**Supplementary data**

**2-Hydroxy-*N*-m-tolyl-acetamide: Optic spectroscopy, X-ray Crystallography and DFT study**

Elyor N. Khurramov

Organic Chemistry Department, National University of Uzbekistan, University Street, 4  
Tashkent, 100174, Uzbekistan  
elyor\_xn@mail.ru

Alisher G. Eshimbetov

Laboratory of Complex Compounds, Institute of Bioorganic Chemistry, Mirzo Ulugbek Street, 83  
Tashkent, 100125, Uzbekistan

Department of Chemistry of Natural Compounds, National University of Uzbekistan, University Str., 4  
Tashkent, 100174, Uzbekistan  
ealisherg@yahoo.com

Shahobiddin M. Adizov

Laboratory of macromolecular plant compounds chemistry, Institute of the Chemistry of Plant Substances, Mirzo Ulugbek Street, 77  
Tashkent, 100170, Uzbekistan  
adizovsh@gmail.com

Khamid U. Khodjaniyazov

Laboratory of Complex Compounds, Institute of Bioorganic Chemistry, Mirzo Ulugbek Street, 83  
Tashkent, 100125, Uzbekistan

Organic Chemistry Department, National University of Uzbekistan, University Street, 4  
Tashkent, 100174, Uzbekistan  
hamidkhodjaniyazov@yandex.ru



**Figure S1**. IR spectrum of 2-hydroxy-*N*-m-tolyl-acetamide (KBr)

**Table S1**. ***The coordinates of amide and imidol tautomers of HTA***

|  |  |
| --- | --- |
| Amide tautomer | Imidol tautomer |
| \* xyz 0 1  O 10.23295 6.60505 8.05358  H 9.86219 5.71090 8.14005  O 8.74720 4.92017 6.68283  N 8.44691 6.33484 4.89482  H 8.69317 7.25890 4.56956  C 7.64056 5.58740 4.00360  C 8.93248 5.98865 6.12234  C 7.27409 6.21008 2.80196  H 7.61412 7.22314 2.60251  C 9.77295 7.06949 6.81553  H 10.61702 7.33706 6.16308  H 9.15324 7.97012 6.94011  C 7.20808 4.28584 4.27152  H 7.48800 3.80575 5.19600  C 6.48327 5.55956 1.85835  C 6.41607 3.63664 3.32588  H 6.07857 2.62677 3.53132  C 6.05405 4.25550 2.13519  H 5.43670 3.72846 1.41461  C 6.09954 6.23965 0.56571  H 5.01271 6.26338 0.44024  H 6.51432 5.70827 -0.29652  H 6.46382 7.26840 0.52970  \* | \* xyz 0 1  C 0.62076 1.79695 -1.43109  C 1.14935 2.93066 -2.07387  C 0.28682 3.91206 -2.55506  C -1.09239 3.79365 -2.40615  C -1.64128 2.67506 -1.76817  C -0.77335 1.69202 -1.29679  N 1.35086 0.71377 -0.90688  C 2.60961 0.62073 -0.81104  O 3.53218 1.54141 -1.17168  C 3.20125 -0.67242 -0.26920  O 4.56514 -0.42164 0.09125  C -3.13446 2.54627 -1.57582  H 2.21662 3.03777 -2.19776  H 0.70011 4.78213 -3.05543  H -1.74683 4.57021 -2.79007  H -1.15981 0.80378 -0.80862  H 3.13470 -1.43704 -1.05266  H 2.60900 -0.99812 0.58914  H 5.07217 -1.23281 0.00384  H -3.68407 2.96521 -2.42318  H -3.46403 3.08196 -0.67819  H -3.43232 1.50143 -1.46168  H 4.39184 1.18962 -0.87660  \* |

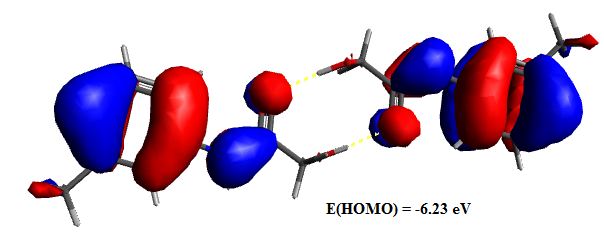
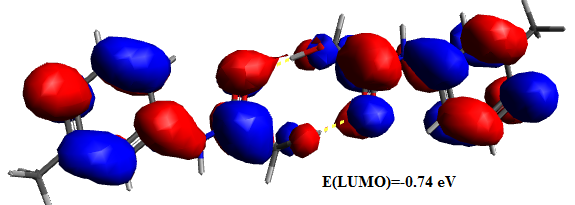
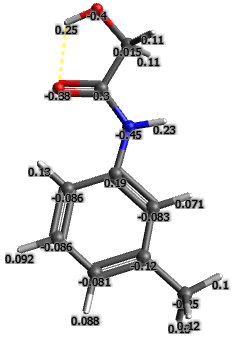
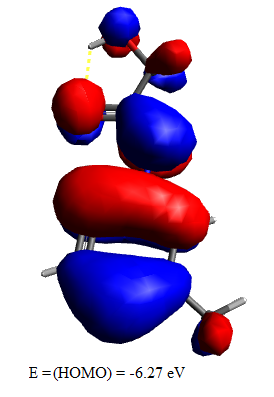
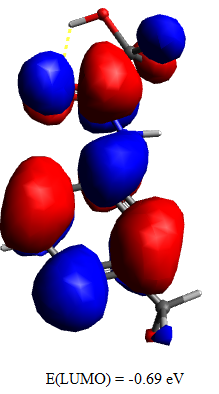


Figure S2. Energy of frontier MOs and frontier electron density

**Figure S3**. Malliken atomic charges on atoms, energy of frontier MOs and frontier electron density of amid ***a***.

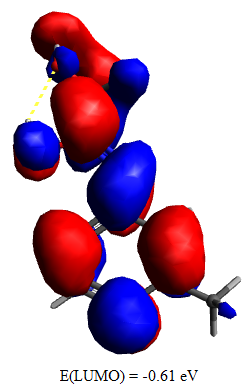
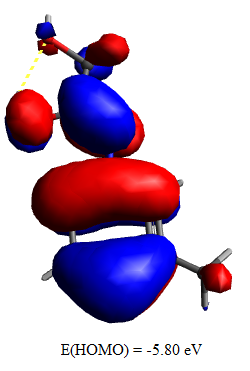
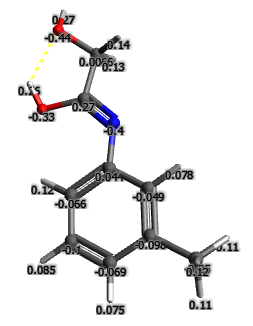


Figure S4. Malliken atomic charges on atoms, energy of frontier MOs and frontier electron density of imidol ***a***.