X-ray structure, hirshfeld surfaces and interaction energy studies of 2,2-diphenyl-1-oxa-3-oxonia-2-boratanaphthalene

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GRAPHICAL ABSTRACT

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ABSTRACT

Single crystal XRD structure of the title compound reveals that the molecule adopt non-planar structure. The molecule is puckered with the total puckering amplitude of (Q) = 0.368(3)Å. Crystals of the title molecules are interconnected by intermolecular O–H⋯O and C–H⋯O interactions to develop 1D chains extending infinitely along the crystallographic a-axis. The intermolecular interactions were explored by Hirshfeld surfaces and their associated fingerprint graphs are obtained which revealed that the H⋯H and H⋯C pairs of inter atomic contacts were pre-dominant in the crystal packing of title compound. The energy of intermolecular interactions are computed using the accurate energy density model of B3LYP/6-31 G(d,p).

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Speciation Table

| Subject area          | X-ray crystallography |
|-----------------------|-----------------------|
| Compound              | 2,2-Diphenyl-1-oxa-3-oxonia-2-boratanaphthalene |
| Data category         | Crystallographic data |
| Data acquisition      | CIF                   |
| Data type             | Analyzed              |
| Procedure             | Crystal structure determination, interpretation and computational analysis |
| Data accessibility    | CCDC: 2064704         |

1. Introduction

Boron fused tri- and tetra-coordinated molecules have found great importance for multifunctional applications such as OLEDs, bio-imaging etc. due to their wide window of electronic properties. Some of the tetra-coordinated boron chelated N, O structures have found to be highly emissive in solid state with colour tunability due to their rigid π-conjugated structures [1, 2]. Crystal structure and molecular packing play major role in the light emissive devices wherein weak π--π interactions greatly helps for enhanced emission [3]. Hence understanding the density wavefunction of B3LYP/6-31G(d,p). With respect to all the above perspectives and in continuation of our ongoing work on structural studies, we now report the structural and Hirshfeld surface studies of the compound 2,2-diphenyl-1-oxa-3-oxonia-2-boratanaphthalene.

2. Procedures

2.1. Experimental

2,2-Diphenyl-1-oxa-3-oxonia-2-boratanaphthalene was synthesized according to the reported procedure [7]. 2-(diphenylboryl)ethanamine (100 mg, 0.96 mmol) was refluxed with 2-hydroxybenzaldehyde (100µl, 0.96 mmol) in 5 ml methanol for 4 h to obtain cream colour solid with 90% yield (Figure 1). Single crystals were grown in ethanol using slow evaporation method.

2.2. Single crystal XRD

The structural and refinement details of the title compound are given in Table 1. A suitable size of block shaped single crystal was selected carefully for X-ray diffraction study. The diffraction data were collected on an Apex Bruker-II diffractometer equipped with MoKa radiation of wavelength 0.71073Å. Complete X-ray intensity data set was processed by SAINT software [8]. The crystal and molecular structure was solved by direct method using SHELXS and refined by full-matrix least squares based on F² SHEXL [9, 10, 11]. All the non-hydrogen atoms were refined anisotropically while the hydrogen atoms were refined isotropically and placed at chemically ideal positions with isotropic displacement parameters as C–H = 0.93Å with Uiso(H) = 1.2Ueq(C) for aromatic rings and O–H = 0.82Å with Uiso(H) = 1.5Ueq(O). The molecular and packing diagram were generated using the MERCURY [12] while PLATON software was used to obtain geometric parameters viz., bond distances, inter-bond angles and torsional angles [13, 14].

Table 1. Crystal, structural and refinement statistics.

| CCDC       | 2064704 |
|------------|---------|
| Chemical formula | C21H19BNO2 |
| Mr         | 328.18  |
| Crystal system, space group | Monoclinic, P21/n |
| Temperature (K) | 290 |
| a, b, c, β (Å⁻¹) | 9.1024(6), 17.8682(15), 10.9790(9), 96.933(2) |
| V (Å⁻³), Z | 1772.62(6), 4 |
| Radiation type | MoKa |
| μ (mm⁻¹) | 0.08 |
| Crystal size (mm) | 0.40 × 0.36 × 0.31 |
| Diffractometer | APEX (Bruker, 2006) |
| No. of measured, independent and observed reflections | 22044, 3649, 1990 |
| R(int) | 0.05 |
| (sin Θ/λ)max (Å⁻¹) | 0.627 |
| Goodness-of-Fit (S) | 1.048 |
| R1(P² > 2σ(P²)), wR2(P²), S | 0.0632, 0.2065, 1.048 |
| No. of reflections | 3649 |
| No. of parameters | 226 |
| Data/Restraints/Parameters | 3649/0/226 |
| H-atom treatment | H-atoms treated by a mixture of independent and constrained refinement |
| Δρmax, Δρmin (eÅ⁻³) | 0.55, -0.34 |
| Index ranges | h = -11→10, k = -22→22, l = -13→13 |
| Theta range (°) | Θmax = 25.2, Θmin = 2.2 |

Figure 1. Schematic diagram of the compound 2,2-diphenyl-1-oxa-3-oxonia-2-boratanaphthalene.
2.3. Computational studies

Three dimensional Hirshfeld surfaces (3D-HS) mapped on both $d_{\text{norm}}$ and electrostatic potentials (ESP), and their associated two dimensional fingerprint graphs are carried out making use of Crystal Explorer 17.5 software and to compute three dimensional interaction energies [15, 16, 17, 18, 19, 20].

3. Results and discussions

3.1. Structural commentary

The molecular structure of the title compound consists of a ten-membered heterocyclic ring [O1–B1–N1–C1/C7] and two phenyl rings [C10/C15] and [C16/C21] which are interlinked such that to have a non-coplanar view, and an -ethoxy group in an extended conformation as given in thermal ellipsoids drawn at 50% probability (Figure 2). The ten-membered ring [O1–B1–N1–C1/C7] displayed a puckering environment at B1 with the total puckering amplitude (Q) of $0.368$ Å and displayed a half-chair conformation. The pseudorotation ($\theta$) and the relative phase ($\phi$) angles are $114.0(3)$$^\circ$ and $136.6(4)$$^\circ$ respectively [21, 22].

In the molecule, the mean planes of phenyl rings [(C10/C15) and (C16/C21)] are inclined with the dihedral angle of $77.05(1)$$^\circ$. The central ten-membered ring (O1–B1–N1–C1/C7) makes the dihedral angle of $85.65(12)$$^\circ$ and $87.55(1)$$^\circ$ with the mean planes of phenyl rings (C10/C15) and (C16/C21) respectively, which reveals that the rings exhibit nearly an orthogonal relation to each other. The chain, N1–C8–C9–O2 adopts a -syn-clinal conformation with the torsional angle of $-75.27$$^\circ$. The bond lengths and inter-bond angle values agree with the standard values [23, 24, 25, 26, 27, 28, 29].

3.1.1. Crystal packing

The crystal of the titled molecule are governed by an intermolecular O2–H2⋯O1 and C14–H14⋯O2 interactions (Table 2), to develop an independent 1D polymeric chains propagating indefinitely along crystallographic $a$-axis, as depicted in Figure 3. In addition to this, the titled molecule also comprise an intra-molecular C7–H7⋯O2 interaction, incorporating a self-assembly closed S(6) loop.

3.2. Computational analysis

The volume of 3D-HS mapped on $d_{\text{norm}}$ (Figure 4) and electrostatic potential (Figure 5) are $369.88$ Å$^2$ and $435.97$ Å$^3$ respectively, with the colour scales of $[-0.5324$ a.u. (red) and $+1.4509$ a.u. (blue)], and $[-0.1112$ a.u. (red) and $+0.1478$ a.u. (blue)] respectively. The surfaces are given in transparent mode to understand the position of all the elements and the functional groups available in the molecule. The $d_{\text{norm}}$ furnishes both the donor and acceptor regions of hydrogen bonding interactions by forming red colour circular spots on its surface with equal brightness.

For instance, the donor and acceptor regions of intermolecular O2–H2⋯O1 interaction can be viewed on the front and rear views of $d_{\text{norm}}$ surfaces, given in Figures 4 a and b respectively. In Figure 4a the red spot surrounding O2–H2 and at the vicinity of O1 in Figure 4b are the indicators of donor and acceptor regions of O2–H2⋯O1 interaction (Table 2) [30, 31, 32, 33]. This is also substantiated by electrostatic

| Interaction      | D-H⋯A | d(H⋯A) | d(D⋯A) | Angle (D-H⋯A) | Symmetry code |
|------------------|-------|--------|--------|---------------|---------------|
| Intra-molecular  | C7–H7–O2 | 2.30   | 2.970(4) | 129           |               |
| Intermolecular   | O2–H2–O1  | 2.08   | 2.900(3) | 176           | $-1/2+x,1/2+y,1/2-z$ |
|                  | C14–H14–O2 | 2.52   | 3.363(4) | 152           | $1+x,y,z$     |

Figure 2. Thermal ellipsoids of a title molecule at 50% of probability.

Table 2. Hydrogen bonding geometry (Å$^\circ$).

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potentials (Fig. 5a and b are front and rear views) by reflecting intense blue coloured patch around O2–H2, while the red coloured patch around O1 represents the electrostatic positive donor and negative acceptor potentials respectively. These electrostatic interactions serve as an important tool in the binding of protein targets [34].

The two-dimensional fingerprint graphs were generated in an expanded mode for all the major contacts, and it is delineated in Figure 6.

Total contribution from all the pairs of inter atomic contacts is given in Figure 6(a). The highest contribution is represented by a pair of H⋯H inter atomic contacts with 60.9%, reflected as a pair of blue coloured spoke like pattern, merged almost in the middle of the graph at de + di = 1.1 Å Figure 6(b). The 29.9% of contribution was made to the Hirshfeld surface from H⋯C pair of inter atomic contacts producing a pair of unique blue coloured wings between the region of 1.12 Å < (de + di) < 1.72 Å Figure 6(c). The pair of H⋯O inter atomic contacts represents only 7.9% of total contribution which is emerged as a characteristic sharp spikes over the region of 0.79 Å < (de + di) < 1.18 Å Figure 6(d). Presence of H⋯O and H⋯C contacts correlates with the intermolecular interactions given in Table 2. Lastly, the C⋯C inter atomic contacts comprise only 2.2% to the crystal packing which is observed as an arrowhead pattern in the region of de + di ≈ 1.70 Å pointing diagonally left downwards Figure 6(e). Overall study of fingerprint graphs reveals that the pair of H⋯H and H⋯C inter atomic contacts are the predominant ones. While H⋯O and C⋯C contacts are less significant in the formation of a three dimensional Hirshfeld surface.

Three-dimensional interaction energies were computed for the title compound using the CrystalExplorer17.5 software [35, 36]. Interaction energy was calculated using an accurate energy density model of B3LYP/6-31G(d,p), during the calculation a cluster of seventeen molecules (comprising a total of 748 atoms) of various colour coding scheme from different Cartesian co-ordinates were surrounding the original one (showed by black coloured ball and stick model) within the default radius of 3.8 Å. The total interaction energy (E_{tot}) in the energy framework have been classified into classic electrostatic (E_{ele}), polarization (E_{pol}), dispersion (E_{dis}) and exchange repulsion (E_{rep}) energies [37].

Further, in the generation of electrostatic, dispersion and total energy frameworks, the tube size of 50 and threshold cut-off energy level of 10 kJ/mol were maintained. The Coloumbic (E_{ele}) energy terms are represented by red coloured solid cylinders (Figure 7), and green coloured solid cylinders in the construction of dispersion energy (E_{dis}) frameworks given in Figure 8. The total energy (E_{tot}) terms are constructed by using the blue coloured solid cylinders (Figure 9). In each of the energy profile the difference in thickness of solid cylinders reveals the relative strength of interaction with the constituent members of a cluster [38, 39], and plays an important role in the integrity of a crystal packing. Also, the red- and orange-coloured dashed lines in all the energy profiles reveal the molecules involved in the hydrogen bonding interactions given in Table 2. The total interacting energies in the cluster of title compound are given in component form (Table 3). Accordingly, the highest total interaction energy (E_{tot} = -67.6 kJ/mol from all the components) was noticed with a pair of symmetric pale-green coloured molecules interacting at the centroid distance of R = 7.76 Å which correlates with the intermolecular O2-H2⋯O1 interaction. The total interaction energy
(\(E_{\text{tot}} = -18.2\ \text{kJ/mol}\)) associated with an intermolecular C14–H14⋯O2 interaction confirms with the red coloured molecules at the centroid distance of \(R = 9.10\AA\). The least total interaction energy was observed as \(E_{\text{tot}} = -1.8\ \text{kJ/mol}\) associated with a couple of pink coloured molecules having the longest molecular centroid distance of \(R = 13.14\AA\). Further, the total energy from all the components in a cluster, the dispersion energy (\(E_{\text{dis}}\)) terms were dominated over the other terms as observed in the reported compounds \([40, 41, 42]\). Further, the total interaction energies are varying with the molecular centroid distances obeying the laws of electrostatics.

### 4. Conclusion

The title compound is crystallized in a monoclinic system with P21/n space group. The molecular structure of the compound was puckered at B1 and adopts half-chair conformation. The packing of molecules were governed by intra- and intermolecular C–H⋯O and O–H⋯O interactions and, they are explored by three dimensional Hirshfeld surfaces and fingerprint calculations, revealing that the H⋯H and H⋯C pairs of inter atomic contacts have made the significant contribution towards the formation of three dimensional...
Hirshfeld surfaces. The interaction energy calculations reveal -67.6 kJ/mol is the highest total interaction energy (from all the components) associated with an intermolecular O2–H⋯O1 interaction. Further, in the energy frameworks, in each case the dispersion energy $E_{\text{dis}}$ term dominated over other components obeying laws of electrostatics.

**Figure 7.** Three-dimensional interaction energy profile for Coulombic ($E_{\text{ele}}$) terms generated with the tube size of 50 and cut-off energy of 10 kJ/mol for clarity purpose.

**Figure 8.** Three-dimensional interaction energy profile for dispersion ($E_{\text{dis}}$) terms generated with the tube size of 50 and cut-off energy of 10 kJ/mol for clarity purpose.
Table 3. Three-dimensional interaction energies (kJ/mol) in component form for the title compound for electron density B3LYP/6-31G(d,p). Colour code: Colour coding scheme of molecules, N: Number of interacting molecules with the reference one, Symop: Rotational symmetry operator, R: Molecular centroid distance. Scale factor: 

\[ E_{\text{tot}} = k_{\text{el}} x E_{\text{el}} + k_{\text{pol}} x E_{\text{pol}} + k_{\text{dis}} x E_{\text{dis}} + k_{\text{rep}} x E_{\text{rep}} \]

Mackenzie et al. [43].

| Colour code | N | Symop     | R       | \( E_{\text{el}} \) | \( E_{\text{pol}} \) | \( E_{\text{dis}} \) | \( E_{\text{rep}} \) | \( E_{\text{tot}} \) |
|-------------|---|-----------|---------|---------------------|---------------------|---------------------|---------------------|---------------------|
| Red         | 2 | \( x, y, z \) | 9.10    | -8.1                | -1.7                | -19.4               | 13.7                | -18.2               |
| Red         | 1 | \(-x, -y, -z\) | 8.40    | -14.1               | -3.6                | -51.8               | 35.7                | -40.7               |
| Green       | 2 | \( x+1/2, -y+1/2, z+1/2 \) | 6.94    | 0.2                 | -2.9                | -42.4               | 18.2                | -27.5               |
| Green       | 2 | \( x+1/2, 0, z+1/2 \) | 7.76    | -46.6               | -15.6               | -44.3               | 51.5                | -67.6               |
| Green       | 2 | \(-x+1/2, y+1/2, -z+1/2 \) | 11.41   | -1.8                | -0.3                | -8.6                | 5.9                 | -6.0                |
| Green       | 2 | \(-x+1/2, y+1/2, -z+1/2 \) | 9.75    | -2.4                | -0.6                | -8.4                | 1.3                 | -9.5                |
| Green       | 1 | \(-x, -y, -z\) | 8.79    | -0.9                | -0.7                | -18.6               | 7.8                 | -12.9               |
| Green       | 1 | \(-x, -y, -z\) | 12.28   | -0.7                | -0.1                | -4.8                | 1.6                 | -4.0                |
| Green       | 1 | \(-x, -y, -z\) | 11.93   | -0.9                | -0.4                | -8.4                | 2.8                 | -6.8                |
| Green       | 2 | \(-x+1/2, y+1/2, -z+1/2 \) | 13.14   | 0.1                 | -0.1                | -2.4                | 0.2                 | -1.8                |

Figure 9. Three-dimensional interaction energy profile for total energy (\( E_{\text{tot}} \)) terms generated with the tube size of 50 and cut-off energy of 10 kJ/mol for clarity purpose.

Table 3. Three-dimensional interaction energies (kJ/mol) in component form for the title compound for electron density B3LYP/6-31G(d,p). Colour code: Colour coding scheme of molecules, N: Number of interacting molecules with the reference one, Symop: Rotational symmetry operator, R: Molecular centroid distance. Scale factor: 

\[ E_{\text{tot}} = k_{\text{el}} x E_{\text{el}} + k_{\text{pol}} x E_{\text{pol}} + k_{\text{dis}} x E_{\text{dis}} + k_{\text{rep}} x E_{\text{rep}} \]

Mackenzie et al. [43].

| Colour code | N | Symop     | R       | \( E_{\text{el}} \) | \( E_{\text{pol}} \) | \( E_{\text{dis}} \) | \( E_{\text{rep}} \) | \( E_{\text{tot}} \) |
|-------------|---|-----------|---------|---------------------|---------------------|---------------------|---------------------|---------------------|
| Red         | 2 | \( x, y, z \) | 9.10    | -8.1                | -1.7                | -19.4               | 13.7                | -18.2               |
| Red         | 1 | \(-x, -y, -z\) | 8.40    | -14.1               | -3.6                | -51.8               | 35.7                | -40.7               |
| Green       | 2 | \( x+1/2, -y+1/2, z+1/2 \) | 6.94    | 0.2                 | -2.9                | -42.4               | 18.2                | -27.5               |
| Green       | 2 | \( x+1/2, 0, z+1/2 \) | 7.76    | -46.6               | -15.6               | -44.3               | 51.5                | -67.6               |
| Green       | 2 | \(-x+1/2, y+1/2, -z+1/2 \) | 11.41   | -1.8                | -0.3                | -8.6                | 5.9                 | -6.0                |
| Green       | 2 | \(-x+1/2, y+1/2, -z+1/2 \) | 9.75    | -2.4                | -0.6                | -8.4                | 1.3                 | -9.5                |
| Green       | 1 | \(-x, -y, -z\) | 8.79    | -0.9                | -0.7                | -18.6               | 7.8                 | -12.9               |
| Green       | 1 | \(-x, -y, -z\) | 12.28   | -0.7                | -0.1                | -4.8                | 1.6                 | -4.0                |
| Green       | 1 | \(-x, -y, -z\) | 11.93   | -0.9                | -0.4                | -8.4                | 2.8                 | -6.8                |
| Green       | 2 | \(-x+1/2, y+1/2, -z+1/2 \) | 13.14   | 0.1                 | -0.1                | -2.4                | 0.2                 | -1.8                |

Declarations

Author contribution statement

N. R. Sreenatha: Analyzed and interpreted the data; Wrote the paper.
D. P. Ganesha: Contributed reagents, materials, analysis tools or data.
A. S. Jeevan Chakravarthy, B. N. Lakshminarayana: Conceived and designed the experiments.
B Suchithra: Performed the experiments.

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Data availability statement

Data associated with this study has been deposited at CCDC under the accession number 2064704.
Declaration of interests statement

The authors declare no conflict of interest.

Additional information

No additional information is available for this paper.

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References

[1] D. Li, H. Zhang, C. Wang, S. Huang, J. Guo, Y. Wang, Construction of full-color tunable and strongly emissive materials by functionalizing a boron-chelate four-fingertipped t-conjugated core, J. Mater. Chem. C 22 (2013) 4319-4328.
[2] V. Khausta, K. Kanathi, H. Takai, K. Funahiki, M. Matsui, Strategy to enhance solid-state fluorescence and aggregation-induced emission enhancement effect in pyrimidine boron complexes, Dalton Trans. 44 (2015) 3326-3341.
[3] S. Feng, S. Gong, G. Feng, Aggregation-induced emission and solid fluorescence of fluororest derivatives, Chem. Commun. 56 (2020) 2531-2534.
[4] S.A. Patel, T. Rajale, E. O'Brien, D.J. Burkhardt, J.K. Nelson, B. Twamley, A. Blumenfeld, M.I. Szabo-Watola, J.M. Gerdes, R.J. Bridges, N.R. Natale, Isoaxole analogs bind the system Y-transporter: structure–activity relationship and pharmacophore model, Bioorg. Med. Chem. 18 (2010) 202-215.
[5] N.M. Silva, J.L.M. Tributino, A.L.P. Miranda, E.J. Barrerio Carlos, F.M. Fraga, New fluorescent derivatization for high-performance liquid chromatography with 2,2'-diphenyl-1-oxa-3-oxa-2-borostannaphlene (DOOB): determination of aminoalkanols, Z. für Anal. Chem. 322 (1985) 343.
[6] D.P. Ganesha, N.R. Sreenatha, B.N. Lakshminarayana, D. P. Ganesha, G.R. Ganendra, S. Nagaraju, S. Madan Kumar, Structural and Hirshfeld surfaces of triphosphine based isoaxazole derivatives: 3-(N-Methylthiophenyl-2-yl)-5,3-(4,5-trimethoxy)isoaxazole and 5-(3-Methylthiophenyl-2-yl)-5,3-(4,5-trimethoxy)isoaxazole, Chem. Data Collect. 17 (2018) 394-403.
[7] N.R. Sreenatha, B.N. Lakshminarayana, D.P. Ganesha, G.R. Ganendra, S. Nagaraju, S. Madan Kumar, Structural and Hirshfeld surfaces of triphosphine based isoaxazole derivatives: 3-(N-Methylthiophenyl-2-yl)-5,3-(4,5-trimethoxy)isoaxazole and 5-(3-Methylthiophenyl-2-yl)-5,3-(4,5-trimethoxy)isoaxazole, Chem. Data Collect. 17 (2018) 394-403.
[8] D.P. Ganesha, N.R. Sreenatha, B.N. Lakshminarayana, D.P. Ganesha, G.R. Ganendra, Crystal structure and Hirshfeld surface analysis of (E)-1-(3,5-dichloro-2-hydroxy-phenyl)-3-0-methyl furan-2-ylprop-2-yl-1-one, Acta Crystallogr. E74 (2018) 1451-1454.
[9] Said Daoiu, Eminne Berrin Cinar, Necmi Dege, Tilik Chiefed, Foud El Kalai, Abdulmalk Abudanina, Khalid Karrouchi, Noureddine Benchat, Cine Millay Bayedere, Necmi Dege, Crystal structure and Hirshfeld surface analysis of 4-(4-methyl-benz-yl)-6-(phenyl-pyridazin-3(2H)-one), Acta Crystallogr. E75 (2019) 1352-1356.
[10] S. Hariprasad, Structural, Computational and 3D Interaction Energy Calculations of (E)-4-methyl-2-(4-aryl-pyrazin-2-yl)benzene-1-Sulfonamide organic compound, Mater. Today Proc. 823 (2020) 823.
[11] S. Hariprasad, D.P. Ganesha, Crystal, spectral characterization, molecular docking, and Hirshfeld surface studies and computation of interaction energies of 4-Amino-N-(3-chloropyrazin-2-yl)benzene-1-Sulfonamide organic compound, Mater. Today Proc. 823 (2020) 823.
[12] S. Hariprasad, D.P. Ganesha, Crystal, spectral characterization, molecular docking, and Hirshfeld surface studies and computation of interaction energies of 4-Amino-N-(3-chloropyrazin-2-yl)benzene-1-Sulfonamide organic compound, Mater. Today Proc. 823 (2020) 823.
[13] S. Hariprasad, D.P. Ganesha, Crystal, spectral characterization, molecular docking, and Hirshfeld surface studies and computation of interaction energies of 4-Amino-N-(3-chloropyrazin-2-yl)benzene-1-Sulfonamide organic compound, Mater. Today Proc. 823 (2020) 823.
[14] S. Hariprasad, D.P. Ganesha, Crystal, spectral characterization, molecular docking, and Hirshfeld surface studies and computation of interaction energies of 4-Amino-N-(3-chloropyrazin-2-yl)benzene-1-Sulfonamide organic compound, Mater. Today Proc. 823 (2020) 823.
[15] S. Hariprasad, D.P. Ganesha, Crystal, spectral characterization, molecular docking, and Hirshfeld surface studies and computation of interaction energies of 4-Amino-N-(3-chloropyrazin-2-yl)benzene-1-Sulfonamide organic compound, Mater. Today Proc. 823 (2020) 823.
[16] S. Hariprasad, D.P. Ganesha, Crystal, spectral characterization, molecular docking, and Hirshfeld surface studies and computation of interaction energies of 4-Amino-N-(3-chloropyrazin-2-yl)benzene-1-Sulfonamide organic compound, Mater. Today Proc. 823 (2020) 823.
[17] S. Hariprasad, D.P. Ganesha, Crystal, spectral characterization, molecular docking, and Hirshfeld surface studies and computation of interaction energies of 4-Amino-N-(3-chloropyrazin-2-yl)benzene-1-Sulfonamide organic compound, Mater. Today Proc. 823 (2020) 823.