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Critical mineral geochemical database development and management

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2022

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Permanent link: https://doi.org/10.4095/329924

This publication is available for free download through GEOSCAN (https://geoscan.nrcan.gc.ca/).

Recommended citation
Gadd, M.G., Lawley, C.J.M., Lauzière, K., Létourneau, F., Pilote, J.-L., Morin, A., and Haji Egeh, A., 2022. Critical mineral geochemical database development and management; Geological Survey of Canada, Open File 8883, 1 .zip file. https://doi.org/10.4095/329924

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Critical mineral geochemical database development and management

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Introduction

Critical minerals and the elements hosted within them are now a focal point in geological survey research. Criticality is based on supply chain stability, element/mineral functionality (most associated with ”green technologies”) and economic importance. Accordingly, Canada has developed a list of 31 critical minerals (i.e., Al, Bi, Co, Cr, Cs, Cu, fluorspar, Ga, Ge, graphite, He, In, Li, Mg, Mn, Mo, Nb, Ni, potash, platinum-group elements (PGE), rare earth elements (REE), Sb, Sc, Sn, Ta, Te, Ti, W, U, V, Zn) that is built on a criteria-based approach that recognizes export opportunities and security requirements, while highlighting the potential to build valuable domestic manufacturing (e.g., battery supply chains). Inclusion on the list satisfy the following criteria: 1) Canada’s geological potential for supplying critical minerals to strategic partners; 2) essential to Canada’s economic security; and/or 3) required for the low-carbon economy.

To tackle climate change and develop carbon-neutral supply chains, Canada has also committed to collaborating with international partners. One such collaboration is the Critical Minerals Mapping Initiative (CMMI), a trilateral agreement among Canada (Geological Survey of Canada), Australia (Geoscience Australia) and the United States (US Geological Survey). The CMMI aims to promote the understanding of critical mineral science (Kelley, 2020; Emsbo et al., 2021; Lawley et al., 2022). This collaboration has produced a web portal that hosts a database of critical minerals in ores and their chemical compositions, as well as a complete set of web-mapping and querying tools to explore the available data (https://criticalminerals.org). The first version of this data repository consists of archival and legacy data from each of the three countries, and it is anticipated that additional geochemical datasets will be added in the future (Emsbo et al., 2021). This group has also designed a deposit classification scheme that can be used to group similar deposits into different environments, groups, and/or types (Hofstra et al., 2021). The classification provides internal consistency to the geochemistry database, such that it can be queried and analyzed. Thus, it can be used to predict critical mineral abundances of different deposit environments, groups, and/or types, and this will be useful to industry to identify exploration and development opportunities. Below we summarize Canada’s contribution to the critical mineral in ores database and the development of novel data structures to facilitate standardized input of geochemical data into future releases.

Column definitions, vocabularies and template descriptions

Each entry (i.e. row) in the database is grouped within several thematic classes providing a broad spectrum of properties about a given sample. The classes are: 1) deposit information, 2) sample information, 3) mineralogy, 4) sample texture(s), 5) sulfide mineral texture(s), 6) alteration, 7) rock-type 1, 8) rock-type 2, and 9) data source information. Each class is divided into subclasses that capture essential geological information for each entry. The definition for each column is provided in Table 1. Compositional data are described below.

Geological province information is based on a spatial join between the Wheeler et al. (1996) dataset and the sample coordinates. All other deposit and sample information are taken directly from each data source. These descriptions are then broken down into several parts, each of which is valuable in understanding some of the most important characteristics of each sample. We developed and implemented a series of vocabularies to standardize sample descriptions from materials collected from modern and legacy datasets. Each vocabulary consists of a list that is called in drop-down menus to select from a pre-defined set of terms in a lookup table (Table 2). We note that none of the vocabularies are exhaustive and the design of the database allows for updates to be made in the future. Constraints in the database are imposed to use the terms within the linked vocabularies to ensure consistency. The "minerals" vocabulary is populated with 371 common rock-forming minerals (Whitney and Evans, 2010). The "sample texture" and "sulphide texture" classes are populated using the "textures" vocabulary. The textural terms build on the definitions provided in Neuendorf et al. (2005). Ores and mineralized samples are commonly altered from their primary composition. The "alteration" vocabulary lists many common alteration types and their definitions closely follow the GeoSciML standard (http://geosciml.org/). Using the same concepts and vocabularies as GeoSciML has the potential to improve interoperability with other online geoscience data sources (Sen and Duffy, 2005). The final vocabulary pertains to "rock types". Although the collector may provide a rock name, the template is used to describe the highest-level rock type information (i.e. igneous, metamorphic, and sedimentary) and subclasses thereof (e.g. intrusive versus extrusive rocks; felsic versus mafic compositions). Specific rock names are not included within the thesauri, but could be added by a user. The original rock names from the data source are also provided for reference. Linkages to published rock name vocabularies from the GSC or international vocabularies could be defined at a later stage of the project.

The database developed for this initial phase is based on a relational model linking together multiple tables using foreign keys. Look-up tables are used to maintain the vocabulary-based fields within the database. Postgresql (with the PostGIS extension) is the database management system used to store the data and manage the geographic information provided. Samples and deposits are georeferenced using latitude and longitude coordinates based on EPSG 4326 SRS. Samples are also georeferenced by using their corresponding UTM coordinated and UTM zone. The SQL views (i.e., virtual tables that are defined by queries) allow reformatting of the data outputs to meet various external data structure requirements. A view was used to provide CMMI with the required information to populate their data repository.

Geochemical data description

We have compiled a database of 'ore' samples from across Canada (Fig. 1). For this report, 'ore' refers to samples defined by the submitter as containing a relatively high abundances of base, precious, or critical elements. The samples may also be referred to as 'mineralized' or 'ore-bearing'. As a result, the compilation contains a variety of rock and mineral samples that range from weakly mineralized (gangue) rocks to ore concentrates. The rationale for creating this compilation was to initiate a Canada-wide database of mineral deposit lithogeochemistry, driven by the need to better constrain the types of critical mineral deposits and their locations.

We also aimed to introduce a data schema, expressed by a unified modeling language model, that will facilitate the incorporation of lithogeochemical data obtained in future studies. Although this report is a 'static' product, the ultimate goal is the creation (and maintenance) of a continually updated critical minerals in ores database that is freely available to the public (http://criticalminerals.org).

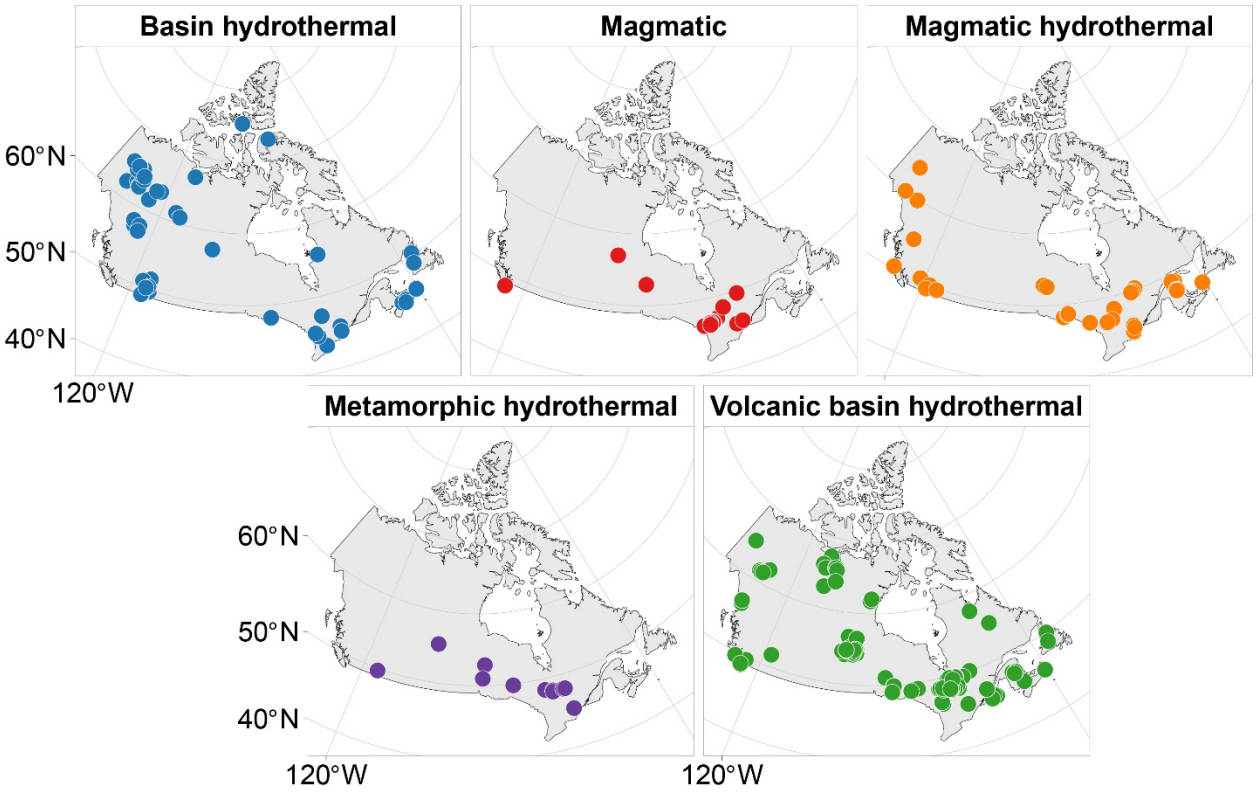

Figure 1: *Deposit environments for samples included in the Canadian critical minerals in ores database.*

The dataset contains 3337 geochemistry samples (Table 3) that are sourced from three previously published multi-component Open Files (i.e., OF5432, OF6578, OF8727). Rock descriptions and other forms of geologically related properties associated with each sample were extracted from the original sources wherever possible, including alteration mineral assemblages (n = 26), sample textures (n > 121), host rock names and types (n > 36), and host rock compositions (n = 4). To improve usability, these attributes are re-classified into a common format using new vocabularies that were generated as part of the current study or adapted from international standards (i.e. GeoSciML). Similarly, each sample has been classified according to a deposit environment (n = 5), deposit group (n = 17), and deposit type (n = 34) by searching for supporting information online (e.g., peer-reviewed papers, government databases and publications, and company documents) using the sample location and the deposit or occurrence name. The deposit classification scheme is described in detail by Hofstra et al. (2021) and a total of 346 deposits or mineral occurrences in Canada were re-classified as part of the current study.

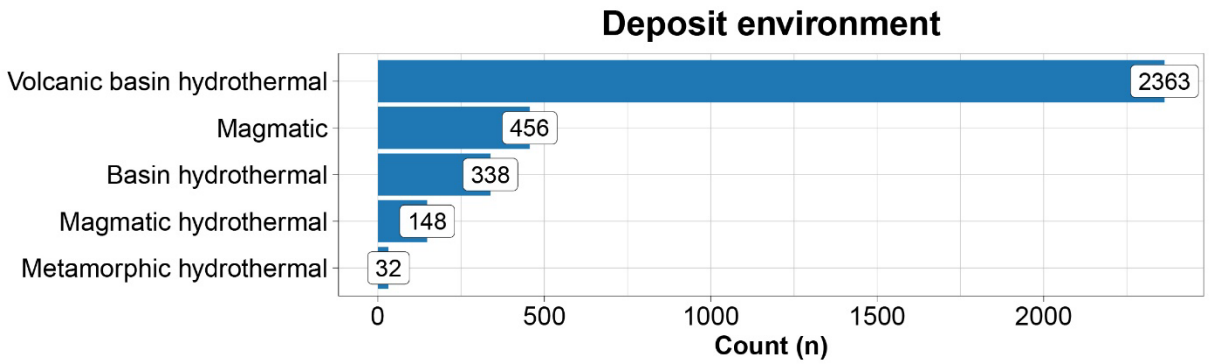

Figure 2: *Sample counts for different deposit environments.*

Overall, the vast majority of samples represent mineral separates (n = 2550) along with lesser core (n = 115), hand sample (n = 329), and unknown sample materials (n = 343). Samples re-classified as "volcanic basin-hydrothermal" are the dominant deposit environment (n = 2363), with bimodal-mafic volcanogenic massive sulphide (VMS) the most abundant deposit type (n = 1786; Figs. 2–3). The geographic distribution of VMS samples are scattered across Canada (Fig. 1). Magmatic deposits are the second most abundant deposit environment (n = 456) with impact-related ultramafic-mafic intrusion Ni-Cu-PGE the major deposit type (n = 434). All of these samples were sourced around the Sudbury Basin (Figs. 1, 3). Basin-hydrothermal deposits are the third most common deposit environment (n = 338) with most of these samples representing Mississippi Valley-type Zn-Pb deposit type (n = 208) from western Canada (Figs. 1, 3).

Compositional data have three informational classes: 1) abundance, 2) analytical method, and 3) detection limit. Abundances are reported in parts per billion (ppb; Au, Hg, Pd, Pt), parts per million (ppm; Ag, As, Ba, Be, Bi, Br, Cd, Ce, Cl, Co, Cr, Cs, Cu, Dy, Er, Eu, F, Ga, Gd, Hf, Ho, In, Ir, La, Lu, Mo, Nb, Nd, Ni, Pb, Pr, Rb, Sb, Sc, Se, Sm, Sn, Sr, Ta, Tb, Te, Th, Tl, Tm, U, V, W, Y, Yb, Zn, Zr) and weight percent [oxide] (pct; Al_2O_3, CaO, CO_2, Fe_2O_3, K_2O, LOI, MgO, MnO, Na_2O, P_2O_5, SiO_2, TiO_2). The analytical methods vary for different elements and the following were used in the reported studies: 1) instrumental neutron activation analysis (INAA); 2) inductively coupled plasma-optical/atomic emission spectrometry (ICP-OES/AES; ICP-ES); 3) inductively coupled plasma-mass spectrometry (ICP-MS); 4) x-ray fluorescence (XRF); 5) ion chromatography (IC); 6) gravimetry (for measuring loss on ignition; LOI). When known, digestion methods are also reported and include $Li_2B_4O_7$ fusion (LBF) and four acid digest (4A). Detection limits are reported for each analyte in the same unit (i.e. ppb, ppm, and weight percent) as the abundance.

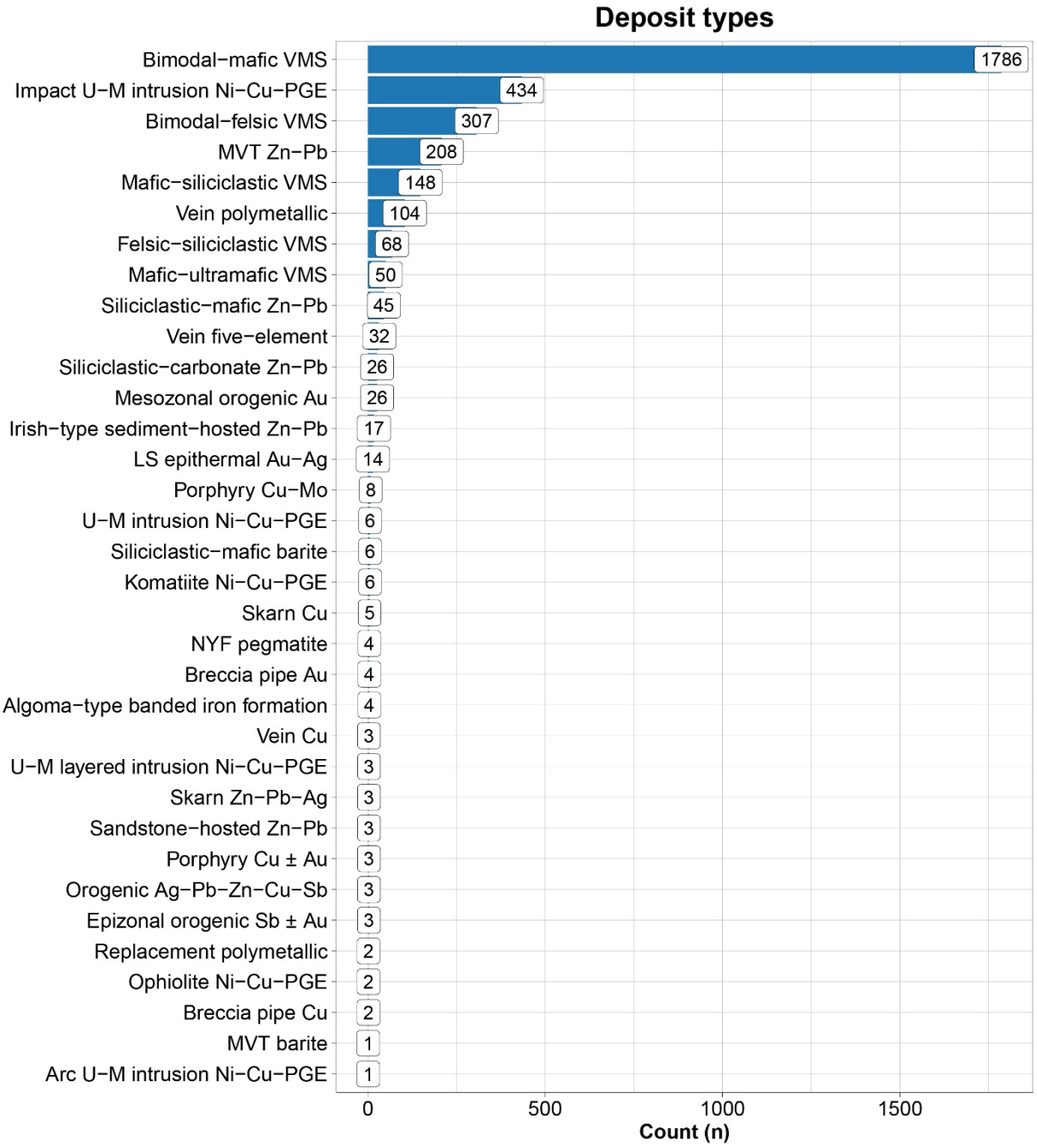

Figure 3: *Sample counts for different deposit types.*

The number of missing values for each element is highly variable (Fig. 4). The ten elements with the most missing values are W (98%), CO_2 (89%), Pd (89%), Pt (89%), Cl (88%), F (88%), Ir (87%), Br (86%), Be (81%), and SiO_2 (76%; Fig. 4a). These missing values may include elements that were not analyzed or measured concentrations that were below the analytical detection limit. The number of missing values per sample suggests that only a few samples are missing concentrations for most elements (Fig. 4b). Elements with the greatest proportion of

missing values tend to be missing for most samples, likely because they were not routinely analyzed and/or because of their low abundance that is below the analytical detection limit. Elements with the greatest proportion of missing values present challenges for further statistical analysis. Missing values for the most abundant elements can be imputed using the half of the provided detection limits or more sophisticated algorithms such as nearest neighbour, self-organizing maps, random forest, and many others (e.g., Grunsky, 2010).

Future directions

This template was developed to streamline and standardize releasing lithogeochemical data. Although the focus here is on ores and ore-bearing rocks, it is equally applicable to any sample that has been analyzed for bulk geochemistry from other mining or mineral exploration environments (e.g. unmineralized rock, sediment, till, etc.). Combined deposit and geochemical information provides a powerful foundation for predicting the most prospective geological settings for each of the critical minerals defined by Natural Resources Canada. Ideally, following the procedure described here will facilitate timely data release and will be integrated with other [digital] sample management tools. The use of a database will allow maintaining the overall integrity of the information and will provide all the supporting mechanisms to implement and enrich the vocabularies linked to the system, while providing at the same time a central location where the critical mineral data can be found, queried and extracted by research groups within the GSC and from external organisations.

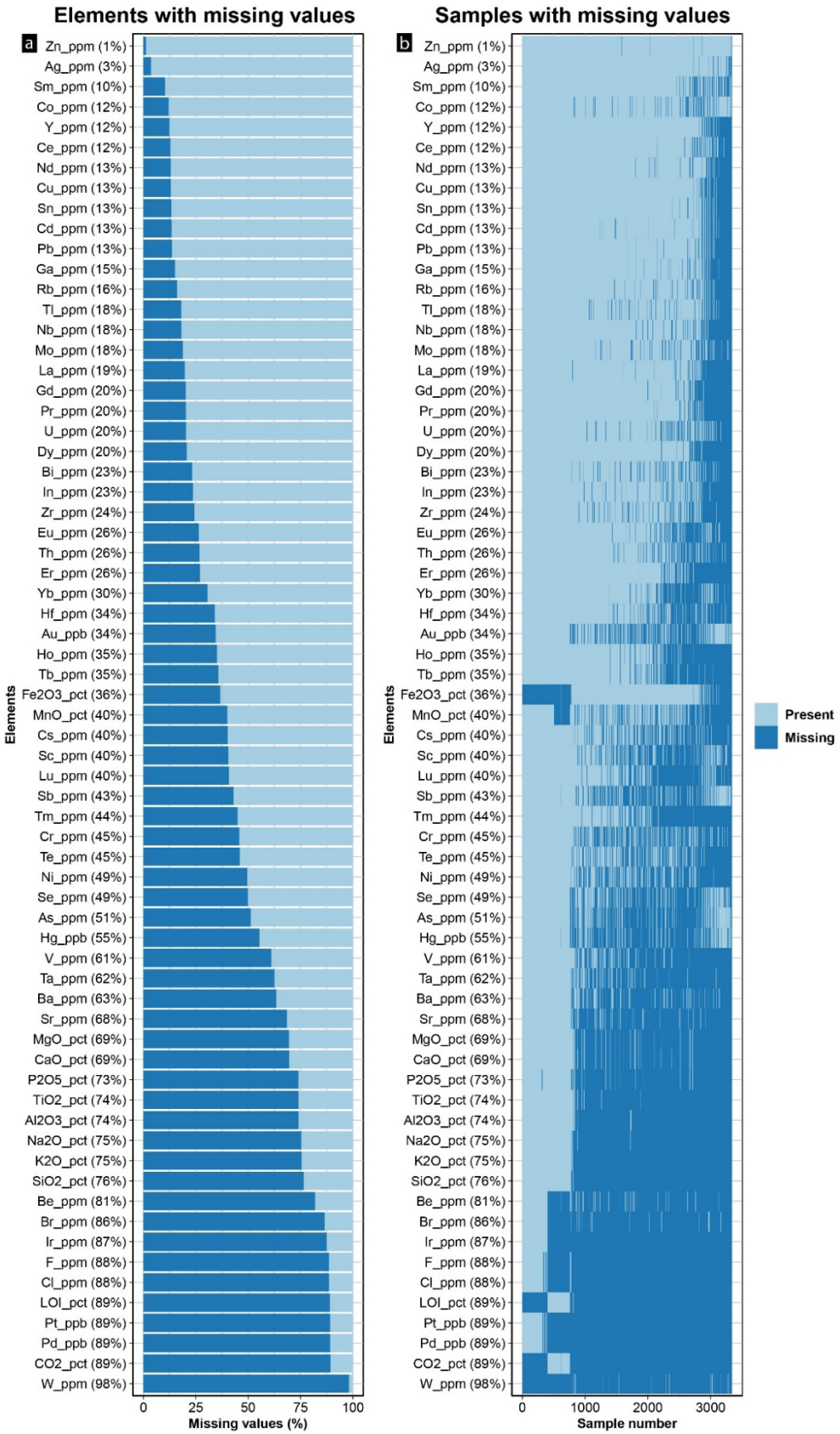

Figure 4: *Proportion of missing values (%) per element (a) and sample (b).*

Acknowledgements
This report was released as part of the Critical Mineral Mapping Initiative collaboration. We would like to thank James Kidder for reviewing this report.

Tables
Table 1 – Column definitions
Table 2 – Vocabularies and empty sample submission template
Table 3 – Canadian contributions to the critical minerals in ore database (this study)

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