Revision 1

word count: 9561

The spatial and temporal evolution of mineral discoveries and their impact on mineral rarity

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Abstract. The paper presents the proceedings of the data analysis of the year and country of mineral discoveries with their Nickel-Strunz classes and rarity to enrich our knowledge of the evolution of mineral discoveries and their spatial distribution during different periods. Based on the dynamic of mineral discovery, three principal periods were identified: 1) Ancient period (up to 1800) of irregular mineral records, 2) Sustainable development period (1800-1949) with regular records and a moderate increase in the total number of minerals, 3) Modern period (1950-present) of rapid development. It is pointed out that the timeline of mineral discoveries exhibits local anomalies. The positive anomalies were linked to the publications of mineralogical encyclopedias and classifications, while the negative ones were caused mainly by historical events, suppressing scientific activity. The majority of rock-forming and widespread minerals were discovered before the 1980s, while the discovery rate of rare and endemic species still progresses due to the study of hard-to-reach locations and the introduction of high-resolution analytical methods. A comparison of Nickel-Strunz class counts throughout mineral history revealed that the fraction of carbonates, oxides, and elements have drastically decreased during the Sustainable development period and the

Modern period with a minor increase of elements during the last period. However, opposite behavior is observed for the phosphates, sulfates, and sulfides, with a sudden decrease in sulfates during the Modern period. On the other hand, the fraction of borates, halides, and silicates remained unchanged during all periods. Spatial analysis of the data showed that the distribution of mineral discoveries on the world map depends not only on the country's geology but also on the area, population, economic development, and general interest in science.

Keywords: minerals distribution; history of mineralogy; minerals discovery; data science; statistics.

Introduction

More than 100 new minerals are discovered yearly, with a total number of over 5,700 minerals approved by the International Mineralogical Association (IMA) as of 3th of February 2022. This number can expand to over 10,000 mineral names, along with numerous synonyms and varieties. Thus, the flow of information in mineralogy is increasing enormously every year due to the discovery of new analytical methods, the study of hard-to-reach locations, including extraterrestrial space, anthropogenic impact on the processes of mineral formation, etc. in addition, the open-source databases on mineral diversity, their properties, and localities shed new light on understanding the patterns between different minerals and have brought mineralogy to a new stage of data-driven discovery.

Several resources control the flow of mineralogical information. Founded in 1958, the International Mineralogical Association (IMA) is the world's largest organization promoting mineralogy, including accepting new minerals and nomenclature (de Fourestier 2002). In cooperation with the RRUFF Project (https://rruff.info/ima/), IMA stores the basic information on mineral chemistry, structure, origins, grouping, and references. All this information, together with some data on physical properties, relationships, and geologic occurrences, is freely distributed by RRUFF, covering about 5,800 mineral names as of August 2022 (Lafuente et al. 2015). Probably, the most complete database resides on https://www.mindat.org (Mindat, Hudson Institute of Mineralogy, accessed 3 Feb 2022) – the world's leading authority on minerals and their localities, deposits, and mines worldwide. Mindat.org collects, organizes, and shares mineral information for the IMA-approved minerals and varieties and synonyms.

Various techniques are used to understand the co-evolution of the geosphere and biosphere – from cluster diagrams and network analysis to frequency spectrum analysis and predictive analytics (Morrison et al. 2017). These modern data-driven strategies deepen our understanding of mineral co-occurrences and even allow us to predict the total number of mineral species occurring on Earth today (Hazen et al. 2019).

Statistical analysis and visualizations in natural sciences are rapidly growing, for example, in biology (Muscente et al. 2019) and ecology (Kondratyeva et al. 2019), but it is still very limited in mineralogy. The first attempts were the works of Hazen and co-authors on the evolution of minerals (Hazen et al. 2008, 2011). The papers present an alternative approach to the systematization and the teaching of the subject of mineralogy through the evolution of minerals.

According to Hystad et al. (2015), mineral species-localities pairs conform to a large number of rare events (LNRE) distribution, similarly to the frequency distribution of words in a book (Baayen 1992, 2002; Evert and Baroni 2008). It is pointed out that the total count of minerals, the so-called "mineral kingdom", is dominated by those of mineral species found at one or two localities. LNRE models are widely used in ecology to estimate the total size of the population and predict the number of new species in a second survey based on the data obtained during the previous survey (Shen et al. 2003). During the last decade, these models and the Bayesian approach have been more frequently used to predict the nature and number of minerals that are yet to be discovered (Hystad et al. 2015a, 2015b, 2018; Hazen et al. 2016, 2019).

The first achievements in statistical analysis of mineralogical data led to the publication of articles on the ecology of mineral groups, where the authors attempted to analyze the distribution and spatial diversity of minerals of cobalt (Hazen et al. 2017), carbon (Hazen et al. 2016; Morrison et. al. 2020), vanadium (Liu et al. 2018), and chromium (Liu et al. 2017), and to predict the number of undiscovered minerals. The most recent studies on predictive analytics indicate that more than 9,300 mineral species occur on Earth (Hystad et al. 2018). The authors highlight that nearly 25% of minerals containing Al, B, C, Cr, P, Si, and Ta, 35% of minerals containing Na, and less than 20% of minerals with Cu, Mg, Ni, S, Te, U, and V remain to be described. It is claimed that sociological factors in the search, discovery, and description of minerals imposed on natural processes lead to these discrepancies in percentages of undiscovered minerals.

The trends in the discovery history of minerals, especially the social and technological aspects, were studied in detail by Barton (2019). The general patterns of mineral discoveries over time were also studied earlier by Bulakh et al. (2003). However, both publications considered only approved species (nearly 4,000 were studied by Bulakh et al. and 4,046 by Barton) and did not consider their varieties and synonyms.

The statistical analysis, prediction, and visualization of data in mineralogy are now in their infancy. The main works are devoted to predicting the number of undiscovered minerals within several chemical groups. A wealth of data has not yet been analyzed, including chemistry, crystallography, geological conditions, and the history of mineral discoveries.

This research aims to develop a robust data warehouse that would allow us to analyze relationships between Nickel-Strunz classes, rarity data, and the country of discovery at various time scales. The latter brings new insight into the distribution of minerals and the temporal and spatial evolution of the discovery process. This paper outlines the first essential step in creating a multidimensional relational mineralogical data model aimed at identifying minerals based on various properties or predicting the probability of new mineral species to be discovered in certain countries or geologic provinces.

Materials and Methods

Initial dataset

The core of the data warehouse consists of IMA-approved minerals with their formulas, discovery years, and Nickel-Strunz classification. The bulk of this data is provided freely by various web resources, while a substantial amount of data on synonyms and varieties is accessible through hard-copy publications. Most information on minerals occurrence and discovery localities was accessed through peer-reviewed publications in American Mineralogist, Canadian Mineralogist, and Mineralogical Magazine journals and reviewed afterward. The IMA list served as a fundamental source of information and was supplemented with several consultations of the original literature.

The IMA List of Minerals. The official list of IMA-approved minerals (https://RRUFF.info/IMA, accessed 10 Jan 2022) is accessible through the RRUFF Project (Lafuente et al. 2015) – a set of relational databases maintained at the Department of Geosciences, The University of Arizona. The IMA list provides information on mineral composition, crystal structure, physical properties, origins, paragenetic mode, IMA status, etc.

Mineral Evolution Database (MED) is hosted under the RRUFF project (https://RRUFF.info/Evolution, accessed 14 Nov 2021) and provides mineral occurrence and age information extracted from original literature sources and the mindat.org database. As of 14

November 2021, the data on 810,907 mineral-locality pairs, of which 210,037 are dated, is available in the MED.

The **Athena** mineral database was published online in 1994 and is now maintained by the Department of Mineralogy of Geneva Natural History Museum. Nickel-Strunz classification used in the current research was kindly provided by Pierre Perroud, the founder of Athena (https://athena.unige.ch/athena/, accessed 12 Dec 2021), with his written permission.

Handbook of Mineralogy (http://www.handbookofmineralogy.org, accessed 28 Dec 2021) is another web resource for accessing data on more than 5,000 minerals (as of 2nd December 2021), maintained by the Mineralogical Society of America (MSA) since 2001. A variety of essential data is provided: crystal data, physical properties, occurrence, association, distribution, name origins, references, and much more.

Webmineral database available at https://webmineral.com (accessed 13 Jan 2022), developed and maintained by David Barthelmy since 1997 provides crucial data on IMA-approved species and more than 2,600 of their synonyms. In addition, a variety of information is provided: name origins, empirical mineral formulas, composition, mineral synonyms, Dana and Nickel-Strunz classification, etc.

Mineralatlas was launched in 2001 (https://www.mineralienatlas.de/, accessed 13 Jan 2022) and was developed primarily for people interested in mineralogy, geology, paleontology, and mining. The resource operates a significant database for minerals, fossils, rocks, and their localities. Additionally, it allows exploring essential mineralogical classifications, e.g., Dana, Nickel-Strunz, Hey, etc.

The final data compilation includes more than 8,160 mineral names, including all currently IMA-approved species and the most relevant synonyms and varieties. Essential fields in our data are "Country of Discovery" and "Year of Discovery", which allows us to track the distribution of minerals by countries with time, assuming possible minor errors in the year of discovery. For instance, the date of discovery of new minerals is immediately published by IMA, suggesting no error. In contrast, the actual year of discovery and the year of publication of this name in the literature may differ for older minerals. Therefore, we are treating the year of the first mention in the literature as the year of discovery if this information is absent. Also, for ancient minerals (in use before 1800), the difference between the discovery and the appearance of the mineral name in the references could be more significant, which requires special processing of this data. For example, it is known that ancient people from the Neolithic period used quartz, but its modern name appeared only in 1505. Similar sources of error apply to the country of discovery as it corresponds to the place of the earliest documentation or description of ancient minerals. For example, many old mineral names were reported from Ancient Egypt or Greece, but the actual geological site is unknown.

Data analysis

The data manipulation of the original raw dataset furthered by basic statistical analysis was performed in Python 3.7.1 (using the software libraries pandas, numpy) with PyCharm IDE and R 3.6.0 (software libraries dplyr, plyr) using RStudio IDE. The visualizations were compiled in Python (library matplotlib) and R (library ggplot2). The data compilation included data processing with further quality control. During the first stage, all data was gathered from external resources, furthered by data wrangling and cleaning to adapt data storage to develop a consistent model. A logical cleaning procedure was employed during the pre-processing to eliminate non-descriptive data and identify the missing data. Consequently, the missing data were screened visually and, in most cases, filled in using hard-copy publications afterward.

Results and discussion

Timeline of mineral discoveries

The timeline of the discovery years or at least the earliest publication of minerals were analyzed, including the distribution between approved and non-approved IMA mineral species, as well as their cumulative curves (Fig. 1). The timeline is set between 1800 and 2019, with 1800 being chosen for convenience since there was no stable record of new minerals before 1800 and their total number was insignificant compared to the current number. It should be noted that similar trends were pointed out by Bulakh et al. (2003).

As shown in Fig. 1, the timeline of mineral discovery is quite heterogeneous, with alternating increases and decreases and local anomalies, both positive and negative. Between 1800 and 1950, the dynamics of mineral discoveries changed a little, fluctuating from year to year. However, the total number of minerals is gradually increasing, leading to an increase in the approved IMA minerals up to ~1,350 and in the total number of minerals up to >1,980.

Since 1950, there has been a sharp increase in the number of discovered or named minerals, with moderate fluctuations of decrease and increase. As a result, the number of approved IMA minerals increased from ~1,350 to ~4,500, and the total number of mineral species climbed from >1,980 to >7,200.

The cumulative curves of discovered/published minerals of each Nickel-Strunz class are displayed in Fig. 2. It shows that the number of sulfides and sulfosalts, sulfates, oxides, and phosphates were approximately the same by 1860. After that, the number of phosphates and sulfides slightly exceeded the number of oxides and sulfates until 1940, when the number of oxides equaled the sulfides and sulfosalts and was bracketed between phosphates and sulfates. In 1970, the number of sulfides and sulfosalts exceeded the number of oxides, and this trend continues. The class of silicates significantly dominated other classes of minerals throughout the described time.

In 1870, the number of carbonates and halides exceeded the number of elements. Until 1940, the total number of borates was less than the number of elements, but this changed in the 2000s. In 1960, the number of carbonates and halides was almost the same, but now the number of carbonates is much higher than that of halides. Minerals of organic compounds have always remained the smallest class. Hazen et al. (2016) predicted that at least 548 undiscovered carbon minerals, of which 118 contain hydrogen. Furthermore, recent studies reveal that the total number of undiscovered carbon minerals is 993 (Morrison et. al. 2020), which increases the number of organic compounds. However, that would not be sufficient to exceed the other mineral classes.

Using the data on where and when the mineral was discovered, we were able to construct a map of the overall distribution of mineral discoveries (Fig. 3). The most significant number of minerals was discovered in the USA (>1,100 minerals, incl. >830 IMA approved) and Russia (975, incl. 828 IMA approved) followed by Germany (426, incl. 367 IMA approved) and Italy (423, incl. 377 IMA approved). In South America, the largest number of minerals was discovered in Chile (>150 minerals, incl. 139 IMA approved). Namibia is the leader in discovered minerals in Africa (123, incl. 106 IMA approved). More than 220 minerals (incl. 172 IMA approved) were discovered in Australia. In Asia, 250 discovered minerals (incl. 140 IMA approved) make China the leader in this group, followed by Japan. It should be noted that the discovery counts per country obtained are generally higher than those estimated by Bulakh et al. (2003). The latter is probably attributed to more than 2x bigger sample size being analyzed within current research.

In general, the number of minerals discovered on the territory of a country depends on its geological conditions, cultural traditions, area, development of science, etc. Central and Northern African countries were identified as “white spots” on the map primarily because most of their territory is covered with the Sahara Desert. The highest number of new minerals was discovered in countries that, in addition to a large area, have solid scientific traditions, stable funding for the fundamental sciences, and/or where large igneous complexes and related geological structures are present.

Therefore, data on the dynamics of mineral discovery (Fig. 1 and Fig. 2) were classified into three distinct periods:

1) Ancient period (before 1800) is characterized by the absence of a stable record or description of mineral discovery and the negligible total number of minerals;

2) Sustainable development period (1800-1949) is characterized by a steady record of mineral discovery and a moderate increase in the total number of minerals;

3) A rapid increase in mineral discoveries characterizes a modern period of rapid development (1950-present) is characterized by due to the development of physical and analytical methods.

Description of periods of mineral discoveries

Ancient period (before 1800). A wide segment of history from the Neolithic until the 1800s was classified as the Ancient period and characterized by the absence of stable records of mineral discoveries and their descriptions. In fact, since the 1780s, a stable record of mineral discovery can be observed, but for convenience, a period up to 1800 has been chosen.

The total number of minerals before 1800 was slightly higher than 100. These are minerals mainly of practical importance, like metals, gems, or decorative stones (Table 1). This period is characterized by a small percentage of approved IMA minerals (about 50% or 70 species) since a big part of minerals are varieties. Table 1 contains 100 of the most ancient mineral names, including their earliest known usage date and country of discovery according to the ancient literature or archeological evidence.

For some native elements, known since ancient times, it is not always clear whether their natural or synthetic form was mentioned. Ancient citations and archeological findings of many elements are likely related to their synthetic varieties, which were obtained by smelting ores (e.g., lead, tin, copper, zinc, arsenic). For example, the first findings of iron date back to nearly 450 BC in China (Lam 2014), but beads made of meteorite iron were found in Gersh, Egypt, and dated 3,200 BC (Rehren et al. 2013). Antimony sulfide, stibnite, has been used since around 3000 BC (Dillis et al. 2019). Later, Pliny the Elder described the native antimony (Mellor 1964), but probably of synthetic origin, and the first description of natural native antimony was made in 1783 in Sweden (Klaproth 1802). The name "phosphorus" was also known in ancient Greece (Parkes and Mellor 1939), but it likely referred to the planet Venus without any relation to elements or minerals because native phosphorus was unknown during ancient times. Phosphorus was discovered by the German alchemist Hennig Brand in 1669 as an element (Weeks 1932), but in nature, it was reported for the first time in 1903 from the Saline Township meteorite (Farrington 1903) (a doubtful mineral species). A similar confusion persists to the present in mining/economic literature among people unfamiliar with the mineralogical literature. Thus, zinc may mean sphalerite, one of the secondary minerals such as the calamine species (see Table 1), or a mixture of all of those.

Varieties of some minerals were known long before their parent minerals were discovered. For example, chiastolite was described in 1754, which predates the description of its parent species andalusite by 44 years. Likewise, sapphire and ruby, as well as other names for aluminum oxide, were known long before the name corundum appeared. Many varieties of quartz were also known since ancient times. Some appeared even before the name quartz was introduced in 1505. Likely, the most ancient name of quartz is "κρύσταλλος" or kristallos that Theophrastus recorded in about 300-325 BCE.

The distribution by Nickel-Strunz classes indicates a significant predominance of silicates and elements. At the same time, organic compounds and phosphates exhibit a minor fraction over the period (Fig. 4). Besides, the Ancient period is characterized by a larger number of minerals from the group of elements and carbonates, as well as a smaller number of phosphates and sulfates, when comparing the distribution of classes with other periods. The latter can be explained by the general appearance of the minerals and the peculiarities of their distribution and use. For instance, elements, although not very common, have found many uses in history, but it is not always known whether the ancient mention of the minerals refers to natural or artificially obtained specimens. Carbonates are widespread and widely used as a building material. On the other hand, besides limited practical significance, the minerals of phosphate and sulfate classes were difficult to identify without chemical analysis due to their dispersed or limited appearance.

Many minerals of the Ancient period do not have a clear link to their discovery locality. The known locations of mineral discoveries of this period by countries are shown in Fig. 5. It should be noted that the discovery sites of ancient minerals are reproduced according to the available literature sources. Consequently, these locations may be tied to the territory of an ancient civilization where the archeological work was concentrated, but not to the actual geological sites.

The map in Fig. 5 notes that the largest number of minerals discovered in Europe before 1800 was in the territories of modern Germany, Italy, The Czech Republic, and Austria, which includes the territory of the former Roman Empire. Also, the territory of modern Great Britain was characterized by the active exploration of minerals.

China, India, and the Middle East territories of modern Afghanistan and Pakistan, which also encompasses the former Persia, occupy a leading position in discovering minerals in Asia. Egypt and South Africa are the only two countries in Africa with minerals discovered before 1800. At the end of the 18th century, the first discoveries of minerals in America were recorded in Canada, the USA, Brazil, etc.

The most prominent persons in mineralogy during this period were Pliny the Elder (AD 23/24-79) – a Roman author, naturalist, and natural philosopher, Theophrastus (371-287 BC) – the successor to Aristotle in the Peripatetic school, Johan Gottschalk Wallerius (1709-1785) – a Swedish chemist and mineralogist, and Georgius Agricola (1494-1555) – a German Humanist scholar, mineralogist, and metallurgist.

Sustainable development period (1800-1949). This period is characterized by the development of regular records of mineral discoveries and their descriptions with insignificant variations from year to year, as well as by the overall moderate increase in the number of minerals. Nearly 2,000 new minerals appeared during this period, of which ~1,350 are now approved by the IMA. Despite the gradual increase in the number of minerals, we have observed several local positive and negative anomalies (demonstrated in Fig. 1). Analysis of the most prominent positive anomalies shows that they can be linked to the publication of the fundamental mineralogical classifications or encyclopedias, for example,

- 1832 – 31 minerals discovered (including 26 IMA approved), a publication of “Basic Mineralogy Trail” by F.S. Beudant (Beudant 1832) and “Vollständige Charakteristik des Mineral-Systems” (“Overview of the Mineral Systems”) of Breithaupt (1832).
- 1845 – 51 minerals discovered (including 44 IMA approved), a publication of “Manual of the determining mineralogy” by Wilhelm Karl von Haidinger (von Haidinger 1845).
- 1868 – 46 minerals discovered (including 34 IMA approved), “A System of Mineralogy: Descriptive Mineralogy, comprising the most recent discoveries (5 ed.)” by James Dwight Dana and George Jarvis Brush (Dana and Brush 1868).

- 1892 – 76 minerals discovered (only 5 IMA approved minerals: baddeleyite, geikielite, marshite, nickelskutterudite, and penfieldite), a publication of "The System of Mineralogy of James D. Dana: Descriptive Mineralogy (6 ed.)" by James Dwight Dana and Edward Salisbury Dana (Dana and Dana 1892), "A catalogue of minerals and synonyms" by Egleston (1892) and "Systematic Mineralogy Based on a Natural Classification" by Hunt (1892).

In contrast, the most prominent negative anomalies have some correlation with historical events, like wars or pandemics. For example,

- 1809 – 1 mineral was discovered (elaeolite - a variety of nepheline). That year was rather eventful with war actions during the Spanish campaign in Peninsular War (1807-1814), War of the Fifth Coalition during Napoleonic Wars (1803-1815), and Finnish War (1808-1809).
- 1917-1918 – 1 mineral (ferrierite) was discovered in 1918 in contrast to 14 (IMA approves only a half) during 1917 since these two years were rather tragic in history, including The Russian Revolution, the outburst of World War I (1914-1918), and an unusually deadly influenza pandemic of the Spanish flu, also known as the 1918 flu pandemic.
- 1936 – 9 minerals (only bermanite and earlandite are approved by IMA) were discovered. The year is known for historical events such as Joseph Stalin's Great Purge in the Soviet Union (1936-1938), Spanish Civil War (1936-1939), West China Famine, and the 1936 North American heatwave.
- 1943 – 8 minerals (including 5 IMA approved) discovered; this was during the middle of World War II (1939-1945).

It is difficult to explain the minima in 1834, 1857, and 1867 years, suggesting the influence of an unknown or random factor on the dynamics of mineral discoveries.

Analysis by classes for the period between 1800 and 1949 showed that the distribution of minerals resembles modern patterns (Fig. 4). Compared with the Ancient period, the largest increase from 2 to 15% occurred in the number of phosphates. The percentage of sulfates also significantly increased from 5% to 10%. The latter may be due to the development of chemical analysis methods during this period, which has improved the identification of minerals. Fig. 4 also indicates a decrease in the percentage of minerals of carbonates and elements since a considerable part of them was known from the previous period.

The distribution of mineral discoveries on the world map shows that the USA obtained unquestionable leadership with 385 discovered minerals (incl. 234 IMA approved) from 1800 to 1949 (Fig. 6). In Latin America, the largest amount of minerals was discovered in Chile (59 minerals with only 8 non-approved by IMA). In Europe, similarly to the Ancient period, Germany (191, incl. 153 IMA approved), Italy (121, incl. 99 IMA approved), and the United Kingdom (107, incl. 70 IMA approved) have the lead in mineral discoveries, together with Sweden, which has discovered approximately 126 minerals (incl. 103 IMA approved). This period is also marked by the development of mineralogical knowledge in Russia, where nearly 81 minerals were discovered (incl. 51 IMA approved). The first mineralogical discoveries took place in Australia.

This period is characterized by a significant interest in mineralogy, resulting in numerous monographs on mineralogy and classifications of minerals by René Just Haüy (1743-1822), Johann Friedrich Ludwig Hausmann (1782-1859), François Sulpice Beudant (1787-1850), Wilhelm Karl von Haidinger (1795-1871). One of the most important works was “A System of Mineralogy” by James Dwight Dana, which was published eight times with the first edition in 1837 and the last in 1997. In January 1916, the first issue of the scientific journal American Mineralogist was published.

Although interest in mineralogy increased significantly during 1800-1949, there was no sharp increase in the number of minerals until the discovery of X-ray powder diffraction in 1916-1917 (Hull 1917) and electron microprobe in 1944 (Hillier and Baker 1944) that had changed the history of mineralogy forever.

The modern period of rapid development (1950-present). The modern period of mineralogical development is characterized by a significant increase in the number of minerals up to ~4,500 of IMA-approved species. The rapid growth is associated with the discovery of new physical methods of mineral identification, such as X-ray powder diffraction in 1916-1917 (Hull 1917), preceded by Bragg's law development in 1912-1913 (Bragg 1913) and electron microprobe introduced in 1944 (Hillier and Baker 1944). According to Fig. 1, the rapid growth of many mineral species started in the 1950s, but X-ray powder diffraction and electron microprobe were discovered several years earlier. Therefore, it takes at least ten years for a new analysis method to reach its full potential. Bulakh et al. (2003) pointed out the uptake of XRD and microprobe, but also the centralization of mineral discoveries among a small group of researchers.

Fig. 1 also indicates that this rapid increase is somewhat uneven and can be described with a waveform curve with peaks at the end of the 1960s, in the 1980s and the 2010s, and with minima in the 1970s and 1990s. These peaks are also mentioned by Barton (2019) and attributed to a variety of factors: the increase of academia role, the evolution of discovery methods, the advent of computers that made crystal structure determination easier, creation of U. S. National Science Foundation (NSF), American uranium exploration boom, etc. The anomaly was in 2012 when a major review article on amphibole nomenclature was published (Hawthorne et al. 2012). Nearly 40% of the discovered minerals in 2012 were silicates (90, incl. 73 IMA approved).

The distribution of minerals by classes after 1950 changed slightly compared with the Sustainable development period (1800-1949). Thus, the contribution of minerals of sulfides and sulfosalts, phosphates, and elements increased by 2-3%, while the percentage of sulfates and oxides decreased correspondingly.

After 1950, many minerals (893, incl. 777 IMA approved) were discovered on the territories of the modern Russian Federation (Fig. 7), while 716 minerals (incl. 599 IMA approved) were discovered in the USA. Contrasted with the previous period, mineral exploration in Canada (250, incl. 218 IMA approved) and Australia (176, incl. 147 IMA approved) has significantly intensified. In addition, almost all countries in Africa and Latin America discovered new minerals, with Chile (91, incl. 87 IMA approved) and Namibia (115, incl. 100 IMA approved) at the top of the leaderboard.

In Europe, the highest number of minerals was discovered in Italy (295, incl. 271 IMA approved), followed by Germany (249, incl. 209 IMA approved), the Czech Republic (103, incl. 90 IMA approved), France (100, incl. 89 IMA approved), and Sweden (96, incl. 81 IMA approved). Consequently, the number of new minerals in the UK decreased prominently compared to the previous period. On the other hand, in Asia, the highest number of new minerals was registered in China (229, incl. 140 IMA approved) and Japan (170, incl. 142 IMA approved).

During this period, there were many essential mineralogy developments triggered by the rapid increase in the number of minerals and, as a result, stimulated new mineral discoveries. First and foremost, it is the foundation of the International Mineralogical Association (IMA), the foundation of the Joint Committee on Powder Diffraction Standards (JCPDS), beginning of the mindat.org database, which went online in October 2000.

Besides the new releases of the Dana classification, many new important works were published, such as "An Index of Mineral Species and Varieties Arranged Chemically" by Max H. Hey (Hey 1950), "Rock-Forming Minerals" series by W.A. Deer, Howie, and J. Zussman (Deer 1962b, 1962a; Deer et al. 1963b, 1963a, 1982, 1997b, 1997a, 2001), "Mineralogical Tables" by H. Strunz and E. Nickel (Strunz and Nickel 2001), "Glossary of Mineral Species" by Michael Fleischer (Fleischer 1995), "Crystal Chemical Classification of Minerals" by A.S. Povarennykh (1972), "Structural mineralogy" (Lima-de-Faria, 2013).

Correlation between discovery rate and mineral rarity

The mineral discovery rate was further analyzed in light of mineral rarity using the taxonomy proposed by Gavryliv et. al. (in preparation) and the mineral occurrence data provided by MED. Accordingly, minerals recorded at exactly one locality are considered endemic, between 2 and 16 localities are considered rare, and those recorded at more than 16 localities are ubiquitous (Fig. 8).

The dominance of rare minerals characterizes the last 50 years of mineral discovery history. The discovery rate of each rarity group shows different patterns depending on its taxonomic position. There were few peaks in the discovery rate of common minerals during the Sustainable development and Modern period of rapid development: 1832 (31 IMA species), 1845 (37 IMA species), 1868 (24 IMA species), and between the 1950s and 1980s (414 IMA species in total). As shown previously, these anomalies are linked to crucial publications in classification mineralogy and the development of new analytical methods.

All the 100 most ancient minerals approved by IMA (Table 1) occur at more than 16 localities, thus being ubiquitous species. The only exception is phosphorus, since the term was used to describe various compounds of phosphorus, but not native phosphorus, which was discovered in the late 20th century in only one location — the Saline Township meteorite. Many other minerals significant as metal ores, such as pyrite, chalcopyrite, bornite, and tetrahedrite, were described and mentioned in the famous book "De Re Metallica" (Agricola 1546) or even before (Table 1).

According to the same data, the most recent ubiquitous minerals are clino-suenoite $\square\{Mn^{2+}_2\}\{Mg_5\}(Si_8O_{22})(OH)_2$, described in 2017, and zincolivenite $CuZn(AsO_4)(OH)$, described in 2006. While these mineral names were created during the last two decades, they are already recorded at nearly 100 different localities. However, prior to the approval of zincolivenite, the names "zinc-olivenite", "Zn-olivenite", "cuproadamite" or "cuprian adamite" were also used for Znbearing olivenites with unspecified Zn:Cu ratios suggesting that the true discovery year of zincolivenite might belong to the period of Sustainable development. Furthermore, clino-suenoite is not a newly discovered species but a new root name that replaces the IMA-discredited manganocummingtonite, initially described in 1966 by Hugo Strunz. Taking into account these discrepancies, the most recent ubiquitous mineral is phosphohedyphane $Ca_2Pb_3(PO_4)_3Cl$ — phosphate analog of hedyphane, approved in 2006 and already recorded at more than 80 localities.

Completely different behavior is observed for rare and endemic species: the discovery rate of rare minerals starts to ascend in the Modern period of rapid development, and the rate of endemic minerals is right-skewed. In contrast, discovery rate of rare species is moderately right-skewed with two significant peaks in the 1980s and 2000s (Fig. 8). The discovery rate of ubiquitous minerals almost completely disappeared after the 1990s. Historically, two of the most ancient endemic species are carbon-hydrogen minerals: phylloretine $C_{18}H_{18}$, described in 1839 by Ørsted (1839), and dinite $C_{20}H_{36}$ — an alicyclic saturated hydrocarbon with three condensed cycles in the formula unit, found within a lignite deposit in the Garfagnana valley (northern Tuscany, Italy) first described by Petri (1852) and redefined later by Franzini et. al. (1991). The other members of the hydrocarbons group — fichtelite $C_{19}H_{34}$, kratochvílite $C_{13}H_{10}$ and evenkite $C_{21}H_{44}$ — occur at less than 9 localities, thus being rare. The other organic minerals containing N or O are also rare: flagstaffite $C_{10}H_{22}O_3$ (1 locality), refikite $C_{20}H_{32}O_2$ (4 localities), guanine $C_5H_5N_5O$ (7 localities), uricite $C_5H_4N_4O_3$ (15 localities). These hydrocarbons have been identified from coal, black shale, or other carbon-rich fossil sources therefore referred to as the biomineralization stage of the Phanerozoic era (Hazen et al. 2008). It is pointed out that during Phanerozoic, biological processes dominated the mineralogical diversification of the Earth’s surface.

While the publications of several fundamental works might explain the general increase in discovery rate after 1950, the KDE (Kernel density estimate) shapes reflect the discovery rate patterns characteristic of each rarity group (Fig. 8). Obviously, the bulk of widespread minerals is already discovered, since there are no significant discoveries of these species observed since the 1990s. On the other hand, the discovery of rare species is still progressing, and the rate of endemic minerals is even higher due to the adoption of new high-resolution analytical techniques and the study of hard-to-reach locations.

Accordingly, the discovery rate during the Sustainable development period is largely dominated by the discovery of ubiquitous minerals. It is suggested that the discovery of these species reflects the publications of significant mineralogical works. This pattern is different for the Modern period of rapid development, where the discovery rate is dictated mainly by rare minerals while the rate of ubiquitous minerals follows this trend at lower grade until the 1980s. The discovery rate of rare minerals is directly correlated with the discovery and adoption of new physical analytical methods. Completely different behavior of the discovery rate is observed for the endemic species — the number of discoveries gradually increased from 1800 until the 2000s, when the number of endemic species discovered started to ascend at an even higher grade. Since most endemic species are of nano- to micro scale with a restricted P-T-X range found within zones of extreme geochemical environments, their discovery rate is probably linked with the acceleration of study of hard-to-reach locations, in addition to the adoption of high-resolution analytical techniques.

Implications

During the last decade, data science has become a tool that allows us to turn raw data into insight and knowledge. Data tidying, transformation, and visualization are the typical steps in obtaining meaningful results and interpretation. However, before going any further with “clean” data, it is an asset to describe the data, identify anomalies, and create a robust data model prototype. Commonly, these scalable models are used to answer precise questions and communicate the results with others. Further, a model with a collection of filtered data may be fitted in and applied to new data for making predictions by machine learning techniques and recently applied LNRE (a large number of rare events) analysis (Hazen et al. 2015; Hystad et al. 2015a, 2015b). In the paper, we used an approach to organize a robust data structure that parallels the relationships within the data and then created a working model, allowing to access these relationships - an essential step before making a prediction analysis which is a work in progress. The data on the dynamics of mineral discovery (Fig. 1 and Fig. 2) was classified into three distinct periods: 1) Ancient period (up to 1800, excluding), characterized by the absence of a stable record of mineral discovery or description, and the negligible total number of minerals; 2) Sustainable development period (1800-1949), during which there was a steady record of mineral discovery and a moderate increase in the number of minerals; 3) Modern period of rapid development (1950-present) when the number of minerals has snowballed as a result of the progress of physical analytical methods. Spatial analysis of the data showed that the distribution of mineral discoveries on the world map is rather heterogeneous, depending not only on the country's geology, but also on the area, population, economic development, and general interest in mineralogy.

The analysis of mineral rarity during each period of the discovery history indicates a direct influence of the introduction of new analytical techniques or significant publications in mineralogy on the discovery of species of particular rarity. Accordingly, the bulk of widespread minerals was discovered during the period of Sustainable development, which is characterized by the publications of fundamental mineralogical classifications or encyclopedias, while the majority of rare and endemic minerals were discovered during the Modern period of rapid development, which is characterized by the introduction of new high-resolution analytical techniques and study of hard-to-reach locations.

To summarize, our research has passed the stage of creating a robust data model - the last step before performing the analysis of mineral rarity as well as predictive analysis that is currently in progress. With the relationships reported in this paper, we aimed to solidify our understanding of the data and achieve meaningful results before analyzing them with the mineral rarity. For predictive modeling, the following studies will focus on chemical data and the Nickel-Strunz class populations. The latter can bring insight into the following topics: which ions are the rarest, which mineral class is the most undiscovered, what is the probability of discovering a mineral with a predefined set of ions, and where it is more likely to be discovered.

Acknowledgments

We sincerely thank Shaunna Morrison, Andrew G. Christy, and two anonymous reviewers for a thorough review, valuable comments, and corrections that helped us improve the paper. The project received funding from the European Union's Horizon 2020 research and innovation Programme based on a grant agreement under the Marie Skłodowska-Curie scheme No. 945478 and was supported by the Slovak Research and Development Agency (contract APVV-19-0065).

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Figure Captions

Fig. 1. Timeline of the mineral discovery process, displaying the year of discovery or at least the earliest year of mineral publication, including the distribution between approved and non-approved IMA mineral species, as well as their cumulative curves.

Fig. 2. Cumulative curves of mineral discoveries by Nickel-Strunz classes.

Fig. 3. Number of minerals discovered by country and the distribution by Nickel-Strunz classes. All political location boundaries are from Plot.ly library (https://plot.ly).

Fig. 4. Distribution of minerals by classes for each period of mineral discoveries and a sum for all periods.

Fig. 5. Map showing the number of minerals discovered by country and the distribution by Nickel-Strunz classes from prehistoric times till 1800 exclusively. All political location boundaries are from Plot.ly library (https://plot.ly). *Note: pie-charts are shown only for top-6 countries which contributed to mineral discoveries.*

Fig. 6. Map showing the number of minerals discovered by country and the distribution by Nickel-Strunz classes from 1800 to 1949. All political location boundaries are from Plot.ly library (https://plot.ly). *Note: pie-charts are shown only for top-10 countries which contributed to mineral discoveries.*

Fig. 7. Map showing the number of minerals discovered by country and the distribution by Nickel-Strunz classes from 1950 till present. All political location boundaries are from Plot.ly library (https://plot.ly). All political location boundaries are from Plot.ly library (https://plot.ly). *Note: pie-charts are shown only for top-15 countries which contributed to mineral discoveries.*

Fig. 8. The discovery rate of endemic (recorded at 1 locality), rare (recorded at 2–16 localities) and ubiquitous (recorded at more than 16 localities) rarity groups with KDE curves.

Tables

Table 1. 100 of the oldest mineral names.

Modern Mineral Name[a]	Named date	First usage date	Status	Country of discovery	First known use
Emerald	Ancient times	1500 BC	Beryl var	Egypt	jewelry
Onyx	Ancient times	2890 – 2686 BC (Egypt as early as the Second Dynasty)	Quartz var	Egypt	carving
Clay	Ancient times	3000 BC	Group name	Japan	ceramics
Tin	Ancient times (mineral name was known since antiquity and predates any formal descriptive publication)	3000 BC (in synthetic form)	Grandfathered, Approved	Central Asia	metal
Bitumen	Ancient times	5000 BC	Mineraloid	Pakistan	waterproofing
Jasper	Ancient times	5000 BC	Quartz var	Pakistan	bow drills
Nephrite	Ancient times	7000 - 5000 BC (Early Neolithic)	Tremolite - Actinolite var	Europe	tools / jewelry
Sapphire	Ancient times	800 BC or earlier	Corundum var	Iran	jewelry
Minium	Ancient times	Ancient times	Grandfathered, Approved	Germany	pigment
Beryl	Ancient times	Ancient times	Grandfathered, Approved	unknown	jewelry
Alabaster	2600 – 2000 BC (Old Egyptian as’"alabastra”)	before 2000 BC (Ancient Egypt)	Gypsum var	Egypt	carving
Niter	3150 - 332 BC (Ancient	3150 - 332 BC (Ancient Egypt - historically, the term “niter” was	Grandfathered,	Egypt	cleaning product

	Egypt)	not well differentiated from “natron”)	Approved		
Natron	3150 - 332 BC (Ancient Egypt)	3150 - 332 BC (Ancient Egypt)	Approved	Egypt	cleaning product
Topaz	Ancient Greece (3000 BC-476 BC)	Ancient times	Grandfathered, Approved	unknown	jewelry
Phosphorus	Ancient Greece (refers to planet Venus, because the element was unknown in ancient time)	Discovered by the German alchemist Hennig Brand in 1669 as element, but in nature first reported in 1903 from the Saline Township meteorite	Grandfathered, Approved	USA (for native phosphorus)	not used in elemental form
Mercury	300-325 BC (first used by Theophrastus)	1500 BC	Grandfathered, Approved	Egypt	cosmetics
Hematite	300-325 BC (first used by Theophrastus)	164000 BC	Approved	South Africa	pigment
Gypsum	300-325 BC (first used by Theophrastus)	3150 - 332 BC Ancient Egypt	Grandfathered, Approved	Egypt	building material
Chrysocolla	300-325 BC (first used by Theophrastus)	Ancient times	Approved	unknown	flux / jewelry
Cinnabar	300-325 BC (first used by Theophrastus)	Antiquity	Grandfathered, Approved	Egypt	cosmetic
Agate	300-325 BC (first used by Theophrastus)	2700 – 1100 BC (Minoan culture)	Quartz var	Italy	carving
Amethyst	323 - 31 BC (from Koine Greek)	3150 - 332 BC Ancient Egypt	Quartz var	Egypt	jewelry
Diamond	16 AD (by Manlius)	4000 BC	Grandfathered, Approved	India	jewelry
Pyrite	50 AD (by Dioscorides)	7000 - 5000 BC (Early Neolithic)	Grandfathered, Approved	unknown	source of ignition / jewelry
Asbestos	60—79 AD (by Pliny the Elder)	2500 BC	Amphibole Group var	Finland	ceramics
Jet	60—79 AD (by Pliny the Elder)	10000 BC	Mineraloid	United Kingdom	jewelry
Opal	60—79 AD (by Pliny the Elder)	4000 BC	Grandfathered, Approved	Ethiopia	jewelry
Lead	60—79 AD (Named plumbum nigrum by Pliny the Elder, but the name was for the chemical element and not a mineral)	7000–6500 BC	Grandfathered, Approved	Sweden	metal
Heliotrope (also known as bloodstone)	60—79 AD (by Pliny the Elder)	3000 BC-476 BC (Ancient Greece)	Quartz var	Greece	jewelry
Galena	60—79 AD (by Pliny the Elder)	3000 BC	Grandfathered, Approved	Egypt	cosmetic / ore
Obsidian	60—79 AD (by Pliny the Elder)	700000 BC	Rock name	Kenya	tools
Malachite	60—79 AD (by Pliny the Elder as 'molochitus')	1800 BC	Grandfathered, Approved	United Kingdom	pigment / decorative stone

Calcite	60—79 AD (by Pliny the Elder)	Ancient Egyptians (but probably earlier)	Grandfathered, Approved	Egypt (?)	carving
Glass	300-500 AD	3600 BC	Mineraloid (usually synthetic)	Western Asia	jewelry
Gold	700–1000 AD (An early mention in the Beowulf)	40000 BC	Grandfathered, Approved	Spain	jewelry
Iron	700–1000 AD (An early mention in the Beowulf)	5000 BC (Beads made from meteoric iron in 3500 BC or earlier were found in Gerzah, Egypt)	Grandfathered, Approved	China (Egypt in native form)	metal
Coal	1253	4000 BC (Neolithic China)	Rock name	China	fuel
Ruby	1300	200 BC or earlier	Corundum var	Asia	jewelry
Arsenic	1310	5000 BC (Bronze Age)	Grandfathered, Approved	Iran	alloys
Garnet	14th-century	3000 BC	Group name	unknown	jewelry / abrasives
Carnelian	14th-century word "cornelian"	10000 - 9000 BC (Early Neolithic)	Quartz var	Bulgaria	jewelry
Amber	14th-century	21000 - 17000 BC (Solutrean culture)	Mineraloid	France, Spain, Portugal (Solutrean region)	jewelry
Sulfur	1390	6000 BC	Grandfathered, Approved	China	medicine
Realgar	1390s	Ancient Greece	Grandfathered, Approved	unknown	pigment
Schorl	1400	Ancient times	Approved, Renamed	Germany	jewelry
Electrum	late 14th-century (The same word was also used for the substance amber)	3000 BC (in Old Kingdom of Egypt)	Gold var	Egypt	metal
Silver	1478	Antiquity	Grandfathered, Approved	unknown	metal
Bismuth	1500 (but was officially discovered in 1753)	Ancient times	Grandfathered, Approved	Germany	metal
Quartz	1505	10000 - 9000 BC (Early Neolithic)	Approved	unknown	jewelry
lodestone	1515	6th century BC	Magnetite var	Greece	uncertain
Zinc	1526	14th to 10th centuries BC	Grandfathered, Approved	Chile (for native zinc)	metal
Copper	1530	8000 BC	Grandfathered, Approved	Iraq	metal
Chalcedony	1546	1800 BC	Quartz var	Turkey	jewelry
Citrine	1546	300 - 150 BC	Quartz var	unknown	jewelry
Salammoniac	1546 (in Pseudo-Geber work “De inventione veritatis”)	3150 - 332 BC Ancient Egypt	Approved, Renamed	Egypt	food
Almandine	1546	Ancient times	Grandfathered,	Turkey	jewelry

			Approved		
Talc	1546 (by Georgius Agricola)	Ancient times	Grandfathered, Approved	Persia (?)	ceramics (?)
Serpentine	1546 (by Georgius Agricola)	7000 - 5000 BC (Early Neolithic)	Group name	unknown	carving
Wolframite	1546 (by Georgius Agricola)	Unknown	Hübnerite-Ferberite var	unknown	ore
Anthracite	16th-century	Ancient times	Mineraloid / Coal var	Wales	fuel
Jade	1565	6000 BC	Nephrite and Jadeite var	China	jewelry
Aquamarine	1590s (?)	Ancient times	Beryl var	unknown	jewelry
Turquoise	17th century	Ancient Egyptians (but probably earlier)	Grandfathered, Approved	Egypt (?)	jewelry
Wood Opal	1601 (?)	Unknown	Opal var	Austria (?)	carving (?)
Lapis Lazuli	1636	7000 BC	Rock name	Afghanistan	jewelry
Kaolinite	1637	Ancient times	Approved	China	ceramics
Ametrine	16th-century (due to legend)	Unknown	Quartz var	Bolivia (due to legend)	jewelry
Rubicelle	1653	Ancient times	Spinel var	unknown	jewelry
Bristol Diamonds	1654	Ancient times	Quart var	United Kingdom	jewelry
Calomel	1655	854–925 AD (by Rhazes)	Grandfathered, Approved	Syria	medicine
Chert	1679	Ancient times	Rock name	unknown	tools
Peridot	1705	300 BC (St. John's Island in the Red Sea)	Forsterite var	Egypt (?)	jewelry
Mica	1706	40000 BC to 10000 BC (the Upper Paleolithic)	Group name	unknown	cave paintings
Tourmaline	1707	1500s (but probably was known in ancient Egypt)	Group name	Brazil	jewelry
Wad	1709	Unknown	Mineraloid	United Kingdom	uncertain
Corundum	1725 (Known by many names in ancient times)	Ancient times	Grandfathered, Approved	India	jewelry
Chalcopyrite	1725	3000 BC (Bronze Age)	Grandfathered, Approved	unknown	ore
Orpiment	1747 (by Wallerius)	1300 BC (Tutankhamun's tomb)	Grandfathered, Approved	Egypt	pigment
Calamine	1747 (by Wallerius)	16th century	Synonym of Hemimorphite, Hydrozincite, Smithsonite	United Kingdom	ore
Selenite	1747 (by Wallerius)	Ancient Greece (but probably earlier)	Gypsum var	unknown	jewelry
Psilomelane	1747 (by Wallerius)	Unknown	General term	unknown	ore
Molybdenite	1747 (by Wallerius)	Unknown	Grandfathered,	unknown	uncertain

			Approved		
Antimony	3000 BC-476 BC	3100 BC (predynastic Egypt in the form of stibnite), Pliny the Elder described the native antimony, but probably of synthetic origin, the first description of natural native antimony was in 1783 in Sweden	Grandfathered, Approved	Sweden (in native form)	cosmetics (in the form of stibnite)
Platinum	1750	600 BC - AD 200	Grandfathered, Approved	Colombia	jewelry
Borax	1753	8th century AD	Grandfathered, Approved	India	uncertain
Oriental Amethyst	1753	Ancient times	Corundum var	Asia	jewelry
Chiastolite	1754 (predates the description of its parental species andalusite by 44 years!)	16th century	Andalusite var	Spain	jewelry
Zeolite	1756	Unknown	Group name	Sweden	uncertain
Flos Ferri	1768	Unknown	Aragonite var	Austria	uncertain
Pitchblende	1770	15th century	Uraninite var	Germany/Czech Republic	ore
Trona	1773	Ancient times	Grandfathered, Approved	Sweden (?)	food (?)
Améthiste Basaltine (of Sage)	1777	Unknown	Apatite var	Germany	jewelry
Spinel	1779	Ancient times	Grandfathered, Approved	unknown	jewelry
Labradorite	1780	1770's	Anorthite var	Canada	jewelry
Adularia	1780	Ancient times	Feldspar var	Switzerland	jewelry
Adamantine Spar	1780 (?)	Unknown	Corundum var	unknown	jewelry
Zircon	1783	Ancient times	Grandfathered, Approved	unknown	jewelry / ceramics
Tiger's Eye	1784	Ancient times	Quartz var	South Africa	jewelry
Alabandite	1784	Ancient Greece (but probably earlier)	Grandfathered, Approved	Romania / Turkey	ceramics
Apatite	1786	Ancient times	Group name	Germany	jewelry

Notes: “var” is a shortcut of variety;

(?) means uncertainty;

[a] the older name correlates with the more modern usage.

Figure 1

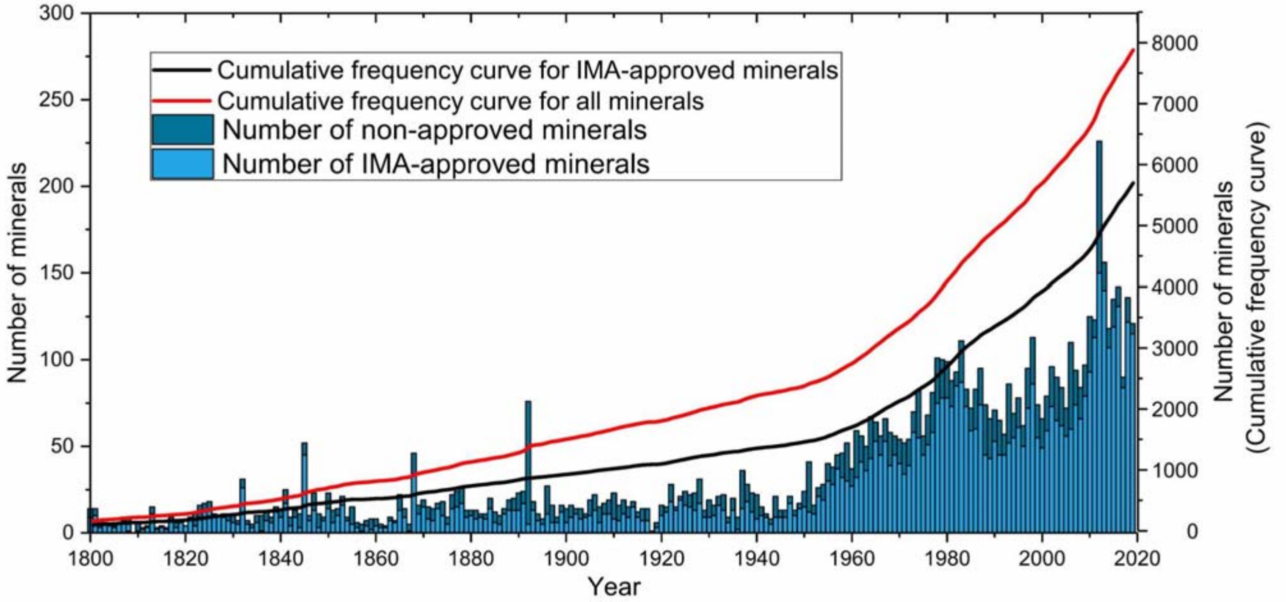

Cumulative frequency curve for IMA-approved minerals
Cumulative frequency curve for all minerals
Number of non-approved minerals
Number of IMA-approved minerals
Number of minerals
0
50
100
150
200
250
300
Number of minerals (Cumulative frequency curve)
0
1000
2000
3000
4000
5000
6000
7000
8000
Year
1800
1820
1840
1860
1880
1900
1920
1940
1960
1980
2000
2020

Figure 2

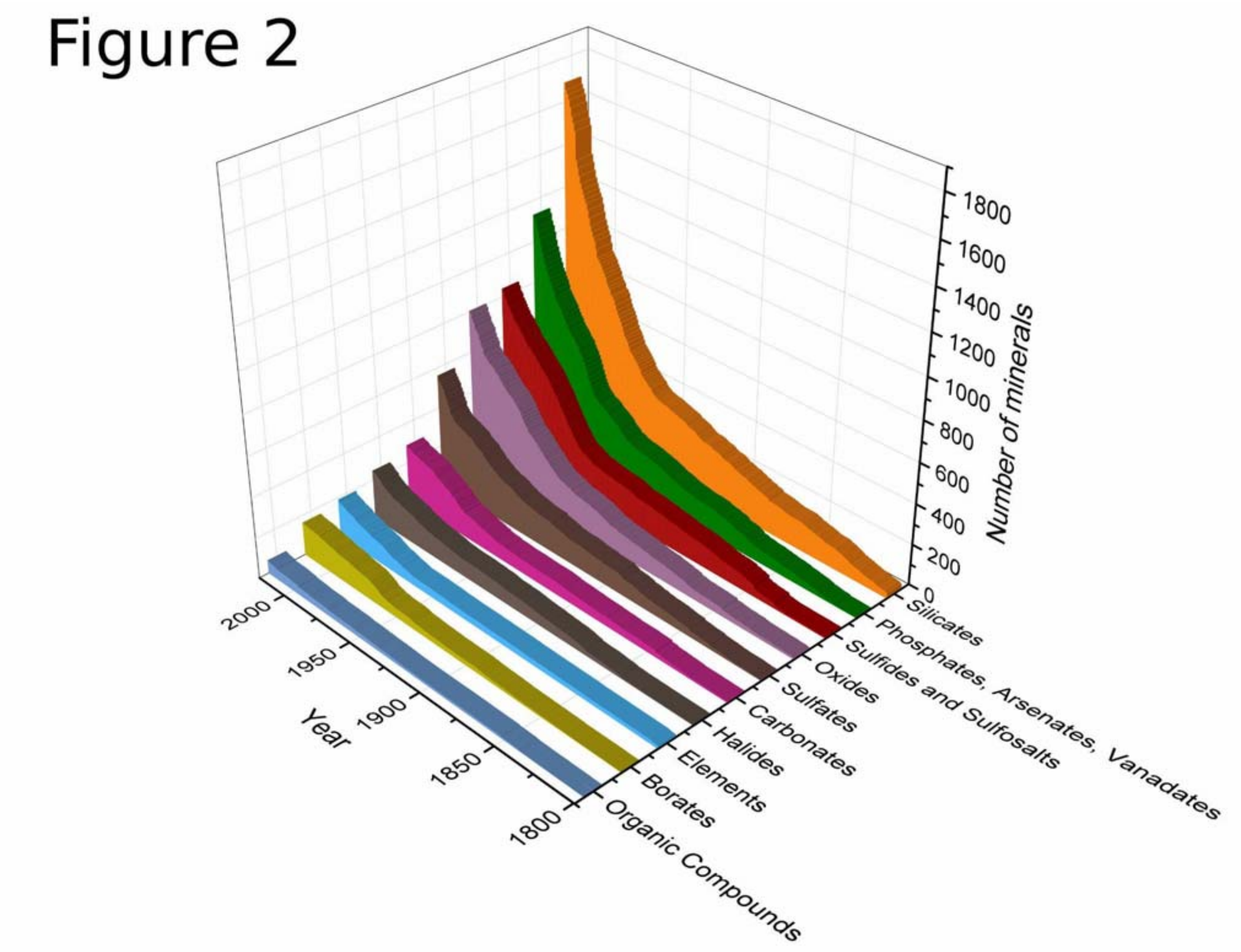


Figure 3

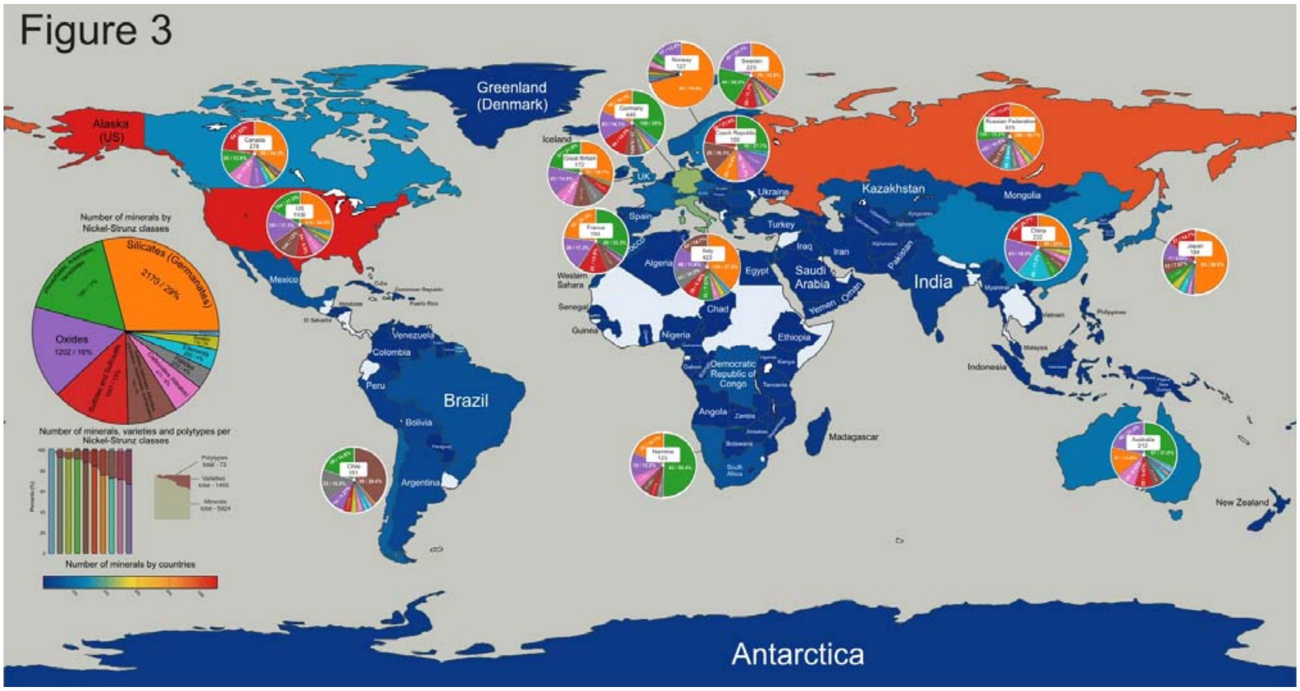


Figure 4

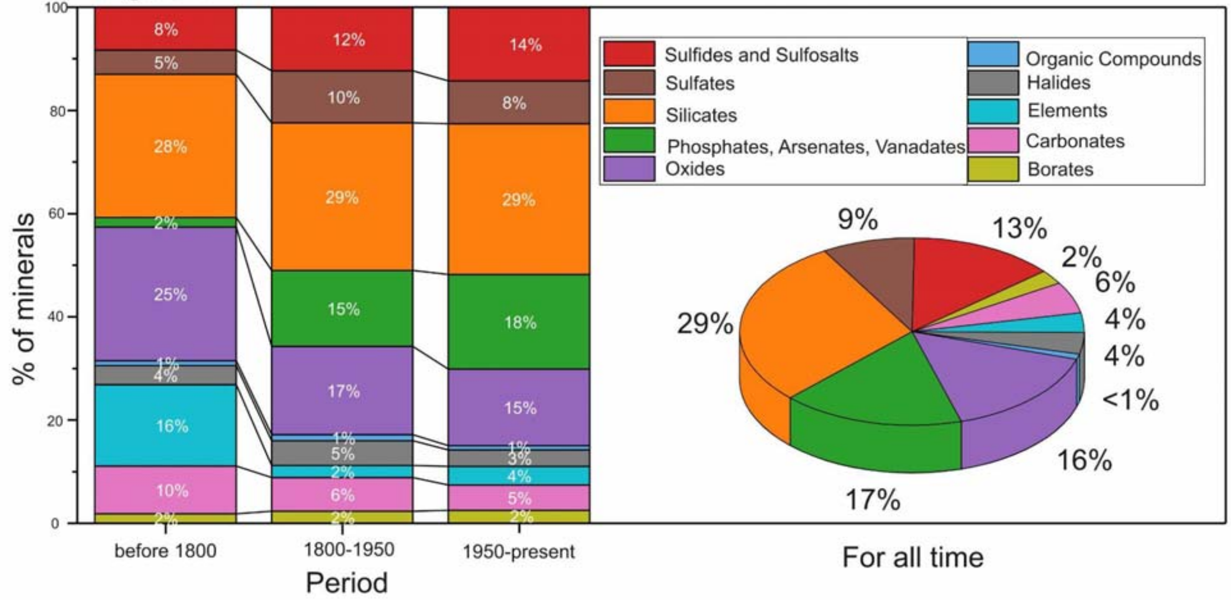


Figure 5

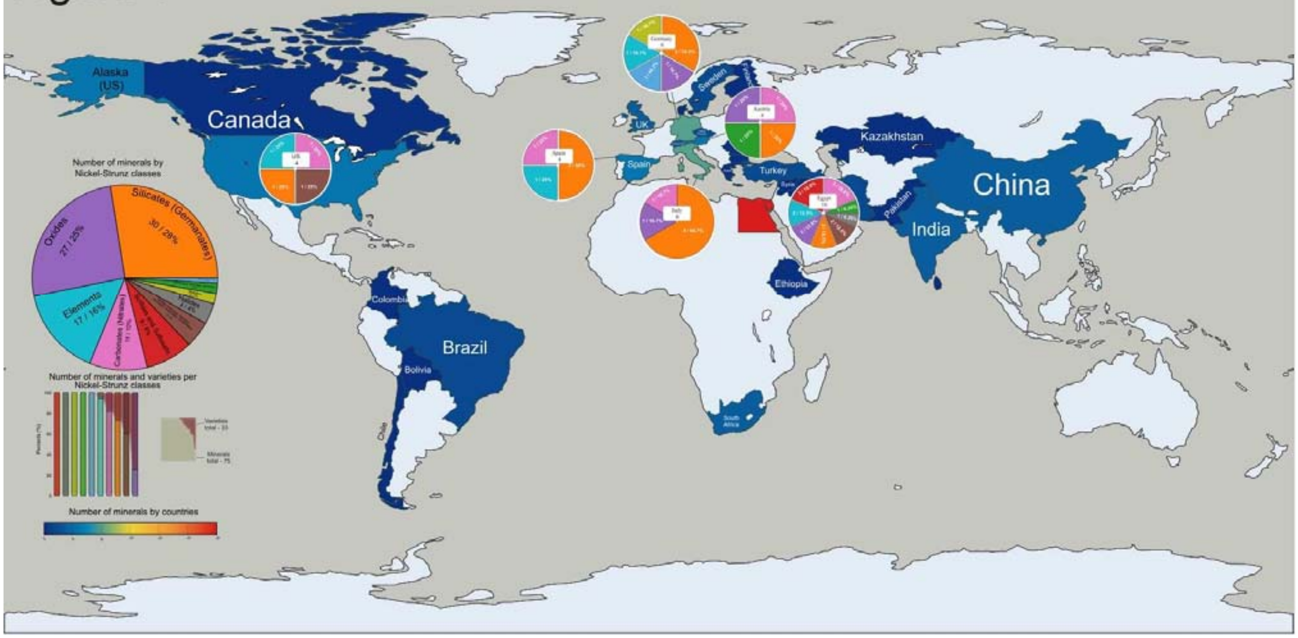


Figure 6

Figure 7

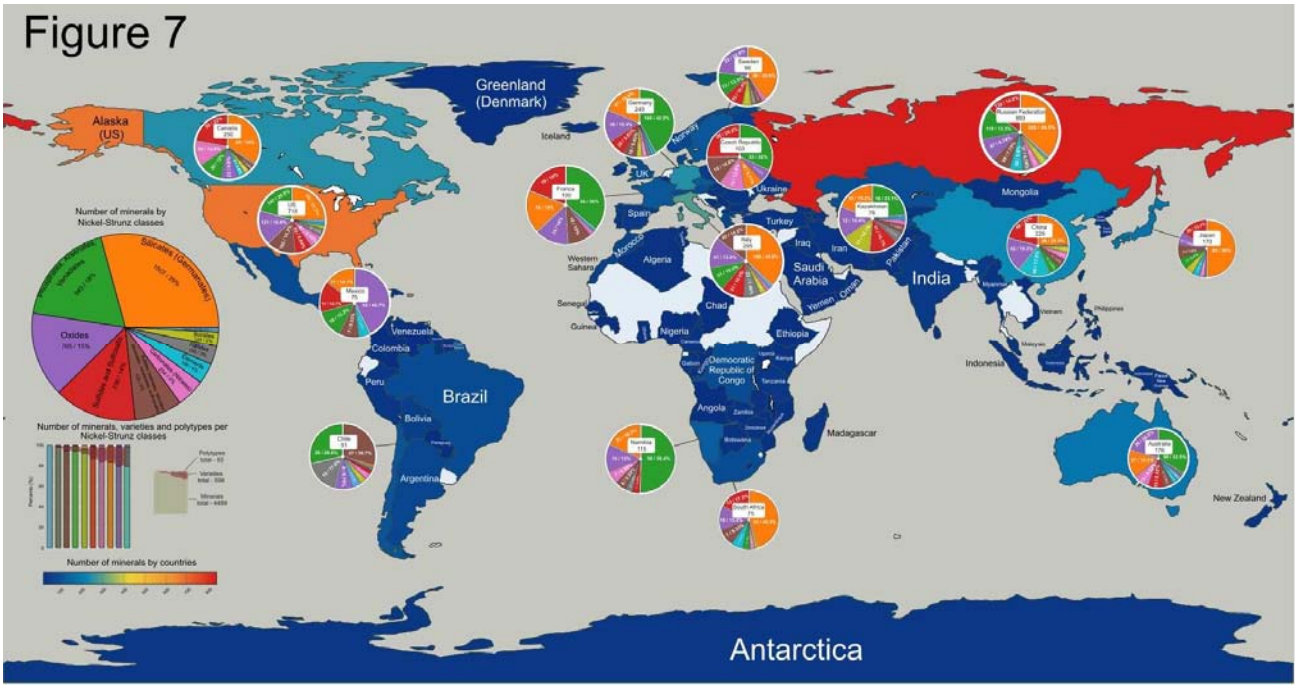
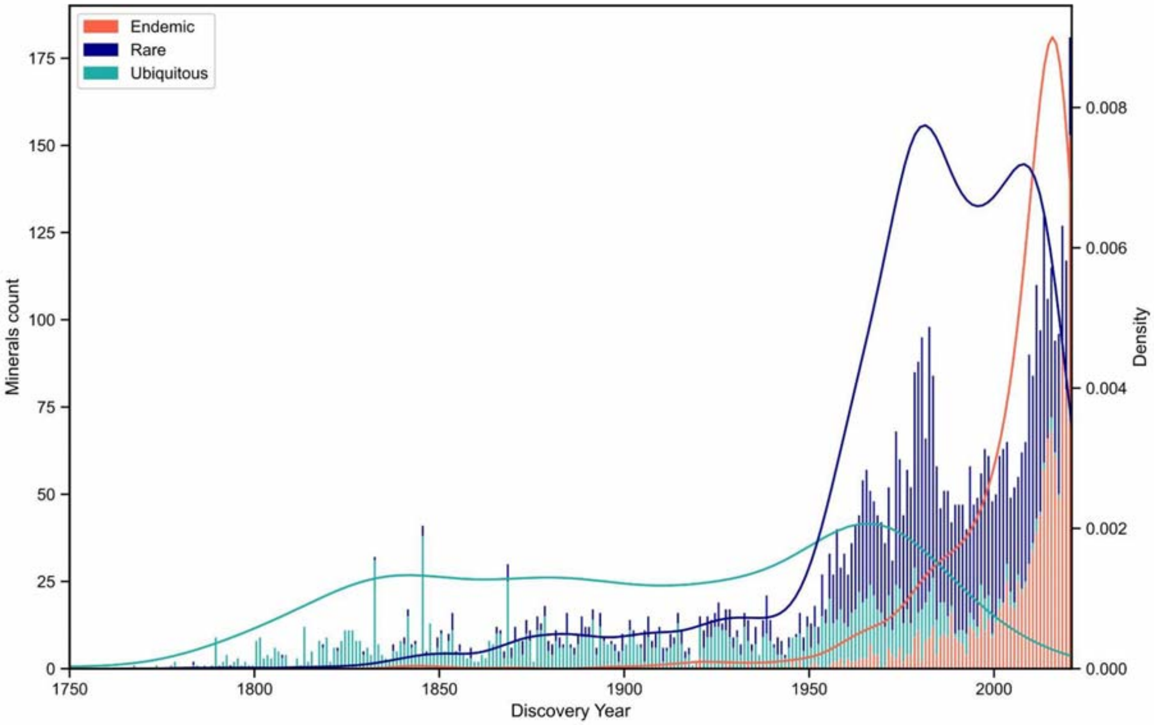


Figure 8


Endemic
Rare
Ubiquitous
Minerals count
0
25
50
75
100
125
150
175
Density
0.000
0.002
0.004
0.006
0.008
1750
1800
1850
1900
1950
2000
Discovery Year

691