HYDROSTATIC PRESSURE STUDIES OF THE NEW ORGANIC CONDUCTOR \( \alpha\)-(BETS)\(_2\)KHg(SCN)\(_4\)

S. A. IVANOV, C. C. AGOSTA, AND T. COFFEY
Physics Dept. Clark University, 950 Main St., Worcester, MA, 01610
USA
E-mail: cagosta@clarku.edu

B. W. FRAVEL, AND L. K. MONTGOMERY
Chemistry Dept. Indiana University, Bloomington, IN 47405
USA

We present the first hydrostatic pressure studies at low temperatures and high magnetic fields of the quasi two dimensional organic metal \( \alpha\)-(BETS)\(_2\)KHg(SCN)\(_4\), where BETS is a cation that has the inner four sulfur atoms of the ET molecule replaced with larger selenium atoms. The material we discuss is a close relative of \((\text{ET})_2\)KHg(SCN)\(_4\), which possesses very interesting electronic properties at low temperatures. In particular, we examine the behavior of beats in the SdH oscillations in the BETS material as a function of pressure up to 14 kBar. These beats can be used to study the interlayer transport, and may be used to test theoretical predictions of coherent and incoherent interlayer transport. We will also discuss effective mass measurements at high pressures that suggest that the screening of electrons increases as the pressure increases, in agreement with theory.

1 Introduction

Electron transport in anisotropic conductors is studied by many groups because of the rich array of ground states that exist in these materials at low temperatures. High temperature superconductivity, the quantum Hall effect and fractional quantum Hall effect, spin density waves and charge density waves all depend on constraining the dimensionality of electron transport. Our measurements of the Shubnikov-de-Haas effect in the quasi 2-dimensional molecular conductor \( \alpha\)-(BETS)\(_2\)KHg(SCN)\(_4\) \([(\text{BETS})\text{K}]\) demonstrate a way to measure the anisotropy in a lower dimensional metal and show that the high compressibility of this molecular conductor system makes it a convenient model to test theories of interlayer transport.

2 Experimental

Magnetoresistance measurements in hydrostatic pressure cells were performed at the NHMFL in fields up to 32.8 tesla, temperatures down to 0.5 K, and pressures up to 13.7 kbar. The high pressures were created using a standard beryllium copper pressure cell. An ac current of 10 \( \mu \)A was flowing perpendicular to the most conducting layers and the resistance was measured using a four lead technique.
3 Results

Fig. 1. shows the magnetic field dependencies of the resistance of (BETS)K divided by a smooth background at different applied hydrostatic pressures. The data at ambient pressure is taken on a different sample using a pulsed field apparatus and high frequency ac detection[3]. The 0.25 kbar field sweep is noisy because it was recorded with only 3 leads attached to the sample.

A low frequency beat visibly appears in the oscillations at an applied pressure of 2.5 kbar. The appearance of the beat is explained by the following. Organic conductors are not ideal 2D or 1D materials, and they always have a nonvanishing transfer integral perpendicular to the conducting layers. This conductivity causes warping of the cylindrical parts of the Fermi Surface into an hour glass shape. When the magnetic field is applied perpendicular to the layers, two extremal areas corresponding to the largest and the smallest diameter cross sections of the Fermi surface contribute to the oscillatory behavior. Mixing of these two frequencies results in the beats seen in the Figure. The fact that we do not observe a beat at ambient pressure does not mean that there is no warping; it suggests that the magnetic field was not high enough for the beat to be noticeable.

A Fast Fourier Transform was applied to the data to create Fig. 2, which clearly shows the two frequencies at the higher pressures. For the lower pressure data, such as the 3.5 kbar data, we can estimate the average frequency of the two fundamentals from Fig. 2 and obtain the difference between the two frequencies from the length of the beat in Fig. 1. The positions of the peaks in Fig 2 allows us to estimate the change of frequency and the cross-sectional area of the Fermi surface as a function of applied pressure. For the lower frequency ($F_1$) it is 6.84 T/kbar, if all the measured pressure range is taken into account, and 9.9 T/kbar for pressures from ambient to 6 kbar. For the higher frequency ($F_2$), it is similar. These numbers are close to values reported by Brooks et al.[1] for ET-based compounds. This
comparison, confirms the similarity in the crystallographic parameters and characteristics between ET and BETS materials.

We can estimate the compressibility coefficients $K_i$ (the diagonal components of the compressibility tensor), if we set $K_x=K_y=K_{xy}$. If $F_0=680$ T, $F=812$ T, and $P=13.7$ kbar, we obtain $K_{xy} \approx 0.006$ kbar$^{-1}$. If $F_0=680$ T, $F=768.2$ T, and $P=6$ kbar, then $K_{xy} \approx 0.0096$ kbar$^{-1}$. These values are close to the ones reported for $\kappa$-(ET)$_2$Cu(As)$_2$: $K_b=0.0025$ kbar$^{-1}$ and $K_a=K_c=0.0036$ kbar$^{-1}$ [2].

The next important parameter of (BETS)$_K$ we can extract from the pressure experiments is the effective mass of the carriers. We used Fourier analysis to determine the amplitude of oscillations at different temperatures. Because the beat frequency is very low, we have to use as large a field range as we can to perform the FFT. If there is a field dependence of the effective mass, we will not be able to see the dependence easily, although in the case of (BETS)$_K$ we did not found any field dependence of the effective mass at ambient pressure[3]. The resulting pressure dependence of the effective masses corresponding to the two frequencies is depicted in Fig. 3.

For the free electron gas, there should not be any band mass dependence on pressure[1]. In a real material however, there are at least contributions from electron-electron and electron-phonon interactions. For organic conductors with their complicated crystallographic structure and associated nontrivial phonon spectra, the change in the electron-phonon interactions with pressure can be complicated. Yet, we have shown in the past that the electron-phonon interactions are small as compared to the band mass [3].

For the contribution of electron-electron interactions the following simple approach can be taken. With increasing pressure the concentration of electrons increases. Generally, the strength of electron-electron (Coulomb) interactions is proportional to the screening length, i.e. the larger the screening length, the larger
the number of electrons that “feel” the screened Coulomb potential, as given in the Thomas-Fermi theory of screening by:

$$\phi(r) = \frac{Q}{r} e^{-k_0 r},$$

where $Q$ is the screened charge and $k_0$ is the Thomas-Fermi wave vector defined by $k_0 = 2e(\pi D(E_F))^{1/2}$ [4].

Because the density of states at the Fermi level $D(E_F)$ is proportional to the lattice constant, $a$, squared, the characteristic screening length, $r_0$, is proportional to the lattice constant: $r_0 \propto 1/k_0 \propto a$. With increasing pressure the screening length should decrease (linearly with pressure in the first approximation) thus decreasing the strength of electron-electron interactions. We observe a decrease in effective masses for (BETS)K (Fig. 3) at rate of about -1.4%/kbar for the first frequency and about -1.5%/kbar for the second.

4 Conclusions.

Beats are seen in the Shubnikov-de-Haas oscillations at high pressures in the molecular conductor $\alpha$-(BETS)$_2$KHg(SCN)$_4$ due to the warping of the Fermi surface. The warping shows that the interplane conduction can be adjusted by the application of pressure. We also suggest that we can see a change in the electron-electron interactions due to a change in the electron density. We acknowledge support from The Petroleum Research Fund #31373-AC6.