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# Computation of Phonon Density of States, Atomic Electrostatic Potential and Electric Field Gradient Tensor Using Single Crystal Data of Six Benzene Sulfonamide Based Compounds

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**ABSTRACT**
Molecular dynamic study of benzene sulfonamide based compounds was carried out to compute several properties like phonon density of states, atomic electric potential and electric field gradient tensor components and then compared. This work establishes the correlation between physical properties and the quantity of carbon atoms in a molecule. The GULP program was used to do all the calculations and reported single crystal data.

**KEYWORDS**
GULP; benzene sulfonamide single crystals; Density of Phonon states; atomic electric potential; electric field gradient tensor

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## INTRODUCTION

Benzyl sulfonamide based compounds were the initial materials for used for curing and preventing bacterial infection in human beings [1]. They exhibit antibacterial [2,3], antifungal [4], anti-inflammatory [5], antitumor[6], anticancer [7], anti-HIV [8] and antitubercular activities [9]. Since there is a continued interest in these Benzene sulfonamide based compounds, we have carried out molecular modeling method to simulate several physical properties like phonon density of states, atomic electric potential and electric field gradient tensor of these materials using General Utility Lattice Program (GULP), freely available software. Six single crystal data of benzene sulfonamide based compounds reported earlier were used in the following investigations. [10-14]

## MATERIAL AND METHOD

Six single crystal data of benzene sulfonamide based compounds were used and they are [10-14]:
1)2,5-Dimethoxy-N-phenylbenzenesulfonamide($C_{14}H_{15}NO_4S$)(Monoclinic, $P_{21/c}$)
2)4-Bromo-N-(4-fluorophenyl)benzenesulfonamide ($C_{12}H_9BrFNO_2S$)(Orthorhombic, $P_{na}2_1$)
3) 3,5-dichloro-N-(2,3-dimethylphenyl)benzenesulfonamide ($C_{14}H_{13}Cl_2NO_2S$)(Monoclinic,$P_{21/n}$)
4) 3,5-dichloro-N-(2,6-dimethylphenyl)benzenesulfonamide ($C_{14}H_{13}Cl_2NO_2S$)(Triclinic, P1)
5) 3,5-dichloro-N-(3,5-dimethylphenyl)benzene-sulfonamide($C_{14}H_{13}Cl_2NO_2S$)(Monoclinic,$P_{21/c}$)
6)4-Bromo-N-(4-bromophenyl)benzenesulfonamide ($C_{12}H_9Br_2NO_2S$)(Monoclinic, $P_{21/n}$)

With experimental single crystal data reported earlier, we have simulated Phonon density of states, atomic electric potential and refractive index and dielectric constant of Prop-2-en-1-one based compounds [15]. For validation of the computed elastic constants in these compounds, we have referred to "Second and Higher Order Elastic Constants" by A. G. Every, A. K. McCurdy (auth.), D. F. Nelson (eds.) [16].

The phonon density of states for a solid as the number of frequencies against frequency value becomes a continuous function when integrated across the Brillouin zone.For carrying out these integrations, GULP employs a standard scheme method [17-19] for selecting grid points. We have employed this procedure to compute the phonon density of states for all the six compounds.

**Atomic electrostatic site potential and electric field gradient tensor**

The Coulombic interaction per unit charge experienced by an ion at a given position in space is measured by atomic electrostatic site potential.For this purpose, we have used Buckingham potential $U(r) = Ae^{-r/\rho} - C/r^6 + q_i q j e^2/r_{ij}$.The optimization of the lattice energy results in the components of the electric field gradient tensor.

## RESULTS

There are six compounds, out of which, 3,4 and 5 compounds have the same composition, but different chemical and crystal structure as reported.

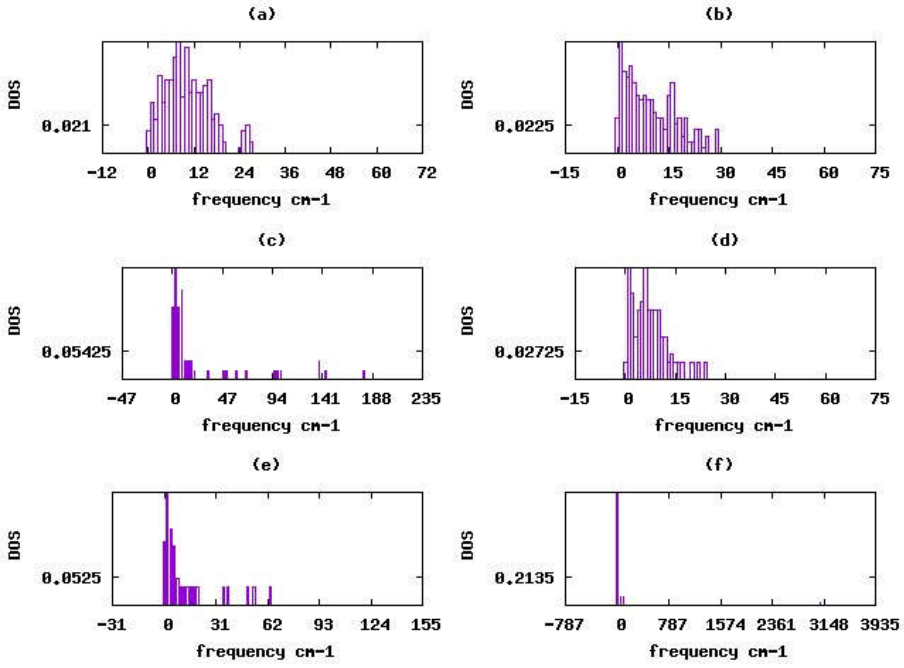


**Figure 1:** Variation of density of phonon states with frequency (a) compd.1 (b) compd.2 (c) compd.3 (d) compd.4 (e) compd.5 and (f) compd.6

**Table 1:** Phonon properties per mole of unit cells at T=300K

| **Sl. No.** | **Compd.1** | **Compd.2** | **Compd.3** | **Compd.4** | **Compd.5** | **Compd.6** |
|---|---|---|---|---|---|---|
| Zero point energy(eV) | 0.158 | 0.134 | 0.189 | 0.059 | 0.085 | 0.512 |
| Entropy(eV/K) | 0.083 | 0.076 | 0.037 | 0.045 | 0.042 | 0.029 |
| Helmholtz free energy(eV) | -23.5 | -28.7 | -10.3 | -12.3 | -13.2 | -6.7 |
| Heat capacity at constant volume(eV/K) | 0.021 | 0.017 | 0.009 | 0.010 | 0.010 | 0.007 |

Figure 1 shows the variation of density of phonons with frequency in all six compounds. We have made a comparison phonon property (per mole of unit cells) at Temperature 300K in Table 1.

In Figure 2 we have compared the atomic site potential of all the six compounds and Table 2 highlights the properties of atomic potential computed. This potential represents the coulomb interaction per unit charge experienced by an ion at a given location in space. Electronegativity of all compounds are approximately same whereas self-energy varies from -1.33 to -10.14 eV.

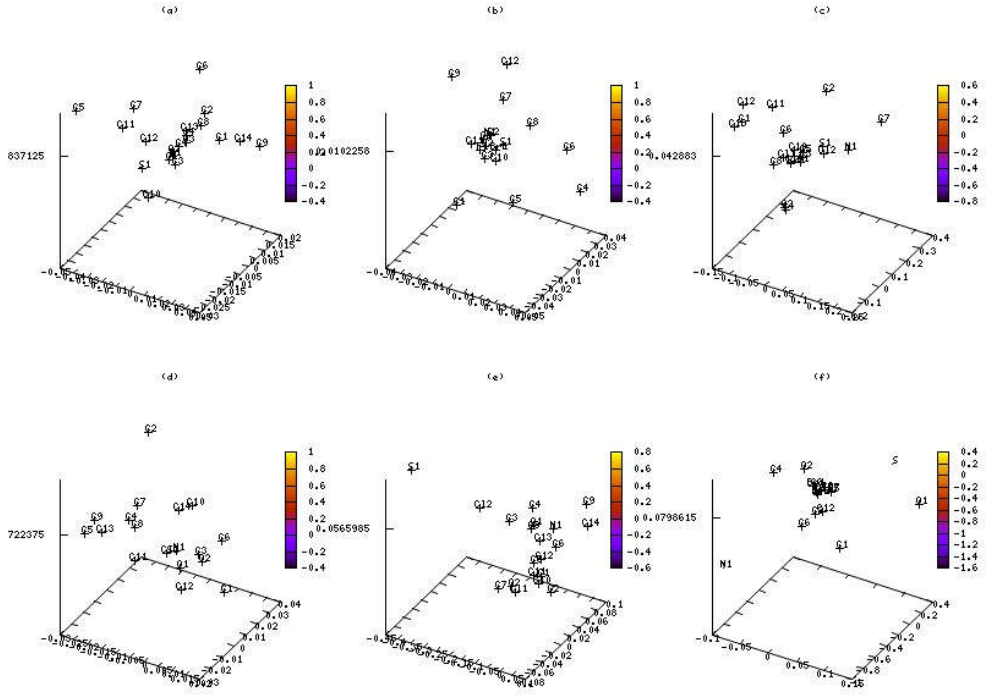

**Figure 2:** Atomic site electric potential of all compounds (a) compd.1 (b) compd.2 (c) compd.3 (d) compd.4 (e) compd.5 and (f) compd.6

T**able 2: Properties of atomic site potential**

| Sl. No. | Compd.1 | Compd.2 | Compd.3 | Compd.4 | Compd.5 | Compd.6 |
|---|---|---|---|---|---|---|
| Electronegativity (eV) | 6.31 | 6.29 | 6.23 | 6.13 | 6.27 | 6.07 |
| Self energy(eV) | -3.43 | -10.14 | -2.71 | -1.33 | -2.39 | -2.49 |

In Figure 3 we have compared the electric field gradients (EFG) at atomic positions of all the six components. Here x-axis refers to 0: xx, 1:xy, 2:yy, 3:xz, 4:yz, 5:zz and y axis refers atoms. For example in Figure 3(a) along y-axis, 0-13 refers to carbon atoms present in the molecule. Figures 2 and 3 do represent the structural optimisation of the lattice energy. Further even though the compounds 3, 4 and 5 have same number of atomic constituents, the higher Vzz component is found in compound 3 and lowest in compound 4. Here we have given a method to quantify the changes in the crystal structure in terms of EFG tensor components.

In Figure 3 EFG is different in each of the six specimens and the presence of heavy elements changes the nature of interatomic interactions. Compds 3,4 and 5 are important since they have same and similar number of atoms but chemical and crystal structures are different. EFG variations in these three compounds are quiet significant which shows that there are different lattice energy minimizations even though one has same molecular weight.

Further, for a better understanding the variations of these tensor components we have plotted higher value diagonalised zz-component of EFG tensor corresponding to the appropriate atom with the volume of the unit cell and we find an interesting result that Nitrogen atom with a reasonably higher volume has higher value.

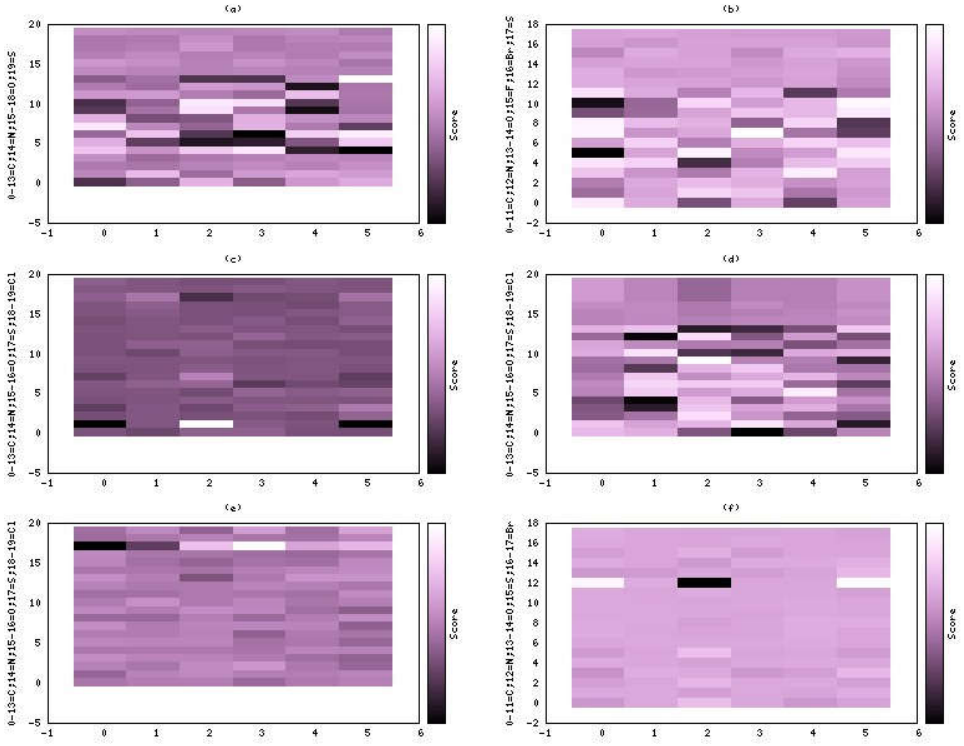


**Figure 3:** Electric field gradients (EFG) at each atomic positions in sulfonamide compounds based on single crystal data. (a) compd.1 (b)compd.2 (c)compd.3 (d) compd.4 (e) compd.5 and (f) compd.6

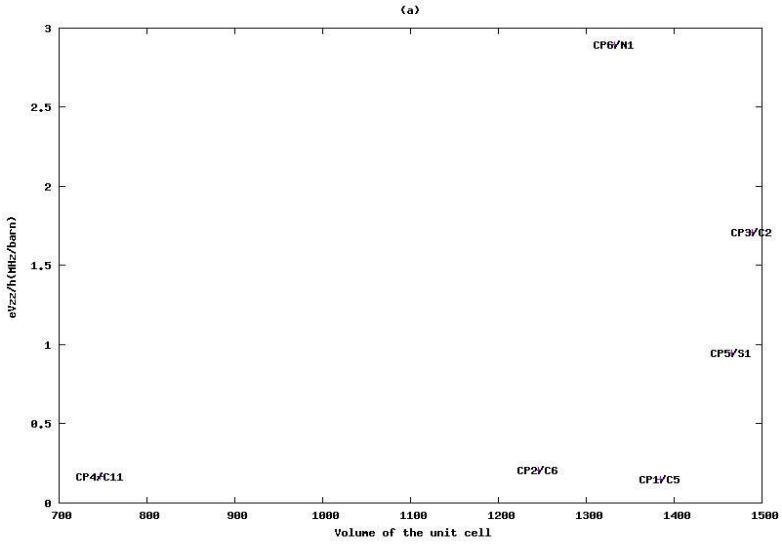


**Figure 4:** Diagonalised zz component of EFG tensor of all six compounds with unit cell volume.(exmaple CP4/C11 refer to compound 4 and carbon atom number 11 in the structure)

## CONCLUSIONS

Using reported single crystal structure data for sulfonamide based compounds, we have computed density of phonon state, atomic site electric potential and electric field gradients at each atomic positions. For lower frequencies, the computed phonon density of states is maximum for compound six and minimum for compound two. This is due to the influence of the functional groups. The variation in electrostatic potential values at atomic positions in these six compounds indicates the sites of molecular interactions with the surroundings. The ESP is a useful tool for studying molecular reactivity in industrial research. In sulfonamide-based compounds, there is a clear representation of EFG for each atomic position, bringing out the atomic interactions in different environments. Figure 4 shows a correlation between one of the predicted physical parameters and molecular weight.

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