



ISSN No: 0975-7384  
CODEN(USA): JCPRC5

*J. Chem. Pharm. Res.*, 2011, 3(1):572-583

---

**Ground state properties: Gross orbital charges, orbital energy and net atomic charges of phenol and its some derivatives**

**Alok Shukla<sup>1</sup>, Rajendra Prasad Tewari<sup>1</sup>, K. D. P. Shukla<sup>1</sup> and Gayasuddin Khan<sup>2\*</sup>**

<sup>1</sup>*Department of Physics, Maharani Lal Kunwari Post Graduate College, Balrampur, (U.P.), INDIA*

<sup>2</sup>*Department of Physics, K. S. Saket Post Graduate College, Ayodhya, Faizabad, (U.P.), INDIA*

---

**ABSTRACT**

*We have studied the ground state properties of a series of phenols. These properties are gross orbital charges, orbital energy and net atomic charges. These properties are calculated by MOPAC software using MINDO/3 methods. The study concluded that the net atomic charges of phenol series as calculated by MINDO/3 are similar to the semi-empirical and ab-initio result, and the flow of charges takes place from less electronegativity to high electronegativity atoms during ortho and para - substitution.*

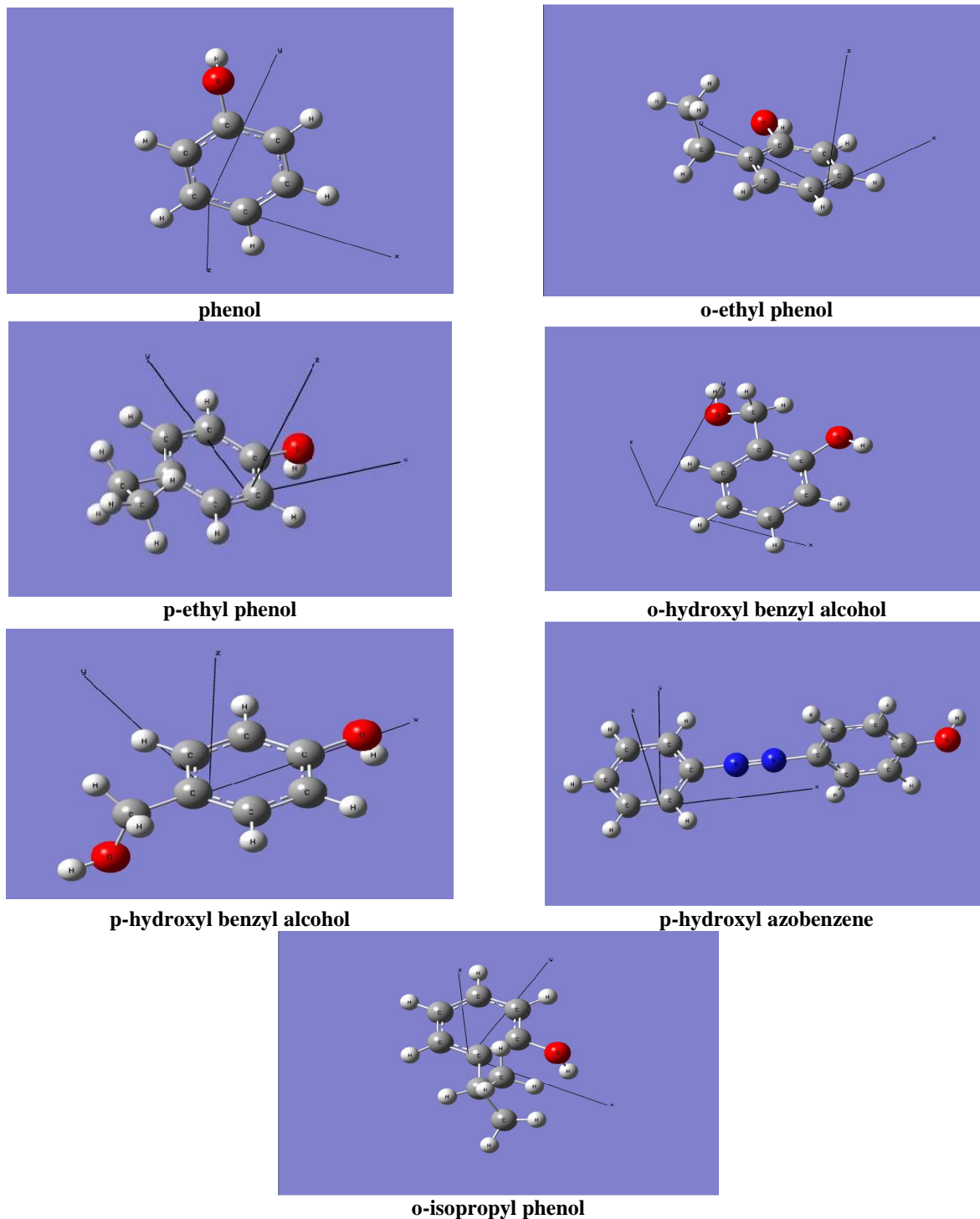
**Key words:** Phenol, MINDO/3, MOPAC, ground state properties.

---

**INTRODUCTION**

People and coworkers developed a series of approximation based on neglect of differential overlap (CNDO) [1-4]. But modification in above method was suggested by Del, Bene and Jaffee and these various versions of the CNDO method, with appropriate parameterization were used to study the electronic structure and spectra of molecules by several workers leading to a moderately successful description of the polarity of substituted benzene [5-9]. But the method discussed above is found no longer suitable for molecular electronic structure calculations. So the electronic structure of some molecule was studied by ab-initio method and semi-empirical method [10-15]. In these methods a single set of parameters allowed the calculation of varied properties of wide range of molecules. One of such treatments (MINDO/3) reported by them and proved successful for calculation giving good results for every ground state properties studied [16, 17]. Thus available evidence suggests that MINDO/3 method may provide better results for

calculating ground state properties such as gross orbital charges, orbital energies, net atomic charges of phenol molecule and some of its derivatives.



**Figure 1.** Coordinates of phenol and its derivatives

## EXPERIMENTAL SECTION

The experimental materials of this paper are phenol and its few derivatives are showing in Fig. 1

For present study the molecular modeling and geometry optimization [18] of all the compounds were carried out with MOPAC software using MINDO/3 methods [19]. The gross orbital charges, orbital energies and net atomic charges of every atom of the derivatives have been calculated by softness calculators.

## RESULT AND DISCUSSION

The gross orbital charges, orbital energies and net atomic charges properties of phenol and its derivatives are described separately as below:

**2.1 Gross orbital charges:** The gross orbital charges of phenol and its derivatives using MINDO/3 method are presented in the Table 1.1 to 1.7 below.

**Table 1: Gross Orbital Charges.**

Table 1.1: Gross orbital charges of phenol.					
Atoms	1s	2s	2p <sub>x</sub>	2p <sub>y</sub>	2p <sub>z</sub>
C <sub>1</sub>		1.235	0.875	0.870	0.949
C <sub>2</sub>		1.241	0.891	0.880	1.114
C <sub>3</sub>		1.209	0.668	0.866	0.862
C <sub>4</sub>		1.247	0.890	1.429	1.137
O <sub>5</sub>		1.787	1.316	0.870	1.914
C <sub>6</sub>		1.234	0.871	0.873	0.945
C <sub>8</sub>		1.234	0.874	0.886	1.079
H <sub>7</sub>	0.988				
H <sub>9</sub>	0.995				
H <sub>10</sub>	1.013				
H <sub>11</sub>	0.971				
H <sub>12</sub>	1.013				
H <sub>13</sub>	0.753				
Table 1.2: Gross orbital charges of o-Ethyl phenol.					
Atoms	1s	2s	2p <sub>x</sub>	2p <sub>y</sub>	2p <sub>z</sub>
C <sub>1</sub>		1.232	0.874	0.872	0.936
C <sub>2</sub>		1.246	0.899	0.884	1.139
C <sub>3</sub>		1.223	0.668	0.869	0.858
C <sub>4</sub>		1.213	0.889	0.867	1.118
O <sub>5</sub>		1.785	1.326	1.430	1.908
C <sub>6</sub>		1.247	0.871	0.876	0.947
C <sub>7</sub>		1.225	0.871	0.849	0.989
C <sub>8</sub>		1.231	0.876	0.888	1.079
C <sub>9</sub>		1.264	0.876	0.889	1.025
H <sub>10</sub>	0.983				
H <sub>11</sub>	1.015				
H <sub>12</sub>	1.015				
H <sub>13</sub>	0.992				
H <sub>14</sub>	0.752				
H <sub>15</sub>	1.040				

H <sub>16</sub>	0.983				
H <sub>17</sub>	0.991				
H <sub>18</sub>	0.999				
H <sub>19</sub>	0.993				
<b>Table 1.3: Gross orbital charges of p-Ethyl phenol.</b>					
<b>Atoms</b>	<b>1s</b>	<b>2s</b>	<b>2p<sub>x</sub></b>	<b>2p<sub>y</sub></b>	<b>2p<sub>z</sub></b>
C <sub>1</sub>		1.194	0.793	1.053	0.815
C <sub>2</sub>		1.284	0.890	0.803	1.085
C <sub>3</sub>		1.217	0.640	0.856	0.829
C <sub>4</sub>		1.385	1.007	0.866	1.025
C <sub>5</sub>		1.778	1.460	1.602	1.591
C <sub>6</sub>		1.266	0.961	0.898	0.932
C <sub>7</sub>		1.215	0.944	0.831	1.010
C <sub>8</sub>		1.213	0.947	0.866	0.916
O <sub>9</sub>		1.265	0.952	0.897	0.915
H <sub>10</sub>	1.088				
H <sub>11</sub>	1.091				
H <sub>12</sub>	0.929				
H <sub>13</sub>	0.955				
H <sub>14</sub>	1.027				
H <sub>15</sub>	0.986				
H <sub>16</sub>	0.990				
H <sub>17</sub>	0.989				
H <sub>18</sub>	1.020				
H <sub>19</sub>	0.745				
<b>Table 1.4: Gross orbital charges of o-Hydroxyl benzyl alcohol.</b>					
<b>Atoms</b>	<b>1s</b>	<b>2s</b>	<b>2p<sub>x</sub></b>	<b>2p<sub>y</sub></b>	<b>2p<sub>z</sub></b>
C <sub>1</sub>		1.216	0.809	0.696	0.840
C <sub>2</sub>		1.239	0.874	0.895	1.241
C <sub>3</sub>		1.229	0.855	0.873	0.946
C <sub>4</sub>		1.244	0.883	0.885	1.099
C <sub>5</sub>		1.219	0.880	0.845	0.864
C <sub>6</sub>		1.231	0.878	0.912	1.245
C <sub>7</sub>		1.241	0.791	0.732	0.814
O <sub>8</sub>		1.780	1.524	1.237	1.882
O <sub>9</sub>		1.787	1.532	1.240	1.909
H <sub>10</sub>	0.977				
H <sub>11</sub>	0.019				
H <sub>12</sub>	0.994				
H <sub>13</sub>	0.971				
H <sub>14</sub>	1.071				
H <sub>15</sub>	0.743				
H <sub>16</sub>	0.072				
H <sub>17</sub>	0.745				
<b>Table 1.5: Gross orbital charges of p-Hydroxyl benzyl alcohol.</b>					
<b>Atoms</b>	<b>1s</b>	<b>2s</b>	<b>2p<sub>x</sub></b>	<b>2p<sub>y</sub></b>	<b>2p<sub>z</sub></b>
C <sub>1</sub>		1.243	0.872	0.866	0.932
C <sub>2</sub>		1.241	0.892	0.882	1.124
C <sub>3</sub>		1.310	0.668	0.870	0.841
C <sub>4</sub>		1.247	0.902	0.885	1.144
O <sub>5</sub>		1.785	1.319	1.431	0.419
C <sub>6</sub>		1.241	0.867	0.867	0.919
C <sub>7</sub>		1.229	0.904	0.895	1.117

C <sub>8</sub>		1.214	0.865	0.821	0.715
O <sub>9</sub>		1.799	1.841	1.501	1.331
H <sub>10</sub>	1.022				
H <sub>11</sub>	0.967				
H <sub>12</sub>	0.982				
H <sub>13</sub>	1.015				
H <sub>14</sub>	0.751				
H <sub>15</sub>	1.114				
H <sub>16</sub>	1.067				
H <sub>17</sub>	0.755				
<b>Table 1.6: Gross orbital charges of p-Hydroxyl azobenzene.</b>					
<b>Atoms</b>	<b>1s</b>	<b>2s</b>	<b>2p<sub>x</sub></b>	<b>2p<sub>y</sub></b>	<b>2p<sub>z</sub></b>
C <sub>1</sub>		1.235	0.883	0.873	1.028
C <sub>2</sub>		1.237	0.882	0.870	0.983
C <sub>3</sub>		1.241	0.869	0.874	1.047
C <sub>4</sub>		1.261	0.881	0.866	0.963
C <sub>5</sub>		1.241	0.867	0.876	1.047
N <sub>6</sub>		1.610	0.999	0.973	1.388
C <sub>7</sub>		1.237	0.865	0.887	0.983
N <sub>8</sub>		1.628	1.045	1.108	1.169
C <sub>9</sub>		1.240	0.887	0.937	0.895
C <sub>10</sub>		1.239	0.876	0.945	0.890
C <sub>11</sub>		1.237	0.890	0.948	0.915
C <sub>12</sub>		1.241	0.878	0.980	0.938
C <sub>13</sub>		1.242	0.919	1.012	0.937
C <sub>14</sub>		1.207	0.855	0.844	0.718
O <sub>15</sub>		1.247	0.920	1.032	0.944
H <sub>16</sub>	1.010				
H <sub>17</sub>	1.012				
H <sub>18</sub>	1.009				
H <sub>19</sub>	1.009				
H <sub>20</sub>	1.102				
H <sub>21</sub>	1.014				
H <sub>22</sub>	0.974				
H <sub>23</sub>	0.989				
H <sub>24</sub>	1.015				
H <sub>25</sub>	0.754				
<b>Table 1.7: Gross orbital charges of o-isopropyl phenol.</b>					
<b>Atoms</b>	<b>1s</b>	<b>2s</b>	<b>2p<sub>x</sub></b>	<b>2p<sub>y</sub></b>	<b>2p<sub>z</sub></b>
C <sub>1</sub>		1.234	0.872	0.871	0.946
C <sub>2</sub>		1.246	0.899	0.883	1.133
C <sub>3</sub>		1.218	0.670	0.863	0.870
C <sub>4</sub>		2.216	0.887	0.874	1.104
O <sub>5</sub>		1.787	1.314	1.433	1.913
C <sub>6</sub>		1.243	0.870	0.875	0.961
C <sub>7</sub>		1.226	0.952	0.881	0.875
C <sub>8</sub>		1.233	0.875	0.886	1.074
C <sub>9</sub>		1.263	0.999	0.911	0.879
C <sub>10</sub>		1.266	0.898	0.900	0.896
H <sub>11</sub>	1.011				
H <sub>12</sub>	0.987				
H <sub>13</sub>	1.012				
H <sub>14</sub>	0.994				
H <sub>15</sub>	0.753				
H <sub>16</sub>	1.023				

H <sub>17</sub>	0.994				
H <sub>18</sub>	0.989				
H <sub>19</sub>	1.008				
H <sub>20</sub>	1.011				
H <sub>21</sub>	1.008				
H <sub>22</sub>	1.012				

The above tables show that the inner most 1s orbital is not significantly involved in the chemical bond. The sp<sup>2</sup> hybridization on a carbon atom required an orbital charge description of following type 2s, 2p<sub>x</sub>, 2p<sub>y</sub>, 2p<sub>z</sub>. This behavior is followed closely in our computed results. The 2s orbitals of all unsubstituted carbons show a population of o-ethyl phenol, p-ethyl phenol, o-hydroxyl benzyl alcohol, p-hydroxyl benzyl alcohol p-hydroxyl azobenzene, o-isopropyl phenol and p-isopropyl phenol approximately 1.234e in phenol so that there is a deficit of 0.776 e. This deficit represents promotion from 2s to 2p orbital. On the other hand that oxygen atom which is not directly attached to the ring carbon is just nearly equal to 1.330 e.

The examination of the charges at various orbitals shows that in phenol charge is seen to migrate from the 2p<sub>x</sub> orbital of C<sub>3</sub> to 2s orbital of O<sub>5</sub>. In o-ethyl phenol the migration of large number of charges take place from 2p<sub>x</sub> orbital of C<sub>3</sub> to 2p<sub>z</sub> orbital of O<sub>5</sub>, from 2p<sub>z</sub> orbital of C<sub>4</sub> to 2s orbital of C<sub>7</sub> and from 2p<sub>y</sub> orbital of C<sub>7</sub> and from 2p<sub>y</sub> orbital of C<sub>7</sub> to 2s orbital of C<sub>4</sub>. In o-hydroxyl benzyl alcohol, the migration of charges take place from 2p<sub>y</sub> orbital of C<sub>1</sub> to 2p<sub>z</sub> orbital O<sub>9</sub> from 2p<sub>y</sub> orbital of C<sub>7</sub> to 2p<sub>z</sub> orbital of O<sub>8</sub> and 2p<sub>y</sub> orbital of C<sub>7</sub> to 2p<sub>z</sub> orbital of C<sub>6</sub>. In p-hydroxyl benzyl alcohol the migration of charges take place from 2p<sub>x</sub> orbital of C<sub>3</sub> to 2p<sub>z</sub> orbital of O<sub>5</sub>, 2p<sub>z</sub> orbital of C<sub>8</sub> to 2p<sub>x</sub> orbital of O<sub>9</sub> and from 2p<sub>z</sub> orbital of C<sub>8</sub> to 2s orbital of C<sub>7</sub>. In p-hydroxyl-azobenzene, migration of large number of charge takes place from 2p<sub>y</sub> orbital of C<sub>4</sub> to 2s orbital of N<sub>6</sub>, from 2p<sub>z</sub> orbital of C<sub>9</sub> to 2s orbital of N<sub>8</sub> and from 2p<sub>z</sub> orbital of C<sub>13</sub> to 2s orbital of O<sub>15</sub>. In o-isopropyl phenol, migration of charges take place from 2p<sub>x</sub> orbital of C<sub>3</sub> to 2p<sub>z</sub> orbital of O<sub>5</sub> and from 2p<sub>y</sub> orbital of C<sub>4</sub> to 2s orbital of C<sub>7</sub> from 2p<sub>z</sub> orbital of C<sub>7</sub> to 2s orbital C<sub>9</sub> and from 2p<sub>z</sub> orbital of C<sub>7</sub> to orbital of C<sub>10</sub>.

Comparisons of charges flowing into different orbital of the substituent (N.C.O.) from carbon atom attached to them in different molecules are found in the order: O > N > C. This is in the order of electro negativity of these atoms.

**2.2 Orbital energies:** The energies of seven highest occupied molecular orbitals (HOMO) and seven lowest unoccupied molecular orbitals (LUMO) of phenol and its derivatives have been presented in Table 2 below.

**TABLE 2: Orbital energy of phenol and its derivatives.**

S.N.	Molecule	MO	Calculated by MINDO/3 (a.u)
1	phenol		-12.09215
			-10.80930
			-10.26367
			-9.32652
		HOMO	-8.46418
		LUMO	+1.15888
			+1.42539
			+1.96183

			+2.83828
			+3.20445
2	o- ethyl phenol		-10.84078
			-10.65982
			-10.05140
			-8.96197
		HOMO	-8.19218
		LUMO	+0.71692
			+1.34158
			+1.87252
			+2.56218
			+2.74285
3	p- ethyl phenol		-10.59512
			-9.61253
			-9.05849
			-8.53382
		HOMO	-8.02638
		LUMO	+0.97992
			+1.48799
			+2.00895
			+2.18332
			+2.50588
4	o- hydroxyl benzyl alcohol		-10.73382
			-10.41223
			-10.18017
			-9.59592
		HOMO	-7.60772
		LUMO	+0.81494
			+1.65973
			+2.1729
			+2.21743
			+2.84049
5	p- hydroxyl benzyl alcohol		-11.19364
			-10.25800
			-10.08001
			-9.46537
		HOMO	-8.52694
		LUMO	+1.03177
			+1.07783
			+1.78459
			+2.32807
			+2.85979
6	p- hydroxyl azobenzene		-9.33381
			-9.14210
			-9.13808
			-7.94307
		HOMO	-7.32529
		LUMO	+0.92885
			+1.16052
			+1.30560
			+1.32805
			+1.48440
	-10.9915		

7	o- isopropyl phenol		-10.04967
			-9.61042
			-9.17768
		HOMO	-8.40289
		LUMO	+0.98829
			+1.36346
			+1.88828
			+2.0846
		+2.69866	

A close look at the above table shows that all the seven HOMO's have negative energies while all the seven LUMO's have positive energies. This result is similar to ab-initio results Yadav *et al.* [9]. The negative values of calculated highest occupied molecular orbital (HOMO) energies an estimate for the molecular ionization potential in accordance with Koopman's theorem [6]. Similarly, the electron affinities can be estimated from the calculated lowest unoccupied molecular orbital (LUMO) energies.

### 2.3 Net atomic charges:

The values of net atomic charges at various atomic sites in units of electron are presented in table 3 below.

**Table 3: Net Charges of phenol and its derivatives**

S.N.	Molecule	Atom	Net atomic charges (a.u.)
1	Phenol	C <sub>1</sub>	0.0708
		C <sub>2</sub>	-0.1269
		C <sub>3</sub>	0.3938
		C <sub>4</sub>	-0.1652
		O <sub>5</sub>	-0.4459
		C <sub>6</sub>	0.0797
		H <sub>7</sub>	-0.1170
		C <sub>8</sub>	-0.0732
		H <sub>9</sub>	0.0046
		H <sub>10</sub>	-0.0128
		H <sub>11</sub>	0.0292
		H <sub>12</sub>	-0.1270
		H <sub>13</sub>	0.2468
2	o- ethyl phenol	C <sub>1</sub>	0.0865
		C <sub>2</sub>	-0.1678
		C <sub>3</sub>	0.3865
		C <sub>4</sub>	-0.0835
		O <sub>5</sub>	-0.4486
		C <sub>6</sub>	0.0586
		C <sub>7</sub>	0.0660
		C <sub>8</sub>	-0.0743
		C <sub>9</sub>	-0.0514
		H <sub>10</sub>	0.0165
		H <sub>11</sub>	-0.0153
		H <sub>12</sub>	-0.0145
		H <sub>13</sub>	-0.0743
H <sub>14</sub>	0.2478		
H <sub>15</sub>	-0.0007		
H <sub>16</sub>	-0.0397		



		H <sub>17</sub>	0.0169
		H <sub>18</sub>	0.0015
		H <sub>19</sub>	-0.0007
3	o- hydroxyl benzyl alcohol	C <sub>1</sub>	0.4385
		C <sub>2</sub>	-0.2896
		C <sub>3</sub>	0.0970
		C <sub>4</sub>	-0.1095
		C <sub>5</sub>	0.1916
		C <sub>6</sub>	-0.2657
		C <sub>7</sub>	0.4222
		O <sub>8</sub>	-0.4235
		O <sub>9</sub>	-0.4673
		H <sub>10</sub>	0.0226
		H <sub>11</sub>	-0.0186
		H <sub>12</sub>	0.0058
		H <sub>13</sub>	-0.0714
		H <sub>14</sub>	0.2577
		H <sub>15</sub>	-0.0725
		H <sub>16</sub>	-0.0070
		4	p- hydroxyl benzyl alcohol
C <sub>1</sub>	0.0876		
C <sub>2</sub>	-0.1395		
C <sub>3</sub>	0.4114		
C <sub>4</sub>	0.1780		
O <sub>5</sub>	-0.4441		
C <sub>6</sub>	0.1063		
C <sub>7</sub>	-0.1457		
C <sub>8</sub>	0.4476		
O <sub>9</sub>	-0.4729		
H <sub>10</sub>	-0.0215		
H <sub>11</sub>	0.0331		
H <sub>12</sub>	0.0179		
H <sub>13</sub>	-0.0153		
H <sub>14</sub>	0.2493		
H <sub>15</sub>	-0.1145		
H <sub>16</sub>	-0.0669		
5	P- hydroxyl azobenzene	H <sub>17</sub>	0.2447
		C <sub>1</sub>	-0.0199
		C <sub>2</sub>	0.0293
		C <sub>3</sub>	-0.0309
		C <sub>4</sub>	0.0284
		C <sub>5</sub>	0.0309
		N <sub>6</sub>	0.0296
		C <sub>7</sub>	0.0292
		N <sub>8</sub>	0.0503
		C <sub>9</sub>	-0.0558
		C <sub>10</sub>	0.0412
		C <sub>11</sub>	0.0487
		C <sub>12</sub>	-0.1094
		C <sub>13</sub>	0.3754
		C <sub>14</sub>	-0.1477
		O <sub>15</sub>	-0.4444
		H <sub>16</sub>	-0.0049

		H <sub>17</sub>	-0.0116
		H <sub>18</sub>	-0.0088
		H <sub>19</sub>	-0.0093
		H <sub>20</sub>	-0.0117
		H <sub>21</sub>	-0.0136
		H <sub>22</sub>	0.2570
		H <sub>23</sub>	0.0106
		H <sub>24</sub>	-0.0155
		H <sub>25</sub>	0.2461
6	o- isopropyl phenol	C <sub>1</sub>	0.0765
		C <sub>2</sub>	-0.1611
		C <sub>3</sub>	0.3789
		C <sub>4</sub>	-0.0808
		O <sub>5</sub>	-0.4465
		C <sub>6</sub>	0.0518
		C <sub>7</sub>	0.0663
		C <sub>8</sub>	-0.0678
		C <sub>9</sub>	0.0521
		C <sub>10</sub>	0.0384
		H <sub>11</sub>	-0.1210
		H <sub>12</sub>	0.0132
		H <sub>13</sub>	0.0123
		H <sub>14</sub>	0.0057
		H <sub>15</sub>	0.2474
		H <sub>16</sub>	-0.0234
		H <sub>17</sub>	0.0580
		H <sub>18</sub>	0.0105
		H <sub>19</sub>	-0.0078
		H <sub>20</sub>	-0.1070
		H <sub>21</sub>	-0.0078
		H <sub>22</sub>	-0.1240

The above table shows that the positive and negative values of the net atomic charges shown at various atomic sites in each molecule are indicative of the fact that the total atomic charges after the molecule is formed, is less or more than the free atomic charges respectively, we observed that in general the result obtained from MINDO/3 method are similar with the other semi-empirical and ab-initio result. At various atomic sites of the ring in phenol and its derivatives taken for the present study, we find that all the carbon atoms attached to-OH group in phenol, (-CH<sub>3</sub>) (-CH<sub>2</sub>) group in o-ethyl and P-ethyl phenol, (-CH<sub>2</sub>) (-OH) group in o-hydroxyl benzyl alcohol, (-N) in p-hydroxyl azobenzene are having positive net charges as observed in earlier semi-empirical and ab initio results. The Positive net charges on the carbon atom attached to substituent group signify that the flow of  $\pi$  changes takes place from these carbons towards the substituent. However, it is observed that the magnitude of the net atomic charges in the present calculation are found to be smaller in comparison to the results obtained by improved 4-31G basis set ab initio SCF calculation. We have seen that the substituent O<sub>5</sub> in phenol and O<sub>5</sub> in O-ethyl phenol O<sub>8</sub> and O<sub>9</sub> in O-hydroxyl benzyl alcohol, O<sub>5</sub> and O<sub>9</sub> in p-hydroxyl benzyl alcohol, O<sub>15</sub> in p-hydroxyl azobenzene are found highly negatively charged in the present study while in the  $\pi$ - electron calculation, each atom carries a net positive charge. This is because of the fact that the  $\pi$ - electrons migrate from these substituent to the ring making the former deficient in  $\pi$ -electron (back donation effect) resulting in a net acquisition of negative charge by the

substituent. A close inspection of the net charges on the oxygen and nitrogen atoms in o-ethyl phenol, o-hydroxyl-benzyl alcohol, p-hydroxyl azobenzene reveals that the huge amount of charges migrates from the ring carbon and hydrogen atoms oxygen and nitrogen atoms making them heavily negative charged. Therefore, may be calculated that the flow of charges takes place from less electronegative atom to more electronegative atoms during the substitution. The magnitudes of the net charges are found in the order: C > O > N. This is not the order of electro negativities among them. Here C has positive charge while O and N have negative charge. It is observed that magnitude of net atomic charges on those carbon atoms which possess substituent like oxygen and nitrogen in different molecules taken for the present study, are found maximum in comparison to other carbon atoms present in the molecules. The predicted charge distributions are generally similar to those given by ab initio SCF calculations.

### CONCLUSION

- ✓ The inner most 1s orbital is not significantly involved in the chemical bond.
- ✓ The sp<sup>2</sup> hybridization on a carbon atom required an orbital charge description of 2s, 2p<sub>x</sub>, 2p<sub>y</sub>, 2p<sub>z</sub>.
- ✓ The E.A. of Oxygen is highest than Nitrogen and Carbon in gross orbital charges of phenol and its derivatives.
- ✓ The I.P. can be estimated from the calculated by HOMO energies which is positive but E.A. can be estimated from the calculated by LUMO energies which is negative.
- ✓ The net atomic charges of phenol and its derivatives, the result from MINDO/3 method are similar with the other semi-empirical and ab-initio result.
- ✓ In the phenol and its derivatives the flow of charges takes place from less electronegative atom to more electronegative atoms during the substitution. The magnitudes of the net charges of carbon is highest than oxygen and nitrogen but this is not the order of electro negativities among them. Here C has positive charge while O and N have negative charge.

### Acknowledgement

This paper is dedicated to the mother of Alok Shukla.

### REFERENCES

- [1] JA Pople, DL Beveridge. Approximate Molecular Orbital Theory, Mc Grath Hill Books Co., Inc., New York, **1970**, 111- 113.
- [2] M Carmen Carreno, Marcos González-López. Antonio Urbano *Angewandte Chemie International Edition*, **2006**, 45, 2737-2741.
- [3] JA Pople; DL Beveridge; PA Dobosh, *J. Chem. Phys.*, **1967**, 47, 2026-2033.
- [4] Manfred Weber, Markus Weber, Michael Kleine-Boymann "Phenol" in Ullmann's Encyclopedia of Industrial Chemistry, Wiley-VCH, 2004.
- [5] J Del Bene; H H Jaffe, *J. Chem. Phys.*, **1968**, 48, 1807-1813.
- [6] Tjalling Kloopman, *Physica (Elsevier)*, **1934**, 1, 104-113.
- [7] JS Yadav; K Singh; D K Rai, *J. Mol. Struct.*, **1991**, 231, 103.
- [8] JS Yadav; PC Mishra; DK Rai, *Ind. J. Pure & Appl. Phys.*, **1970**, 8, 70.
- [9] JS Yadav; PC Mishra; DK Rai., *Mol. Struct. (Theo. chem.)*, 1972, 13, 253.
- [10] E Clementi, *J. Chem. Phys.*, **1967**, 46, 4731-4737.

- [11] Pedro J Silva, *J. Org. Chem.*, **2009**, 74, 914-916.
- [12] OP Singh; JS Yadav, *J. Chem. Sci.*, **1985**, 95, 427-436.
- [13] LS Yadav; J S Yadav; DK Rai, *J. Chem. Sci.*, **1988**, 100, 315-321.
- [14] OP Singh; LS Yadav; PNS Yadav; LS Yadav, *J. Mol. Struct. (Theochem.)*, **1987**, 151, 227-232.
- [15] Corwin Hanscha; Susan C. Mckarnsb; Carr J. Smith; David J. Doolittle. *Chemico-Biological Interactions*, **2000**, 127 (1), 61-72.
- [16] RC Bingham et al., *J. Am. Chem. Soc.*, **1975**, 97, 1285-1293.
- [17] A Komornicki; J W Mclever, *Chem. Phys. Lett.*, **1971**, 10, 303-306.
- [18] JJP Stewart, *I. J. Comp. Chem.*, **1989**, 10, 209-220.
- [19] A Svobodova; J Psotova; D A Walterova, *Review. Biomed. Papers*, **2003**, 147,137-145.