Supplementary information

Effect of terminal substituents of 2-aminobenzimidazoles on non-covalent molecular interactions in their transition metal coordination compounds. Evaluation of their biological activity.

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Table S1. Crystallographic data of sfabz, seabz and compound 1.

|  |  |  |  |
| --- | --- | --- | --- |
| Compounds | sfabz | seabz | 1 |
| Chemical formula | C15H15N3O2S | C11H15N3O2S | NiC30H30N6O4S2Cl2 |
| Formula weight (g mol-1) | 301.36 | 253.32 | 732.33 |
| Crystal size (mm) | 0.5x0.09x0.01 | 0.48x0.21x0.19 | 0.39x0.18x0.07 |
| Crystal color | Colourless | Colopurless | Blue |
| Crystal system | Monoclinic | Monoclinic | Triclinic |
| Space group | P 21/n | P 21/n | P-1 |
| a (Å) | 9.9313(12) | 5.6408(8) | 9.5656(13) |
| b (Å) | 5.4217(5) | 18.453(3) | 9.9837(9) |
| c (Å) | 26.904(3) | 11.1532(15) | 17.3370(19) |
| α (°) | 90 | 90 | 83.852(9) |
| β (°) | 99.497(12) | 97.747(13) | 87.640(10) |
| γ (°) | 90 | 90 | 78.220(10) |
| V (Å3) | 1428.8(3) | 1150.3(3) | 1611.2(3) |
| Z | 4 | 4 | 2 |
| Dcalc (mg cm-3) | 1.401 | 1.463 | 1.51 |
| μ (mm-1) | 0.235 | 0.275 | 0.944 |
| F(000) | 632 | 536 | 756 |
| Temp. (K) | 130(2) | 130(2) | 130(2) |
| θ range (°) data collection | 3.836-29.631 | 3.687-29.73 | 3.417-29.598 |
| Index range |  |  |  |
| h | -13-13 | -6-7 | -12-13 |
| k | -7-7 | -25-25 | -13-13 |
| l | -35-35 | -15-14 | -22-23 |
| Measured reflections | 18416 | 6496 | 21425 |
| Independent reflections | 3697 | 2754 | 7779 |
| Reflections observed [I>2σ(I)] | 2836 | 1922 | 5740 |
| Rint | 0.0494 | 0.0629 | 0.0627 |
| Parameters | 196 | 155 | 406 |
| R [F2 > 2σ(F2)] | 0.0445 | 0.0527 | 0.0549 |
| wR2 (F2) | 0.102 | 0.1255 | 0.1495 |
| S | 1.068 | 1.078 | 1.072 |
| (Δ/σ)max | 0.001 | 0 | 0.001 |
| Δρmax (eÅ-3) | 0.403 | 0.424 | 1.024 |
| Δρmin (eÅ-3) | -0.454 | -0.593 | -0.514 |

Table S2. Crystallographic data of 2, 3 and 5.

|  |  |  |  |
| --- | --- | --- | --- |
| Compounds | 2 | 3 | 5 |
| Chemical formula | Ni2C63H64N12O9S4Br4 | NiC22H30N6O4S2Cl2 | CuC30H30N6O4S2Cl2 |
| Formula weight (g mol-1) | 1698.56 | 636.25 | 737.16 |
| Crystal size (mm) | 0.42x0.38x0.23 | 0.49x0.21x0.13 | 0.242x0.192x0.089 |
| Crystal color | Dark green | Blue | Green |
| Crystal system | Triclinic | Monoclinic | Triclinic |
| Space group | P-1 | P 21/c | P-1 |
| a (Å) | 10.6925(6) | 16.9816(12) | 10.365(2) |
| b (Å) | 11.1876(6) | 15.3376(8) | 11.384(2) |
| c (Å) | 14.4961(9) | 10.2625(7) | 13.918(3) |
| α (°) | 76.685(5) | 90 | 100.833(4) |
| β (°) | 89.622(5) | 100.987(7) | 94.543(4) |
| γ (°) | 89.579(4) | 90 | 97.599(4) |
| V (Å3) | 1687.39(17) | 2623.9(3) | 1589.8(5) |
| Z | 1 | 4 | 2 |
| Dcalc (mg cm-3) | 1.672 | 1.611 | 1.540 |
| μ (mm-1) | 3.115 | 1.145 | 1.033 |
| F(000) | 858 | 1320 | 758 |
| Temp. (K) | 130(2) | 130(2) | 298(2) |
| θ range (°) data collection | 3.452-30.163 | 3.61-29.496 | 1.498-26.022 |
| Index range |  |  |  |
| h | -14-14 | -16-23 | -12-12 |
| k | -15-14 | -21-19 | -14-14 |
| l | -19-20 | -13-10 | -17-17 |
| Measured reflections | 24487 | 13678 | 39236 |
| Independent reflections | 8685 | 6288 | 6231 |
| Reflections observed [I>2σ(I)] | 7059 | 4365 | 3167 |
| Rint | 0.032 | 0.0518 | 0.1178 |
| Parameters | 433 | 336 | 620 |
| R [F2 > 2σ(F2)] | 0.0334 | 0.0486 | 0.0682 |
| wR2 (F2) | 0.0781 | 0.1035 | 0.1744 |
| S | 1.034 | 1.048 | 0.96 |
| (Δ/σ)max | 0.002 | 0.001 | 0 |
| Δρmax (eÅ-3) | 0.567 | 0.592 | 0.501 |
| Δρmin (eÅ-3) | -0.593 | -0.501 | -0.0435 |

Table S3. Crystallographic data of 9 and 10.

|  |  |  |
| --- | --- | --- |
| Compounds | 9 | 10 |
| Chemical formula | ZnC30H30N6O4S2Cl2 | ZnC32H32N6O5S2Br2 |
| Formula weight (g mol-1) | 738.99 | 869.94 |
| Crystal size (mm) | 0.433x0.248x0.070 | 0.28x0.25x0.19 |
| Crystal color | colourless | Colourless |
| Crystal system | Triclinic | Triclinic |
| Space group | P-1 | P-1 |
| a (Å) | 10.367(11) | 10.6872(5) |
| b (Å) | 10.928(12) | 11.2000(5) |
| c (Å) | 14.556(15) | 14.5708(7) |
| α (°) | 78.18(2) | 76.451(4) |
| β (°) | 89.19(2) | 89.503(4) |
| γ (°) | 85.37(2) | 89.511(4) |
| V (Å3) | 1609(3) | 1695.44(14) |
| Z | 2 | 2 |
| Dcalc (mg cm-3) | 1.526 | 1.704 |
| μ (mm-1) | 1.105 | 5.342 |
| F(000) | 760 | 876 |
| Temp. (K) | 150(2) | 130(2) |
| θ range (°) data collection | 2.432-26.414 | 4.060-73.656 |
| Index range |  |  |
| h | -12-12 | -13-13 |
| k | -13-13 | -13-13 |
| l | -18-18 | -18-18 |
| Measured reflections | 33661 | 36795 |
| Independent reflections | 6549 | 6720 |
| Reflections observed [I>2σ(I)] | 3903 | 5824 |
| Rint | 0.1339 | 0.0435 |
| Parameters | 418 | 433 |
| R [F2 > 2σ(F2)] | 0.0586 | 0.0394 |
| wR2 (F2) | 0.1087 | 0.1106 |
| S | 1.022 | 1.081 |
| (Δ/σ)max | 0 | 0.001 |
| Δρmax (eÅ-3) | 0.449 | 0.637 |
| Δρmin (eÅ-3) | -0.619 | -1.329 |

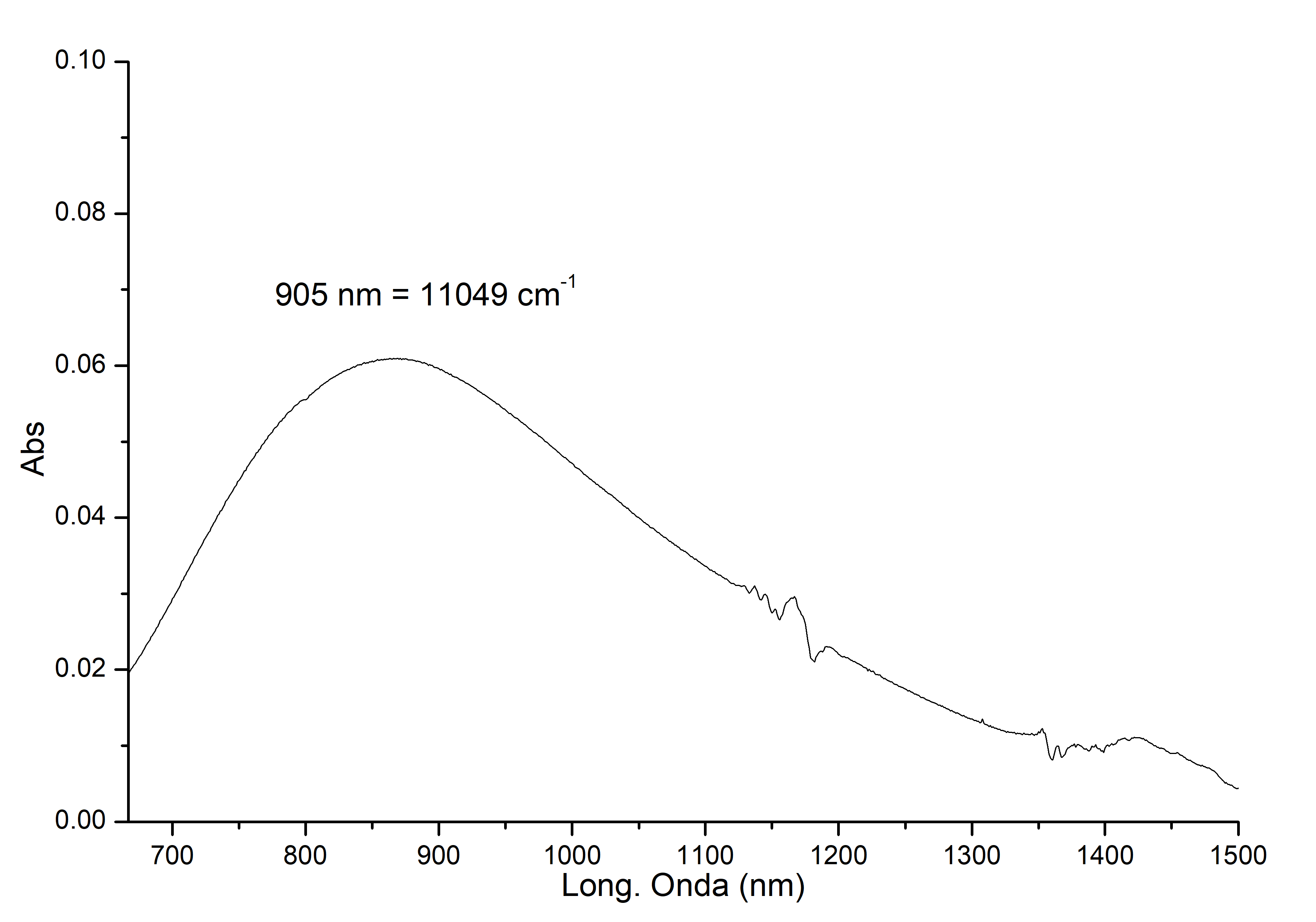
nm

Figure S1. Solution spectrum of [Cu(sfabz)2Cl2] in DMSO, 1x10-3 M.

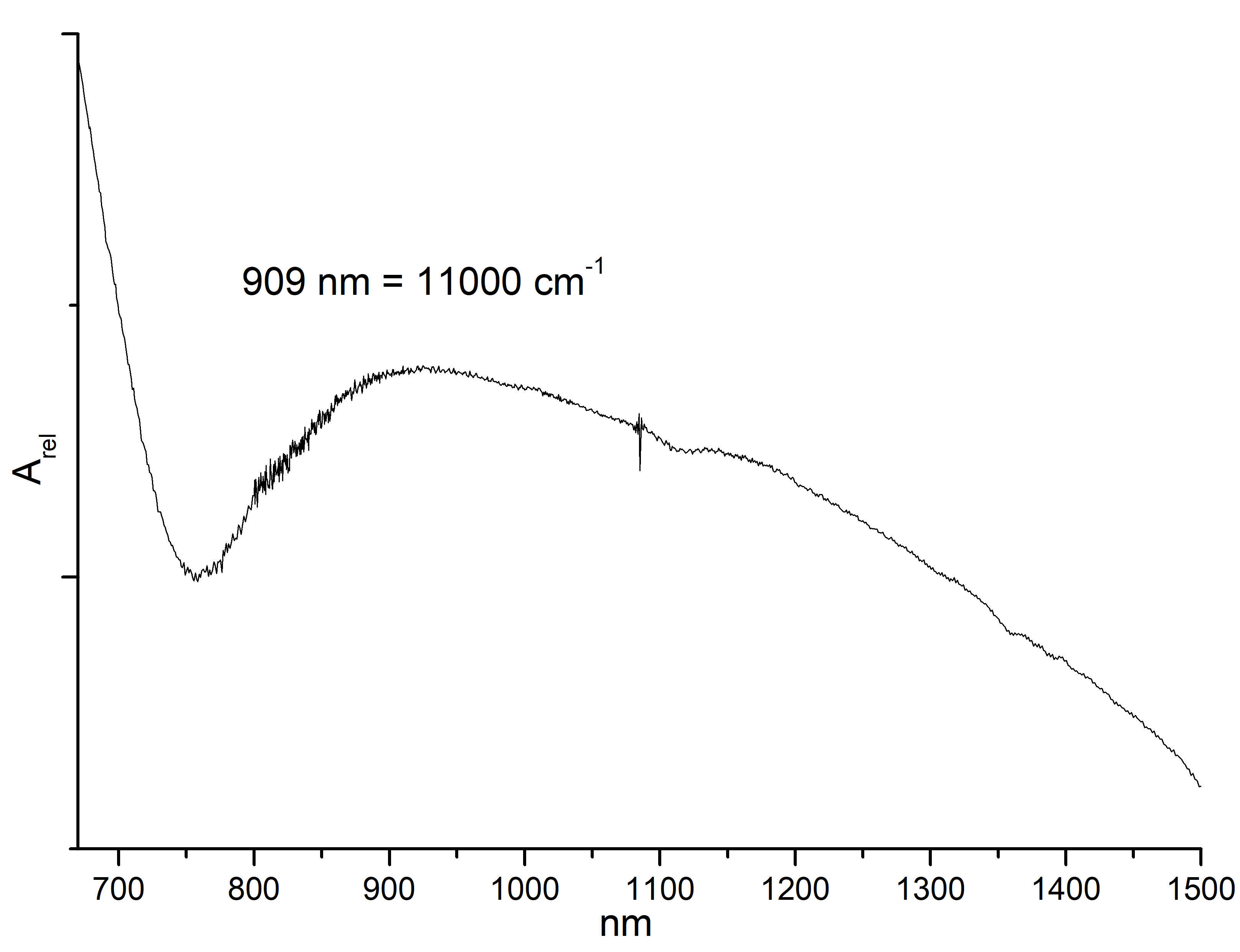
nm

Figure S2. Diffuse reflectance spectrum of [Cu(sfabz)2Cl2].

Table S4. 1H-NMR for sfabz and its coordination compounds (DMSO d6).

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Signal | sfabz | [Zn(sfabz)2Cl2] (9) | [Zn(sfabz)2Br2] (10) | [Cd(sfabz)2Cl2] (13) | [Hg(sfabz)2Cl2] (15) |
| 4 | 7.05 ppm (d) | 7.21 ppm (s, broad) | 7.23 ppm (d) | 7.22 ppm (d) | 7.22 ppm (d) |
| 5 | 6.89 ppm (t) | 6.94 ppm (m) | 6.94 ppm (t) | 6.92 ppm (t) | 6.98 ppm (m) |
| 6 | 6.79 ppm (t) | 6.92 ppm (m) | 6.92 ppm (m) | 6.85 ppm (t) | 6.94 ppm (m) |
| 7 | 6.74 ppm (d) | 6.92 ppm (m) | 6.92 ppm (m) | 6.82 ppm (d) | 6.94 ppm (m) |
| 10 (2H) | 6.43 ppm (s, broad) | 7.21 ppm (s, broad) | 7.10 ppm (s, broad) | 6.75 ppm (s, broad) | 7.12 ppm (s, broad) |
| 11 (2H) | 4.28 ppm (t) | 4.40 ppm (t) | 4.40 ppm (t) | 4.32 ppm (t) | 4.39 ppm (t) |
| 12 (2H) | 3.72 ppm (t) | 3.81 ppm (t) | 3.81 ppm (t) | 3.74 ppm (t) | 3.81 ppm (t) |
| 17 (2H) | 7.86 ppm (d) | 7.84 ppm (m) | 7.84 ppm (d) | 7.85 ppm (d) | 7.85 ppm (d) |
| 18 (2H) | 7.58 ppm (t) | 7.55 ppm (m) | 7.56 ppm (t) | 7.58 ppm (t) | 7.52 ppm (t) |
| 19 | 7.71 ppm (t) | 7.67 ppm (m) | 7.68 ppm (t) | 7.69 ppm (t) | 7.63 ppm (t) |

Table S5. 13C-NMR for sfabz and its coordination compounds (DMSO d6).

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Signal | sfabz | [Zn(sfabz)2Cl2] (9) | [Zn(sfabz)2Br2] (10) | [Cd(sfabz)2Cl2] (13) | [Hg(sfabz)2Cl2] (15) |
| 2 | 154.82 ppm | 154.92 ppm | 154.76 ppm | 154.97 ppm | 155.06 ppm |
| 4 | 115.27 ppm | 114.62 ppm | 114.81 ppm | 115.43 ppm | 114.36 ppm |
| 5 | 121.10 ppm | 122.24 ppm | 122.16 ppm | 121.54 ppm | 122.21 ppm |
| 6 | 118.66 ppm | 120.62 ppm | 120.55 ppm | 119.62 ppm | 120.57 ppm |
| 7 | 107.73 ppm | 108.98 ppm | 108.90 ppm | 108.25 ppm | 109.08 ppm |
| 8 | 133.91 ppm | 132.33 ppm | 132.43 ppm | 133.09 ppm | 132.49 ppm |
| 9 | 142.92 ppm | 139.08 ppm | 139.10 ppm | 140.91 ppm | 139.29 ppm |
| 11 | 36.08 ppm | 36.37 ppm | 36.36 ppm | 36.21 ppm | 36.58 ppm |
| 12 | 53.18 ppm | 52.54 ppm | 52.59 ppm | 52.86 ppm | 52.52 ppm |
| 16 | 136.17 ppm | 138.70 ppm | 138.87 ppm | 139.10 ppm | 139.05 ppm |
| 17 (2C) | 127.96 ppm | 127.80 ppm | 127.83 ppm | 127.91 ppm | 127.73 ppm |
| 18 (2C) | 129.84 ppm | 129.83 ppm | 129.86 ppm | 129.88 ppm | 129.78 ppm |
| 19 | 134.44 ppm | 134.49 ppm | 134.51 ppm | 134.50 ppm | 134.43 ppm |

Table S6. 1H-NMR for seabz and its coordination compounds (d6 DMSO).

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Signal | seabz | [Zn(seabz)2Cl2] (11) | [Zn(seabz)2Br2] (12) | [Cd(seabz)2Cl2] (14) | [Hg(seabz)2Cl2] (16) |
| 4 | 7.13 ppm (dd, overlapped) | 7.28 ppm (m, overlapped) | 7.28 ppm (dd, overlapped) | 7.33 ppm (dd) | 7.29 ppm (m, overlapped) |
| 5 | 6.88 ppm (td) | 7.01 ppm (m, overlapped) | 6.99 ppm (m, overlapped) | 6.98 ppm (m, overlapped) | 7.02 ppm (m, overlapped) |
| 6 | 6.94 ppm (td) | 6.99 ppm (m, overlapped) | 7.02 ppm (m, overlapped) | 6.97 ppm (m, overlapped) | 7.02 ppm (m, overlapped) |
| 7 | 7.15 ppm (dd, overlapped) | 7.26 ppm (m, overlapped) | 7.29 ppm (dd, overlapped) | 7.22 ppm (dd) | 7.28 ppm (m, overlapped) |
| 10 (2H) | 6.48 ppm (s, broad) | 7.32 ppm (s, broad) | 7.18 ppm (s, broad) | 6.86 ppm (s, broad) | 7.13 ppm (s, broad) |
| 11 (2H) | 4.39 ppm (t) | 4.49 ppm (t) | 4.49 ppm (t) | 4.42 ppm (t) | 4.46 ppm (t) |
| 12 (2H) | 3.46 ppm (t) | 3.55 ppm (t) | 3.55 ppm (t) | 3.48 ppm (t) | 3.52 ppm (t) |
| 16 (2H) | 3.08 ppm (q) | 3.14 ppm (q) | 3.14 ppm (q) | 3.12 ppm (q) | 3.13 ppm (q) |
| 17 (3H) | 1.15 ppm (t) | 1.17 ppm (t) | 1.17 ppm (t) | 1.16 ppm (t) | 1.16 ppm (t) |

Table S7. 13C-NMR for seabz and its coordination compounds (d6 DMSO).

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Signal | seabz | [Zn(seabz)2Cl2] (11) | [Zn(seabz)2Br2] (12) | [Cd(seabz)2Cl2] (14) | [Hg(seabz)2Cl2] (16) |
| 2 | 155.05 ppm | 155.10 ppm | 154.92 ppm | 155.12 ppm | 155.25 ppm |
| 4 | 115.40 ppm | 114.65 ppm | 114.84 ppm | 115.59 ppm | 114.57 ppm |
| 5 | 121.17 ppm | 122.37 ppm | 122.29 ppm | 121.70 ppm | 122.20 ppm |
| 6 | 118.78 ppm | 120.81 ppm | 120.74 ppm | 119.92 ppm | 120.55 ppm |
| 7 | 108.12 ppm | 109.36 ppm | 109.29 ppm | 108.70 ppm | 109.26 ppm |
| 8 | 134.05 ppm | 132.45 ppm | 132.55 ppm | 133.11 ppm | 132.78 ppm |
| 9 | 143.19 ppm | 138.81 ppm | 138.99 ppm | 140.74 ppm | 139.78 ppm |
| 11 | 35.60 ppm | 35.78 ppm | 35.78 ppm | 35.70 ppm | 35.91 ppm |
| 12 | 49.62 ppm | 49.04 ppm | 49.07 ppm | 49.30 ppm | 49.16 ppm |
| 16 | 47.29 ppm | 47.34 ppm | 47.35 ppm | 47.31 ppm | 47.32 ppm |
| 17 | 6.34 ppm | 6.28 ppm | 6.30 ppm | 6.32 ppm | 6.30 ppm |