Vibrational investigation on pharmaceutical activity of m-xylene-4-sulphonic acid by quantum computational and experimental support

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ABSTRACT
Detailed physical, chemical, thermal and circular vibrational investigations have been made on FT-IR, FT-Raman, NMR and UV–Visible spectra of m-xylene-4-sulphonic acid. The modification of the basic property of the base compound favoured by the asymmetric orientation of the charge levels among the atoms of the compound has been discussed in detail. The transitional pattern among the natural bond orbitals emphasized the inducement of the antibacterial and antifungal activity in the compound. Strong interpretations of the physical and chemical properties by intense observation using excitations between the electronic energy levels within the molecule have been carried out. The arrangement of the dipole moment of the bonds and the change of the resultant magnetic moment were observed from the average polarizability first-order diagonal hyperpolarizability. The receptor and inhibition property of the molecule were interpreted by the identification of reactive sites from the molecular electrostatic potential contour map. The chemical reaction continuity is keenly observed from thermodynamic analysis.

1. Introduction
m-Xylene-4-sulphonic acid is an organo-sulphur compound also called dimethylbenzene sulphonic acid. This is the simplest aromatic sulphonic acid which is a combination of dimethyl benzene and sulphonic acid. Sulphonic acid is from an important group of compounds in medicinal and pharmaceutical chemistry with several biological applications [1–4]. Basically, when sulphonic groups are adopted with the benzene ring, the pharmaceutical potential is induced in the compound. Apart from that, if benzene sulphonic acid is associated with dimethyl groups, the antibacterial and antifungal activity will be induced in the compound. Some chemotherapeutically important sulpha drugs are supported by SO2OH moiety which is an important toxophoric function [5]. Benzene sulphonic acid is also used as an acidic catalyst in esterification and dehydration reactions and its groups can be bound to the surface of inert support materials to form solid acid catalysts [6]. Sulphonic acids with methyl groups are often used during manufacture of pharmaceuticals [7].

Usually, the structure activity of the base compound is altered with respect to the substitutional groups. Here, the base is benzene sulphonic acid and substitutional group is a couple of methyl groups. According to the structure activity, the benzene sulphonic acid has antifungal properties and after the substitution of methyl groups, the structure activity is found to be enhanced and the compound obtains antibacterial and antifungal properties. In this work, the structure activity related to the above-mentioned groups has been investigated by examining the IR, Raman, NMR and UV–Visible spectra along with the theoretical interpretation.

2. Experimental profile
The compound m-xylene-4-sulphonic acid is purchased from Sigma–Aldrich Chemicals, USA, which is of spectroscopic grade and hence used for recording the spectra as such without any further purification.

- The FT-IR spectrum of the compound was recorded using a Bruker IFS 66 V spectrometer with different scanning [8].
- The FT-Raman spectrum of the same compound was also recorded using the same instrument with an FRA 106 Raman module equipped with an Nd:YAG laser source operating at 1.064 µm line widths with 200 mW power.
- The high-resolution 1HNMR and 13CNMR spectra were recorded using 300 and 75 MHz NMR spectrometer [9].
- The UV–Vis spectra were recorded in the liquid phase dissolved in methanol solvent in the range
of 200–800 nm, with the scanning interval of 0.2 nm, using the UV-1700 series instrument.

3. Computational profile

In theoretical part, the entire quantum chemical computations were performed using the Gaussian 09 D. 01 version software program in a core i7 computer [10]. The wave numbers and geometrical parameters were computed at the optimized geometry which was found after performing a scan. The desirable properties related with electronic spectra; natural bond orbital (NBO) and high occupied molecular orbitals (HOMO)–low unoccupied molecular orbitals (LUMO) were calculated using the time-dependent SCF method with best fit basis set. In the same way, the $^1H$ and $^{13}C$ NMR chemical shifts were calculated by the gauge independent atomic orbital method using an I-PCM model in combination with B3LYP/6-311+ +G(2d,p). The Mulliken charge orientation among all the molecular orbitals is mapped and the values were intensely analysed for the identification of the key factor for pharmaceutical function of the compound. The dipole moment, linear polarizability and the first-order hyperpolarizability in different coordinates of the compound have been computed using the B3LYP method with the 6-3111++G(d,p) basis set. The ECD and VCD spectra were simulated, the enantiomer of the compound was identified and the side effect property was interpreted.

4. Results and discussion

4.1. Structural deformation analysis

The present compound is a tri-substituted benzene ring and basically it is a strong hexagonal ring. Normally, the hexagonal ring is broken by the substitution and its CC bond lengths are compressed or stretched out which depends upon its mass and strong polarity. Here, the benzene ring was substituted by two symmetrical methyl groups along with the sulphonic acid. Owing to the holding of different ligand groups, particularly, the injection of methyl groups, the ring was found to be twisted out of shape. The bond length of the ring $C2–C3$ is 0.004 Å to 0.018 Å and differed from all the remaining bond lengths. As the ligands reserved at the place of C1, C4 and C5, the bond length C4–C5 was more stretched than others in the ring. The entire hexagonal frame of the benzene ring was found to be distorted on par with the dissimilar substitutional group. From this observation, it was clear that, whenever the benzene ring was broken, the corresponding molecular property of the same will be changed. Here, the same effect was observed and apart from that, the holding of sulphonic acid in the ring was stabilized by the adjacent methyl group. This is the key reason for the inducement of antifungal activity in the compound. In the sulphonic group, the bond lengths of $S=O19$ and $S=O20$ are slightly differed by 0.002 Å with one another since one side of O was attracted by H of the acid group. The largest bond length was found between the ring and the sulphonic group (C–S = 1.792 Å) due to the existence of a strong dipole moment. Except for one, all the bond lengths C–H of two methyl groups were observed to be the same (1.091 Å). This difference of bond length was not marked much in the role of methyl group in pharmaceutical activity. The enlargement bond angle of C1–C6–C5 (123.1°) of the ring showed the consistent repulsion between two methyl groups whereas the bond angle C2–C3–C4 illustrated the compression of the bottom moiety. From the bond angle changes explained the reception of the ligand groups by the ring and it was also confirmed that, the structure modification insisted the changes of the physical and chemical properties of the compound (Table 1 and Figure 1).

4.2. Mulliken charge population analysis

The Mulliken charge levels are depicted in Table 2 and the corresponding sketch is displayed in Figure 2. The present compound was made up of a benzene ring, couple of methyl groups and sulphonic acid groups. Usually, in a benzene ring, the negative charges accumulated on all CC bonds and the protonic region occupied over H bonds. In this case, the C1, C2, C4 and C6 were found to be more negative whereas C3 and C5 were identified as neutral. From this condition, it can be inferred that, since the negative charges have been forced to displace away from the ring to the ligand groups, the benzene ring acted as a precise base for the preparation of the present compound with a novel property. The boundary of the compound was found to be in the protonic region which was due to the hydrogen atoms. In the case of methyl groups, the negative charges were directed towards C10 and C11 from the ring and moderately strong dipoles were expressed which caused the stabilization of the existing physico-chemical property.

In the sulphonic group, there were three strong dipoles created by two $\pi$ bonding and one $\sigma$ bonding orbitals. The sulphur atom was determined to be more positive while the surrounding O atoms were found to be more negative asymmetrically. The negative flavour fluctuated among the O atoms of sulphonic groups which was due to the H as well as in order to make an irrational dipole moment. By the formation of the strong dipole moment in the sulphonic acid group, it was ensured that the antifungal and antibacterial properties were induced. From this discussion, it is clear that due to the asymmetric charge orientation towards the ligand groups, the active sulphonic acid domain existed and this is the root cause of stimulation of the novel property.
Table 1. Optimized geometrical parameters for m-xylene-4-sulphonic acid computed at HF/DFT (B3LYP&B3PW91) with 6-311++G(d, p) and 6-311++G(d,p) basis sets.

| Geometrical parameters | HF 6-311++G (d,p) | B3LYP 6-311++G (d,p) | B3PW91 6-311++G (d,p) |
|------------------------|-------------------|----------------------|----------------------|
| Bond length (Å)        |                   |                      |                      |
| C1−C2                  | 1.382             | 1.398                | 1.395                |
| C1−C6                  | 1.393             | 1.401                | 1.399                |
| C1−C10                 | 1.508             | 1.509                | 1.508                |
| C2−C3                  | 1.384             | 1.392                | 1.389                |
| C2−H7                  | 1.074             | 1.086                | 1.084                |
| C3−C6                  | 1.382             | 1.393                | 1.393                |
| C3−H8                  | 1.072             | 1.083                | 1.082                |
| C4−C5                  | 1.403             | 1.409                | 1.407                |
| C4−S18                 | 1.763             | 1.789                | 1.792                |
| C5−C11                 | 1.382             | 1.398                | 1.395                |
| C5−C11                 | 1.511             | 1.509                | 1.507                |
| C6−H9                  | 1.076             | 1.087                | 1.085                |
| C10−H12                | 1.083             | 1.093                | 1.091                |
| C10−H13                | 1.085             | 1.093                | 1.092                |
| C10−H14                | 1.085             | 1.093                | 1.095                |
| C11−H15                | 1.082             | 1.093                | 1.091                |
| C11−H16                | 1.082             | 1.094                | 1.092                |
| C11−H17                | 1.083             | 1.094                | 1.093                |
| H15−O21                | 2.572             | 3.467                | 3.475                |
| S18−O21                | 1.419             | 1.463                | 1.455                |
| S18−O20                | 1.582             | 1.545                | 1.447                |
| S18−O21                | 1.411             | 1.651                | 1.649                |
| O20−H22                | 0.946             | 0.972                | 0.968                |

| Bond angle (°)         |                   |                      |                      |
| C2−C1−C6               | 118.7             | 118.4                | 118.4                |
| C2−C1−C10              | 121.4             | 121.0                | 121.1                |
| C6−C1−C10              | 119.9             | 120.5                | 120.5                |
| C1−C2−C3               | 120.1             | 120.5                | 120.4                |
| C2−C3−H7               | 119.5             | 119.6                | 119.5                |
| C2−C3−C4               | 120.2             | 119.7                | 119.8                |
| C2−C3−H8               | 120.3             | 120.9                | 120.9                |
| C3−C4−H8               | 119.5             | 119.3                | 119.4                |
| C3−C4−C5               | 121.3             | 121.8                | 121.8                |
| C3−C4−S18              | 116.9             | 116.5                | 116.5                |
| C3−C4−S18              | 121.8             | 121.7                | 121.6                |
| C4−C5−C6               | 116.9             | 116.5                | 116.5                |
| C4−C5−C11              | 123.5             | 123.4                | 123.4                |
| C5−C6−C11              | 119.6             | 120.1                | 120.1                |
| C6−C6−C5               | 122.8             | 123.0                | 123.1                |
| C6−C6−H9               | 118.8             | 118.9                | 118.9                |
| C5−C6−H9               | 118.4             | 118.1                | 118.1                |
| C10−C10−H12            | 111.3             | 111.5                | 111.5                |
| C10−C10−H13            | 110.8             | 111.5                | 111.5                |
| C10−C10−H14            | 110.6             | 110.7                | 110.7                |
| H12−C10−H13            | 108.2             | 108.3                | 108.3                |
| H12−C10−H14            | 108.1             | 107.4                | 107.6                |
| H13−C10−H14            | 107.7             | 107.2                | 107.3                |
| C5−C11−H15             | 110.6             | 111.0                | 111.0                |
| C5−C11−H16             | 110.6             | 110.4                | 110.3                |
| C5−C11−H17             | 111.4             | 111.3                | 111.2                |
| H15−C11−H16            | 109.0             | 108.8                | 108.9                |
| H15−C11−H17            | 107.5             | 106.8                | 106.8                |
| H16−C11−H17            | 108.4             | 108.5                | 108.4                |
| C4−S18−O20             | 108.5             | 108.9                | 108.7                |
| C4−S18−O20             | 103.4             | 109.9                | 110.1                |
| C4−S18−O21             | 110.3             | 102.6                | 102.7                |
| O19−S18−O20            | 106.5             | 121.5                | 121.6                |
| O19−S18−O21            | 120.9             | 106.7                | 106.9                |
| O20−S18−O21            | 105.8             | 105.9                | 105.1                |
| S18−O20−H22            | 110.5             | 106.2                | 107.5                |

| Dihedral angle (°)     |                   |                      |                      |
| C6−C1−C2−C3            | 0.05              | 0.16                 | 0.11                 |
| C6−C1−C2−C7            | −179.86           | 179.73               | 179.83               |
| C10−C1−C2−C3           | 179.74            | 178.72               | 178.82               |
| C10−C1−C2−C7           | −0.16             | −1.38                | −1.24                |
| C2−C1−C6−C5            | 0.25              | 0.46                 | 0.40                 |
| C2−C1−C6−H9            | −179.97           | −179.56              | −179.63              |
| C10−C1−C6−C5           | −179.45           | −178.43              | −178.54              |
| C10−C1−C6−H9           | −179.97           | −179.63              | −179.66              |

(Continued)
4.3. Vibrational analysis

The existence of fundamental modes of vibrations along with group frequencies for m-xylene-4-sulphonic acid is presented in Table 3. The multiple scanning FT-IR and FT-Raman vibrational pattern of observed and simulated spectra by different methods are displayed in Figures 3 and 4, respectively. The resultant compound was architected by the combination of benzene ring, two methyl and a sulphonic acid group which consisted of 22 atoms and the total confinement belongs to the C5 point group. The 60 fundamental modes of vibrations were distributed as:

$$\Gamma_{ vib} = 41\Gamma' + 19\Gamma''.$$  

The quantum mechanical calculations using density force fields equations offered by Pulay and Rauhut were used to check the reliability of fitting the scaling factors for theoretical harmonic frequencies and verified with the experimental data [11,12]. The calculated wave numbers at the HF level were scaled by the factor 0.902, 0.885 and 0.890. Similarly, wavenumber calculated at B3LYP were scaled by 0.882, 0.921, 0.932 and 0.857 and in the same way B3PW91 was scaled by the factors 0.910, 0.934, 0.896 and 0.865, respectively. After the scaling, the difference between Expt. and theoretical was found to be reduced.

4.3.1. Ring C–H vibrations

Usually, the base compound is coupled with ligand groups, making a final product and each and every

### Table 1. Contained.

| Geometrical parameters | HF 6-31+G (d,p) | B3LYP 6-31+G (d,p) | B3PW91 6-31+G (d,p) |
|------------------------|-----------------|--------------------|---------------------|
| C2-C1-C10-H13          | 124.33          | 146.31             | 141.43              |
| C2-C1-C10-H14          | -176.45         | -155.92            | -160.69             |
| C6-C1-C10-H14          | -55.98          | -34.83             | -39.66              |
| C6-C1-C10-H14          | 63.33           | 84.54              | 79.64               |
| C1-C2-C3-C4            | -0.12           | -0.01              | -0.01               |
| C1-C3-C4-H8            | -179.76         | 179.94             | -179.98             |
| H1-C2-C3-C4            | 179.97          | 179.91             | -179.95             |
| H7-C2-C3-H8            | 0.15            | 0.05               | 0.08                |
| C2-C3-C4-C5            | -0.09           | -0.09              | -0.13               |
| C2-C3-C4-S18           | -179.08         | -178.73            | -178.67             |
| H8-C3-C4-S5            | 179.55          | 179.95             | 179.84              |
| H8-C3-C4-S18           | 0.56            | 1.31               | 1.30                |
| C3-C4-C5-C6            | 0.36            | 0.36               | 0.39                |
| C3-C4-C5-C11           | -179.52         | 179.96             | -179.93             |
| S18-C4-C5-C6           | 179.30           | 178.93             | 178.85              |
| S18-C4-C5-C11          | -0.58           | -1.47              | -1.47               |
| C3-C4-S18-O19          | -2.03           | -5.69              | -5.01               |
| C3-C4-S18-O20          | -114.89         | 129.72             | 130.70              |
| C3-C4-S18-O21          | 132.42          | -117.95            | -117.78             |
| C5-C4-S18-O19          | 178.99          | 175.67             | 176.45              |
| C5-C4-S18-O20          | 66.13           | -48.93             | -47.84              |
| C5-C4-S18-O21          | -46.56          | 63.41              | 63.68               |
| C4-C5-C6-C1            | -0.44           | -0.54              | -0.53               |
| C4-C5-C6-H9            | 179.78          | 179.47             | 179.50              |
| C11-C5-C6-C1           | 179.44          | 179.84             | 179.78              |
| C11-C5-C6-H9           | -0.34           | -0.14              | -0.19               |
| C4-C5-C11-H15          | 65.02           | 62.34              | 62.55               |
| C4-C5-C11-H16          | -174.58         | -176.90            | -176.68             |
| C4-C5-C11-H17          | -54.52          | -56.51             | -56.24              |
| C6-C5-C11-H15          | -114.85         | -118.07            | -117.78             |
| C6-C5-C11-H16          | 5.55            | 2.69               | 2.99                |
| C6-C5-C11-H17          | 125.61          | 123.08             | 123.43              |
| C4-S18-O20-H22         | 92.32           | 102.79             | 92.40               |
| O19-S18-O20-H22        | -21.99          | -11.42             | -21.84              |
| O21-S18-O20-H22        | -151.76         | -141.92            | -152.39             |

### Table 2. Mulliken charge levels of m-xylene-4-sulphonic acid.

| Atoms | Charge level | Colour code |
|-------|--------------|-------------|
| C1    | -0.095       | Black (neutral) |
| C2    | -0.060       | Dark red    |
| C3    | -0.022       | Dark red    |
| C4    | -0.362       | Dark red    |
| C5    | 0.003        | Black (neutral) |
| C6    | -0.035       | Dark red    |
| C10   | -0.257       | Visible red |
| C11   | -0.277       | Visible red |
| S18   | -0.050       | Visible red |
| O19   | -0.465       | Visible red |
| O20   | -0.461       | Visible red |
| H7    | 0.095        | Dark green  |
| H8    | 0.134        | Dark green  |
| H9    | 0.086        | Dark green  |
| H12   | 0.116        | Dark green  |
| H13   | 0.22         | Dark green  |
| H14   | 0.136        | Dark green  |
| H16   | 0.102        | Dark green  |
| H17   | 0.147        | Dark green  |
| H22   | 0.301        | Dark green  |
group in the compound is emphasized by their active vibrations such as stretching and bending. If the benzene is used as base to construct the compound, its presence will be ensured by the ring vibrations. Here, the benzene ring is a base ring and over that the entire ligand groups are attached in suitable positions. There were three remaining C–H bonds in the ring found after the ligand pairing. The related C–H stretching bands have been found with medium intensity at 3050, 3010 and 3000 cm\(^{-1}\) in both IR and Raman spectra. Normally, the C–H stretching vibrations were observed in the region 3000–3100 cm\(^{-1}\) for benzene derivatives [13–15]. Though these vibrations were found within the expected region, two of three appeared at the lower end of the limited region. This view showed the ligand influence on the ring. Here, the C–H in-plane and out-of-plane bending modes was found at 1225, 1190 and 1160 cm\(^{-1}\) and 1000, 990 and 910 cm\(^{-1}\), respectively. Usually, those vibrational bands were identified in the region 1300–1000 cm\(^{-1}\) and 1000–750 cm\(^{-1}\), respectively [16,17]. The out-of-plane vibrations were pushed to the top end whereas in-plane vibrations were pulled down to the lower end of the expected region which was mainly due to the existence of chemical equilibrium forces for making dipole interaction over the ring.

Figure 1. Crystal view.

4.3.2. Methyl C–H vibrations

The present compound possesses two methyl groups at ortho and para positions in the ring. Usually, if the ligand is at the ortho position in the ring, it will be effective and play an important role in the modification of the property of the compound [18]. The ligand groups in the ring emphasized their presence by active vibrational motion in the expected level. In this case, six C–H bonds of two methyl groups have expressed stretching and bending vibrations. Accordingly, the C–H stretching vibrational bands were found at 2990, 2970, 2955, 2945, 2940 and 2910 cm\(^{-1}\). In fact, the C–H stretching modes of methyl group are observed in the region 3000–2850 cm\(^{-1}\) [19,20]. Hence, all these vibrations were found at the top end of the allotted region of the spectra which implies that the components of the methyl group are identified to be active and they were involved primarily in the pharmaceutical activity.

The C–H in-plane and out-of-plane bending vibrations for methyl groups were formally observed in the region 1250–900 and 950–750 cm\(^{-1}\), respectively [21–23]. Here, in-plane and out-of-plane bending motions were observed at 1140, 1080, 1060, 1055, 1045 and 1035 cm\(^{-1}\) and 875, 840, 815, 715, 710 and 690 cm\(^{-1}\), respectively. All these in-plane and out-of-plane bending modes appeared moderately...
inside the allotted region of the spectrum. This view strongly described that the methyl groups proved their active presence in the pharmaceutical phase of the compound.

4.3.3. CC vibrations
In this case, CC bonds were positioned at two different places, inside the ring and at the methyl point. Normally, the ring C=C and C–C stretching vibrational peaks are identified in the region 1400–1625 cm\(^{-1}\) [24,25]. At this point, the C=C stretching multiple absorption crest appeared at 1580, 1485 and 1460 cm\(^{-1}\) and consequently the C–C stretching modes have been observed at 1410, 1400 and 1395 cm\(^{-1}\). The CCC in-plane and out-of-plane vibrations are usually behind the mid infrared vibrational region [26]. Here, two such vibrational peaks were found at 590, 580 and 570 cm\(^{-1}\) and 560, 530 and 525 cm\(^{-1}\), respectively. These vibrations were found to be far behind the observed range which

Figure 2. FTIR spectrum.

Figure 3. FTIRaman spectrum.
was mainly by the holding of the ligand in the ring. The C–C bridge stretching vibrations were identified at 1310 and 1290 cm\(^{-1}\). The corresponding in-plane and out-of-plane bending modes have been exposed at 640 and 620 and 480 and 380 cm\(^{-1}\), respectively. Along with the methyl group vibrational modes, those signals showed good appearance in the spectrum.

### 4.3.4. \(\text{O–H} \) and \(\text{S–O} \) vibrations

The \(\text{O–H} \) vibrations are generally measured between 3600 and 3200 cm\(^{-1}\) in acid derivative compounds.
Here the acid group was assembled along with the sulphonic group and a moderate influence on such a group was expected. The broadness of the band due to the O–H stretching vibration may be used to distinguish between the hydrated and anhydrous forms of sulphonic acids. The O–H stretching vibration appeared at 3450 cm$^{-1}$ as rather broad band and its corresponding in-plane and out-of-plane bending modes were found with very strong intensity at 1610 cm$^{-1}$ and with medium intensity at 1010 cm$^{-1}$, respectively. The in-plane O–H deformation vibration can provide a medium to strong band in the region of 1440–1260 cm$^{-1}$ [28]. In the same way, the out-of-plane vibrations are generally observed at 900–700 cm$^{-1}$ [29]. Accordingly, the entire O–H vibrations are elevated to the higher region of the spectra and actually the vibrations have been improved by the sulphonic group. This means that the hydroxyl group was

![Figure 4. NMR spectra.](image)

![Figure 5. FMO view.](image)
completely bonded with the sulphonic group and it was synchronized to bring out a favourable pharmaceutical property.

The bands observed due to the \( \text{SO}_3 \) stretching vibration for both the anhydrous and hydrated forms are strong and usually broad. In general, these two bands together form a broad absorption with two maxima and may thus be distinguished from the acid salts which have two separate bands. The \( \text{S}=\text{O} \) asymmetric stretching for anhydrous sulphonic acid occurs in the region 1355–1340 cm\(^{-1}\) \(^{[30,31]}\). Here, the \( \text{S}=\text{O} \) stretching modes have been found at 1440 and 1420 cm\(^{-1}\) in IR and Raman spectra. The \( \text{S}=\text{O} \) stretching vibrational signal was observed at 1285 cm\(^{-1}\) and normally such a vibration is located in the region 1165–1150 cm\(^{-1}\). The in-plane and out-of-plane deformations have been found to appear at 660 and 600 cm\(^{-1}\) and 315 and 230 cm\(^{-1}\), respectively. All those vibrations have proved to be pure and appeared at the top end of the allowed region which showed and ensured their presence in the role of drug action and particularly antifungal activity.

### 4.3.5. C–S vibrations

The alkyl sulphonic acids (anhydrous) give rise to their \( \text{S}–\text{C} \) stretching vibration in the region 700–600 cm\(^{-1}\) \(^{[30]}\). The consecutive in-plane and out-of-plane deformations are observed in the far infrared region. Here, the stretching vibration was found at 680 cm\(^{-1}\) and in-plane and out-of-plane bending vibrations were identified at 565 and 340 cm\(^{-1}\), respectively. All those vibrations have proved to be pure and appeared at the top end of the allowed region which showed and ensured their presence in the role of drug action and particularly antifungal activity.

### Table 4. Experimental and calculated 1H and 13C NMR chemical shifts of \( m \)-xylene-4-sulphonic acid.

| Atom position | Solvent phase | TMS-B3LYP/6-311++G(2d,p) | Experimental shift (ppm) |
|---------------|---------------|--------------------------|--------------------------|
| C1            | Gas           | DMSO                     | CCl4                     | 153.99 | 156.28 | 154.42 | 144.0 |
| C2            | 131.15        | 131.35                   | 130.74                   | 135.0 |
| C3            | 131.34        | 129.08                   | 130.11                   | 128.0 |
| C4            | 147.44        | 143.78                   | 144.67                   | 152.0 |
| C5            | 146.15        | 146.11                   | 145.42                   | 145.0 |
| C6            | 135.01        | 135.62                   | 134.71                   | 140.0 |
| C10           | 20.16         | 19.94                    | 19.91                    | 20.0  |
| C11           | 21.40         | 20.90                    | 20.91                    | 22.0  |
| H7            | 7.14          | 7.33                     | 7.19                     | 7.50  |
| H8            | 7.38          | 7.20                     | 7.23                     | 7.40  |
| H9            | 7.13          | 7.33                     | 7.16                     | 7.20  |
| H12           | 1.53          | 1.58                     | 1.51                     | 2.30  |
| H13           | 1.55          | 1.60                     | 1.52                     | 2.20  |
| H14           | 1.87          | 1.84                     | 1.81                     | 2.20  |
| H15           | 6.43          | 6.18                     | 6.23                     | 7.00  |
| H16           | 1.12          | 1.17                     | 1.07                     | –     |
| H17           | 1.55          | 1.46                     | 1.43                     | –     |
| H22           | 5.37          | 5.95                     | 5.46                     | 6.90  |
| O19           | 317.93        | 288.99                   | 300.80                   | –     |
| O20           | 315.89        | 285.87                   | 297.65                   | –     |
| O21           | 260.04        | 256.86                   | 254.56                   | –     |
| S18           | 101.64        | 98.54                    | 101.71                   | –     |

### 4.4. NMR assessment

The \(^{13}\text{C}\) and \(^{1}\text{H}\) NMR spectra via observation and simulation by a computational program are presented in Figure 5 and their results are depicted in Table 4. The \(^{13}\text{C}\) is particularly important in the analysis of large, biochemically significant molecules since the \(^{13}\text{C}\) NMR spectra can be much simpler than the corresponding proton spectra \(^{[32]}\). Normally, the \( \text{sp}^3 \) hybridized carbons of the benzene ring absorbs over 100 ppm downfield \(^{[33]}\). Here, the chemical shift of carbon was found to be located in two separate regions, below and above 100 ppm. The observed chemical shifts of C2, C3 and C6 were 135, 128 and 140 ppm and the calculated 131, 129 and 135 ppm, respectively. These are the carbons in the ring which were not substituted anymore and bonded with the H proton. C1 and C5 have been substituted by methyl groups and the chemical shift of the same was chemical shift of 144 and 145 ppm, respectively. Such higher values of shift showed the methyl group injection and correspondingly the chemical properties were changed on par with the groups. The NMR spectra of the present compound showed the very huge chemical shift for C4 (Expt. 152 ppm and cal. 147 ppm) which is the substituted place of sulphonic groups. The large dislocation of such chemical shift inferred clearly that C4 is the bridge point which is also the pathway to exchange the chemical properties between ring and sulphonic groups.

The C10 and C11 showed less chemical shift (Expt. 20 and 22 ppm) which was purely due to the symmetrical shielding of the surrounding electrons. The proton of the H atoms around the ring showed the chemical shift range from 7.20 to 7.50 ppm whereas the chemical shift of H12, H13, H14, H15, H16 and H17 of the methyl group appeared at a low level which implies the involvement of the methyl group in the ring for the modification of the pharmaco-chemical property such as antifungal activity. The chemical shift of H22 of the hydroxyl group was found to be 6.90 ppm which was due to the asymmetrical Van der Waals attraction of O in the sulphonic group. There was no substantial difference observed in the chemical shifts in the different solvents’ phases. Hence, the impact of the solvents on the chemical shifts of various atoms was negligibly diminutive.

### 4.5. Frontier molecular interaction profile

Frontier Molecular Orbital theory uses molecular orbital interaction to explain the structure and reactivity of molecules, and in organic chemistry, the theory has been insanely successful. Normally, the chemical activity of the compound is predicted from the overlapping of orbitals among various atoms of the compound \(^{[34]}\). The \( \sigma \) and \( \pi \) orbitals of the nearby molecular group with the same energy (degenerate energy levels) are
overlapped and blended with one another. Such a type of interaction often appeared between the molecular orbitals and leads to the asymmetrical delocalization of molecular orbitals.

The transition between bonding and antibonding orbitals plays an important role in the manifestation of the physico-chemical property of the compound. Here, in the case of LUMO, the antibonding orbitals were found to be overlapped between carbon atoms of the ring. The same energy antibonding orbitals appeared in one methyl group, whereas there was no antibonding orbitals found in the rest of the methyl group and the sulphonic group. In the case of HOMO, two semicircular $\pi$-bonding orbital lobes were found to overlap. There were two additional $\sigma$-bonding orbitals found in the methyl and sulphonic groups. Usually, according to the selection rule, the transition was not possible between HOMO and LUMO. Hence, in the case of HOMO$^{-1}$, the $\pi$-bonding orbital lobes overlapping takes place between C2–C3 and C5–C6 via C4 which is the substitutional place of the sulphonic group. In addition to that, the positive sign orbitals appeared to overlap in the composition of the sulphonic group whereas the negative sign lobe overlapped with ring carbons with the same sign. From this overlapping process, it was clear that the overlapped region was able to supply electrons to various regions among the atoms for producing a new chemical property. The HOMO–LUMO energy values were presented in the Table 5.

In the case of LUMO$^{-1}$, the antibonding lobes were present in the C–S of the sulphonic group and ring, C–C of the methyl group and ring, C–C of the ring and O–H of the hydroxyl groups. From this vacancy environment, the location that was able to receive the electron density was clear. The possible transitions were found to be taking place in and around the location where the bonding orbital lobes interconnected. At the HOMO+2 ring, the bonding lobes overlap in the ring, one methyl group and sulphonic group of the compound. In this case, one methyl group was exempted, which implies that one methyl group was needed for the inducement of pharmacological activity in the compound. The formation of a charge-transfer complex occurs when filled $\pi$-orbitals in the donor overlap with the depleted orbitals in the acceptor, resulting in the production of two new molecular orbitals. The transition between these newly formed orbitals is responsible for the new absorption bands observed in the charge-transfer complexes and thus leads to the new physico-chemical property of the compound. According to the charge-transfer spectra [37,38], electron transfer from the donor to the acceptor is more complete in the excited state than in the ground state and the wavelength of absorption can, in fact, be correlated with electron affinity of the acceptor and the ionization potential of the donor.

In the present case, the electronic excitation absorption CT band was found at 256 nm with oscillator strength of 0.008 at the energy gap of 4.83 eV and the absorption band is assigned to $\pi\rightarrow\pi^*$ transition in charge distributions over the molecule. The colour coding charge level map visualized various charged regions with respect to the ligand and base component of the molecule. In the figure, the potential energy for the charge distributions was spread to be plane on the surface of the molecule. In this case, according to the Cartesian coordinate system, the C4 of the ring acts as the centre in which x cuts the sulphonic group and y cuts the methyl group, whereas z is perpendicular to the plane of the molecule. From this orientation, it is clear that a strong dipole moment was found at the sulphonic group which contains large electron density and also it was more reactive than other parts of the molecule.

The molecular electrostatic potential (MEP) is used to determine a receptor-reactive site of the molecular surface and it is also used to determine the nature of the orientation of a chemical bond [35,36]. The figure shows that the negative charges are asymmetrically oriented over the Os’ of the sulphonic group, whereas the blue region is spread around the hydrogen atoms of the phenyl ring and methyl groups. The opposite region is highly positive (nucleophilic) and located on C–H bonds of the ring. The colour code of the MEP map is in the range from ~6.824 a.u. (deepest red) to 6.824 a.u. (faded blue) in the compound. From this observation, it is clear that the charges were found to be depleted enough to induce a saturated chemical property and the sulphonic group acts as the main receptor branch for binding the compound with the protein.

### 4.7. Electronic excitation analysis

The formation of a charge-transfer complex occurs between the base and substitutional groups which when blended allow transfer of electronic charge through space from an electron-rich molecule (a Lewis-base donor) to an electron-deficient molecule (a Lewis-acid acceptor). The bond formation between complexes occurs when filled $\pi$-orbitals in the donor overlap with the depleted orbitals in the acceptor, resulting in the production of two new molecular orbitals. The transition between these newly formed orbitals is responsible for the new absorption bands observed in the charge-transfer complexes and thus leads to the new physico-chemical property of the compound. According to the charge-transfer spectra [37,38], electron transfer from the donor to the acceptor is more complete in the excited state than in the ground state and the wavelength of absorption can, in fact, be correlated with electron affinity of the acceptor and the ionization potential of the donor.

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### 4.6. Molecular electrostatic potential maps

The molecular electrical potential surface shown in Figure 7 illustrates the three-dimensional asymmetrical
the gas phase. The energy of the CT complex is found to be 4.83 eV and is enough to ensure the transition between acceptor (sulphonic and methyl groups) and donor (phenyl ring). In the solvent phase, the CT band is identified at the same nanometre with oscillator strength of 0.012 at the same energy gap. The result obtained for the CT complex in gas as well as solvent phases showed the strong interaction between donor and acceptor. The absorption band of m-xylene transparently occurs in the UV spectrum in the R-band (German, radikalartig) and naturally has antibacterial and antifungal activity. In this case, the absorption band is found at the quartz-UV region which indicates that the formation of the sulphonic acid segment with xylene is the root cause of such pharmaceutical activity. The electronic excitation parameters are presented in Table 6 and the absorption band is displayed in Figure 8.

The electronic displacement causing the creation of new molecular orbitals gives rise to Circular Dichroism called ECD which is directed via the orbital overlap interaction path which implies an instantaneous transformation and polarization of dipoles in the molecule. The proton and electronic clouds are redistributed during the transition, causing asymmetric charge displacement. Frequently, the electron redistribution takes place among Frontier molecular orbitals due to the presence of chromophores in the compound; thus, the electronic orientation modifies the chemical activity of the compound which can be identified easily by the ECD. According to Figure 8, the ECD absorption band is identified at 220 nm which honestly precise the rich chemical reactivity. The energy values of frontier molecular orbitals of the present molecule are obtained in Table 7 and its energy level diagram is displayed in Figure 8. According to the energy level values, it was identified that the saturation (degeneracy) was found from H+8 and L−8 levels. From this view, it was clear that the production of new molecular orbitals was stabilized at that level (Figure 9).

4.8. Polarizability and first-order hyperpolarizability analysis

The stabilization of polarized orbitals is the root cause of the strong physico-chemical property of the compound which was investigated by computing polarizability – first-order hyperpolarizability and the values are presented in Table 8. The calculated value of the dipole moment is found to be 5.41 Debye. The highest value of the dipole moment is observed for component $\mu_x$, which is equal to −4.788 D and the lowest value of the dipole moment of the molecule for the component $\mu_g$ is 0.22 D. The calculation shows the intense orientation of the charge levels in the negative $x$ component of the coordinate of the compound which points out the direction of the sulphonic group. The calculated average polarizability and anisotropy of the polarizability are $150.65 \times 10^{-30}$ esu and $211.13 \times 10^{-30}$ esu, respectively. The hyperpolarizability $\beta$ is one of the key factors of stabilization of the frontier molecular orbital interaction system. The calculated B3LYP/6-311+G(d,p) first hyperpolarizability value ($\beta$) is $16.9 \times 10^{-33}$ esu. From this observation, it was clear that hyper asymmetrical polarization was taking place in order to emphasize the formation of new frontier molecular orbitals for the creation of a new pharmaceutical property.

Figure 6. Frontier molecular analysis graph.
4.9. Thermodynamic functions’ analysis

The thermodynamic properties of entropy, specific heat capacity and enthalpy of the organic compound are very significant since they play an important role in physical as well as chemical properties [39]. In this case, the calculated thermodynamic parameters are depicted in Table 9. The calculated entropy, specific heat capacity and enthalpy were found to vary linearly with respect to temperature in optimistic mode. When the temperature increased from 100 to 1000 K, the thermodynamic functions established to swing as linear pattern and sustained up at maximum temperature. This view of variation showed the consistent chemical stability of the present compound. The Gibbs free energy always has a negative temperature coefficient if the organic compound has a strong and unique chemical property. In this case, it was found to be true and also it was inferred that the negative coefficient established by the chemical reaction is endless.

4.10. NBO transition analysis

NBO analysis is very important for the determination of interactions between the filled orbital of one subsystem and vacant orbital of another subsystem within the compound which is used to predict the consistent electronic structure and the chemical property of the compound [28]. NBO calculations were performed using the NBO 6.0 program [40] as implemented in the Gaussian09 package and the corresponding

Table 5. Frontier molecular orbital energy levels of m-xylene-4-sulphonic acid.

| Energy levels | B3LYP/6-311++G(d,p) |
|---------------|----------------------|
|               | IR region (eV)       | UV–Visible region (eV) |
| H+10          | 12.72                | 12.799               |
| H+9           | 12.31                | 12.193               |
| H+8           | 12.09                | 12.063               |
| H+7           | 11.96                | 11.462               |
| H+6           | 10.38                | 10.457               |
| H+5           | 10.01                | 10.186               |
| H+4           | 9.851                | 9.884                |
| H+3           | 9.729                | 9.647                |
| H+2           | 9.649                | 9.582                |
| H+1           | 9.548                | 9.212                |
| H             | 9.128                | 9.020                |
| L             | 4.284                | 4.443                |
| L−1           | 4.261                | 4.164                |
| L−2           | 0.871                | 1.306                |
| L−3           | 0.585                | 0.764                |
| L−4           | 0.223                | 0.248                |
| L−5           | 0.429                | 0.665                |
| L−6           | 0.641                | 0.797                |
| L−7           | 0.905                | 0.949                |
| L−8           | 1.152                | 1.310                |
| L−9           | 1.495                | 1.517                |
| L−10          | 1.678                | 1.775                |
values are depicted in Table 9. The transition among inter-molecular donor and acceptor of base and substitutional groups causes asymmetrical electron delocalization between the hyper-conjugated species in the molecule which leads to the confinement of the new property.

A number of transitions were observed among the various orbitals within the molecule, some of which caused asymmetrical electron orientation between base and ligand groups and some important transitional motions occurred with large stabilization energy and such that main source of the new property. Here, the $\sigma-\sigma^*$ transition takes place from C1–C2 to C5–C6 by consuming 17.35 kcal/mol of energy from CH$_3$. Similarly, the $\sigma-\sigma^*$ transitional motion was observed from C3–C4 to C1–C2 and C5–C6 by inhaling 14.39 and 21.54 kcal/mol of energy from another CH$_3$. From this observation, it was clear that the energy was exchanged by both the methyl groups via the ring. In the ligand group, the $\pi-\pi^*$ transition was identified from C10–H12 to S18–O20 and S18–O21. The same $\sigma-\sigma^*$ transition was found from

![Figure 8. ECD UV-visible spectra.](image)

Table 6. Theoretical electronic absorption spectra of $m$-xylene-4-sulphonic acid (absorption wavelength $\lambda$ (nm), excitation energies $E$ (eV) and oscillator strengths ($f$)) using the TD-DFT/B3LYP/6-311++G(d,p) method.

| $\lambda$ (nm) | $E$ (eV) | $f$ | Major contribution | Assignment | Region | Bands |
|---------------|---------|-----|--------------------|------------|--------|-------|
| Gas           |         |     |                    |            |        |       |
| 256.32        | 4.837   | 0.008 | H$\rightarrow$L (92%) | $n\rightarrow\pi^*$ | Quartz UV | R-band (German, radikalartig) |
| 256.16        | 4.936   | 1.599 | H$\rightarrow$L (89%) | $n\rightarrow\pi^*$ | Quartz UV |       |
| 256.07        | 5.208   | 0.0421 | H$\rightarrow$L-1 (86%) | $n\rightarrow\pi^*$ | Quartz UV |       |
| DMSO          |         |     |                    |            |        |       |
| 256.18        | 4.839   | 0.0128 | H$\rightarrow$L (90%) | $n\rightarrow\pi^*$ | Quartz UV | R-band (German, radikalartig) |
| 251.95        | 4.920   | 0.2251 | H$\rightarrow$L-1 (90%) | $n\rightarrow\pi^*$ | Quartz UV |       |
| 251.45        | 5.288   | 0.0027 | H$\rightarrow$L-1 (87%) | $n\rightarrow\pi^*$ | Quartz UV |       |
| CCl$_4$       |         |     |                    |            |        |       |
| 256.54        | 4.833   | 0.013 | H$\rightarrow$L (86%) | $n\rightarrow\pi^*$ | Quartz UV | R-band (German, radikalartig) |
| 252.29        | 4.914   | 0.223 | H$\rightarrow$L-1 (85%) | $n\rightarrow\pi^*$ | Quartz UV |       |
| 237.37        | 5.223   | 0.00 | H+1$\rightarrow$L-1 (78%) | $n\rightarrow\pi^*$ | Quartz UV |       |

Note: $H$: HOMO; $L$: LUMO
O21–H22 to S18–O19 and S18–O20 in the sulphonic groups. From this, it was inferred that the transition energy was exchanged from the sulphonic group to ring and vice versa, in order to stabilize the structure for providing pharmaceutical applications.

4.11. Vibrational circular dichroism

The chirality of the compound manifests the chemical property of the same which is very important to determine the pharmaceutical activity processes. The positive and negative circularly polarized infrared radiation during a vibrational transition is called vibrational circular dichroism [41,42]. The VCD can be used for many types of analysis related to the structure and conformations of molecules of biological interest, determining the enantiomeric purity of a sample relative to a known standard, determining absolute configurations and determining the solution conformations of large and small biological molecules.

The VCD spectrum of the title compound is displayed in Figure 10. The present compound has more than one conformational structure and confirmed mirror enantiomers which emphasize the chemical purity and the compounds are free from unwanted side effects. In this case, in the enantiomer, the significant functional group (sulphonic acid group) was rather differentiated between the mirror images. This condition may affect the fundamental application of the compound. But this was not so in this case, since any sulphonic group position could not affect the basic property of the compound.

4.12. Chemical properties

The physico-chemical properties and different reactivity descriptors of the compound have been determined from intra-molecular charge transfer among the Frontier molecular energy levels (HOMO–LUMO) and are presented in Table 10. The electron affinity of the various regions of the molecule is very important for the determination of the reaction ability of the organic compound and the same was found to be 9.128 which is very high and the reaction capability
of the present compound is active even when inert. The ionization potential of the compound is significant to evaluate chemical-bond reorganization. The ionization potential was found to be 4.284 which is very huge and enough to sustain the chemical-bond stability.

Generally, chemical hardness is a measure of resistance to charge transfer while electronegativity is a measure of the tendency to attract electrons by an atom in a chemical bond [43]. Here, the values of both parameters were found to be 2.421 and 6.706 respectively and they appeared in an elevated phase which showed the present compound to be a good reactive molecule for further additive properties. The total dipole moment reproduced the ability of interaction of compounds with the surrounding medium and have more binding ability, resulting in enhancement of the biological effects. In this case, the dipole moment was identified as 5.410 Debye which is also adequate to have rich biological activity. The electrophilicity index is a measure of energy fluctuation with respect to maximal charge flow among the frontier molecular orbitals. The electrophilicity index was identified to be 9.287 eV whereas that of the benzene ring was 2.09 eV. The energy of 7.197 eV is higher than the base compound which was mainly due to the addition of sulphonic groups at appropriate positions along with the methyl group. From this observation, it was concluded that the maximum energy flow takes place for creating the pronounced pharmaceutical application. Here, the present compound was composed of a couple of methyl species and sulphonic groups in symmetrical form and the electrophilicity charge transfer of the compound was found to be +2.769 which established the charge flows from ligand groups to benzene after the completion of the Frontier molecular orbitals. This caused par ligand groups to obtain the chemical property of being an antifungal agent.

### Table 8. Thermodynamic functions at different temperatures for m-xylene-4-sulphonic acid.

| Temperature (K) | $S_0^0$ (cal mol$^{-1}$ K$^{-1}$) | $C_{p, ref}^0$ (cal mol$^{-1}$ K$^{-1}$) | $\Delta G_0^0$ (kcal mol$^{-1}$) | Gibbs free energy $\Delta G = \Delta H - T \Delta S$ (kJ mol$^{-1}$) |
|-----------------|-----------------------------|-----------------------------|------------------|----------------------------------|
| 100             | 5.95                        | 314.28                      | 89.62            | -31,338.4                       |
| 200             | 17.83                       | 394.36                      | 146.70           | -78,725.3                       |
| 298.15          | 34.79                       | 462.68                      | 198.57           | -137,740.0                      |
| 300             | 35.16                       | 463.91                      | 199.53           | -138,973.0                      |
| 400             | 57.60                       | 528.13                      | 248.29           | -211,004.0                      |
| 500             | 84.57                       | 588.14                      | 289.70           | -293,780.0                      |
| 600             | 115.28                      | 644.04                      | 323.45           | -386,101.0                      |
| 700             | 149.65                      | 696.04                      | 350.89           | -486,877.0                      |
| 800             | 185.30                      | 744.42                      | 373.53           | -595,162.0                      |
| 900             | 223.63                      | 789.54                      | 392.48           | -710,194.0                      |
| 1000            | 263.70                      | 831.74                      | 408.53           | -831,331.0                      |

### Table 9. NBO analytical data of m-xylene-4-sulphonic acid.

| Type of transition | Donor (i) | Acceptor (j) | Energy difference $E_{ij} - E_i$ (a.u.) | Polarized energy $F(j|i)$ (a.u.) |
|--------------------|-----------|--------------|------------------------------------------|-----------------------------------|
| $\sigma-\sigma^*$  | C1-C2     | C2-C3        | 3.52                                     | 1.28                              |
|                    | C3-C4     | 27.29        | 0.27                                     | 0.077                             |
|                    | C5-C6     | 17.35        | 0.29                                     | 0.064                             |
|                    | C7-C8     | 4.17         | 1.27                                     | 0.061                             |
|                    | C9-C10    | 3.92         | 0.86                                     | 0.054                             |
|                    | C11-C12   | 3.18         | 1.26                                     | 0.065                             |
|                    | C13-C14   | 4.45         | 1.09                                     | 0.062                             |
|                    | C15-C16   | 4.13         | 1.08                                     | 0.060                             |
|                    | C17-C18   | 5.90         | 1.28                                     | 0.078                             |
|                    | C19-C20   | 3.69         | 1.14                                     | 0.058                             |
|                    | C21-C22   | 14.39        | 0.31                                     | 0.050                             |
|                    | C23-C24   | 21.54        | 0.31                                     | 0.073                             |
|                    | C25-C26   | 3.83         | 1.10                                     | 0.058                             |
|                    | C27-C28   | 5.43         | 1.28                                     | 0.074                             |
|                    | C29-C30   | 3.55         | 1.29                                     | 0.061                             |
|                    | C31-C32   | 2.89         | 1.27                                     | 0.054                             |
|                    | C33-C34   | 3.22         | 0.77                                     | 0.048                             |
|                    | C35-C36   | 4.68         | 1.25                                     | 0.066                             |
|                    | C37-C38   | 4.96         | 0.85                                     | 0.060                             |
|                    | C39-C40   | 2.36         | 0.29                                     | 0.074                             |
|                    | C41-C42   | 17.92        | 0.27                                     | 0.062                             |
|                    | C43-C44   | 3.23         | 1.19                                     | 0.055                             |
|                    | C45-C46   | 2.66         | 1.19                                     | 0.050                             |
|                    | C47-C48   | 4.42         | 1.09                                     | 0.062                             |
|                    | C49-C50   | 4.79         | 1.07                                     | 0.064                             |
|                    | C51-C52   | 0.54         | 1.74                                     | 0.027                             |
|                    | C53-C54   | 4.23         | 1.08                                     | 0.061                             |
|                    | C55-C56   | 0.76         | 1.30                                     | 0.029                             |
|                    | C57-C58   | 0.80         | 1.29                                     | 0.030                             |
|                    | C59-C60   | 2.36         | 1.07                                     | 0.049                             |
|                    | C61-C62   | 2.15         | 1.11                                     | 0.045                             |
|                    | C63-C64   | 2.62         | 1.12                                     | 0.050                             |
|                    | C65-C66   | 0.89         | 1.08                                     | 0.029                             |
|                    | C67-C68   | 1.06         | 1.09                                     | 0.031                             |

### Table 10. Calculated chemical parameters of m-xylene-4-sulphonic acid.

| Chemical parameter | B3LYP/6-311++G(d,p) | Electrophilicity charge transfer ($\Delta N_{max-h} - \Delta N_{max-h}$) |
|--------------------|----------------------|-------------------------------------------------|
| $\delta_{HOMO}$ (eV) | 9.128               | 9.020                                           |
| $\delta_{LUMO}$ (eV) | 4.284               | 4.390                                           |
| $\Delta \delta_{HOMO-LUMO}$ (eV) | 4.843 | 4.630 +2.769                                     |
| $\delta_{HOMO-1}$ (eV) | 9.548               | 9.212                                           |
| $\delta_{LUMO+1}$ (eV) | 4.284               | 4.164                                           |
| $\Delta \delta_{HOMO-1-LUMO+1}$ (eV) | 5.263 | 5.047                                           |
| Chemical hardness | 2.421               | 2.315                                           |
| Electronegativity ($\mu$) | 6.706               | 6.705                                           |
| Chemical potential | 6.706               | 6.705                                           |
| Dipole moment | 5.410               | 6.003                                           |
5. Conclusion

The FT-IR and FT-Raman vibrational pattern sequences emphasized the active part of the composition of the molecule for creating an active pharmaceutical application of the compound. The NMR analysis showed the different chemical environment of the carbons present in the molecule which opened the cause of such antibacterial and antifungal property. From the Mulliken discussion, it was clear that due to the asymmetric charge orientation towards the ligand groups, the active sulphonic acid domain existed and this is the root cause for the stimulation of a novel property. The chemical-bond stability of the compound was proved by observing the rich ionization potential. The chemical hardness and electronegativity appeared in an elevated phase which showed the present compound to be a good reactive molecule for further additive properties.

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Disclosure statement

No potential conflict of interest was reported by the authors.

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