Spin-canting driven Weyl physics in EuCd$_2$As$_2$

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Though rare, magnetic Weyl semimetals stand as the best platform to study elusive Weyl physics as they can host the minimal allowable number of Weyl points. Here we present neutron diffraction and density functional theory work elucidating the magnetic structure realized in the magnetic Weyl semimetal EuCd$_2$As$_2$. Our work shows an unanticipated magnetic structure (magnetic space group $C2'/m'$) with an in-plane [210] moment direction and a slight out-of-plane canting. This canted structure indicates that subtle tuning (rather than a phase transition) may be able to stabilize the sought c-polarized state. Our density functional theory work shows that though Weyl physics should exist for a purely in-plane [210] structure, even a slight canting drastically alters the relevant bands leading to well defined Weyl points. Furthermore, we find that relative to the c-polarized state the [210] order with a small canting brings the Weyl points closer to the Fermi level and thus may lead to clearer signatures of the Weyl physics.

I. INTRODUCTION

Despite implying (along with long-range entangled states) the presence of classifications beyond Landau theory, symmetry protected topological states (SPT) are delightfully enumerable in suitable materials and toy models via familiar and intuitive symmetry considerations. For instance, starting from a Dirac semimetal (DSM) with a single Dirac point (DP), one may break inversion-symmetry (IS), time-reversal symmetry (TRS), both or even combinations of either with crystal symmetries to break the DP into varying numbers of Weyl points (WP). Alternatively, one could instead shift the DP off a crystal symmetry operation to render the DSM instead a topological insulator [1][3].

Enticingly, each of these situations leads to different materials’ properties and, for some of the cases, different emergent physics heralding in a ‘zoo’ of exotic topological quasi-particles [1][4]. Of these, the chiral Weyl quasiparticle is especially interesting both as a unique realization of a solution to relativistic wave-equations and as a tool for enabling new or enhancing existing technologies such as photovaltics, valleytronics and quantum computers [6][10]. Yet the numerous routes to and realizations of Weyl semimetals (WSM) are not all equal, with TRS breaking providing the only route to a minimal number of WP and thus providing their clearest signatures. However, magnetic WSM have proven somewhat rare with several of the candidate materials encumbered by less than ideal symmetries leading to numerous WP [11][15].

Recently, an analysis of magnetic space groups (MSG) led to the prediction that EuCd$_2$As$_2$ (centrosymmetric space group $P\overline{3}m1$) when coupled with an out-of-plane A-type antiferromagnetism (AFM) should exhibit a single pair of WP [10][17]. However, experimental work has generated conflicting stories, with early reports of the desired magnetic structure giving way to suggestions of a less ideal in-plane AFM arrangement or even DSM rather than WSM physics [18][20]. This conflict is in-part due to the highly neutron absorbing Eu and Cd which prevent the use of neutron scattering to provide a definitive magnetic structure solution leaving less comprehensive techniques as the only available probes [18][19]. As a further complication, several recent papers have shown that different synthesis procedures can lead to different magnetic orders with new seemingly purely ferromagnetic (FM) EuCd$_2$As$_2$ samples appearing [21][22]. Nonetheless, throughout its study EuCd$_2$As$_2$ has shown promising hints at topological physics such as WP in ARPES measurements, the quantum anomalous Hall Effect, effective TRS breaking in the paramagnetic phase, and a large negative transverse magnetoresistance indicating the need for more work settling the actual magnetic structure [17][22][24].

In this communication, using isotopic $^{153}$Eu and $^{116}$Cd we report the zero field and 2 T magnetic structures of FM EuCd$_2$As$_2$ determined by neutron diffraction and analyze the topology of the resulting band structures. Our data reveal a \textit{k} = (0, 0, 0) type FM order for both the zero field and 2 T structures. Qualitative analysis of the magnetic intensities suggests that for the zero field structure the Eu moments point along the in-plane [210] direction with a slight out-of-plane canting (MSG $C2'/m'$) while the 2 T structure exhibits the expected c-polarized state. Using this canted magnetic structure to perform DFT calculations we find that the band structure is extraordinarily sensitive to the moment canting with even small canting angles enhancing the Weyl physics. For a $10^\circ$ canting we find a well-defined WP with a close proximity to the Fermi level. As the canting is further

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increased, the WP is pushed higher in energy, indicating the best signature of the Weyl physics might exist not in the \(c\)-polarized structure but for an in-plane model with slight canting. These results suggest that the Weyl physics might be optimized in EuCd\(_2\)As\(_2\) by tuning the canting angle - a gambit allowed by the symmetry of the MSG.

Single crystals of EuCd\(_2\)As\(_2\) were grown following the procedure reported in Ref. [22]. To mitigate the neutron absorption of naturally occurring Eu and Cd (absorption cross-sections of 2520 b and 4530 b respectively,) isotopic \(^{116}\)Cd and \(^{153}\)Eu (of purity \(\sim 99\%\)) were used in the reactions (with neutron absorption cross-sections of 0.075 b and 312 b respectively) [25]. Doing so improves the transmitted signal for a 2 mm diameter crystal, and 1.48 Å neutrons from 0.0003% to 66%. To further mitigate neutron absorption (and the need for the associated corrections) a nominally isotropically shaped crystal of mass \(< 1\) mg, with a diameter of \(\sim 1\) mm and thickness of \(< 0.1\) mm was used. Neutron diffraction experiments were carried out on the WAND\(^2\) diffractometer of Oak Ridge National Laboratory’s High Flux Isotope reactor with incident wavelength 1.48 Å [26, 27]. Data were collected by rotating the sample in the crystallographic \(ab\) plane allowing for peaks in the (HK0) plane to be observed. Temperature and field dependent data sets were collected using a cryomagnet. To monitor for absorption artifacts, each data set was collected over a broad range of \(H\) and \(K\) for data collected at (a) 50 K, 0 T. To monitor for absorption effects, each data set was collected over a broad range of \(H\) and \(K\) for data collected using a cryomagnet. To monitor for absorption artifacts, each data set was collected over a broad range of \(H\) and \(K\) for data collected above 0 T.

To start our analysis we consider data collected above 0 T (i.e. > 30 K) to identify the nuclear peaks and check for any absorption effects. In Fig. (a) we show the obtained (HK0) slice collected at 50 K over a broad range of \(H\) and \(K\). We note that the small size and high quality of our sample led to resolution limited peaks which have very slight extent in reciprocal space complicating their visualization. Nonetheless peaks are seen which are consistent with the \(P3m1\) space group. Comparing the peak intensity in \(Q\) constant rings (e.g. the \{110\} set of reflections) we see no significant modulation over the plotted 180° of rotation indicating no significant anisotropic absorption effect [31].

Shown in Fig. (b) is a region centering on the \{100\} series of reflections which are accidentally forbidden in the nuclear structure. As the sample is cooled below \(T_c\) we observe an increase in intensity on this series as...

**FIG. 1.** Neutron diffraction patterns of the HK0 plane for an isotopic EuCd\(_2\)As\(_2\) single crystal over a broad range of \(H\) and \(K\) for data collected at (a) 50 K, 0 T; (b) 5 K, 0 T; and (d) 5 K, 2 T.
shown in the data collected at 5 K (Fig. 1(c)), no additional new reflections are seen at fractional coordinates (including along the L direction which the out-of-plane detector coverage allows us to check to L = 0 ± 0.7 (r.l.u.).) The appearance of scattering intensity on these peaks below $T_c$ is indicative of a magnetic transition with ordering vector $k = (0, 0, 0)$.

Due to the single 1a Wyckoff position of the Eu site in the $P3m1$ space group, a $k = (0, 0, 0)$ order is purely FM. This is consistent with the descriptions of the magnetic structure arising from magnetic susceptibility measurements but inconsistent with the previous results from resonant elastic x-ray scattering experiments which suggested AFM order with $k = (0, 0, 1)$ [19, 21, 22]. However, as discussed in Refs. 21 and 22, this disagreement is likely due to specifics of the sample growth which can produce either AFM or FM samples.

To identify the magnetic structure we performed symmetry analysis and considered all allowed subgroups of $P3m1$ with $k = (0, 0, 0)$ which produced unique magnetic structures (Fig. 2). Of the four allowed MSG $P3m1$ is a purely $c$-polarized state, $C2/m$ is a purely $b$-polarized state and the remaining two allow mixing between in-plane and out-of-plane components with $C2'/m'$ locking the in-plane moment component to the crystallographic [210] direction and the final, and lowest symmetry, MSG $P\overline{T}$ leaving the moment direction unconstrained.

In order to discriminate between these, we remember that for magnetic neutron scattering only moment components perpendicular to the scattering vector contribute to the measured intensity. As such, models with different in-plane moment directions should produce different intensity modulations around the $\{100\}$ series. In Fig. 3(a) we plot the integrated intensity of the $\{100\}$ reflections and in Fig. 3(b) we do the same but for simulated scattering from the various possible magnetic structures with a magnetic moment of $6.7 \mu_B$ per Eu [21, 22]. In panel (a) we see that there is an intensity modulation where the $(100)$ and $(\overline{1}00)$ reflections are weaker than the $(010)$ and $(\overline{1}0\overline{1})$ reflections. This observation alone rules out the purely $c$-polarized state which has equivalent scattering intensities for the $(100)$ series (Fig. 3(b)).

Next, we compare the relative peak intensities of the $(100)$ series to those predicted by the various magnetic structures. For the $b$-polarized $C2'/m'$ structure we find the six reflections bifurcate into a doublet with four reflections ($(010), (1\overline{1}0), (\overline{1}0\overline{1}), (0\overline{1}\overline{1})$) having a smaller intensity than the remaining two ($(100), (\overline{1}00)$) (Fig. 3(b)). While our data do not contain all six reflections, we can see from the four we do observe that this pattern does not hold - our peaks appear split in the opposite manner with four reflections having larger intensity than the $(100)$ and $(\overline{1}00)$ reflections. This observation is consistent with the $C2'/m'$ MSG, whose [210] moment direction weakens $(100)$ and $(\overline{1}00)$ peaks. The final MSG ($P\overline{T}$), by nature of its lower symmetry, can also replicate this bipartite intensity. However, as it is of lower symmetry and does not provide a better model we use the higher symmetry $C2'/m'$.

Looking closer at the purely in-plane $C2'/m'$ model, we see a discrepancy between the simulated and observed intensities - while the model predicts a $(010)/(100)$ intensity ratio of $\sim 10$, our measured intensities have a ratio of $\sim 2$. Considering the magnetic model, we can identify two possible causes for this disagreement. The first is that the moment is not purely in-plane but canted towards the $c$-axis. This would increase the intensity on the $(100)$ and $(\overline{1}00)$ reflections by increasing the moment component perpendicular to their scattering vector. The second possibility is that this increased intensity is due to multiple magnetic domains (associated with the nuclear $C_3$ symmetry) with unequal populations.

This second possibility merits deeper discussion. The
symmetry allowed magnetic domains transform the in-plane moment constraint of $M_{\text{domain}_1} = (2M_y, M_y)$ to $M_{\text{domain}_2} = (M_x, -M_x)$ and $M_{\text{domain}_3} = (M_x, 2M_x)$. This permutes which set of reflections has the lower intensity from (100), (T00) to (T10), (1T0) and (010), (0T0). It is therefore, possible to achieve the observed (010)/(100) intensity ratio by carefully tuning the domain populations with 63% of the sample in domain 1 and an equal split of the remaining sample into 18.5% of domain 2 and of domain 3. While such a situation is not impossible, it is unlikely that the sample would tune so carefully the domain populations - domain 2 and 3 must balance near perfectly to give the observed intensity split. Furthermore, while this is able to produce the intensity ratio, in our modeling it was unable to adequately capture simultaneously both the ratios between the magnetic reflections and the magnetic and nuclear reflections. We therefore, favor the simpler explanation of a spin-canting.

This discussion might bring up the question of why we apparently see only a single magnetic domain, or at least one largely dominant domain. Indeed in Ref. 21 multiple domains were optically imaged in the magnetically ordered state of a FM sample. To explain this we point out the previously reported sensitivity of these samples to field cooling protocols. In Refs. 19 and 22 magnetization measurements on EuCd$_2$As$_2$ revealed a significant splitting between field-cooled and zero-field cooled protocols where even a small cooling field of tens of Oe produced large 50% value changes in the base temperature signal ostensibly due to domain alignment effects. In our experiment, a cryomagnet was used which is known to exhibit remnant fields on the order of dozens of Oe providing a plausible explanation for this observation.

In Fig. 3(b) we show the simulated intensities of the C$^2$m'/m' model with a moment canting of 30° (Fig. 2(c).) As discussed, this increases the intensities on the (100) and (T00) reflections and gives a (010)/(100) intensity ratio close to that observed. We therefore continue with the assumption that EuCd$_2$As$_2$'s magnetic structure includes a canting of the moments out of the ab plane. Admittedly we are unable to unequivocally rule out some contribution from secondary domains and so refrain reporting a firm canting angle, instead giving a range of θ = 5 – 35° based on the simulated relative magnetic reflection intensities and the relative magnetic/nuclear Bragg intensities. It is important to emphasize that even in the absence of this observation, since a c-direction component is allowed by the MSG then by symmetry arguments some finite (albeit possibly small) moment along c should be expected.

If we turn to the data collected under a 2 T applied field, we see a different story (Fig. 4). While we similarly see intensity on the {100} series, we do not observe any statistically significant intensity modulation around the series (this also functions as evidence that our sample exhibits no significant anisotropic absorption (Fig. 3a.).) This indicates a metamagnetic transition which must be to the c-polarized P$^{3}$m'$^1$ MSG as has been previously suggested. We label this as a metamagnetic transition rather than a spin-reorientation within the C$^2$/m due to suggestion of a phase transition in previous studies 21 22.

To predict the topological properties we performed DFT calculations of the electronic band structure for the purely in-plane [210] direction, the [001] direction as well as for several canting angles in between (Fig. 4). Starting with the [001] structure (Fig. 4(a) and (g)), our results are consistent with previous calculations showing a WP ~0.05 eV above the Fermi level along the Γ-A direction in the Brillouin zone 21 42. As reported in Ref. 21 our calculations show only a single set of WPs indicating an ideal situation to study Weyl physics.
For the purely in-plane [210] order (Fig. 4(b)) the band structure looks largely similar except for along the Γ-A line. Here we still find a WP which is actually closer to the Fermi level however, it is also slightly off of the protected Γ-A line (this was also reported for the [100] structure [21, 42]). Additionally, the previously steep valence band between the WP and Γ becomes nearly flat creating a less ideal situation for the isolation of Weyl physics.

As the moment tilts out of the ab-plane, we find that this flat band quickly drops away and begins to resemble the [001] band structure. For even a minor 10° canting (Fig. 4(d)) the dispersion in the immediate vicinity of the WP closely resembles the [001] structure. As the moment is further canted, we find this trend continues. Looking at the position of the WP relative to the Fermi level, we find that the [210] structure is closest at ~0.03 eV above the Fermi level. As the canting is increased to 10° the WP moves up in energy to ~0.04 eV with further increases moving the WP to higher energies until it resides at ~0.06 eV in the [001] structure.

The results of canting on the electronic structure are compelling. Though the [001] state has been thought the preferred structure for realizing Weyl physics in EuCd₂As₂ our results suggest otherwise. As shown, one likely does not need to stabilize the fully c-polarized state to realize a single set of WP - this appears to be achieved with an in-plane [210] type order. Furthermore, while the band structure for the purely in-plane order is less than ideal, our neutron data suggest that the moment is canted by 5 – 35°. This canting creates a situation similar to the [001] band structure while also moving the WP closer to the Fermi level. This seemingly indicates that the ideal configuration is closer to the realized zero-field ground state magnetic structure without any need for significant tuning.

In summary, we report that EuCd₂As₂ orders in the FM C2'/m' MSG with Eu moments pointing along the crystallographic [210] direction with a slight out-of-plane canting. DFT analysis of this structure shows that the well defined WPs previously reported for the purely c-polarized structure are achieved by the slight out-of-plane canting of the moment. Furthermore, we find that the WP lies closest to the Fermi level for the in-plane structure and so the minimal canting possible which leads to a well-defined WP is the ideal magnetic structure for optimizing the Weyl physics. Notably, the identified MSG allows canting by symmetry and so continuous tuning of the canting angle should be possible via small perturbations which tune the magnetic interactions. This result increases the intrigue of our recent report on Ba substitution (i.e. Eu₁₋ₓBaₓCd₂As₂) which suggested small Ba substitutions led to moment canting and enhanced Weyl physics as identified by transport measurements [22]. This indicates that routes such as Ba substitution may be valid approaches to tune the Weyl physics in EuCd₂As₂. Our results confirm the interest in this material as a magnetic WSM with a single pair of WP and present a route forward for optimizing the desired physics.

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[1] N. P. Armitage, E. J. Mele, and A. Vishwanath, Weyl and Dirac semimetals in three-dimensional solids, Rev. Mod. Phys. 90, 015001 (2018).
[2] A. Burkov, Topological semimetals, Nature materials 15, 1145 (2016).
[3] B. Yan and C. Felser, Topological materials: Weyl semimetals, Annual Review of Condensed Matter Physics 8, 337 (2017).
[4] X.-G. Wen, Colloquium: Zoo of quantum-topological phases of matter, Rev. Mod. Phys. 89, 041004 (2017).
[5] G. B. Osterhoudt, L. K. Diebel, M. J. Gray, X. Yang, J. Stancio, X. Huang, B. Shen, N. Ni, P. J. Moll, Y. Ran, et al., Colossal mid-infrared bulk photovoltaic effect in a type-I Weyl semimetal, Nature materials 18, 471 (2019).
[6] C.-K. Chan, P. A. Lee, K. S. Burch, J. H. Han, and Y. Ran, When Chiral Photons Meet Chiral Fermions: Photoinduced Anomalous Hall Effects in Weyl Semimetals, Phys. Rev. Lett. 116, 026805 (2016).
[7] C.-K. Chan, N. H. Lindner, G. Refael, and P. A. Lee, Photocurrents in Weyl semimetals, Phys. Rev. B 95, 041104 (2017).
[8] S. A. Parameswaran, T. Grover, D. A. Abanin, D. A. Pesin, and A. Vishwanath, Probing the chiral anomaly with nonlocal transport in three-dimensional topological semimetals, Phys. Rev. X 4, 031035 (2014).
[9] D. E. Kharzeev and Q. Li, The chiral qubit: quantum computing with chiral anomaly, arXiv (2019).
[10] S. Jia, S.-Y. Xu, and M. Z. Hasan, Weyl semimetals, fermi arcs and chiral anomalies, Nature materials 15, 1140 (2016).
[11] D. Liu, A. Liang, E. Liu, Q. Xu, Y. Li, C. Chen, D. Pei, W. Shi, S. Mo, P. Dudin, et al., Magnetic Weyl semimetal phase in a Kagomé crystal, Science 365, 1282 (2019).
[12] G. Chang, B. Singh, S.-Y. Xu, G. Bian, S.-M. Huang, C.-H. Hsu, I. Belopolski, N. Alidoust, D. S. Sanchez, H. Zheng, H. Lu, X. Zhang, Y. Bian, T.-R. Chang, H.-T. Jeng, A. Bansil, H. Hsu, S. Jia, T. Neupert, H. Lin, and M. Z. Hasan, Magnetic and noncentrosymmetric Weyl fermion semimetals in the RAlGe family of compounds (R=rare earth), Phys. Rev. B 97, 041104 (2018).
[13] J.-R. Soh, H. Jacobsen, B. Ouladdiaf, A. Ivanov, A. Piovano, T. Tejsner, Z. Feng, H. Wang, H. Su, Y. Guo, Y. Shi, and A. T. Boothroyd, Magnetic structure and excitations of the topological semimetal YbMnBi$_2$, Phys. Rev. B 100, 144431 (2019).

[14] C. Shekhar, N. Kumar, V. Grinenko, S. Singh, R. Sarkar, H. Luetteken, S.-C. Wu, Y. Zhang, A. C. Komarek, E. Kampert, Y. Skourski, J. Wosnitza, W. Schnelle, A. McCollam, U. Zeitler, J. Kibbler, B. Yan, H.-H. Klauss, S. S. P. Parkin, and C. Felser, Anomalous Hall effect in Weyl semimetal half-Heusler compounds RPtBi (R = Gd and Nd), Proc. Natl. Acad. Sci. 115, 9140 (2018).

[15] Y. Xu, J. Zhao, C. Yi, Q. Wang, Q. Yin, Y. Wang, X. Hu, L. Wang, E. Liu, G. Xu, et al., Electronic correlations and flattened band in magnetic Weyl semimetal candidate Co$_3$Sn$_2$S$_2$, Nat. Comm. 11, 1 (2020).

[16] G. Hua, S. Nie, Z. Song, R. Yu, G. Xu, and K. Yao, Dirac semimetal in type-IV magnetic space groups, Phys. Rev. B 98, 201116 (2018).

[17] J.-R. Soh, F. de Juan, M. G. Vergniory, N. B. M. Schröter, M. C. Rahn, D. Y. Yan, J. Jiang, M. Bristow, P. A. Reiss, J. N. Bandy, Y. F. Guo, Y. G. Shi, T. K. Kim, A. McCollam, S. H. Simon, Y. Chen, A. I. Coldea, and A. T. Boothroyd, Ideal Weyl semimetal induced by magnetic exchange, Phys. Rev. B 100, 214102 (2019).

[18] Z. Wang, W. Yi, Q. Wu, V. A. Sidorov, J. Bao, Z. Tang, J. Guo, Y. Zhou, S. Zhang, H. Li, Y. Shi, X. Xu, W. L. Zhang, K. Yang, A. Li, G. Cao, J. Hu, L. Sun, and Z. Zhao, Correlation between superconductivity and bond angle of CrAs chain in non-centrosymmetric compounds A(2)Cr(3)As(3) (A = K, Rb), Sci. Rep. 6, 37878 (2016).

[19] M. Rahn, J.-R. Soh, S. Francoual, L. Veiga, J. Stremper, J. Mardegan, D. Yan, Y. Guo, Y. Shi, and A. Boothroyd, Coupling of magnetic order and charge transport in the candidate Dirac semimetal EuCd$_2$As$_2$, Phys. Rev. B 97, 214422 (2018).

[20] J. Ma, H. Wang, S. Nie, C. Yi, Y. Xu, H. Li, J. Jandke, W. Wulfhekel, Y. Huang, D. West, et al., Emergence of Nontrivial Low-Energy Dirac Fermions in Antiferromagnetic EuCd$_2$As$_2$, Adv. Mater. 32, 1907565 (2020).

[21] N. H. Jo, B. Kuthanazhi, Y. Wu, E. Timmons, T.-H. Kim, L. Zhou, L.-L. Wang, B. G. Ueland, A. Palasyuk, D. H. Ryan, R. J. McQueeney, K. Lee, B. Schrunk, A. A. Burkov, R. Prozorov, S. L. Bud’ko, A. Kaminski, and P. C. Canfield, Manipulating magnetism in the topological semimetallic EuCd$_2$As$_2$, Phys. Rev. B 101, 140402 (2020).

[22] L. D. Sanjeeva, J. Xing, K. M. Taddei, D. Parker, R. Custelcean, C. dela Cruz, and A. S. Sefat, Evidence of Ba-substitution induced spin-canting in the magnetic Weyl semimetal EuCd$_2$As$_2$, Phys. Rev. B 102, 104404 (2020).

[23] C. Niu, N. Mao, X. Hu, B. Huang, and Y. Dai, Quantum anomalous Hall effect and gate-controllable topological phase transition in layered EuCd$_2$As$_2$, Phys. Rev. B 99, 235119 (2019).

[24] Y. Xu, L. Das, J. Ma, C. Yi, Y. Shi, A. Tiwari, S. Tsirkin, T. Neupert, M. Medarde, M. Shi, et al., Topological transverse transport in the presence and absence of long-range magnetic order in EuCd$_2$As$_2$, arXiv preprint arXiv:2008.05300 (2020).

[25] H. Börner, J. Brown, C. Carlile, R. Cubitt, R. Currat, A. Dianoux, B. Farago, A. Hewat, J. Kulda, E. Lelièvre-Berna, et al., Neutron Data Booklet (2003).

[26] S. Calder, K. An, R. Boehler, C. Dela Cruz, M. Frontzek, M. Guthrie, B. Haberl, A. Huq, S. A. Kimber, J. Liu, et al., A suite-level review of the neutron powder diffraction instruments at oak ridge national laboratory, Review of Scientific Instruments 89, 092701 (2018).

[27] M. Frontzek, R. Whitfield, K. Andrews, A. Jones, M. Bobrek, K. Vodopivec, B. Chakoumakos, and J. Fernandez-Baca, WAND—A versatile wide angle neutron powder/single crystal diffractometer, Review of Scientific Instruments 89, 092801 (2018).

[28] M. Aroyo, J. Perez-Mato, C. Capillas, E. Kroumova, S. Ivantchev, G. Madariaga, A. Kirov, and H. Wondratschek, Bilbao crystallographic server: I. Databases and crystallographic computing programs, Z. Kristallogr. 221, 15 (2006).

[29] M. Aroyo, A. Kirov, C. Capillas, J. Perez-Mato, and H. Wondratschek, Bilbao Crystallographic Server. II. Representations of crystallographic point groups and space groups, Acta Crystallogr. Sec. A 62, 115 (2006).

[30] M. Aroyo, J. Perez-Mato, D. Orobenega, E. Tasci, G. De La Flor, and A. Kirov, Crystallography online: Bilbao crystallographic server, Bulg. Chem. Commun. 43, 183 (2011).

[31] A. Wills, A new protocol for the determination of magnetic structures using simulated annealing and representation analysis (SARAh), Phys. B 276-278, 680 (2000).

[32] H. Stokes, D. Hatch, and B. Campbell, Isodistort, isotropy software suite (2019).

[33] B. J. Campbell, H. T. Stokes, D. E. Tanner, and D. M. Hatch, ISODISPLACE: a web-based tool for exploring structural distortions, Journal of Applied Crystallography 39, 607 (2006).

[34] J. Rodríguez-Carvajal, Recent advances in magnetic structure determination by neutron powder diffraction, Physica B: Condensed Matter 192, 55 (1993).

[35] K. Momma and F. Izumi, VESTA 3 for three dimensional visualization of crystal, volumetric and morphology data, J. Appl. Crystallogr. 44, 1272 (2011).

[36] G. Kresse and J. Furthmuller, Efficient iterative schemes for ab initio total-energy calculations using a plane-wave basis set, Phys. Rev. B 54, 11169 (1996).

[37] G. Kresse and J. Furthmüller, Efficiency of ab-initio total energy calculations for metals and semiconductors using a plane-wave basis set, Computational materials science 6, 15 (1996).

[38] P. E. Blöchl, Projector augmented-wave method, Phys. Rev. B 50, 17953 (1994).

[39] G. Kresse and D. Joubert, From ultrasoft pseudopotentials to the projector augmented-wave method, Phys. Rev. B 59, 1758 (1999).

[40] L.-L. Wang, N. Jo, B. Kuthanazhi, Y. Wu, R. McQueeney, A. Kaminski, and P. Canfield, Single pair of Weyl fermions in the half-metallic semimetal EuCd$_2$As$_2$, Phys. Rev. B 99, 245147 (2019).

[41] H. Zhang, Y. L. Zhu, Y. Qiu, W. Tian, H. B. Cao, Z. Q. Mao, and X. Ke, Field-induced magnetic phase transitions and the resultant giant anomalous Hall effect in the antiferromagnetic half-Heusler compound DyPtBi, Phys. Rev. B 102, 094424 (2020).

[42] J.-Z. Ma, S. Nie, C. Yi, J. Jandke, T. Shang, M. Yao, M. Naamneh, L. Yan, Y. Sun, A. Chikina, V. Stro-
cov, M. Medarde, M. Song, Y.-M. Xiong, G. Xu, W. Wulfhekel, J. Mesot, M. Reticcioli, C. Franchini, C. Mudry, M. Müller, Y. Shi, T. Qian, H. Ding, and M. Shi, Spin fluctuation induced Weyl semimetal state in the paramagnetic phase of EuCd$_2$As$_2$, Science Advances 5, 10.1126/sciadv.aaw4718 (2019).