Band structure and superconductivity in Lu at high pressures

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We report here the effect of pressure on the band structure and the superconducting behavior of the hcp metal lutetium. The present work shows that the average of the square of the phonon frequency is considerably increased under pressure and this effect is taken into account while calculating T_c. The calculated T_c values are in fairly good agreement with the experimental trends. The question of $s \rightarrow d$ valence transfer under pressure as well as Heine's fifth-power law are discussed. We also report the variation of other parameters such as the electronic specific heat and conduction bandwidth with pressure.

INTRODUCTION

We will attempt to explain the pressure-induced superconductivity and the experimentally observed variation in the superconducting transition temperature at high pressures for the hcp metal lutetium. The band-structure results, and hence the T_c values, determined in the present work should be more reliable as they are based on the experimental observation of Lin-Gun Liu[1] which shows that the metal retains its hcp structure up to pressures for which the calculations have been done. Further, the more recent theoretical work of Skriver[2] also confirms the earlier experimental result, namely, that Lu stays in the hcp structure up to 230 kbar. Similar high-pressure studies have been reported[3-5] for other lanthanides such as La and Pr. But in these works, the authors assume them to be fcc at normal pressure to start with. But they can exist either in fcc or dhcp forms. At high pressures Pr undergoes a series of structural transitions (Jayaraman *et al.*[6]), whereas La undergoes an isostructural transition. In the case of Pr the authors[5] have not taken into account the structural changes in their calculations. Such ambiguities with respect to the crystalline structure are absent in the present calculation.

Lu is not a superconductor at ambient pressure and becomes one around 45 kbar. Probst[7] measured the superconducting transition temperature experimentally, and the values vary from 20 mK around 45 kbar to approximately 1.1 K at 180 kbar. Wittig[8] proposed that there should be an $s \rightarrow d$ valence transfer to promote superconductivity in a pressure-induced superconductor such as the one under consideration. This possibility is tested in the present work using the Friedel[9] sum rule which makes use of the phase shifts at the Fermi energy at different pressures. Our calculation lends strong support to Wittig's[8] argument on valence transfer.

Heine's[10] fifth-power law which states that the width of the d band should be inversely proportional to the fifth power of the Wigner-Seitz sphere radius is tested for Lu at high pressures. The d-band width is a difficult quantity to determine for hcp metals because of sd hybridization.[11] Therefore, we have adopted Wigner-Seitz[12] boundary conditions to determine this parameter.

The outline of the paper is as follows: Section I deals with the band-structure calculations done at different pressures by the relativistic augmented plane wave (RAPW) method. The variation of the electronic specific-heat coefficient and the conduction bandwidth with pressure is also dealt with in this section. The calculation of T_c using McMillan's[13] formula is discussed in Sec. II. We also discuss in this section the effect of pressure on Θ_D and $\langle \omega^2 \rangle$, and hence on T_c. $\langle \omega^2 \rangle$ is the average of the square of the phonon frequency. In Sec. III the possibility of a $s \rightarrow d$ electron transfer under pressure is discussed. Section IV deals with the behavior of Heine's[10] fifth-power law at high pressures. Finally, the results and discussion are given in Sec. V.

I. BAND STRUCTURE BY RAPW METHOD

Lu being a high-Z metal, the RAPW method is used and the band structures are calculated for six different pressures from 0 to 230 kbar. The band structures are done for all the pressures for which the lattice constants are available from the experimental work.[1] The c and a values corresponding to different pressures are given in Table I. The c/a ratio ranges from 1.589 to 1.547 when the pressure is varied from 0 to 230 kbar. The band-structure calculations have been done for all the pressures assuming the hcp structure as the values do not differ much from the ideal value of 1.633. The crystal potential is constructed using Libermann's[14] free-atom charge density which has been calculated for the electronic configuration $5d^16s^2$. Libermann proposed a new potential func-

TABLE I. Cell parameters.

Pressure (kbar)	c (Å)	a (Å)
0	5.5805	3.5176
36	5.409	3.440
103	5.213	3.341
157	5.067	3.259
191	4.987	3.217
230	4.921	3.179

tion which incorporates a constant λ, which is a function of the charge density, to the Hartree-Fock formalism. The potential function which is derived by means of a variational principle has the correct asymptotic form at large radii in the case of atoms and ions. The muffin-tin (MT) potential includes exchange and correlation contributions calculated using the Vashishta and Singwi scheme which has been dealt with in detail elsewhere.[15] The exchange correlation expression is

$$V_{vs}(r)=\beta(r_s)\left[-\frac{2}{\pi}\right][3\pi^2\rho(r)]^{1/3}, \quad (1)$$

with

$$\beta(r_s)=1+0.031r_s\ln\left[1+\frac{24.3}{r_s}\right], \quad (2)$$

where r_s is the electron gas parameter. The band structures are obtained using this potential by computing the eigenvalues for 1824 points uniformly distributed in the entire Brillouin zone. The band structure of Lu along the symmetry directions Γ-K-M-Γ and A-H-L-A is shown in Figs. 1–4 for 36 and 230 kbar. We now compare the Fermi surface changes between 36 and 230 kbar. At the symmetry point K, the IV band is close to the Fermi energy for 36 kbar, whereas it comes down for 230 kbar. But at point M the IV band moves up gradually with increase in pressure, and eventually at 230 kbar the band goes above the Fermi energy. The changes in the Fermi surface topology arising from the ALH plane are more drastic compared to that of ΓKM plane. For 36 kbar, as well as for other pressures, we find electron pockets due to III and IV bands and their sizes remain the same even up to 191 kbar. But at 230 kbar these electron pockets disappear as the bands at H move well above the Fermi level. The band structure and T_c calculation for 103 kbar have already been reported.[16] The Fermi energy, the density of states corresponding to the Fermi energy, the electronic specific-heat coefficients, and the conduction bandwidths for the above pressures are given in Table II. The density of states corresponding to the Fermi energy at zero pressure is 1.80 electrons/eV atom which is in agreement with those obtained by other theoretical workers (Tsang *et al.*[17]). They are 1.88, 1.74, and 1.74 electrons/eV atom. As expected, the conduction bandwidths increase with increase of pressure.

In most of the rare earths the $4f$ electrons are found to be highly localized with a minor direct influence on the valence electrons.[18] In these rare earths the localized magnetic moments due to $4f$ electrons prevent the forma-

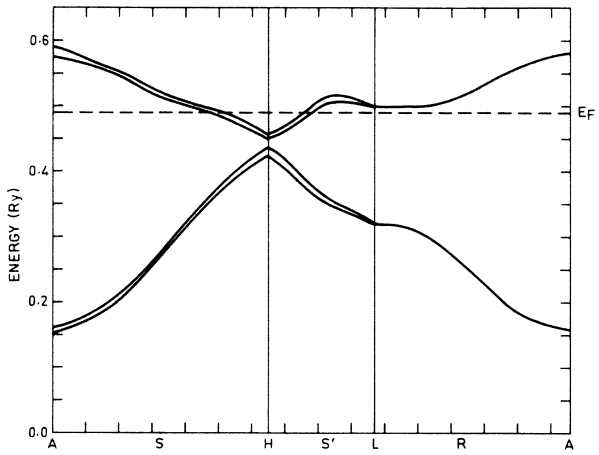

FIG. 2. Band structure along A-H-L-A for 36 kbar.

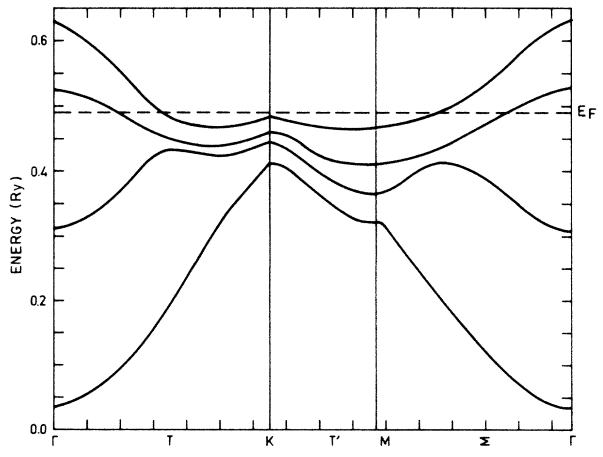

FIG. 1. Band structure along Γ-K-M-Γ for 36 kbar.

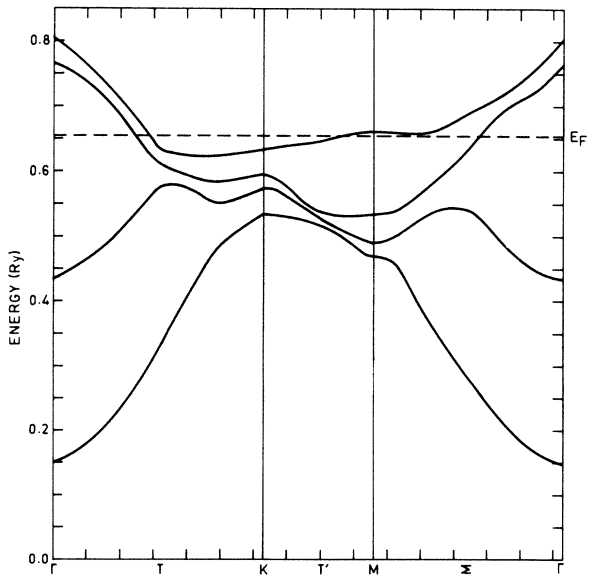

FIG. 3. Band structure along Γ-K-M-Γ for 230 kbar.

TABLE II. E_F, $N(E_F)$, electronic specific-heat coefficient and conduction bandwidth.

Pressure (kbar)	E_F (Ry)	$N(E_F)$ [states/eV atom]	γ [mJ/(mol K^2)]	Conduction bandwidth (eV)
0	0.455	1.800	4.239	6.00
36	0.488	1.799	4.237	6.14
157	0.597	1.511	3.558	6.61
191	0.627	1.455	3.427	6.72
230	0.654	1.283	3.022	6.82

tion of superconducting phase. To account for high value of transition temperature in La when compared to Lu and Y, Wittig argued that the high value was an enhancement effect and this enhancement is due to the presence of $4f$ bands. These $4f$ electrons form a narrow band located a few eV below the conduction band, and this band is very sensitive to potential.[19] These states do not form a band, but they are highly localized and atomiclike. The recent calculation of Strange *et al.*[20] on thulium also shows that $4f$ states are well below the conduction band and the levels are sensitive to the potential used as observed by Dimmock[19] earlier. In our calculation for Lu the $4f$ bands do not interfere with the s-d bands. The f levels are well below the bottom of the conduction band.

II. CALCULATION OF SUPERCONDUCTING TRANSITION TEMPERATURE

A. Θ_D and $\langle\omega^2\rangle$ as constants

In this section we present the calculation of electron-phonon mass enhancement factor λ and the superconducting transition temperature. The superconducting transition temperature is calculated in the same manner as has been done in our earlier work[21] using McMillan's[13] formula which is

$$T_c=\frac{\Theta_D}{1.45}\exp\left[\frac{-1.04(1+\lambda)}{\lambda-\mu^*(1+0.62\lambda)}\right], \tag{3}$$

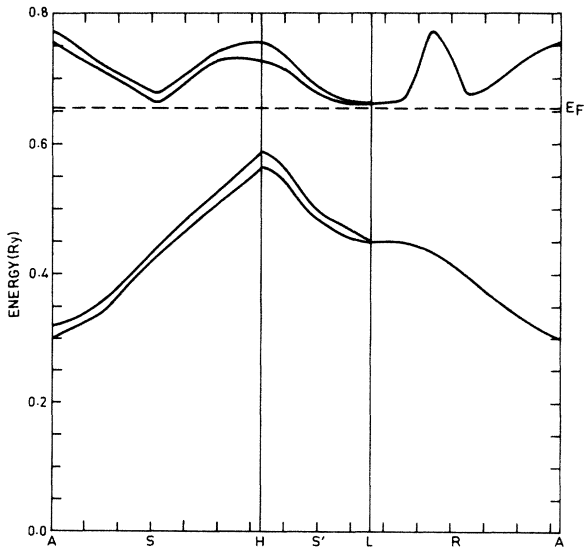

FIG. 4. Band structure along A-H-L-A for 230 kbar.

where λ is given by

$$\lambda=\frac{N(E_F)\langle I^2\rangle}{M\langle\omega^2\rangle}. \tag{4}$$

$N(E_F)$ is the spin density of the states at the Fermi energy. $\langle I^2\rangle$ is the square of the electron-phonon matrix element averaged over the Fermi surface, M is the atomic mass, and $\langle\omega^2\rangle$ is the average of the square of the phonon frequency. Following the work of Papaconstantopoulos *et al.*[22] the average of the square of the phonon frequency $\langle\omega^2\rangle$ to be used in Eq. (4) is calculated from the Debye temperature by setting

$$\langle\omega^2\rangle=0.5\Theta_D^2. \tag{5}$$

The value of the Debye temperature at 0 K and ambient pressure is taken from the recent work of Tsang *et al.*[17] as 183 K. The electron-phonon coupling constant was calculated employing the Gaspari-Gyorffy[23] formula using nonrelativistic phase shifts obtained from the MT potential. Generally, nonrelativistic phase shifts are used to calculate T_c even for high-Z materials. For instance, the work of Pickett *et al.*[3] on La and Dakshinamoorthy *et al.*[24] on Ac can be cited. Moreover, Pickett[25] has calculated the value of $\eta_{l,l+1}$ with and without relativistic phase shifts for La, γ-Ce, and Th, and the two values show negligible difference. The values of T_c along with the other parameters that are involved in the calculation of T_c are given in Table III.

B. Variation of Θ_D and $\langle\omega^2\rangle$ with pressure

The existing theoretical calculations of Pickett *et al.*[3] and Dakshinamoorthy *et al.*[4] which try to explain the experimentally observed variation of T_c with pressure in the case of a metal like La which has a high dT_c/dp value do not take into account the variation of Θ_D and $\langle\omega^2\rangle$ with pressure. But Neve *et al.*[26] while trying to explain the observed variation of electrical resistivity as a function of pressure calculates the variation of λ as a function of pressure employing a suitable expression for the variation

TABLE III. Parameters to calculate T_c (keeping $\Theta_D=183$ K).

Pressure (kbar)	λ	T_c (K)
157	0.537	1.558
191	0.611	2.605
230	0.682	3.738

TABLE IV. T_c calculation by taking $\langle\omega^2\rangle = 0.5\Theta_D^2$.

Pressure (kbar)	γ_G	$\langle\omega^2\rangle^{1/2}$	Θ_D	λ	T_c (K)
0	0.750	129.43	183.0	0.276	
36	0.699	136.52	193.0	0.308	
103	0.679	145.85	206.2	0.371	0.167
157	0.616	153.96	217.7	0.427	0.524
191	0.602	157.37	222.5	0.465	0.913
230	0.591	160.91	227.5	0.496	1.333

of Θ_D with pressure. The references cited by Narlikar[27] also emphasize the fact that the variation of Θ_D with pressure cannot be ignored. There has been no phonon band-structure calculation done at high pressures. If such studies could be made, $\langle\omega\rangle$ could be known as a function of pressure and Dyne's[28] formula could be used as such to calculate T_c. In the absence of phonon band-structure studies at high pressures we resort to the calculation of the average of the square of the phonon frequency using the Grüneisen parameter. Such a calculation has been tried by us[29,30] for La, which gives a better agreement with experimental T_c values in comparison with the earlier theoretical work.[3] We have observed $\langle\omega^2\rangle$ to increase by 20% when the pressure is raised by 120 kbar in La. It should be noted that $\langle\omega^2\rangle$ is found inside the exponential of Eq. (3) through Eq. (4). Hence, even a small variation in $\langle\omega^2\rangle$ will lead to a drastic change in T_c. The considerable change in $\langle\omega^2\rangle$ that we have observed in our calculation at high pressures strongly suggests that the effect of pressure on Θ_D and $\langle\omega^2\rangle$ should definitely be incorporated in high-pressure studies of superconductivity.

The method employed by us to calculate the effect of pressure on Θ_D and $\langle\omega^2\rangle$, and hence on T_c, is described here. The average of the square of the phonon frequency and the thermodynamic Grüneisen parameter γ_G are connected by the relation (Smith and Shelton[31]):

$$\gamma_G = -\frac{d\ln\langle\omega^2\rangle^{1/2}}{d\ln V} . \tag{6}$$

The existing relations connecting γ_G with pressure are due to Ramakrishnan *et al.*[32] and Godwal *et al.*[33] They are

$$\gamma_G = \gamma_0 \left[\frac{V}{V_0}\right]^S , \tag{7}$$

$$\gamma_G = \gamma_0 \frac{\rho_0}{\rho} + \frac{2}{3}\left[1-\frac{\rho_0}{\rho}\right]^2 , \tag{8}$$

TABLE V. Comparions of T_c values.

Pressure (kbar)	$T_c^{(1)}$ (K)	$T_c^{(2)}$ (K)	$T_c^{(\text{expt})}$ (K)
45			0.02
103		0.167	
157	1.56	0.524	
180			1.1
191	2.61	0.913	
230	3.74	1.333	

$$\gamma_G = \frac{\gamma_0\rho_0}{\rho} + \frac{2}{3}\left[1-\frac{\rho_0}{\rho}\right] , \tag{9}$$

where ρ_0 and ρ are the densities at ambient and high pressures. γ_0 is the zero pressure Grüneisen parameter. We used all three relations to study the variation of γ_G with pressure for a number of metals. This was done in particular to In, Al, Pb, and Cu as the value of S required in Eq. (7) is available only for the above metals. The V/V_0 values corresponding to the pressures were taken from the work of Vaidya and Kennedy.[34] To make a comparison between Eqs. (7), (8), and (9), γ_G values are calculated for pressures up to 45 kbar. It was found that all the relations give almost consistent values.[29,30] As the parameter S occurring in Eq. (7) is not available for Lu, Eq. (8) was chosen which obviously gives consistent values compared with that obtained by using Eq. (9). The Grüneisen parameter for Lu at ambient pressure is taken as 0.75 (Gschneidner[35]). The V/V_0 values are calculated from the cell parameters given in Table I. The above values are interpolated by numerical techniques at every 10 kbar. They agree well with the values compiled by Kennedy.[36] The values of γ_G and $\langle\omega^2\rangle^{1/2}$ are calculated using Eqs. (8) and (6). The value of $\langle\omega^2\rangle^{1/2}$ is obtained using numerical interpolations for the pressures for which the band structures have been done. All the above values along with the other parameters required to calculate T_c are given in Table IV. In this calculation we have taken into account the variation of Θ_D and $\langle\omega^2\rangle$ with pressure unlike in Sec. II A, where the values of Θ_D and $\langle\omega^2\rangle$ have been kept constant.

As has been done by Pickett *et al.*[3] for La, wherein the μ^* value was kept as 0.13 for all pressures, we have also calculated T_c for both cases, keeping μ^* as 0.13, for it is usual to have $\mu^* = 0.13$ for the transition metals instead of using the Benneman-Garland formula. In Table V we compare the theoretically calculated T_c values with the experimental values. The experimental values are 20 mK around 45 kbar and $\simeq$1.1 K at 180 kbar. It is obvious from the table that both theoretical calculations are in accord with the experimental trend.

III. $s \rightarrow d$ ELECTRON TRANSFER

In this section we investigate Wittig's[8] proposal of $s \rightarrow d$ electron transfer in materials like Lu which become superconductors at high pressures. The proposal of Wittig is tested in the following two ways: First the d electron phase shifts corresponding to Fermi energies are calculated from the MT potential for different pressures.

TABLE VI. d electron number.

Pressure (kbar)	Z_d
36	1.13
103	1.22
157	1.29
191	1.33
230	1.36

The muffin-tin spheres are taken so as to touch each other, obviously to reduce the interstitial region. As the MT sphere radius is small, compared to Wigner-Seitz radius, the number of electrons inside the MT radius will be slightly less than 3. In the absence of self-consistency, we opt for the sum rule to study the $s \rightarrow d$ electron transfer under pressure. The calculation has been done in the same spirit as was done by Ratti *et al.*[37] in the calculation of E_F for Nb from the Friedel sum rule which gives a good agreement with that obtained from a direct band-structure calculation. By invoking the Friedel[9] sum rule, the d electron number Z_d is calculated using the expression

$$Z_d = \frac{10}{\pi}\delta_2(E_F) . \tag{10}$$

The d phase shifts corresponding to E_F which are used in the calculation of λ, and hence T_c and the calculated Z_d values as a function of pressure are given in Table VI. The observation that Z_d value increases shows that the d electron number increases with pressure. This is in agreement with the proposal of Wittig. Further, it is well known that for a material to be a superconductor $\delta_2(E_F)$ should preferably be large. For a pressure-induced superconductor if T_c increases with pressure, obviously $\delta_2(E_F)$ should increase at the expense of $\delta_0(E_F)$ and $\delta_1(E_F)$ as a function of pressure. This fact again follows from the Friedel sum rule whose general form is

$$Z_v = \frac{2}{\pi}\sum_l (2l+1)\delta_l(E_F) , \tag{11}$$

and Eq. (10) is a special case of the above equation. The values of δ_2 as a function of pressure are given in Table VII. δ_2 is found to increase with pressure. These results clearly indicate that there should be $s \rightarrow d$ transfer in Lu as proposed by Wittig.

TABLE VII. d phase shifts at Fermi energy.

Pressure (kbar)	$\delta_2(E_F)$
0	0.344
36	0.357
103	0.384
157	0.406
191	0.418
230	0.429

IV. HEINE'S FIFTH-POWER LAW

The validity of Heine's[10] fifth-power law is checked at high pressures by showing that the width of d band changes with pressure as r_s^{-5} where r_s is the Wigner-Seitz sphere radius. From the bonding and antibonding conditions given by Wigner and Seitz[12] the d-band width is obtained using the expression

$$W_d = E_t - E_b , \tag{12}$$

where E_t and E_b are the top and bottom of the d band. They are calculated by determining the energies for which the logarithmic derivative SR_l'/R_l becomes minus infinity and zero, respectively. S is the MT sphere radius. By making use of the MT potentials constructed for different pressures, E_t and E_b are fixed. Hence the d-band widths are calculated using the above expression. The d-band width, the Wigner-Seitz sphere radius r_s, as well as the values of $W_d r_s^5$ are given in Table VIII. The dependence of r_s^{-5} is good up to 25%. We observe that the value of $W_d r_s^5$ dips at 191 kbar and increases at 230 kbar. At present we are not sure whether this may be due to the anticipated structural transition after 230 kbar.

V. RESULTS AND DISCUSSIONS

The main objective of the paper is to explain first the occurrence of superconductivity and then its subsequent increase of T_c with pressure in the metal Lu. As has been described in Sec. II, T_c has been calculated keeping Θ_D as constant and also taking into account the variation of $\langle\omega^2\rangle$ with pressure. Both procedures confirm that the metal should become a superconductor under pressure as has been reported experimentally. The values of T_c obtained by both procedures reproduce the experimental trend, namely, that the values of T_c increase with increase of pressure. We are unable to compare our results with the experimental results as the latter are available only for certain pressures as shown in Table V. The experimental T_c value is 1.1 K at 180 kbar. The theoretical value calculated at 191 kbar is 2.60 K when pressure effects are not taken into account explicitly, and it is 0.91 K when pressure effects are taken into account. Even though the experimental value at 157 kbar is not given, T_c versus the pressure graph given by Probst was used to obtain the T_c value at that pressure. The value so obtained is 0.64 K. The theoretical value calculated taking into account the pressure effect is 0.52 K which is in close agreement compared to 1.56 K obtained by the other method. These findings show that T_c calculations, determined by taking into account the pressure effects, agree well with the ex-

TABLE VIII. Heine's fifth-power law.

Pressure (kbar)	W_d (Ry)	r_s (Å)	$W_d r_s^5$
36	0.755	1.877	18.05
103	0.875	1.818	17.37
157	0.975	1.772	17.03
191	1.025	1.747	16.67
230	1.102	1.734	17.27

perimental values. But it should be admitted that the magnitude in the variation of T_c is very sensitive to the variation in λ. However, we strongly feel that the pressure effects on $\langle\omega^2\rangle$ should be taken into account as our calculation shows a variation of 24% in $\langle\omega^2\rangle$ for a rise in pressure of 230 kbar. Such a large change in the $\langle\omega^2\rangle$ value makes us to conclude that in all high-pressure investigations on T_c apart from calculating the electron band structure alone at high pressures, the pressure effects on phonons should also be taken into account.

Next we investigate Wittig's proposal of $s \rightarrow d$ valence transfer to explain pressure-induced superconductivity. The theoretical work of Pickett *et al.* which aims at explaining the variation of T_c with pressure in the metal La lends support to this view. As our calculation is nonself-consistent we follow an indirect procedure to test this in the metal under consideration. Employing the Friedel sum rule we calculate the d electron number Z_d at different pressures. We observe Z_d to increase with pressure. This, together with the fact that $\delta_2(E_F)$ increases with pressure, go to strengthen our belief that the much anticipated $s \rightarrow d$ transfer proposed by Wittig takes place in Lu also. In our case the electronic specific-heat coefficient decreases with pressure since $N(E_F)$ decreases with pressure.

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