Bonds lengths, valence and torsion angles in the Mn(II), Fe(II) and Co(II)) phthalocyanine metal chelates. The **bold font** in brackets specifies experimental values, regular font, calculated by DFT B3LYP 6-31G(d), OPBE/TZVP, B3PW91/TZVP and wB97XD/TZVP (first, second, third and fourth value, respectively) *.

| M | Mn | Fe | Co |
|---|---|---|---|
| M–N bond lengths, *pm* | | | |
| (M1N1) | 195.9; 195.5; 195.9; 194.1; (**193.9**) | 193.8; 190.8; 194.0; 200.3; (**192.7**) | 189.6; 191.5; 192.7; 192.9; (**191.0**) |
| (M1N2) | 193.7; 193.7; 194.1; 195.8; (**193.8**) | 193.8; 190.8; 194.0; 200.3; (**192.6**) | 189.6; 191.5; 192.7; 192.9; (**191.0**) |
| (M1N3) | 195.9; 195.5; 195.9; 194.1; (**193.9**) | 193.8; 190.8; 194.0; 200.4; (**192.7**) | 189.6; 191.5; 192.7; 192.9; (**191.0**) |
| (M1N4) | 193.7; 193.7; 194.1; 195.8; (**193.8**) | 193.8; 190.8; 194.0; 200.3; (**192.6**) | 189.6; 191.5; 192.7; 192.9; (**191.0**) |
| C–N bond lengths, *pm* | | | |
| (N1C3) | 138.5; 138.1; 137.5; 137.9; (**138.9**) | 138.0; 138.2; 137.0; 136.2; (**138.1**) | 138.8; 137.8; 137.0; 136.6; (**138.4**) |
| (N1C4) | 138.5; 138.1; 137.5; 137.9; (**139.7**) | 138.1; 138.3; 137.2; 136.2; (**137.5**) | 138.8; 137.8; 137.0; 136.6; (**137.1**) |
| (N2C1) | 139.5; 138.9; 138.4; 137.0; (**139.1**) | 138.1; 138.3; 137.2; 136.2; (**137.5**) | 138.8; 137.8; 137.0; 136.6; (**137.1**) |
| (N2C2) | 139.5; 138.9; 138.4; 137.0; (**139.2**) | 138.0; 138.3; 137.0; 136.1; (**138.2**) | 138.8; 137.8; 137.0; 136.6; (**138.4**) |
| (N3C7) | 138.5; 138.1; 137.5; 137.9; (**138.9**) | 138.0; 138.2; 137.0; 136.1; (**138.1**) | 138.8; 137.8; 137.0; 136.6; (**137.0**) |
| (N3C8) | 138.5; 139.1; 137.5; 137.9; (**139.7**) | 138.1; 138.3; 137.2; 136.1; (**137.5**) | 138.8; 137.8; 137.0; 136.6; (**138.7**) |
| (N4C5) | 139.5; 138.9; 138.4; 137.0; (**139.1**) | 138.1; 138.3; 137.2; 136.1; (**137.5**) | 138.8; 137.8; 137.0; 136.6; (**138.0**) |
| (N4C6) | 139.5; 138.9; 138.4; 137.0; (**139.2**) | 138.0; 138.2; 137.0; 136.2; (**138.2**) | 138.8; 137.8; 137.0; 136.6; (**138.0**) |
| (N5C2) | 131.2; 131.1; 130.6; 132.3; (**131.4**) | 132.2; 131.9; 131.6; 132.3; (**132.1**) | 131.9; 131.7; 131.4; 131.2; (**131.9**) |
| (N5C3) | 133.1; 132.7; 132.3; 130.4; (**132.5**) | 132.2; 131.9; 131.6; 132.2; (**132.2**) | 131.9; 131.7; 131.4; 131.2; (**132.6**) |
| (N6C6) | 131.2; 131.1; 130.6; 132.3; (**131.4**) | 132.2; 131.9; 131.6; 132.1; (**132.1**) | 131.9; 131.7; 131.4; 131.2; (**131.9**) |
| (N6C7) | 133.1; 132.7; 132.3; 130.4; (**132.5**) | 132.2; 131.9; 131.6; 132.4; (**132.2**) | 131.9; 131.7; 131.4; 131.2; (**132.6**) |
| (N7C4) | 133.1; 132.7; 132.3; 130.4; (**132.4**) | 132.2; 131.9; 131.6; 132.2; (**132.0**) | 131.9; 131.7; 131.4; 131.2; (**132.3**) |
| (N7C5) | 131.2; 132.8; 130.6; 132.3; (**132.8**) | 132.2; 131.9; 131.6; 132.3; (**132.4**) | 131.9; 131.7; 131.4; 131.2; (**132.5**) |
| (N8C1) | 131.2; 131.1; 130.6; 132.3; (**132.8**) | 132.2; 131.9; 131.6; 132.1; (**132.4**) | 131.9; 131.7; 131.4; 131.2; (**132.3**) |
| (N8C8) | 133.1; 132.7; 132.3; 130.4; (**132.4**) | 132.2; 131.9; 131.6; 132.4; (**132.0**) | 131.9; 131.7; 131.4; 131.2; (**132.5**) |

| C–C bond lengths, *pm* | | | |
|---|---|---|---|
| (C9C10) | 141.2; 141.0; 140.5; 139.1; (**140.8**) | 140.4; 140.0; 139.9; 140.0; (**139.0**) | 139.9; 140.1; 139.7; 139.2; (**139.2**) |
| (C11C12) | 140.3; 140.2; 139.7; 139.9; (**140.7**) | 140.4; 140.0; 139.9; 140.0; (**139.3**) | 139.9; 140.1; 139.7; 139.2; (**139.8**) |
| (C13C14) | 141.2; 141.0; 140.5; 139.1; (**140.8**) | 140.4; 140.0; 139.9; 140.1; (**139.0**) | 139.9; 140.1; 139.7; 139.2; (**139.2**) |
| (C15C16) | 140.3; 140.2; 139.7; 139.9; (**140.7**) | 140.4; 140.0; 139.9; 140.0; (**139.3**) | 139.9; 140.1; 139.7; 139.2; (**139.8**) |
| (C9C17) | 140.1; 139.9; 139.4; 138.6; (**139.2**) | 139.6; 139.2; 139.0; 138.7; (**139.5**) | 139.2; 139.5; 138.9; 138.8; (**139.3**) |
| (C17C25) | 138.8; 138.8; 138.2; 138.6; (**139.4**) | 139.3; 139.7; 138.7; 138.5; (**138.7**) | 139.8; 139.2; 138.7; 138.4; (**139.4**) |
| (C25C26) | 141.5; 141.0; 140.7; 139.8; (**140.9**) | 140.9; 140.1; 140.2; 140.0; (**139.4**) | 140.4; 140.5; 140.2; 140.1; (**139.1**) |
| (C26C18) | 138.8; 138.8; 138.2; 138.6; (**139.6**) | 139.3; 139.7; 138.7; 138.5; (**139.7**) | 139.8; 139.2; 138.7; 138.4; (**139.4**) |
| (C18C10) | 140.1; 139.9; 139.4; 138.6; (**140.0**) | 139.6; 139.2; 138.9; 138.7; (**139.4**) | 139.2; 139.5; 138.9; 138.8; (**139.0**) |
| C–H bond lengths, *pm* | | | |
| (C17H1) | 108.5; 108.8; 108.3; 108.2; (**109.5**) | 108.5; 108.9; 108.3; 108.2; ( **–** ) | 108.5; 108.8; 108.3; 108.2; (**95.3**) |
| (C25H9) | 108.7; 109.0; 108.4; 108.3; (**107.8**) | 108.7; 109.0; 108.4; 108.3; ( **–** ) | 108.6; 109.0; 108.4; 108.3; (**95.8**) |
| (C26H10) | 108.7; 109.0; 108.4; 108.3; (**109.4**) | 108.7; 109.0; 108.4; 108.3; ( **–** ) | 108.6; 109.0; 108.4; 108.3; (**96.3**) |
| (C18H2) | 108.5; 108.8; 108.3; 108.2; (**108.0**) | 108.5; 108.9; 108.3; 108.2; ( **–** ) | 108.5; 108.8; 108.3; 108.2; (**95.1**) |
| ∠NMN bond angles in the $MN_4$ chelate node, *deg* | | | |
| (N1M1N4) | 90.0; 90.0; 90.0; 90.0; (**91.3**) | 90.0; 90.0; 89.9; 90.0; (**90.9**) | 90.0; 90.0; 90.0; 90.0; (**90.0**) |
| (N4M1N3) | 90.0; 90.0; 90.0; 90.0; (**88.7**) | 90.0; 90.0; 90.1; 90.0; (**89.1**) | 90.0; 90.0; 90.0; 90.0; (**90.0**) |
| (N3M1N2) | 90.0; 90.0; 90.0; 90.0; (**91.3**) | 90.0; 90.0; 89.9; 90.0; (**90.9**) | 90.0; 90.0; 90.0; 90.0; (**90.0**) |
| (N2M1N1) | 90.0; 90.0; 90.0; 90.0; (**88.7**) | 90.0; 90.0; 90.1; 90.0; (**89.1**) | 90.0; 90.0; 90.0; 90.0; (**90.0**) |
| ***VAS*** | 360.0; 360.0; 360.0; 360.0; (**360.0**) | 360.0; 360.0; 360.0; 360.0; (**360.0**) | 360.0; 360.0; 360.0; 360.0; (**360.0**) |
| ∠NNN non-bond angles in the $MN_4$ chelate node, *deg* | | | |
| (N1N4N3) | 90.7; 90.5; 90.5; 89.5; (**90.5**) | 90.0; 90.0; 90.0; 90.0; (**90.0**) | 90.0; 90.0; 90.0; 90.0; (**90.0**) |
| (N4N3N2) | 89.3; 89.5; 89.5; 90.5; (**89.5**) | 90.0; 90.0; 90.0; 90.0; (**90.0**) | 90.0; 90.0; 90.0; 90.0; (**90.0**) |
| (N3N2N1) | 90.7; 90.5; 90.0; 89.5; (**90.5**) | 90.0; 90.0; 90.0; 90.0; (**90.0**) | 90.0; 90.0; 90.0; 90.0; (**90.0**) |
| (N2N1N4) | 89.3; 90.5; 89.5; 90.5; (**89.5**) | 90.0; 90.0; 90.0; 90.0; (**90.0**) | 90.0; 90.0; 90.0; 90.0; (**90.0**) |
| NVAS | 360.0; 360.0; 360.0; (**360.0**) | 360.0; 360.0; 360.0; 360.0; (**360.0**) | 360.0; 360.0; 360.0; 360.0; (**360.0**) |

| | | | |
|---|---|---|---|
| Bond angles in the 6-numbered ring (M1N1C4N7C5N4), *deg* | | | |
| (N1M1N4) | 90.0; 90.0; 90.0; 90.0; (**91.3**) | 90.0; 90.0; 89.9; 90.0; (**90.9**) | 90.0; 90.0; 90.0; 90.0; (**90.0**) |
| (M1N4C5) | 126.2; 126.1; 126.0; 125.6; (**125.2**) | 126.3; 126.7; 126.0; 124.7; (**125.4**) | 127.0; 126.4; 126.1; 126.1; (**127.8**) |
| (N4C5N7) | 127.5; 127.6; 127.5; 127.3; (**127.9**) | 127.5; 127.6; 127.5; 127.6; (**128.0**) | 127.6; 127.8; 127.6; 127.7; (**126.2**) |
| (C5N7C4) | 123.1; 123.0; 123.6; 123.7; (**122.7**) | 122.5; 121.4; 123.0; 125.4; (**122.2**) | 120.8; 121.5; 122.5; 122.6; (**121.1**) |
| (N7C4N1) | 127.2; 127.4; 127.2; 127.5; (**127.7**) | 127.5; 127.6; 127.5; 127.5; (**127.9**) | 127.6; 127.8; 127.6; 127.6; (**128.4**) |
| (C4N1M1) | 125.9; 125.8; 125.7; 125.9; (**125.2**) | 126.2; 126.7; 126.0; 124.8; (**125.5**) | 127.0; 126.4; 126.1; 126.0; (**125.8**) |
| VAS[1] | 719.9; 719.9; 720.0; 720.0; (**720.0**) | 720.0; 720.0; 719.9; 720.0; (**719.9**) | 720.0; 719.9; 719.9; 720.0; (**719.3**) |
| Bond angles in the 5-numbered ring (C3N1C4C9C10), *deg* | | | |
| (C3N1C4) | 108.2; 108.4; 108.7; 108.2; (**107.5**) | 107.6; 106.6; 108.1; 110.4; (**107.3**) | 106.1; 107.1; 107.7; 107.9; (**107.3**) |
| (N1C4C9) | 109.2; 109.1; 108.9; 109.1; (**109.5**) | 109.8; 110.4; 109.5; 108.1; (**110.0**) | 110.6; 110.1; 109.8; 109.7; (**109.3**) |
| (C4C9C10) | 106.7; 106.7; 106.7; 106.8; (**106.6**) | 106.4; 106.3; 106.4; 106.7; (**106.6**) | 106.3; 106.3; 106.3; 106.3; (**106.2**) |
| (C9C10C3) | 106.7; 106.7; 106.7; 106.8; (**107.0**) | 106.4; 106.3; 106.5; 106.7; (**106.5**) | 106.3; 106.3; 106.3; 106.4; (**106.5**) |
| (C10C3N1) | 109.2; 109.1; 108.9; 109.1; (**109.3**) | 109.8; 110.4; 109.5; 109.7; (**109.6**) | 110.6; 110.1; 109.8; 110.0; (**108.2**) |
| VAS[2] | 540.0; 540.0; 539.9; 540.0; (**539.9**) | 540.0; 540.0; 540.0; 540.0; (**540.0**) | 539.9; 539.9; 539.9; 540.0; (**537.5**) |
| Bond angles in the 6-numbered ring (C9C10C18C26C25C17), *deg* | | | |
| (C9C10C18) | 121.0; 120.1; 121.0; 121.3; (**120.8**) | 121.2; 121.2; 121.1; 121.1; (**121.4**) | 121.4; 121.3; 121.3; 121.4; (**119.6**) |
| (C10C18C26) | 117.7; 117.8; 117.7; 117.5; (**117.5**) | 117.6; 117.7; 117.6; 117.7; (**117.0**) | 117.5; 117.5; 117.5; 117.4; (**119.2**) |
| (C18C26C25) | 121.3; 121.3; 121.3; 121.2; (**121.3**) | 121.2; 121.1; 121.3; 121.2; (**121.2**) | 121.1; 121.2; 121.2; 121.2; (**119.4**) |
| (C26C25C17) | 121.3; 121.3; 121.3; 121.2; (**121.3**) | 121.2; 121.1; 121.1; 121.2; (**121.8**) | 121.1; 121.2; 121.2; 121.2; (**120.0**) |
| (C25C17C9) | 117.7; 117.8; 117.7; 117.5; (**117.3**) | 117.6; 117.7; 117.6; 117.7; (**116.9**) | 117.5; 117.5; 117.5; 117.4; (**119.7**) |
| (C17C9C10) | 121.0; 121.0; 121.0; 121.3; (**121.8**) | 121.2; 121.2; 121.3; 121.1; (**121.7**) | 121.4; 121.3; 121.3; 121.4; (**119.6**) |
| VAS[3] | 720.0; 719.3; 720.0; 720.0; (**720.0**) | 720.0; 720.0; 720.0; 720.0; (**720.0**) | 720.0; 720.0; 720.0; 720.0; (**717.5**) |
| Selected torsion angles, *deg* | | | |
| (M1N1C4N7) | 0.0; 0.0; 0.0; 0.0; 0.0; (**1.1**) | 0.0; 0.0; 0.0; 0.0; (**0.0**) | 0.0; 0.0; 0.0; 0.0; (**11.0**) |
| (N1C4C9C17) | 180.0; 180.0; 180.0; 180.0; (**176.9**) | 180.0; 180.0; 180.0; 180.0; (**178.8**) | 180.0; 180.0; 180.0; 180.0; (**175.8**) |
| (N1C3C10C18) | 180.0; 180.0; 180.0; 180.0; (**177.3**) | 180.0; 180.0; 180.0; 180.0; (**178.6**) | 180.0; 180.0; 180.0; 180.0; (**157.8**) |
| (N7C4C9C17) | 0.0; 0.0; 0.0; 0.0; (**1.9**) | 0.0; 0.0; 0.0; 0.0; (**0.0**) | 0.0; 0.0; 0.0; 0.0; (**3.4**) |

| | | | |
|---|---|---|---|
| (N5C3C10C18) | 0.0; 0.0; 0.0; 0.0; (**3.5**) | 0.0; 0.0; 0.0; 0.0; (**1.9**) | 0.0; 0.0; 0.0; 0.0; (**2.6**) |
| (H1C17C9C10) | 180.0; 180.0; 180.0; 180.0; (**178.9**) | 180.0; 180.0; 180.0; 180.0; ( **–** ) | 180.0; 180.0; 180.0; 180.0; (**165.0**) |
| (H10C26C18C10) | 180.0; 180.0; 180.0; 180.0; (**178.9**) | 180.0; 180.0; 180.0; 180.0; ( **–** ) | 180.0; 180.0; 180.0; 180.0; (**153.4**) |
| (H2C18C10C9) | 180.0; 180.0; 180.0; 180.0; (**179.4**) | 180.0; 180.0; 180.0; 180.0; ( **–** ) | 180.0; 180.0; 180.0; 180.0; (**180.0**) |
| (C9C4N1M1) | 180.0; 180.0; 180.0; 180.0; (**177.6**) | 180.0; 180.0; 180.0; 180.0; (**178.1**) | 180.0; 180.0; 180.0; 180.0; (**168.1**) |
| (C10C3N1M1) | 180.0; 180.0; 180.0; 180.0; (**177.5**) | 180.0; 180.0; 180.0; 180.0; (**177.9**) | 180.0; 180.0; 180.0; 180.0; (**159.9**) |
| (H1C17C9C4) | 0.0; 0.0; 0.0; 0.0; (**3.3**) | 0.0; 0.0; 0.0; 0.0; ( **–** ) | 0.0; 0.0; 0.0; 0.0; (**4.6**) |
| (H2C18C10C3) | 0.0; 0.0; 0.0; 0.0; (**2.1**) | 0.0; 0.0; 0.0; 0.0; ( **–** ) | 0.0; 0.0; 0.0; 0.0; (**7.0**) |

* The sign (**–**) means that there is no corresponding experimental data.

Bonds lengths, valence and torsion angles in the Ni(II), Cu(II) and Zn(II) phthalocyanine metal chelates. The **bold font** in brackets specifies experimental values, regular font, calculated by DFT B3LYP 6-31G(d), OPBE/TZVP, B3PW91/TZVP and wB97XD/TZVP (first, second, third and fourth value, respectively) *.

| M | Ni | Cu | Zn |
|---|---|---|---|
| M–N bond lengths, *pm* | | | |
| (M1N1) | 190.4; 190.3; 191.0; 191.1; (**183.0**) | 196.0; 196.2; 196.0; 195.7; (**195.3**) | 199.1; 199.6; 199.3; 199.1; (**201.4**) |
| (M1N2) | 190.4; 190.3; 191.0; 191.1; (**183.1**) | 195.0; 196.2; 196.0; 195.7; (**195.0**) | 199.1; 199.6; 199.3; 199.1; (**201.4**) |
| (M1N3) | 190.4; 190.3; 191.0; 191.1; (**183.0**) | 196.0; 196.2; 196.0; 195.7; (**195.3**) | 199.1; 199.6; 199.3; 199.1; (**202.0**) |
| (M1N4) | 190.4; 190.3; 191.0; 191.1; (**183.1**) | 195.0; 196.2; 196.0; 195.7; (**195.0**) | 199.1; 199.6; 199.3; 199.1; (**202.0**) |
| C–N bond lengths, *pm* | | | |
| (N1C3) | 138.1; 137.7; 137.1; 136.7; (**137.9**) | 137.5; 137.0; 136.6; 136.3; (**138.8**) | 137.4; 136.9; 136.5; 136.1; (**136.9**) |
| (N1C4) | 138.1; 137.7; 137.1; 136.7; (**139.0**) | 137.6; 137.0; 136.6; 136.3; (**138.9**) | 137.4; 136.9; 136.5; 136.1; (**136.6**) |
| (N2C1) | 138.1; 137.7; 137.1; 136.7; (**137.1**) | 138.3; 137.0; 136.6; 136.3; (**137.9**) | 137.4; 136.9; 136.5; 136.1; (**136.4**) |

| | | | |
|---|---|---|---|
| (N2C2) | 138.0; 137.7; 137.1; 136.7; (**137.7**) | 138.3; 137.0; 136.6; 136.3; (**138.1**) | 137.4; 136.9; 136.5; 136.1; (**136.8**) |
| (N3C7) | 138.1; 137.7; 137.1; 136.7; (**137.9**) | 137.5; 137.0; 136.6; 136.3; (**138.8**) | 137.4; 136.9; 136.5; 136.1; (**136.5**) |
| (N3C8) | 138.1; 137.7; 137.1; 136.7; (**139.0**) | 137.6; 137.0; 136.6; 136.3; (**138.9**) | 137.4; 136.9; 136.5; 136.1; (**136.3**) |
| (N4C5) | 138.0; 137.7; 137.1; 136.7; (**139.5**) | 138.3; 137.0; 136.6; 136.3; (**137.9**) | 137.4; 136.9; 136.5; 136.1; (**136.7**) |
| (N4C6) | 138.1; 137.7; 137.1; 136.7; (**137.7**) | 138.3; 137.0; 136.6; 136.3; (**138.1**) | 137.4; 136.9; 136.5; 136.1; (**136.3**) |
| (N5C2) | 131.8; 131.5; 131.1; 131.0; (**136.8**) | 130.9; 132.3; 131.9; 131.6; (**135.4**) | 133.0; 132.9; 132.4; 132.1; (**133.5**) |
| (N5C3) | 131.8; 131.5; 131.1; 131.0; (**137.7**) | 135.0; 132.3; 131.9; 131.6; (**137.1**) | 133.0; 132.9; 132.4; 132.1; (**134.4**) |
| (N6C6) | 131.8; 131.5; 131.1; 131.0; (**136.8**) | 130.9; 132.3; 131.9; 131.6; (**135.4**) | 133.0; 132.9; 132.4; 132.1; (**132.9**) |
| (N6C7) | 131.8; 131.5; 131.1; 131.0; (**137.7**) | 135.0; 132.3; 131.9; 131.6; (**137.1**) | 133.0; 132.9; 132.4; 132.1; (**133.7**) |
| (N7C4) | 131.8; 131.5; 131.1; 131.0; (**138.0**) | 134.9; 132.3; 131.9; 131.6; (**134.4**) | 133.0; 132.9; 132.4; 132.1; (**133.4**) |
| (N7C5) | 131.8; 131.5; 131.1; 131.0; (**137.3**) | 130.8; 132.3; 131.9; 131.6; (**134.9**) | 133.0; 132.9; 132.4; 132.1; (**132.9**) |
| (N8C1) | 131.8; 131.5; 131.1; 131.0; (**137.3**) | 130.8; 132.3; 131.9; 131.6; (**134.9**) | 133.0; 132.9; 132.4; 132.1; (**133.6**) |
| (N8C8) | 131.8; 131.5; 131.1; 131.0; (**138.0**) | 134.9; 132.3; 131.9; 131.6; (**134.4**) | 133.0; 132.9; 132.4; 132.1; (**133.9**) |
| C–C bond lengths, *pm* | | | |
| (C9C10) | 140.0; 139.9; 139.5; 138.9; (**138.3**) | 141.2; 140.6; 140.1; 139.5; (**140.7**) | 141.0; 141.0; 140.5; 139.9; (**140.1**) |
| (C11C12) | 140.0; 139.9; 139.5; 138.9; (**138.9**) | 139.9; 140.6; 140.1; 139.5; (**140.7**) | 141.0; 141.0; 140.5; 139.9; (**139.2**) |
| (C13C14) | 140.0; 139.9; 139.5; 138.9; (**138.3**) | 141.2; 140.6; 140.1; 139.5; (**140.7**) | 141.0; 141.0; 140.5; 139.9; (**140.0**) |
| (C15C16) | 140.0; 139.9; 139.5; 138.9; (**138.9**) | 139.9; 140.6; 140.1; 139.5; (**140.7**) | 141.0; 141.0; 140.5; 139.9; (**138.4**) |
| (C9C17) | 139.6; 139.5; 139.0; 138.9; (**139.4**) | 139.7; 139.4; 138.9; 138.8; (**137.9**) | 139.6; 139.4; 138.9; 138.8; (**137.8**) |
| (C17C25) | 139.3; 139.2; 138.7; 138.3; (**139.2**) | 139.4; 139.3; 138.7; 138.4; (**137.2**) | 139.4; 139.3; 138.8; 138.4; (**138.5**) |
| (C25C26) | 140.9; 140.6; 140.2; 140.2; (**140.7**) | 141.0; 140.5; 140.1; 140.1; (**141.2**) | 140.8; 140.4; 140.1; 140.0; (**139.6**) |
| (C26C18) | 139.3; 139.2; 138.7; 138.3; (**139.5**) | 139.4; 139.3; 138.7; 138.4; (**137.9**) | 139.4; 139.3; 138.8; 138.4; (**138.1**) |
| (C18C10) | 139.6; 139.5; 139.0; 138.9; (**138.5**) | 139.7; 139.4; 138.9; 138.8; (**137.9**) | 139.6; 139.4; 138.9; 138.9; (**138.2**) |
| C–H bond lengths, *pm* | | | |
| (C17H1) | 108.5; 108.8; 108.3; 108.2; ( – ) | 108.6; 108.8; 108.3; 108.2; (**102.8**) | 108.5; 108.9; 108.3; 108.2; (**92.9**) |
| (C25H9) | 108.7; 109.0; 108.4; 108.3; ( – ) | 108.7; 109.0; 108.4; 108.3; (**102.3**) | 108.7; 109.0; 108.4; 108.3; (**93.0**) |
| (C26H10) | 108.7; 109.0; 108.4; 108.3; ( – ) | 108.7; 109.0; 108.4; 108.3; (**102.5**) | 108.7; 109.0; 108.4; 108.3; (**93.0**) |
| (C18H2) | 108.5; 108.8; 108.3; 108.2; ( – ) | 108.6; 108.8; 108.3; 108.2; (**102.8**) | 108.5; 108.9; 108.3; 108.2; (**93.0**) |

| ∠NMN bond angles in the $MN_4$ chelate node, *deg* | | | |
|---|---|---|---|
| (N1M1N4) | 90.0; 90.0; 90.0; 90.0; (**89.3**) | 90.0; 90.0; 90.0; 90.0; (**89.0**) | 90.0; 90.0; 90.0; 90.0; (**87.9**) |
| (N4M1N3) | 90.0; 90.0; 90.0; 90.0; (**90.7**) | 90.0; 90.0; 90.0; 90.0; (**91.0**) | 90.0; 90.0; 90.0; 90.0; (**87.6**) |
| (N3M1N2) | 90.0; 90.0; 90.0; 90.0; (**89.3**) | 90.0; 90.0; 90.0; 90.0; (**89.0**) | 90.0; 90.0; 90.0; 90.0; (**88.0**) |
| (N2M1N1) | 90.0; 90.0; 90.0; 90.0; (**90.7**) | 90.0; 90.0; 90.0; 90.0; (**91.0**) | 90.0; 90.0; 90.0; 90.0; (**88.2**) |
| ***VAS*** | 360.0; 360.0; 360.0; 360.0; (**360.0**) | 360.0; 360.0; 360.0; 360.0; (**360.0**) | 360.0; 360.0; 360.0; 360.0; (**351.9**) |
| ∠NNN non-bond angles in the $MN_4$ chelate node, *deg* | | | |
| (N1N4N3) | 90.0; 90.0; 90.0; 90.0; (**90.2**) | 90.2; 90.0; 90.0; 90.0; (**90.1**) | 90.0; 90.0; 90.0; 90.0; (**89.8**) |
| (N4N3N2) | 90.0; 90.0; 90.0; 90.0; (**89.8**) | 89.8; 90.0; 90.0; 90.0; (**89.9**) | 90.0; 90.0; 90.0; 90.0; (**90.2**) |
| (N3N2N1) | 90.0; 90.0; 90.0; 90.0; (**90.2**) | 90.2; 90.0; 90.0; 90.0; (**90.1**) | 90.0; 90.0; 90.0; 90.0; (**89.8**) |
| (N2N1N4) | 90.0; 90.0; 90.0; 90.0; (**89.8**) | 89.8; 90.0; 90.0; 90.0; (**89.9**) | 90.0; 90.0; 90.0; 90.0; (**90.2**) |
| NVAS | 360.0; 360.0; 360.0; 360.0; (**360.0**) | 360.0; 90.0; 360.0; 360.0; (**360.0**) | 360.0; 360.0; 360.0; 360.0; (**360.0**) |
| Bond angles in the 6-numbered ring (M1N1C4N7C5N4), *deg* | | | |
| (N1M1N4) | 90.0; 90.0; 90.0; 90.0; (**89.3**) | 90.0; 90.0; 90.0; 90.0; (**89.0**) | 90.0; 90.0; 90.0; 90.0; (**87.9**) |
| (M1N4C5) | 126.7; 126.6; 126.4; 126.3; (**130.4**) | 125.9; 125.6; 125.5; 125.5; (**127.5**) | 125.3; 125.1; 125.1; 125.0; (**124.6**) |
| (N4C5N7) | 127.7; 127.9; 127.7; 127.8; (**126.9**) | 128.5; 127.9; 127.7; 127.7; (**127.2**) | 127.5; 127.6; 127.5; 127.5; (**128.1**) |
| (C5N7C4) | 121.2; 121.0; 121.8; 121.9; (**116.0**) | 122.1; 123.0; 123.5; 123.6; (**122.0**) | 124.4; 124.6; 124.9; 125.0; (**123.4**) |
| (N7C4N1) | 127.7; 127.9; 127.7; 127.7; (**126.9**) | 127.6; 127.9; 127.7; 127.7; (**126.5**) | 127.5; 127.6; 127.5; 127.5; (**127.9**) |
| (C4N1M1) | 126.7; 126.6; 126.4; 126.3; (**130.5**) | 125.9; 125.6; 125.5; 125.5; (**127.8**) | 125.3; 125.1; 125.0; 125.0; (**124.7**) |
| VAS[1] | 720.0; 720.0; 720.0; 720.0; (**720.0**) | 720.0; 720.0; 719.9; 720.0; (**720.0**) | 720.0; 720.0; 720.0; 720.0; (**716.6**) |
| Bond angles in the 5-numbered ring (C3N1C4C9C10), *deg* | | | |
| (C3N1C4) | 106.5; 106.8; 107.2; 107.4; (**99.9**) | 108.0; 108.8; 108.9; 108.9; (**106.1**) | 109.4; 109.8; 109.9; 110.0; (**108.8**) |
| (N1C4C9) | 110.5; 110.3; 110.1; 110.0; (**115.9**) | 109.6; 109.2; 109.1; 109.1; (**111.4**) | 108.8; 108.6; 108.5; 108.4; (**109.1**) |
| (C4C9C10) | 106.3; 106.3; 106.3; 106.3; (**102.6**) | 106.4; 106.4; 106.4; 106.4; (**106.5**) | 106.5; 106.5; 106.6; 106.6; (**106.1**) |
| (C9C10C3) | 106.3; 106.3; 106.3; 106.3; (**106.5**) | 106.4; 106.4; 106.4; 106.5; (**105.5**) | 106.5; 106.5; 106.5; 106.6; (**106.7**) |
| (C10C3N1) | 110.4; 110.3; 110.1; 110.0; (**115.1**) | 109.6; 109.2; 109.1; 109.1; (**110.4**) | 108.8; 108.6; 108.5; 108.4; (**109.3**) |
| VAS[2] | 540.0; 540.0; 540.0; 540.0; (**540.0**) | 540.0; 540.0; 540.0; 540.0; (**539.9**) | 540.0; 540.0; 540.0; 540.0; (**540.0**) |

| Bond angles in the 6-numbered ring (C9C10C18C26C25C17), *deg* | | | |
|---|---|---|---|
| (C9C10C18) | 121.4; 121.3; 121.3; 121.4; (**119.9**) | 121.0; 121.1; 121.2; 121.3; (**120.0**) | 121.1; 121.0; 121.1; 121.2; (**120.4**) |
| (C10C18C26) | 117.4; 117.5; 117.4; 117.3; (**120.9**) | 117.8; 117.7; 117.6; 117.5; (**118.0**) | 117.7; 117.8; 117.7; 117.6; (**118.4**) |
| (C18C26C25) | 121.2; 121.2; 121.2; 121.3; (**119.0**) | 121.2; 121.2; 121.2; 121.2; (**120.7**) | 121.2; 121.2; 121.2; 121.2; (**120.7**) |
| (C26C25C17) | 121.2; 121.2; 121.2; 121.3; (**119.9**) | 121.2; 121.2; 121.2; 121.2; (**119.7**) | 121.2; 121.2; 121.2; 121.1; (**121.4**) |
| (C25C17C9) | 117.4; 117.5; 117.4; 117.3; (**119.9**) | 117.8; 117.7; 117.6; 117.5; (**118.5**) | 117.7; 117.8; 117.7; 117.7; (**117.7**) |
| (C17C9C10) | 121.4; 121.3; 121.3; 121.4; (**120.4**) | 121.0; 121.1; 121.2; 121.3; (**120.8**) | 121.1; 121.0; 121.1; 121.2; (**121.4**) |
| VAS[3] | 720.0; 720.0; 719.8; 720.0; (**720.0**) | 720.0; 720.0; 720.0; 720.0; (**720.0**) | 720.0; 720.0; 720.0; 720.0; (**720.0**) |
| Selected torsion angles, *deg* | | | |
| (M1N1C4N7) | 0.0; 0.0; 0.0; 0.0; (**0.0**) | 0.0; 0.0; 0.0; 0.0; (**2.7**) | 0.0; 0.0; 0.0; 0.0; (**13.4**) |
| (N1C4C9C17) | 180.0; 180.0; 180.0; 180.0; (**180.0**) | 180.0; 180.0; 180.0; 180.0; (**172.9**) | 180.0; 180.0; 180.0; 180.0; (**179.0**) |
| (N1C3C10C18) | 180.0; 180.0; 180.0; 180.0; (**180.0**) | 180.0; 180.0; 180.0; 180.0; (**180.0**) | 180.0; 180.0; 180.0; 180.0; (**177.4**) |
| (N7C4C9C17) | 0.0; 0.0; 0.0; 0.0; (**0.0**) | 0.0; 0.0; 0.0; 0.0; (**0.0**) | 0.0; 0.0; 0.0; 0.0; (**0.2**) |
| (N5C3C10C18) | 0.0; 0.0; 0.0; 0.0; (**0.0**) | 0.0; 0.0; 0.0; 0.0; (**0.0**) | 0.0; 0.0; 0.0; 0.0; (**3.0**) |
| (H1C17C9C10) | 180.0; 180.0; 180.0; 180.0; ( – ) | 180.0; 180.0; 180.0; 180.0; (**178.5**) | 180.0; 180.0; 180.0; 180.0; (**178.3**) |
| (H10C26C18C10) | 180.0; 180.0; 180.0; 180.0; ( – ) | 180.0; 180.0; 180.0; 180.0; (**180.0**) | 180.0; 180.0; 180.0; 180.0; (**179.7**) |
| (H2C18C10C9) | 180.0; 180.0; 180.0; 180.0; ( – ) | 180.0; 180.0; 180.0; 180.0; (**180.0**) | 180.0; 180.0; 180.0; 180.0; (**179.8**) |
| (C9C4N1M1) | 180.0; 180.0; 180.0; 180.0; (**180.0**) | 180.0; 180.0; 180.0; 180.0; (**176.5**) | 180.0; 180.0; 180.0; 180.0; (**165.3**) |
| (C10C3N1M1) | 180.0; 180.0; 180.0; 180.0; (**180.0**) | 180.0; 180.0; 180.0; 180.0; (**176.3**) | 180.0; 180.0; 180.0; 180.0; (**165.1**) |
| (H1C17C9C4) | 0.0; 0.0; 0.0; 0.0; ( – ) | 0.0; 0.0; 0.0; 0.0; (**0.0**) | 0.0; 0.0; 0.0; 0.0; (**2.5**) |
| (H2C18C10C3) | 0.0; 0.0; 0.0; 0.0; ( – ) | 0.0; 0.0; 0.0; 0.0; (**0.0**) | 0.0; 0.0; 0.0; 0.0; (**2.0**) |

* The sign (–) means that there is no corresponding experimental data.

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**NBO Analysis Data**

Complex [Fe**L**$(O)_2$]

**<S**2> = 0.0000**

**Summary of Natural Population Analysis:**

| Atom | No | Natural Charge | Natural Population | | | |
|---|---|---|---|---|---|---|
| | | | Core | Valence | Rydberg | Total |
| Fe | 1 | -0.15472 | 17.99274 | 8.13861 | 0.02336 | 26.15472 |
| N | 2 | -0.29718 | 1.99915 | 5.27150 | 0.02653 | 7.29718 |
| N | 3 | -0.29700 | 1.99915 | 5.27133 | 0.02652 | 7.29700 |
| N | 4 | -0.30612 | 1.99914 | 5.27959 | 0.02739 | 7.30612 |
| N | 5 | -0.30617 | 1.99914 | 5.27963 | 0.02740 | 7.30617 |
| C | 6 | 0.33114 | 1.99926 | 3.64910 | 0.02050 | 5.66886 |
| C | 7 | 0.33083 | 1.99926 | 3.64938 | 0.02053 | 5.66917 |
| C | 8 | 0.33085 | 1.99926 | 3.64935 | 0.02053 | 5.66915 |
| C | 9 | 0.33115 | 1.99926 | 3.64908 | 0.02051 | 5.66885 |
| C | 10 | 0.33106 | 1.99926 | 3.64888 | 0.02081 | 5.66894 |
| C | 11 | 0.33216 | 1.99926 | 3.64779 | 0.02080 | 5.66784 |
| C | 12 | 0.33218 | 1.99926 | 3.64777 | 0.02079 | 5.66782 |
| C | 13 | 0.33104 | 1.99926 | 3.64890 | 0.02080 | 5.66896 |
| N | 14 | -0.36249 | 1.99937 | 5.34850 | 0.01462 | 7.36249 |
| N | 15 | -0.36236 | 1.99937 | 5.34840 | 0.01459 | 7.36236 |
| N | 16 | -0.36227 | 1.99937 | 5.34831 | 0.01459 | 7.36227 |
| N | 17 | -0.36228 | 1.99937 | 5.34832 | 0.01459 | 7.36228 |
| C | 18 | -0.21913 | 1.99911 | 4.20836 | 0.01166 | 6.21913 |
| C | 19 | -0.22058 | 1.99911 | 4.20981 | 0.01166 | 6.22058 |
| C | 20 | -0.21914 | 1.99911 | 4.20837 | 0.01166 | 6.21914 |
| C | 21 | -0.22054 | 1.99911 | 4.20976 | 0.01166 | 6.22054 |
| C | 22 | -0.22034 | 1.99911 | 4.20960 | 0.01163 | 6.22034 |
| C | 23 | -0.21899 | 1.99911 | 4.20826 | 0.01162 | 6.21899 |
| C | 24 | -0.22032 | 1.99911 | 4.20958 | 0.01163 | 6.22032 |
| C | 25 | -0.21898 | 1.99911 | 4.20825 | 0.01162 | 6.21898 |
| H | 26 | 0.24384 | 0.00000 | 0.75460 | 0.00156 | 0.75616 |
| H | 27 | 0.24386 | 0.00000 | 0.75458 | 0.00156 | 0.75614 |
| H | 28 | 0.24386 | 0.00000 | 0.75458 | 0.00156 | 0.75614 |
| H | 29 | 0.24385 | 0.00000 | 0.75459 | 0.00156 | 0.75615 |
| H | 30 | 0.24353 | 0.00000 | 0.75490 | 0.00157 | 0.75647 |
| H | 31 | 0.24355 | 0.00000 | 0.75489 | 0.00157 | 0.75645 |
| H | 32 | 0.24354 | 0.00000 | 0.75489 | 0.00157 | 0.75646 |
| H | 33 | 0.24353 | 0.00000 | 0.75491 | 0.00157 | 0.75647 |
| O | 34 | -0.01567 | 1.99993 | 6.00866 | 0.00708 | 8.01567 |
| O | 35 | -0.01567 | 1.99993 | 6.00866 | 0.00708 | 8.01567 |
| * Total * | | -0.00000 | 69.97364 | 131.55170 | 0.47467 | 202.00000 |

**NATURAL POPULATIONS: Natural atomic orbital occupancies**

| NAO | Atom | No | lang | Type(AO) | Occupancy | Energy |
|---|---|---|---|---|---|---|
| 1 | Fe | 1 | S | Cor( 1S) | 2.00000 | -248.80150 |
| 2 | Fe | 1 | S | Cor( 2S) | 2.00000 | -34.15938 |
| 3 | Fe | 1 | S | Cor( 3S) | 1.99589 | -4.77747 |
| 4 | Fe | 1 | S | Val( 4S) | 0.31906 | 0.39481 |
| 5 | Fe | 1 | S | Ryd( 6S) | 0.00183 | 1.06961 |
| 6 | Fe | 1 | S | Ryd( 5S) | 0.00047 | 0.92269 |
| 7 | Fe | 1 | px | Cor( 2p) | 2.00000 | -25.55408 |
| 8 | Fe | 1 | px | Cor( 3p) | 1.99861 | -2.26490 |
| 9 | Fe | 1 | px | Val( 4p) | 0.27972 | 0.35377 |
| 10 | Fe | 1 | px | Ryd( 5p) | 0.00083 | 1.80077 |
| 11 | Fe | 1 | py | Cor( 2p) | 2.00000 | -25.55431 |
| 12 | Fe | 1 | py | Cor( 3p) | 1.99863 | -2.26536 |
| 13 | Fe | 1 | py | Val( 4p) | 0.27920 | 0.35191 |
| 14 | Fe | 1 | py | Ryd( 5p) | 0.00083 | 1.80182 |
| 15 | Fe | 1 | pz | Cor( 2p) | 2.00000 | -25.57739 |
| 16 | Fe | 1 | pz | Cor( 3p) | 1.99963 | -2.29914 |
| 17 | Fe | 1 | pz | Val( 4p) | 0.27236 | 0.23256 |
| 18 | Fe | 1 | pz | Ryd( 5p) | 0.00267 | 1.85818 |
| 19 | Fe | 1 | dxy | Val( 3d) | 1.18925 | -0.29477 |
| 20 | Fe | 1 | dxy | Ryd( 4d) | 0.00298 | 1.90634 |
| 21 | Fe | 1 | dxy | Ryd( 5d) | 0.00003 | 2.81730 |
| 22 | Fe | 1 | dxz | Val( 3d) | 1.27137 | -0.30196 |
| 23 | Fe | 1 | dxz | Ryd( 4d) | 0.00077 | 0.95595 |
| 24 | Fe | 1 | dxz | Ryd( 5d) | 0.00009 | 3.14484 |
| 25 | Fe | 1 | dyz | Val( 3d) | 1.26856 | -0.30146 |
| 26 | Fe | 1 | dyz | Ryd( 4d) | 0.00052 | 0.95090 |
| 27 | Fe | 1 | dyz | Ryd( 5d) | 0.00008 | 3.14367 |
| 28 | Fe | 1 | dx2y2 | Val( 3d) | 1.98422 | -0.26719 |
| 29 | Fe | 1 | dx2y2 | Ryd( 4d) | 0.00497 | 1.17051 |
| 30 | Fe | 1 | dx2y2 | Ryd( 5d) | 0.00033 | 3.07837 |
| 31 | Fe | 1 | dz2 | Val( 3d) | 1.27486 | -0.37794 |
| 32 | Fe | 1 | dz2 | Ryd( 4d) | 0.00691 | 1.86049 |
| 33 | Fe | 1 | dz2 | Ryd( 5d) | 0.00004 | 3.09693 |

==========

Complex [Co**L**$(O)_2$]

**<S**2>= 0.7609**

**Summary of Natural Population Analysis:**

| Atom | No | Natural Charge | Natural Population | | | |
|---|---|---|---|---|---|---|
| | | | Core | Valence | Rydberg | Total |
| Co | 1 | 0.06473 | 17.99367 | 8.91985 | 0.02174 | 26.93527 |
| N | 2 | -0.29894 | 1.99910 | 5.27449 | 0.02535 | 7.29894 |
| N | 3 | -0.29053 | 1.99909 | 5.26516 | 0.02627 | 7.29053 |
| N | 4 | -0.29384 | 1.99910 | 5.26706 | 0.02769 | 7.29384 |
| N | 5 | -0.29052 | 1.99909 | 5.26516 | 0.02627 | 7.29052 |
| C | 6 | 0.33170 | 1.99926 | 3.64805 | 0.02099 | 5.66830 |
| C | 7 | 0.33009 | 1.99926 | 3.64966 | 0.02100 | 5.66991 |
| C | 8 | 0.32872 | 1.99926 | 3.65118 | 0.02083 | 5.67128 |
| C | 9 | 0.32872 | 1.99926 | 3.65118 | 0.02083 | 5.67128 |
| C | 10 | 0.33009 | 1.99926 | 3.64966 | 0.02100 | 5.66991 |
| C | 11 | 0.33170 | 1.99926 | 3.64805 | 0.02099 | 5.66830 |
| C | 12 | 0.32590 | 1.99924 | 3.65338 | 0.02148 | 5.67410 |
| C | 13 | 0.32590 | 1.99924 | 3.65338 | 0.02148 | 5.67410 |
| N | 14 | -0.35770 | 1.99937 | 5.34356 | 0.01478 | 7.35770 |
| N | 15 | -0.35708 | 1.99936 | 5.34297 | 0.01475 | 7.35708 |
| N | 16 | -0.35770 | 1.99937 | 5.34356 | 0.01478 | 7.35770 |
| N | 17 | -0.35708 | 1.99936 | 5.34297 | 0.01475 | 7.35708 |
| C | 18 | -0.21780 | 1.99911 | 4.20702 | 0.01167 | 6.21780 |
| C | 19 | -0.21780 | 1.99911 | 4.20702 | 0.01167 | 6.21780 |
| C | 20 | -0.21680 | 1.99910 | 4.20606 | 0.01164 | 6.21680 |
| C | 21 | -0.21878 | 1.99910 | 4.20801 | 0.01166 | 6.21878 |
| C | 22 | -0.21122 | 1.99911 | 4.20050 | 0.01161 | 6.21122 |
| C | 23 | -0.21122 | 1.99911 | 4.20050 | 0.01161 | 6.21122 |
| C | 24 | -0.21878 | 1.99910 | 4.20801 | 0.01166 | 6.21878 |
| C | 25 | -0.21680 | 1.99910 | 4.20606 | 0.01164 | 6.21680 |
| H | 26 | 0.24501 | 0.00000 | 0.75344 | 0.00155 | 0.75499 |
| H | 27 | 0.24501 | 0.00000 | 0.75344 | 0.00155 | 0.75499 |
| H | 28 | 0.24460 | 0.00000 | 0.75385 | 0.00156 | 0.75540 |
| H | 29 | 0.24452 | 0.00000 | 0.75392 | 0.00156 | 0.75548 |
| H | 30 | 0.24524 | 0.00000 | 0.75321 | 0.00155 | 0.75476 |
| H | 31 | 0.24524 | 0.00000 | 0.75321 | 0.00155 | 0.75476 |
| H | 32 | 0.24452 | 0.00000 | 0.75392 | 0.00156 | 0.75548 |
| H | 33 | 0.24460 | 0.00000 | 0.75385 | 0.00156 | 0.75540 |
| O | 34 | -0.16184 | 1.99994 | 6.15611 | 0.00579 | 8.16184 |
| O | 35 | -0.16184 | 1.99994 | 6.15611 | 0.00579 | 8.16184 |
| * Total * | | 0.00000 | 69.97427 | 132.55353 | 0.47220 | 203.00000 |

**NATURAL POPULATIONS: Natural atomic orbital occupancies**

| NAO | Atom | No | lang | Type(AO) | Occupancy |
|---|---|---|---|---|---|
| 1 | Co | 1 | S | Cor( 1S) | 2.00000 |
| 2 | Co | 1 | S | Cor( 2S) | 2.00000 |
| 3 | Co | 1 | S | Cor( 3S) | 1.99638 |
| 4 | Co | 1 | S | Val( 4S) | 0.32018 |
| 5 | Co | 1 | S | Ryd( 5S) | 0.00182 |
| 6 | Co | 1 | S | Ryd( 6S) | 0.00048 |
| 7 | Co | 1 | px | Cor( 2p) | 2.00000 |
| 8 | Co | 1 | px | Cor( 3p) | 1.99882 |
| 9 | Co | 1 | px | Val( 4p) | 0.28745 |
| 10 | Co | 1 | px | Ryd( 5p) | 0.00078 |
| 11 | Co | 1 | py | Cor( 2p) | 2.00000 |
| 12 | Co | 1 | py | Cor( 3p) | 1.99880 |
| 13 | Co | 1 | py | Val( 4p) | 0.28544 |
| 14 | Co | 1 | py | Ryd( 5p) | 0.00080 |
| 15 | Co | 1 | pz | Cor( 2p) | 2.00000 |
| 16 | Co | 1 | pz | Cor( 3p) | 1.99968 |
| 17 | Co | 1 | pz | Val( 4p) | 0.28726 |
| 18 | Co | 1 | pz | Ryd( 5p) | 0.00292 |
| 19 | Co | 1 | dxy | Val( 3d) | 1.98796 |
| 20 | Co | 1 | dxy | Ryd( 4d) | 0.00270 |
| 21 | Co | 1 | dxy | Ryd( 5d) | 0.00041 |
| 22 | Co | 1 | dxz | Val( 3d) | 1.71518 |
| 23 | Co | 1 | dxz | Ryd( 4d) | 0.00483 |
| 24 | Co | 1 | dxz | Ryd( 5d) | 0.00015 |
| 25 | Co | 1 | dyz | Val( 3d) | 1.49330 |
| 26 | Co | 1 | dyz | Ryd( 4d) | 0.00077 |
| 27 | Co | 1 | dyz | Ryd( 5d) | 0.00010 |
| 28 | Co | 1 | dx2y2 | Val( 3d) | 1.22011 |
| 29 | Co | 1 | dx2y2 | Ryd( 4d) | 0.00167 |
| 30 | Co | 1 | dx2y2 | Ryd( 5d) | 0.00002 |
| 31 | Co | 1 | dz2 | Val( 3d) | 1.32299 |
| 32 | Co | 1 | dz2 | Ryd( 4d) | 0.00426 |
| 33 | Co | 1 | dz2 | Ryd( 5d) | 0.00002 |

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Complex [Ni**L**$(O)_2$]

**<S**2>= 2.0122**

**Summary of Natural Population Analysis:**

| Atom | No | Natural Charge | Natural Population | | | |
|---|---|---|---|---|---|---|
| | | | Core | Valence | Rydberg | Total |
| Ni | 1 | 0.30150 | 17.99487 | 9.68782 | 0.01581 | 27.69850 |
| N | 2 | -0.30525 | 1.99905 | 5.28043 | 0.02576 | 7.30525 |
| N | 3 | -0.30521 | 1.99905 | 5.28039 | 0.02576 | 7.30521 |
| N | 4 | -0.30523 | 1.99905 | 5.28042 | 0.02576 | 7.30523 |
| N | 5 | -0.30527 | 1.99905 | 5.28046 | 0.02576 | 7.30527 |
| C | 6 | 0.32850 | 1.99925 | 3.65083 | 0.02142 | 5.67150 |
| C | 7 | 0.32850 | 1.99925 | 3.65083 | 0.02142 | 5.67150 |
| C | 8 | 0.32850 | 1.99925 | 3.65083 | 0.02142 | 5.67150 |
| C | 9 | 0.32850 | 1.99925 | 3.65083 | 0.02142 | 5.67150 |
| C | 10 | 0.32851 | 1.99925 | 3.65083 | 0.02142 | 5.67149 |
| C | 11 | 0.32850 | 1.99925 | 3.65083 | 0.02142 | 5.67150 |
| C | 12 | 0.32851 | 1.99925 | 3.65083 | 0.02142 | 5.67149 |
| C | 13 | 0.32850 | 1.99925 | 3.65083 | 0.02142 | 5.67150 |
| N | 14 | -0.35651 | 1.99937 | 5.34220 | 0.01495 | 7.35651 |
| N | 15 | -0.35651 | 1.99937 | 5.34220 | 0.01495 | 7.35651 |
| N | 16 | -0.35651 | 1.99937 | 5.34220 | 0.01495 | 7.35651 |
| N | 17 | -0.35651 | 1.99937 | 5.34220 | 0.01495 | 7.35651 |
| C | 18 | -0.21363 | 1.99910 | 4.20287 | 0.01166 | 6.21363 |
| C | 19 | -0.21363 | 1.99910 | 4.20287 | 0.01166 | 6.21363 |
| C | 20 | -0.21363 | 1.99910 | 4.20287 | 0.01166 | 6.21363 |
| C | 21 | -0.21363 | 1.99910 | 4.20287 | 0.01166 | 6.21363 |
| C | 22 | -0.21363 | 1.99910 | 4.20287 | 0.01166 | 6.21363 |
| C | 23 | -0.21363 | 1.99910 | 4.20287 | 0.01166 | 6.21363 |
| C | 24 | -0.21363 | 1.99910 | 4.20287 | 0.01166 | 6.21363 |
| C | 25 | -0.21363 | 1.99910 | 4.20287 | 0.01166 | 6.21363 |
| H | 26 | 0.24616 | 0.00000 | 0.75229 | 0.00155 | 0.75384 |
| H | 27 | 0.24616 | 0.00000 | 0.75229 | 0.00155 | 0.75384 |
| H | 28 | 0.24616 | 0.00000 | 0.75229 | 0.00155 | 0.75384 |
| H | 29 | 0.24616 | 0.00000 | 0.75229 | 0.00155 | 0.75384 |
| H | 30 | 0.24616 | 0.00000 | 0.75229 | 0.00155 | 0.75384 |
| H | 31 | 0.24616 | 0.00000 | 0.75229 | 0.00155 | 0.75384 |
| H | 32 | 0.24616 | 0.00000 | 0.75229 | 0.00155 | 0.75384 |
| H | 33 | 0.24616 | 0.00000 | 0.75229 | 0.00155 | 0.75384 |
| O | 34 | -0.27139 | 1.99995 | 6.26686 | 0.00458 | 8.27139 |
| O | 35 | -0.27139 | 1.99995 | 6.26686 | 0.00458 | 8.27139 |
| * Total * | | -0.00000 | 69.97522 | 133.55996 | 0.46482 | 204.00000 |

**NATURAL POPULATIONS: Natural atomic orbital occupancies**

| NAO | Atom | No | lang | Type(AO) | Occupancy |
|---|---|---|---|---|---|
| 1 | Ni | 1 | S | Cor( 1S) | 2.00000 |
| 2 | Ni | 1 | S | Cor( 2S) | 2.00000 |
| 3 | Ni | 1 | S | Cor( 3S) | 1.99705 |
| 4 | Ni | 1 | S | Val( 4S) | 0.32548 |
| 5 | Ni | 1 | S | Ryd( 5S) | 0.00165 |
| 6 | Ni | 1 | S | Ryd( 6S) | 0.00046 |
| 7 | Ni | 1 | px | Cor( 2p) | 2.00000 |
| 8 | Ni | 1 | px | Cor( 3p) | 1.99899 |
| 9 | Ni | 1 | px | Val( 4p) | 0.28588 |
| 10 | Ni | 1 | px | Ryd( 5p) | 0.00077 |
| 11 | Ni | 1 | py | Cor( 2p) | 2.00000 |
| 12 | Ni | 1 | py | Cor( 3p) | 1.99899 |
| 13 | Ni | 1 | py | Val( 4p) | 0.28588 |
| 14 | Ni | 1 | py | Ryd( 5p) | 0.00077 |
| 15 | Ni | 1 | pz | Cor( 2p) | 2.00000 |
| 16 | Ni | 1 | pz | Cor( 3p) | 1.99985 |
| 17 | Ni | 1 | pz | Val( 4p) | 0.30078 |
| 18 | Ni | 1 | pz | Ryd( 5p) | 0.00259 |
| 19 | Ni | 1 | dxy | Val( 3d) | 1.28538 |
| 20 | Ni | 1 | dxy | Ryd( 4d) | 0.00090 |
| 21 | Ni | 1 | dxy | Ryd( 5d) | 0.00004 |
| 22 | Ni | 1 | dxz | Val( 3d) | 1.90891 |
| 23 | Ni | 1 | dxz | Ryd( 4d) | 0.00226 |
| 24 | Ni | 1 | dxz | Ryd( 5d) | 0.00011 |
| 25 | Ni | 1 | dyz | Val( 3d) | 1.90891 |
| 26 | Ni | 1 | dyz | Ryd( 4d) | 0.00226 |
| 27 | Ni | 1 | dyz | Ryd( 5d) | 0.00011 |
| 28 | Ni | 1 | dx2y2 | Val( 3d) | 1.98031 |
| 29 | Ni | 1 | dx2y2 | Ryd( 4d) | 0.00119 |
| 30 | Ni | 1 | dx2y2 | Ryd( 5d) | 0.00038 |
| 31 | Ni | 1 | dz2 | Val( 3d) | 1.40629 |
| 32 | Ni | 1 | dz2 | Ryd( 4d) | 0.00231 |
| 33 | Ni | 1 | dz2 | Ryd( 5d) | 0.00003 |

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