The crystal structure of meteoritic schreibersite: refinement of the absolute crystal structure

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Abstract

Schreibersite is an iron-nickel phosphide mineral $(Fe,Ni)_3P$ and is found in many iron and stony meteorites. Due to its abundance in meteorites and the inclusion of phosphorus it its crystal structure, schreibersite has significant implications for life on Earth. Schreibersite has a tetragonal crystal structure, crystalizing with the $I\bar{4}$ space group. This space group is non-centrosymmetric, allowing for two different crystal structures that are related to one another by an inversion symmetry operation, termed the "normal" and "inverse" structures. In previous studies, only one atomic arrangement was observed and all crystal structure refinements were based off that one structure. This means the less commonly observed crystal structure has not been as well refined. Crystal structure atom positions, occupancy and displacement parameters were refined from single crystals and were based on X-ray diffraction data using 2500 to 8000 individual intensity refinements. Four crystals were tested from the Seymchan iron meteorite, and one crystal from the Campo del Cielo meteorite. Three crystals, two from Seymchan and the one from Campo del Cielo, had the inverted crystal structure. The remaining two crystals from Seymchan possessed the normal atomic arrangement. More accurate crystal structure refinements were obtained for the normal crystal structure because of its abundance in the samples. It appears that the two enantiomorphic forms are equally and randomly distributed among the natural crystals measured.

Introduction

The iron-nickel phosphide solid solution Fe_3P-Ni_3P is a common component in many iron-rich meteorites (Buchwald 1975), and is also found as an accessory mineral in many silicate-rich meteorites (Brearley and Jones 1998; Mittlefehldt et al. 1998). The solid solution is known more commonly by its mineral name "schreibersite", and it is given the general chemical equation $(Fe,Ni)_3P$. Though schreibersite is considered a "rare" mineral because of the few environments where it is found, the implications it might have for life on Earth are quite profound. It is believed that Earth's source of phosphorus is ultimately derived from schreibersite and other meteoritic phosphide minerals (University of Arizona 2004). On Earth, phosphorus is necessary for life in the form PO_4^{3-}, or as phosphate. The phosphorus in the phosphate compound has been oxygenated and has a positive five charge. In meteorites, the phosphorus atom has no charge because meteorites are reducing environments. The iron and nickel atoms in schreibersite also have no charge because they have not been oxygenated, either. Schreibersite occurs naturally in one location on Earth: Disko Island off the coast of Greenland (Bryant et al. 2013). In Disko Island there is a basaltic intrusion into a coal seam, which creates a highly reduced environment in which schreibersite can form. Along with Disko Island, the Earth's inner core is thought to be composed of an iron-nickel alloy in which schreibersite could be an important component (Alfè et al. 2002).

In the late 1960s, the crystal structure of schreibersite was solved and refined by Doenitz (1968, 1970) using X-ray diffraction data. The schreibersite crystals Doenitz used were from the North Chile hexahedrite (IIA iron), which impacted Earth near Tocopilla, Chile. The structure that Doenitz found in schreibersite was identical to the structures of synthetic Fe_3P (Aronsson 1955; Rundqvist et al. 1962; Larsson 1965) and Ni_3P (Rundqvist et al. 1962), whose crystal structures had been solved previously. It was concluded that all members of the schreibersite-nickelphosphide

Table 1 Summary of the *I*-4 space group

Multiplicity	Wyckoff Letter	Site Symmetry	Coordinates			Reflection Conditions
			(0, 0, 0)+	(1/2, 1/2, 1/2)+		General:
8	*g*	1	(1) *x*, *y*, *z*	(2) -*x*, -*y*, *z*	(3) y, -*x*, -*z* (4) -y, *x*, -*z*	*hkl* : *h* + *k* + *l* = 2*n* *hk*0 : *h* + *k* = 2*n* 0*kl* : *k* + *l* = 2*n* *hhl* : *l* = 2*n* 00*l* : *l* = 2*n* *h*00 : *h* = 2*n*

series have a tetragonal lattice system and belong to the $I\bar{4}$ space group (Skála and Císařová 2005). This space group is listed as number 82 in the International Tables for Crystallography, and its properties are summarized in Table 1. In the $I\bar{4}$ space group, there are four atoms which lie in 8 *g* sites. These atoms are all in general positions because they do not lie on symmetry operators, and they are all crystallographically non-equivalent. There are four different occupied sites, three of which are occupied by a non-definite metallic atom (either Fe or Ni), and one by a P atom. For the purposes of this paper, the three metallic atoms will be abbreviated M1, M2 and M3. Since the $I\bar{4}$ space group is non-centrosymmetric, chiral and has no polar axis, it allows two different spatial arrangements of the atoms in the unit cell that have the inverse symmetry from one another (Skála and Císařová 2005). Doenitz (1970) observed these two different atomic arrangements, and he assigned the standard, or regular, crystal structure, and the inverse structure. The normal structure is depicted in Figure 1a, and the inverse structure is depicted in Figure 1b.

While schreibersite has been the focus of

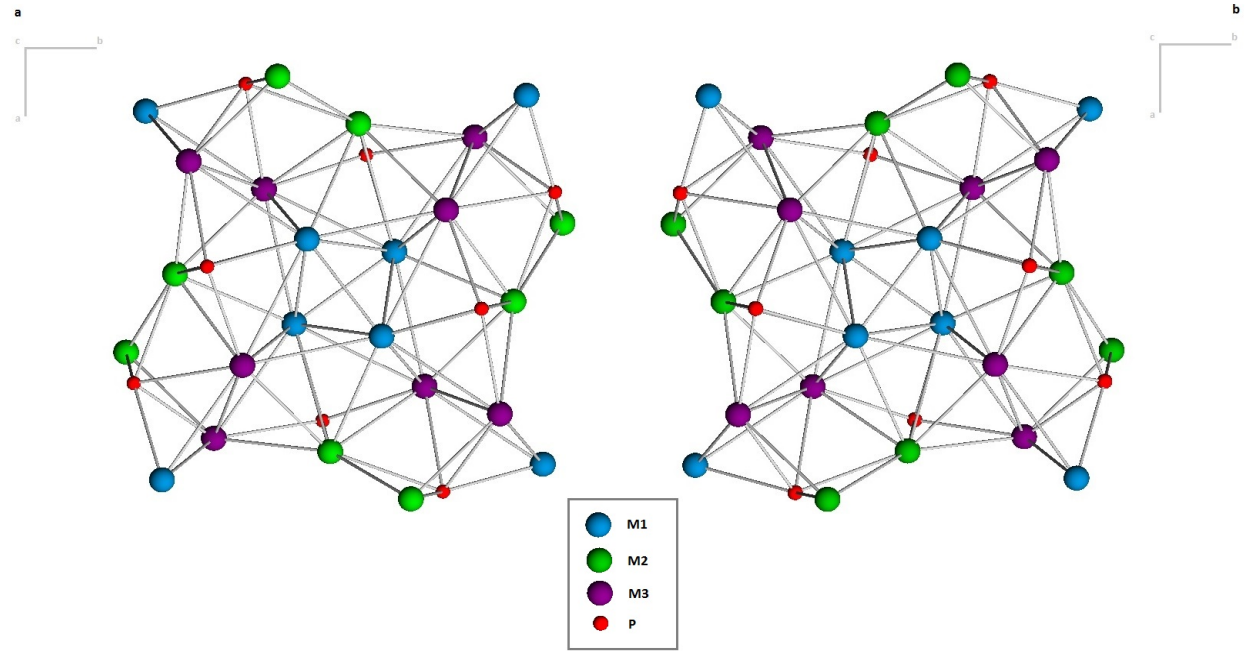

Figure 1 The regular and inverse crystal structures of schreibersite depicted using the XTALDRAW program. **a** is the normal crystal structure which is less commonly observed. **b** is the inverse crystal structure which has been reported before. The data for the normal structure

numerous crystal refinement studies (Aronsson 1955; Rundqvist et al. 1962; Rundqvist 1962; Larsson 1965; Doenitz 1968, 1970) and in more recent powder diffraction studies (Skála and Frýda 1996; Liu et al. 1998; Skála and Drábek 2003), the absolute crystal structure was not determined. Skála and Císařová (2005) was the first attempt at solving schreibersite's absolute crystal structure. For their experiments, eight samples of schreibersite were tested from five different meteorites by single-crystal X-ray diffraction. In the $I\bar{4}$ space group there are two possible enantiomorphic forms, known as the normal and inverse structures, and the two may be distinguished by X-ray diffraction data based on anomalous dispersion. In centric space groups, Friedel's Law says that $F^2_{hkl}=F^2_{-h-k-l}$. For acentric space groups, such as the $I\bar{4}$ space group, this does not hold and anomalous dispersion causes small differences between F^2_{hkl} and F^2_{-h-k-l}.

Skála and Císařová (2005) concluded with no ambiguity that all of their crystals exhibited the inverse atomic arrangement when compared to the standard set by Doenitz (1970). There were some crystals in which were racemic twins were seen, and these twins had the normal structure dominate over the inverse structure. There were no crystals with purely a normal structure however like they found with the inverse structure. This is not what is expected when compared to other minerals that also have two symmetrical crystal structures. For example, quartz also has two different atomic arrangements that are commonly known as left and right-handed quartz. It appears as though quartz crystals do not prefer one atomic arrangement over the other as both arrangements are seen in equal abundance (Gault 1949). This means that the left or right crystal structure of quartz is determined by chance. Schreibersite should behave the same way with the regular and inverse structures appearing in equal proportion.

Since the only pure samples of schreibersite whose absolute crystal structures have been studied are inverse atomic arrangements (Skála and Císařová 2005), the crystallographic data could be different for the normal structure. The purpose of this project was to try and find a normal crystal structure and refine its atomic arrangement.

Samples, Data Collection and Evaluation

For this study, five samples were selected from two different iron meteorites: one sample from Campo del Cielo (coarse octahedrite,

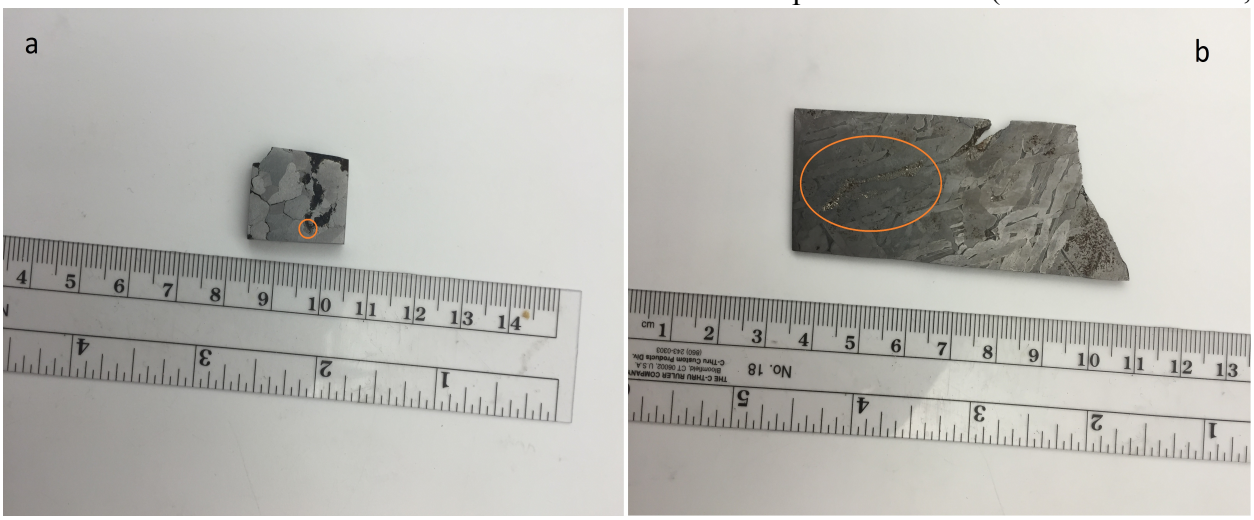

Figure 2 Photos of the slabs from which the crystals of schreibersite were extracted. **a** shows the slab from the Campo del Cielo meteorite. **b** shows the slab from the Seymchan meteorite.

IAB-MG, shown in Figure 2a) and four samples from Seymchan (coarse octahedrite, PMG, shown in Figure 2b). Single crystals were extracted mechanically from pieces of these meteorites as opposed to using chemical solution extraction processes.

Data for the structure determination were collected using the X-ray diffractometer at the Department of Geological Sciences at the University of Colorado at Boulder. The instrument has a Bruker APEX-II CCD X-ray detector on a Bruker P4 four-circle diffractometer. The X-ray generator is a Bruker/MAC Science rotating anode operated at 50 Kv and 250 mA. The crystal structures were solved using the SHELXS97 (Sheldrick 1997) program, and were then refined using the SHELXL97 (Sheldrick 1997) program. The two SHELX97 programs were run through the WinGX graphical interface (Farrugia 1999). The Ni_3P end-member of schreibersite was used for all SHELXL97 refinements, but then the nickel occupancy was subsequently refined using the SHELSL97 program.

Results

To determine the absolute orientation of the studied schreibersite crystals, we fixed the structures to both the normal orientation from Doenitz (1970) and the inverse arrangement. Both of those arrangements were refined using SHELXL97. The correct structure was determined by comparing Flack's *x* parameter (Flack 1983; Flack and Bernardinelli 1999, 2000) found in the SHELXL program. These results are summarized in Table 2. The atomic arrangement was determined by looking at the values of *x*. If *x* is equal to 0 or within one standard deviation from 0, then it means that is the correct crystal structure (Flack and Bernardinelli 2000). Racemates are present when *x* is outside one standard deviation from 0. Using this information, it can be concluded that crystals 1 and 2a from Seymchan and the one crystal evaluated from Campo del Cielo have absolute crystal structures that correspond to the inverse atomic arrangement that has been exclusively observed in schreibersite (Skála and Císařová 2005). Crystals 3 and 5 from Seymchan have the absolute crystal structure that agrees with the normal atomic arrangement, however.

A summary of the coordinates of atoms based off of the correct absolute structure is summarized in Table 3. Just like was done previously (Skála and Císařová 2005), the coordinates of equivalent atoms are determined by the following equations: $x_I=y_N$; $y_I=1-x_N$; $z_I=z_N$. In these equations, subscript "N" refers to the normal atomic arrangement and "I" to the inverted one. Table 3 also includes equivalent isotropic displacement parameters and nickel occupancies for all metallic atoms. Anisotropic displacement parameters for the metallic atoms and phosphorus are summarized in Table 4. Finally, bond lengths between the various metallic atoms and phosphorus are summarized in Table 5.

In addition to the tables listed above, crystallographic information files for each of the evaluated samples are attached as it is normally required for crystallographic publications.

Discussion and Conclusion

While the number of samples evaluated is small, it can be concluded that half of them have normal absolute atomic arrangements and the other half are inverted. This is observed in other minerals (Gault 1949) and makes logical sense. This is the first time that the normal absolute atomic arrangement of schreibersite has been observed in such abundance, and it is quite exciting. Even though the samples with the normal crystal structure were only seen from the Seymchan

Table 2 Results of absolute structure tests of the studied schreibersite crystals

Sample	Seymchan, cr #1		Seymchan, cr #2a		Seymchan, cr #3		Seymchan, cr #5		Campo del Cielo	
Structural Model	Normal	Inverse	Normal	Inverse	Normal	Inverse	Normal	Inverse	Normal	Inverse
SHELX-97, refinement agianst F^2										
R_{all}	0.0405	0.0334	0.0356	0.0291	0.0415	0.0438	0.0557	0.0579	0.0463	0.0438
wR_{all}	0.1403	0.1136	0.1218	0.0970	0.1192	0.1273	0.1638	0.1679	0.1379	0.1279
GooF	1.105	0.893	0.931	0.740	0.813	0.868	1.076	1.104	0.979	0.907
Flack's *x* parameter	0.95 (5)	0.03 (4)	0.83 (4)	0.14 (3)	0.18 (8)	0.77 (8)	0.06 (22)	0.87 (23)	0.75 (9)	0.22 (8)
Interpretation	Inverse		Inverse, some racemic twin		Normal, some racemic twin		Normal		Inverse, some racemic twin	

Table 3 Atomic coordinates, equivalent isotropic displacement paramters (in $Å^2$), and nickel occupancies of M1-M3 sites in the studied schreibersite crystals

Site	Seymchan, cr #1	Seymchan, cr #2a	Seymchan, cr #3	Seymchan, cr #5	Campo del Cielo
M1, 8g					
x	0.92101 (8)	0.92100 (8)	0.07908 (1)	0.07882 (3)	0.92103 (1)
y	0.10727 (8)	0.10728 (7)	0.89297 (1)	0.89209 (3)	0.10751 (1)
z	0.76990 (1)	0.76958 (1)	0.23078 (3)	0.22945 (7)	0.77013 (3)
U_{eq}	0.00739 (6)	0.00825 (1)	0.00805 (4)	0.01237 (9)	0.00819 (4)
Ni occ	28.00000 (1)	25.86752 (8)	25.75776 (9)	25.65276 (8)	26.20240 (1)
M2, 8g					
x	0.03252 (8)	0.03229 (7)	0.96766 (1)	0.96751 (3)	0.03291 (1)
y	0.36095 (8)	0.36095 (7)	0.63898 (1)	0.63923 (3)	0.36120 (1)
z	0.98309 (1)	0.98325 (1)	0.01553 (3)	0.01742 (7)	0.98232 (3)
U_{eq}	0.00654 (2)	0.00769 (1)	0.00844 (4)	0.00979 (9)	0.00795 (3)
Ni occ	28.00000 (1)	25.76056 (9)	26.10867 (8)	26.49836 (8)	26.75764 (1)
M3, 8g					
x	0.82984 (7)	0.82963 (7)	0.17028 (1)	0.17016 (3)	0.83018 (1)
y	0.21911 (7)	0.21911 (7)	0.78097 (1)	0.78105 (3)	0.21886 (1)
z	0.24902 (1)	0.24876 (1)	0.75157 (3)	0.75028 (7)	0.24945 (3)
U_{eq}	0.00867 (6)	0.00861 (1)	0.00862 (3)	0.01625 (8)	0.00879 (3)
Ni occ	28.00000 (9)	27.46548 (8)	27.23952 (8)	28.00000 (0)	28.00000 (1)
P, 8g					
x	0.04761 (1)	0.04726 (1)	0.95263 (2)	0.95289 (6)	0.04873 (2)
y	0.29231 (1)	0.29240 (1)	0.70745 (2)	0.70683 (6)	0.29265 (2)
z	0.48723 (3)	0.48689 (2)	0.51273 (6)	0.51608 (1)	0.48571 (6)
U_{eq}	0.00704 (9)	0.00768 (2)	0.00760 (6)	0.01053 (1)	0.00612 (4)
Interpretation	Inverse	Interted	Normal	Normal	Inverse

The data refined wih the SHELXL-97.2 program

U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor

Coordiates of normal (N) and Inverse (I) structure relates to xI=yN; yI=1-xN; zI=zN

Table 4 Anisotropic displacment parameters (in $Å^2$) in the studied schreibersite crystals

Site	Seymchan, cr #1	Seymchan, cr #2a	Seymchan, cr #3	Seymchan, cr #5	Campo del Cielo
M1					
U_{11}	0.00726 (3)	0.00868 (2)	0.00743 (5)	0.01386 (1)	0.00773 (5)
U_{22}	0.00772 (3)	0.00901 (2)	0.00777 (5)	0.01911 (1)	0.00885 (5)
U_{33}	0.00720 (3)	0.00705 (2)	0.00894 (6)	0.00412 (1)	0.00798 (7)
U_{12}	–0.00020 (2)	–0.00033 (2)	–0.00021 (4)	0.00055 (1)	0.00004 (4)
U_{13}	–0.00070 (3)	–0.00063 (2)	–0.00079 (5)	–0.00019 (1)	–0.00034 (5)
U_{23}	0.00025 (3)	0.00032 (2)	0.00035 (5)	–0.00111 (1)	0.00032 (5)
M2					
U_{11}	0.00646 (3)	0.00870 (2)	0.00922 (6)	0.01162 (1)	0.00896 (5)
U_{22}	0.00654 (3)	0.00798 (2)	0.00774 (5)	0.01160 (1)	0.00837 (5)
U_{33}	0.00661 (3)	0.00640 (3)	0.00836 (7)	0.00613 (1)	0.00650 (7)
U_{12}	0.00005 (2)	0.00041 (2)	0.00041 (4)	–0.00194 (1)	–0.00015 (3)
U_{13}	0.00005 (3)	–0.00031 (2)	–0.00012 (5)	–0.00127 (1)	–0.00013 (5)
U_{23}	0.00051 (3)	0.00036 (2)	0.00078 (5)	–0.00027 (1)	0.00090 (5)
M3					
U_{11}	0.00953 (3)	0.00986 (2)	0.97100 (8)	0.02253 (1)	0.00958 (5)
U_{22}	0.00804 (3)	0.00865 (2)	0.00869 (5)	0.01963 (1)	0.00860 (4)
U_{33}	0.00844 (3)	0.00733 (2)	0.00852 (5)	0.00659 (1)	0.00819 (6)
U_{12}	–0.00079 (2)	–0.00104 (1)	–0.00122 (4)	–0.00192 (1)	–0.00049 (3)
U_{13}	0.00000 (2)	–0.00023 (2)	–0.00053 (5)	0.00147 (1)	–0.00180 (5)
U_{23}	0.00079 (3)	0.00063 (2)	–0.00010 (5)	0.00279 (1)	0.00007 (5)
P					
U_{11}	0.00864 (6)	0.00879 (4)	0.00992 (1)	0.01524 (3)	0.00737 (9)
U_{22}	0.00657 (6)	0.00879 (4)	0.00702 (1)	0.00480 (2)	0.00620 (8)
U_{33}	0.00592 (5)	0.00632 (4)	0.00586 (1)	0.01154 (2)	0.00479 (1)
U_{12}	0.00133 (5)	0.00067 (3)	0.00062 (7)	0.00547 (2)	0.00008 (6)
U_{13}	0.00011 (5)	0.00015 (3)	–0.00150 (9)	–0.00008 (3)	–0.00140 (9)
U_{23}	–0.00064 (6)	–0.00038 (4)	–0.00200 (1)	–0.00052 (2)	–0.00245 (1)

The data refined wih the SHELXL-97.2 program

Anisotropic displacement factor takes the form $-2\pi[h^2a^2*U_{11} + \ldots + 2*hka*b*U_{12}]$

Table 5 Bond lenghts (in Å) for M_3P polyhedron in the studied schreibersite crystals

I	C	J	Seymchan, cr #1	Seymchan, cr #2a	Seymchan, cr #3	Seymchan, cr #5	Campo del Cielo
M1	–	P	2.3121 (1)	2.3144 (1)	2.3153 (2)	2.3092 (6)	2.3114 (2)
M1	–	P	2.3904 (1)	2.3930 (1)	2.3958 (2)	2.3919 (6)	2.4024 (2)
M1	–	M1	2.4128 (1)	2.4171 (1)	2.4160 (2)	2.4137 (6)	2.4183 (2)
M1	–	M3	2.5053 (1)	2.5096 (1)	2.5100 (2)	2.4976 (4)	2.5071 (2)
M1	–	M3	2.6659 (1)	2.6700 (1)	2.6702 (2)	2.6579 (4)	2.6667 (2)
M1	–	M1	2.6689 (1)	2.6757 (1)	2.6773 (2)	2.6623 (5)	2.6731 (2)
M1	–	M1	2.6689 (1)	2.6757 (1)	2.6773 (2)	2.6623 (5)	2.6731 (2)
M1	–	M2	2.6845 (1)	2.6880 (1)	2.6951 (1)	2.6676 (4)	2.6861 (1)
M1	–	M3	2.7608 (1)	2.7653 (9)	2.7675 (1)	2.7488 (4)	2.7594 (1)
M1	–	M3	2.7662 (1)	2.7672 (9)	2.7711 (1)	2.7553 (4)	2.7696 (1)
M1	–	M3	2.8175 (1)	2.8223 (9)	2.8209 (1)	2.8135 (4)	2.8168 (1)
M1	–	M2	2.8639 (1)	2.8677 (1)	2.8672 (1)	2.8557 (4)	2.8681 (1)
M2	–	P	2.3013 (1)	2.3069 (1)	2.3100 (3)	2.3066 (8)	2.3092 (3)
M2	–	P	2.3227 (1)	2.3244 (1)	2.3248 (2)	2.3093 (6)	2.3259 (2)
M2	–	P	2.3324 (1)	2.3337 (1)	2.3337 (2)	2.3206 (6)	2.3301 (2)
M2	–	P	2.3367 (1)	2.3382 (1)	2.3341 (3)	2.3180 (8)	2.3383 (3)
M2	–	M3	2.5358 (1)	2.5381 (9)	2.5367 (1)	2.5307 (4)	2.5430 (1)
M2	–	M3	2.5631 (1)	2.5689 (9)	2.5686 (1)	2.5568 (4)	2.5649 (1)
M2	–	M2	2.5875 (1)	2.5897 (1)	2.5907 (2)	2.5822 (5)	2.5860 (2)
M2	–	M3	2.6301 (1)	2.6335 (9)	2.6367 (1)	2.6208 (4)	2.6311 (1)
M2	–	M1	2.6845 (1)	2.6880 (1)	2.6951 (1)	2.6676 (4)	2.6861 (1)
M2	–	M2	2.7695 (1)	2.7742 (1)	2.7825 (2)	2.7612 (5)	2.7669 (2)
M2	–	M2	2.7695 (1)	2.7742 (1)	2.7825 (2)	2.7612 (5)	2.7669 (2)
M2	–	M1	2.8639 (1)	2.8677 (1)	2.8672 (1)	2.8557 (4)	2.8681 (1)
M3	–	P	2.2413 (1)	2.2472 (1)	2.2480 (2)	2.2470 (6)	2.2402 (2)
M3	–	P	2.3368 (1)	2.3389 (1)	2.3425 (2)	2.3209 (6)	2.3423 (2)
M3	–	P	2.3859 (1)	2.3904 (1)	2.3914 (2)	2.3780 (6)	2.3786 (2)
M3	–	M1	2.5053 (1)	2.5096 (1)	2.5100 (2)	2.4976 (4)	2.5071 (2)
M3	–	M2	2.5358 (1)	2.5381 (9)	2.5367 (1)	2.5307 (4)	2.5430 (1)
M3	–	M2	2.5631 (1)	2.5689 (9)	2.5686 (1)	2.5568 (4)	2.5649 (1)
M3	–	M2	2.6301 (1)	2.6335 (9)	2.6367 (1)	2.6208 (4)	2.6311 (1)
M3	–	M1	2.6659 (1)	2.6700 (1)	2.6702 (2)	2.6579 (4)	2.6667 (2)
M3	–	M3	2.7164 (9)	2.7185 (7)	2.7199 (1)	2.7112 (3)	2.7249 (1)
M3	–	M3	2.7164 (9)	2.7185 (7)	2.7199 (1)	2.7112 (3)	2.7249 (1)
M3	–	M1	2.7608 (1)	2.7653 (9)	2.7675 (1)	2.7488 (4)	2.7594 (1)
M3	–	M1	2.7662 (1)	2.7672 (9)	2.7711 (1)	2.7553 (4)	2.7696 (1)
P	–	M3	2.2413 (1)	2.2473 (1)	2.2480 (2)	2.2470 (6)	2.2402 (2)
P	–	M2	2.3013 (1)	2.3069 (1)	2.3100 (3)	2.3066 (8)	2.3092 (3)
P	–	M1	2.3121 (1)	2.3144 (1)	2.3153 (2)	2.3092 (6)	2.3114 (2)
P	–	M2	2.3227 (1)	2.3244 (1)	2.3248 (2)	2.3093 (6)	2.3259 (2)
P	–	M2	2.3324 (1)	2.3337 (1)	2.3337 (2)	2.3206 (6)	2.3301 (2)
P	–	M3	2.3368 (1)	2.3389 (1)	2.3425 (2)	2.3209 (6)	2.3423 (2)
P	–	M2	2.3367 (1)	2.3382 (1)	2.3341 (3)	2.3180 (8)	2.3383 (3)
P	–	M3	2.3859 (1)	2.3904 (1)	2.3914 (2)	2.3780 (6)	2.3786 (2)
P	–	M1	2.3904 (1)	2.3930 (1)	2.3958 (2)	2.3919 (6)	2.4024 (2)

The data refined wih the SHELXL-97.2 program

meteorite, it does not mean that there were not normal crystals in the Campo del Cielo meteorite, or in previously studied examples for that matter (Skála and Císařová 2005). The anisotropic displacement parameters and bond lengths found in these refinements were similar to one another and to the values found in previous schreibersite absolute crystal structure refinements (Skála and Císařová 2005). This means that the crystalline properties did not change between the regular and inverse atomic structures, and previously published crystal structure refinements for schreibersite were correct. The prevalence of nickel and iron did not change from one atomic arrangement to the next, which is expected. Finally, nickel prefers the M3 site, iron the M1 site and the M2 site is a mixture between the two. The ordering of iron and nickel into different sites is curious at first glance because it was originally thought that each site was equivalent to one another. There are actually minor energy differences between each of the three sites that were created as the iron meteorites cooled and equilibrated slowly. This ordering means that there could be more nickel and less iron in schreibersite than was previously believed. While the empirical formula for schreibersite varies from one publication to the next, they all list iron as having a much higher presence than nickel. For example, this empirical formula was found for the schreibersite in the Toluca meteorite: $Fe_{2.1}Ni_{0.9}P$ (Skála and Císařová 1999). Our data suggests there is a more even amount of iron and nickel, and there may even be more nickel than there is iron. These values could vary depending on the sample though and the amount of nickel in the meteorite.

In the future, more samples from a wider array of better-studied meteorites could be used for these same tests. These types of tests could also help determine if one structure is preferred over the other depending on the conditions in which the meteorite formed. Using an electron microprobe would determine the exact amounts of iron and nickel in the schreibersite to further refine the empirical formula, as well.

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Appendix 1 Crystallographic information file for Seymchan, cr #1

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'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
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F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
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Appendix 2 Crystallographic information file for Seymchan, cr #2a

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 'Fe'  'Fe'   0.3463   0.8444
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'Ni'  'Ni'   0.3393   1.1124
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

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_symmetry_space_group_name_H-M    I-4

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Refinement of F^2^ against ALL reflections.  The weighted R-factor wR and
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on F, with F set to zero for negative F^2^. The threshold expression of
F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
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_atom_sites_solution_secondary    difmap
_atom_sites_solution_hydrogens    geom
_refine_ls_hydrogen_treatment     mixed
_refine_ls_extinction_method      SHELXL
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Appendix 3 Crystallographic information file for Seymchan, cr #3

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 'Fe'  'Fe'   0.3463   0.8444
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'Ni'  'Ni'   0.3393   1.1124
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

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 Refinement of F^2^ against ALL reflections.  The weighted R-factor wR and
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Appendix 4 Crystallographic information file for Seymchan, cr #5

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 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'Ni'  'Ni'   0.3393   1.1124
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

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 Refinement of F^2^ against ALL reflections.  The weighted R-factor wR and
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 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
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_atom_sites_solution_secondary    difmap
_atom_sites_solution_hydrogens    geom
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_refine_ls_extinction_coef        0.012(2)
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 'Fe'  'Fe'   0.3463   0.8444
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'Ni'  'Ni'   0.3393   1.1124
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

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 Refinement of F^2^ against ALL reflections.  The weighted R-factor wR and
 goodness of fit S are based on F^2^, conventional R-factors R are based
 on F, with F set to zero for negative F^2^. The threshold expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
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_atom_sites_solution_secondary    difmap
_atom_sites_solution_hydrogens    geom
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_refine_ls_extinction_method      SHELXL
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 'Fc^*^=kFc[1+0.001xFc^2^\l^3^/sin(2\q)]^-1/4^'
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 and torsion angles; correlations between esds in cell parameters are only
 used when they are defined by crystal symmetry.  An approximate (isotropic)
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