**Supplementary Table 1**  The different optimized parameters (bond lengths and bond angles) of organometallic Schiff base ligand (H2L).

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| **Bond length (Å)** |
| C(1)-C(2) | 1.4436 | C(14)-H(18) | 1.0808 |
| C(1)-C(5) | 1.4429 | C(16)-C(17) | 1.4350 |
| C(1)-H(6) | 1.0811 | C(16)-H(19) | 1.0801 |
| C(1)-Fe(11) | 2.1180 | C(17)-H(20) | 1.0808 |
| C(2)-C(3) | 1.4432 | C(21)-C(22) | 1.5199 |
| C(2)-H(7) | 1.0811 | C(21)-N(26) | 1.2979 |
| C(2)-Fe(11) | 2.1201 | C(22)-H(23) | 1.0973 |
| C(3)-C(4) | 1.4427 | C(22)-H(24) | 1.0983 |
| C(3)-H(8) | 1.0814 | C(22)-H(25) | 1.0918 |
| C(3)-Fe(11) | 2.1213 | N(26)-C(27) | 1.3978 |
| C(4)-C(5) | 1.4433 | C(27)-C(28) | 1.4294 |
| C(4)-H(9) | 1.0810 | C(27)-C(29) | 1.4104 |
| C(4)-Fe(11) | 2.1208 | C(28)-C(30) | 1.3900 |
| C(5)-H(10) | 1.0810 | C(28)-H(31) | 1.0853 |
| C(5)-Fe(11) | 2.1179 | C(29)-C(32) | 1.4032 |
| Fe(11)-C(12) | 2.1155 | C(29)-H(33) | 1.0845 |
| Fe(11)-C(13) | 2.1152 | C(30)-C(34) | 1.4208 |
| Fe(11)-C(14) | 2.1286 | C(30)-H(35) | 1.0853 |
| Fe(11)-C(16) | 2.1101 | C(32)-C(34) | 1.4328 |
| Fe(11)-C(17) | 2.1285 | C(32)-O(40) | 1.3768 |
| C(12)-C(13) | 1.4550 | C(34)-C(36) | 1.4532 |
| C(12)-C(14) | 1.4353 | C(36)-O(37) | 1.2673 |
| C(12)-H(15) | 1.0777 | C(36)-O(38) | 1.3827 |
| C(13)-C(16) | 1.4553 | O(38)-H(39) | 0.9836 |
| C(13)-C(21) | 1.4822 | O(40)-H(41) | 0.9992 |
| C(14)-C(17) | 1.4431 |  |  |
| **Bond angle (°)** |
| C(2)-C(1)-C(5) | 107.9887 | Fe(11)-C(12)-H(15) | 125.0209 |
| C(2)-C(1)-H(6) | 126.0294 | C(13)-C(12)-C(14) | 108.2354 |
| C(5)-C(1)-H(6) | 125.9788 | C(13)-C(12)-H(15) | 126.1827 |
| H(6)-C(1)-Fe(11) | 124.8504 | C(14)-C(12)-H(15) | 125.5818 |
| C(1)-C(2)-C(3) | 107.9242 | Fe(11)-C(13)-C(21) | 124.6037 |
| C(1)-C(2)-H(7) | 125.9641 | C(12)-C(13)-C(16) | 106.9621 |
| C(3)-C(2)-H(7) | 126.1113 | C(12)-C(13)-C(21) | 128.6351 |
| H(7)-C(2)-Fe(11) | 125.5637 | C(16)-C(13)-C(21) | 124.3930 |
| C(2)-C(3)-C(4) | 108.1122 | Fe(11)-C(14)-H(18) | 125.3070 |
| C(2)-C(3)-H(8) | 126.0340 | C(12)-C(14)-C(17) | 108.3387 |
| C(4)-C(3)-H(8) | 125.8511 | C(12)-C(14)-H(18) | 125.6395 |
| H(8)-C(3)-Fe(11) | 125.0177 | C(17)-C(14)-H(18) | 126.0185 |
| C(3)-C(4)-C(5) | 107.9048 | Fe(11)-C(16)-H(19) | 125.5060 |
| C(3)-C(4)-H(9) | 126.0210 | C(13)-C(16)-C(17) | 108.4307 |
| C(5)-C(4)-H(9) | 126.0727 | C(13)-C(16)-H(19) | 125.9283 |
| H(9)-C(4)-Fe(11) | 125.0672 | C(17)-C(16)-H(19) | 125.6358 |
| C(1)-C(5)-C(4) | 108.0701 | Fe(11)-C(17)-H(20) | 125.7768 |
| C(1)-C(5)-H(10) | 125.9879 | C(14)-C(17)-C(16) | 108.0302 |
| C(4)-C(5)-H(10) | 125.9391 | C(14)-C(17)-H(20) | 126.0745 |
| H(10)-C(5)-Fe(11) | 124.8516 | C(16)-C(17)-H(20) | 125.8952 |
| C(1)-Fe(11)-C(3) | 66.8218 | C(13)-C(21)-C(22) | 116.9237 |
| C(1)-Fe(11)-C(4) | 66.8846 | C(13)-C(21)-N(26) | 126.3818 |
| C(1)-Fe(11)-C(12) | 158.3470 | C(22)-C(21)-N(26) | 116.6922 |
| C(1)-Fe(11)-C(13) | 159.8498 | C(21)-C(22)-H(23) | 110.9765 |
| C(1)-Fe(11)-C(14) | 123.4913 | C(21)-C(22)-H(24) | 110.7208 |
| C(1)-Fe(11)-C(16) | 123.9779 | C(21)-C(22)-H(25) | 109.2524 |
| C(1)-Fe(11)-C(17) | 108.8960 | H(23)-C(22)-H(24) | 107.5778 |
| C(2)-Fe(11)-C(4) | 66.8607 | H(23)-C(22)-H(25) | 109.4182 |
| C(2)-Fe(11)-C(5) | 66.8692 | H(24)-C(22)-H(25) | 108.8511 |
| C(2)-Fe(11)-C(12) | 160.2095 | N(26)-C(27)-C(28) | 119.9179 |
| C(2)-Fe(11)-C(13) | 124.7591 | N(26)-C(27)-C(29) | 120.0711 |
| C(2)-Fe(11)-C(14) | 159.2140 | C(28)-C(27)-C(29) | 119.7091 |
| C(2)-Fe(11)-C(16) | 109.9255 | C(27)-C(28)-C(30) | 119.8234 |
| C(2)-Fe(11)-C(17) | 124.5365 | C(27)-C(28)-H(31) | 119.1204 |
| C(3)-Fe(11)-C(5) | 66.7917 | C(30)-C(28)-H(31) | 121.0546 |
| C(3)-Fe(11)-C(12) | 124.5295 | C(27)-C(29)-C(32) | 120.3808 |
| C(3)-Fe(11)-C(13) | 109.8357 | C(27)-C(29)-H(33) | 120.7534 |
| C(3)-Fe(11)-C(16) | 125.3604 | C(32)-C(29)-H(33) | 118.8609 |
| C(3)-Fe(11)-C(17) | 160.2581 | C(28)-C(30)-C(34) | 121.2400 |
| C(4)-Fe(11)-C(12) | 108.8506 | C(28)-C(30)-H(35) | 120.4425 |
| C(4)-Fe(11)-C(13) | 124.2894 | C(34)-C(30)-H(35) | 118.3175 |
| C(4)-Fe(11)-C(14) | 123.4105 | C(29)-C(32)-C(34) | 120.2248 |
| C(4)-Fe(11)-C(16) | 160.4953 | C(29)-C(32)-O(40) | 117.5504 |
| C(5)-Fe(11)-C(12) | 123.1982 | C(34)-C(32)-O(40) | 122.2244 |
| C(5)-Fe(11)-C(13) | 159.1654 | C(30)-C(34)-C(32) | 118.6139 |
| C(5)-Fe(11)-C(14) | 108.3310 | C(30)-C(34)-C(36) | 122.3206 |
| C(5)-Fe(11)-C(17) | 123.2579 | C(32)-C(34)-C(36) | 119.0634 |
| C(12)-Fe(11)-C(16) | 67.2135 | C(34)-C(36)-O(37) | 124.7097 |
| C(12)-Fe(11)-C(17) | 66.7152 | C(34)-C(36)-O(38) | 115.3791 |
| C(13)-Fe(11)-C(14) | 66.9824 | O(37)-C(36)-O(38) | 119.9112 |
| C(13)-Fe(11)-C(17) | 67.0772 | C(36)-O(38)-H(39) | 110.0013 |
| C(14)-Fe(11)-C(16) | 66.6542 | C(32)-O(40)-H(41) | 110.0769 |

**Supplementary Table 3** Main calculated optical transitions with composite ion in terms of molecular orbitals.

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| **Compound** | **Transition** | **Excitation energy (eV)** | **λmax calc.****nm (eV)** | **λmax exp.****nm (eV)** | **Oscillator strength** |
| **Ligand (H2L)** | HOMO-4 LUMO (68%) | 5.04 | 277 (4.48) | 271 (4.57) | 0.005 |
| HOMO LUMO+3 (48%)HOMO-2 LUMO (38%) | 5.324.40 | 312 (3.98) | 314 (3.95) | 0.3211 |