### **Findings from Complete Review:**

## Nina's thoughts:

Overall, I haven't looked at this paper in quite a number of years, but I do apologize for my past typos and errors. I appreciate you picking up on them and making this paper better!

It seems that there would be value in talking to a mineralogist to get feedback on the whole structure of the database, given our lack of expertise in mineralogy. For example, in the actual paper about Niningerite, it says:

"a new meteoritic sulfide ranging in composition from  $(Fe_{0.19}Mg_{0.66}Mn_{0.14}Ca_{0.007}Cr_{0.002})S$  to  $(Fe_{0.52}Mg_{0.33}Mn_{0.06}Ca_{0.06}Cr_{0.03}Zn_{0.004})S$ "

It's unclear to me whether just putting MgS is accurate or if it's overly reductive. Similarly for questions around whether to include the 2+ and what might be going on when the same mineral is listed differently in different places.

#### Table 1:

- I believe "Allendite" is misspelled, according to C Ma 2014 it is spelled "Allendeite".
  - Yep, it was spelled correctly in other places, so this is just a typo.
- I believe the chemical formula for Niningerite is wrong, it is given as "MnS" and mindat.org gives the formula as either "(Mg,Fe2+,Mn2+)S" or MgS. Either way I think in the paper, "Mg" was accidentally transcribed as "Mn". PubChem also gives the formula as MgS.
  - Yep, I suspect that was a typo
- I believe the chemical formula for Osbornite is wrong, it is given as "TiNi" and LF Dobrzhinetskaya 2009 gives the formula as "TiN". I think "TiN" was accidentally transcribed in the paper as "TiNi".
  - Yep, another typo
- Both the IMA and nondescript formulae listed for Panethite use "Fe<sup>2+</sup>" instead of "Fe" in the formula...(Na,Ca)<sub>2</sub>(Mg,Fe)<sub>2</sub>(PO<sub>4</sub>)<sub>2</sub>. I don't know if this is important but I noted it anyway.
  - I'm not sure either. I'm not a mineralogy expert, but it might be worth asking one of them. Either way, probably best to put the 2+ to be more precise.
- The paper gives the formula for Keilite as "(Fe,Mn,Mg,Ca,Cr)S" which I think comes from webmineral.com. I don't know why the contradiction exits (or even if it is a true contradiction) but I found the formula given by M. Shimizu as "(Fe,Mg)S", the formula given by the handbook of mineralogy as "(Fe2+,Mg)S" and the formula given by the IMA as FeS.

- Very curious... I don't have a good answer to this, other than to say that it's possible I found the formula on web mineral (although, I did try to avoid it) and think it's best to go with what was published by M. Shimizu.
- For Kangite, C Ma lists the formula as "(Sc,Ti,Al,Zr,Mg,Ca,□)2O3" and in the paper it is listed with a "C" instead of "Ca". I think the "Ca" may have been mistyped and transcribed as a "C" in the paper.
  - Yep, I agree
- The IMA formula and nondescript formulae for Cohenite are listed as "Fe<sub>3</sub>C" with the annotation "May contain minor Ni or Co replacing Fe". I don't know if this means the formula should be listed as it appears in our paper, "(Fe,Ni,Co)<sub>3</sub>C", or as "Fe<sub>3</sub>C" with impurities.
  - Hmm.. I'm not sure about this. I just did a quick search online and found this conference paper from 2019: <a href="https://www.hou.usra.edu/meetings/lpsc2019/pdf/2510.pdf">https://www.hou.usra.edu/meetings/lpsc2019/pdf/2510.pdf</a> which uses (Fe,Ni,Co)<sub>3</sub>C as well, so that might be a good reference to add. It also refers to Cohenite it as "cementite" which we might need to get to the bottom of.
- I believe the mineral name "Moniptite" is misspelled. According to Mindat, J. Becket and C. Ma, I believe it should be spelled "Monipite." I note this in a later section, if it should be spelled "monipite" then it is misspelled throughout the whole paper.
  - Yep, looks like I was just saying it in my head in a certain way and never picked up on the misspelling haha.
- I'm just wondering, Khatyrkite appears in table six but not table 1 or 5. Are we not including Khatyrkite in tables 1 or 5? -- Actually I looked into this further and I think Khatyrkite is a typo (in table six) and should really be Kryachkoite. I talk about this more in table six edits, but if Khatyrkite doesn't appear in our database at all, should we add it?
  - There is actually a mineral called Khatyrkite that's only been found in meteorites, but it seems like I may have gotten the two names mixed and therefore made some mistakes about what's presented in what table. It would be good to include both of them.

#### Table 5:

- No other occurrence is listed for Adrianite in the paper; according to mindat.org and RRUFF, Adrianite has also been detected in the Qutrixpileo meteorite.
  - I haven't heard of that meteorite before, so that discovery may have been after my work, or I just missed it entirely. Let's add it!
- No other occurrence is listed for Allendeite in the paper; according to mindat.org and RRUFF, Adrianite has also been detected in the Qutrixpileo meteorite.
  - Same as above
- Decagonite is said to be found in fragments  $\sim$ 60 mm across this is actually confusing because two publications of the same paper by L Bindi state this dimension as 60  $\mu$ m

across (1, 2) but another on research gate states it as 60mm. I wonder if the paper that uses "mm" had a preprint error.

- Ooh, very confusing. I think it's quite unlikely to be mm, that would be huge. I'd bet on μm.
- No other occurrence is listed for Grossite in the paper; according to mindat.org
  Grossite has also been detected in Acfer 182 (CH3).
  - Let's add it, I'm unfamiliar with that meteorite.
- No other occurrence is listed for Hexamolybdenum in the paper; according to mindat.org and Chi Ma 2011 it has also been detected in NWA 1934 (CV3).
  - Let's add it
- Lonsdaleite's crystal behavior is described to be cubic with side lengths of 0.25mm, but the handbook of mineralogy states it also forms cubes and "cubo-octahedra, to 0.7 mm." I don't know if this is noteworthy (and I don't really trust the handbook), though I noted it. Per width, P. Németh 2014 states: "The twins in the Canyon Diablo sample divide the grains into domains that are 1- to 3-nm wide (Fig. 2), and the stacking faults produce domains two to four layers across (0.4–0.8 nm wide; Fig. 3). The synthetic sample shows a similar domain structure, although the domains are wider (2–20 nm)."
  - Might be good to ask a mineralogist about this. I also general don't trust these handbooks (you can see how many typos I've made trying to compile all this info, so it's highly feasible that they make just a number of errors too if they aren't being reviewed thoroughly).
- I believe I believe Monipite is spelled wrong, as it appears in the paper as "Monipite" and C. Ma has it as "Monipite."
  - Yep, addressed in the previous section.
- Stolperite is described to form irregular grains up to 3mm in size, the handbook of mineralogy puts this figure as  $3\mu$ m, but I couldn't actually verify the handbook's claim externally so I think the original figure is good.
  - Curious. I'd also default to the original figure (just reviewed this publication with the graphic showing the mineral: <a href="https://phys.org/news/2017-03-minerals-unique-meteorite.html">https://phys.org/news/2017-03-minerals-unique-meteorite.html</a>)
- No other occurrence is listed for Troilite, according to SS Hontsova 2016, it has also been detected in Seymchan (PMG).
  - Sounds good, let's add that the paper came out after I finished my work on this paper.

## Table 6:

- No density is listed for Adrianite; according to C. Ma 2019, it has a density of 3.03 g/cm<sup>3</sup>.
  - Let's add that, I must have missed it.
- No cell parameters or information about crystal structure are provided for Cohenite; H...Bhadeshia states it "has an orthorhombic unit cell and the common convention is to set the order of the lattice parameters as a=0.50837 nm,

b=0.67475 nm and c=0.45165 nm." Granted, Bhadeshia refers to it as *Cementite*, but goes on to refer to it as: "In mineralogy, the carbide is known as cohenite (Fe,Ni,Co)3C."

- The conference paper I linked above (repeated here: <a href="https://www.hou.usra.edu/meetings/lpsc2019/pdf/2510.pdf">https://www.hou.usra.edu/meetings/lpsc2019/pdf/2510.pdf</a>) also refers to it as Cementite and has that formula. My hunch is that it's reasonable to use the crystallographic structure from Bhadeshia.
- Daubreelite is listed to be in the space group Fm3m, according to M. R. M. Izawa 2010, RRUFF, and mindat, it's in the group Fd3m.
  - Likely a typo, let's change that.
- Droninoite is said to be Rhombohedral, but N. V. Chukanov 2009 states
  "Droninoite is trigonal." However, ALS Costa 2017 and ES Zhitova 2015 state it is rhombohedral, so I think the original description is correct.
  - Curious. It has definitely happened that minerals have been mischaracterized in original findings,
- No cell parameters are listed for Grossite; D. Weber 1994 gives them as "a = 12.94Å, b = 8.910Å, c = 5.446 Å, β = 107.0°" Also, D Weber 1994 states Grossite is monoclinic.
  - Ok, great! Let's add that data in.
- Hexamolybdenum is listed as having a density of 11.99g/cm<sup>3</sup>; according to C. Ma 2014, the density should be 11.90 g/cm<sup>3</sup>.
  - Likely just a typo, let's change that!
- I believe in this table, Kryachkoite is mislisted as "Khatyrkite." First of all, in the paper Khatyrkite is listed as having a density of 3.79 g/cm³ (calc); according to Springer Minerals it has a density of 4.36 g/cm³. Also, P. Steinhardt 2012 states "As first reported by Razin et al (1985), khatyrkite...is a tetragonal crystal." Additionally, Khatyrkite is listed with the group "Cmc21," M. Mehl lists the space group I4/mcm. All of these properties listed are in conflict with Khatyrkite's properties but match Kryachkoite's properties perfectly. I checked C. Ma 2017 which lists the properties of Kryachkoite: "Kryachkoite occurs with khatyrkite and aluminum, having an empirical formula of Al5.45Cu0.97Fe0.55Cr0.02Si0.01 and an orthorhombic Cmc21 structure with a = 7.460 Å, b = 6.434 Å, c = 8.777 Å, V = 421.3 Å3, Z = 4." The properties listed for "Khatyrkite" in the paper match Kryachkoite's true properties perfectly. Additionally, Khatyrkite does not appear anywhere else in the paper whereas Kryachkoite does; I believe Khatyrkite is wrongly used in place of Kryachkoite in table 6.
  - As mentioned above, both are meteorite minerals, so we should put them both in all the tables I must have just mixed them up across the tables, causing these inconsistencies you picked up on.
- I believe "Linguite" is misspelled in table six, according to LG Liu 2007, I think it should be spelled as "Lingunite."
  - Yep, let's change that

- According to J. Beckett 2009 & C. Ma 2014, I believe "moniptite" is spelled wrong throughout the whole paper, I believe it should be spelled: "monipite."
  - Likely just a typo I didn't catch and perpetuated, thanks for picking up on it.
- Murchisite is listed as having hexagonal crystal behavior; when discussing Crystallography, C. Ma 2011 states it has a "trigonal structure." I read on and found that the hexagonal reference relates to a later sentence in the same paper which states: "The structure consists of close-packed S layers in hexagonal stacking with Cr in octahedral voids and ordered vacancies in every second interlayer."
  - Sounds like I must have transcribed that incorrectly.
- Oldhamite is listed as being part of the space group "Pm3m," I believe it should be part of the space group Fm3m. In his book Applied Mineralogy of Cement & Concrete, M. Broekmans states oldhamite is in the space group Fm3m. Also, A. S. Povarennykh in the book Crystal Chemical Classification of Minerals lists Oldhamite under the Galena group which is stated to be of the space group Fm3m. MRM Izawa 2010 supports this.
  - Sounds good, let's change that.
- J. Lima-de-Faria states in the *Structural Classification of Minerals* that Osbornite is in the space class of Fm3m.
  - Awesome, let's add that.
- I. Steele 1992 states Stanfieldite's cell parameters *c* and *B* as "17.09 Å" and "99.96°," respectively.
  - Sounds good.
- The value for Tetrataenite's Unit Cell V is calculated from cell parameters on mindat to be 22.92 ų I can't find where 313.61 comes from, though I am suspicious because that is the exact unit cell volume for Tistarite, so I wonder if Tistarite's unit cell volume was accidentally used for Tetrataenite as well. I also found some extra information about Tetrataenite's cell parameters from T. Tagai 1995: it has "β = 90.04° and y = 90.00°."
  - That seems likely to me too, I would have just copied out the whole block of data to preserve the formatting and then probably just forgot to change the V value.
- I found different cell parameters for Wadsleyite in J. Smyth 1997 but that particular paper discussed *Hydrous* wadsleyite so I don't think the difference matters.
  - Hmm.. I'm not sure about that. Might be good to talk to a mineralogist about this.

#### Table 7:

- As a general note, I found different colors from the handbook of mineralogy than what are listed for a couple of the minerals, but I don't really trust the handbook of mineralogy as I've (not infrequently) seen discrepancies between it and published literature so I didn't note them, however I can run through them all and get the ones that have different colors as described by the handbook if you would like.
  - Yeah, it's an interesting resource, lots of mistakes. Unclear who's maintaining it and why there are so many discrepancies. Probably not worth it if their colors are

different than the literature but if they have colors that aren't mentioned in the paper

- According to B. Pracejus 2014, Daubreelite is opaque.
  - Sounds good
- According to the Chromium(VI) Handbook edited by J. Guertin, Krinovite has a sub-adamantine lustre and it's diaphaneity is semi transparent to opaque.
  - Sounds good
- According to Si Silicon: System Si-C. SiC: Natural Occurrence. Preparation..., the "Optical character of moissanite is uniaxially positive...but anomalously biaxial crystals were found."
  - Ok, let's add "uniaxial (+), anomalously biaxial"
- If "moniptite" should be spelled "monipite" then it might be spelled wrong here too.
  - Yep!

# Other Correction Suggestions:

- On Page 10, ¶ 1, line 2, in the sentence that states: "Three examples are listed below;" I think "Three" should be replaced with "Four" because four minerals are described in § 4.3.
  - Yep, I must have forgotten to update that.
- On Page 11,¶ 5, line 6, a sentence starts "Otherwise The..."; I think the "The" should be written as "the" because the "T" should not be capitalized.
  - Yep!