**Supplementary Materials**

DFT Analysis and Bioactivity of 2-((E)-(4-methoxybenzylimino)methyl)phenol and its Ni(II) and Pd(II) Complexes

Amalina Mohd Tajuddina\*, El Hassane Anouarb, \*, Kalavathy Ramasamyc, Abdulrahman I Alharthib, Hadariah Bahrona

aFaculty of Applied Sciences, Universiti Teknologi MARA, 40450 Shah Alam, Selangor, Malaysia.

*b*College of Science and Humanities, The Department of Chemistry, Prince Sattam bin Abdulaziz University, Al‐Kharj, Saudi Arabia.

*c*Faculty of Pharmacy, Universiti Teknologi MARA, 40450 Shah Alam, Selangor, Malaysia.

Table 1S Chemical Shifts of 1H NMR for L1c and PdL1c

|  |  |
| --- | --- |
| **Assignments** | **Chemical Shift (ppm)** |
| **L1c** | **PdL1c** |
| C-**C**H2 | 4.74*(s)* | 4.93*(s)* |
| N=**C**7H | 8.40*(s)* | 7.69*(s)* |
| **C**2-H (Ar) | 6.94-6.97*(m)* | 6.55-6.58*(d)* (J*HH* = 9 Hz) |
| **C**3-H (Ar) | 7.27-7.30*(m)* | 7.24-7.26*(t)* (J*HH* = 6 Hz) |
| **C**4-H (Ar) | 7.24-7.27*(m)* | 7.13-7.16*(t)* (J*HH* = 9 Hz) |
| **C**5-H (Ar) | 7.30-7.33*(m)* | 7.34-7.37*(d)* (J*HH* = 9 Hz) |
| **C**11,**C**13-H (Ar) | 6.84-6.87*(m)* | 6.52-6.55*(d)* (J*HH* = 9 Hz) |
| **C**10, **C**14-H (Ar) | 7.20-7.23*(m)* | 7.21-7.22*(d)* (J*HH* = 9 Hz) |
| Ar-O**C**H3 | 3.80*(s)* | 3.78*(s)* |
| **C**1-OH | 13.48*(b)* | - |

Note: *(s)* = singlet; *(d)* = doublet; *(t)* = triplet; *(b)* = broad; Ar = aromatic

Table 2S Chemical Shifts of 13C NMR for L1c and Pd(L1c)2

|  |  |
| --- | --- |
| **Assignments** | **Chemical Shift (ppm)** |
| **L1c** | **PdL1c** |
| C-**C**H2 | 62.5*(s)* | 58.5*(s)* |
| N=**C**7H | 161.1*(s)* | 162.8*(s)* |
| **C**2-H (Ar) | 117.0*(s)* | 120.3*(s)* |
| **C**3-H (Ar) | 132.2*(s)* | 134.7*(s)* |
| **C**4-H (Ar) | 118.6*(s)* | 129.6*(s)* |
| **C**5-H (Ar) | 131.4*(s)* | 134.2*(s)* |
| **C**10, **C**14-H (Ar) | 114.0*(s)* | 114.0*(s)* |
| **C**11, **C**13-H (Ar) | 130.2*(s)* | 130.9*(s)* |
| Ar-O**C**H3 | 55.3*(s)* | 55.2*(s)* |
| **C**1-OH | 165.1*(s)* | - |

Note: *(s)* = singlet; Ar = aromatic

**Table 3S**. NMR correlation coefficient between predicted and experimental chemical shifts of L1c.

|  |  |  |  |
| --- | --- | --- | --- |
| Method | 1H-NMR |  | 13C-NMR |
| Gas | PCM |  | Gas | PCM |
| B3LYP | 98.76 | 99.33 |  | 93.09 | 92.84 |
| B3P86 | 97.18 | 98.27 |  | 92.99 | 92.75 |
| CAM-B3LYP | 98.6 | 99.5 |  | 93.05 | 92.74 |
| M06-2X | 96.65 | 99.42 |  | 93.07 | 92.69 |
| PBE0 | 98.32 | 98.85 |  | 93.01 | 92.74 |

**Table 4S**. NMR correlation coefficient between predicted and experimental chemical shifts of Pd(L1c)2.

|  |  |  |  |
| --- | --- | --- | --- |
| Method | 1H-NMR |  | 13C-NMR |
| Gas | PCM |  | Gas | PCM |
| B3LYP | 74.47 | 82.71 |  | 76.83 | 76.4 |
| B3P86 | 71.08 | 90.32 |  | 76.83 | 76.41 |
| CAM-B3LYP | 73.79 | 89.42 |  | 76.24 | 75.79 |
| M06-2X | 80.03 | 90.29 |  | 78.62 | 78.45 |
| PBE0 | 72.41 | 90.4 |  | 76.85 | 76.44 |

**Table 5S** Calculated interatomic bond distances (Å), bond and torsion angles (degrees) for L1c and its complexes Ni(L1c)2 and Pd(L1c)2 calculated at B3LYP in gas and PCM.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
|  | **L1c** |  | **Ni(L1c)2** |  | **Pd(L1c)2** |
|  | Gas | PCM | Exp |  | Gas | PCM | X-Ray |  | Gas | PCM | X-Ray |
| Bond |  |  |  |  |  |  |  |  |  |  |  |
| C1-O1 | 1.3684 | 1.3738 | 1.3671 ± |  | 1.33649 | 1.33804 | 1.30847 ± |  | 1.33925 | 1.34139 | 1.31044 ±  |
| O1-H | 1.0369 | 1.0472 | 0.9719 ± |  |  |  |  |  |  |  |  |
| C1-C2 | 1.4116 | 1.4107 | 1.4144 ± |  | 1.42669 | 1.42744 | 1.42145 ± |  | 1.42852 | 1.42861 | 1.41298 ± |
| C1-C6 | 1.4328 | 1.4323 | 1.4081 ± |  | 1.42942 | 1.43141 | 1.41364 ± |  | 1.43504 | 1.43497 | 1.41588 ± |
| C6-C7 | 1.4579 | 1.4596 | 1.4665 ± |  | 1.43771 | 1.43957 | 1.43576 ± |  | 1.44337 | 1.44495 | 1.4284 ± |
| C7=N | 1.3079 | 1.3083 | 1.2878 ± |  | 1.31544 | 1.31498 | 1.29746 |  | 1.31203 | 1.31238 | 1.28573 ± |
| C7-H | 1.0994 | 1.0971 | 1.1159 ± |  | 1.09476 | 1.09395 | 0.95024 ± |  | 1.09482 | 1.09406 | 0.92968 ± |
| N-C8 | 1.4766 | 1.4775 | 1.4394 ± |  | 1.51239 | 1.51218 | 1.48657 |  | 1.50781 | 1.50745 | 1.48594 ± |
| C8-C9 | 1.5241 | 1.5238 | 1.5014 ± |  | 1.5217 | 1.52176 | 1.51316 ± |  | 1.52149 | 1.52233 | 1.50541 ± |
| C9-C10 | 1.4161 | 1.4166 | 1.4052 ± |  | 1.41373 | 1.41363 | 1.39924 ± |  | 1.41376 | 1.41414 | 1.39031 ± |
| C9-C14 | 1.4043 | 1.4053 | 1.3942 ± |  | 1.41004 | 1.41072 | 1.38838 ± |  | 1.40959 | 1.41027 | 1.37229 ± |
| C12-O | 1.3982 | 1.3993 | 1.3818 ± |  | 1.39845 | 1.39896 | 1.3735 ± |  | 1.39803 | 1.39844 | 1.37408 ± |
| O-C15 | 1.4559 | 1.4619 | 1.4227 ± |  | 1.45581 | 1.46205 | 1.4269 ± |  | 1.45601 | 1.46217 | 1.41608 ± |
| Bond angles (°) |  |  |  |  |  |  |  |  |  |  |  |
| C1-O1-H | 107.4 | 106.8 | 109.9 ± |  | 120.7 | 121.0 | 120.5 ± |  | 123.5 | 123.6 | 122.8 ± |
| C1-C6-C7 | 119.8 | 119.8 | 125.0 ± |  | 115.0 | 115.2 | 116.8 ± |  | 114.3 | 114.3 | 115.9 ± |
| C6-C7-H | 117.0 | 117.3 | 113.2 ± |  | 127.8 | 127.5 | 126.4 ± |  | 129.1 | 128.9 | 128.3 ± |
| C6-C7-N | 119.8 | 121.2 | 124.0 ± |  | 114.3 | 114.8 | 114.7 ± |  | 116.6 | 116.6 | 117.3 ± |
| C7-N-C8 | 119.8 | 119.6 | 120.2 ± |  | 113.2 | 113.2 | 110.5 ± |  | 112.7 | 112.5 | 111.0 ± |
| N-C8-C9 | 113.9 | 113.9 | 114.6 ± |  | 118.6 | 118.6 | 117.3 ± |  | 118.6 | 118.6 | 118.5 ± |
| C12-O-C15 | 118.5 | 118.4 | 116.1 ± |  | 120.7 | 121.0 | 120.5 ± |  | 123.5 | 123.6 | 122.8 ± |
| Torsion angles (°) |  |  |  |  |  |  |  |  |  |  |  |
| C1-C6-C7-N | 0.0 | 0.0 | 0.0 ± |  | -2.6 | -4.4 | 7.0 ± |  | 0.4 | 2.1 | 8.2 ± |
| C6-C7-N-C8 | 180.0 | 180.0 | 180.0 ± |  | 178.1 | 177.5 | -170.4 ± |  | 178.9 | -177.3 | -171.8 ± |
| C7-N-C8-C9 | 180.0 | 180.0 | 180.0 ± |  | 76.8 | 69.2 | 99.9 ± |  | 79.0 | 82.6 | 99.4 ± |
| N-C8-C9-C14 | 0.0 | 0.0 | 0.0 ± |  | 66.7 | 62.6 | 95.4 ± |  | 74.2 | 76.0 | 95.2 ± |
| C13-C12-O-C15 | 0.0 | 0.0 | 0.0 ± |  | -0.2 | -0.3 | 3.8 ± |  | -0.3 | -0.4 | 2.9 ± |

**Table 6S**

Correlation coefficients between calculated and experimental internal coordinates (Bond lengths, bond angles, and torsion angles) of L1c and its complexes Ni(L1c)2 and Pd(L1c)2.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
|  | L1c |  | Ni(L1c)2 |  | Pd(L1c)2 |
| **Bond lengths** | Gas | PCM |  | Gas | PCM |  | Gas | PCM |
| B3LYP | 97.95 | 97.49 |  | 98.13 | 98.08 |  | 98.03 | 97.96 |
| B3P86 | 97.34 | 96.50 |  | 98.36 | 98.28 |  | 98.15 | 98.10 |
| CAM-B3LYP | 98.38 | 98.00 |  | 98.04 | 98.04 |  | 97.83 | 97.79 |
| M06-2X | 98.45 | 98.04 |  | 98.83 | 98.08 |  | 97.74 | 97.79 |
| PBE0 | 79.79 | 97.18 |  | 98.04 | 98.27 |  | 98.08 | 98.04 |
|  |  |  |  |  |  |  |  |  |
| **Bond Angles** |  |  |  |  |  |  |  |  |
| B3LYP | 66.03 | 67.79 |  | 91.68 | 92.79 |  | 96.38 | 96.81 |
| B3P86 | 65.10 | 61.33 |  | 94.80 | 94.55 |  | 97.29 | 97.78 |
| CAM-B3LYP | 69.77 | 68.88 |  | 92.50 | 94.11 |  | 97.07 | 97.51 |
| M06-2X | 72.66 | 69.15 |  | 95.14 | 96.57 |  | 98.60 | 98.80 |
| PBE0 | 67.15 | 63.60 |  | 95.95 | 94.83 |  | 97.17 | 97.74 |
|  |  |  |  |  |  |  |  |  |
| **Torsion Angles** |  |  |  |  |  |  |  |  |
| B3LYP | 100.00 | 100.00 |  | 33.28 | 36.88 |  | 31.17 | 99.76 |
| B3P86 | 100.00 | 100.00 |  | 38.82 | 37.57 |  | 99.63 | 99.72 |
| CAM-B3LYP | 100.00 | 100.00 |  | 37.48 | 99.53 |  | 99.70 | 99.74 |
| M06-2X | 100.00 | 100.00 |  | 37.34 | 99.82 |  | 99.76 | 99.91 |
| PBE0 | 100.00 | 100.00 |  | 99.82 | 37.25 |  | 99.64 | 99.72 |