Bull. Mater. Sci., Vol. 21, No. 6, December 1998, pp. 451–456. © Indian Academy of Sciences.

Two-component model for optical conductivity in Y–Ba–CuO superconductors

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MS received 1 July 1998

Abstract. The optical conductivity of optimized doped $YBa_2Cu_3O_{7-\delta}$ ($\delta = 0{\cdot}0$, $T_c = 92$ K) superconductors, which are frequency dependent, has been theoretically investigated based on two-component (Drude and mid infrared terms) approach within the Fermi liquid description. Our approach incorporates the Drude contribution as well as hopping of charge carriers in the model dielectric function along with the structure factor. It explains the anomalies observed in the optical measurements for the normal state as the frequency dependence of optical conductivity using the Drude term which gives a sharp peak at zero frequency, and a long tail at higher frequencies, i.e. in the infrared region. The extra term (hopping carriers) gives a peak value in the optical conductivity centred in the mid infrared region. The two species of charge carriers contribution to the conduction in the CuO chain layer as well as CuO_2 layer will account for the optical conductivity in the mid infrared as well as infrared frequency regions. The analysis reveals an interesting relation $\sigma_{CuO_2\ layer} \approx 3\sigma_{chain\ layer}$, and the nature for optical conduction with energy is similar qualitatively, the only difference is quantitatively. It is shown that the analysis is consistent with the published data on optical conductivity in optimized-doped $YBa_2Cu_3O_{7-\delta}$ superconductors.

Keywords. Optical conductivity; Drude term; hopping; YBCO superconductors.

1. Introduction

Since the discovery of high temperature superconductivity in cuprates, attempts have been made to identify the superconducting energy gap and other features responsible for the pairing mechanism, using infrared spectroscopy. Infrared spectroscopy provides valuable information on optical conduction of the charge carriers in the normal as well as superconducting states, which are not clearly understood and controversies remain to be unresolved (Tanner and Timusk 1992). Among various cuprates, 90 K Y–Ba–CuO system has been widely analysed experimentally, since good crystals with a very sharp superconducting transition at T_c can be prepared from it. However, 90 K Y–Ba–CuO system has complex crystal structure as there exists single one-dimensional (1-D) CuO chain layer, two-dimensional (2-D) CuO_2 layer, and metal oxide layers. It is generally believed that superconductivity occurs primarily in the 2-D CuO_2 layer, and that the 1-D CuO chains are not so crucial. Recent experiments have indicated that the chain layer is metallic and contributes significantly to the transport of charge carriers (Bernhard and Tallon 1996). Exact mechanism of the binding of holes into Cooper pairs remains elusive and this concept has to be taken into account in attempting a theoretical discussion of this system.

Optical conductivity measurements in the mid- and near-infrared regimes can give valuable information regarding the properties of low-lying charge excitations in the metallic system. For optimized-doped 90 K YBCO, the optical conductivity, $\sigma(\omega)$, spectra shows a sharp peak at $\omega = 0$, and a long tail extending to higher frequencies in the infrared region where $\sigma(\omega)$ falls as ω^{-1} slower than ω^{-2} decay in the Drude spectrum. The origin of the mid-infrared (MIR) band is still unclear. When a Drude model is used, an extremely short mean free path should be used to fit the optical data, and the temperature dependence is much weaker than expected due to dc conductivity. It has been argued that the anomaly in MIR band may be caused by the coupling between the mid-infrared carriers and phonons. Furthermore, the optical spectra is mainly due to the 2-D CuO_2 layers (Tanner and Timusk 1992). While some authors attribute MIR band in part to trapped holes near dopant atoms, others claim that it is from the Cu–O chains of YBCO that most of the weight originates. It is therefore important to establish the role of CuO chain layer as well as CuO_2 layers in the optical conduction mechanism.

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Extending the scenario, the idea of phonon-mediated force alone to meet high transition temperature in cuprates seems to be difficult, and the observed high T_c may be associated with charge fluctuations other than the phonon, proposed earlier (Kresin *et al* 1993). Examples to support this include low energy plasmons, or excitons which might play an important role in realizing high T_c superconductivity. Optical conductivity measurements (Uchida *et al* 1991) and Raman scattering experiments (Sugai *et al* 1990) have suggested the strong density fluctuations in the mid-infrared region of optical spectra.

Optical conductivity can be obtained after a Krammers Kroning analysis of the reflectance spectra, and many experimental studies of YBCO superconductors have been carried out in the recent past (Thomas *et al* 1988; Kamaras *et al* 1990; Orenstein *et al* 1990). While the far-infrared region depends strongly on temperature, especially below T_c, the mid-infrared region is temperature independent. There is a clear minimum at $\sim 2000\,\mathrm{cm}^{-1}$ that can be easily seen at $T = 100$ K (Orenstein *et al* 1990). It is remarkable in this connection that the real part of the conductivity, which describes the absorption, provides a measure of the size of the superconducting gap. There has been an ongoing debate as to whether or not a superconducting gap is observable in the in-plane reflectivity spectrum. Conventional superconductors display an *s*-wave gap and are in dirty limit, while the high T_c cuprates are different. Using the two-component model in which a spectrum is decomposed into a *T*-dependent Drude part and a *T*-independent mid-infrared absorption part, Kamaras *et al* (1990) claimed that a gap cannot be observed in the in-plane spectrum because of clean limit of superconductivity. Experimental results for optical conductivity (Terasaki *et al* 1990; Uchida *et al* 1991) in the superconducting copper oxides suggest that these exists as at least two species of carriers, contributing to the conduction in CuO_2 layer over the infrared and the lower frequency regimes in the light of conductivity sum rules.

On the theoretical side, it may be noted that the normal state $\sigma(\omega)$ does not follow an ordinary Drude law in the infrared region. Schlesinger *et al* (1990) have analysed the $\sigma(\omega)$ data using one component model which considers the frequency dependent parameters $m(\omega)$ and $1/\tau(\omega)$, and obtained a gap of $500\,\mathrm{cm}^{-1}$. The two-component analysis in which the $\sigma(\omega)$ spectrum is decomposed into an ordinary term (where all parameters are independent of frequency) at $\omega = 0$ plus an extra Drude contribution modelled by one or more lorentz oscillators centred at ω in the MIR region. Recently, Stevens *et al* (1997) have investigated the electronic excitations contribution to the superconducting gap function in YBCO systems using the Femto second time resolved spectroscopy. The optical response favours the two-component model of high T_c superconductivity in the YBCO systems. As mentioned earlier, the mid-infrared in the optical spectra is mainly due to the CuO_2 layers (Tanner and Timusk 1992). Guided by these experimental and analytical work, the role of 1-D CuO chain layer and 2-D CuO_2 layer contribution to optical conductivity as well as the underlying physics of observed MIR anomaly was investigated.

In § 2, we have discussed a model which we have developed using two species of charge carriers. The first channel to the conductivity is the coherent Drude component with temperature dependent damping. Secondly the hopping of charge carriers from one site to another site of the CuO_2 layer will contribute to the conductivity. Moreover, we assumed that in the metallic normal phase, $\sigma(\omega)$ consists of a Drude term centred at zero frequency whose shape depends on temperature, and the hopping term will contribute a peak value in the mid-infrared region. Role of chains and layers are well approximated, forming a layer stacking sequence structure of YBCO. § 3 deals with the estimation of parameter, along with results and discussion.

2. The model

The peculiarity of the high T_c superconducting cuprates are in their structural complexity as well as topology of Fermi surface associated with the electronic band energy. For the calculation of the transport property, knowledge is required of both hole and phonon bands, construction of the Fermi surface, in addition to the operating superconducting mechanism. The high T_c cuprates are layered, low-dimensional structures with anisotropic Fermi surface. The single crystal of Y-based cuprate superconductors can be modelled as an infinite array of two-dimensional (2-D) conducting CuO_2 planes and 1-D CuO chains, which have a significant number of charge carriers (holes) and are well separated by metal oxide reservoirs with interlayer distance $d_c \gg d_a, d_b$. In a unit cell, the layer stacking sequence is Y, CuO_2, BaO, oxygen deficient CuO (chain), CuO_2, BaO, CuO_2, Y.... The layers in the x–y plane possess a relatively weak coupling between the planes in the perpendicular z direction. To a first approximation, these layers are well separated and treated as non-interacting. We may regard such a system as a 2-D hole liquid which may be characterized as a collection of strongly correlated, but with the itinerant Fermi particles confined along *ab* axis. Furthermore, these two species of carriers contribute to the conduction along the *ab* axis, which is consistent with the earlier observations.

The free charge carriers, as developed from the chemical doping in the parent compound, are constrained to move within this 2D CuO_2 layer and hence the electron gas lies in this plane. We assume that for a non-interacting

system, copper and oxygen electrons are within the Fermi surface. The Fermi surface is anisotropic and is considered as open in the k_z direction perpendicular to the layer plane, i.e. in the z-axis. Regarding the construction of the Fermi surface, we assume that the 2-D electron system contains a subgroup with a high density of states near the Fermi level. In this case, the Fermi curve has sections which are almost linear, and has a number of nesting states. As a result of the nesting of the Fermi surface, the scattering processes involve $2k_F$ scattering across the Fermi surface which dissipates momentum effectively. The energy of a particle with open Fermi surface has the following form,

$$\varepsilon(k) = (\hbar^2 k^2/2m^{\parallel}) + (\hbar^2/m^{\perp}d^2)[1 - \cos(k_z d)] - \mu,$$

where k and k_z are the 2-D momentum wave vector along and perpendicular to the CuO_2 plane. It appears that one can estimate the effective mass of the electron for their motion in respective directions using the band structure parameters based on local density approximation. The Fermi liquid picture provides the information along the plane only, as it utilizes the experimental data on electronic specific heat coefficient for the estimation of effective mass. We restrict ourselves to the case $|k_{z,\max}| = \pi/c$. The interplanar separation, d, is half of the lattice parameter 'c', and μ represents the chemical potential. Within this Fermi liquid picture (Varshney and Singh 1995; Varshney *et al* 1996), one can estimate the normal and superconducting state parameters using experimental information in a self consistent way.

As was said above, the electrons below the Fermi surface do interact with nearby charges and the resulting potential have a particularly strong influence in the long wavelength limit. We consider the screened Coulomb potential for a series of identical CuO_2 planes. Furthermore, we speculate that two species of carriers contribute to the electrical conduction along the *ab* axis, which is consistent with the earlier observations (Timusk and Tanner 1989). The distance between two consecutive layers is $d(=2d_1+d_2)$, between a CuO chain and a CuO_2 layer is d_1, and d_2 denotes the separation of two consecutive chains. The charged quasi particles are being scattered by the phonons as well as the electronic excitations (plasmons) and the impurities possess a finite damping rate Σ. The effective interaction potential between the electrons can be conveniently described by the perturbation approach. Performing the Fourier transformation and keeping in mind the periodicity of the layers, the q_z integration ranges from $-\pi/d$ to $+\pi/d$, one does write the effective interaction potential as (Varshney and Singh 1995):

$$V(q, q_z, \omega) = \frac{2\pi e^2}{q\varepsilon_\infty \varepsilon(q, q_z, \omega)} S(q, q_z), \tag{1}$$

where, $\varepsilon(q, q_z, \omega)$ is the model dielectric function for a single band of charge carriers. $S(q, q_z)$ represents the static structure factor. The contribution from core electrons is ε_∞ and in the frequency region of interest it is independent of frequency.

The dielectric function, $\varepsilon(q, q_z, \omega)$ in terms of polarizability is expressed as

$$\varepsilon(q, q_z, \omega) = 1 + P(q, \omega)S(q, q_z), \tag{2}$$

with

$$P(q, \omega) = \frac{-2\pi e^2}{q\varepsilon_\infty} \Pi(q, \omega), \tag{3}$$

and

$$S(q, q_z) = \frac{\sinh(qd_1)\sinh(qd_2)}{\cosh(qd_1)\cosh(qd_2) - \cos(q_z d)}, \tag{4}$$

where, q is the in-plane 2-D wave vector and q_z is in the z direction. The elastic properties along and perpendicular to the conducting planes are considerably different. To have the conduction along the *a–b* plane, it is suffice to average (1) to get

$$V(q, \omega) = \frac{d}{2\pi} \int_{-\pi/d}^{+\pi/d} V(q, q_z, \omega)\, dq_z. \tag{5}$$

The integral can thus be evaluated by using (1) and (5) to obtain

$$V(q,\omega) = \frac{2\pi e^2}{q\varepsilon_\infty} \frac{D(q, \omega)\sinh(qd_1)\sinh(qd_2)}{|D(q, \omega)|\,[|D^2(q, \omega) - 1|]^{1/2}}, \tag{6}$$

with

$$D(q, \omega) = \cosh(qd) + P(q, \omega)\sinh(qd_1)\sinh(qd_2). \tag{7}$$

The two-dimensional electronic polarizability in long wavelength limit ($q \to 0$) is

$$P(q, \omega) = -\frac{2\pi e^2 Z^2 n}{\varepsilon_\infty m^* \omega\,[\omega + i\Sigma(\omega)]}, \tag{8}$$

with $\Sigma(\omega)$ being the frequency dependent relaxation rate.

We thus write the model dielectric function for two species of charge carriers as:

$$D(q, \omega) = 1 - \frac{2\pi e^2 q\alpha}{\varepsilon_\infty} \sum_\mu \frac{Z_\mu^2 n_\mu}{m_\mu^* \omega[\omega + i\Sigma(\omega)]}, \tag{9}$$

where n_μ is the 2-D charge carrier contribution and m_μ^* the effective mass of the carriers. The sum of electronic and ionic bound charge is denoted as Ze. We represent

$$\alpha = q^2 d_1 d_2.$$

The frequency dependent relaxation rates are expressed in terms of memory functions as:

$$\Sigma_\mu(\omega) = \Sigma_\mu(0) + [\Sigma_\mu(\infty) - \Sigma_\mu(0)][-i\omega\Gamma_\mu(\omega)], \quad (10)$$

in terms of memory functions $\Gamma_\mu(\omega)$ (Yoshida and Takeno 1989). Here, we denote $\Sigma_\mu(0) = \gamma_{1\mu}$ and $\Sigma_\mu(\infty) = \gamma_{2\mu}$ as the low and high frequency limits of the relaxation rates, respectively. In order to satisfy the requirements of casuality, the memory functions are:

$$\Gamma_\mu(\omega) = \int_0^\infty \Gamma_\mu^*(t) e^{i\omega t} dt, \quad (11)$$

where $\Gamma_\mu(t=0) = 1$ and $\Gamma_\mu(t=\infty) = 0$. Using the Gaussian forms of Γ (Yoshida and Takeno 1989) for the memory function

$$\Gamma_\mu^*(t) = \exp(-t^2/\gamma_{c\mu}^2), \quad (12)$$

with $\gamma_{c\mu}$ being the characteristic relaxation rates.

Using (9) and (10), the imaginary part of the dielectric function is

$$\mathrm{Im}D(q,\omega) = 1 - \frac{2\pi e^2 q\alpha}{\varepsilon_\infty} \times \sum_\mu \frac{Z_\mu^2 n_\mu \gamma_{1\mu}}{m_\mu^* \omega[\omega^2 - (\gamma_{2\mu} - \gamma_{1\mu})^2 + \gamma_{1\mu}^2]}. \quad (13)$$

The optical conductivity is expressed as:

$$\sigma(\omega) = \lim_{q\to 0}\left[\frac{\omega 1}{2\pi q}\,\mathrm{Im}\varepsilon(q,\omega)\right] \quad (14)$$

$$= \alpha \sum_{\mu=1}^{2} \frac{\omega_{p\mu}^2}{2\pi} \frac{\gamma_{1\mu}}{[\omega^2 - (\gamma_{2\mu} - \gamma_{1\mu})^2 + \gamma_{1\mu}^2]}, \quad (15)$$

where 1 is the number density of CuO_2 layers along c axis.

Using the developed expression for optical conductivity assuming two channels of optical within CuO chain layer as well as CuO_2 layer, we have computed optical conductivity for YBCO superconductors at $T = 100$ K. Deduced results along with discussions are presented in the following section.

3. Results and discussion

We have estimated the optical conductivity of $YBa_2Cu_3O_{7-\delta}$ superconductors at $T = 100$ K based on the experimental observations within the Fermi liquid description in the reciprocal space. Such a technique is of vital importance as the structural information of the system, i.e. lattice parameters as well as the specific heat measurements can be performed well on high quality single crystals, and the data yielded for any theoretical description are more reliable. For the YBCO superconductors, a stack of 2-D layers and 1-D chains which are well separated by average distances, the condition for optimized pairing suggests that 2-D charge carrier density in the layers will follow $n_L d^2 = 1$, and for 1-D chains $n_C d_2 = 1$. Thus the volume concentration of the charge carriers will be $n = n_C n_L/3$. The Fermi wave vector for the 2-D plane is $K_{FL} = (2\pi n_L)^{1/2}$, and for 1-D chain it is $K_{FC} = (2\pi n_C)^{1/2}$.

Furthermore, the effective mass of the charge carriers can be well estimated from the electronic specific heat coefficient (γ) value for 2-D layers as $m_L = 3\hbar^2\pi\gamma d K_B^{-2}$, and $m_C = 12\hbar^2\pi\gamma d^2 d_2^2 n K_B^{-2}$ are used for the 1-D chains, respectively (Varshney *et al* 1996). It has been pointed out that incorporation of the realistic physical parameters, based on experimental observations in the Fermi liquid description, will lead to a clearer picture of the properties in the YBCO systems. The lattice parameter and separational distance of the YBCO unit cell are $a = 3{\cdot}81$ Å, $b = 3{\cdot}88$ Å, $c = 11{\cdot}88$ Å, $d \cong 6$ Å, $d_1 = 4{\cdot}129$ Å and $d_2 = 3{\cdot}422$ Å to deduce $n = 2{\cdot}82 \times 10^{21}$ cm^{-3}. Taking $\gamma = 12{\cdot}6$ mJ–mol^{-1}–K^{-2} (Inderhees *et al* 1987), the effective mass $m_L = 6m_e$, and $m_C = 2m_e$ are deduced. With these realistic parameters based on experimental information, we attempted to estimate the plasma frequency in chain layer, using $\omega_C^2 = 4\pi e^2 \bar{n}_C/m_C = 4\pi e^2 n_C/m_C A_C$. Here, $n_C = N/d_2$, and area of unit cell A_C is 'ca' to obtain ω_C as 1·146 eV. Similarly for 2-D CuO_2 layer, $\omega_L^2 = 4\pi e^2 \bar{n}_L/m_L$, with $\bar{n}_L = 2n_L/c$ and $n_L = N/d^2$. Assuming that one hole N (= 1) enters into the number of holes in chain layer of length d_2 as well as area A_C of 2-D CuO_2 layer.

From the above, it can be inferred that frequency of plasmons, as developed in 2-D CuO_2 layer, is enhanced by a factor of 1·7 than that in 1-D CuO chain layer. The low value of plasma frequency in CuO chain layer is attributed to the reduced effective mass of holes as well as the hole carrier concentration in the one-dimensional conduction process. For the two-component model of optical conductivity, the effective mass (m_μ) follows the relation $m_2 = 8m_1$ for two species of charge carriers. The effective mass of charge carrier participating in hopping process is much larger due to weak Josephson coupling, and is difficult to determine because of short mean free path. The background dielectric constant, ε_∞, is taken as 4·5. The sum of ionic and bound electronic charge is Ze, and is $-2e$. The optical conductivity essentially depends on the value of relaxation rates representing the life time of free charge carriers, and are roughly estimated as $\gamma_1 \approx \gamma_2 \approx 2$–$5\ K_B T$ (Timusk and Tanner 1989).

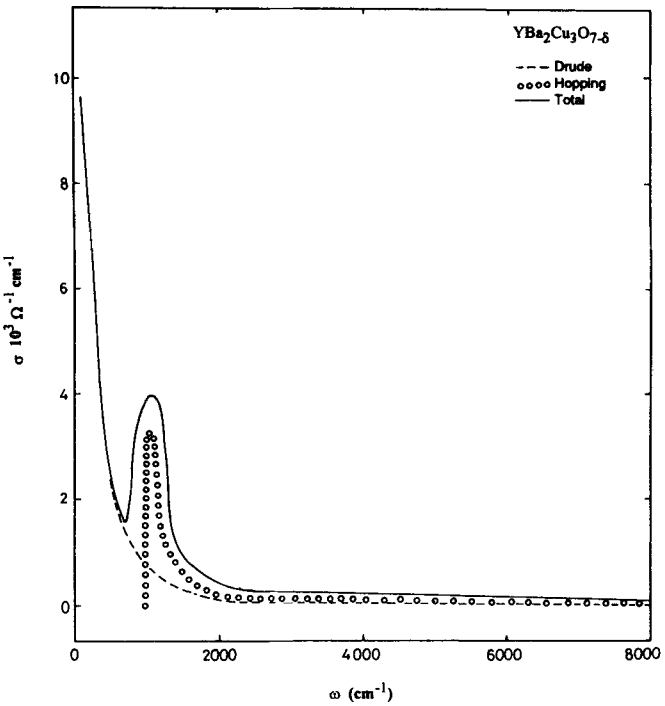

Figure 1. Calculated result of optical conductivity for CuO_2 layer with CuO chain layer for $YBa_2Cu_3O_{7-\delta}$ at $T = 100$ K. Dashed curve is from Drude ($\mu = 1$) and dotted curve refers to hopping component ($\mu = 2$). Solid line represents the sum of both species of charge carriers.

With these realistic parameters based on experimental information, we have plotted the optical conductivity of chain layer and CuO_2 layer for two species of charge carriers in figure 1. We find that $\sigma_{CuO_2\ layer} \approx 3\sigma_{chain\ layer}$. While qualitatively the nature for optical conduction with energy is similar, the difference is only quantitatively. The relaxation rates are temperature dependent, and for $T = 100$ K we use $\gamma_{11}(\gamma_{21})$ as 300(400) cm^{-1}, respectively. Physically this corresponds to the case of ordinary Drude model. A peak value of $\sigma(\omega)$ at zero frequency is observed which develops from the 2-D plasmon modes and a tail at higher frequencies. Furthermore, for the second component, we used $\gamma_{12}(\gamma_{22})$ as 2000 (1000) cm^{-1} and obtained a peak value at $\omega = 1000$ cm^{-1}. Indeed this non-Drude behaviour is interpreted in terms of hopping of the charge carriers from one site to another along the layer. It may be pointed out that the relaxation rates γ_{12} and γ_{22} are involved in the hopping process, and in cuprate superconductors γ_{12} and $\gamma_{22} \geq \varepsilon_F$, so the motion of charge carriers within the layer and chain are no doubt hopping like. Both contributions are then clubbed and the resultant optical conductivity is consistent with the reported data on $YBa_2Cu_3O_{7-\delta}$ superconductors (Thomas *et al* 1988).

4. Conclusion

In this communication we have devoted our efforts to understand: (i) role of chain layer and CuO_2 layer in the optical conduction process, and (ii) the observed anomalous behaviour in the mid-infrared region of YBCO superconductors. To elucidate the contribution of chain layer and CuO_2 layer, proper structure factor for layer stacking sequence of YBCO has been constructed which utilizes the information of structural data within the Fermi liquid description. We speculate that phonons as well as low energy plasmons perhaps contribute to the superconducting pairing. Physically, the Drude carriers couple only weakly with phonons or low energy plasmons, giving rise to a sharp value at zero frequency. Using the memory function approach for frequency-dependent relaxation rates, we have systematically obtained the characteristic relaxation rates. In a true sense, the scattering rates are very large, and of the order of T_c in high T_c cuprates. Specific heat data is used to estimate the effective mass of the charge carriers (holes) participating in the *a–b* plane conduction process. The effective mass of the charge carrier in CuO chain layer is nearly 3-times smaller than that of CuO_2 layer because of its one-dimensional characteristic.

Assuming two-channel of optical conduction, i.e. (i) Drude component with temperature-dependent relaxation rates which essentially describes the peak value centred at $\omega = 0$ as well as the long tail in the infrared region, and (ii) the hopping of the charge carrier from one site to another within the CuO_2 layer—the interlayer effects, we interpret the anomalies observed in the optical measurements. Within this framework, we are able to understand the observed anomaly in the mid-infrared region. In principle, CuO chain layer as well as CuO_2 layer actively participate in the optical conduction process and they differ in only the magnitude. The analysis reveals that $\sigma_{layer} \approx 3\sigma_{chain}$. In conclusion, the two species of charge carriers, which were earlier observed experimentally, can describe the anomalies observed in the $\sigma(\omega)$ spectrum as a sharp one at $\omega = 0$, a long tail in the infrared region and a peak value centred at mid-infrared region ($\omega = 1000\ cm^{-1}$).

Acknowledgements

DV thanks the Madhya Pradesh Council of Science and Technology, Bhopal, for financial assistance.

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