functional theory (DFT), with the Local density approximation (LDA) [20] to the exchange correlation energy of electrons and ultrasoft pseudopotentials [21], to represent the interaction between ionic cores and valence electrons. Kohn-Sham wave functions have been represented with a plane wave basis with an energy cutoff of 30 Ry and charge density cutoff of 180 Ry.

Integration over Brillouin zone was sampled with the Monkhorst-Pack scheme [22] with appropriate k point mesh and occupation numbers have been smeared using Methfessel-Paxton scheme [23] with a broadening of 0.03 Ry. The structure has been relaxed to minimize energy.

III. RESULTS AND DISCUSSION

A. Structure of L-Arginine Semimalonate

In the present investigation, the Triclinic unit cell of L-arginine semimalonate was first simulated using the "Avogadro" [24]. Later, atomic positions of the molecules have been used in the plane wave self consistent field calculations. The structure has been relaxed and the optimized values of the unit cell parameters so arrived through minimization of energy are; a = *5.353 Å*, *b = 6.931 Å*, *c = 9.922 Å*, *α = 69.53°*, *β = 89.03°*, *γ = 71.12°*. "scf'" calculation was done using the final atomic positions obtained after relaxing the structure using the program 'pw.x' code of Quantum espresso.

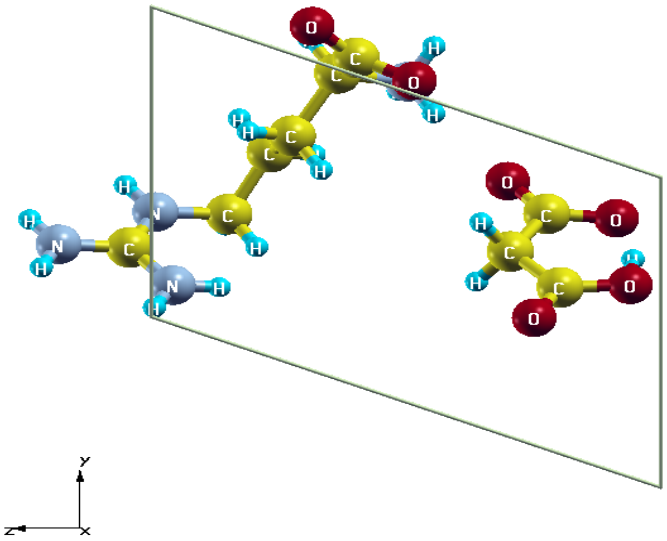

Fig. 1 Structure of the unit cell of L-arginine semimalonate as viewed along X axis

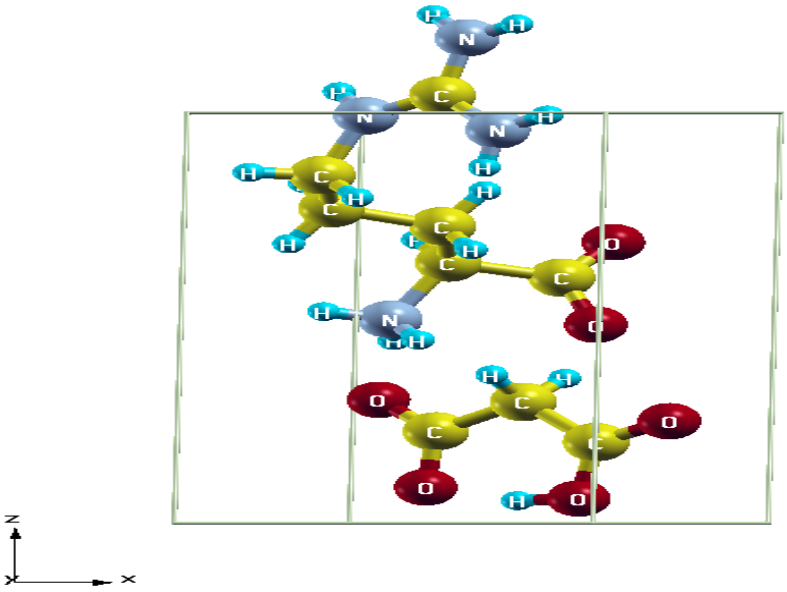

Fig. 2 Structure of the unit cell of L-arginine semimalonate as viewed along Y axis

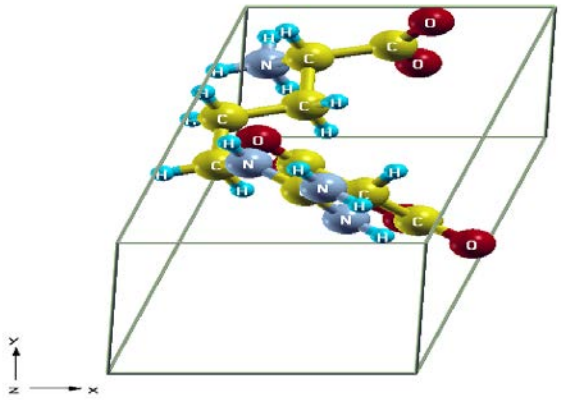

Fig. 3 Structure of the unit cell of L-arginine semimalonate as viewed along Z axis

The completely relaxed structure of the unit cell was visualized using the program "XcrysDen" [25] and the structure of L-arginine semimalonate as viewed along X, Y, and Z axes are shown in Figures 1, 2 and 3 respectively. The values of bond lengths and bond angles in the relaxed structure of L-arginine semimalonate are tabulated in tables I and II respectively.

TABLE I BOND LENGTHS IN L-ARGININE SEMIMALONATE

Bond	Bond length (Å)
C – H	1.00
C – C	1.51
C – O	1.25
N – H	1.00

TABLE II BOND ANGLES IN L-ARGININE SEMIMALONATE

Bond	Bond angle (deg)
H – N – H	120
O – C – O	124
N – C – N	119, 122
C – C – C	110 – 117

It is found that the structural parameters of L-arginine semimalonate are matching very well with the XRD studies found in the literature [26].

IV. EDOS CALCULATION

Electron Density of States (EDOS) are computed in L-arginine semimalonate using the Electronic structure calculation code of Quantum espresso. EDOS in L-arginine semimalonate has been shown in Figure 4. The band gap is found to be 2.35eV. The band gap is found to be similar to that exhibited by semiconductors and photonic band gap materials. Bang gap lies in the range of values exhibited by the Non-Linear Optical (NLO) materials [27] and the liquid crystalline materials [28]. It has been observed that several inorganic NLO materials show a band gap in the range 2eV to 4eV. For example, a band gap of 4eV has been observed in Lithium niobate. A band gap of 3.2eV has been observed in Barium titanate. BSO crystals show a value of 4.02eV and also KTN nanoparticles show a band gap of 3.26eV. An optical band gap of 3.65eV has been observed in the organic NLO material L-Tartaric acid. It is found that the tuning of the band gap plays an important role in the field of photonic crystals.

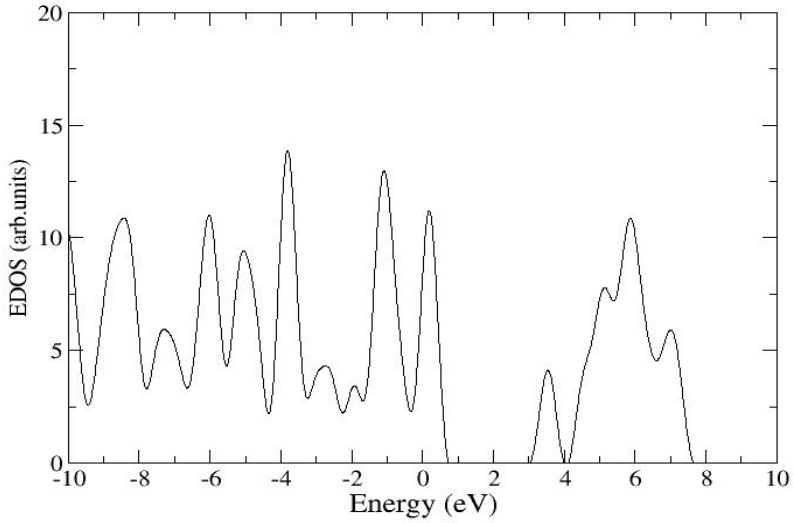

Fig. 4 Electron Density of States in L-arginine semimalonate

V. POLARIZABILITY AND PHONON MODES

The polarizability volume has also been calculated using the phcg.x code of Quantum espresso software. Its value comes out to be 77.40 $Å^3$, 77.08 $Å^3$, 76.55 $Å^3$ along X, Y and Z axes respectively with an average value of 77.01 $Å^3$. Values of phonon modes have also been computed using the ph.x program of quantum espresso software. The computed phonon modes so computed range from 0 cm^{-1} to 8012 cm^{-1}.

VI. CONCLUSION

The structure of the unit cell of L-arginine semimalonate crystal is found to be triclinic. Band gap in L-arginine semimalonate is found to be 2.35 eV. This value is close to the values exhibited by NLO materials and liquid crystalline materials. The polarizability value comes out to be 77.40 $Å^3$, 77.08 $Å^3$, 76.55 $Å^3$ along X, Y and Z axes respectively with an average value of 77.01 $Å^3$. Values of phonon modes range from 0 cm^{-1} to 8012 cm^{-1}.

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