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## Structural Properties of Bioactive Molecule Naphthalene 2-Sulfonic Acid

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**ABSTRACT.** Naphthalene 2-sulfonic acid (NSA) and its derivatives are the most important class of organic compounds and are important products of industrial chemical processes. . Bioactive molecule NSA was performed by means of Density Functional Theoretical (DFT) method using standard B3LYP/6-31G (d,p) basis set implemented with Gaussian'09 software package. NBO analysis were performed to provide valuable information about various intermolecular interactions. Optical properties of the NSA molecule were studied using UV-Vis spectral analysis. In addition, Molecular docking was performed for the different receptors for calculating binding affinities and predicting binding sites.

**Introduction.** Bioactive substance is experiencing a growing interest of phytomedicines, including their clinical applications, standardization, quality control, mode of action and potential drug interactions have emerged as one of the most exciting developments in modern therapeutics and medicine. Bioactive compounds are still regarded as a valuable pool for discovering novel mode of action. [1] Substituted sulfonic acid is used as analytical reagent in the manufacture of disinfectants, antiseptics, deodorants and medicines. It is also used for disinfecting skin and for the treatment of minor wounds and purification of drinking water in case of amoebicidal and bactericidal emergencies [2]. Naphthalene is used to make dyes, explosives, plastics and lubricants. Naphthalene is very dangerous to human health especially children who may mistake naphthalene balls for candy. It enters human through inhalation or passing through the skin. Because of their spectroscopic properties and chemical significance of NSA have been studied extensively by spectroscopic and theoretical methods. A systematic study on the molecule structure and vibrational spectra will help in understanding the property of NSA molecule. Present study intends to fully exploit the structural and biological characterization of NSA along with DFT calculations to investigate the spectral investigations using UV-vis, Docking and NBO analysis of NSA molecule.

### Experimental and Computational details

UV-visible absorption spectrum of the sample was measured, using UV-vis JASCO (V-570) UV/VIS/NIR spectrometer. DFT Computation were carried out using Gaussian'09 program [3] at B3LYP/6-311G(d,p) level. Natural bond orbital (NBO) analysis [4] have been using NBO 3.1 program to understand inter- and intra-molecular delocalization. Optimized structure was docked using Auto Dock Tools (ADT) Version 1.5.4 revision 30[5].

### Results and Discussion

**Geometrical structures.** Structure parameters of the NSA molecule were calculated using DFT / B3LYP/6-311++G(d,p) basis set has been listed in Table.1 . and the molecular structure with atom

numbering scheme adopted in this study is shown in Fig. 1. Bond length of S<sub>18</sub>-O<sub>21</sub> (1.6497Å) is higher than other S-O bond lengths S<sub>18</sub>-O<sub>19</sub> and (1.4575Å) and S<sub>18</sub>-O<sub>20</sub> (1.4643Å) which is due to the attachment of hydrogen atom with it. Hydrogen sulfate anion is highly distorted from its tetrahedral arrangement which is manifested from its bond angles O<sub>19</sub>-S<sub>18</sub>-O<sub>20</sub> (121.07°), O<sub>19</sub>-S<sub>18</sub>-O<sub>21</sub>(108.43°), S<sub>18</sub>-O<sub>21</sub>-O<sub>22</sub>(106.04°) and O<sub>20</sub>-S<sub>18</sub>-O<sub>21</sub>(106.19°). Presence of strong intra-molecular hydrogen bond interactions C<sub>11</sub>-H<sub>16</sub>...O<sub>19</sub> has been confirmed by the measured distances C<sub>11</sub>...O<sub>19</sub> which is 2.9431Å lying within the range <3 Å for hydrogen interaction [6].

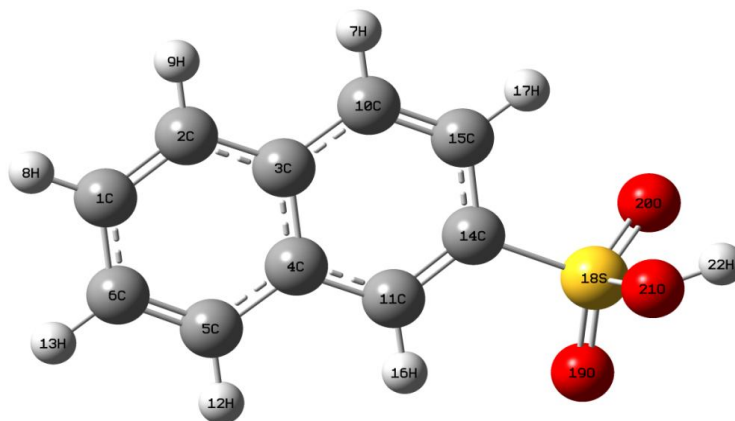


Fig. 1. Optimized structure of Naphthalene-2-sulfonic acid.

Table 1. Optimized Bond lengths (Å), Bond angles (°) and Dihedral angle (°) of Naphthalene 2-sulfonic acid by B3LYP/6-31g(d,p) basis sets.

Bond Length	Theo. (Å)	Bond angle	Theo. (°)	Dihedral angle (°)	Theo. (°)
S <sub>18</sub> -O <sub>19</sub>	1.4575	O <sub>19</sub> -S <sub>18</sub> -O <sub>20</sub>	121.07	C <sub>6</sub> -C <sub>1</sub> -C <sub>2</sub> -C <sub>3</sub>	-0.06
S <sub>18</sub> -O <sub>20</sub>	1.4643	O <sub>19</sub> -S <sub>18</sub> -O <sub>21</sub>	108.43	C <sub>2</sub> -C <sub>1</sub> -C <sub>6</sub> -C <sub>5</sub>	0.03
S <sub>18</sub> -O <sub>21</sub>	1.6497	O <sub>20</sub> -S <sub>18</sub> -O <sub>21</sub>	106.19	C <sub>1</sub> -C <sub>2</sub> -C <sub>3</sub> -C <sub>4</sub>	-0.01
C <sub>1</sub> -C <sub>6</sub>	1.4163	S <sub>18</sub> -O <sub>21</sub> -O <sub>22</sub>	106.03	C <sub>1</sub> -C <sub>2</sub> -C <sub>3</sub> -C <sub>10</sub>	179.69
C <sub>1</sub> -H <sub>8</sub>	1.0859	C <sub>1</sub> -C <sub>2</sub> -C <sub>6</sub>	120.52	C <sub>1</sub> -C <sub>2</sub> -C <sub>3</sub> -C <sub>4</sub>	-0.003
C <sub>2</sub> -C <sub>3</sub>	1.4196	C <sub>2</sub> -C <sub>1</sub> -H <sub>8</sub>	119.97	C <sub>1</sub> -C <sub>2</sub> -C <sub>3</sub> -C <sub>10</sub>	179.69
C <sub>2</sub> -H <sub>9</sub>	1.0865	C <sub>6</sub> -C <sub>1</sub> -H <sub>8</sub>	119.51	C <sub>2</sub> -C <sub>3</sub> -C <sub>4</sub> -C <sub>5</sub>	0.09
C <sub>3</sub> -C <sub>4</sub>	1.4336	C <sub>1</sub> -C <sub>2</sub> -C <sub>3</sub>	120.69	C <sub>2</sub> -C <sub>3</sub> -C <sub>4</sub> -C <sub>11</sub>	-179.97
C <sub>3</sub> -C <sub>10</sub>	1.4228	C <sub>1</sub> -C <sub>2</sub> -H <sub>9</sub>	120.45	C <sub>10</sub> -C <sub>3</sub> -C <sub>4</sub> -C <sub>5</sub>	-179.60
C <sub>4</sub> -C <sub>5</sub>	1.4206	C <sub>3</sub> -C <sub>2</sub> -H <sub>9</sub>	118.85	C <sub>10</sub> -C <sub>3</sub> -C <sub>4</sub> -C <sub>11</sub>	0.32
C <sub>4</sub> -C <sub>11</sub>	1.419	C <sub>2</sub> -C <sub>3</sub> -C <sub>4</sub>	118.73	C <sub>2</sub> -C <sub>3</sub> -C <sub>10</sub> -C <sub>15</sub>	-179.94
C <sub>5</sub> -C <sub>6</sub>	1.3761	C <sub>2</sub> -C <sub>3</sub> -C <sub>10</sub>	122.17	C <sub>4</sub> -C <sub>3</sub> -C <sub>10</sub> -C <sub>15</sub>	-0.25
C <sub>5</sub> -H <sub>12</sub>	1.0864	C <sub>4</sub> -C <sub>3</sub> -C <sub>10</sub>	119.10	C <sub>3</sub> -C <sub>4</sub> -C <sub>5</sub> -C <sub>6</sub>	-0.13
C <sub>6</sub> -H <sub>13</sub>	1.0856	C <sub>3</sub> -C <sub>4</sub> -C <sub>5</sub>	119.21	C <sub>11</sub> -C <sub>4</sub> -C <sub>5</sub> -C <sub>6</sub>	179.97
H <sub>7</sub> -C <sub>10</sub>	1.0863	C <sub>3</sub> -C <sub>4</sub> -C <sub>11</sub>	118.99	C <sub>5</sub> -C <sub>4</sub> -C <sub>11</sub> -C <sub>14</sub>	179.96
C <sub>10</sub> -C <sub>15</sub>	1.3734	C <sub>5</sub> -C <sub>4</sub> -C <sub>11</sub>	121.81	C <sub>4</sub> -C <sub>5</sub> -C <sub>6</sub> -C <sub>1</sub>	0.06
C <sub>11</sub> -C <sub>14</sub>	1.3755	C <sub>4</sub> -C <sub>5</sub> -C <sub>6</sub>	120.57	C <sub>3</sub> -C <sub>10</sub> -C <sub>15</sub> -C <sub>14</sub>	-0.18
C <sub>11</sub> -H <sub>16</sub>	1.0849	C <sub>4</sub> -C <sub>5</sub> -H <sub>12</sub>	118.81	C <sub>4</sub> -C <sub>11</sub> -C <sub>14</sub> -C <sub>15</sub>	-0.49
C <sub>14</sub> -C <sub>15</sub>	1.4169	C <sub>6</sub> -C <sub>5</sub> -H <sub>12</sub>	120.62	C <sub>11</sub> -C <sub>14</sub> -C <sub>15</sub> -C <sub>10</sub>	0.57

## Natural Bond Orbital Analysis

To interpret the presence of intermolecular and intramolecular charge transfer interactions, the second order perturbation energies were calculated using NBO analysis. Electron occupancies of lone pair and anti-bonding orbitals of NSA molecule are given in Table .2. To investigate energy features of intramolecular non-bonded S···O interactions. Existence of C-S···O interactions is confirmed due to interaction between lone pair oxygen atoms O<sub>19</sub> and O<sub>20</sub> with C<sub>14</sub>-S<sub>18</sub> having stabilization energies of 16.48 and 16.62 kJ/mol respectively. Central sulphur atom is SP<sup>2</sup> hybridised with 26.89% s character and 71.67% p character that shortens bond length of C-S (1.78 Å). Intramolecular charge transfer is obtained by orbital overlapping within ring system between  $\pi$  C<sub>1</sub> - C<sub>2</sub> and  $\pi^*$ C<sub>5</sub>-C<sub>6</sub> having a stabilization energy of 17.07 kJ/mol.

Table 2. Second order perturbation theory analysis of Fock matrix in NBO basis.

Donor (i)	ED(i) (e)	Acceptor (j)	ED(j) (e)	E(2) <sup>a</sup> (kJ mol <sup>-1</sup> )	E(j)- E(i) <sup>b</sup> (a.u)	F(i,j) <sup>c</sup> (a.u)
LP <sub>2</sub> O <sub>19</sub>	1.80507	$\sigma^*$ C <sub>14</sub> -S <sub>18</sub>	0.18460	16.48	0.45	0.077
LP <sub>2</sub> O <sub>19</sub>	1.80507	$\sigma^*$ S <sub>18</sub> -O <sub>20</sub>	0.14000	12.72	0.59	0.078
LP <sub>3</sub> O <sub>19</sub>	1.77036	$\sigma^*$ S <sub>18</sub> -O <sub>21</sub>	0.30690	31.07	0.37	0.097
LP <sub>2</sub> O <sub>20</sub>	1.80871	$\sigma^*$ C <sub>14</sub> - S <sub>18</sub>	0.18460	13.56	0.45	0.070
LP <sub>2</sub> O <sub>20</sub>	1.80871	$\sigma^*$ S <sub>18</sub> - O <sub>19</sub>	0.14067	16.62	0.59	0.090
LP <sub>3</sub> O <sub>20</sub>	1.78564	$\sigma^*$ S <sub>18</sub> - O <sub>21</sub>	0.30690	31.70	0.37	0.099
LP <sub>2</sub> O <sub>21</sub>	1.93961	$\sigma^*$ S <sub>18</sub> - O <sub>19</sub>	0.14067	7.72	0.65	0.065
$\pi$ C <sub>11</sub> -C <sub>14</sub>	1.76297	$\pi^*$ C <sub>10</sub> -C <sub>15</sub>	0.22653	17.47	0.32	0.067
$\pi$ C <sub>10</sub> - C <sub>15</sub>	1.73639	$\pi^*$ C <sub>11</sub> - C <sub>14</sub>	0.02239	17.22	0.28	0.063
$\pi$ C <sub>1</sub> - C <sub>2</sub>	1.72875	$\pi^*$ C <sub>5</sub> - C <sub>6</sub>	0.24118	17.07	0.30	0.064

*a*-E(2) means energy of hyperconjugative interactions; *b*-Energy difference between donor and acceptor *i* and *j* NBO orbitals; *c*-F(*i,j*) is the Fock matrix element between *i* and *j* NBO orbitals.

### UV-visible spectra

To investigate UV-vis absorption spectrum of NSA molecule dissolved in D<sub>2</sub>O is shown in Fig. 2 and theoretical values with combined experimental values in Table.3. In maximum absorption values are 309 and 302 nm and computed at 307 and 299 nm. Experimental band at 309 nm is attributed mainly to HOMO→LUMO transition with 74% contribution. This transition is predicted as  $\pi$ → $\pi^*$  transition. In this case the energy transitions are in reasonable agreement with experimental results. Calculated value of electrophilicity index describes the biological activity. Electronic band transitions can be well understood from the plot of  $(\alpha h\nu)^2$  verses photon energy as depicted in Fig 3. The wide optical band gap of NSA is found to be 4.7 eV suggesting its suitability for electronics applications.



**Summary.** NSA molecule under investigation has wide biological applications. Natural bond orbital analysis performed in this study gives information about the molecular species which are responsible for more chemical stability. In UV spectra maximum absorption wavelengths and their excitation energies predicted in this study belong to  $\pi \rightarrow \pi^*$  transition. Moreover, molecular docking simulations have been done to test the biological inhibition activity against inflammation. The results showed that NSA molecule has potential activity against inflammation.

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