Theory of the Metal-Insulator Transition in PrRu$_4$P$_{12}$ and PrFe$_4$P$_{12}$

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All symmetry allowed couplings between the $4f^2$-electron ground state doublet of trivalent praseodymium in PrRu$_4$P$_{12}$ and PrFe$_4$P$_{12}$ and displacements of the phosphorus, iron or ruthenium ions are considered. Two types of displacements can change the crystal lattice from body-centred cubic to simple orthorhombic or to simple cubic. The first type lowers the point group symmetry from tetrahedral to orthorhombic, while the second type leaves it unchanged, with corresponding space group reductions $\text{Im} \bar{3} \rightarrow \text{Pmmm}$ and $\text{Im} \bar{3} \rightarrow \text{Pn} \bar{3} \bar{m}$ respectively. In former case, the lower point-group symmetry splits the degeneracy of the $4f^2$ doublet into states with opposite quadrupole moment, which then leads to anti-quadrupolar ordering, as in PrFe$_4$P$_{12}$. Either kind of displacement may conspire with nesting of the Fermi surface to cause the metal-insulator or partial metal-insulator transition in PrFe$_4$P$_{12}$ and PrRu$_4$P$_{12}$. We investigate this scenario using band-structure calculations, and it is found that displacements of the phosphorus ions in PrRu$_4$P$_{12}$ (with space group reduction $\text{Im} \bar{3} \rightarrow \text{Pn} \bar{3}$) open a gap everywhere on the Fermi surface.

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I. INTRODUCTION

The rare earth-filled skutterudites (RT$_4$P$_{12}$; R=rare earth; T = Fe, Ru or Os; P$_n$ = P, As or Sb) exhibit a wide range of phenomena, including superconductivity in nearly all of the La-compounds$^{12,13}$, as well as PrRu$_4$As$_{12}$$^{24}$ and PrRu$_4$Sb$_{12}$$^{25}$, heavy fermion superconductivity in PrOs$_4$Sb$_{12}$$^{15}$, semiconducting or semimetallic behaviour in the Ce-compounds$^{16,17}$ and ferromagnetism in several of the Nd- and Eu-compounds$^{18,15,16}$ and UFe$_4$P$_{12}$$^{26}$. PrRu$_4$P$_{12}$ undergoes a metal-insulator (M-I) transition at approximately $T_{MI} = 60 \text{K}$$^{20}$ while in PrFe$_4$P$_{12}$ there is a partial M-I transition at a much lower temperature, seen as a sharp upturn in the resistivity at $T_{MI} = 6.7 \text{K}$$^{27}$ which then tends to zero at low temperatures. In both cases, the M-I transition is accompanied by a structural phase transition which doubles the volume of the primitive cell$^{22,23}$.

In PrFe$_4$P$_{12}$, a peak in the magnetic susceptibility is observed at $T_{MI}$$^{28}$ and $T_{MI}$ is field-dependent, but there is no magnetic ordering. However, in-field neutron diffraction experiments found direct evidence of anti-quadrupolar ordering below $T_{MI}$$^{28}$. In contrast, $T_{MI}$ of PrRu$_4$P$_{12}$ is not field dependent (as seen in the specific heat$^{22}$ and thermal expansion$^{27}$) and no peak is observed in the susceptibility either$^{28}$ which suggests that there is no ordering of any kind at $T_{MI}$. An upturn in the susceptibility at very low temperatures hints that there may be some kind of ordering below $T = 0.35 \text{K}$$^{28}$ and is likely related to the low-temperature magnetic field dependent peaks found in the thermal expansion and specific heat, whose positions decrease in temperature with decreasing field$^{16,17}$.

Nesting of the Fermi surface may be the common feature of the M-I transition in both of these materials. Band-structure calculations for LaFe$_4$P$_{12}$$^{16}$ PrFe$_4$P$_{12}$ and PrRu$_4$P$_{12}$$^{28}$ found an approximately cubed-shaped hole-like Fermi surface, with nesting wavevector $q = (1,0,0)$ (due to the 48th band in LaFe$_4$P$_{12}$ and the 49th band in PrFe$_4$P$_{12}$ and PrRu$_4$P$_{12}$). The band itself has a roughly flat dispersion, which means that slight differences can cause substantially different Fermi surface topologies. Thus, in PrRu$_4$Sb$_{12}$ and LaRu$_4$Sb$_{12}$ the resulting FS does not have the nesting property$^{20}$.

LaFe$_4$P$_{12}$ and PrFe$_4$P$_{12}$ possess an additional smaller hole-like spherical Fermi surface, so that the M-I transition in PrFe$_4$P$_{12}$ is incomplete, and it remains a metal at low temperatures. It has been suggested that a nested Fermi surface is also a possible cause of the resistivity upturns seen in NdFe$_4$P$_{12}$, SmRu$_4$P$_{12}$, GdRu$_4$P$_{12}$ and TbRu$_4$P$_{12}$$^{21}$.

If nesting is a prerequisite for the M-I transition, then so is a cell-doubling structural instability, which halves the Brillouin zone (BZ) at the nesting wave vector. All of the rare earth-filled skutterudites crystallise in the body-centred cubic (bcc) lattice with space group $\text{Im} \bar{3}$ (#204), except for the low-temperature phases of PrFe$_4$P$_{12}$ and PrRu$_4$P$_{12}$. In these cases, superlattice reflections are a clear indication of doubling of the primitive cell$^{12,13}$. The change in structure appears to be due to a displacement of Fe ions in PrFe$_4$P$_{12}$ and both of Ru and P ions in PrRu$_4$P$_{12}$, with space groups Pmmm (#47) and Pn$\bar{3}$.
In Section II, all symmetry allowed couplings of Pr$^{3+}$ 4$f^2$ electrons to the lattice are considered. It is shown that anti-quadrupolar ordering of the 4$f^2$ electrons follows when the point group symmetry at the Pr site is lowered from tetrahedral to orthorhombic (as is the case in the Im3 → Pnmm transition). In Section III we present band structure calculations which show that a gap opens everywhere at the Fermi energy when P ion displacements (with space group reduction Im3 → Pn3) are considered in PrRu$_4$P$_{12}$ [24]. We summarise our results in Section IV.

### II. STRUCTURAL PHASE TRANSITION AND ANTI-QUADRUPOLAR ORDERING

According to XANES studies on PrRu$_4$P$_{12}$ [21] and susceptibility measurements on PrFe$_2$P$_{12}$ [19], the valency of the Pr ion is +3, i.e., a 4$f^2$ configuration with total angular momentum $J = 4$. The Ru/Fe ions form a crystal field with $O_h$ symmetry with respect to the Pr ions, but the P ions lower the symmetry to $T_h$. Under $O_h$ symmetry, the $J = 4$ state splits into a singlet, a doublet and a triplet, corresponding to the representations $\Gamma_1 \oplus \Gamma_3 \oplus \Gamma_4 \oplus \Gamma_5$ of $O$ respectively. Under the actual symmetry $T_h$, the $\Gamma_3$ doublet is split into states related by time reversal symmetry (complex conjugates). Crystal field splitting alone cannot determine the ground state, but specific heat measurements on PrFe$_2$P$_{12}$ [19] and PrRu$_4$P$_{12}$ [24] favour the doublet, which is

$$\Gamma_{4h}^+ = \sqrt{7/24} (1 + i) + \sqrt{17/24} (1 - i)$$

$$\Gamma_{4h}^- = \sqrt{7/24} (1 - i) + \sqrt{17/24} (1 + i)$$

These states carry quadrupole moment $\langle J_z^2 \rangle = \pm 8\hbar^2$.

On the other hand, a singlet ground state,

$$\Gamma_1 = \sqrt{5/24} (1 + i) + \sqrt{19/24} (1 - i)$$

with a low lying triplet first excited state has not been conclusively ruled out. The exact form of the triplets is unknown in $T_h$, because in general they are linear combinations of

$$\Gamma_{4h}^+ = \sqrt{7/24} (1 + i) + \sqrt{17/24} (1 - i)$$

$$\Gamma_{4h}^- = \sqrt{7/24} (1 - i) + \sqrt{17/24} (1 + i)$$

$$\Gamma_1 = \sqrt{5/24} (1 + i) + \sqrt{19/24} (1 - i)$$

$$\Gamma_3 = \sqrt{5/24} (1 - i) + \sqrt{19/24} (1 + i)$$

These states carry quadrupole moment $\langle J_z^2 \rangle = \pm 8\hbar^2$.

In the following discussion, we often refer to the representations of $O_h$ respectively. Under the actual crystal field symmetry, there is only one coupling for each of the $\Gamma_1$ and $\Gamma_3$ modes, since the identity ($\Gamma_1$) only appears once in the decompositions $\Gamma_1 \otimes \Gamma_3 \otimes \Gamma_3 = \Gamma_1 \oplus \Gamma_2 \oplus \Gamma_3$ and $\Gamma_3 \otimes \Gamma_3 \otimes \Gamma_3 = \Gamma_1 \oplus \Gamma_2 \oplus 3\Gamma_3$. Under the actual symmetry $T_h$, $\Gamma_2$ reduces to $\Gamma_a$, and there are two couplings...
for each mode instead of one. There are more choices of coupling to the P ion displacements. There are two different \( \Gamma_3 \) modes, represented by \( v = (1, 1, 1) \), and each of these has two couplings to the \( 4f^2 \) doublet. Also there are two kinds of \( \Gamma_h \oplus \Gamma_c \) modes, represented by \( v = (1, 1, -2) \) and \( v = (1, -1, 0) \), which altogether have four different couplings to the \( 4f^2 \) doublet.

Although any of the above couplings might lead to a M-I transition via coupling to the conduction electrons, there is a significantly different consequence for those distortions which lower the point group symmetry (namely the \( \Gamma_3 \) or \( \Gamma_h \oplus \Gamma_c \) modes) compared to those which do not (the \( \Gamma_1 \) or \( \Gamma_a \) modes). When the point group symmetry is lowered by the \( \Gamma_3 \) or \( \Gamma_h \oplus \Gamma_c \) modes, the degeneracy of the \( 4f^2 \) doublet is lifted, and as we shall show next, the result is anti-quadrupolar ordering.

We consider first the \( \Gamma_3 \) or \( \Gamma_h \oplus \Gamma_3 \) modes. The general form of the Hamiltonian which describes the coupling between Fe/Ru ion or P ion displacements and the \( 4f^2 \) doublet in the bcc conventional cell is

\[
H = \epsilon(f^1 f + f^{*1} f^* + f^1 f' + f^{*1} f'^*) \\
+ \frac{1}{2}[T(f^1 f^* A^* - f^{*1} f'^* A') + \text{h.c.}] + \frac{\omega}{2}|A|^2 \\
+ \frac{B}{4}|A|^4 + C_1 \frac{1}{6}|A|^6 + C_2 \frac{1}{12}(A^4 + A^6) \\
+ C_3 \frac{1}{12}(A^6 - A^6).
\]

The operators \( f^1 \) and \( f'^1 \) act on the two neighbouring Pr sites and correspond to the complex wavefunctions \( |f\rangle = (|\Gamma_3^+\rangle - i|\Gamma_3^-\rangle)/\sqrt{2} \) and \( |f^*\rangle = (|\Gamma_3^+\rangle + i|\Gamma_3^-\rangle)/\sqrt{2} \). \( A \) is the complex amplitude of the displacement \( \vec{v} = \vec{v}_0 + \chi \vec{v}_2 + \chi^2 \vec{v}_1 \) of either eight Fe/Ru ions or 24 P ions, where \( \chi = \exp(i\frac{2\pi}{3}) \), and the displacement vectors are \( \vec{v}_0 = (1, 0, 0), \vec{v}_1 = (0, 1, 0), \text{and} \vec{v}_2 = (0, 0, 1) \). The actual displacement is then \( 2Re A \vec{v} \). \( A \) corresponds to the anti-phase mode as described above, therefore it changes sign under the bcc lattice translation \( t = (\frac{a}{2}, \frac{a}{2}, \frac{a}{2}) \). Since odd order in \( A \) terms do not appear in \( H \), (Note that under the same translation \( f \rightarrow f' \)). All of the coupling constants are real, except for \( T \), which is real in \( \Omega_h \), but complex in \( T_h \). When the coupling constant \( T \) is prohibited in \( \Omega_h \) but allowed in \( T_h \). \( C_1 \) should be greater than \( C_2 \) and \( C_3 \) for stability.

We begin by diagonalising \( H \) with respect to \( f \). Writing \( A = \alpha e^{i \alpha} \) and \( T = e^{i \tau} \), the eigenvalues are \( \epsilon = \pm \tau \alpha \) with eigenvectors \( e^{i((\alpha+\tau)\alpha)} |f\rangle \pm |f^*\rangle \). Then the ground state projection of \( H \) is

\[
H_{eff} = -\alpha \tau + \frac{\omega}{2} \alpha^2 + \frac{B}{4} \alpha^4 + \frac{C_1}{6} \alpha^6 + \frac{C_2}{6} \alpha^6 \cos 6 \alpha + \frac{C_3}{6} \alpha^6 \sin 6 \alpha.
\]

We will assume for the moment that \( \tau = 0 \) and \( C_3 = 0 \) (as in \( \Omega_h \) symmetry). Then, for \( C_2 < 0 \), \( H_{eff} \) has minima at \( \alpha = 0, \pi/3, 2\pi/3, \pi, 4\pi/3, 5\pi/3 \). The corresponding displacements are proportional to \( \pm(-1, -1, 2), \pm(-1, 2, -1) \), and \( \pm(2, -1, -1) \). These displacements reduce the crystal field symmetry from \( \Omega_h \) to \( D_{4h} \), thereby splitting the \( 4f^2 \) doublet, so that now the ground state is non-degenerate. For example, for the \((-1, -1, 2) \) displacement (\( \alpha = 0 \)), the \( 4f^2 \) ground state is \( \Gamma_3^+ \). The \( 4f^2 \) ground state on the neighbouring site is orthogonal to this (because of the change of sign on \( T \)), therefore the \( 4f^2 \) ground state alternates between \( \Gamma_4^+ \) and \( \Gamma_3^- \) from site to site. Since the states \( \Gamma_3^+ \) carry opposite quadrupole moments, it follows that the ground state will have anti-quadrupolar ordering. The displacement doubles the primitive cell and changes the structure from bcc to simple orthorhombic (Im\( \bar{3} \) to Pmmm).

When \( C_2 > 0 \), \( H_{eff} \) has minima at \( \alpha = \pi/6, \pi/2, 5\pi/6, 7\pi/6, 3\pi/2, 11\pi/6 \). This leads to domains with displacements of the form \( \pm(1, -1, 0), \pm(1, 0, 1) \), and \( \pm(0, 1, 1) \). The corresponding \( 4f^2 \) ground states carry quadrupole moments \( J_2^+ - J_2^- \) etc. which alternate sign from site to site in the same way as for \( C_2 < 0 \). The space group reduction is also the same: Im\( \bar{3} \) to Pmmm.

When the coupling constant \( T \) is complex and \( C_3 \) is non-zero (as they are in general in \( T_h \) symmetry), the angle \( \tau \) is non-zero and the angle \( \alpha \) is no longer fixed. The ground state can be a mixture of \( \Gamma_3^+ \) and \( \Gamma_3^- \) and the displacements are a mixture of \((2, 1, 1)\) and \((-1, -1, 0)\) modes. However, for the case when the \( 4f^2 \) doublet is more strongly coupled to the Fe/Ru displacements, the \( \Omega_h \) symmetry is broken only by the presence of the P ions, which interact indirectly through their contribution to the crystal field. Therefore, in this case, it may be appropriate to take the \( \Omega_h \rightarrow T_h \) symmetry lowering as a perturbative effect, and then the resulting anti-quadrupole moment should be close to the maximum value which is found under \( \Omega_h \) symmetry.

Now we consider the \( \Gamma_1 \) or \( \Gamma_a \) modes. The Hamiltonian is

\[
H = \epsilon(f^1 f + f^{*1} f^* + f^1 f' + f^{*1} f'^*) \\
+ TA(f^1 f - f^{*1} f' + \text{h.c.}) + \omega A^2 \\
+ \frac{B}{4} A^4 + \frac{C}{6} A^6,
\]

where \( A \) is now the operator for the displacement \( v = (1, 1, 1) \) and all of the coupling constants are real. In this case, the \( 4f^2 \) ground state remains degenerate and there is no lattice distortion. Therefore, in order for this type of distortion to occur, the source of the instability must be something else, such as coupling to conduction electrons, as we show in Section III.

The assumption that the doublet is the ground state of the Pr\(^{3+} \) ion is not a strict requirement. In the alternate scenario of a singlet ground state and low-lying triplet excited state, Kiss and Fazekas showed how to couple the \( \Gamma_3 \) lattice distortion mode to the quadrupole moment of the triplet. In this case, the Hamiltonian takes the same form as in [10] except that the operator \( f \) corresponds to the wavefunction \( |f\rangle = (|\Gamma_4^+\rangle + \chi|\Gamma_3^+\rangle + \chi^2|\Gamma_4^-\rangle)/\sqrt{3} \). Diagonalising \( H \) breaks the degeneracy of the triplet; the
energy of one state is lowered by $TA$, and another is raised by the same amount. If $TA$ is large enough then the state $e^{i\alpha + \tau}|f\rangle - |f^*\rangle$ is the ground state of the system. Note that this state carries no magnetic moment, but in general has a quadrupole moment. Anti-quadrupolar ordering follows as before.

Thus, beginning with all possible couplings between the $\text{Pr}^{3+}$ $4f^2$ doublet and the lattice, we find that there are only two types of lattice distortions that are consistent with a cell-doubling structural phase transition. In the first case ($\Gamma_3$), the point group symmetry is lowered from $T_h$ to $D_{2h}$, and the doublet is split into states carrying opposite quadrupole moment. Anti-quadrupolar ordering is a consequence of the lower point group symmetry and doubling of the primitive cell. For the second kind of cell-doubling distortion ($\Gamma_1$), the point group symmetry remains $T_h$, and there is no quadrupole ordering. Experimental evidence suggests that the first scenario applies to PrFe$_3$P$_{12}$ and while the second one applies to PrRu$_4$P$_{12}$.

III. BAND STRUCTURE CALCULATIONS

Band structure calculations were performed using the FLAPW-LDA+U method$^{39}$ to investigate the origin of the M-I transition in PrRu$_4$P$_{12}$. The LDA+U method has described the non-magnetic localized $f$ electron system$^{19}$.

Various $\Gamma_1$-type lattice distortions involving P ion displacements were considered. The space group is lowered from Im3 to Pm3 as the primitive cell is doubled. In Im3, we used the observed lattice parameters, i.e. the lattice constant $a = 8.0424\, \text{Å}$ and the internal parameters $u = 0.3576$ and $v = 0.1444$ for P positions$^{22}$. In Pm3, the positions of Ru ions are equivalent as $8i$, $(1/2 + \delta_T, 1/2 + \delta_T, 1/2 + \delta_T)$. While the P ions occupy the inequivalent positions $12j$, $(0, u + \delta_u^A, v + \delta_v^A)$ and $12k$, $(1/2, 1/2 + u + \delta_u^B, 1/2 + v + \delta_v^B)$. When $\delta_T = 0$, $\delta_u^A = \delta_v^B$ and $\delta_u^B = \delta_v^A$, the space group has the higher symmetry Im3 with the smaller primitive cell. The site of Pr ions is split to two sites (1a $(0,0,0)$ and 1b $(1/2,1/2,1/2)$) in Pm3 due to the inequivalent surroundings. However, since the local symmetry m3 for the both sites is unchanged, any kind of lifting the degeneracy of the localized $4f^2$ state is not expected in Pm3. Here the singlet $\Gamma_1$ states for $4f^2$ electrons as the starting state were assumed and found after the self-consistent steps.

Although Ru ions are experimentally distorted to minimize the total energy, the position of Ru ions does not affect the Fermi surface, because the Fermi surface of PrRu$_4$P$_{12}$ consists of mainly P-p band. Therefore $\delta_T = 0$ is assumed in the calculations. Moreover, the anti-phase distortion of P ions are considered. Several values of the two parameters $\delta_u = \delta_u^A = -\delta_u^B$ and $\delta_v = \delta_v^A = -\delta_v^B$ with $\delta_u \delta_v < 0$ were considered in the calculations, and are listed in Table I.

Optimal results were obtained for $\delta_u = 0.003a$ and $\delta_v = -0.004a$. This distortion produced a gap across the entire Fermi surface, as shown in Fig. 1. Fig. 2 shows the density of states in the vicinity of the Fermi level both for Pm3 and Im3 corresponding to Fig 1.

| $\delta_u$ | $\delta_v$ | $\Delta E$ (eV) |
|----------|----------|----------------|
| 0.001    | 0.001    | 0.002          |
| 0.002    | 0.002    | 0.003          |
| 0.003    | 0.003    | 0.004          |
| 0.004    | 0.004    | 0.005          |
| 0.005    | 0.005    | 0.006          |

FIG. 1: Insulating band structure for PrRu$_4$P$_{12}$ obtained with $\delta_u = 0.003a$ and $\delta_v = -0.004a$. 

TABLE I: The calculated band gaps $\Delta E$ in eV with distortions. The minus sign means that the valence and conduction bands are overlapped. The asterix indicates that a self-consistent solution was not obtained.
and P-dotted line and dashed line indicates total, Ru-

4 phase transition in PrFe

4 modulus, with

I transition temperatures differ by an order of magni-

4 structural phase transition, the lattice instability may be

4 similarities in the shape of the Fermi surface and in the

4 transition between PrFe

4 magnetic fields

4 transition of structural phase transition in PrFe

4 density of states (states/Ry cell)

The observation of anti-quadrupolar ordering below

4 component, respectively. Note that there are two P-p components in (b).

IV. DISCUSSION AND SUMMARY

There are significant differences in the nature of the transition between PrFe$_4$P$_{12}$ and PrRu$_4$P$_{12}$. The M-I transition temperatures differ by an order of magnitude, with $T_{MI} = 6.7$K for PrFe$_4$P$_{12}$ versus $T_{MI} = 60$K for PrRu$_4$P$_{12}$. In addition, $T_{MI}$ of the Fe-compound decreases in temperature with increasing magnetic field, while the Ru-compound shows no magnetic field dependence of $T_{MI}$ (seen as a jump in the specific heat) and no anomaly in the magnetic susceptibility at $T_{MI}$ either. This suggests that, in spite of the similarities in the shape of the Fermi surface and in the structural phase transition, the lattice instability may be of a quite different character between the two materials.

The observation of anti-quadrupolar ordering below $T_{MI}$ in PrFe$_4$P$_{12}$ is strong evidence that the structural phase transition in PrFe$_4$P$_{12}$ involves lattice distortion modes which lower the point group symmetry from $T_h$ to $D_{2h}$ (the $\Gamma_3$ modes). Moreover, the experiments indicate that it is the Fe ions which are displaced in this mode. As for PrRu$_4$P$_{12}$, the absence of magnetic anomalies mentioned at the beginning of this section, as well as Raman studies and electron diffraction, indicate that the structural phase transition at $T_{MI}$ does not change the local Pr site symmetry and is not accompanied by quadrupole ordering, hence it involves those modes which do not lower the point group symmetry (the $\Gamma_1$ modes). Our band structure calculations favour P ion displacements over Ru ion displacements since the former are shown to be a source of the M-I transition.

The low temperature upturn in the susceptibility and the magnetic field dependence of the thermal expansion and specific heat in PrRu$_4$P$_{12}$ at low temperatures suggest that there may be an ordering at a lower temperature. It could be due to a second structural phase transition which lowers the point group and lifts the degeneracy of the doublet, but so far there are no experimental clues about the type of deformation involved. There are two possibilities, either in-phase or anti-phase modes of the $\Gamma_3$ type distortions described in detail above. In-phase modes were excluded as a source of the MI transition because they do not double the primitive cell. Since the cell is already doubled below the first transition, exclusion of the in-phase modes is no longer necessary. Then the space group is lowered through the sequence Im$\bar{3}$ → Pm$\bar{3}$ → Pmmm, but now the 4$f^2$ state has quadrupolar ordering below the second transition. Only the P-ions participate in the in-phase modes, but the anti-phase modes may involve either P ions or Fe/Ru ions. The anti-phase modes lead to anti-quadrupolar ordering and lower the space group through the same sequence Im$\bar{3}$ → Pm$\bar{3}$ → Pmmm. Given the similarities between the transition temperatures and the magnetic field dependences of structural phase transition in PrFe$_4$P$_{12}$ and the proposed second transition in PrRu$_4$P$_{12}$, it seems more likely that the second transition in PrRu$_4$P$_{12}$ would be due to displacements of the Ru ions, rather than either in-phase or anti-phase modes of P ions.

To summarise, we have studied structural phase transitions coupled to localised 4$f^2$ states and to band electrons in PrFe$_4$P$_{12}$ and PrRu$_4$P$_{12}$. In both cases the source of the structural instability is identified, but the mechanisms are quite different. In PrFe$_4$P$_{12}$, a Jahn-Teller type mechanism occurs, as coupling between $\Gamma_3$ type displacements and the 4$f^2$ electrons lifts the degeneracy and lowers the energy of the ground state of the 4$f^2$ electrons. The space group is reduced from Im$\bar{3}$ to Pm$\bar{3}$m. Coupling to the band electrons removes part of the Fermi surface. In PrRu$_4$P$_{12}$, our bandstructure calculations show that coupling between lattice displacements and band electrons will remove the Fermi surface everywhere and produce a metal-insulator transition. The space group is lowered from Im$\bar{3}$ to Pm$\bar{3}$. This produces no change in symmetry at the Pr sites, hence no orbital ordering occurs.
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