**Supplementary Information**

**Cytotoxicity evaluation and DNA binding studies of 1,3-dihydroxy-2-(4-methoxyphenyl)-4,5-dimethyl-1*H*-imidazol-3-ium chloride beyond its structural and Hirshfeld surface analysis, spectroscopic investigations, vibrational assignments, and theoretical characterizations**

Munna Mukhia [1], Sumiran Tamang [1], Koushik Chakraborty [1], Imran Habib [2], Koustav Singha [2], Sangita Dey [3], Anoop Kumar [3], Dhiraj Brahman [4], Mossaraf Hossain [2,*], Kiran Pradhan [1,**]

[1] Department of Chemistry, University of North Bengal, Raja Rammohunpur, District- Darjeeling, 734013, India
[2] Synthetic Organic Research Laboratory, University Grants Commission-Human Resource Development Centre (Chemistry), University of North Bengal, District Darjeeling, 734013, India
[3] Department of Biotechnology, University of North Bengal, Raja Rammohunpur, District-Darjeeling, 734013, India
[4] Department of Chemistry, St. Joseph's College, Post Office-North Point, District-Darjeeling, 734104, India
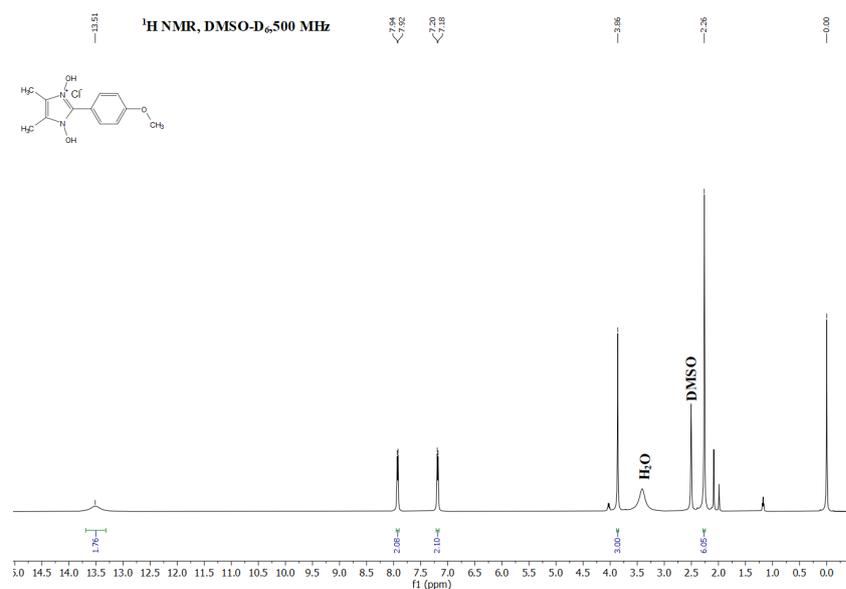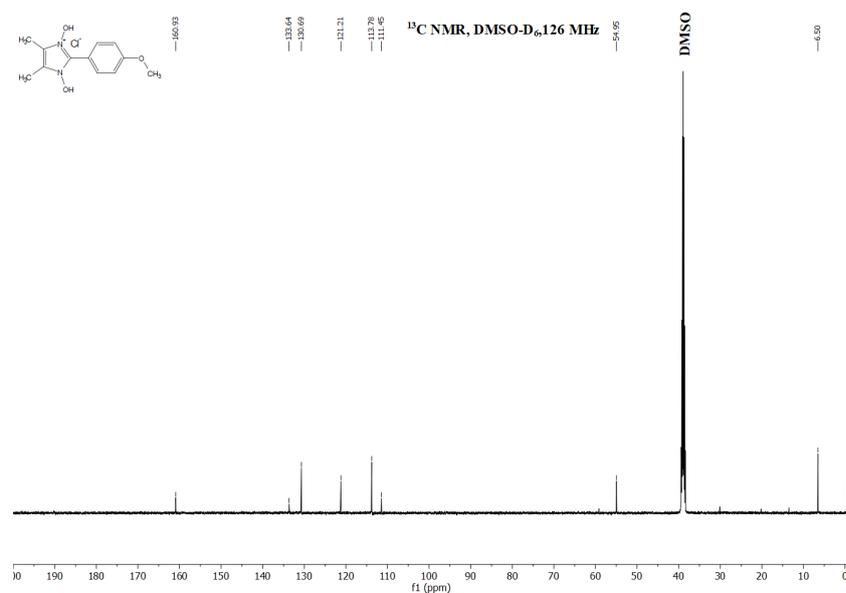
**Figure S1.** 1H NMR spectrum of DMPDI.
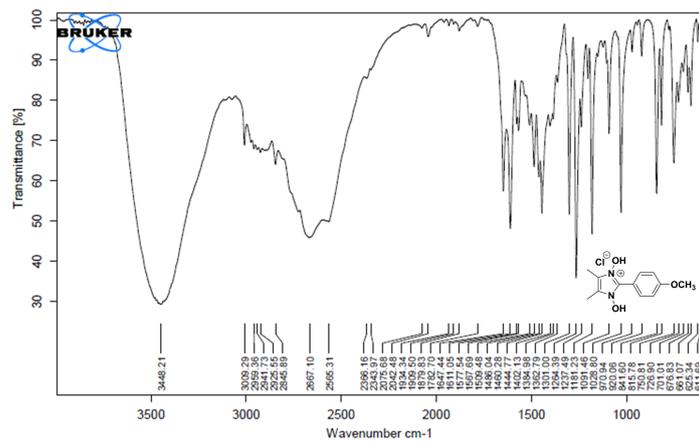


**Figure S2.** 13C NMR spectrum of DMPDI.

**Figure S3.** IR spectrum of DMPDI in KBr.

**Table S1.** Anisotropic displacement parameters (ADPs) for non-H atoms of DMPDI.

| Atom | U11 (Å²) | U22 (Å²) | U33 (Å²) | U23 (Å²) | U13 (Å²) | U12 (Å²) |
|------|----------|----------|----------|----------|----------|----------|
| Cl1  | 0.0585   | 0.0534   | 0.0661   | -0.0118  | 0.0041   | -0.0003  |
| O1   | 0.0521   | 0.0526   | 0.0388   | -0.0042  | -0.0112  | -0.0072  |
| O2   | 0.0521   | 0.0401   | 0.0489   | -0.0054  | -0.0069  | -0.0138  |
| O3   | 0.0536   | 0.0858   | 0.0432   | 0.0137   | 0.0125   | -0.0029  |
| N1   | 0.0354   | 0.0368   | 0.0341   | -0.0018  | -0.0031  | -0.0014  |
| N2   | 0.0368   | 0.0308   | 0.0374   | -0.0025  | -0.0017  | -0.0036  |
| C1   | 0.0388   | 0.0325   | 0.0364   | 0.0013   | 0.0038   | -0.0010  |
| C2   | 0.0436   | 0.0481   | 0.0383   | 0.0084   | 0.0018   | 0.0036   |
| C3   | 0.0385   | 0.0527   | 0.0454   | 0.0071   | 0.0057   | 0.0026   |
| C4   | 0.0479   | 0.0459   | 0.0381   | 0.0017   | 0.0084   | -0.0023  |
| C5   | 0.0529   | 0.0623   | 0.0331   | 0.0074   | -0.0010  | -0.0031  |
| C6   | 0.0421   | 0.0548   | 0.0407   | 0.0019   | -0.0032  | -0.0005  |
| C7   | 0.0529   | 0.0792   | 0.0627   | 0.0125   | 0.0178   | -0.0002  |
| C8   | 0.0352   | 0.0304   | 0.0364   | 0.0021   | -0.0019  | 0.0021   |
| C9   | 0.0329   | 0.0341   | 0.0430   | 0.0010   | 0.0036   | 0.0038   |
| C10  | 0.0380   | 0.0306   | 0.0402   | 0.0006   | 0.0048   | 0.0035   |
| C11  | 0.0375   | 0.0521   | 0.0631   | 0.0008   | 0.0074   | -0.0042  |
| C12  | 0.0625   | 0.0466   | 0.0405   | -0.0018  | 0.0080   | 0.0041   |

**Table S2**. Vibrational assignments of DMPDI (with proposed assignments).

| ν(cm⁻¹) B3LYP/6-31G+(d,2p) | IRᵢ | R_A | IR ν(cm⁻¹) | Raman ν(cm⁻¹) | Assignments |
|---|---|---|---|---|---|
| 3764 | 25.2875 | 40.5139 | 3448 | | ν (s) O-H -OH group |
| 3738 | 51.2234 | 110.8269 | | | ν (s) O-H -OH group |
| 3218 | 10.8673 | 134.2613 | 3009 | | ν (s) C-H Ben + ν (as) C-H methoxy |
| 3215 | 15.3567 | 80.7769 | 2845 | | ν (as) C-H Ben |
| 3198 | 10.1270 | 100.3025 | for C-H | | ν (as) C-H Ben |
| 3191 | 9.3484 | 28.7846 | stretching | | ν (as) C-H Ben |
| 3147 | 22.7854 | 166.1333 | | 3012 2849 for C-H stretching | ν (as) C-H methyl |
| 3132 | 10.4385 | 81.6981 | | | ν (as) C-Hmethyl |
| 3125 | 8.5435 | 44.8128 | | | ν (as) C-Hmethyl |
| 3094 | 17.2739 | 81.4575 | | | ν (as) C-Hmethyl |
| 3079 | 35.1632 | 58.8277 | | | ν (as) C-Hmethoxy |
| 3076 | 13.3282 | 122.3187 | | | ν (as) C-Hmethyl |
| 3034 | 41.9100 | 252.4264 | | | ν (s) C-Hmethyl |
| 3023 | 53.9626 | 378.6023 | | | ν (s) C-Hmethyl |
| 3015 | 65.6914 | 173.5073 | | | ν (s) C-Hmethoxy + ν (s) C-H Ben |
| 1658 | 114.5055 | | 1647 | 1566 | ν (s) C=C-C=C Ben + ν (s) C=N imid + ν (s) C-N imid + ν (δ) C-H Ben + ν(w) C-Hmethyl |
| 1642 | 43.8207 | 825.4187 | 1611 | 1614 | ν (s) C=C-C=C Ben + ν (s) C-N-C=C-N imid + ν (w+τ) C-Hmethyl+ ν (δ) C-H Ben |
| 1614 | 9.4273 | 52.5699 | 1577 | 1597 | ν (as) C=C-C=C Ben + ν (p) C-H Ben |
| 1571 | 100.4624 | 98.4347 | 1567 | | ν (s) C-N-C=C-N imid + ν (as) C=C-C=C Ben + ν (p) C-H Ben + ν (s) C-C Ben-Imid + ν (s) C-Omethoxy + ν (w) C-Hmethoxy |
| 1514 | 60.5088 | 921.1845 | 1509 | | ν (as) C=C-C=C Ben + ν (p) C-H Ben + ν (s) C-C Ben-Imid + ν (s) C-N-C=C-N imid + ν (s) C-Omethoxy + ν (w+τ) C-Hmethoxy + ν (w+τ) C-Hmethyl |
| 1504 | 59.1594 | 567.6697 | - | | ν (w+τ) C-Hmethoxy |
| 1498 | 1.0767 | 67.4273 | - | | ν (w+τ) C-Hmethyl + ν (w) O-H group |
| 1495 | 25.5979 | 23.7814 | - | | ν (w+τ) C-Hmethyl + ν (w) O-H group |
| 1493 | 7.4096 | 96.2881 | - | | ν (w+δ) C-Hmethoxy |
| 1479 | 11.5427 | 13.7063 | - | | ν (δ+p) C-Hmethyl |
| 1476 | 19.1520 | 23.7341 | - | 1450 | ν (w) C-Hmethoxy + ν (p) C-H Ben + ν (as) C=C-C=C Ben + ν (w+τ) C-Hmethyl |
| 1475 | 9.1363 | 11.8984 | - | | ν (δ+τ) C-Hmethyl + ν (w) C-Hmethoxy + ν (p) C-H Ben |
| 1468 | 16.7903 | 18.2275 | 1486 | 1480 | ν (as) C=C-C=C Ben + ν (δ) C-H Ben + ν (s) C-N-C=C-N imid + ν (w) C-Hmethoxy + ν (w) O-H group + ν (δ) C-Hmethyl + ν (s) N-O imid |
| 1438 | 29.2777 | 14.7851 | 1460 | 1450 | ν (w) O-H group + ν (s) N-O imid + ν (w) C-Hmethyl + ν (as) C=C-C=C Ben + ν (δ) C-H Ben |
| 1428 | 16.7316 | 14.8674 | 1444 | 1423 | ν (w) C-Hmethyl + ν (s) C=C-C=C Ben + ν (δ) C-H Ben + ν (s) C-N-C=C-N imid + ν (w) O-H group + ν (s) N-O imid |
| 1420 | 12.2954 | 95.7366 | - | 1425 | ν (w) C-Hmethyl + ν (s) C=C-C=C Ben + ν (δ) C-H Ben + ν (s) C-N-C=C-N imid + ν (w) O-H group + ν (s) N-O imid |
| 1402 | 2.3918 | 23.3178 | - | | ν (w) C-Hmethyl + ν (s) C=C-C=C Ben + ν (δ) C-H Ben + ν (s) C-N-C=C-N imid + ν (w) O-H group + ν (s) N-O imid |
| 1369 | 25.7626 | 1.0455 | 1362 | 1359 | ν (w) O-H group + ν(s) C=C-C=C Ben + ν (δ) C-H Ben + ν (s) C-N-C=C-N imid + ν (w) C-Hmethyl + ν (τ) C-Hmethoxy |
| 1345 | 7.4937 | 113.9564 | - | | ν (p) C-H Ben + ν (τ) C-Hmethoxy + ν (w) O-H group + ν(as) C=C-C=C Ben |
| 1328 | 11.0698 | 10.8393 | - | | ν (p) C-H Ben + ν(as) C=C-C=C Ben + ν (τ) C-Hmethoxy + ν (w) O-H group |
| 1309 | 11.9326 | 4.7320 | | | ν (s) C-N-C=C-N imid + ν (w) O-H group + ν (δ+τ) C-Hmethyl |
| 1291 | 333.8784 | 116.4204 | 1301 | 1302 | ν (s) C-O Ben-methoxy + ν (s) C-Omethoxy + ν(as) C=C-C=C Ben + ν (p) C-H Ben + ν (w+τ) C-Hmethyl |
| 1241 | 31.9715 | 8.6081 | 1264 | 1265 | ν (as) C-N-C=C-N imid + ν (s) C-N imid + ν (w) O-H group + ν (w+τ) C-Hmethyl + ν (w) C-Hmethyl + ν(as) C=C-C=C Ben + ν (p) C-H Ben |
| 1209 | 77.0217 | 4.7270 | - | | ν (δ) C-H Ben + ν (w) C-Hmethoxy |
| 1204 | 4.0071 | 75.0813 | 1202 | | ν (w+τ) C-Hmethoxy + ν (δ) C-H Ben |
| 1169 | 0.9289 | 4.8804 | | | ν (τ+p) C-Hmethoxy |
| 1168 | 11.0249 | 1.2488 | 1181 | 1185 | ν (s) C-N imid +ν (w+τ) C-Hmethyl + ν (as) C-N-C=C-N imid + ν(as) C=C-C=C Ben + ν (p) C-H Ben |
| 1143 | 7.9264 | 55.6914 | 1091 | | ν (δ) C-H Ben + ν (w+τ) C-Hmethoxy |
| 1103 | 11.9629 | 6.5822 | - | 1106 | ν (w+τ) C-Hmethyl + ν (s) O-N imid + ν (as) C-N-C=C-N imid + ν (p) C-H Ben + ν(as) C=C-C=C Ben |
| 1065 | 1.6671 | 47.0726 | - | | ν (τ) C-Hmethyl + ν (δ) C-H Ben |
| 1063 | 60.1674 | 1.6067 | - | | ν (s) O-Cmethoxy + ν (as) C-N-C=C-N imid + ν (p) C-H Ben + ν (τ) C-Hmethyl |
| 1054 | 5.4585 | 8.1666 | - | 972 | ν (τ) C-Hmethyl |
| 1026 | 0.4747 | 8.1688 | - | | ν(as) C=C-C=C Ben + ν (δ) C-H Ben + ν (τ) C-Hmethyl + ν (τ) C-Hmethoxy |
| 1012 | 1.7491 | 3.0063 | - | | ν (τ) C-Hmethyl + ν (as) C-N-C=C-N imid + ν (p) C-H Ben + ν (w) C-H Ben + ν(as) C=C-C=C Ben |
| 1000 | 2.4929 | 11.8717 | - | | ν (τ) C-Hmethyl + ν (w) C-H Ben |
| 974 | 5.5465 | 2.1455 | 970 | | ν (s) C-N imid + ν (τ) C-Hmethyl + ν (as) C-N-C=C-N imid + ν(as) C=C-C=C Ben |
| 948 | 0.2863 | 45.4993 | - | | ν (w) C-H Ben |

| | | | | | |
|---|---|---|---|---|---|
| 844 | 43.5197 | 0.1797 | 841 | 837 | ν (w+τ) C-H Ben |
| 831 | 5.5717 | 1.9835 | - | | ν (τ) C-Hmethyl + ν (as) C-N-C=C-N imid + ν(as) C-C=C Ben + ν (τ) C-Hmethoxy + ν (s) C-C imid-methyl + ν (s) C-O Ben-methoxy |
| 819 | 5.2454 | 22.8314 | - | 823 | ν (w) C-H Ben |
| 783 | 5.6863 | 5.9319 | 750 | 776 | ν(as) C=C-C=C Ben + ν (τ) C-Hmethyl + ν (as) C-N-C=C-N imid + ν (s) O-N imid + ν (τ) C-Hmethoxy + ν (s) C-C imid-methyl + ν (s) C-O Ben-methoxy |
| 750 | 1.7666 | 16.0100 | - | | ν (τ) C-Hmethyl + ν (as) C-N-C=C-N imid + ν (s) O-N imid + ν (s) C-C imid-methyl + ν(as) C=C-C=C Ben + ν (τ) C-Hmethoxy |
| 732 | 2.2935 | 20.8888 | - | | ν (as) C-N-C=C-N imid + ν(as) C=C-C=C Ben + ν (w) C-H Ben |
| 697 | 7.1140 | 9.6732 | 702 | | ν (τ) C-Hmethyl + ν (p) O-H group + ν (w) C-H Ben |
| 651 | 2.1335 | 12.5841 | - | | ν (τ) C-Hmethyl + ν (as) C-N-C=C-N imid + ν(as) C=C-C=C Ben + ν (τ) C-Hmethoxy |
| 636 | 3.1375 | 5.3950 | - | | ν (τ) C-Hmethyl + ν (as) C-N-C=C-N imid + ν(as) C=C-C=C Ben |
| 608. | 3.0455 | 4.1405 | - | | ν (τ) C-Hmethyl + ν (as) C-N-C=C-N imid + ν(as) C=C-C=C Ben + ν (τ) C-Hmethoxy + ν (p) C-H Ben |
| 600 | 29.7066 | 1.5614 | - | | ν (τ) C-Hmethyl + ν (τ) C-Hmethoxy + ν(as) C=C-C=C Ben |
| 576 | 7.9286 | 9.4270 | - | | ν (s) C-C imid-methyl + ν (s) N-O imid + ν (τ) C-Hmethoxy + ν (as) C-N-C=C-N imid |
| 527 | 9.0366 | 12.7153 | - | | ν (τ) C-Hmethyl + ν (τ) C-Hmethoxy + ν (w) C-H Ben |

**Table S3.** Theoretical calculated NLO properties of 1, 3-dihydroxy-2-(4-methoxyphenyl)-4, 5-dimethyl-1*H*-imidazol-3-ium chloride.

| Parameter | Urea (Standard) | DMPDI |
|---|---|---|
| **Electric dipole moment ($\mu$)** | | |
| $\mu_x$ | 0 | -4.2254 |
| $\mu_y$ | -4.06 | 1.6453 |
| $\mu_z$ | 0.0018 | 2.9311 |
| $\mu_{total}$ (debye) | 4.06 | 5.3993 |
| **Polarizability ($\alpha_{total}$)** | | |
| $\alpha_{xx}$ | -2.463084 | -12.6093006 |
| $\alpha_{yy}$ | -3.651648 | -13.70306106 |
| $\alpha_{zz}$ | -4.005846 | -15.19774698 |
| $\alpha_{xy}$ | -0.00004446 | 0.70845528 |
| $\alpha_{xz}$ | -0.010374 | -0.0060021 |
| $\alpha_{yz}$ | 0.001482 | 0.19449768 |
| $<\alpha>$ x10$^{-24}$ (esu) | -3.373526 | -13.83670288 |
| Anisotropy of polarisation $\Delta\alpha$ x10$^{-24}$ (esu) | 1.399806076 | 2.585449491 |
| **First-order hyperpolarizability ($\beta_{total}$)** | | |
| $\beta_{xxx}$ | -2.24622 x10$^{-5}$ | -0.142238299 |
| $\beta_{xyy}$ | -3.45572 x10$^{-6}$ | -0.138069837 |
| $\beta_{xzz}$ | 8.6393 x10$^{-6}$ | -0.063794319 |
| $\beta_{yyy}$ | -0.146349742 | 0.126087128 |
| $\beta_{xxy}$ | -0.005442759 | 0.306556057 |
| $\beta_{yzz}$ | 0.017710565 | -0.064239243 |
| $\beta_{zzz}$ | -0.000086393 | 0.034068216 |
| $\beta_{xxz}$ | -0.000777537 | 0.129036585 |
| $\beta_{yyz}$ | -0.000259179 | 0.174101765 |
| $\beta_{xyz}$ | 0.000431965 | 0.050748976 |
| $<\beta>$ x10$^{-30}$ (esu) | 0.134086641 | 0.606495039 |
| **Second-order hyperpolarizability ($\gamma_{total}$)** | | |
| $\gamma_{xxxx}$ | -0.060776852 | -2.595617612 |
| $\gamma_{yyyy}$ | -0.059382693 | -0.54206834 |
| $\gamma_{zzzz}$ | -0.014802861 | -0.109676711 |
| $\gamma_{xxyy}$ | -0.022175331 | -0.565234189 |
| $\gamma_{yyzz}$ | -0.01411233 | -0.103788708 |
| $\gamma_{xxzz}$ | -0.020076286 | -0.515345071 |
| $\gamma_{total}$ x10$^{-36}$ (esu) | -0.04953806 | -1.12321972 |