**An *in vitro* Investigation of the Cytotoxic Activity Supported by the Quantum Chemical Analyses and Molecular Docking of the Novel Ag(I)-NHC complex**

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**3. 1. Preparation of NHC (1) precursor and Ag(I)-NHC (2) complex**



**Figure S1.**LC-MS spectrum of **2**

***3.2. Molecular Geometry and Stability***

|  |  |
| --- | --- |
| NHC precursor **(1)** | Ag(I)-NHCcomplex **(2)** |
| **L6**  **L5**  **L4**  **L3**  **L2**  **L1** | **C4**  **C3**  **C2**  **C1** |
| **L8**  **L7**  **L14** | **C8**  **C6**  **C7**  **C5** |
| **L11**  **L10**  **L14**  **L8**  **L9** | **C12**  **C10**  **C11**  **C9** |
| **L14**  **L9**  **L11**  **L8** | **C8**  **C8**  **C14**  **C13** |
| **L14**  **L13**  **L12**  **L8** | **C8**  **C14**  **C13**  **C8** |

**Figure S2.** Potential Energy Surface scan as a function the dihedral angles:τ1 (C13-N12-C14-C17); τ2 (N12-C14-C17-C19), τ3 (C1-N11-C40-C49); τ4 (N11-C40-C49-C50); τ5 (N11-C40-C49-C43) for NHC precursor **(1)** and τ5 (C1-C40-C49-C43) for Ag(I)-NHC complex (**2**)

**Table S1a.** The PES scan as a function of each torsion angle for the NHC precursor **(1)** at the B3LYP/6-31G(d,p) level of the theory, in vacuum

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **τ1 (C13-N12-C14-C17)** | | |  | **τ2 (N12-C14-C17-C19)** | | |  | **τ3 (C1-N11-C40-C49)** | | |  | **τ4 (N11-C40-C49-C50)** | | |  | **τ5 (N11-C40-C49-C43)** | | |
| Dihedral angle | Energy (au) | ΔE/  kcalmol-1 |  | Dihedral angle | Energy (au) | ΔE/  kcalmol-1 |  | Dihedral angle | Energy (au) | ΔE/  kcalmol-1 |  | Dihedral angle | Energy (au) | ΔE/  kcalmol-1 |  | Dihedral angle | Energy (au) | ΔE/  kcalmol-1 |
| **89** | **-3535.8647** | **0.5864** |  | 71 | -3535.8678 | 0.5864 |  | 35 | -3535.8615 | 4.9659 |  | **0** | **-3535.8687** | **0.4385** |  | **-180** | **-3535.8687** | **1.4658** |
| 104 | -3535.8638 | 2.4911 |  | **86** | **-3535.8687** | **0.0000** |  | 50 | -3535.8646 | 3.0394 |  | 15 | -3535.8680 | 0.8781 |  | -165 | -3535.8679 | 1.9650 |
| 119 | -3535.8638 | 2.4672 |  | 101 | -3535.8685 | 0.1470 |  | 65 | -3535.8668 | 1.6694 |  | 30 | -3535.8665 | 1.8303 |  | -150 | -3535.8663 | 3.0015 |
| **134** | **-3535.8641** | **2.2941** |  | 116 | -3535.8666 | 1.3433 |  | 80 | -3535.8680 | 0.8691 |  | 45 | -3535.8646 | 3.0019 |  | -135 | -3535.8643 | 4.2132 |
| 149 | -3535.8639 | 2.4138 |  | 131 | -3535.8630 | 3.5797 |  | 95 | -3535.8686 | 0.5149 |  | 60 | -3535.8630 | 4.0137 |  | -120 | -3535.8633 | 4.8771 |
| 164 | -3535.8628 | 3.0811 |  | 146 | -3535.8588 | 6.2113 |  | **110** | **-3535.8687** | **0.4220** |  | 75 | -3535.8618 | 4.7425 |  | -105 | -3535.8691 | 1.1947 |
| 179 | -3535.8614 | 4.0000 |  | 161 | -3535.8577 | 6.8777 |  | 125 | -3535.8686 | 0.5285 |  | 90 | -3535.8673 | 1.3469 |  | -90 | -3535.8708 | 0.1310 |
| 194 | -3535.8619 | 3.6638 |  | 176 | -3535.8569 | 7.3864 |  | 140 | -3535.8681 | 0.8367 |  | 105 | -3535.8680 | 0.8707 |  | **-75** | **-3535.8710** | **0.0000** |
| 209 | -3535.8648 | 1.8620 |  | 191 | -3535.8620 | 4.2342 |  | **155** | **-3535.8687** | **0.4585** |  | 120 | -3535.8689 | 0.3202 |  | -60 | -3535.8697 | 0.8286 |
| 224 | -3535.8670 | 0.4430 |  | 206 | -3535.8644 | 2.6690 |  | 170 | -3535.8685 | 0.5945 |  | **135** | **-3535.8694** | **0.0000** |  | -45 | -3535.8681 | 1.8420 |
| 239 | -3535.8675 | 0.1511 |  | 221 | -3535.8665 | 1.3828 |  | 185 | -3535.8666 | 1.7714 |  | 150 | -3535.8680 | 0.9106 |  | -30 | -3535.8663 | 2.9881 |
| **254** | **-3535.8678** | **0.0000** |  | **236** | **-3535.8677** | **0.6280** |  | **200** | **-3535.8671** | **1.4406** |  | 165 | -3535.8660 | 2.1484 |  | -15 | -3535.8645 | 4.0950 |
| 269 | -3535.8670 | 0.4480 |  | 251 | -3535.8674 | 0.7943 |  | 215 | -3535.8668 | 1.6606 |  | 180 | -3535.8639 | 3.4627 |  | 0 | -3535.8638 | 4.5574 |
| 284 | -3535.8651 | 1.6502 |  | 266 | -3535.8655 | 1.9949 |  | 230 | -3535.8659 | 2.1868 |  | 195 | -3535.8637 | 3.5834 |  | 15 | -3535.8645 | 4.0938 |
| 299 | -3535.8623 | 3.4106 |  | 281 | -3535.8627 | 3.7846 |  | 245 | -3535.8657 | 2.3310 |  | 210 | -3535.8649 | 2.8550 |  | 30 | -3535.8663 | 2.9923 |
| 314 | -3535.8617 | 3.7898 |  | 296 | -3535.8593 | 5.8743 |  | **260** | **-3535.8657** | **2.3238** |  | 225 | -3535.8657 | 2.3244 |  | 45 | -3535.8678 | 2.0510 |
| 329 | -3535.8631 | 2.9115 |  | 311 | -3535.8584 | 6.4456 |  | 275 | -3535.8647 | 2.9753 |  | **240** | **-3535.8671** | **1.4472** |  | **60** | **-3535.8681** | **1.8469** |
| **344** | **-3535.8638** | **2.5046** |  | 326 | -3535.8579 | 6.7563 |  | 290 | -3535.8691 | 0.1849 |  | 255 | -3535.8668 | 1.6651 |  | 75 | -3535.8671 | 2.4530 |
| 359 | -3535.8635 | 2.6697 |  | 341 | -3535.8578 | 6.8087 |  | 305 | -3535.8692 | 0.1141 |  | 270 | -3535.8657 | 2.3308 |  | 90 | -3535.8655 | 3.4877 |
| **374** | **-3535.8644** | **2.0932** |  | 356 | -3535.8583 | 6.5478 |  | **320** | **-3535.8694** | **0.0000** |  | 285 | -3535.8686 | 0.5171 |  | 105 | -3535.8686 | 1.5491 |
| 389 | -3535.8633 | 2.7733 |  | 371 | -3535.8591 | 6.0385 |  | 335 | -3535.8686 | 0.5165 |  | **300** | **-3535.8689** | **0.3485** |  | **120** | **-3535.8689** | **1.3705** |
| 404 | -3535.8609 | 4.2862 |  | 386 | -3535.8645 | 2.6060 |  | 350 | -3535.8665 | 1.8191 |  | 315 | -3535.8687 | 0.4320 |  | 135 | -3535.8687 | 1.4683 |
| 419 | -3535.8634 | 2.7410 |  | 401 | -3535.8665 | 1.3500 |  | 365 | -3535.8638 | 3.5519 |  | 330 | -3535.8680 | 0.8577 |  | 150 | -3535.8680 | 1.8846 |
| 434 | -3535.8640 | 2.3399 |  | **416** | **-3535.8675** | **0.7415** |  | 380 | -3535.8621 | 4.6137 |  | 345 | -3535.8685 | 0.5476 |  | 165 | -3535.8685 | 1.5823 |
| **449** | **-3535.8644** | **2.0906** |  | 431 | -3535.8671 | 1.0156 |  | 395 | -3535.8619 | 4.7320 |  | 360 | -3535.8687 | 0.4384 |  | 180 | -3535.8687 | 1.4658 |

**Table S1b.** The PES scan as a function of each torsion angle for the Ag(I)-NHC complex (**2**) complex at the B3LYP/6-31G(d,p)/LANL2DZ level of the theory, in vacuum

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **τ1 (C13-N12-C14-C17)** | | |  | **τ2 (N12-C14-C17-C19)** | | |  | **τ3 (C1-N11-C40-C49)** | | |  | **τ4 (N11-C40-C49-C50)** | | |  | **τ5 (C1-C40-C49-C43)** | | |
| Dihedral angle | Energy (au) | ΔE/  kcalmol-1 |  | Dihedral angle | Energy (au) | ΔE/  kcalmol-1 |  | Dihedral angle | Energy (au) | ΔE/  kcalmol-1 |  | Dihedral angle | Energy (au) | ΔE/  kcalmol-1 |  | Dihedral angle | Energy (au) | ΔE/  kcalmol-1 |
| 91 | -3680.7797 | 0.6116 |  | 69 | -3680.7795 | 0.7788 |  | 35 | -3680.7730 | 4.4256 |  | **0** | **-3680.7795** | **0.6027** |  | -165 | -3680.7789 | 1.0416 |
| **106** | **-3680.7807** | **0.0000** |  | 84 | -3680.7795 | 0.7811 |  | 50 | -3680.7766 | 2.1768 |  | 15 | -3680.7793 | 0.7388 |  | **-150** | **-3680.7795** | **0.6459** |
| 121 | -3680.7806 | 0.0593 |  | 99 | -3680.7799 | 0.5385 |  | 65 | -3680.7789 | 0.7269 |  | 30 | -3680.7782 | 1.4160 |  | -135 | -3680.7790 | 0.9681 |
| 136 | -3680.7796 | 0.6518 |  | 114 | -3680.7806 | 0.0732 |  | 80 | -3680.7795 | 0.3162 |  | 45 | -3680.7766 | 2.3966 |  | -120 | -3680.7775 | 1.8780 |
| 151 | -3680.7777 | 1.8740 |  | **129** | **-3680.7807** | **0.0000** |  | **95** | **-3680.7800** | **0.0000** |  | 60 | -3680.7752 | 3.2703 |  | -105 | -3680.7760 | 2.8476 |
| 166 | -3680.7752 | 3.4446 |  | 144 | -3680.7803 | 0.2648 |  | 110 | -3680.7787 | 0.8004 |  | 75 | -3680.7751 | 3.3653 |  | -90 | -3680.7750 | 3.4815 |
| 181 | -3680.7739 | 4.2511 |  | 159 | -3680.7795 | 0.7359 |  | 125 | -3680.7771 | 1.8565 |  | 90 | -3680.7764 | 2.5292 |  | -75 | -3680.7753 | 3.2692 |
| 196 | -3680.7752 | 3.4317 |  | 174 | -3680.7786 | 1.3007 |  | 140 | -3680.7752 | 3.0561 |  | 105 | -3680.7779 | 1.6243 |  | -60 | -3680.7767 | 2.3932 |
| 211 | -3680.7776 | 1.8924 |  | 189 | -3680.7781 | 1.6299 |  | 155 | -3680.7732 | 4.2974 |  | **120** | **-3680.7784** | **1.2965** |  | -45 | -3680.7780 | 1.5868 |
| 226 | -3680.7795 | 0.7344 |  | 204 | -3680.7781 | 1.6348 |  | 170 | -3680.7739 | 3.8509 |  | 135 | -3680.7779 | 1.6110 |  | **-30** | **-3680.7784** | **1.3464** |
| **241** | **-3680.7804** | **0.1526** |  | 219 | -3680.7785 | 1.3585 |  | 185 | -3680.7757 | 2.7158 |  | 150 | -3680.7765 | 2.4687 |  | -15 | -3680.7776 | 1.8177 |
| 256 | -3680.7803 | 0.2050 |  | 234 | -3680.7791 | 0.9985 |  | 200 | -3680.7772 | 1.7422 |  | 165 | -3680.7749 | 3.4594 |  | 0 | -3680.7761 | 2.7525 |
| 271 | -3680.7794 | 0.7681 |  | **249** | **-3680.7795** | **0.7651** |  | 215 | -3680.7782 | 1.1291 |  | 180 | -3680.7747 | 3.5874 |  | 15 | -3680.7748 | 3.5951 |
| 286 | -3680.7792 | 0.9420 |  | 264 | -3680.7795 | 0.7823 |  | 230 | -3680.7787 | 0.8049 |  | 195 | -3680.7766 | 2.3932 |  | 30 | -3680.7748 | 3.6076 |
| 301 | -3680.7783 | 1.4968 |  | 279 | -3680.7798 | 0.5871 |  | 245 | -3680.7792 | 0.4993 |  | 210 | -3680.7790 | 0.8758 |  | 45 | -3680.7767 | 2.4247 |
| 316 | -3680.7778 | 1.7866 |  | 294 | -3680.7805 | 0.1341 |  | **260** | **-3680.7796** | **0.2800** |  | **225** | **-3680.7804** | **0.0000** |  | 60 | -3680.7792 | 0.8369 |
| **331** | **-3680.7779** | **1.7215** |  | **309** | **-3680.7806** | **0.0977** |  | 275 | -3680.7789 | 0.7145 |  | 240 | -3680.7804 | 0.0066 |  | **75** | **-3680.7805** | **0.0000** |
| 346 | -3680.7775 | 1.9576 |  | 324 | -3680.7802 | 0.3418 |  | 290 | -3680.7764 | 2.2899 |  | 255 | -3680.7791 | 0.8458 |  | 90 | -3680.7803 | 0.1322 |
| 361 | -3680.7771 | 2.2219 |  | 339 | -3680.7794 | 0.8026 |  | **305** | **-3680.7786** | **0.8940** |  | 270 | -3680.7769 | 2.2232 |  | 105 | -3680.7788 | 1.0980 |
| 376 | -3680.7771 | 2.2312 |  | 354 | -3680.7787 | 1.2772 |  | 320 | -3680.7753 | 2.9623 |  | 285 | -3680.7753 | 3.2041 |  | 120 | -3680.7766 | 2.4581 |
| **391** | **-3680.7773** | **2.0983** |  | 369 | -3680.7782 | 1.5848 |  | 335 | -3680.7718 | 5.1399 |  | 300 | -3680.7751 | 3.3568 |  | 135 | -3680.7752 | 3.3079 |
| 406 | -3680.7773 | 2.1030 |  | 384 | -3680.7781 | 1.6300 |  | 350 | -3680.7713 | 5.4623 |  | 315 | -3680.7760 | 2.8179 |  | 150 | -3680.7751 | 3.4000 |
| 421 | -3680.7783 | 1.4594 |  | 399 | -3680.7784 | 1.4247 |  | 365 | -3680.7729 | 4.4863 |  | 330 | -3680.7774 | 1.9106 |  | 165 | -3680.7760 | 2.8424 |
| 436 | -3680.7792 | 0.8923 |  | 414 | -3680.7790 | 1.0585 |  | 380 | -3680.7754 | 2.8890 |  | 345 | -3680.7787 | 1.0730 |  | 180 | -3680.7775 | 1.9211 |
| 451 | -3680.7797 | 0.6116 |  | **429** | **-3680.7795** | **0.7788** |  | **395** | **-3680.7783** | **1.1023** |  | **360** | **-3680.7794** | **0.6243** |  | **195** | **-3680.7789** | **1.0417** |

|  |  |  |  |
| --- | --- | --- | --- |
|  |  |  |  |
| **L1** | **L2** | **L3** | **L4** |
|  |  |  |  |
| **L5** | **L6** | **L7** | **L8** |
|  |  |  |  |
| **L9** | **L10** | **L11** | **L12** |
|  |  |  |  |
| **L13** | **L14** |  |  |

**Figure S3a.** The conformational structures predicted in PES scan of the NHC precursor **(1)** at B3LYP/6-31G(d,p) in vacuum.

|  |  |  |  |
| --- | --- | --- | --- |
|  |  |  |  |
| **C1** | **C2** | **C3** | **C4** |
|  |  |  |  |
| **C5** | **C6** | **C7** | **C8** |
|  |  |  |  |
| **C9** | **C10** | **C11** | **C12** |
|  |  |  |  |
| **C13** | **C14** |  |  |

**Figure S3b.** The conformational structures predicted in PES scan of the Ag(I)-NHC complex (**2**) complex at B3LYP/6-31G(d,p) in vacuum

**Table S2a.** The relative energies for the stable conformers of the NHC precursor **(1)** at 6-31+G(d,p) basis set

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | **Vacuum** | | | |  | **CHCl3** | | | |
| **Conf.** | **Tot. energy/ hartree** | **ΔE/**  **kcalmol-1** | **Free energy/ hartree** | **ΔG/ kcalmol-1** |  | **Tot. energy/ hartree** | **ΔE/ kcalmol-1** | **Free energy/ hartree** | **ΔG/ kcalmol-1** |
| **L1** | -3535,483194 | 0,83145 | -3535,540943 | 1,05422 |  | -3535,50241 | 0,23218 | -3535,56191 | 0,00000 |
| **L2** | -3535,478061 | 4,05246 | -3535,535145 | 4,69252 |  | -3535,49931 | 2,17432 | -3535,55921 | 1,69490 |
| **L3** | **-----** | **-----** | **-----** | **-----** |  | -3535,50047 | 1,44641 | -3535,55943 | 1,55748 |
| **L4** | -3535,474407 | 6,34538 | -3535,532296 | 6,48029 |  | -3535,49848 | 2,69766 | -3535,55577 | 3,85354 |
| **L5** | -3535,474680 | 6,17407 | -3535,532348 | 6,44766 |  | -3535,49890 | 2,43160 | -3535,55703 | 3,06287 |
| **L6** | -3535,473869 | 6,68298 | -3535,533160 | 5,93812 |  | -3535,50088 | 1,19352 | -3535,56017 | 1,09375 |
| **L7** | -3535,478703 | 3,64960 | -3535,537468 | 3,23481 |  | -3535,50011 | 1,67545 | -3535,55896 | 1,85492 |
| **L8** | -3535,475505 | 5,65637 | -3535,533421 | 5,77434 |  | -3535,49976 | 1,89194 | -3535,55786 | 2,54141 |
| **L9** | -3535,478010 | 4,08446 | -3535,535750 | 4,31287 |  | -3535,49854 | 2,66190 | -3535,55639 | 3,46322 |
| **L10** | -3535,479906 | 2,89470 | -3535,537634 | 3,13064 |  | -3535,49913 | 2,28853 | -3535,55706 | 3,04656 |
| **L11** | -3535,484519 | 0,00000 | -3535,542623 | 0,00000 |  | -3535,50278 | 0,00000 | -3535,56108 | 0,52334 |
| **L12** | -3535,482136 | 1,49536 | -3535,540988 | 1,02598 |  | -3535,50214 | 0,40223 | -3535,56094 | 0,60806 |

**Table S2b.** The relative energies for the stable conformers of the Ag(I)-NHC complex (**2**) molecule at 6-31+G(d,p)/LANL2DZ basis set

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | **Vacuum** | | | |  | **CHCl3** | | | |
| **Conf.** | **Tot. energy/ hartree** | **ΔE/**  **kcalmol-1** | **Free energy/ hartree** | **ΔG/ kcalmol-1** |  | **Tot. energy/ hartree** | **ΔE/ kcalmol-1** | **Free energy/ hartree** | **ΔG/ kcalmol-1** |
| **C1** | -3680.382530 | 0.19139 | -3680.445251 | 0.32568 |  | -3680402801 | 0.06401 | -3680.465458 | 0.79066 |
| **C2** | -3680.382526 | 0.19390 | -3680.446599 | 0.00000 |  | -3680.402903 | 0.00000 | -3680.466718 | 0.00000 |
| **C3** | **-----** | **-----** | **-----** | **-----** |  | -3680.401402 | 0.94189 | -3680.464451 | 1.42256 |
| **C4** | -3680.382333 | 0.31501 | -3680.445016 | 0.99335 |  | -3680.402603 | 0.18825 | -3680.465172 | 0.97013 |
| **C5** | -3680.380741 | 1.31400 | -3680.443696 | 1.82166 |  | -3680.400872 | 1.27447 | -3680.464016 | 1.69553 |
| **C6** | -3680.382598 | 0.14872 | -3680.446041 | 0.35015 |  | -3680.402852 | 0.03200 | -3680.465718 | 0.62751 |
| **C7** | -3680.382835 | 0.00000 | -3680.445770 | 0.52021 |  | -3680.402569 | 0.20959 | -3680.465209 | 0.94691 |
| **C8** | -3680.380844 | 1.24937 | -3680.443738 | 1.79530 |  | -3680.400938 | 1.23306 | -3680.463316 | 2.13479 |
| **C9** | -3680.381857 | 0.61370 | -3680.444416 | 1.36985 |  | -3680.400843 | 1.29267 | -3680.462577 | 2.59852 |

**Table S3.** The Boltzmann population (%) calculated from the relative electronic (**ΔE**) and free energy values (**ΔG)** of the conformers

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | NHC precursor **(1)** | | | | |  | Ag(I)-NHC complex (**2**) | | | | | |
|  | **Vacuum** | |  | **CHCl3** | |  |  | **Vacuum** | |  | **CHCl3** | |
| **Conf.** | *Bolt.dist./*  *%(ΔE)* | *Bolt.dist./*  *%(ΔG)* |  | *Bolt.dist./*  *%(ΔE)* | *Bolt.dist./*  *%(ΔG)* |  | **Conf.** | *Bolt.dist./*  *%(ΔE)* | *Bolt.dist./*  *%(ΔG)* |  | *Bolt.dist./*  *%(ΔE)* | *Bolt.dist./*  *%(ΔG)* |
| **L1** | 0.091 | 0.090 |  | 0.083 | 0.083 |  | **C1** | 0.125 | 0.125 |  | 0.111 | 0.111 |
| **L2** | 0.091 | 0.091 |  | 0.083 | 0.083 |  | **C2** | 0.125 | 0.125 |  | 0.111 | 0.111 |
| **L3** | **-----** | **-----** |  | 0.083 | 0.083 |  | **C3** | **-----** | **-----** |  | 0.111 | 0.111 |
| **L4** | 0.091 | 0.091 |  | 0.083 | 0.084 |  | **C4** | 0.125 | 0.125 |  | 0.111 | 0.111 |
| **L5** | 0.090 | 0.091 |  | 0.083 | 0.083 |  | **C5** | 0.125 | 0.125 |  | 0.111 | 0.111 |
| **L6** | 0.091 | 0.091 |  | 0.083 | 0.083 |  | **C6** | 0.125 | 0.125 |  | 0.111 | 0.111 |
| **L7** | 0.091 | 0.091 |  | 0.083 | 0.083 |  | **C7** | 0.125 | 0.125 |  | 0.111 | 0.111 |
| **L8** | 0.091 | 0.091 |  | 0.083 | 0.083 |  | **C8** | 0.125 | 0.125 |  | 0.111 | 0.111 |
| **L9** | 0.091 | 0.091 |  | 0.083 | 0.084 |  | **C9** | 0.125 | 0.125 |  | 0.111 | 0.111 |
| **L10** | 0.091 | 0.090 |  | 0.083 | 0.083 |  |  |  |  |  |  |  |
| **L11** | 0.091 | 0.090 |  | 0.083 | 0.083 |  |  |  |  |  |  |  |
| **L12** | 0.091 | 0.090 |  | 0.083 | 0.083 |  |  |  |  |  |  |  |

***3. 3. FT-IR Spectral Analysis***

**Table S4.** The observed and calculated vibrational frequencies (in cm-1) of NHC precursor **(1)** salt and Ag(I)-NHC complex (**2**) complex at B3LYP/6-31+G(d,p)/LANL2DZ level in CHCl3

|  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  |  |  |  |  | NHC precursor **(1)** |  |  |  |  |  | Ag(I)-NHC complex (**2**) |
| *Exp.* | *Mod nos* | *Unscal.* | *Scal.* | *IIR* | *PED %*a | *Exp.* | *Mod nos.* | *Unscal* | *Scal.* | *IIR* | *PED %*a |
|  | 150 | 3336 | 3218 | 39 | νC13H (99) | 3062 | 150 | 3248 | 3079 | 17 | νasC50H2 (99) |
| 3104 | 149 | 3245 | 3131 | 17 | νasC50H2 (100) |  | 149 | 3231 | 3063 | 5 | νCH R**A** (85) |
|  | 148 | 3228 | 3114 | 4 | νCH R**A** (92) |  | 148 | 3225 | 3057 | 10 | νasCH R**A** (80) |
|  | 147 | 3225 | 3111 | 8 | νasCH R**A** (89) |  | 147 | 3222 | 3054 | 10 | νCH R**C** (92) |
|  | 146 | 3220 | 3107 | 13 | νCH R**C** (96) |  | 146 | 3212 | 3045 | 15 | νasCH R**A** (86) |
|  | 145 | 3213 | 3100 | 13 | νasCH R**A** (95) |  | 145 | 3200 | 3033 | 3 | νasCH R**A** (89) |
|  | 144 | 3203 | 3091 | 13 | νCH R**C** (91) |  | 144 | 3199 | 3033 | 22 | νasCH R**C** (99) |
|  | 143 | 3202 | 3089 | 2 | νasCH R**A** (91) |  | 143 | 3186 | 3021 | 13 | νasCH R**C** (94) |
|  | 142 | 3188 | 3076 | 4 | νasCH R**C** (92) |  | 142 | 3174 | 3009 | 15 | νasCH R**C** (96) |
|  | 141 | 3175 | 3063 | 17 | νasCH R**C** (96) |  | 141 | 3164 | 2999 | 6 | νC50H2 (99) |
|  | 140 | 3162 | 3051 | 5 | νC50H2 (99) |  | 140 | 3133 | 2970 | 24 | νasC43H2 (90) |
|  | 139 | 3137 | 3026 | 4 | νasC14H2 (94) |  | 139 | 3116 | 2954 | 6 | νasC14H2 (95) |
|  | 138 | 3133 | 3023 | 23 | νasC43H2 (93) | 2965 | 138 | 3116 | 2954 | 66 | νasC36H2 (81) |
|  | 137 | 3116 | 3007 | 68 | νas (C27H2+ C36H2) (91) |  | 137 | 3113 | 2951 | 25 | νasC27H2 (79) |
|  | 136 | 3114 | 3004 | 18 | νas (C27H2+ C36H2) (89) | 2960 | 136 | 3109 | 2948 | 81 | νasC31H2 (90) |
|  | 135 | 3108 | 2999 | 116 | νasC31H2 (87) |  | 135 | 3108 | 2947 | 80 | νasC31H2 (87) |
|  | 134 | 3107 | 2997 | 47 | νasC31H2 (91) |  | 134 | 3102 | 2941 | 19 | νas (C27H2+ C31H2+ C36H2) (77) |
|  | 133 | 3103 | 2994 | 6 | νasC40H2 (93) |  | 133 | 3101 | 2940 | 9 | νasC36H2 (80) |
|  | 132 | 3101 | 2992 | 15 | νas (C27H2+ C36H2) (74) |  | 132 | 3094 | 2933 | 6 | νasC40H2 (95) |
|  | 131 | 3100 | 2991 | 14 | νasC36H2 (80) |  | 131 | 3078 | 2918 | 21 | νasC43H2 (98) |
|  | 130 | 3080 | 2972 | 19 | νasC43H2 (98) |  | 130 | 3069 | 2909 | 27 | νC14H2 (99) |
|  | 129 | 3077 | 2968 | 15 | νC14H2 (94) |  | 129 | 3052 | 2893 | 44 | νC40H2 (95) |
| 2953 | 128 | 3058 | 2950 | 21 | νC40H2 (93) |  | 128 | 3042 | 2884 | 39 | ν(C27H3+ C31H3+ C36H3) (87) |
|  | 127 | 3041 | 2934 | 40 | ν(C27H2+ C31H3+ C36H3) (91) |  | 127 | 3034 | 2876 | 43 | ν(C31H3+ C36H3) (85) |
|  | 126 | 3033 | 2926 | 45 | ν(C27H3+ C36H3) (84) | 2867 | 126 | 3033 | 2875 | 50 | ν(C27H3+ C36H3) (85) |
|  | 125 | 3032 | 2925 | 46 | νC36H3 (90) |  | 125 | 3029 | 2871 | 33 | νC43H3 (90) |
| 2865 | 124 | 3030 | 2923 | 31 | νC43H3(94) | 1656 | 124 | 1721 | 1721 | 19 | νC49C50 (80) |
| 1834 | 123 | 1720 | 1720 | 24 | νC49C50(80) |  | 123 | 1659 | 1659 | 5 | νCCR**C** (50) |
| 1664 | 122 | 1663 | 1663 | 17 | νCCR**A** (62) |  | 122 | 1654 | 1654 | 8 | νCCR**A** (65)+ ipb HCC R**A** (11) |
|  | 121 | 1659 | 1659 | 14 | νCCR**C** (60)+ νCCR**C** (14) |  | 121 | 1651 | 1651 | 0 | νCCR**AB** (69) |
|  | 120 | 1648 | 1648 | 11 | νCCR**A** (69) |  | 120 | 1615 | 1615 | 2 | νCCR**C** (61) |
|  | 119 | 1614 | 1614 | 0 | νCCR**C** (71)+ (α+ β) R**C** (11) |  | 119 | 1551 | 1551 | 30 | ipb HCC R**C** (78) |
| 1555 | 118 | 1599 | 1599 | 146 | νNC (50) |  | 118 | 1518 | 1518 | 15 | σ(C31H2+ C36H2) (64) |
|  | 117 | 1552 | 1552 | 27 | ipb HCC R**C** (59)+ τC40H2 (12) |  | 117 | 1518 | 1518 | 1 | νCC R**A** (32)+ ipb HCC R**A** (21) |
|  | 116 | 1521 | 1521 | 14 | νCC R**A** (37)+ ipb HCC R**A** (17) |  | 116 | 1513 | 1513 | 48 | νCC R**A**+ νNC (32)+ ipb HCC R**C** (21)+ α (R**A**+CNC)(19) |
|  | 115 | 1519 | 1519 | 15 | σ(C27H2+ C31H2+ C36H2) (72) |  | 115 | 1507 | 1507 | 11 | σ(C27H2+ C31H2) (63) |
|  | 114 | 1517 | 1517 | 6 | ν(NC+ CC) (36)+ ipb HCC R**A** (34) |  | 114 | 1501 | 1501 | 14 | σ(C27H2+C36H2) (42)+ τ (C27H2+ C36H2) (27) |
|  | 113 | 1508 | 1508 | 11 | σ(C27H2+ C31H2+ C36H2) (68) |  | 113 | 1491 | 1491 | 34 | σ(C43H2+ C50H2) (69)+ σ C40H2 (14) |
|  | 112 | 1502 | 1502 | 13 | σ (C27H2+ C36H2) (69) |  | 112 | 1490 | 1490 | 0 | τ (C27H2+ C31H2+ C36H2) (66) |
|  | 111 | 1495 | 1495 | 56 | σ (C14H2+ C40H2+ C43H2+ C50H2) (71) |  | 111 | 1487 | 1487 | 25 | σ C14H2 (75) |
|  | 110 | 1492 | 1492 | 21 | σ(C14H2+ C43H2) (69) |  | 110 | 1485 | 1485 | 0 | σ(C27H2+ C36H2) (66) |
|  | 109 | 1490 | 1490 | 1 | σ(C27H2+C31H2) (66) |  | 109 | 1483 | 1483 | 0 | τ (C27H2+ C36H2) (29)+ σ(C27H2+C36H2) (37) |
|  | 108 | 1486 | 1486 | 0 | σ(C27H2+ C31H2+ C36H2) (53) |  | 108 | 1482 | 1482 | 16 | σ C40H2 (66)+ σ(C43H2+ C50H2) (14) |
|  | 107 | 1485 | 1485 | 2 | σ C40H2 (52) | 1475 | 107 | 1477 | 1477 | 10 | σ C43H2 (92) |
|  | 106 | 1483 | 1483 | 0 | τ(C27H2+C36H2) (65) |  | 106 | 1450 | 1450 | 8 | ipb HCC R**C** (62) |
|  | 105 | 1479 | 1479 | 5 | τ C43H2 (61) | 1443 | 105 | 1446 | 1446 | 5 | σ(C43H2+ C50H2) (72)+ νC49C50 (10) |
| 1427 | 104 | 1465 | 1465 | 132 | νNC (35) |  | 104 | 1431 | 1431 | 6 | sb(C27H3+ C31H3+ C36H3) (65) |
|  | 103 | 1449 | 1449 | 17 | νCC R**C** (46)+ ipb HCC R**C** (25) |  | 103 | 1428 | 1428 | 147 | νNC (44) |
|  | 102 | 1447 | 1447 | 1 | σ(C43H2+C50H2) (64) |  | 102 | 1427 | 1427 | 87 | νNC (41)+ τ(C14H2+C40H2) (10) |
|  | 101 | 1432 | 1432 | 3 | sb(C27H3+ C31H3+ C36H3) (81) |  | 101 | 1418 | 1418 | 9 | sbC43H3 (89) |
|  | 100 | 1419 | 1419 | 6 | sbC43H3(91) |  | 100 | 1404 | 1404 | 15 | sb(C27H3+ C31H3)(76) |
|  | 99 | 1409 | 1409 | 1 | ω(C14H2+C40H2) (21)+ νCC R**A** (34) |  | 99 | 1400 | 1400 | 25 | sb(C27H3+ C31H3)+ ω(C14H2+C40H2) (58)+ ipb HCC R**A** (19) |
|  | 98 | 1403 | 1403 | 10 | sbC33H3 (72)+ ω(C27H2+C36H2) (11) |  | 98 | 1399 | 1399 | 5 | sb(C27H3+ C31H3) (63) |
|  | 97 | 1401 | 1401 | 9 | ω(C27H2+C36H2) (65)+ τ (C27H2+C36H2) (10) |  | 97 | 1395 | 1395 | 42 | ωC40H2 (48) |
|  | 96 | 1399 | 1399 | 4 | νCC R**A** (33)+ ω(C14H2+C40H2) (35)+ ipb HCC R**A** (11) |  | 96 | 1387 | 1387 | 53 | ω(C14H2+C40H2) (50) |
|  | 95 | 1387 | 1387 | 10 | ω(C14H2+C40H2) (23)+ ipb HCC R**AC** (33)+ νNC (14) | 1387 | 95 | 1380 | 1380 | 41 | νNC (38)+ ωC40H2 (13) |
| 1375 | 94 | 1370 | 1370 | 42 | ipb HCC R**AC**+τC14H2 (73)+ νCC R**C** (13) |  | 94 | 1368 | 1368 | 18 | ipb HCC R**AC**+τ(C14H2+C40H2) (34)+ νCC R**C** (11) |
|  | 93 | 1363 | 1363 | 44 | ipb HCC R**AC** (16)+ ω(C14H2+C40H2) (10) | 1345 | 93 | 1340 | 1340 | 12 | ipb HCC R**C** (61)+ νCCR**C** (13) |
|  | 92 | 1345 | 1345 | 26 | ipb HCC R**AC** (23) |  | 92 | 1331 | 1331 | 24 | ωC14H2+ νCC R**C** (46) |
|  | 91 | 1339 | 1339 | 4 | ipb HCC R**AC** (56) |  | 91 | 1303 | 1303 | 5 | τ(C14H2+C40H2)+ νCC R**A** (53)+ νNC (13)+ ipb HCC R**A** (10) |
|  | 90 | 1299 | 1299 | 30 | ipb HCC R**A** (39)**+** ω(C14H2+ C40H2) (12) |  | 90 | 1287 | 1287 | 29 | νCCR**C**+ νC24C35 (22) |
| 1270 | 89 | 1286 | 1286 | 27 | (ω+ τ) (C27H2+C31H2+ C36H2) (46)+ νCC (11) | 1266 | 89 | 1258 | 1258 | 22 | ν(C40C49+ C43C49) (30)+ (ρ+τ) (C27H2+C36H2) (46) |
|  | 88 | 1258 | 1258 | 14 | ν(C43C49+ C49C50) (63)+ ωC43H2+ ρC50H2 (14) |  | 88 | 1245 | 1245 | 20 | τ(C14H2+C40H2) (51) |
|  | 87 | 1254 | 1254 | 12 | τC14H2 (49)+ ipb HCC R**AC** (14) |  | 87 | 1233 | 1233 | 1 | ipb HCC R**C+** αR**C** (33)+ νCCR**C** (10) |
|  | 86 | 1241 | 1241 | 21 | ipb HCC R**C+** τC40H2 (47)+ νNC (10) |  | 86 | 1228 | 1228 | 1 | ν(C27C35+ C31C35) (22)+ (ρ+τ) (C27H2+C36H2) (13) |
|  | 85 | 1238 | 1238 | 11 | νNC (19)+ α R**A** (12)+ (α+ β) (CCC+ CNC) (10) |  | 85 | 1223 | 1223 | 4 | ν(C27C35+ C35C36) (42)+ (ρ+τ) (C27H2+C36H2) (24) |
|  | 84 | 1227 | 1227 | 2 | νC31C35 (11)+ σ(C27H2+C31H2) (38) |  | 84 | 1215 | 1215 | 4 | ipb HCC R**C** (63)+ νCCR**C** (19) |
|  | 83 | 1222 | 1222 | 6 | (ρ+ τ) (C27H2+ C31H2+ C36H2) (51) |  | 83 | 1213 | 1213 | 32 | τ(C14H2+C40H2) (44)+ ipb HCC R**AC** (17) |
|  | 82 | 1220 | 1220 | 3 | ipb HCC R**C**+νCC R**A** (60)+ νCCR**C** (21) |  | 82 | 1191 | 1191 | 0 | ipb HCC R**A**+νCC R**A** (55) |
| 1181 | 81 | 1218 | 1218 | 136 | ipb HCN (47)+ νNC (19) | 1178 | 81 | 1169 | 1169 | 0 | ipb HCC R**A**+ νCC R**A** (71) |
|  | 80 | 1187 | 1187 | 1 | ipb HCC R**A** (66) |  | 80 | 1149 | 1149 | 9 | ipb HCC R**C** (58) |
|  | 79 | 1154 | 1154 | 10 | ipb HCC R**A** (38)+ νCC R**A** (27) |  | 79 | 1148 | 1148 | 5 | ipb HCC R**A** (41)+ νCC R**A** (21)+ τ(C14H2+C40H2) (10) |
|  | 78 | 1151 | 1151 | 7 | ipb HCC R**C** (48)+ νCCR**C** (32) |  | 78 | 1129 | 1129 | 20 | νCCR**C**+ νC24C35 (42) |
|  | 77 | 1145 | 1145 | 8 | νNC (11)+ α CNC (15) | 1108 | 77 | 1080 | 1080 | 2 | ρ(C40H2+C43H2) (71) |
| 1129 | 76 | 1128 | 1128 | 22 | νCC (41)+ ω(C27H2+C31H2+ C36H2) (21) |  | 76 | 1050 | 1050 | 20 | ν(CC+NC) (27)+ α R**A** (33) |
|  | 75 | 1080 | 1080 | 2 | τC43H2 (70) |  | 75 | 1048 | 1048 | 1 | τC27H2+ ρC36H2 (50) |
|  | 74 | 1050 | 1050 | 0 | (ω+ τ) (C27H2+C36H2) (60) |  | 74 | 1043 | 1043 | 2 | τC27H2+ ρC36H2 (69) |
|  | 73 | 1043 | 1043 | 4 | (ρ+ω+ τ) (C27H2+C31H2+ C36H2) (68) |  | 73 | 1039 | 1039 | 13 | ipb HCC R**A**+ α R**A** (71) |
| 1086 | 72 | 1039 | 1039 | 13 | ν(CC+ NC) (41) | 1025 | 72 | 1031 | 1031 | 15 | ipb HCC R**C**+ α R**C** (66) |
|  | 71 | 1038 | 1038 | 9 | νCC R**A** (52) |  | 71 | 1023 | 1023 | 3 | ρ(C43H2+C50H2) (50) |
|  | 70 | 1033 | 1033 | 10 | νCCR**C** (61)+ ipb HCC R**C** (10) |  | 70 | 994 | 994 | 2 | ρC14H2+ opb HCC R**C** (36) |
| 1017 | 69 | 1021 | 1021 | 11 | ωC43H2+ ρC50H2 (29)+ ν(CC+ NC) (16) |  | 69 | 991 | 991 | 0 | opb HCC R**A** (82) |
|  | 68 | 998 | 998 | 3 | opb HCC R**C** (66)+ νCC R**C** (16) |  | 68 | 988 | 988 | 0 | opb HCC R**C** (88) |
|  | 67 | 985 | 985 | 0 | opb HCC R**A** (81) |  | 67 | 985 | 985 | 2 | ρ(C14H2+C40H2) (42) |
|  | 66 | 983 | 983 | 1 | ρ(C14H2+C40H2) (36)+ τC43H2 (15) |  | 66 | 969 | 969 | 2 | opb HCC R**C** (52)+ ρ(C14H2+C40H2) (16) |
|  | 65 | 973 | 973 | 0 | ρC14H2+ opb HCC R**C** (70) |  | 65 | 961 | 961 | 0 | (ρ+τ) (C27H2+C36H2) (42)+ ν(C27C35+ C31C35) (14) |
|  | 64 | 970 | 970 | 2 | opb HCC R**C** (81) |  | 64 | 960 | 960 | 3 | ρC50H2 (48)+ ν(C40C49+ C43C49) (27) |
|  | 63 | 963 | 963 | 1 | τ (C27H2+ C31H2+ C36H2) (52) |  | 63 | 948 | 948 | 3 | opb HCC R**A** (92) |
|  | 62 | 962 | 962 | 3 | ρC50H2 (75) |  | 62 | 941 | 941 | 1 | ν(C27C35+ C31C35) (60)+ χ CCCC (11) |
|  | 61 | 947 | 947 | 2 | opb HCC R**A** (90) |  | 61 | 929 | 929 | 1 | ν(C27C35+ C35C36) (72) |
|  | 60 | 941 | 941 | 1 | ω (C27H2+ C31H2+ C36H2) (68)+ (α+ β) CCC (12) | 918 | 60 | 924 | 924 | 60 | ωC50H2 (96) |
|  | 59 | 929 | 929 | 2 | (ρ+ τ) (C27H2+ C31H2+ C36H2) (77) |  | 59 | 862 | 862 | 1 | opb HCC R**A** (70) |
| 938 | 58 | 922 | 922 | 60 | ωC50H2 (94) |  | 58 | 859 | 859 | 17 | opb HCC R**C** (48) |
|  | 57 | 881 | 881 | 40 | opb HCC R**C** (63)+ νCC R**C** (18) |  | 57 | 854 | 854 | 1 | opb HCC R**C** (86)+ ν(C40C49+ C49C50) (11) |
|  | 56 | 860 | 860 | 5 | νCC R**C+** opb HCC R**C** (38) |  | 56 | 854 | 854 | 3 | ν(C40C49+ C49C50) (52) |
|  | 55 | 858 | 858 | 1 | opb HCC R**A** (81) |  | 55 | 848 | 848 | 21 | opb HCC R**C** (61)+ νCC R**C** (11) |
|  | 54 | 853 | 853 | 12 | νCC (49) |  | 54 | 826 | 826 | 7 | νCC R**C** (43) |
|  | 53 | 849 | 849 | 5 | opb HCC R**C** (69) |  | 53 | 811 | 811 | 34 | νCC R**C** (20) |
| 833 | 52 | 827 | 827 | 41 | opb HCN (76) | 802 | 52 | 800 | 800 | 12 | α (R**A**+CNC)(16) |
|  | 51 | 826 | 826 | 18 | νCC R**C+** opb HCC R**C** (29)+ α R**C** (13) |  | 51 | 770 | 770 | 1 | β R**A** (32)+ opb HCC R**AC** (26) |
|  | 50 | 817 | 817 | 15 | α R**A** (33)+ ν(CC+ NC) (19) | 742 | 50 | 757 | 757 | 106 | opb HCC R**A** (91) |
| 794 | 49 | 794 | 794 | 10 | ν(CC+ NC) (57) |  | 49 | 751 | 751 | 1 | opb HCC R**AC** (14)+ α CNC (11)+ (α+ β) CCC (19) |
|  | 48 | 759 | 759 | 15 | opb HCC R**AC** (29) |  | 48 | 721 | 721 | 13 | α CNC (12)+ ν(CC+NC) (19) |
| 755 | 47 | 753 | 753 | 100 | opb HCC R**A** (84) |  | 47 | 699 | 699 | 1 | τC50H2 (77) |
|  | 46 | 722 | 722 | 2 | opb HCC R**A** (59) | 682 | 46 | 688 | 688 | 3 | νCCR**C** (27)+ opb HCC R**A** (15) |
|  | 45 | 706 | 706 | 11 | α CNC (13) |  | 45 | 656 | 656 | 4 | opb HCC R**A+** χ CCNC (33)+ α CCN (15) |
|  | 44 | 695 | 695 | 4 | τC50H2 (65)+ τC43H2 (16) |  | 44 | 651 | 651 | 0 | α R**C** (65) |
|  | 43 | 685 | 685 | 3 | α R**C** (41) | 612 | 43 | 607 | 607 | 23 | α CCN (25) |
|  | 42 | 654 | 654 | 0 | (α+ β) R**C** (77) |  | 42 | 589 | 589 | 0 | opb HCC R**A** (66) |
| 679 | 41 | 625 | 625 | 17 | (α+ β) R**A** (37)+ νCCR**A** (12) |  | 41 | 579 | 579 | 3 | α (R**A**+CNC) (60) |
|  | 40 | 601 | 601 | 45 | opb HCN (57) | 561 | 40 | 571 | 571 | 9 | α R**A** (30)+ opb HCC R**C** (20) |
|  | 39 | 574 | 574 | 2 | α R**A** (33)+ opb HCC R**A** (11) |  | 39 | 551 | 551 | 9 | opb HCC R**C** (31)+ α R**A** (14) |
|  | 38 | 567 | 567 | 9 | opb HCC R**A** (47)+ α R**A** (10) |  | 38 | 525 | 525 | 3 | β (R**C**+CNC) (15) |
| 558 | 37 | 559 | 559 | 33 | opb HCC R**C** (35)+ α CCN (10) |  | 37 | 477 | 477 | 6 | α C43C49C50 (48)+ ν(C40C49+ C43C49) (10) |
|  | 36 | 549 | 549 | 3 | α CCN (21) |  | 36 | 465 | 465 | 1 | χ CCCC (49) |
|  | 35 | 511 | 511 | 0 | α CCC (14) |  | 35 | 439 | 439 | 4 | opb HCC R**A** (86) |
|  | 34 | 472 | 472 | 4 | ρC50H2+ τ(C40H2+ C43H2) (59)+ ν(C43C49+ C49C50) (11)+ χ CCCC (12) |  | 34 | 423 | 423 | 14 | ρC40H2+ τC43H2 (78) |
|  | 33 | 467 | 467 | 0 | (α+ β) CCC (58) |  | 33 | 418 | 418 | 1 | (α+ β) CCC (25) |
|  | 32 | 423 | 423 | 7 | χ CCCC (43) |  | 32 | 416 | 416 | 0 | opb HCC R**C** (61) |
|  | 31 | 422 | 422 | 7 | χ CCCC (52) |  | 31 | 389 | 389 | 3 | χ CCCC (34)+ (α+ β) CCC (12) |
|  | 30 | 417 | 417 | 18 | χ CCCC (67)+ τC43H2 (11) |  | 30 | 368 | 368 | 1 | χ CCCC (22) |
|  | 29 | 414 | 414 | 1 | χ CCCC (71) |  | 29 | 356 | 356 | 1 | ρC14H2 (47) |
|  | 28 | 379 | 379 | 4 | χ CCCC (15)+ (α+ β) CCC (37) |  | 28 | 335 | 335 | 2 | (α+ β) CCC (32)+ β (R**C**+CNC) (11)+ χ CCCN (16) |
|  | 27 | 363 | 363 | 1 | (α+ β) CCC (34)+ ρC14H2 (12) |  | 27 | 327 | 327 | 1 | α R**C** (34) |
|  | 26 | 359 | 359 | 2 | (α+ β) CCC (46) |  | 26 | 325 | 325 | 0 | ρC31H3 (84) |
|  | 25 | 341 | 341 | 2 | α CCC (37) |  | 25 | 308 | 308 | 2 | α CCC (34) |
|  | 24 | 329 | 329 | 0 | ρC31H3 (93) |  | 24 | 290 | 290 | 0 | χ CCCN (19)+ (α+ β) CCN (25) |
|  | 23 | 313 | 313 | 1 | α CCC (48) |  | 23 | 279 | 279 | 1 | β CNC (24)+ ρ(C27H3+ C36H3) (17) |
|  | 22 | 306 | 306 | 2 | ρC14H2 (39)+ α CCN (11) |  | 22 | 274 | 274 | 0 | ρ(C27H3+ C36H3) (81) |
|  | 21 | 286 | 286 | 23 | χ CCCN (37)+ α CCN (14) |  | 21 | 255 | 255 | 1 | (α+ β) (R**A**+CNC) (11)+ ρ(C27H3+ C36H3) (16)+ χ CCCC (10) |
|  | 20 | 270 | 270 | 0 | ρ(C27H3+ C36H3) (89) |  | 20 | 239 | 239 | 1 | ρ(C27H3+ C36H3) (72)+ χ CCCC (16) |
|  | 19 | 258 | 258 | 0 | α CNC (23)+ ρ(C27H3+ C36H3) (10) |  | 19 | 229 | 229 | 20 | ν (AgBr+ AgC) (81) |
|  | 18 | 244 | 244 | 0 | ρ(C27H3+ C36H3) (33) |  | 18 | 221 | 221 | 2 | (α+ β) CCN (23) |
|  | 17 | 217 | 217 | 4 | α CCN (17) |  | 17 | 199 | 199 | 1 | χ CCCC (22) |
|  | 16 | 213 | 213 | 0 | ρ(C27H3+ C36H3) (51) |  | 16 | 178 | 178 | 0 | ρC43H3 (91) |
|  | 15 | 209 | 209 | 1 | (α+ β) CCC (16) |  | 15 | 169 | 169 | 0 | (α+ β) (R**A**+CNC) (33) |
|  | 14 | 181 | 181 | 0 | ρC43H3 (95) |  | 14 | 142 | 142 | 2 | χ CCCC (30)+ ν (AgBr+ AgC) (15) |
|  | 13 | 149 | 149 | 2 | (α+ β) (CCC+ CNC) (33) |  | 13 | 132 | 132 | 7 | ν (AgBr+ AgC) (67)+ χ CCCC (11) |
|  | 12 | 135 | 135 | 3 | χ CCCC (28)+ ΝBrC (12) |  | 12 | 107 | 107 | 1 | α N-C-Ag (55)+ χ NCAgBr (16) |
|  | 11 | 100 | 100 | 5 | α (CCN+ CNC) (19)+ χ CCCC (40) |  | 11 | 87 | 87 | 3 | χ (CCCN+ CNNAg) (51) |
|  | 10 | 99 | 99 | 17 | ΝBrC (47)+ χ CCCC (10) |  | 10 | 79 | 79 | 0 | χ (CCCN+ CCCC) (47) |
|  | 9 | 72 | 72 | 10 | α NCBr (35)+ χ CCNC (24) |  | 9 | 65 | 65 | 0 | χ CCCN (77) |
|  | 8 | 56 | 56 | 2 | χ (CCCC+ CCCN) (65) |  | 8 | 59 | 59 | 0 | χ CNCAg (40)+ α C-AgBr (16) |
|  | 7 | 55 | 55 | 3 | χ (CCCC+ CCNC) (65) |  | 7 | 51 | 51 | 0 | χ CCCC (74) |
|  | 6 | 51 | 51 | 4 | χ CCCN (50) |  | 6 | 45 | 45 | 1 | χ CCNC (82) |
|  | 5 | 39 | 39 | 5 | α CNCBr+ BrNNC (54)+ χ CCCN (10) |  | 5 | 33 | 33 | 2 | α C-AgBr (30)+ χ (CCCN+ CNNAg) (42) |
|  | 4 | 28 | 28 | 2 | χ CCNC (65) |  | 4 | 29 | 29 | 2 | χ NCAgBr (58)+ α N-C-Ag (17)+ χ CCNC (13) |
|  | 3 | 24 | 24 | 4 | χ CCNC (52) |  | 3 | 21 | 21 | 0 | χ CCCN (48) |
|  | 2 | 20 | 20 | 1 | χ (CCCN+ CCNC) (42) |  | 2 | 15 | 15 | 1 | χ CCCN (68) |
|  | 1 | 14 | 14 | 0 | χ (CCCN+ CCNC) (63) |  | 1 | 6 | 6 | 1 | χ CCCN (77) |

*\* I*IR,IR intensity. The abbreviations are ν,symmetric stretching; νas,asymmetric stretching; ω, wagging; τ, twisting; ρ, rocking; σ, scissoring; α, in-plan ring deformation; β, non-planar ring deformation; ipb. in-plane bending; opb, out-plane bending; sb, symmetric bending (umbrella); χ, torsion; R, ring.

**500**

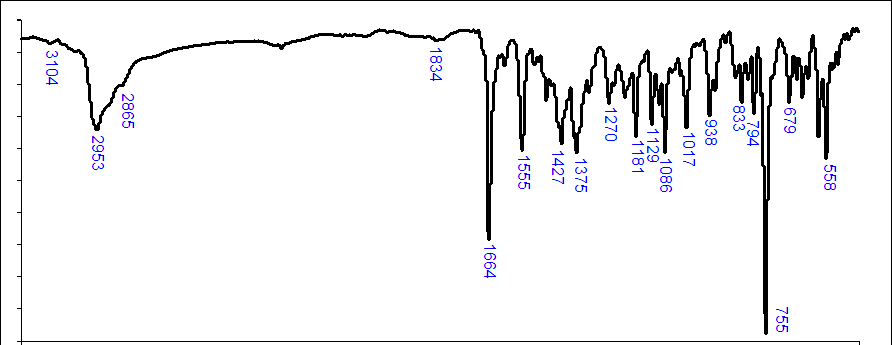
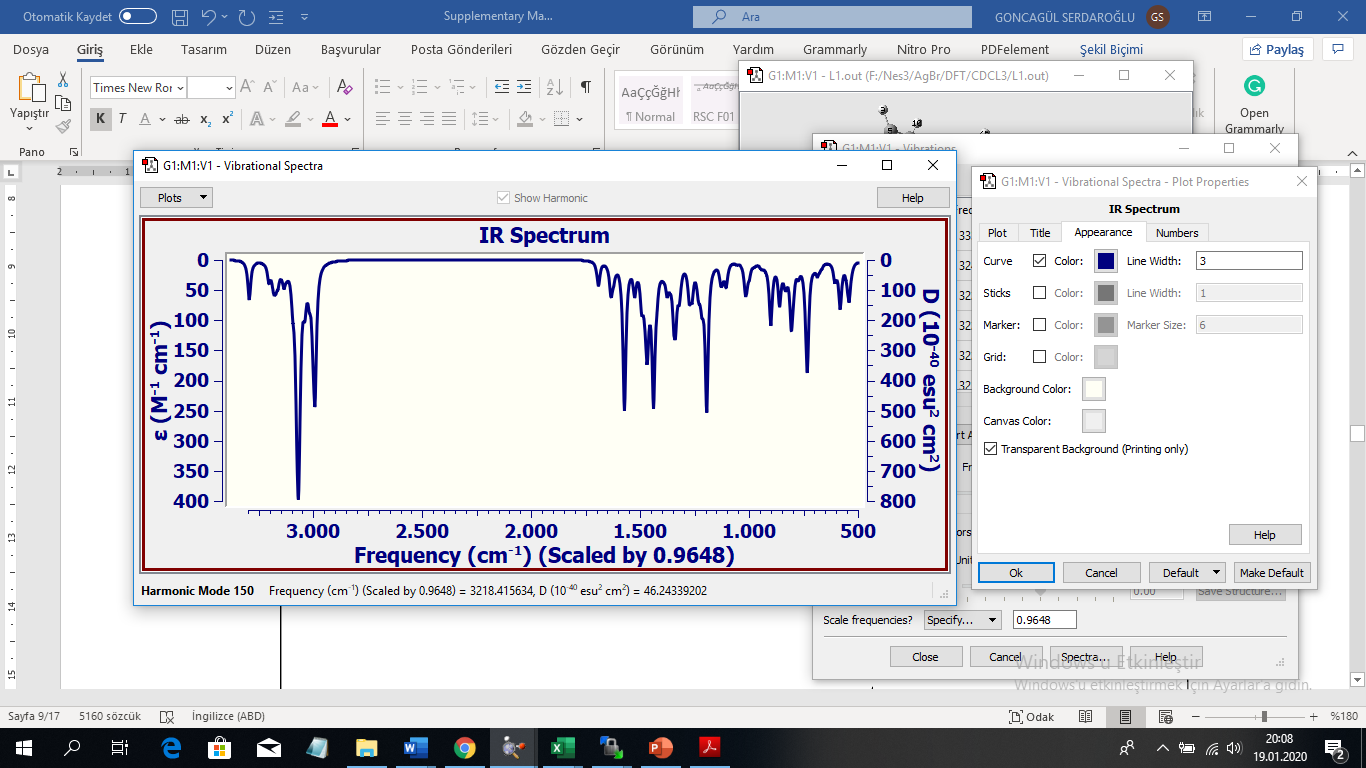
**Wavenumbers (cm-1)**

**3200**

**(a)**

**Transmittance (%)**

**(b)**



**Figure S4a.**The experimental (a) and simulated (b) *FT-IR*spectrum of the NHC precursor **(1)**

**500**

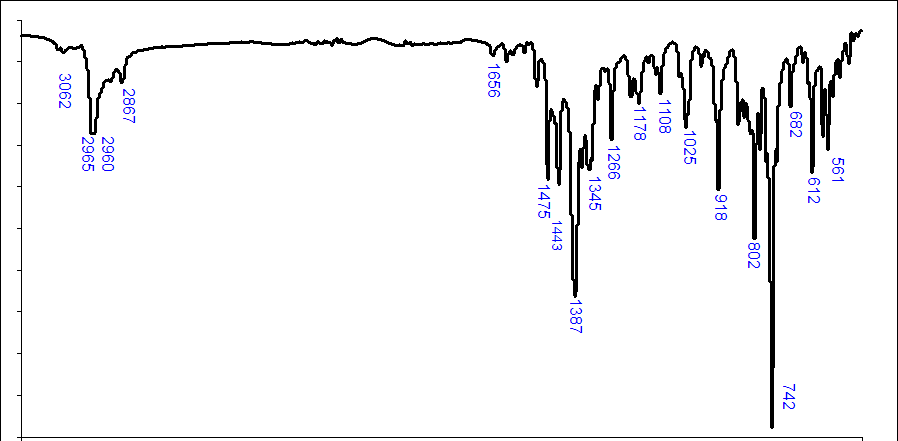
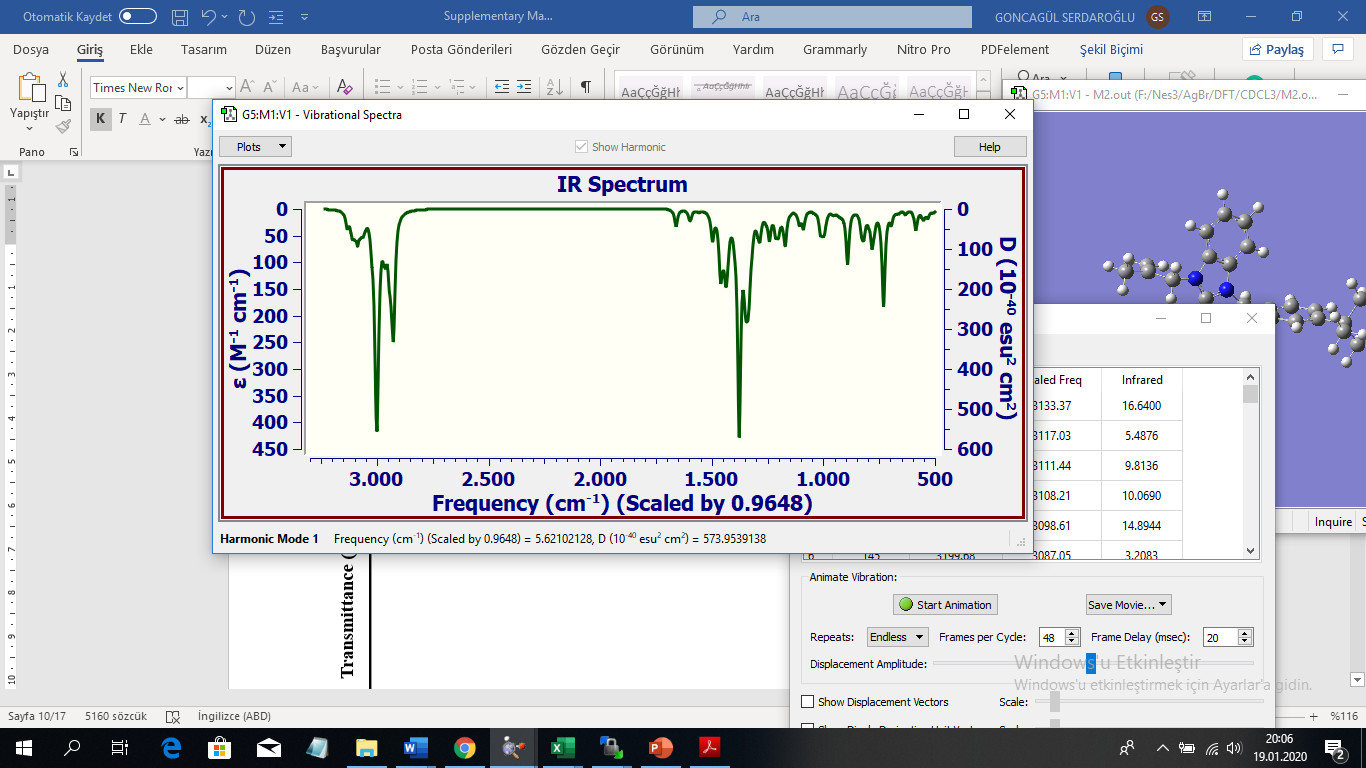
**3200**

**Wavenumbers (cm-1)**

**Transmittance (%)**

**(a)**

**(b)**



**Figure S4b.**The experimental (a) and simulated (b) *FT-IR*spectrum of the Ag(I)-NHCcomplex **(2)**

***3. 4. 1H and 13C{1H}******NMR spectral analysis***

**Table S5a.** The observed and calculated 1H and 13C{1H} NMR isotropic chemical shifts (with respect to TMS, all values in ppm) for three lower energy conformers of NHC precursorat B3LYP/6-31+G(d,p) level of the theory

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  |  | Vacuum | | |  | Chloroform | | |
| ***13C*** | **Exp.** | **L1** | **L2** | **L12** |  | **L1** | **L2** | **L12** |
| 1-C | 137.37 | 131.51 | 131.63 | 131.26 |  | 130.46 | 130.72 | 130.60 |
| 2-C | 131.29 | 130.08 | 129.96 | 131.39 |  | 129.53 | 129.03 | 130.28 |
| 3-C | 113.81 | 108.11 | 109.72 | 108.20 |  | 109.87 | 110.93 | 110.02 |
| 4-C | 127.19 | 120.36 | 120.03 | 120.59 |  | 123.09 | 123.20 | 123.08 |
| 5-C | 127.25 | 120.63 | 120.22 | 120.52 |  | 123.39 | 123.61 | 123.11 |
| 6-C | 113.72 | 107.30 | 106.61 | 108.08 |  | 109.54 | 109.84 | 109.79 |
| 13-C | 143.24 | 131.58 | 127.51 | 130.87 |  | 140.07 | 139.72 | 137.61 |
| 14-C | 51.21 | 52.25 | 55.12 | 52.09 |  | 52.57 | 54.19 | 52.62 |
| 17-C | 129.62 | 128.36 | 131.53 | 128.48 |  | 128.07 | 130.05 | 127.87 |
| 18-C | 131.63 | 130.36 | 124.29 | 130.63 |  | 130.34 | 126.15 | 130.40 |
| 19-C | 128.04 | 126.41 | 122.89 | 126.41 |  | 126.93 | 124.15 | 127.11 |
| 20-C | 128.04 | 125.34 | 124.70 | 125.21 |  | 125.76 | 125.35 | 125.78 |
| 22-C | 126.35 | 121.26 | 122.23 | 121.10 |  | 122.59 | 122.82 | 122.34 |
| 24-C | 162.57 | 149.91 | 148.85 | 149.83 |  | 151.68 | 150.82 | 151.58 |
| 27-C | 31.18 | 33.10 | 33.50 | 33.14 |  | 33.19 | 33.14 | 33.18 |
| 31-C | 31.18 | 29.08 | 28.98 | 29.08 |  | 29.05 | 28.99 | 29.05 |
| 35-C | 34.67 | 40.48 | 40.21 | 40.51 |  | 41.08 | 40.76 | 41.07 |
| 36-C | 31.18 | 33.27 | 33.21 | 33.30 |  | 33.28 | 33.49 | 33.25 |
| 40-C | 53.62 | 53.45 | 53.14 | 53.79 |  | 53.39 | 54.02 | 54.33 |
| 43-C | 19.86 | 22.87 | 23.16 | 22.26 |  | 22.58 | 22.76 | 21.38 |
| 49-C | 152.45 | 143.65 | 144.38 | 137.58 |  | 144.53 | 144.91 | 139.71 |
| 50-C | 116.29 | 104.17 | 103.95 | 120.24 |  | 104.06 | 104.15 | 119.01 |
|  |  |  |  |  |  |  |  |  |
| ***1H*** |  |  |  |  |  |  |  |  |
| 7-H | 7.44 | 7.60 | 7.08 | 7.57 |  | 8.00 | 7.82 | 7.97 |
| 8-H | 7.56 | 7.57 | 7.24 | 7.57 |  | 7.87 | 7.68 | 7.87 |
| 9-H | 7.58 | 7.51 | 7.38 | 7.53 |  | 7.82 | 7.74 | 7.83 |
| 10-H | 7.46 | 7.36 | 7.31 | 7.41 |  | 7.71 | 7.70 | 7.80 |
| 15-H | 5.86 | 4.77 | 4.80 | 4.74 |  | 5.24 | 5.08 | 5.14 |
| 16-H | 5.86 | 5.39 | 5.45 | 5.49 |  | 5.32 | 5.66 | 5.40 |
| 21-H | 7.71 | 9.34 | 7.64 | 9.33 |  | 8.83 | 7.84 | 8.98 |
| 23-H | 7.37 | 7.44 | 7.32 | 7.42 |  | 7.57 | 7.48 | 7.55 |
| 25-H | 7.67 | 7.88 | 7.78 | 7.86 |  | 7.96 | 7.85 | 7.96 |
| 26-H | 7.39 | 7.45 | 7.40 | 7.43 |  | 7.57 | 7.51 | 7.55 |
| 28-H | 1.27 | 1.16 | 1.17 | 1.16 |  | 1.19 | 1.15 | 1.19 |
| 29-H | 1.27 | 1.15 | 1.12 | 1.15 |  | 1.12 | 1.01 | 1.12 |
| 30-H | 1.27 | 1.66 | 1.57 | 1.66 |  | 1.65 | 1.55 | 1.65 |
| 32-H | 1.27 | 1.48 | 1.47 | 1.46 |  | 1.47 | 1.48 | 1.47 |
| 33-H | 1.27 | 1.50 | 1.44 | 1.50 |  | 1.50 | 1.37 | 1.50 |
| 34-H | 1.27 | 1.07 | 1.06 | 1.07 |  | 1.10 | 1.06 | 1.10 |
| 37-H | 1.27 | 1.18 | 1.18 | 1.19 |  | 1.21 | 1.18 | 1.22 |
| 38-H | 1.27 | 1.64 | 1.60 | 1.65 |  | 1.64 | 1.55 | 1.65 |
| 39-H | 1.27 | 1.11 | 1.18 | 1.10 |  | 1.08 | 1.12 | 1.09 |
| 41-H | 5.29 | 4.30 | 4.34 | 4.11 |  | 4.62 | 4.69 | 4.60 |
| 42-H | 5.29 | 5.42 | 5.19 | 5.15 |  | 5.09 | 5.51 | 4.91 |
| 44-H | 1.80 | 1.90 | 2.04 | 1.63 |  | 1.96 | 2.11 | 1.66 |
| 45-H | 1.80 | 2.08 | 2.26 | 1.72 |  | 1.93 | 2.10 | 1.74 |
| 46-H | 1.80 | 1.79 | 1.87 | 1.61 |  | 1.88 | 2.01 | 1.41 |
| 47-H | 11.60 | 9.02 | 9.93 | 8.95 |  | 8.67 | 9.84 | 8.73 |
| 51-H | 4.99 | 4.60 | 5.09 | 6.41 |  | 4.20 | 4.39 | 5.85 |
| 52-H | 5.13 | 4.94 | 5.28 | 5.50 |  | 4.97 | 5.18 | 5.48 |

**Table S5b.** The observed and calculated 1H and 13C{1H} NMR isotropic chemical shifts (with respect to TMS, all values in ppm) for three lower energy conformers of Ag(I)-NHC complex at B3LYP/6-31+G(d,p)/LANL2DZ level of the theory

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  |  | **Vacuum** | | |  | **CHCl3** | | |
| ***13C*** | **Exp.** | **C1** | **C2** | **C12** |  | **C1** | **C2** | **C12** |
| 1-C | 134.17 | 132.57 | 132.58 | 132.09 |  | 133.08 | 133.13 | 132.51 |
| 2-C | 133.82 | 131.35 | 131.20 | 131.88 |  | 131.69 | 131.42 | 132.28 |
| 3-C | 112.12 | 109.33 | 109.56 | 109.25 |  | 109.86 | 109.96 | 109.80 |
| 4-C | 124.09 | 120.41 | 120.33 | 120.53 |  | 121.26 | 121.18 | 121.34 |
| 5-C | 124.14 | 120.58 | 120.57 | 120.30 |  | 121.45 | 121.43 | 121.07 |
| 6-C | 111.97 | 108.67 | 108.53 | 109.50 |  | 109.30 | 109.16 | 110.26 |
| 13-C | 191.46 | 185.44 | 185.74 | 184.43 |  | 185.12 | 185.41 | 184.09 |
| 14-C | 53.03 | 56.92 | 56.99 | 56.83 |  | 56.96 | 57.03 | 56.79 |
| 17-C | 132.08 | 130.63 | 130.57 | 130.62 |  | 131.70 | 131.74 | 131.76 |
| 18-C | 125.96 | 123.49 | 123.82 | 123.49 |  | 123.21 | 124.71 | 123.08 |
| 19-C | 126.93 | 124.22 | 123.25 | 124.36 |  | 124.99 | 122.70 | 125.05 |
| 20-C | 126.93 | 125.19 | 124.09 | 125.10 |  | 125.20 | 124.76 | 125.15 |
| 22-C | 125.96 | 121.16 | 122.61 | 121.15 |  | 121.78 | 122.60 | 121.79 |
| 24-C | 151.46 | 149.31 | 149.30 | 149.33 |  | 149.79 | 149.76 | 149.78 |
| 27-C | 31.24 | 32.63 | 33.07 | 32.61 |  | 32.84 | 33.21 | 32.86 |
| 31-C | 31.24 | 28.80 | 28.64 | 28.78 |  | 28.88 | 28.75 | 28.86 |
| 35-C | 34.57 | 39.92 | 39.91 | 39.93 |  | 40.36 | 40.37 | 40.37 |
| 36-C | 31.24 | 32.92 | 32.92 | 32.92 |  | 32.86 | 32.91 | 32.83 |
| 40-C | 55.46 | 56.81 | 56.65 | 59.96 |  | 56.88 | 56.65 | 60.17 |
| 43-C | 21.10 | 22.40 | 22.42 | 20.87 |  | 22.62 | 22.61 | 21.07 |
| 49-C | 139.34 | 140.74 | 140.51 | 142.82 |  | 143.39 | 143.36 | 143.28 |
| 50-C | 114.50 | 106.49 | 106.60 | 112.00 |  | 105.51 | 105.42 | 112.64 |
|  |  |  |  |  |  |  |  |  |
| ***1H*** |  |  |  |  |  |  |  |  |
| 7-H | 7.32 | 7.55 | 7.49 | 7.53 |  | 7.64 | 7.57 | 7.61 |
| 8-H | 7.21 | 7.43 | 7.40 | 7.42 |  | 7.53 | 7.51 | 7.52 |
| 9-H | 7.31 | 7.50 | 7.49 | 7.47 |  | 7.61 | 7.60 | 7.57 |
| 10-H | 7.46 | 7.40 | 7.40 | 7.70 |  | 7.56 | 7.56 | 7.81 |
| 15-H | 5.63 | 4.95 | 6.18 | 4.94 |  | 5.16 | 6.01 | 5.15 |
| 16-H | 7.34 | 6.13 | 4.99 | 6.13 |  | 5.96 | 5.22 | 5.96 |
| 21-H | 7.44 | 7.74 | 7.62 | 7.74 |  | 7.68 | 7.77 | 7.65 |
| 23-H | 7.44 | 7.57 | 7.54 | 7.56 |  | 7.72 | 7.45 | 7.70 |
| 25-H | 7.23 | 7.69 | 7.75 | 7.68 |  | 7.73 | 7.83 | 7.70 |
| 26-H | 1.27 | 7.49 | 7.42 | 7.49 |  | 7.56 | 7.43 | 7.56 |
| 28-H | 1.27 | 1.15 | 1.18 | 1.15 |  | 1.15 | 1.17 | 1.15 |
| 29-H | 1.27 | 1.17 | 1.21 | 1.17 |  | 1.11 | 1.13 | 1.10 |
| 30-H | 1.27 | 1.58 | 1.53 | 1.58 |  | 1.56 | 1.55 | 1.55 |
| 32-H | 1.27 | 1.47 | 1.37 | 1.47 |  | 1.48 | 1.36 | 1.46 |
| 33-H | 1.27 | 1.53 | 1.51 | 1.52 |  | 1.52 | 1.47 | 1.52 |
| 34-H | 1.27 | 1.09 | 1.03 | 1.09 |  | 1.09 | 1.03 | 1.08 |
| 37-H | 1.27 | 1.13 | 1.15 | 1.12 |  | 1.12 | 1.14 | 1.11 |
| 38-H | 1.27 | 1.44 | 1.53 | 1.43 |  | 1.46 | 1.56 | 1.44 |
| 39-H | 1.27 | 0.99 | 1.06 | 0.99 |  | 0.97 | 1.02 | 0.95 |
| 41-H | 5.04 | 4.64 | 4.64 | 4.78 |  | 4.84 | 4.85 | 4.96 |
| 42-H | 5.04 | 5.38 | 5.39 | 5.64 |  | 5.20 | 5.22 | 5.43 |
| 44-H | 1.74 | 2.12 | 2.12 | 1.78 |  | 2.13 | 2.13 | 1.82 |
| 45-H | 1.74 | 2.13 | 2.11 | 1.33 |  | 2.06 | 2.05 | 1.37 |
| 46-H | 1.74 | 1.89 | 1.88 | 2.18 |  | 2.00 | 2.00 | 2.05 |
| 51-H | 5.02 | 4.27 | 4.28 | 5.57 |  | 4.26 | 4.22 | 5.66 |
| 52-H | 4.86 | 5.22 | 5.23 | 5.37 |  | 5.22 | 5.20 | 5.43 |



**Figure S5a.**The recorded*1H* NMRspectrum of the NHC precursor **(1)**



**Figure S5b.**The recorded13C{1H}NMRspectrum of the NHC precursor **(1)**



**Figure S5c.**The recorded*1H* NMRspectrum of Ag(I)-NHCcomplex **(2)**



**Figure S5d.**The recorded13C{1H}NMRspectrum of Ag(I)-NHCcomplex **(2)**

***3.6. FMO (Frontier Molecular Orbital) Analysis***

**Table S6a.** The calculated quantum chemical parameters for the confirmed conformers of NHC precursor **(1)** after re-optimization performed by 6-31+G(d,p) basis set

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | **Vacuum** | | | | | | | | | | | |
|  | **L1** | **L2** | **L3** | **L4** | **L5** | **L6** | **L7** | **L8** | **L9** | **L10** | **L11** | **L12** |
| HOMO (*-I*) | -0.2045 | -0.2050 | **-----** | -0.1823 | -0.1846 | -0.1871 | -0.2010 | -0.1875 | -0.1975 | -0.2002 | -0.2024 | -0.2019 |
| LUMO (*-A*) | -0.0510 | -0.0489 | **-----** | -0.0749 | -0.0763 | -0.0747 | -0.0567 | -0.0745 | -0.0553 | -0.0546 | -0.0507 | -0.0503 |
| *ΔE* (Energy Gap) | 4.1775 | 4.2477 | **-----** | 2.9209 | 2.9486 | 3.0591 | 3.9255 | 3.0760 | 3.8708 | 3.9628 | 4.1280 | 4.1233 |
| *χ* | -3.4754 | -3.4550 | **-----** | -3.4994 | -3.5500 | -3.5628 | -3.5062 | -3.5647 | -3.4399 | -3.4671 | -3.4433 | -3.4312 |
| *η* | 2.0887 | 2.1238 | **-----** | 1.4604 | 1.4743 | 1.5296 | 1.9628 | 1.5380 | 1.9354 | 1.9814 | 2.0640 | 2.0617 |
| *ω* | 2.8914 | 2.8103 | **-----** | 4.1925 | 4.2740 | 4.1494 | 3.1317 | 4.1311 | 3.0570 | 3.0335 | 2.8722 | 2.8553 |
| *ΔNmax* | 1.6639 | 1.6268 | **-----** | 2.3961 | 2.4079 | 2.3293 | 1.7864 | 2.3178 | 1.7774 | 1.7498 | 1.6683 | 1.6643 |
|  |  |  |  |  |  |  |  |  |  |  |  |  |
|  | **CHCl3** | | | | | | | | | | | |
|  | **L1** | **L2** | **L3** | **L4** | **L5** | **L6** | **L7** | **L8** | **L9** | **L10** | **L11** | **L12** |
| HOMO (-I) | -0.2187 | -0.2190 | -0.2198 | -0.2153 | -0.2154 | -0.2219 | -0.2199 | -0.2190 | -0.2148 | -0.2179 | -0.2181 | -0.2179 |
| LUMO (-A) | -0.0587 | -0.0611 | -0.0652 | -0.0685 | -0.0684 | -0.0694 | -0.0652 | -0.0685 | -0.0630 | -0.0632 | -0.0577 | -0.0590 |
| *ΔE* (Energy Gap) | 4.3522 | 4.2967 | 4.2072 | 3.9957 | 4.0003 | 4.1503 | 4.2072 | 4.0948 | 4.1307 | 4.2088 | 4.3636 | 4.3236 |
| *χ* | -3.7739 | -3.8110 | -3.8786 | -3.8605 | -3.8623 | -3.9633 | -3.8788 | -3.9119 | -3.7791 | -3.8247 | -3.7525 | -3.7670 |
| *η* | 2.1761 | 2.1483 | 2.1036 | 1.9979 | 2.0002 | 2.0751 | 2.1036 | 2.0474 | 2.0653 | 2.1044 | 2.1818 | 2.1618 |
| *ω* | 3.2725 | 3.3801 | 3.5757 | 3.7298 | 3.7289 | 3.7848 | 3.5762 | 3.7372 | 3.4575 | 3.4757 | 3.2269 | 3.2821 |
| *ΔNmax* | 1.7343 | 1.7739 | 1.8438 | 1.9323 | 1.9310 | 1.9099 | 1.8439 | 1.9107 | 1.8298 | 1.8175 | 1.7199 | 1.7425 |

\**ΔE* (Energy Gap), *χ, η, ω* and *ΔNmax* are in eV; HOMO and LUMO energies are in au.

**Table S6b.** The calculated quantum chemical parameters for the confirmed conformers of Ag(I)-NHC complex (**2**) molecule after re-optimization performed by 6-31+G(d,p)/LANL2DZ basis set

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | **Vacuum** | | | | | | | | |
|  | **C1** | **C2** | **C3** | **C4** | **C5** | **C6** | **C7** | **C8** | **C9** |
| HOMO (*-I*) | -0.2147 | -0.2144 | **-----** | -0.2146 | -0.2141 | -0.2146 | -0.2161 | -0.2144 | -0.2177 |
| LUMO (*-A*) | -0.0636 | -0.0635 | **-----** | -0.0635 | -0.0636 | -0.0635 | -0.0637 | -0.0638 | -0.0640 |
| *ΔE* (Energy Gap) | 4.1114 | 4.1084 | **-----** | 4.1122 | 4.0956 | 4.1116 | 4.1489 | 4.0980 | 4.1821 |
| *χ* | -3.7858 | -3.7808 | **-----** | -3.7843 | -3.7790 | -3.7824 | -3.8065 | -3.7837 | -3.8315 |
| *η* | 2.0557 | 2.0542 | **-----** | 2.0561 | 2.0478 | 2.0558 | 2.0745 | 2.0490 | 2.0911 |
| *ω* | 3.4860 | 3.4793 | **-----** | 3.4825 | 3.4869 | 3.4795 | 3.4923 | 3.4936 | 3.5103 |
| *ΔNmax* | 1.8416 | 1.8405 | **-----** | 1.8405 | 1.8454 | 1.8398 | 1.8349 | 1.8466 | 1.8323 |
|  |  |  |  |  |  |  |  |  |  |
|  | **CHCl3** | | | | | | | | |
|  | **C1** | **C2** | **C3** | **C4** | **C5** | **C6** | **C7** | **C8** | **C9** |
| HOMO (-I) | -0.2441 | -0.2440 | -0.2434 | -0.2441 | -0.2434 | -0.2440 | -0.2447 | -0.2434 | -0.2443 |
| LUMO (-A) | -0.0541 | -0.0540 | -0.0540 | -0.0540 | -0.0540 | -0.0540 | -0.0540 | -0.0540 | -0.0541 |
| *ΔE* (Energy Gap) | 5.1710 | 5.1704 | 5.1718 | 5.1718 | 5.1541 | 5.1710 | 5.1881 | 5.1533 | 5.1764 |
| *χ* | -4.0568 | -4.0538 | -4.0553 | -4.0553 | -4.0465 | -4.0541 | -4.0635 | -4.0452 | -4.0606 |
| *η* | 2.5855 | 2.5852 | 2.5859 | 2.5859 | 2.5771 | 2.5855 | 2.5941 | 2.5766 | 2.5882 |
| *ω* | 3.1827 | 3.1783 | 3.1799 | 3.1799 | 3.1769 | 3.1784 | 3.1826 | 3.1754 | 3.1853 |
| *ΔNmax* | 1.5691 | 1.5681 | 1.5682 | 1.5682 | 1.5702 | 1.5680 | 1.5665 | 1.5700 | 1.5689 |

\**ΔE* (Energy Gap), *χ, η, ω* and *ΔNmax* are in eV; HOMO and LUMO energies are in au.