**Table 2. Mass spectra of ligand (1) and Cu(II), complex (2, 4)**

|  |  |  |  |
| --- | --- | --- | --- |
| **Complex No.** | **Fragment** | **m/z** | **Rel. Int.** |
| **(1)** | C4H3N2 | 79 | 15 |
| C4H4N3 | 94 | 19 |
| C4H4N3O2S | 158 | 20 |
| C10H8N3O3S | 234 | 23 |
| C10H8N4O2S | 248 | 18 |
| C11H10N6O2S | 290 | 22 |
| C14H14N6O2S | 330 | 29 |
| C15H15N6O2S | 343 | 26 |
| C17H20N6O4S | 404 | 45 |
| **(2)** | C4H3N2 | 79 | 18 |
| C4H4N3 | 94 | 25 |
| C4H4 N3SO2 | 158 | 27 |
| C10H8N3SO2 | 234 | 19 |
| C11H10N5SO2 | 276 | 24 |
| C11H12N6SO4Cu | 387.5 | 30 |
| C15H20N6 SO9Cu | 523.5 | 32 |
| C19H25N6SO9Cu | 576.5 | 20 |
| C21H30N6SO10Cu | 621.5 | 55 |
| **(4)** | H2O | 18 | 27 |
| C4H5N2O | 97 | 22 |
| C4H6N3O | 112 | 19 |
| C4H6N3SO3 | 176 | 25 |
| C10H10N3SO3 | 252 | 26 |
| C11H12N5SO3 | 294 | 15 |
| C13H14N6SO4Cl2Cu | 460.5 | 30 |
|  | C11H16N6SO6Cl2Cu | 494.5 | 24 |
| C15H21N6SO6Cl2Cu | 547.5 | 35 |
| C17H26N6SO7Cl2Cu | 592.5 | 53 |

**Table 4. The electronic absorption spectral bands (nm) and magnetic moment (B.M) for the**

 **ligand [L] and its metal complexes.**

|  |  |  |
| --- | --- | --- |
| **No.** | **λmax\* ()** | **μeff in BM** |
| **(1)** | 255, 270, 330 | - |
| **(2)** | 290, 306, 382, 452, 530, 630 | 1.72 |
| **(3)** | 296, 310, 395, 455, 535, 645 | 1.71 |
| **(4)** | 285, 305, 383, 460, 533, 655 | 1.68 |
| **(5)** | 292, 312, 385, 445, 585, 648 | 1.74 |
| **(6)** | 285, 290, 392, 555, 620, 715 | 4.7 |
| **(7)** | 286, 306, 380, 495, 620, 735 | 2.77 |
| **(8)** | 265, 325, 385, 466, 592, 640 | 5.2 |
| **(9)** | 285, 305, 380, 465, 562, 634 | 3.8 |
| **(10)** | 285, 300, 386, 496, 618, 736 | 2.9 |
| **(11)** | 260, 310, 340 | Dia. |

 \* in nm

**Table 5. Thermal data for some of metal complexes**

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Complex No.** | **Temp.****(oC)** | **DTA (peak)** | **TGA(wt.loss)** | **Assignments** |
| Endo Exo Calc. Found |
|  **(2)** | 45 | endo | - | - | - | Broken of H-bondings |
| 120 | endo | - | 9.01 | 8.96 | Loss of (2H2O) coordinated water molecules |
| 170 | endo | - | 20.78 | 20.84 | Loss of two coordinated (OAc) groups |
| 355 | - | Exo | - | - | Melting point |
| 465 - 650 | - | Exo | 17.77 | 17.33 | Decomposition process with formation of CuO |
|  **(3)** | 45 | endo | - | - | - | Broken of H-bondings |
| 83 | endo | - | 8.57 | 8.65 | Loss of (2H2O) hydrated water molecules |
| 135 | endo | - | 9..04 | 9.03 | Loss of (3H2O) coordinated water molecules |
| 215 | endo | - | 17.66 | 17.55 | Loss of one coordinated (SO4)group |
| 320 | exo | - | - | - | Melting point |
| 440 - 660 | - | Exo | 17.76 | 17.88 | Decomposition process with the formation of CuO |
|  **(4)** | 48 | endo | - | - | - | Broken of H-bondings |
| 85 | endo | - | 3.04 | 3.08 | Loss of (H2O) hydrated water molecule |
| 145 | endo | - | 6.27 | 6.46 | Loss of (2H2O) coordinated water molecules |
| 177 | endo | - | 13.18 | 13.27 | Loss of coordinated one chloride molecule |
| 345 | endo | - | - | - | Melting point |
| 455 – 670 | - | Exo | 17.00 | 17.02 | Decomposition process with the formation of NiO |
| (**5)** | 45 | endo | - | - | - | Broken of H-bondings |
| 87 | endo | - | 5.69 | 5.75 | Loss of(2H2O) hydrated water molecules |
| 135 | endo |  | 6.04 | 6.06 | Loss of (2H2O) coordinated water molecules |
| 165 | endo | - | 22.14 | 22.18 | Loss of two (NO3) groups |
| 310 | exo | - | - | - | Melting Point |
| 440 - 680 | - | Exo | 18.32 | 18.42 | Decomposition process with the formation of CuO |
|  **(6)** | 46 | endo | - | - | - | Broken of H-bondings |
| 87 | endo | - | 5.51 | 5.57 | Loss of(2H2O) hydrated water molecules |
| 137 | endo |  | 5.84 | 5.86 | Loss of (2H2O) coordinated molecules |
| 186 | endo | - | 20.3 | 20.35 | Loss of two coordinated (OAc) groups |
| 326 | exo | - | - | - | Melting Point |
| 460 - 680 | - | Exo | 16.18 | 16.13 | Decomposition process with the formation of CoO |
| **(7)** | 46 | endo | - | - | - | Broken of H-bondings |
| 89 | endo | - | 8.73 | 8.86 | Loss of (3H2O) hydrated water molecules |
| 125 | endo | - | 6.38 | 6.34 | Loss of two coordinated (H2O) molecules |
| 180 | endo | - | 22.32 | 22.03 | Loss of two coordinated (OAc) groups |
| 350 | - | Exo | - | - | Melting point |
| 465 - 660 | - | Exo | 18.17 | 18.23 | Decomposition process with formation of Ni O |
| **(8)** | 47 | Endo | - | - | - | Broken of H-bondings |
| 86 | Endo | - | 5.57 | 5.77 | Loss of(2H2O) hydrated water molecules |
| 120 | Endo | - | 8.86 | 8.55 | Loss of (3H2O) coordinated molecules |
| 185 | Endo | - | 17.27 | 17.03 | Loss of one coordinated (SO4) group |
| 359 | - | Exo | - | - | Melting Point |
| 460- 650 | - | Exo | 15.62 | 15.54 | Decomposition process with the formation of Fe2O3 |
| **(9)** | 45 | Endo | - | - | 0 | Broken of H-bondings |
| 84 | Endo | - | 8.18 | 8.06 | Loss of(3H2O) hydrated water molecules |
| 130 | Endo | - | 8.91 | 8.76 | Loss of (3H2O) coordinated molecules |
| 180 | Endo | - | 17.39 | 17.22 | Loss of one coordinated (SO4) group |
| 350 | - | Exo | - | - | Melting Point |
| 450- 670 | - | Exo | 14.89 | 14.67 | Decomposition process with the formation of Cr2O3 |
| **(10)** | 44 | Endo | - | - | - | Broken of H-bondings |
| 87 | Endo | - | 5.55 | 5.34 | Loss of(2H2O) hydrated water molecules |
| 129 | Endo | - | 8.81 | 8.45 | Loss of (3H2O) coordinated molecules |
| 184 | Endo | - | 17.24 | 17.23 | Loss of one coordinated (SO4) group |
| 352 | - | Exo | - | - | Melting Point |
| 440- 650 | - | Exo | 16.13 | 16.22 | Decomposition process with the formation of NiO |
| **(11)** | 48 | Endo | - | - | - | Broken of H-bondings |
| 80 | Endo | - | 2.73 | 2.67 | Loss of one (H2O) hydrated water molecule |
| 137 | Endo | - | 5.61 | 5.47 | Loss of (2H2O) coordinated molecules |
| 175 | Endo | - | 19.49 | 19.23 | Loss of two coordinated (OAc) groups |
| 335 | - | Exo | - | - | Melting Point |
| 440- 660 | - | Exo | 16.69 | 16.56 | Decomposition process with the formation of ZnO |

**Table 6. ESR data for the metal (II/ III) complexes**

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **No.** | **g||** | **g⊥** | **gisoa** | **A||****(G)** | **A⊥****(G)** | **Aisob****(G)** | **G c** | **ΔExy** | **ΔExz** | **K⊥2** | **K||2** | **K** | **g||/A||** | **α 2** | **ß 2** | **ß12** | **-2 ß** | **ad2****(%)** |
| **(2)** | 2.13 | 2.08 | 2.15 | 155 | 15 | 19 | 2.19 | 19620 | 23817 | 0.82 | o.36 | o.67 | 0.81 | 137 | 0.62 | 1.35 | 185 | 69 |
| **(4)** | 2.15 | 2.07 | 2.10 | 145 | 23 | 65 | 4.0 | 15445 | 19272 | 0.56 | 0.44 | 0.71 | 155.6 | 0.64 | 0.88 | 0.73 | 310 | 88 |
| **(9)** | - | - | 2.09 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |

**a) giso = (2g┴ + g||)/3, b) Aiso = (2A┴ + A||)/3, c) G= (g|| - 2)/ (g┴ - 2)**

**Table 7.** IC50 values of the ligand and the 9 complexes and their cytotoxic reactivity against human mononuclear cells.

|  |  |
| --- | --- |
| **Ligand and complexes concentrations** | **Cell count after incubation with ligand 1 and its complexes** |
| **Ligand 1** | **Complex 2** | **Complex 3** | **Complex 4** | **Complex 5** | **Complex 6** | **Complex 7** | **Complex 8** | **Complex 9** |
| **1000 µg/mL** |  |  |  |  |  |  |  |  |  |
| **500 µg/mL** |  |  | 90 |  |  |  |  |  |  |
| **250 µg/mL** | 210 | 120 | 180 | 90 | 210 |  | 150 | 120 | 120 |
| **125 µg/mL** | 240 | 180 | 210 | 180 | 240 | 150 | 180 | 210 | 120 |
| **62.5 µg/mL** | 200 | 210 | 330 | 210 | 240 | 150 | 210 | 240 | 150 |
| **31.2 µg/mL** |  | 210 |  | 240 | 270 | 150 | 180 | 270 | 210 |
| **Control** | 330 | 330 | 330 | 330 | 330 | 330 | 330 | 330 | 330 |
|  | **IC50 values (**µg/mL) |
| 216.88  | 159.19 | 235.16  | 148 | 228.89  | 150 | 170.42 | 178 | 134 |
| **Toxicity** |
| rare | weak | rare | weak | rare | weak | weak | weak | weak |