Theoretical insights into the metal chelating and antimicrobial properties of the Chalcone based Schiff bases

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**Supplementary Table Captions**

**Table S1** Occupancies of electron Donor and Acceptor NBOs and Bond stabilization energy E(2) (in kcal/mol) of (a) isolated HL1 Schiff base (b) HL1-Co\textsuperscript{2+} (c) HL1-Ni\textsuperscript{2+} (d) HL1-Cu\textsuperscript{2+} and (e) HL1-Zn\textsuperscript{2+} calculated at CAM-B3LYP/LANL2DZ level of theory.

**Table S2** Occupancies of electron Donor and Acceptor NBOs and Bond stabilization energy E(2) (in kcal/mol) of (a) isolated HL1 Schiff base (b) HL2-Co\textsuperscript{2+} (c) HL2-Ni\textsuperscript{2+} (d) HL2-Cu\textsuperscript{2+} and (e) HL2-Zn\textsuperscript{2+} calculated at CAM-B3LYP/LANL2DZ level of theory.

**Table S3** Occupancies of electron Donor and Acceptor NBOs and Bond stabilization energy E(2) (in kcal/mol) of (a) isolated HL1 Schiff base (b) HL3-Co\textsuperscript{2+} (c) HL3-Ni\textsuperscript{2+} (d) HL3-Cu\textsuperscript{2+} and (e) HL3-Zn\textsuperscript{2+} calculated at CAM-B3LYP/LANL2DZ level of theory.
Table S1 Occupancies of electron Donor and Acceptor NBOs and Bond stabilization energy E(2) (in kcal/mol) of (a) isolated HL1 Schiff base (b) HL1-Co2+ (c) HL1-Ni2+ (d) HL1-Cu2+ and (e) HL1-Zn2+ calculated at CAM-B3LYP/LANL2DZ level of theory.

(a)

| Donor NBO       | Acceptor NBO | Donor NBO Occupancy | Acceptor NBO Occupancy | E(2)  |
|-----------------|--------------|---------------------|------------------------|-------|
| Alpha Spin      |              |                     |                        |       |
| BD (1)N2 - C3   | LP*(8) Co1   | 0.98949             | 0.06673                | 3.03  |
| BD (1)N2 - C5   | LP*(8) Co1   | 0.99123             | 0.06673                | 3.76  |
| BD (1)N10 - C18 | LP*(9) Co1   | 0.99212             | 0.06509                | 2.89  |
| BD (1)O11 - C14 | LP*(7) Co1   | 0.9956              | 0.08435                | 3.35  |
| LP (1)N2        | LP*(8) Co1   | 0.93941             | 0.06673                | 15.25 |
| LP (1)N10       | LP*(9) Co1   | 0.92153             | 0.06509                | 15.36 |
| LP (2)O11       | LP*(7) Co1   | 0.92252             | 0.08435                | 27.5  |
| LP (1)Cl27      | LP*(7) Co1   | 0.99461             | 0.08435                | 4.83  |
| LP (2)Cl27      | LP*(8) Co1   | 0.97873             | 0.06673                | 5.52  |
| LP (3)Cl27      | LP*(9) Co1   | 0.97834             | 0.06509                | 4.83  |
| LP (4)Cl27      | LP*(6) Co1   | 0.8817              | 0.14572                | 56.8  |

| Beta spin       |              |                     |                        |       |
| BD (1)N10 - C18 | LP*(6) Co1   | 0.99172             | 0.06037                | 1.66  |
| BD (1)O11 - C14 | LP*(6) Co1   | 0.99365             | 0.06037                | 2.39  |
| LP (2) Co1      | BD*(1) Co1- N10 | 0.96233             | 0.12166                | 5.38  |
| LP (1)N2        | BD*(1) Co1- N2 | 0.9148              | 0.0495                 | 17.74 |
| LP (1)N10       | LP*(5) Co1   | 0.85934             | 0.10456                | 26.71 |
| LP (2)O11       | LP*(4) Co1   | 0.86651             | 0.13471                | 40.78 |
| LP (1)Cl27      | LP*(3) Co1   | 0.98544             | 0.16345                | 6.05  |
| LP (2)Cl27      | LP*(7) Co1   | 0.96972             | 0.04045                | 4.02  |
| LP (3)Cl27      | LP*(6) Co1   | 0.95371             | 0.06037                | 5.24  |
| LP (4)Cl27      | LP*(3) Co1   | 0.83512             | 0.16345                | 83.31 |

(b)

| Donor NBO       | Acceptor NBO | Donor NBO Occupancy | Acceptor NBO Occupancy | E(2)  |
|-----------------|--------------|---------------------|------------------------|-------|
| BD (1) N1 - C2  | BD*(1)C4 - H 28 | 1.9804             | 0.01923                | 5.96  |
| BD (1) N1 - C4  | BD*(1)N5 - C6 | 1.98532             | 0.03409                | 5.02  |
| BD (2) N1 - C4  | BD*(2)C2 - C3 | 1.89647             | 0.2706                 | 23.33 |
| BD (1) C8 - N9  | BD*(1)C16 - C17 | 1.98077             | 0.03755                | 5.58  |
| BD (1) N9 - C17 | BD*(1)C16 - C17 | 1.98508             | 0.03755                | 2.55  |
| BD (2) N9 - C17 | BD*(2)C18 - C19 | 1.92458             | 0.08331                | 6.34  |
| BD (1)O10 - C13 | BD*(1)C14 - C16 | 1.99047             | 0.02205                | 2.49  |
| LP (1)N1        | BD*(1)C4 - N5 | 1.93633             | 0.04467                | 10.87 |
| LP (1)N9        | BD*(1)C17 - C18 | 1.90824             | 0.05382                | 18.92 |
| LP (2)O10       | BD*(1)C12 - C13 | 1.91635             | 0.04313                | 15.86 |
| LP (3)O10       | BD*(2)C13 - C16 | 1.62793             | 0.48628                | 103.03|
| Donor NBO | Acceptor NBO | Donor NBO Occupancy | Acceptor NBO Occupancy | E(2) |
|-----------|--------------|----------------------|------------------------|------|
| **Alpha Spin** |
| LP (1)Ni1 | BD*(1)N2 - C3 | 0.99865 | 0.00887 | 0.09 |
| LP (4)Ni1 | BD*(2)N2 - C3 | 0.99822 | 0.32312 | 0.33 |
| BD (1)N2 - C3 | LP*(8)Ni1 | 0.9895 | 0.06849 | 3 |
| BD (1)N2 - C5 | LP*(8)Ni1 | 0.99121 | 0.06849 | 3.64 |
| BD (1)N10 - C18 | LP*(9)Ni1 | 0.99203 | 0.06264 | 2.84 |
| BD (1)O11 - C14 | LP*(7)Ni1 | 0.99558 | 0.0867 | 3.94 |
| LP (1)N2 | LP*(8)Ni1 | 0.93564 | 0.06849 | 17.1 |
| LP (1)N10 | LP*(9)Ni1 | 0.92311 | 0.06264 | 15.71 |
| LP (2)O11 | LP*(7)Ni1 | 0.92132 | 0.0867 | 34.53 |
| LP (1)Cl27 | LP*(7)Ni1 | 0.99474 | 0.0867 | 4.85 |
| LP (2)Cl27 | LP*(8)Ni1 | 0.97876 | 0.06849 | 5.32 |
| LP (3)Cl27 | LP*(9)Ni1 | 0.97711 | 0.06264 | 4.44 |
| LP (4)Cl27 | LP*(6)Ni1 | 0.87536 | 0.15092 | 61.31 |
| **Beta Spin** |
| LP (1)Ni1 | BD*(1)C9 - N10 | 0.99858 | 0.01351 | 0.12 |
| LP (2)Ni1 | BD*(2)N10 - C18 | 0.99706 | 0.01516 | 0.29 |
| BD (1)N2 - C3 | LP*(8)Ni1 | 0.98921 | 0.06431 | 2.99 |
| BD (1)N2 - C5 | LP*(8)Ni1 | 0.99111 | 0.06431 | 3.56 |
| BD (1)N10 - C18 | LP*(9)Ni1 | 0.99176 | 0.05247 | 3.13 |
| BD (1)O11 - C14 | LP*(7)Ni1 | 0.99473 | 0.08945 | 3.84 |
| LP (1)N2 | LP*(6)Ni1 | 0.90099 | 0.11981 | 24 |
| LP (1)N10 | LP*(5)Ni1 | 0.8374 | 0.15256 | 51.56 |
| LP (1)O11 | LP*(7)Ni1 | 0.95709 | 0.08945 | 13.64 |
| LP (2)O11 | LP*(4)Ni1 | 0.87242 | 0.2286 | 19.82 |
| LP (1)Cl27 | LP*(7)Ni1 | 0.98947 | 0.08945 | 6.42 |
| LP (2)Cl27 | LP*(9)Ni1 | 0.96773 | 0.05247 | 4.01 |
| LP (3)Cl27 | LP*(8)Ni1 | 0.96354 | 0.06431 | 3.54 |
| LP (4)Cl27 | LP*(4)Ni1 | 0.84227 | 0.2286 | 46.89 |
| Donor NBO | Acceptor NBO | Occupancy Donor NBO | Occupancy Acceptor NBO | E(2) |
|-----------|--------------|---------------------|------------------------|------|
| Alpha Spin |
| LP (2)Cu1 | BD*(2)N2 - C3 | 0.3049              | 0.99902                | 0.23 |
| LP (3)Cu1 | BD*(1)N10 - C18 | 0.0156              | 0.99858                | 0.16 |
| BD (1)C9 - N10 | LP*(8)Cu1 | 0.99022              | 0.06274                | 3.09 |
| BD (1)N10 - C18 | LP*(8)Cu1 | 0.99205              | 0.06274                | 3.49 |
| BD (1)O11 - C14 | LP*(7)Cu1 | 0.99562              | 0.08349                | 4.03 |
| LP (1)N10 | LP*(8)Cu1 | 0.92419              | 0.06274                | 16.9 |
| LP (2)O11 | LP*(7)Cu1 | 0.92514              | 0.08349                | 34.22 |
| LP (1)Cl27 | LP*(7)Cu1 | 0.99362              | 0.08349                | 5.61 |
| LP (2)Cl27 | LP*(8)Cu1 | 0.97809              | 0.06274                | 4.9  |
| LP (3)Cl27 | LP*(9)Cu1 | 0.97672              | 0.0559                 | 4.56 |
| LP (4)Cl27 | LP*(6)Cu1 | 0.87446              | 0.15226                | 63.6 |

| Beta Spin |
| BD (1)N10 - C18 | LP*(7)Cu1 | 0.99161              | 0.06387                | 2.87 |
| BD (1)O11 - C14 | LP*(6)Cu1 | 0.99538              | 0.11369                | 2.92 |
| LP (1)N10 | LP*(5)Cu1 | 0.814                | 0.15449                | 37.34 |
| LP (1)O11 | LP*(6)Cu1 | 0.94921              | 0.11369                | 11.47 |
| LP (1)Cl27 | LP*(6)Cu1 | 0.98704              | 0.11369                | 8.33 |
| LP (2)Cl27 | LP*(8)Cu1 | 0.97773              | 0.05715                | 3.26 |
| LP (3)Cl27 | LP*(6)Cu1 | 0.95616              | 0.11369                | 7.75 |
| LP (4)Cl27 | LP*(6)Cu1 | 0.82131              | 0.11369                | 40.28 |

(d)

| Donor NBO | Acceptor NBO | Occupancy Donor NBO | Occupancy Acceptor NBO | E(2) |
|-----------|--------------|---------------------|------------------------|------|
| BD (1)N10 - C18 | LP*(9)Zn1 | 1.9856               | 0.12038                | 3.57 |
| BD (1)O11 - C14 | LP*(7)Zn1 | 1.99076              | 0.15592                | 4.05 |
| LP (1)N2 | LP*(8)Zn1 | 1.87079              | 0.13067                | 27.93 |
| LP (1)N10 | LP*(6)Zn1 | 1.84454              | 0.32549                | 30.16 |
| LP (2)O11 | LP*(7)Zn1 | 1.84501              | 0.15592                | 45.22 |
| LP (1)Cl27 | LP*(7)Zn1 | 1.9891               | 0.15592                | 10.02 |
| LP (2)Cl27 | LP*(8)Zn1 | 1.95753              | 0.13067                | 10.24 |
| LP (3)Cl27 | LP*(9)Zn1 | 1.95511              | 0.12038                | 10.23 |
| LP (4)Cl27 | LP*(6)Zn1 | 1.75548              | 0.32549                | 98.14 |

(e)
Table S2 Occupancies of electron Donor and Acceptor NBOs and Bond stabilization energy $E(2)$ (in kcal/mol) of (a) isolated HL2 Schiff base (b) HL2-Co$^{2+}$ (c) HL2-Ni$^{2+}$ (d) HL2-Cu$^{2+}$ and (e) HL2-Zn$^{2+}$ calculated at CAM-B3LYP/LANL2DZ level of theory.

(a)

| Donor NBO | Acceptor NBO | Donor NBO Occupancy | Acceptor NBO Occupancy | $E(2)$ |
|-----------|--------------|----------------------|------------------------|--------|
| BD (1)N1 - C2 | BD*(1)C4 - H 28 | 1.9803 | 0.01853 | 5.62 |
| BD (1)N2 - C4 | BD*(1)N5 - C6 | 1.9852 | 0.0533 | 5.11 |
| BD (2)N1 - C4 | BD*(2)C2 - C3 | 1.8839 | 0.29054 | 26.18 |
| BD (1)C8 - N9 | BD*(1)C16 - C17 | 1.9805 | 0.03617 | 5.77 |
| BD (1)N9 - C17 | BD*(1)C16 - C17 | 1.985 | 0.03617 | 2.51 |
| BD (2)N9 - C17 | BD*(2)C13 - C16 | 1.9353 | 0.48579 | 6.32 |
| BD (1)O10 - C13 | BD*(1)C14 - C16 | 1.9904 | 0.02224 | 2.54 |
| LP (1)N1 | BD*(1)C4 - N5 | 1.9367 | 0.04325 | 10.82 |
| LP (1)N9 | BD*(1)C17 - C18 | 1.9084 | 0.0439 | 16.56 |

(b)

| Donor NBO | Acceptor NBO | Donor NBO Occupancy | Acceptor NBO Occupancy | $E(2)$ |
|-----------|--------------|----------------------|------------------------|--------|
| LP (4) Co1 | BD*(2)N2 - C3 | 0.9948 | 0.3188 | 0.48 |
| BD (1)N2 - C3 | LP*(8) Co1 | 0.9894 | 0.0667 | 3.17 |
| BD (1)N2 - C5 | LP*(8) Co1 | 0.9912 | 0.0667 | 3.92 |
| BD (1)O11 - C14 | LP*(7) Co1 | 0.9955 | 0.0843 | 3.44 |
| LP (1)N10 | LP*(9) Co1 | 0.9214 | 0.0651 | 15.79 |
| LP (1)Cl27 | LP*(7) Co1 | 0.9946 | 0.0843 | 4.86 |
| LP (2)Cl27 | LP*(8) Co1 | 0.9787 | 0.0667 | 5.51 |
| LP (3)Cl27 | LP*(9) Co1 | 0.9783 | 0.0651 | 4.83 |

Alpha Spin

| Donor NBO | Acceptor NBO | Donor NBO Occupancy | Acceptor NBO Occupancy | $E(2)$ |
|-----------|--------------|----------------------|------------------------|--------|
| LP (1)Co1 | BD*(1)N10 - C18 | 0.9976 | 0.0144 | 0.19 |
| BD (1)N2 - C5 | LP*(7) Co1 | 0.9908 | 0.04 | 2.73 |
| BD (1)N10 - C18 | LP*(4) Co1 | 0.9917 | 0.1343 | 1.21 |
| LP (1)N2 | LP*(6) Co1 | 0.9146 | 0.0602 | 20.37 |
| LP (1)N10 | LP*(4) Co1 | 0.8591 | 0.1343 | 33.63 |
| LP (2)O11 | LP*(5) Co1 | 0.8665 | 0.1047 | 38.19 |
| LP (1)Cl27 | LP*(7) Co1 | 0.9854 | 0.04 | 4.29 |
| LP (4)Cl27 | LP*(3) Co1 | 0.8353 | 0.1633 | 77.47 |
| Donor NBO | Acceptor NBO | Donor NBO Occupancy | Acceptor NBO Occupancy | E(2) |
|----------|--------------|---------------------|------------------------|------|
| Alpha Spin |
| LP (1)Ni1 | BD*(1)N2 - C3 | 0.9986 | 0.0088 | 0.09 |
| LP (4)Ni1 | BD*(2)N10 - C18 | 0.9962 | 0.13 | 0.4 |
| BD (1)N2 - C3 | LP*(8)Ni1 | 0.9895 | 0.0688 | 3.26 |
| BD (1)N2 - C5 | LP*(8)Ni1 | 0.9911 | 0.0688 | 4.1 |
| BD (1)N10 - C18 | LP*(9)Ni1 | 0.9921 | 0.0633 | 3.16 |
| BD (1)O11 - C14 | LP*(7)Ni1 | 0.9955 | 0.0862 | 3.81 |
| LP (1)N2 | LP*(8)Ni1 | 0.9355 | 0.0688 | 18.34 |
| LP (1)N10 | LP*(9)Ni1 | 0.9242 | 0.0633 | 17.49 |
| LP (2)O11 | LP*(7)Ni1 | 0.9201 | 0.0862 | 33.51 |
| LP (1)Cl27 | LP*(7)Ni1 | 0.9948 | 0.0862 | 4.66 |
| LP (2)Cl27 | LP*(8)Ni1 | 0.9786 | 0.0688 | 5.12 |
| LP (4)Cl27 | LP*(6)Ni1 | 0.8757 | 0.1495 | 60.98 |
| Beta Spin |
| BD (1)N2 - C3 | LP*(8)Ni1 | 0.9892 | 0.068 | 3.19 |
| BD (1)N2 - C5 | LP*(8)Ni1 | 0.8461 | 0.068 | 3.88 |
| BD (1)N10 - C18 | LP*(9)Ni1 | 0.9918 | 0.0538 | 3.03 |
| BD (1)O11 - C14 | LP*(7)Ni1 | 0.9949 | 0.0893 | 3.72 |
| LP (1)N2 | LP*(6)Ni1 | 0.9026 | 0.1197 | 23 |
| LP (1)N10 | LP*(5)Ni1 | 0.8398 | 0.1536 | 50.73 |
| LP (1)O11 | LP*(7)Ni1 | 0.9566 | 0.0893 | 12.42 |
| LP (2)O11 | LP*(7)Ni1 | 0.8838 | 0.0893 | 19.76 |
| LP (1)Cl27 | LP*(7)Ni1 | 0.9897 | 0.0893 | 6.44 |
| LP (2)Cl27 | LP*(8)Ni1 | 0.9696 | 0.068 | 3.7 |
| LP (3)Cl27 | LP*(9)Ni1 | 0.963 | 0.0538 | 3.33 |
| LP (4)Cl27 | LP*(4)Ni1 | 0.8438 | 0.2286 | 48.61 |
### Alpha Spin

| Donor NBO | Acceptor NBO | Donor NBO Occupancy | Acceptor NBO Occupancy | E(2) |
|-----------|--------------|---------------------|------------------------|------|
| LP (1)Cu1 | BD*(2)N10 - C18 | 0.9992              | 0.1201                 | 0.07 |
| LP (2)Cu1 | BD*(2)N2 - C3  | 0.999               | 0.3042                 | 0.26 |
| LP (3)Cu1 | BD*(1)N10 - C18| 0.9985              | 0.0156                 | 0.15 |
| BD (1)N10 - C18 | LP*(8)Cu1 | 0.992               | 0.0625                 | 3.26 |
| BD (1)O11 - C14 | LP*(7)Cu1 | 0.9956              | 0.0833                 | 3.88 |
| BD (1)N10 | LP*(8)Cu1     | 0.9242              | 0.0625                 | 15.97|
| LP (2)O11 | LP*(7)Cu1     | 0.9251              | 0.0833                 | 33.44|
| LP (1)Cl27 | LP*(7)Cu1    | 0.9935              | 0.0833                 | 5.5  |
| LP (2)Cl27 | LP*(8)Cu1     | 0.978               | 0.0625                 | 3.41 |
| LP (3)Cl27 | LP*(9)Cu1     | 0.9767              | 0.0555                 | 2.98 |
| LP (4)Cl27 | LP*(6)Cu1     | 0.8744              | 0.1522                 | 63.77|

### Beta Spin

| Donor NBO | Acceptor NBO | Donor NBO Occupancy | Acceptor NBO Occupancy | E(2) |
|-----------|--------------|---------------------|------------------------|------|
| BD (1)N10 - C18 | LP*(7)Cu1 | 0.99163             | 0.06364                | 2.88 |
| BD (1)O11 - C14 | LP*(6)Cu1 | 0.99539             | 0.11329                | 2.88 |
| LP (2)Cu1 | BD*(2)N2 - C3  | 0.99921             | 0.30483                | 0.28 |
| LP (1)N10 | LP*(5)Cu1     | 0.81257             | 0.15497                | 32.92|
| LP (1)O11 | LP*(6)Cu1     | 0.94913             | 0.11329                | 11.7 |
| LP (1)Cl27 | LP*(6)Cu1     | 0.98712             | 0.11329                | 7.92 |
| LP (2)Cl27 | LP*(8)Cu1     | 0.97767             | 0.05686                | 3.33 |
| LP (3)Cl27 | LP*(6)Cu1     | 0.95606             | 0.11329                | 7.07 |
| LP (4)Cl27 | LP*(6)Cu1     | 0.82207             | 0.11329                | 36.43|

### (d)

### (e)
Table S3 Occupancies of Electron Donor and Acceptor NBOs and Bond stabilization energy E(2) (in kcal/mol) of (a) isolated HL3 Schiff base (b) HL3-Co^{2+} (c) HL3-Ni^{2+} (d) HL3-Cu^{2+} and (e) HL3-Zn^{2+} calculated at CAM-B3LYP/LANL2DZ level of theory.

| Donor NBO   | Acceptor NBO          | Donor NBO Occupancy | Acceptor NBO Occupancy | E(2) |
|-------------|-----------------------|---------------------|------------------------|------|
| BD (1)N1 - C2 | BD*(1)C4 - H          | 1.9803              | 0.01845                | 5.65 |
| BD (1)N1 - C4 | BD*(1)N5 - C6         | 1.9851              | 0.0305                 | 5.1  |
| BD (2)N1 - C4 | BD*(2)C2 - C3         | 1.8828              | 0.29172                | 25.92|
| BD (1)C8 - N9 | BD*(1)C16 - C17       | 1.9804              | 0.03643                | 5.67 |
| BD (1)N9 - C17 | BD*(1)C13 - C16      | 1.9847              | 0.0519                 | 2.49 |
| BD (2)N9 - C17 | BD*(2)C13 - C16      | 1.936               | 0.47937                | 6.22 |
| BD (1)O10 - C13 | BD*(1)C14 - C16    | 1.9902              | 0.02248                | 2.44 |
| LP (1)N1     | BD*(1)C4 - N5         | 1.9366              | 0.0432                 | 10.79|
| LP (1)N9     | BD*(1)C17 - C18       | 1.909               | 0.0451                 | 15.9 |
| LP (3)O10   | BD*(2)C13 - C16       | 1.6468              | 0.47937                | 99.81|

(a)

| Donor NBO   | Acceptor NBO          | Donor NBO Occupancy | Acceptor NBO Occupancy | E(2) |
|-------------|-----------------------|---------------------|------------------------|------|
| LP (4)Co1   | BD*(2)N2 - C3         | 0.9979              | 0.3188                 | 0.44 |
| BD (1)N2 - C3 | LP*(8) Co1           | 0.9894              | 0.0668                 | 3.05 |
| BD (1)N2 - C5 | LP*(8) Co1           | 0.9912              | 0.0668                 | 3.79 |
| BD (1)N10 - C18 | LP*(9) Co1        | 0.992               | 0.0646                 | 2.92 |
| BD (1)O11 - C14 | LP*(7) Co1      | 0.9956              | 0.0843                 | 3.33 |
| LP (1)N2    | LP*(8) Co1           | 0.939               | 0.0668                 | 15.32|
| LP (1)N10   | LP*(9) Co1           | 0.9218              | 0.0646                 | 15.51|
| LP (2)O11   | LP*(7) Co1           | 0.9226              | 0.0843                 | 27.2 |
| LP (1)C27   | LP*(7) Co1           | 0.9945              | 0.0843                 | 4.81 |
| LP (2)C27   | LP*(8) Co1           | 0.9785              | 0.0668                 | 5.52 |
| LP (3)C27   | LP*(9) Co1           | 0.9781              | 0.0646                 | 4.85 |
| LP (4)C27   | LP*(6) Co1           | 0.8812              | 0.1459                 | 56.54|

(b)

Alpha Spin

Beta Spin

BD (1)N10 - C18 | LP*(6) Co1 | 0.9917 | 0.0932 | 1.67 |
BD (1)O11 - C14 | LP*(6) Co1 | 0.9937 | 0.0932 | 2.37 |
LP (1)N10      | LP*(5) Co1 | 0.8606 | 0.1111 | 26.96|
LP (1)O11      | LP*(6) Co1 | 0.9609 | 0.0932 | 10.27|
LP (2)O11      | LP*(4) Co1 | 0.8672 | 0.1428 | 41.85|
LP (2)C27      | LP*(7) Co1 | 0.9693 | 0.0688 | 4.01 |
LP (3)C27      | LP*(6) Co1 | 0.9522 | 0.0932 | 5.2  |
LP (4)C27      | LP*(3) Co1 | 0.8339 | 0.1868 | 83.24|
| Donor NBO | Acceptor NBO | Donor NBO Occupancy | Acceptor NBO Occupancy | E(2) |
|-----------|-------------|---------------------|------------------------|------|
| **Alpha Spin** | | | | |
| BD (1)N2 - C3 | LP*(8)Ni1 | 0.9895 | 0.0688 | 3.13 |
| BD (1)N2 - C5 | LP*(8)Ni1 | 0.9911 | 0.0688 | 3.97 |
| BD (1)N10 - C18 | LP*(9)Ni1 | 0.992 | 0.0628 | 3.13 |
| BD (1)O11 - C14 | LP*(7)Ni1 | 0.9955 | 0.0863 | 3.77 |
| LP (1)N2 | LP*(8)Ni1 | 0.9351 | 0.0688 | 17.82 |
| LP (1)N10 | LP*(9)Ni1 | 0.9242 | 0.0628 | 17.43 |
| LP (2)O11 | LP*(7)Ni1 | 0.9203 | 0.0863 | 32.63 |
| LP (1)Cl27 | LP*(7)Ni1 | 0.9948 | 0.0863 | 4.61 |
| LP (2)Cl27 | LP*(8)Ni1 | 0.9785 | 0.0688 | 5.08 |
| LP (4)Cl27 | LP*(6)Ni1 | 0.8753 | 0.15 | 60.06 |
| **Beta Spin** | | | | |
| LP (1)Ni1 | BD*(1)N10 - C18 | 0.9986 | 0.0145 | 0.1 |
| BD (1)N2 - C3 | LP*(8)Ni1 | 0.9892 | 0.0673 | 3.17 |
| BD (1)N2 - C5 | LP*(8)Ni1 | 0.991 | 0.0673 | 3.89 |
| BD (1)N10 - C18 | LP*(9)Ni1 | 0.9917 | 0.0531 | 3.07 |
| BD (1)O11 - C14 | LP*(7)Ni1 | 0.9949 | 0.0894 | 3.68 |
| LP (1)N2 | LP*(6)Ni1 | 0.9011 | 0.1211 | 22.07 |
| LP (1)N10 | LP*(5)Ni1 | 0.8412 | 0.1512 | 50.23 |
| LP (1)O11 | LP*(7)Ni1 | 0.9571 | 0.0894 | 12.31 |
| LP (2)O11 | LP*(7)Ni1 | 0.8807 | 0.0894 | 18.56 |
| LP (1)Cl27 | LP*(7)Ni1 | 0.9894 | 0.0894 | 6.33 |
| LP (2)Cl27 | LP*(8)Ni1 | 0.9685 | 0.0673 | 4.37 |
| LP (3)Cl27 | LP*(9)Ni1 | 0.963 | 0.0531 | 4.11 |
| LP (4)Cl27 | LP*(4)Ni1 | 0.8412 | 0.229 | 44.87 |
| Donor NBO | Acceptor NBO | Donor NBO Occupancy | Acceptor NBO Occupancy | E(2) |
|-----------|--------------|---------------------|------------------------|------|
| **Alpha Spin** | | | | |
| LP (2)Cu1 | BD*(2)N2 - C3 | 0.9989 | 0.306 | 0.22 |
| LP (3)Cu1 | BD*(1)N10 - C18 | 0.9984 | 0.0149 | 0.17 |
| LP (5)Cu1 | BD*(2)N10 - C18 | 0.9955 | 0.1276 | 0.44 |
| BD (1)C9 - N10 | LP*(8)Cu1 | 0.99 | 0.0622 | 3.12 |
| BD (1)N10 - C18 | LP*(8)Cu1 | 0.992 | 0.0622 | 3.53 |
| BD (1)O11 - C14 | LP*(7)Cu1 | 0.9956 | 0.0834 | 4.01 |
| LP (1)N10 | LP*(8)Cu1 | 0.9242 | 0.0622 | 17.06 |
| LP (2)O11 | LP*(7)Cu1 | 0.9243 | 0.0834 | 34.06 |
| LP (1)Cl27 | LP*(7)Cu1 | 0.9936 | 0.0834 | 5.64 |
| LP (2)Cl27 | LP*(8)Cu1 | 0.9776 | 0.0622 | 4.89 |
| LP (3)Cl27 | LP*(9)Cu1 | 0.9767 | 0.0575 | 4.6 |
| LP (4)Cl27 | LP*(6)Cu1 | 0.8735 | 0.1517 | 63.49 |
| **Beta Spin** | | | | |
| BD (1)N10 - C18 | LP*(7)Cu1 | 0.9914 | 0.063 | 2.91 |
| BD (1)O11 - C14 | LP*(6)Cu1 | 0.9954 | 0.1113 | 2.89 |
| LP (4)Cu1 | BD*(2)N10 - C18 | 0.9991 | 0.131 | 0.54 |
| LP (1)N2 | LP*(7)Cu1 | 0.9437 | 0.063 | 4.42 |
| LP (1)N10 | LP*(5)Cu1 | 0.8247 | 0.1517 | 37.71 |
| LP (1)O11 | LP*(6)Cu1 | 0.9489 | 0.1113 | 11.4 |
| LP (1)Cl27 | LP*(6)Cu1 | 0.9874 | 0.1113 | 8.35 |
| LP (2)Cl27 | LP*(8)Cu1 | 0.9776 | 0.0593 | 3.47 |
| LP (3)Cl27 | LP*(6)Cu1 | 0.9544 | 0.1113 | 7.74 |
| LP (4)Cl27 | LP*(6)Cu1 | 0.8234 | 0.1113 | 40.42 |

| Donor NBO | Acceptor NBO | Donor NBO Occupancy | Acceptor NBO Occupancy | E(2) |
|-----------|--------------|---------------------|------------------------|------|
| **(d)** | | | | |
| LP (3)Zn1 | BD*(2)N2 - C5 | 1.9979 | 0.4252 | 0.21 |
| LP (4)Zn1 | BD*(2)N10 - C18 | 1.9975 | 0.0289 | 0.25 |
| LP (5)Zn1 | BD*(2)N2 - C5 | 1.9964 | 0.4252 | 0.7 |
| BD (1)N10 - C18 | LP*(9)Zn1 | 1.9855 | 0.1193 | 3.57 |
| BD (1)O11 - C14 | LP*(7)Zn1 | 1.9908 | 0.1567 | 4.04 |
| LP (1)N2 | LP*(8)Zn1 | 1.8693 | 0.1311 | 27.8 |
| LP (1)N10 | LP*(6)Zn1 | 1.8453 | 0.3259 | 30.36 |
| LP (2)O11 | LP*(6)Zn1 | 1.8447 | 0.3259 | 29.34 |
| LP (1)Cl27 | LP*(7)Zn1 | 1.9891 | 0.1567 | 10.03 |
| LP (2)Cl27 | LP*(8)Zn1 | 1.9572 | 0.1311 | 10.24 |
| LP (3)Cl27 | LP*(9)Zn1 | 1.9547 | 0.1193 | 10.22 |
| LP (4)Cl27 | LP*(6)Zn1 | 1.7539 | 0.3259 | 97.82 |

| Donor NBO | Acceptor NBO | Donor NBO Occupancy | Acceptor NBO Occupancy | E(2) |
|-----------|--------------|---------------------|------------------------|------|
| **(e)** | | | | |

(d) 

(e)