potential for numerous new combinations, even as the complexities of formulas—in terms of both the number of coexisting elements, k_{max}, and their largest coefficients, n—added new permutational possibilities. The results (Table 1; Figure 1) are a monotonic increase in the functional information through nine chronological stages of mineral evolution. Indeed, we observe relatively equally spaced increases in functional information over the 12 parts of the evolutionary system of mineralogy (Figure 1).

Intriguingly, when functional information is plotted versus the cumulative number of IMA-CNMNC-approved mineral species (Figure 2), the functional information appears to be approaching an asymptotic limit. Such behavior suggests that mineral evolution is not open-ended (1–5). Rather, there is a limit to the degree to which mineral systems can increase in diversity, because the mineral kingdom is sculpted by selection for static persistence in a system of large but finite chemical possibilities. If so, then Earth may
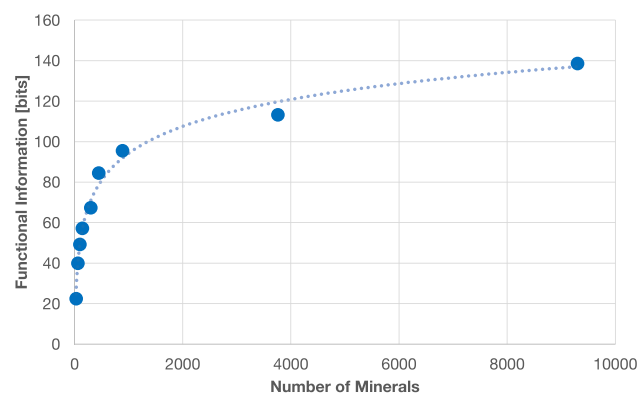
Fig. 2. A plot of functional information versus cumulative number of minerals reveals an asymptotic limit, suggesting that mineral evolution is not open-ended.
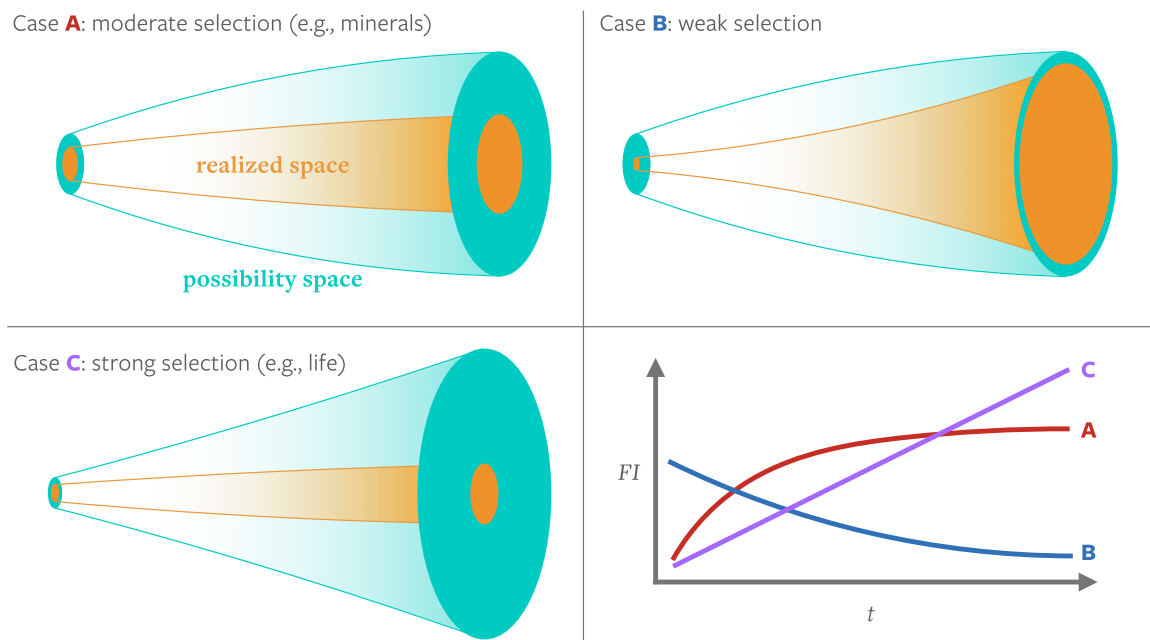
Fig. 3. Example types of evolving systems. A) Nonopen-ended system (e.g. minerals), characterized by an expanding possibility space and a moderate degree of selection. B) Nonopen-ended system characterized by expanding possibility space but little or no selection. C) Open-ended system (e.g. life?), characterized by a rapidly expanding possibility space and a strong degree of selection. D) The behavior of functional information vs. time for all three cases.

have already sampled a significant fraction of the combinatorially rich formula space possible with the current inventory of 72 mineral-forming elements, as illustrated in Figure 3A.

In this context, it is interesting to compare and contrast different possible modes of evolution. For example, a system's possibility space might expand in a manner similar to mineral evolution, yet under extremely weak or nonexistent selection pressures. In such a case, the functional information of that system may remain constant or even decrease with time (Figure 3B).

A third plausible mode is open-ended evolution in a system for which the possibility space expands indefinitely (1, 2, 5)—a situation that may be exemplified by the evolution of life (Figure 3C). Kauffman and colleagues, who have explored this concept in several works (40–44), suggest that the complexity of Earth's biosphere is greater than the entire abiotic universe (40, 41). Their "Theory of the Adjacent Possible" (42) posits that an evolving system occupies an ever-smaller subset of the total possible—an idea equivalent to the proposed law of increasing functional information (9). Kauffman and Roli (43, 44) further demonstrate that biological evolution is likely open-ended and not deducible via the Newtonian paradigm.

Life, in contrast to the mineral realm, is shaped by selective pressures for dynamic persistence and novelty generation, reflective of the active feedback loops and ongoing exchange of information between biological systems and their environments (45). These additional selective forces, as well as the enormous combinatorial space of biomolecules, cells, and ecosystems, mean that the configurational space of life's realized forms may become vanishingly small compared to the space of all possible configurations, both viable and nonviable. Although such a calculation has yet to be performed, we speculate that the functional information of living systems does not approach an asymptote with time (Figure 3D), which would be a result consistent with the hypothesis of life's open-endedness (1, 4).

With more than 6,000 different mineral species approved by the IMA-CNMNC and 100 new species discovered yearly (46), it might seem that Earth's mineral kingdom is remarkably well endowed. However, that view misses a key property of evolving systems: As with all other evolving systems, the known mineral kingdom represents only a miniscule fraction of all conceivable configurations—by our rough estimation fewer than one stable mineral occurs in every 10^{42} possible element combinations. We conclude that minerals constitute a bounded evolving system, with monotonic increasing functional information approaching an asymptote—a finding that is consistent with the proposed law of increasing functional information (9).

Author Contributions

R.M.H. and M.L.W. contributed equally to conceptualization, methodology, validation, formal analysis, investigation, writing—original draft, reviewing and editing, and supervision. R.M.H. was involved in data curation, project administration, and funding acquisition. M.L.W. was involved in visualization.

Data Availability

The authors do not report any new data in this manuscript. All mineralogical data underlying our calculations can be found in published tabulations of mineral formulas and paragenetic modes in reference (13).

References

1   Bedau MA, Snyder E, Packard NH. 1998. A classification of long-term evolutionary dynamics. In: Adami C, Belew RK, Kitano H, Taylor CE, editors. *Artificial life VI: proceedings of the sixth international conference on artificial life*. Cambridge (MA): MIT Press. p. 228–237.

2   Adams A, Zenil H, Davies PCW, Walker SI. 2017. Formal definitions of unbounded evolution and innovation reveal universal mechanisms for open-ended evolution in dynamical systems. *Sci Rep*. 7:997.

3   Sayama H. 2019. Cardinality leap for open-ended evolution. Arxiv 1806.06628. https://doi.org/10.48550/arXiv.1806.06628, preprint: not peer reviewed.

4   Packard N, *et al*. 2018. An overview of open-ended evolution: editorial introduction to the open-ended evolution II special issue. *Artif Life*. 25:93–103.

5   Taylor T. 2018. Evolutionary innovations and where to find them. *Artif Life*. 25:207–224.

6   Marshall SM, Murray ARG, Cronin LA. 2017. A probabilistic framework for identifying biosignatures using pathway complexity. *Phil Trans Royal Soc A*. 375:20160342.

7   Marshall SM, *et al*. 2021. Identifying molecules as biosignatures with assembly theory and mass spectrometry. *Nat Commun*. 12: 3033.

8   Sharma A, *et al*. 2023. Assembly theory explains and quantifies selection and evolution. *Nature*. 622:321–328.

9   Wong ML, *et al*. 2023. On the roles of selection and function in evolving systems. *Proc Natl Acad Sci U S A*. 120:e2310223120.

10 Szostak JW. 2003. Functional information: molecular messages. *Nature*. 423:689–689.

11 Hazen RM, Griffin PL, Carothers JM, Szostak JW. 2007. Functional information and the emergence of biocomplexity. *Proc Natl Acad Sci U S A*. 104:8574–8581.

12 Hazen RM, Ferry JM. 2010. Mineral evolution: mineralogy in the fourth dimension. *Elements*. 6:9–12.

13 Hazen RM, Morrison SM, Prabhu A. 2023. The evolution of mineral evolution. In: Bindi L, Cruciani G, editors. *Celebrating the international year of mineralogy*. Cham (Switzerland): Springer. p. 15–37.

14 Hazen RM, *et al*. 2008. Mineral evolution. *Am Min*. 93:1693–1720.

15 Hazen RM. 2019. An evolutionary system of mineralogy: proposal for a classification based on natural kind clustering. *Am Min*. 104: 810–816.

16 Hazen RM, Morrison SM. 2022. On the paragenetic modes of minerals: a mineral evolution perspective. *Am Min*. 107:1262–1287.

17 Hazen RM, *et al*. 2021. On the attributes of mineral paragenetic modes. *Can J Min Petrol*. 61:653–673.

18 Hazen RM. 2012. *The story of earth: the first 4.5 billion years, from stardust to living planet*. New York (NY): Viking.

19 Hazen RM. 2007. The emergence of chemical complexity: an Introduction. *Amer Chem Soc Symp*. 981:2–14.

20 Krivovichev S. 2012. Topological complexity of crystal structures: quantitative approach. *Acta Cryst A68*. 68:393–398.

21 Krivovichev SV. 2013. Structural complexity of minerals: information storage and processing in the mineral world. *Min Mag*. 77:275–326.

22 Krivovichev SV. 2016. Structural complexity and configurational entropy of crystalline solids. *Acta Cryst*. B72:274–276.

23 Grew ES, Krivovichev SV, Hazen RM, Hystad G. 2016. Evolution of structural complexity in boron minerals. *Can Min*. 54:125–143.

24 Krivovichev SV, Krivovichev VG, Hazen RM. 2018. Structural and chemical complexity of minerals: correlations and time evolution. *Eur J Min*. 30:231–236.

25 Krivovichev SV, *et al*. 2022. StarovaStructural and chemical complexity of minerals: an update. *Min Mag*. 86:183–204.

26 Hazen RM, Morrison SM. 2020. An evolutionary system of mineralogy, part I: stellar mineralogy (>13 to 4.6 Ga). *Am Min*. 105: 627–651.

27 Morrison SM, Hazen RM. 2020. An evolutionary system of mineralogy, part II: interstellar and solar nebula primary condensation mineralogy (> 4.565 Ga). *Amer Min*. 105:1508–1535.

28 Hazen RM, Morrison SM, Prabhu A. 2021. An evolutionary system of mineralogy, part III: primary chondrule mineralogy (4.566 to 4.561 Ga). *Am Min*. 106:325–350.

29 Morrison SM, Hazen RM. 2021. An evolutionary system of mineralogy, part IV: planetesimal differentiation and impact mineralization (4.566 to 4.560 Ga). *Am Min*. 106:730–761.

30 Hazen RM, Morrison SM. 2021. An evolutionary system of mineralogy, part V: planetesimal aqueous and thermal alteration of planetesimals (4.565 to 4.550 Ga). *Am Min*. 106:1388–1419.

31 Morrison SM, Prabhu A, Hazen RM. 2023. An evolutionary system of mineralogy, part VI: earth's earliest hadean crust (> 4370 Ma). *Am Min*. 108:42–58.

32 Hazen RM, Morrison SM, Prabhu A, Walter MJ, Williams JR. 2023. An evolutionary system of mineralogy, part VII: the evolution of the igneous minerals (> 2500 Ma). *Am Min*. 108:1620–1641.

33 Morrison SM, Prabhu A, Hazen RM. 2024. An evolutionary system of mineralogy. Part VIII. The evolution of metamorphic minerals. *Am Min*. 109. https://doi.org/10.2138/am-2023-9004

34 Burke EAJ. 2006. The end of CNMMN and CCM—long live the CNMNC! *Elements*. 2:388.

35 Mills SJ, Hatert F, Nickel EH, Ferrais G. 2009. The standardization of mineral group hierarchies: application to recent nomenclature proposals. *Eur J Min*. 21:1073–1080.

36 Schertl H-P, Mills SJ, Maresch WV. 2018. *A compendium of IMA-approved mineral Nomenclature*. Stuttgart (Germany): International Mineralogical Association.

37 Bermanec M, *et al*. 2023. The evolution of mineral hardness reveals both changing parageneses and preservational bias in the mineralogical record. *Minerals*. 13(8):1089.

38 Hazen RM, Grew ES, Downs RT, Golden J, Hystad G. 2015. Mineral ecology: chance and necessity in the mineral diversity of terrestrial planets. *Can Min*. 53:295–323.

39 Hystad G, Eleish A, Downs RT, Morrison SM, Hazen RM. 2019. Bayesian estimation of Earth's undiscovered mineralogical diversity using noninformative priors. *Math Geosci*. 51:401–417.

40 Cortes M, Kauffman SA, Liddle AR, Smolin L. 2022. Biocosmology: Biology from a cosmological perspective. arXiv:2204.09379. https://doi.org/10.48550/arXiv.2204.09379, preprint: not peer reviewed.

41 Cortês M, Kauffman S, Liddle A, Smolin L. 2022. Biocosmology: Towards the birth of a new science. arXiv:2204.09378. https://doi.org/10.48550/arXiv.2204.09378, preprint: not peer reviewed.

42 Kauffman S. 2022. Is there a 4th law of thermodynamics for systems that do work to construct their expanding phase space? *Entropy*. 24(10):1383.

43 Kauffman S, Roli A. 2023. A third transition in science? *Interface Focus*. 13:20220063.

44 Kauffman S, Roli A. 2024. Is the emergence of life an expected phase transition in the evolving universe? arXiv 2401.09514. https://doi.org/10.48550/arXiv.2401.09514, preprint: not peer reviewed.

45 Wong ML, Prabhu A. 2023. Cells as the first data scientists. *J Royal Soc Interface*. 20(199):20220810.

46 Barton IE. 2019. Trends in the discovery of new minerals over the last century. *Am Min*. 104:641–651.