Inorganic Chemistry

Flux Synthesis of a Metal Carbide Hydride Using Anthracene As a Reactant

Tate O. Engstrand, Emily M. Cope, Guillermo Vasquez, Jo W. Haddock, Mary B. Hertz, Xiaoping Wang, and Susan E. Latturner*



ABSTRACT: $La_{15}(FeC_6)_4H$ was synthesized from the reaction of iron and anthracene in La/Ni eutectic flux. Anthracene was the source of both the carbon and hydrogen in the product. The structure of this metal carbide hydride features hydride ions in tetrahedral interstitial sites surrounded by lanthanum ions, which was confirmed by single-crystal neutron diffraction studies. The trigonal planar FeC₆ units in which the central iron atom is coordinated by three ethylenide groups are similar to those found in $La_{3,67}FeC_{67}$, a previously reported compound that is formed in the absence of a hydride source. Magnetic susceptibility data confirm that the iron sites do not have magnetic moments. Density of states



Article

calculations indicate that $La_{15}(FeC_6)_4H$ is metallic and is stabilized by the incorporation of hydride anions.

INTRODUCTION

Metal carbides and metal hydrides are two classes of compounds that have been heavily explored in recent years. Transition-metal carbides such as WC are utilized for their hardness; multinary rare earth transition-metal carbides exhibit complex structures and properties ranging from strong magnetism $(Pr_2Fe_{14}C)$ to semiconductivity $(LaRhC_2)$.¹⁻ Metal hydrides, previously of interest as hydrogen storage materials as exemplified by $LaNi_5H_6$, are undergoing a research renaissance due to superconductivity observed in LaH_{10} superhydrides at high pressure.^{4,5} There are very few compounds located at the intersection of these classes, e.g., the metal carbide hydrides, or metal carbohydrides. Ternary $M_x C_y H_z$ phases are known for M = early transition metals or rare earth metals. These disordered compounds such as ZrC_{0.44}H_{0.89} and YbCH_{0.5} are typically made from reacting metal carbides with hydrogen gas, or reacting metal and carbon under an atmosphere of hydrogen.^{6–8} The hydride and carbide ions randomly occupy interstitial sites surrounded by 4-6 metal cations.

Metal flux synthesis offers a different method for the synthesis of complex intermetallic hydrides and carbides. Flux reactions enable reactants to be brought into solution, overcoming diffusion barriers and enabling elements with very different melting points to interact. Slow cooling of the solution allows products to be isolated as crystals.⁹ Our group has explored synthesis in a variety of rare earth/transition metal (R/T) eutectic flux mixtures; these fluxes are excellent solvents for carbon and have yielded metal carbides such as $La_{21}Fe_8Sn_7C_{12}$, $Ce_{33}Fe_{13}B_{18}C_{34}$, and $Pr_{62}Fe_{21}Si_{16}C_{32}$.^{10–12} Complex metal hydrides can be readily synthesized in fluxes containing alkaline earth metals, as indicated by the formation

of LiCa₇Ge₃H₃ and Ca₅₄In₁₃H₂₇ from reactions of CaH₂ with other elements in Ca/Li melts.^{13,14} Alkaline-earth-based fluxes have also yielded metal carbide hydrides, including LiCa₂C₃H from Ca/Li and Ba₁₂InC₁₈H₄ from Ba/Li melts.^{15,16}

In this work we report the synthesis of $La_{15}(FeC_6)_4H$, a new metal carbide hydride that grows as large crystals from the reaction of iron and anthracene in La/Ni eutectic flux. The anthracene ($C_{14}H_{10}$) conveniently acts as both a carbon and hydrogen source. Its decomposition during the flux reaction was anticipated from a previous report on the pyrolysis of methane over molten metals.¹⁷ The presence of hydride in the product structure was indicated by single-crystal neutron diffraction studies. This suggests the possibility that the nearly infinite variety of organic molecules may be useful reactants for metal flux synthesis of new metal carbide hydrides.

EXPERIMENTAL PROCEDURE

Synthesis. The title compound was grown from reactions in lanthanum/nickel eutectic melts. The La/Ni eutectic (88:12 wt %, Alfa Aesar, 99.9%; ingot pieces) was stored under nitrogen until it was used. Iron powder (Strem Chemicals, 99.9%) and anthracene powder ($C_{14}H_{10}$, Sigma-Aldrich, 97%) were weighed out in a 1:0.2 mmol ratio and placed in an alumina crucible. Pieces of La/Ni eutectic weighing a total of 1.5 g were then added into the crucible. The crucible was placed in a fused silica tube with a wad of fiberfrax ceramic fiber below and above it. A piece of iron mesh was placed between the crucible

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and the fiberfrax to act as a filter during centrifugation and to prevent pieces of the brittle fiberfrax from falling into the reaction mixture. The tube was immediately evacuated and flame-sealed under a pressure of 10⁻³ Torr. This ampule was then placed into a furnace and heated to 950 °C in 3 h, held at this temperature for 12 h, and then cooled to 600 °C in 120 h at which point it was removed from the furnace, inverted, and centrifuged to remove the excess molten flux. The inside of the reaction ampule was typically discolored by deposition of carbon due to the decomposition of anthracene vapor. CAUTION! Decomposition of anthracene generates gaseous products which may result in elevated pressures in the sealed ampules. While very small amounts of anthracene were used in this work and there were no signs of excessive hydrogen gas pressure generated (no tubes ruptured during heating), suitable safety precautions for handling potentially pressurized vessels were taken during the centrifugation process, including use of face shields and insulated gloves.

Synthesis of the title compound by stoichiometric reaction of its elements was also attempted. Lanthanum powder, iron powder, carbon powder, and anthracene (as both a carbon and hydrogen source) were combined in a 3:0.8:4.52:0.2 mmol ratio in an alumina crucible which was sealed under vacuum in a silica tube. This reaction was heated to 1000 $^{\circ}$ C in 3 h, held at this temperature for 12 h, and cooled to room temperature in 36 h. The resulting solid was a mixture of a black powder surrounding silvery chunks.

Elemental Analysis. Elemental analysis was carried out using a FEI Nova 400 NanoSEM scanning electron microscope with energy dispersive spectroscopy capabilities (SEM-EDS). Samples of the product crystals were placed on an aluminum puck using double-sided carbon tape. To avoid artifacts from flux residue on the sample surface, the crystals were cleaved (with some difficulty as they are somewhat hard) to expose their interiors to be analyzed. An average atomic ratio of 78.0(7)% La and 22.0(7)% Fe was observed. This method is not sensitive to light elements such as hydrogen and carbon; the presence of these elements was confirmed using other methods (vide infra). No incorporation of aluminum from the crucible or nickel from the flux was observed.

Crystallographic Studies. Samples of $La_{15}(FeC_6)_4H$ were covered in Parabar oil and examined under a microscope to select crystals for diffraction studies. Suitable pieces were cut from larger crystals and were mounted in a MiTeGen microloop. Single-crystal Xray diffraction data were collected at 200 K using a Bruker APEX 2 CCD diffractometer with a Mo-K α radiation source. Absorption corrections were applied to the data sets using the SADABS program. Refinement of the structures were performed using the SHELXTL package. ^{18,19} The $La_{15}(FeC_6)_4H$ structure was solved in the hexagonal $P\overline{6}$ space group. Lanthanum and iron atoms were located via direct methods; positions of carbon atoms were found from analysis of residual electron density peaks in the difference Fourier maps and consideration of interatomic distances (vide infra). Thermal parameters were refined anisotropically. Crystallographic data and X-ray diffraction collection parameters for this compound are shown in Table 1.

Neutron Diffraction. To determine the location and occupancy of hydride ions in the sample, single-crystal neutron diffraction data were collected on the TOPAZ diffractometer at the Spallation Neutron Source at Oak Ridge National Laboratory.²⁰ A large $La_{15}(FeC_6)_4H$ crystal (1 × 1 × 0.4 mm) was coated with a thin film of Krytox fluorinated grease and adhered to a MiTeGen loop. This was attached to the goniometer head inside the TOPAZ sample chamber and then cooled to 100 K under a nitrogen stream. Data were collected using 19 crystal orientations determined using the CrystalPlan software for an estimated 98% coverage of reflections of the hexagonal cell.²¹ Each orientation was exposed to 9-10 C of proton charge at a neutron beam power of 1.4 MW (for approximately 2 h). The integrated peak intensities were determined using the 3D ellipsoidal q-space integration in the Mantid platform. The neutron absorption coefficient is $0.04792 + 0.013583\lambda$ (in mm⁻¹; λ ranges from 0.4–3.5 Å). Data reduction (including detector efficiency, neutron TOF spectrum, and absorption corrections) was carried out with the ANVRED3 program.²³ The reduced data were

Table 1. Crystallographic Data Collection Parameters for $La_{15}(FeC_6)_4H$

diffraction type	X-ray	neutron
formula	$La_{15}(FeC_6)_4H$	
$M_{\rm r}$ (g/mol)	2596.30	
crystal system, space group	hexagonal, P 6	
Ζ	1	
temperature (K)	200	100
a, c (Å)	8.7890(4), 10.7691(5)	8.7764(5), 10.7355(9)
V (Å ³)	720.42 (7)	716.1(1)
radiation type	Mo- $K\alpha$	neutron TOF
$\mu (\text{mm}^{-1})$	23.63	0.04792 + 0.013583 \times λ
crystal size (mm)	$0.15 \times 0.15 \times 0.14$	$1 \times 1 \times 0.4$
no. of measured, independent, and observed $[I > 2\sigma(I)]$ reflections	8021, 1232, 1231	12379, 2730
R _{int}	0.022	
θ values (deg)	$\theta_{\min} = 1.891^{\circ}, \\ \theta_{\max} = 28.358^{\circ}$	$\theta_{\min} = 7.32^{\circ}, \\ \theta_{\max} = 78.497^{\circ}$
no. of reflections	1232	2730
no. of parameters	66	80
R_1 , wR_2 (all data)	0.0112, 0.0248	0.0238, 0.0504
$R_1, wR_2 (I > 2\sigma(I))$	0.0111, 0.0248	0.0238, 0.0504
$\Delta \langle_{ m max'} \Delta \langle_{ m min}$	0.91, $-0.72~(e~{\rm \AA}^{-3})$	1.412, -1.328 (f Å ⁻³)
${}^{a}R_{1} = \Sigma(F_{0} - F_{c})/\Sigma F_{0} ; wR_{2} = \left[\Sigma[w(F_{0}^{2} - F_{c}^{2})^{2}]/\Sigma(w F_{0} ^{2})^{2}\right]^{1/2}.$		

then refined in the SHELXTL suite of programs; resulting parameters are shown in Table 1.¹⁸ Additional crystallographic data including tables of atom positions and thermal parameters and bond lengths can be found in the Supporting Information (Tables S1 and S2) and are deposited as a CIF file with the Cambridge Crystallographic Data Centre (CCDC), under the deposition no. 2005299.

Electronic Structure Calculations. Density of states (DOS) calculations were performed using the tight-binding linear muffin tin orbitals-atomic sphere approximation implemented in the Stuttgart TB-LMTO-ASA software package (ver. 47.1b).²⁴⁻²⁷ Calculations were carried out on a nonhydrided model $(La_{15}(FeC_6)_4)$ and fully hydrided model $(La_{15}(FeC_6)_4H_2)$ in space group $P\overline{6}$ to explore the effects of addition of hydrogen to the structure. The $P\overline{6}$ structural models were based on unit cell parameters and atomic coordinates experimentally determined by neutron diffraction at 100 K. Since the neutron diffraction data indicated that the hydride site was halfoccupied, we derived another model in the lower symmetry space group P3, which splits the hydride 2g Wyckoff site into two 1a Wyckoff sites (see Tables S1 and S2). This allows the creation of a model in which only one of those 1a hydride sites is occupied, yielding a $La_{15}(FeC_6)_4H$ stoichiometry. DOS calculations were performed for this P3 model. For all three models, empty spheres were added to fill the interstitial spaces of the unit cell. An improved tetrahedron method was used to integrate a $18 \times 18 \times 6 \kappa$ -space, giving 440 irreducible κ points in the first Brillouin zone the model hexagonal phase. The basis set of the calculation consisted of 6s/ (6p)/5d/4f for La, 4s/4p/3d for Fe, 2s/2p/(3d) for C, and 1s/(2p)/(3d)(3d) for H, with parenthetical orbitals downfolded.

Magnetic Susceptibility. Magnetic susceptibility measurements were collected using a Quantum Design MPMS SQUID magnetometer. A single large crystal of $La_{15}(FeC_6)_4H$ was sandwiched between two 4 cm pieces of Kapton tape which was then placed inside a plastic sample holder for insertion into the magnetometer. Field-cooled (FC) and zero-field-cooled (ZFC) measurements were collected at a 10000 G applied field strength over a temperature range from 1.8 to 300 K.

RESULTS AND DISCUSSION

Synthesis. Synthesis and crystal growth of rare earth transition-metal carbides has been carried out in metal fluxes with great success. Eutectics formed from early rare earth metals (La, Ce, Pr, Nd) and late transition metals (Co, Ni, Cu) are excellent solvents for carbon; we have used such eutectics as growth media for carbides including $La_{21}Fe_8Sn_7C_{12}$, $Ce_{33}Fe_{13}B_{18}C_{34}$, $Pr_{62}Fe_{21}Si_{16}C_{32}$, and Nd_2Co_2SiC .^{10–12,28} All these reactions used amorphous carbon (acetylene carbon black) as a precursor. We are now investigating the use of organics as a source of carbon, and possibly of hydrogen. This is inspired by a report by McFarland et al. in which methane gas was decomposed into carbon and hydrogen by flowing it through a bath of molten metals.¹⁷ Given this behavior, it is possible that other C_xH_y compounds will also act as sources of carbon and potentially hydrogen when heated in the presence of metal fluxes.

Anthracene ($C_{14}H_{10}$, mp = 215 °C and bp = 340 °C at 760 mmHg) was used in this experiment because of its stability, low cost, and ease in handling and weighing. This compound enters the vapor phase before the flux melts; La/Ni eutectic (68 mol % La/32 mol % Ni) has a melting point of 517 $^{\circ}$ C.²⁵ When the La/Ni flux melts, the anthracene vapor will be decomposed into carbon and hydrogen. This was evidenced by the fact that the inner surface of the silica reaction ampules was coated with carbon when removed from the furnace. The carbon is highly soluble in the metal melt; this experiment indicates that the hydrogen gas is also reactive toward the flux, as both elements were incorporated into the $La_{15}(FeC_6)_4H$ product. Changing the amounts (in mmol) of Fe and anthracene to 0.5:0.2 or 1:0.4 produced similar results. This product is also produced if pyrene $(C_{16}H_{10})$ is used in place of anthracene. When a similar reaction was carried out using only carbon (instead of anthracene), the products were unreacted carbon powder and small silver crystals of La3,67FeC6. An attempt at stoichiometric synthesis led to formation of carbon powder and silvery chunks identified by PXRD as being La_{3.67}FeC₆.³⁰

This new quaternary carbide hydride grows as very large faceted silver crystals (see Figure 1), along with a greyish powder byproduct that was not identified. The $La_{15}(FeC_6)_4H$ crystals are air and water sensitive; the surface becomes black when exposed to air. The yield is approximately 20% based on



Figure 1. Microscope image of $La_{15}(FeC_6)_4H$ crystals on 1 mm grid paper.

anthracene, likely due to the loss of some of this reactant through vapor phase decomposition and deposition of carbon on the ampule surface. Attempts to make analogs of this new phase by replacing iron with other transition metals (including Mn and Ru) were not successful. Reactions with manganese yielded well-formed crystals, with elemental analysis indicating atomic percentages of 79% La and 21% Mn. Preliminary single-crystal diffraction studies indicated a rhombohedral unit cell with *a* = 15.28 Å and *c* = 16.02 Å. These atomic ratios and unit cell parameters are identical to those reported for La₁₁(MnC₆)₃, which was previously synthesized from reactions of Mn and carbon in La/Ni flux and exhibits a structure that is an ordered supercell of the La_{3.67}FeC₆ type.³¹

Structure. The title compound crystallizes with a new structure type in hexagonal space group $P\overline{6}$. The structure is shown in Figure 2, in comparison to a related compound La_{3.67}FeC₆. Both compounds feature roughly trigonal planar FeC₆ units, which are comprised of a central iron atom coordinated by three ethylenide (C=C) species. Similar TC₆ building blocks have been observed in other $R_xT_yC_z$ carbometalate compounds (R = rare earth, T = transition metal), including La_{3.67}FeC₆, La₁₁(MnC₆)₃, and RE₁₅Fe₈C₂₅ (RE = Y, Dy, Ho, Er).^{30–32} The double bond between the carbon atoms is implied by the bond length (in the range of 1.30–1.34 Å for these compounds) which compares well to the 1.334–1.337 Å double bond lengths seen in ethylene.³³ The Fe–C distances in La₁₅(FeC₆)₄H are within 1.80–1.85 Å, similar to those observed in other iron carbide phases such as La_{3.67}FeC₆ (1.814 Å), Y₂Fe₁₇C (1.824–1.939 Å), and Gd₁₃Fe₁₀C₁₃ (1.804–1.876 Å).^{30,34,35}

The initial report on La3,67FeC6 indicated one crystallographically unique iron site, although a reinvestigation of the structure revealed a supercell with two Fe sites.³⁰ The associated FeC₆ units are rigorously trigonal planar and perfectly eclipsed along the *c*-axis (Figure 2); the C-Fe-C angle is 120° , and the Fe-C-C bonding is linear. $La_{15}(FeC_6)_4H$, on the other hand, has three unique iron sites. While the FeC_6 units centered by Fe(1) and Fe(3) are trigonal planar, they have bent Fe-C-C bonds with angles of 162–168° and are rotationally offset in their stacking along the *c*-axis. The Fe(2) site centers FeC_6 units that are eclipsed along the c-axis, with slight distortion from planarity (the C-Fe-Cangle is 118°), possibly due to repulsion from the lanthanum ion positioned between them. All of the FeC₆ units are wellseparated from each other by surrounding La³⁺ ions (see Figure 3); the closest Fe–Fe distances between these species is 4.945(2) Å.

The incorporation of hydride in $La_{15}(FeC_6)_4H$ was postulated due to the synthesis in the presence of anthracene and the resulting formation of a new structure; in the absence of a hydrogen source, $La_{3,67}FeC_6$ is formed. The presence of a hydride was clearly indicated by the negative scattering of this element in the neutron diffraction data collected on a single crystal of $La_{15}(FeC_6)_4H$. During refinement, the site occupancy approached 50%, so it was fixed at 0.50. It is located on a (0,0,z) position (2g Wyckoff site), surrounded by four lanthanum cations in a tetrahedral geometry. The distances of 2.456(6)Å to three lanthanum sites and 2.648(15)Å to the fourth La site along the *c*-axis are similar to those reported for lanthanum hydrides. La-H distances in LaH2 and LaH3 are 2.455 and 2.433 Å, respectively; a 2.428 Å distance is observed in LaCo₅H₃.³⁶⁻³⁸ The La₁₅(FeC₆)₄H hydride site is 1.98 Å from its symmetry equivalent along the *c*-axis (see Figure 3).



Figure 2. Structures of $La_{15}(FeC_6)_4H$ and $La_{3,67}FeC_6$ viewed down the [110] and [001] directions. Lanthanum, iron, carbon, and hydrogen atoms are represented by green, red, black, and yellow spheres, respectively. Trigonal planar FeC₆ groups are shown in polyhedral mode, as is the coordination of hydride site.



Figure 3. Local coordination environments of iron and hydride sites in $La_{15}(FeC_6)_4H$. La, Fe, C, and H are represented by green, red, black, and yellow spheres, respectively. (a) Fe(1) site viewed down the *c*-axis, and the (b) Fe(2) site and (c) H(1) site viewed perpendicular to the *c*-axis.

Given the typical behavior in metal hydrides where occupied interstitial sites should be separated by at least 2.1 Å, the observed half-occupancy is therefore logical, i.e., if one of the 2g sites is occupied, its symmetry equivalent must be vacant.³⁹

Magnetic Properties. $La_{15}(FeC_6)_4H$ behaves as a Pauli paramagnet. Field-cooled and zero-field-cooled plots exhibited the identical susceptibility behavior at the same temperatures; the field-cooled curve is pictured in Figure 4. The susceptibility of La₁₅(FeC₆)₄H is very weakly temperature dependent between 300 and 1.8 K, increasing from 5.0×10^{-4} to $1.2 \times$ 10^{-3} emu/La³⁺ when cooled through this range. However, this is likely due to magnetic impurities from residual flux remaining on the crystal. The magnitude of the Pauli paramagnetism is similar to values reported for intermetallic compounds with no localized or itinerant moments, such as La_2BiNi and $La_2Au_3Sn_6$.^{40,41} This behavior is consistent with a metallic compound containing nonmagnetic La³⁺ ions and iron atoms strongly coordinated by carbon eliminating the magnetic moment on this atom; the only contribution to the susceptibility (aside from very small core diamagnetism) is the Pauli paramagnetism due to the conduction electrons.⁴



Figure 4. Field-cooled magnetic susceptibility data for $La_{15}(FeC_6)_4H$ between 300 and 1.8 K.

Electronic Structure Calculations. Density of states calculations were carried out for three models of the title compound. The partial occupancy of the hydride site in the P6 space group was modeled either as completely empty $(La_{15}(FeC_6)_4 \mod e)$ or completely full $(La_{15}(FeC_6)_4H_2)$ model) to compare the relative stabilities of the compound with and without the presence of the hydride interstitials. The third model is derived from lowering the symmetry to P3, which splits the hydride 2g Wyckoff site into two 1a sites. Assigning only one of these 1*a* sites as occupied yields a model $(La_{15}(FeC_6)_4H \text{ model in } P3)$ that is more reflective of the actual P-6 structure in which the hydride site is half-occupied. The DOS diagrams of all three models are shown in Figure 5. For all models, the iron-carbon bonding in the FeC₆ units predominates in the region immediately below the Fermi level, particularly between -1 and -2.5 eV. Lanthanum-carbon bonding is accounted for in the region between -3.5 to -5.5eV. Fe-d states provide the majority contribution from iron at all pictured energy levels. Lanthanum states increase in prominence above the Fermi level. While the DOS data for



Figure 5. Density of states diagrams for three models of $La_{15}(FeC_6)_4H$. States for H are represented with yellow, C with black, Fe in red, and La in green, with total DOS represented by a dashed gray line. The Fermi level is set at 0 eV (blue dashed line), and a pseudogap is indicated by an arrow.

the hydrided and nonhydrided models in $P\overline{6}$ are very similar, it is notable that the nonhydrided model yields a sharp lanthanum-based peak at the Fermi level (indicative of instability) which is not present for the hydride.

The hydride states in $La_{15}(FeC_6)_4H_2$ (in P-6) and $La_{15}(FeC_6)_4H$ (in P3) are well below the Fermi level (at -3and -3.5 eV), very narrow, and overlap with narrow La states, supporting a stable, localized, and ionic nature. In the $P\overline{6}$ structure, the hydride site is half-occupied; this partial occupancy and corresponding fewer electrons will shift the Fermi level lower, positioning it in a small pseudogap. The density of states calculated for La₁₅(FeC₆)₄H in P3 to model this half-occupancy confirms that $E_{\rm F}$ is shifted even closer to the small pseudogap. These data indicate that incorporation of hydride into the structure stabilizes the compound. Similar formation of a pseudogap at $E_{\rm F}$ has been observed for other intermetallic hydrides such as LaGa₂H and Ca₅Sb₃H.^{43,44} These reports explored this pseudogap formation from a Zintl phase electron counting perspective; hydride incorporation enabled these compounds to achieve a charge balanced state. While identification of local charges in metallic phases is often

unrealistic, a useful comparison can be made to the related compounds $Ln_{3.67}TC_6$ (Ln = lanthanides; T = Fe, Ru, Os).⁴⁵ The rare earth cations are trivalent (supported by magnetic susceptibility measurements), and their partial occupancy is consistent. This indicates a -11 charge for the TC₆ group to balance the (Ln^{3+})_{3.67} cation charge. The title compound can therefore be viewed as (La^{3+})₁₅([FeC₆]⁻¹¹)₄(H⁻); the incorporation of the hydride (and its half-occupancy) balances the overall electron count and positions the Fermi level in a pseudogap.

CONCLUSIONS

The metal flux synthesis of La₁₅(FeC₆)₄H provides a new addition to the library of reported metal carbide hydrides. Because it contains carbon as part of a Fe_xC_y species, the title compound can actually be viewed as a carbometallate hydride, the first reported to our knowledge. The use of organic molecules in metal flux synthesis introduces a vast array of new reactants for metal carbide hydride growth. Another intriguing avenue to explore is the use of metal cyanides or C_xH_yN_z compounds as reactants in metal flux syntheses of complex metal carbide nitrides. In these investigations, care must be taken to ensure that gaseous decomposition products do not generate sufficient pressure to rupture the reaction vessel at high temperatures.

ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available free of charge at https://pubs.acs.org/doi/10.1021/acs.inorgchem.0c01505.

Tables of atomic positions and bond lengths for $La_{15}(FeC_6)_4H$ in $P\overline{6}$ from neutron diffraction and table of atomic positions for $La_{15}(FeC_6)_4H$ in lower symmetry space group P3 (PDF)

Accession Codes

CCDC 2005299 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge via www.ccdc.cam.ac.uk/data_request/cif, or by emailing data_request@ccdc.cam.ac.uk, or by contacting The Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, UK; fax: +44 1223 336033.

AUTHOR INFORMATION

Corresponding Author

Susan E. Latturner – Department of Chemistry and Biochemistry, Florida State University, Tallahassee, Florida 32306, United States; o orcid.org/0000-0002-6146-5333; Email: slatturner@fsu.edu

Authors

- **Tate O. Engstrand** Department of Chemistry and Biochemistry, Florida State University, Tallahassee, Florida 32306, United States
- **Emily M. Cope** Department of Chemistry and Biochemistry, Florida State University, Tallahassee, Florida 32306, United States
- **Guillermo Vasquez** Department of Chemistry and Biochemistry, Florida State University, Tallahassee, Florida 32306, United States
- Jo W. Haddock Department of Chemistry and Biochemistry, Florida State University, Tallahassee, Florida 32306, United States

- **Mary B. Hertz** Department of Chemistry and Biochemistry, Florida State University, Tallahassee, Florida 32306, United States
- Xiaoping Wang Neutron Scattering Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, United States; ¹⁰ orcid.org/0000-0001-7143-8112

Complete contact information is available at: https://pubs.acs.org/10.1021/acs.inorgchem.0c01505

Notes

The authors declare no competing financial interest.

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