**Supplementary materials**

**Figures**

**Figure S1:** ORTEP drawing with the atom-labeling scheme.

**Figure S2:** Projection of the title molecule along the axis a.

**Figure S3:** The correlation between the experimental and theoretical (a) bond length and (b)bond angles for C8 H12 N2 O5 calculated from DFT / B3LYP / 6-311++G (d, p).

**Figure S4:** AIM graph ofC8 H12 N2 O5: (a) monomer and (b) dimer.

**Figure S5:** The Mulliken charges distribution designed by color change on the atoms with scale range ( red for negative charge and green for positive charge).

**Figure S6:** Histogramof Mulliken atomic charges in C8 H12 N2 O5.

**Figure S7:** Molecular electrostatic potential (MEP) of 2-(3, 4-dihydroxyphenyl)ethanaminium nitrate.

**Figure S8:** Surface minima and maxima of MEP.

**Figure S9:** Surface area in each ESP range on the VDW surface of C8 H12 N2 O5.

**Figure S10:** Molecular orbital HOMO-LUMO of our compound at B3LYP / 6-311++G(d, p) level.

**Figure S11:** Dos plots of the title compound.

**Figure S12:** The DTA/TGA curves of 2-(3, 4-dihydroxyphenyl) ethanaminium nitrate.

**Figure S13:** Different types of interactions between ligand and proteins.

**Tables**

**Table S1:** Crystal data and experimental parameters used for the intensity data collection strategy and final results for the structure determination.

**Table S2:** The Mulliken charge distribution calculated by B3LYP / 6-311 ++ G(d. p).

**Table S3:** Second order perturbation theory analysis of Fock matrix in NBO analysis.

**Table S4:** Summary of surface analysis of2-(3, 4-dihydroxyphenyl) ethanaminium nitrate.

**Table S5:**  Calculated global reactive energy descriptor of C8 H12 N2 O5.

**Table S6:** dipole moment (µ), polarizability (α) and first hyperpolarisability (β) for the title compound.

**Table S1**

|  |  |
| --- | --- |
| Temperature | 150 K |
| Empirical formula | C8H12N2O5 |
| Crystal system | Triclinic |
| Space group | *P1* |
| *a* | 8.3066 (4) Å |
| *b* | 10.4856 (5) Å |
| *c* | 11.2303 (7) Å |
| *β* | 89.868 (2) ° |
| *α* | 79.623 (2) ° |
| z | 4 |
| v | 953.37 (9) Å3 |
| F(000) | 456 |
| μ(Mo Kα) | 0.13 mm-1 |
| Reflections collected | 10787 |
| Independent reflections | 4339 |
| Reflections with I > 2σ(I) | 3583 |
| Rint | 0.038 |
| Absorption correction: multi-scan | Tmin = 0.870, Tmax = 0.966 |
| Refined parameters | 312 |
| *R[F2> 2σ(F2)]* | 0.043 |
| *wR(F2)* | 0.113 |
| Δρmax = 0.31 e Å-3 | Δρmin = 0.31 e Å-3 |

**Table S2:**

|  |  |  |  |
| --- | --- | --- | --- |
| **Atoms** | **Mulliken charges** | **Atoms** | **Mulliken charges** |
| O1 | -0.262 | C14 | -0.228 |
| O2 | -0.329 | C15 | 0.190 |
| N3 | -0.306 | H16 | 0.158 |
| C4 | -0.637 | C17 | -0.896 |
| H5 | 0.194 | H18 | 0.159 |
| H6 | 0.201 | H19 | 0.313 |
| C7 | -0.113 | H20 | 0.397 |
| H8 | 0.196 | H21 | 0.319 |
| H9 | 0.212 | H22 | 0.292 |
| C10 | 0.878 | H23 | 0.284 |
| C11 | -0.216 | O24 | -0.165 |
| H12 | 0.198 | O25 | -0.151 |
| C13 | -0.296 | O26 | -0.026 |
|  |  | N27 | -0.364 |

**Table S3:**

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Donor (i)** | **Acceptor (j)** | **E(2) kcal/mol** | **E(j)-E(i) (a.u)** | **F(i. j) (a.u)** |
| σ (C10-C11) | σ\*(O1-C13) | 3.98 | 1.02 | 0.057 |
| σ (C10-C11) | σ\*(C7-C10) | 1.51 | 1.11 | 0.037 |
| σ (C10-C11) | σ\*(C10-C17) | 3.22 | 1.27 | 0.057 |
| σ (C10-C11) | σ\*(C11-C13) | 2.95 | 1.96 | 0.055 |
| σ (C10-C17) | σ\*(C7-C10) | 1.79 | 1.11 | 0.040 |
| σ (C10-C17) | σ\*(C10-C11) | 3.28 | 1.26 | 0.058 |
| σ (C10-C17) | π\*(C11-C13) | 18.44 | 0.28 | 0.065 |
| σ (C10-C17) | π \*(C14-C15) | 19.88 | 0.27 | 0.067 |
| π (C14-C15) | π \*(C10-C17) | 17.90 | 0.30 | 0.067 |
| π (C14-C15) | π \*(C11-C13) | 18.97 | 0.29 | 0.068 |
| π (C14-C15) | π \*(C10-C17) | 224.69 | 0.01 | 0.080 |
| π (C11-C13) | π \*(C10-C17) | 20.95 | 0.29 | 0.071 |
| π (C11-C13) | π \*(C14-C15) | 19.71 | 0.28 | 0.067 |
| LP1 (O24) | σ\*(N3-H21) | 1.97 | 1.13 | 0.042 |
| LP2 (O24) | σ\*(N3-H19) | 0.14 | 0.60 | 0.008 |
| LP2 (O24) | σ\*(N3-H20) | 0.11 | 0.57 | 0.007 |
| LP2 (O24) | σ\*(N3-H21) | 6.97 | 0.60 | 0.058 |
| LP1 (O25) | σ\*(N3-H20) | 5.98 | 1.01 | 0.071 |
| LP2 (O25) | σ\*(N3-H19) | 0.07 | 0.69 | 0.007 |
| LP2 (O25) | σ\*(N3-H20) | 47.14 | 0.67 | 0.160 |
| LP3 (O25) | σ\*(N3-H19) | 0.07 | 0.59 | 0.006 |
| LP3 (O25) | σ\*(C7-H9) | 0.14 | 0.66 | 0.009 |

**Table S4:**

|  |  |  |  |
| --- | --- | --- | --- |
| **Number of surface minima** | **Minimal value (kcal/mol)** | **Number of surface maxima** | **Maximal value (Kcal/mol)** |
| 1 | 114.88 | 1 | 122.86 |
| 2 | -95.18 | 2 | 122.11 |
| 3 | -101.12 | 3 | 120.05 |
| 4 | -89.17 | 4 | 48.87 |
| 5 | -101.57 | 5 | 17.79 |
|  |  | 6 | -69.42 |

**Table S5:**

|  |  |
| --- | --- |
| **Parameters** | **B3LYP / 6-311 ++ G(d. p)** |
| E HOMO (eV) | - 6.17 |
| E LUMO (eV) | - 0.61 |
| │ΔE HOMO-LUMO│(eV) | 5.56 |
| electronic affinity (A) (eV) | 0.61 |
| ionization potential (I) (eV) | 6.17 |
| electronegativity (eV) | 3.39 |
| chemical potential (μ) ( eV) | -3.39 |
| Chemical hardness (η) (eV) | 2.75 |
| softness (eV)-1 | 0.18 |
| electrophilicity (eV) | 2.09 |
| Additional electronic charges ΔΝ max | 1.23 |

I=- EHOMO . A=- ELUMO . χ=(I+A)/2 . μ=-(I+A)/2 . η=(I-A)/2 . ΔN max=- μ/ η .

**Table S6:**

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Dipole moment (Debye)** | | **Polarizability (**× 10-23) esu | | **Hyperpolarizability (**× 10-29) | |
| **µx** | 2.172 | **αxx** | 1.4227 | **βxxx** | 4.2588 |
| **µy** | -13.113 | **αxy** | 0.3603 | **βxxy** | -16.3131 |
| **µz** | 4.936 | **αyy** | 2.4740 | **βxyy** | 1.7175 |
| **µtot** | 14.179 | **αxz** | -0.0866 | **βyyy** | -167.1564 |
|  |  | **αyz** | -0.0560 | **βxxz** | 11.2995 |
|  |  | **αzz** | 1.9448 | **βxyz** | -7.7453 |
|  |  | **αtot (a.u)** | 131.39 | **βyyz** | 29.4625 |
|  |  | **αtot (e.s.u)** | 1.9471 | **βxzz** | 4.2191 |
|  |  |  |  | **βyzz** | -37.1175 |
|  |  |  |  | **βzzz** | 34.9721 |
|  |  |  |  | **βtot (a.u)** | 2702.172 |
|  |  |  |  | **βtot (e.s.u)** | 2.3344 |

α: 1a.u = 0.1482 ×10-24 esu. β: 1a.u = 8.6393×10-33