The calculations of the electronic and the optical properties of CeSb and LaSb, using the full potential augmented plane wave (FP-LAPW) method including spin orbit coupling within local spin density (LSDA) approximation as implemented in WIEN2K code have been performed. The reflectivity and the real part of the optical conductivity of CeSb and LaSb have been calculated. The real part of the optical conductivity of these compounds is deduced from Kramers-Kronig transformation. The calculated spectra of the real part of the optical conductivity and reflectivity of LaSb and CeSb are in the agreement with the available experimental data. Our calculations give the value of specific heat constant of CeSb and LaSb 23.4 mJmol\(^{-1}\)K\(^{-2}\) and 0.37 mJmol\(^{-1}\)K\(^{-2}\), respectively, which are very close to experimental value.

Keywords: Rare earth compound, Optical properties, Reflectivity
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1 Introduction
The study of materials which have extremely low carrier concentration like rare earth monopnictides is gaining momentum due to the presence of some anomalous properties, e.g. metal-insulator transition, heavy fermionic behaviour, magnetic polaron, magnetic excitations. These phenomena originate from the electronic structure of the compounds due to the presence of the magnetic energy levels near the Fermi level. Optical spectra are very useful for studying these excited magnetic energy levels. The 14° Kerr rotation first discovered in CeSb by Reim et al.\(^2\) in the late eighties and the even more astonishing 90° Kerr rotation in the same compound by Pittini et al.\(^3\) ten years later evoked a lot of excitement. The occurrence of such a large magneto-optical Kerr rotation in materials that are at the borderline between well localized and itinerant f electron states also attracted much interest from the theoretical side\(^3-8\). Hence, among the cerium pnictides, CeSb is believed to be one of the most fascinating rare-earth compounds owing to its variety of anomalous electronic and magnetic properties. It shows a Kondo state in a semi metal, despite the rather simple rock salt structure and has been well studied both experimentally and theoretically. The optical conductivity and reflectivity spectra were measured at 300 K on single crystals of CeSb and LaSb by Kwon et al.\(^9\) Uspenskii et al.\(^10\) pointed out that a 90° rotation can occur only when the absorptive part of the diagonal and off-diagonal permittivities are zero. The maximum Kerr rotation can be achieved at energy with zero reflectivity. We have performed the calculations of the electronic and the optical properties of CeSb and LaSb. We present here the full potential calculations, using the standard local spin density approximation (LSDA), of the reflectivity and the real part of the optical conductivity of CeSb and LaSb, and compare these with the experimental data.

2 Computational Details
CeSb and LaSb crystallize in a simple NaCl structure (space group Fm\(_{3m}\)) with experimental lattice constant\(^11\) of 6.399 Å and 6.475 Å, respectively. The calculations have been performed by employing the full potential linearized augmented plane wave (FPLAPW) method, within LSDA, as implemented in the WIEN2K code\(^12\). In the calculations reported here, we used \(R_{MT}K_{\text{max}}=7\), which determines matrix size, where \(K_{\text{max}}\) is the plane wave cut-off and \(R_{MT}\) is the smallest of all atomic sphere radii. We used 20,000 \(k\) points in whole Brillouin zone for obtaining self consistency, and the \(k\) space integration was performed using modified tetrahedron method\(^13\). Convergence with respect to the number of \(k\) points has been thoroughly checked. For the optical properties we have used broadening of 0.1 eV to simulate experimental broadening.
3 Theory
We use the Kubo formula\(^{14}\) for the optical conductivity:

\[
\sigma_{\alpha\beta}(\omega) = \frac{e^2}{8\pi^2 \eta m^2 \omega} \sum_{nn'} \int d^3k |p_{\alpha}|^2 \\
\times \langle kn | p_{\beta} | kn' \rangle f_{kn}(1-f_{kn'}) \delta(\varepsilon_{kn} - \varepsilon_{kn'} - \eta \omega)
\]

where \(e\) is the electronic charge, \(m\) the electron mass, \(\omega\) the frequency of incoming/outgoing electromagnetic radiation, \(p\) the momentum operator, |\(kn\rangle\) the crystal wave function, corresponding to eigenvalue \(E_{kn}\), and \(f_{kn}\) is Fermi distribution function ensuring that only transitions from occupied to unoccupied state are counted.

4 Results and Discussion
Our LSDA calculations give the total magnetic moment 0.81 \(\mu_B\) of CeSb which is very close to measured value of magnetic moment of \(\Gamma_7\) ground state (\(gJ = 0.71 \mu_B\)) of CeSb. The calculations show the value of the coefficient of electronic specific heat as 23.4 \(\text{mJ mol}^{-1}\text{K}^{-2}\) for CeSb and 0.37 \(\text{mJ mol}^{-1}\text{K}^{-2}\) for LaSb is in good agreement with the experimental value of 25.0 and 1.0 \(\text{mJ mol}^{-1}\text{K}^{-2}\), respectively.

Fig. 1 shows calculated frequency-dependent reflectivity and real part of the optical conductivity spectra of CeSb and LaSb along with corresponding experimental data\(^9\). The energy is plotted on logarithmic scale because available experimental data is also on logarithmic scale. We note that the characteristic features of the calculated reflectivity and conductivity are similar for CeSb and LaSb. The slight difference at low energies is due to the presence of the f electron in CeSb for which the spin-up bands lie right at the Fermi level. The calculated reflectivity for CeSb is in fairly good agreement with experimental data with a slight shifting of the broad peak near 1 eV. The calculated reflectivity for LaSb also shows good agreement, with 1 eV structure being represented faithfully, with the experimental data (available only up to 5 eV) though with less pronounced structures. Lack of experimental data for LaSb at energies above 5 eV hampers the comparison.

We note that larger value of broadening brings the reflectivity spectrum of CeSb magnitude wise very close to the experimental curve.

The experimental spectra of optical conductivity (right panel of Fig. 1) show high value at low energies followed by fast drop and thereafter some peaks at high energies. The calculated spectra of the real part of the optical conductivity show similar trends as in the experimental data though with a slight shifting towards lower energies for CeSb. The real part of the

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**Fig. 1**—Reflectivity and real part of optical conductivity (\(\text{Re } \sigma_{xx}\)) spectra of CeSb and LaSb (Energy is plotted on logarithmic scale)
optical conductivity spectrum of CeSb shows peaks, due to the transitions from the valence band, formed by the Sb-5p states and Ce-f states, to the conduction band formed predominately by the Ce-5d states. The transitions from Sb-5p to Ce-5d are dominant in the energy range from 1 - 8 eV. In the real part of the optical conductivity spectrum of LaSb peaks arise mainly due to the transitions between Sb-5p states and La-5d.

The disagreement in the form of slight shifting of peaks (in CeSb) and magnitude wise (in both CeSb and LaSb) with respect to the experimental data can be attributed to the fact that density functional theory (DFT) is not suitable for the excited states. This shortcoming may be removed to some extent by using better approximations for exchange correlation potential in the calculations e.g by using LSDA+U or GGA+U approximations where Coulomb correlations are explicitly taken care of.

5 Conclusion

We have performed full potential calculations of the optical properties of CeSb and LaSb within LSDA. The calculated magnetic moment and coefficient of electronic specific heat are in good agreement with experimental data. The characteristic features of the optical spectra for CeSb and LaSb are quite similar, the slight difference arising out of the presence of f electron in CeSb. The calculated reflectivity and optical conductivity spectra of CeSb and LaSb are in good agreement with the experiment, with almost all the features reproduced in the calculated spectra. The features at low energies in the calculated reflectivity are less sharp as compared to the experimental curves. This discrepancy is likely to be removed to some extent with the use of better approximations for exchange and correlations. Analysis of the calculated spectra shows that the peaks arise mainly due to the transitions from Sb-p states to R-5d states.

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