

Revised version - R1

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3 **Steinhardtite, a new body-centered-cubic allotropic form of aluminum from the**
4 **Khatyrka CV3 carbonaceous chondrite**

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6 LUCA BINDI^{1*}, NAN YAO², CHANEY LIN³, LINCOLN S. HOLLISTER⁴, GLENN J. MACPHERSON⁵,
7 GERALD R. POIRIER^{2,‡}, CHRISTOPHER L. ANDRONICOS⁶, VADIM V. DISTLER⁷, MICHAEL P. EDDY⁸,
8 ALEXANDER KOSTIN⁹, VALERY KRYACHKO⁷, WILLIAM M. STEINHARDT¹⁰ and MARINA
9 YUDOVSKAYA⁷

10
11 ¹Dipartimento di Scienze della Terra, Università di Firenze, Via La Pira 4, I-50121 Florence, Italy

12 ²Princeton Institute for the Science and Technology of Materials, Bowen Hall, Princeton University, Princeton, NJ
13 08544, USA

14 ³Department of Physics, Princeton University, Jadwin Hall, Princeton, NJ 08544, USA

15 ⁴Department of Geosciences, Princeton University, Guyot Hall, Princeton, NJ 08544, USA

16 ⁵Department of Mineral Sciences, National Museum of Natural History, Smithsonian Institution, Washington DC,
17 20560, USA

18 ⁶Division of Earth and Atmospheric Sciences, Purdue University, West Lafayette, IN 47907, USA

19 ⁷Institute of Geology of Ore Deposits, Petrography, Mineralogy, and Geochemistry (IGEM), Russian Academy of
20 Sciences, Staromonetny per. 35, Moscow, 119017 Russia

21 ⁸Department of Earth, Atmospheric, and Planetary Sciences, Massachusetts Institute of Technology, Cambridge, MA
22 02139, USA

23 ⁹Geoscience Technology, BHP Billiton, Houston, TX 77056, USA

24 ¹⁰Department of Earth and Planetary Sciences, Harvard University, 20 Oxford Street, Cambridge, MA 02138, USA

25
26 *E-mail: luca.bindi@unifi.it

27
28 ‡ Present address: Advanced Material Characterization Laboratory, University of Delaware, Newark, Delaware 19716,
29 USA

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32 **ABSTRACT**

33 Steinhardtite is a new mineral from the Khatyrka meteorite; it is a new allotropic form of
34 aluminum. It occurs as rare crystals up to ~10 μm across in meteoritic fragments that contain
35 evidence of a heterogeneous distribution of pressures and temperatures during impact shock, in
36 which some portions of the meteorite reached at least 5 GPa and 1200 °C. The meteorite fragments
37 contain the high-pressure phases ahrensitite, coesite, stishovite, and an unnamed spinelloid with
38 composition $\text{Fe}_{3-x}\text{Si}_x\text{O}_4$ ($x \approx 0.4$). Other minerals include trevorite, Ni-Al-Mg-Fe spinels, magnetite,
39 diopside, forsterite, clinoenstatite, nepheline, pentlandite, Cu-bearing troilite, icosahedrite,
40 khatyrkite, cupalite, taenite and Al-bearing taenite. Given the exceedingly small size of
41 steinhardtite, it was not possible to determine most of the physical properties for the mineral.

42 A mean of 9 electron microprobe analyses (obtained from two different fragments) gave the
43 formula $\text{Al}_{0.38}\text{Ni}_{0.32}\text{Fe}_{0.30}$, on the basis of 1 atom. A combined TEM and single-crystal X-ray
44 diffraction study revealed steinhardtite to be cubic, space group $Im\bar{3}m$, with $a = 3.0214(8)$ Å, and V
45 $= 27.58(2)$ Å³, $Z = 2$. In the crystal structure [$R_1 = 0.0254$], the three elements are disordered at the

46 origin of the unit cell in a body-centered-cubic packing (α -Fe structure type). The five strongest
47 powder-diffraction lines [d in Å (I/I_0) (hkl)] are: 2.1355 (100) (110); 1.5100 (15) (200); 1.2329 (25)
48 (211); 0.9550 (10) (310); 0.8071 (30) (321).

49 The new mineral has been approved by the IMA-NMNC Commission (2014–036) and named
50 in honor of Paul J. Steinhardt, Professor at the Department of Physics of Princeton University, for
51 his extraordinary and enthusiastic dedication to the study of the mineralogy of the Khatyrka
52 meteorite, a unique CV3 carbonaceous chondrite containing the first natural quasicrystalline phase
53 icosahedrite.

54 The recovery of the polymorph of Al described here that contains essential amounts of Ni and
55 Fe suggests that Al could be a contributing candidate for the anomalously low density of the Earth's
56 presumed Fe-Ni core.

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58 **Keywords:** aluminum, chemical composition, TEM, X-ray diffraction, new mineral, steinhardtite.

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INTRODUCTION

61 In the course of a detailed investigation of fragments belonging to the Khatyrka meteorite
62 (Steinhardt and Bindi 2012; MacPherson et al. 2013; Bindi and Steinhardt 2014), we found a
63 metallic AlNiFe mineral (Hollister et al. 2014) which turned out to have the characteristics of a new
64 mineral species.

65 Here we report the structural and chemical study leading to the description of this new
66 mineral, which was named steinhardtite after Paul J. Steinhardt, Professor at the Department of
67 Physics of Princeton University and Director of the Princeton Center for Theoretical Science, for
68 his extraordinary and enthusiastic dedication to the study of the mineralogy of the Khatyrka
69 meteorite, a unique CV3 carbonaceous chondrite hosting the first natural quasicrystal icosahedrite
70 (Bindi et al. 2009, 2011, 2012). Moreover, decagonal quasicrystalline alloys have been described in
71 the Al-Ni-Fe system (e.g., Lemmerz et al. 1994; Parshin et al. 2009), thus representing an added
72 reason for the dedication: Steinhardt's pioneering contribution to the theoretical development of
73 quasiperiodic structures (e.g., Levine and Steinhardt 1984).

74 The mineral and its name have been approved by the Commission on New Minerals,
75 Nomenclature and Classification, IMA (2014–036). The holotype material is deposited in the
76 mineralogical collections of the Museo di Storia Naturale, Università di Firenze (Italy), under
77 catalogue number 3142/I.

78

OCCURRENCE

79 Steinhardtite was found in one of the meteoritic fragments (labeled number 126; see
80 Hollister et al. 2014 for more details) recovered from an expedition to the Koryak Mountains in far
81 eastern Russia in 2011 (Steinhardt and Bindi 2012; Bindi and Steinhardt 2014) as a result of a
82 search for material that would provide information on the origin of the quasicrystal mineral
83 icosahedrite (Bindi et al. 2009, 2011, 2012; Hollister et al. 2014). The recovered fragments have
84 meteoritic (CV3-like) oxygen isotopic compositions (MacPherson et al. 2013; Hollister et al. 2014).

85 In the meteoritic fragments, which present a range of evidence indicating that an impact shock
86 generated a heterogeneous distribution of pressures and temperatures in which some portions of the
87 meteorite reached at least 5 GPa and 1200 °C, steinhardtite occurs as small grains, one of which is
88 surrounded by trevorite (Fig. 1a). The grains of steinhardtite are generally anhedral and do not
89 contain inclusions or intergrowths of other minerals. The maximum grain size of steinhardtite
90 identified so far is about 10 μm . Given the exceedingly small size, it was not possible to determine
91 properties like color, streak, luster, hardness, cleavage, parting, fracture or density. The calculated
92 density (for $Z = 2$), using the empirical formula and the unit-cell volume from single-crystal data
93 (see below), is 5.52 g/cm^3 . Other minerals identified in the meteorite fragments include trevorite,
94 diopside, forsterite, ahrensite, clinoenstatite, nepheline, coesite, stishovite, pentlandite, Cu-bearing
95 troilite, icosahedrite, khatyrkite, cupalite, taenite, Al-bearing taenite, Ni-Al-Mg-Fe spinels,
96 magnetite, and an unnamed spinelloid with composition $\text{Fe}_{3-x}\text{Si}_x\text{O}_4$ ($x \approx 0.4$).

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EXPERIMENTAL METHODS

99 X-ray diffraction and structure refinement

100 A crystal of steinhardtite $8 \times 9 \times 10 \mu\text{m}$ across (Fig. 1c) was mounted on a 0.005 mm
101 diameter carbon fiber (which was, in turn, attached to a glass rod) and checked on a CCD-equipped
102 Oxford Diffraction Excalibur 3 single-crystal diffractometer. Despite the extremely small size of the
103 crystal (to the limit for conventional in-house experiments), the diffraction quality was satisfactory
104 and several reflections were collected. The refined unit-cell dimensions are: $a = 3.0214(8) \text{ \AA}$ and V
105 $= 27.58(2) \text{ \AA}^3$. Intensity integration and standard Lorentz-polarization corrections were done with
106 the *CrysAlis* RED software package (Oxford Diffraction 2006). The program ABSPACK in
107 *CrysAlis* RED (Oxford Diffraction 2006) was used for the absorption correction.

108 The systematic absences indicated the space group $Im\bar{3}m$ and the structure was refined
109 starting from the atomic coordinates reported $\alpha\text{-Fe}$ (Wilburn and Bassett 1978) using the full-matrix

110 least-squares program SHELXL-97 (Sheldrick 2008). The scattering curve for neutral Ni was taken
111 from the *International Tables for X-ray Crystallography* (Ibers and Hamilton 1974). The scattering
112 power was allowed to vary (Ni vs. structural vacancy) at the (0,0,0) position. The refined value
113 (21.8 e⁻) is in excellent agreement with the mean electron number calculated from the empirical
114 formula (21.7 e⁻). Refinement of the anisotropic atomic displacement parameters led to an R_1 index
115 of 0.0208 [for 11 reflections with $F_o > 4\sigma(F_o)$] and 0.0254 (for all 12 independent reflections) with
116 3 refined parameters. Details on the data collection and refinement are given in Table 1 and in the
117 deposited CIF¹.

118 **Chemical analyses**

119 The same crystal used for the structural study (Fig. 1c) together with another grain of
120 steinhardtite showing an almost tabular morphology (Fig. 1b) were analyzed by means of a JEOL
121 JXA-8600 electron microprobe analysis in wavelength dispersion mode at 15 kV, 20 nA beam
122 current, and 1 μ m beam diameter. Variable counting times were used: 30 s for Al, Ni and Fe, and 60
123 s for the minor elements Mg, Si, Cr, P, Co, Cu, Cl, Ca, Zn, and S. Replicate analyses of synthetic
124 Al₅₃Ni₄₂Fe₅ were used to check accuracy and precision. The crystal fragments were found to be
125 homogeneous within analytical error. The standards used were: metal-Al (Al), synthetic Ni₃P (Ni,
126 P), synthetic FeS (Fe), metal-Mg (Mg), metal-Si (Si), metal-Cr (Cr), metal-Co (Co), metal-Cu (Cu),
127 synthetic CaCl₂ (Ca, Cl) and synthetic ZnS (Zn, S). Magnesium, Si, Cr, P, Co, Cu, Cl, Ca, Zn, and S
128 were found to be equal to or below the limit of detection (0.01 wt%).

129 Nine point analyses on different spots were performed on the two fragments. Table 2 reports
130 the chemical analyses (means and ranges in wt% of elements), standard deviations and atomic ratios
131 calculated on 1 atom per formula unit.

132 **Transmission electron microscopy**

133 Because of the small size of the grains, the single-crystal X-ray investigation was combined
134 with a structural study done by transmission electron microscopy. The instrument was a Philips
135 CM200-FEG TEM operating at 200 KeV with a vacuum pressure of $\sim 2 \times 10^{-7}$ Torr. The electron
136 beam size ranged from 30 nm to 0.2 μ m. The sample was placed on an Au mesh TEM grid (300
137 mesh, 3mm in diameter) that was previously covered by a thin carbon layer (support film). Energy
138 Dispersive (EDS) data were obtained using Evex NanoAnalysis System IV attached to the Philips

¹ For a copy of the CIF, document item AMxxxxx, contact the Business Office of the Mineralogical Society of America (see inside front cover of recent issue) for price information. Deposit items may also be available on the American Mineralogist web site at <http://www.minsocam.org>.

139 CM200-FEG TEM. A small probe diameter of 20-100 nm was used, with a count rate of 100-300
140 cps and an average collection time of 180 s. The quantitative analyses were taken at 200 kV and are
141 based on using pure elements and the NIST 2063a standard sample as a reference under the
142 identical TEM operating conditions.

143 The measurement of the cubic unit-cell parameter from both the selected area diffraction
144 patterns (Fig. 2) and the diffraction rings (Fig. 3) is only about 1% different and led to a value of
145 3.02(1) Å, in excellent agreement with the value measured by single-crystal X-ray diffraction
146 [3.0214(8) Å].

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RESULTS AND DISCUSSION

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Crystal structure considerations

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In the crystal structure of steinhardtite, Al, Ni and Fe are disordered at the origin of the unit-
151 cell (0,0,0) in a body-centered-cubic (bcc) packing (α -Fe structure type). The metal-metal bond
152 distance observed is 2.6166(7) Å ($\times 8$). Taking into account the site population and the unit-cell
153 parameters observed for the face-centered-cubic (fcc) polymorphs of pure Ni and Fe (Wyckoff
154 1963; Nishihara et al. 2012), and assuming the same V/atom ratio for fcc and bcc structure for Ni,
155 Fe, and ideality, the following unit-cell value for the pure Al polymorph (Ni- and Fe-free
156 steinhardtite) can be derived: $a = 3.218$ Å. Such a value is in excellent agreement with that
157 predicted ($a = 3.230$ Å) by Lechermann et al. (2005) for the bcc allotropic form of Al under room
158 conditions.

159

Potential new natural quasicrystals?

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Decagonal quasicrystalline alloys have been described in the Al-Ni-Fe system (e.g., Lemmerz
161 et al. 1994; Parshin et al. 2009). The decagonal phase is thermodynamically stable in a narrow
162 compositional range around $\text{Al}_{71}\text{Ni}_{24}\text{Fe}_5$. At a temperature of about 940 °C it transforms to
163 $\text{Al}_{13}(\text{Fe},\text{Ni})_4$, $\text{Al}_3(\text{Ni},\text{Fe})_2$ and the liquid phase, and between 800 and 850 °C to $\text{Al}_{13}(\text{Fe},\text{Ni})_4$,
164 $\text{Al}_3(\text{Ni},\text{Fe})$ and $\text{Al}_3(\text{Ni},\text{Fe})_2$. For comparison to the decagonal quasicrystal, based on 100 atoms the
165 composition of steinhardtite is $\text{Al}_{38}\text{Ni}_{32}\text{Fe}_{30}$, quite far from the theoretical composition for a
166 decagonal quasicrystal; but it should be kept in mind that a large variation of the Al/(Ni+Fe) ratio
167 has been observed among the spinel phases of the Khatyrka fragments (see Hollister et al. 2014).
168 This implies that the decagonal quasicrystal may yet be found in the Khatyrka meteorite.

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171 **Steinhardtite in the Al-Ni-Fe system**

172 The composition of steinhardtite within the Al-Ni-Fe system (Chumak et al. 2008) suggests
173 that it should exhibit the B2 structure (CsCl-type; space group $Pm\bar{3}m$) and not the A2 structure
174 (space group $Im\bar{3}m$) as observed for the new mineral. The B2 structure is typically observed for
175 stoichiometric composition, such as (Ni,Fe)Al. In this structure, Ni and Fe atoms share the
176 structural positions at the cell corners (0,0,0) and Al atoms are at the centers ($\frac{1}{2},\frac{1}{2},\frac{1}{2}$) (Rennhofer et
177 al. 2003; Lechermann et al. 2005; Zhang and Du 2007). On the other hand, in the A2 structure there
178 is a complete disorder of the three atoms (i.e., Al, Ni and Fe) at the origin (and, consequently, at
179 $\frac{1}{2},\frac{1}{2},\frac{1}{2}$ given the I lattice) of the unit cell.

180 To the best of our knowledge, nothing is known about the effects of pressure on the Al-Ni-Fe
181 system. Recent investigations on high pressure torsion (HPT) processing of B2-ordered Fe-Al
182 (Gammer et al. 2011) and Ni-Al (Klöden et al. 2008) alloys showed that when a pressure of 4-6
183 GPa is applied during the process an incipient cation disorder in the original B2 structure toward the
184 formation of either nanosized domains with persistent B2 order (Gammer et al. 2011) or even of the
185 A2 structure is observed (Sergiy Divinski, personal communication). The structural disorder of
186 steinhardtite (pointing to the A2 structure) may have been induced by shock. At ambient pressure the
187 B2 structure would be stable.

188 **Origin**

189 The incorporation of metallic Al in steinhardtite as well as in taenite has been tentatively
190 explained by Hollister et al. (2014) with one of the two possible scenarios: (i) the Al-bearing FeNi
191 phases might have been the initial source of the Al-bearing alloys khatyrkite, cupalite and
192 icosahedrite; or (ii) the Al-metals may have had a pre-accretion nebular origin and steinhardtite and
193 Al-bearing taenite observed in the sample formed by reaction of shock-produced Al-melt and pre-
194 existing taenite.

195 In the first hypothesis, the shock features observed locally for grains 125 and 126 of the
196 Khatyrka meteorite (Hollister et al. 2014) would be generated by a strong increase of heat and
197 pressure sufficient to extract Al from the FeNi metals and to initiate the local melting of metals and
198 silicates. In the second hypothesis, the Al metals would form in some nebular process before the
199 impact, with the impact resulting in the remelting, rapid cooling (about $10^2 - 10^3$ °C s⁻¹) and
200 solidification of the Al metals. In both scenarios, the sequence of events leading to the exchange of
201 metallic Al that formed steinhardtite and Al-taenite can only be plausibly imagined to occur in
202 space under low fO_2 solar nebular conditions.

203

IMPLICATIONS

204 Our investigation of the different fragments of the thus far unique and remarkable Khatyrka
205 carbonaceous chondrite (MacPherson et al. 2013) has revealed the heretofore unobserved metallic
206 Al bearing minerals (Hollister et al. 2014) for a carbonaceous chondrite: khatyrkite, cupalite,
207 icosahedrite, and steinhardtite. These unique phases existed at the birth of our solar system 4.5
208 billion years ago. The fact that metallic Al can be incorporated in nebular FeNi to form new mineral
209 species like steinhardtite is a striking discovery.

210 It is currently accepted that the phase considered stable in the Earth's core is a body-centered-
211 cubic structured alloy of Fe-Ni doped with lighter elements (e.g., Dubrovinsky et al. 2007; Luo et
212 al. 2010). Moreover, first-principle theoretical (Friedli and Ashcroft 1975; Moriarty and McMahan
213 1982; Boettger and Trickey 1996; Pickard and Needs 2010) and experimental studies (Roy and
214 Steward 1969; Akahama et al. 2006; Vailionis et al. 2011) have shown that pure Al converts from a
215 face-centered-cubic to a hexagonal-close-packed structure at multimegabar pressures, and, at 0.38
216 TPa, a pressure slightly above that found at the center of the Earth, to a body-centered-cubic
217 structure. Such a bcc polymorph of Al, successfully synthesized with ultrafast explosions, also has
218 been found to be quenchable at room conditions (Vailionis et al. 2011).

219 These considerations, together with the presence of essential amounts of Ni and Fe in
220 steinhardtite might reveal an additional light element, Al (beside C, O, Si, and S; Allègre et al.
221 2001; Côté et al. 2008) to contribute to the anomalously low density of the Earth's presumed Fe-Ni
222 core.

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FIGURE CAPTIONS

314 FIGURE 1. SEM-BSE images of three small steinhardtite grains. In (a) steinhardtite (STE) is
315 enclosed by trevorite (TRE); in (b) it is a separate grain exhibiting tabular morphology; in
316 (c) it is a small grain attached to a carbon fiber that was used for the X-ray single-crystal
317 diffraction study.

318

319 FIGURE 2. TEM image of steinhardtite. Electron diffraction patterns (zone axes are indicated) were
320 obtained from a thin region of this granule (indicated with the white dotted circle).

321

322 FIGURE 3. TEM image of another granule of steinhardtite. On the right are the diffraction rings,
323 obtained from a thin region (indicated with the white dotted circle), which were indexed
324 according to a body-centered-cubic structure, space group $Im\bar{3}m$, with $a = 3.02(1)$ Å
325 (indexing as 110, 200, 211, 220, 310, 222, 321).

326

TABLE 1. Data and experimental details for the selected steinhardtite crystal

Crystal data	
Formula	Al _{0.38} Ni _{0.32} Fe _{0.30}
Crystal size (mm)	0.008 × 0.009 × 0.010
Form	block
Colour	black
Crystal system	cubic
Space group	$Im\bar{3}m$ (#229)
a (Å)	3.0214(8)
V (Å ³)	27.58(2)
Z	2
Data collection	
Instrument	Oxford Diffraction Xcalibur 3
Radiation type	MoK α ($\lambda = 0.71073$)
Temperature (K)	298(3)
Detector to sample distance (cm)	5
Number of frames	115
Measuring time (s)	350
Maximum covered 2θ (°)	70.37
Absorption correction	multi-scan (<i>ABSPACK</i> ; Oxford Diffraction 2006)
Collected reflections	465
Unique reflections	12
Reflections with $F_o > 4\sigma(F_o)$	11
R_{int}	0.0285
Range of h, k, l	$0 \leq h \leq 4, 0 \leq k \leq 4, 0 \leq l \leq 4$
Refinement	
Refinement	Full-matrix least squares on F^2
Final R_1 [$F_o > 4\sigma(F_o)$]	0.0209
Final R_1 (all data)	0.0254
Number of least squares parameters	3
$\Delta\rho_{\text{max}}$ (e Å ⁻³)	0.22
$\Delta\rho_{\text{min}}$ (e Å ⁻³)	-0.38

$$R_{\text{int}} = (n/n-1)^{1/2} [F_o^2 - F_o(\text{mean})^2] / \sum F_o^2$$

$$R_1 = \sum ||F_o| - |F_c|| / \sum |F_o|$$

TABLE 2. Electron microprobe analyses (means, ranges and standard deviations in wt% of elements) and atomic ratios (on the basis of one atom) for steinhardtite.

element	wt %	ranges	σ	atom	atomic ratios
Al	22.41	21.94 – 23.30	0.16	Al	0.38
Ni	40.90	40.01 – 42.10	0.26	Ni	0.32
Fe	36.23	35.06 – 37.29	0.19	Fe	0.30
total	99.54	98.45 – 101.62			





