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Supporting Information

## **Running in the Family: Molecular Factors controlling Spin Crossover of Iron(II) Complexes with Schiff-base like Ligands**

Sophie Schönfeld, Wolfgang Bauer<sup>†</sup>, Sebastian Thallmair<sup>†</sup>, Gerald Hörner,<sup>\*</sup> and Birgit Weber<sup>\*</sup>

# Supporting Information for

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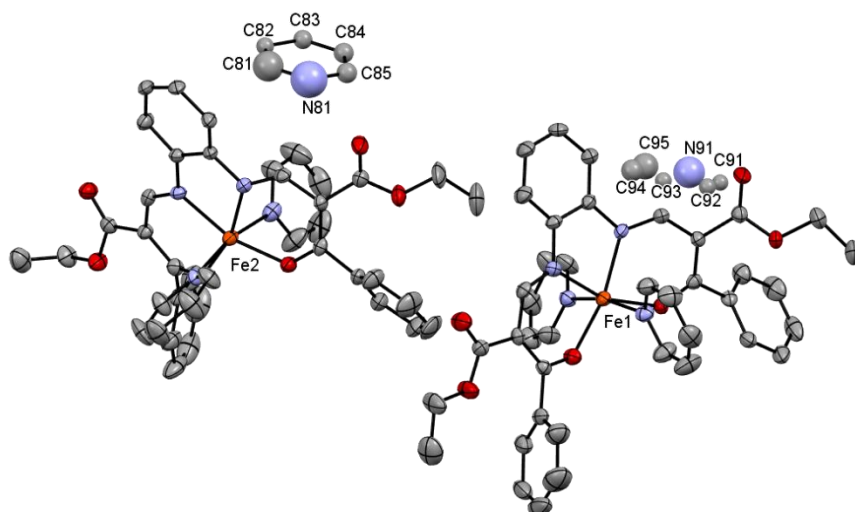
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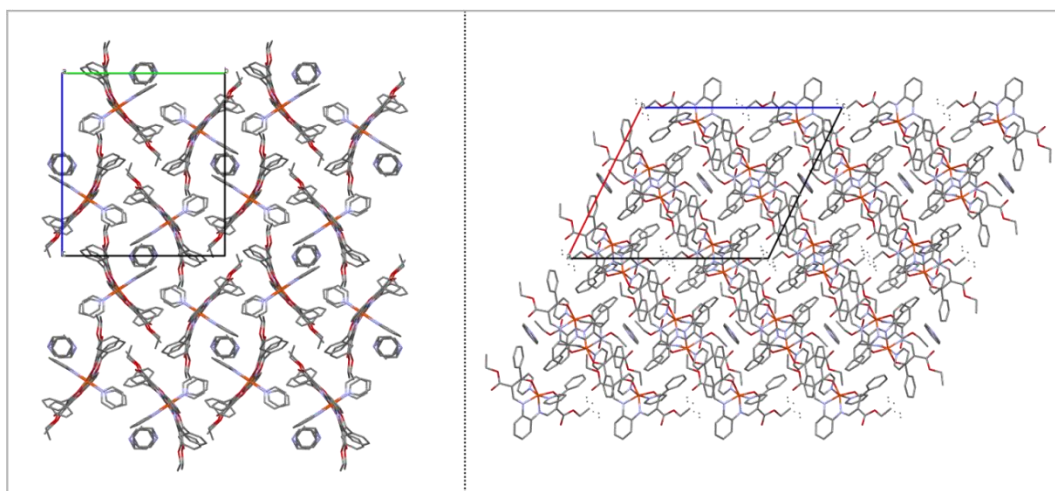
**Table S1** Crystallographic data of  $\{[\text{Fe6}(\text{py})_2]\cdot\text{py}\}$  and  $[\text{Fe7}(\text{py})_2]$ 

| Compound                               | $\{[\text{Fe6}(\text{py})_2]\cdot\text{py}\}$                                       | $[\text{Fe7}(\text{py})_2]$                        |  |
|--|---|--|--|
|  | 173 K   | 170 K  | 220 K  |
| Formula                                | $2(\text{C}_{40}\text{H}_{36}\text{FeN}_4\text{O}_6), \text{C}_5\text{H}_5\text{N}$ | $\text{C}_{28}\text{H}_{28}\text{FeN}_4\text{O}_6$ | $\text{C}_{28}\text{H}_{28}\text{FeN}_4\text{O}_6$ |
| CCDC                                   | –   | 2041117  | 2041118  |
| $M_r / \text{g mol}^{-1}$              | 1528.26   | 572.30   | 572.59   |
| $N / \text{\AA}$                       | 0.70930   | 0.71073  | 0.71073  |
| $T / \text{K}$                         | 173   | 170  | 220  |
| Crystal system                         | monoclinic  | triclinic  | triclinic  |
| Space group                            | $P2_1/n$  | $P\bar{1}$   | $P\bar{1}$   |
| $a / \text{\AA}$                       | 19.438(6)   | 8.8320(4)  | 9.0668(2)  |
| $b / \text{\AA}$                       | 18.651(9)   | 15.0013(7)   | 15.3564(4)   |
| $c / \text{\AA}$                       | 23.287(6)   | 20.0953(8)   | 19.7077(5)   |
| $\alpha / ^\circ$                      | 90  | 86.245(4)  | 92.321(2)  |
| $\beta / ^\circ$                       | 116.144(18)   | 85.661(3)  | 97.259(2)  |
| $\gamma / ^\circ$                      | 90  | 88.490(4)  | 93.322(2)  |
| $V / \text{\AA}^3$                     | 7579(5)   | 2648.5(2)  | 2714.23(12)  |
| $Z$                                    | 4   | 4  | 4  |
| $d_{\text{calcd}} / \text{Mg cm}^{-3}$ | 1.339   | 1.435  | 1.401  |
| $\mu / \text{mm}^{-1}$                 | 0.452   | 0.620  | 0.605  |
| $\Theta$ range/ $^\circ$               | 4.2–26.3  | 2.3–28.6   | 2.3–28.5   |
| Reflections collected                  | 32679   | 36827  | 38958  |
| Indep. reflections                     | 15303   | 12613  | 12926  |
| $R_{\text{int}}$                       | 0.050   | 0.134  | 0.062  |
| $R(F)$                                 | 0.0477  | 0.0819   | 0.0465   |
| $wR2(F2)$                              | 0.0998  | 0.2156   | 0.0947   |
| Goof                                   | 0.75  | 0.88   | 0.89   |

**Figure S1:** ORTEP drawing of the asymmetric unit of the motif of  $\{[\text{Fe6}(\text{py})_2]\cdot\text{py}\}$  (173 K) with the atom numbering scheme used for the co-crystallized solvent. Hydrogen atoms are omitted for clarity. Thermal ellipsoids are presented at 50% level.



**Figure S2:** Molecular packing of the  $\{[\text{Fe}_6(\text{py})_2]\cdot\text{py}\}$  motif in the crystal at 173 K. Left: view along axis **a** and right: view along axis **b**. Hydrogen atoms have been omitted for clarity.



In Figure S2 the packing of  $\{[\text{Fe}_6(\text{py})_2]\cdot\text{py}\}$  is displayed. The independent iron centers Fe1 and Fe2 alternate along axis **a**. As a result, all the front iron centers shown on the left in Figure S2 belong to one type of iron sites. Co-crystallized pyridine plays a crucial role in the packing. A view along the **b**-axis shows that pairs of Fe1 and Fe2 alternately form a diagonal strand. Between these strands, always at the height of an iron pair, there is one of the pyridine molecules, which results in a chessboard-like arrangement of the pyridine molecules in the crystal. Although no classical hydrogen bonds could be identified, there are some intra and intermolecular short contacts, which are summarized in Table S2. Particularly the oxygens of the ester groups are involved in these contacts. Short contacts between the coordinated pyridine molecules and the phenyl backbone are certainly a reason for the unique packing of the molecule.

**Table S2:** Short contacts observed in the crystal structure of  $\{[\text{Fe}_6(\text{py})_2]\cdot\text{py}\}$  with relevant distances (Å) and angles (°).

| Donor–H⋯acceptor                 | D–H  | H⋯A  | D⋯A      | D–H⋯A |
|----------------------------------|------|------|----------|-------|
| C(3)–H(3)⋯O(13)                  | 0.95 | 2.31 | 2.716(4) | 105   |
| C(6)–H(6)⋯O(22) <sup>[a]</sup>   | 0.95 | 2.52 | 3.442(5) | 164   |
| C(10)–H(10)⋯O(15)                | 0.95 | 2.36 | 2.748(4) | 104   |
| C(33)–H(33)⋯O(24) <sup>[b]</sup> | 0.95 | 2.54 | 3.266(5) | 133   |
| C(36)–H(36)⋯O(11)                | 0.95 | 2.44 | 3.039(5) | 121   |
| C(43)–H(43)⋯O(25)                | 0.95 | 2.37 | 2.749(4) | 103   |
| C(46)–H(46)⋯O(11) <sup>[c]</sup> | 0.95 | 2.51 | 3.409(5) | 158   |
| C(50)–H(50)⋯O(23)                | 0.95 | 2.37 | 2.755(4) | 104   |
| C(72)–H(72)⋯O(25) <sup>[d]</sup> | 0.95 | 2.43 | 3.170(5) | 134   |
| C(74)–H(74)⋯O(23) <sup>[e]</sup> | 0.95 | 2.46 | 3.295(5) | 147   |
| C(75)–H(75)⋯O(22)                | 0.95 | 2.52 | 3.064(5) | 117   |
| C(78)–H(78)⋯O(16) <sup>[f]</sup> | 0.95 | 2.53 | 3.214(5) | 129   |

[a]:  $x, -1/2-y, 1/2+z$ ; [b]:  $-x, -1/2+y, -1/2-z$ ; [c]:  $-1+x, -1/2-y, -1/2+z$ ; [d]:  $-1-x, -1/2+y, -3/2-z$ ;  
[e]:  $x, -1/2-y, -1/2+z$ ; [f]:  $-x, 1/2+y, -1/2-z$

**Figure S3:** Molecular packing of  $[\text{Fe7}(\text{py})_2]$  in the crystal at top: 170 K and bottom 220 K. Left: view along axis  $a$  and right: view along axis  $a^*$ . Hydrogen atoms have been omitted for clarity.

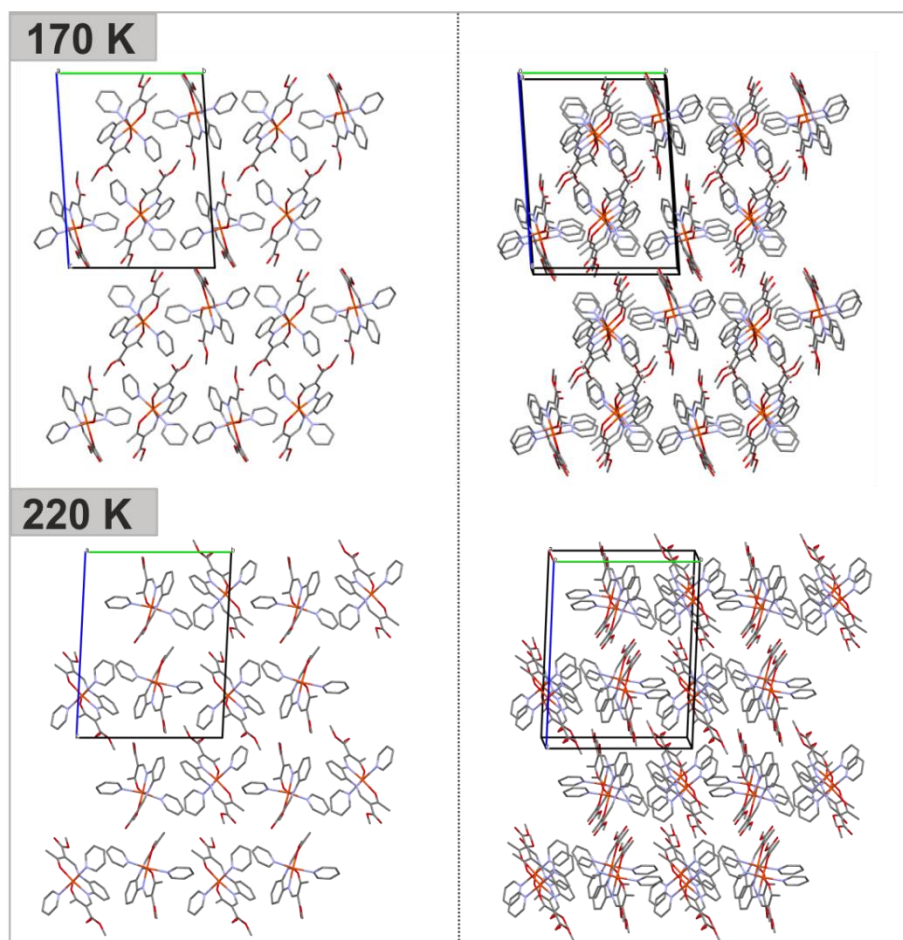


Figure S3 displays the packing of  $[\text{Fe7}(\text{py})_2]$  in the crystal at two different temperatures. A view along the  $a$  axis reveals that Fe1 and Fe2 always alternate horizontally from left to right. As a result, there is a vertical line from top to bottom, of either Fe1 in a row or Fe2 underneath each other. Consequently, the iron centers are arranged in a chessboard like pattern in the crystal. Again, some inter- and intramolecular short contacts can be identified, which are summarized in Tables S3 and S4. At 170 K significantly more short contacts can be observed. On closer examination, it becomes clear that there is a short contact between the equatorially coordinated oxygen O8 of the iron center in the LS state and the H21 of the pyridine coordinating Fe1 in the HS state. In magnetic susceptibility measurements, a plateau is observed at 170 K. It may be argued that only one of the two iron center can reach the diamagnetic LS state at this temperature due to the large number of occurring short contacts.

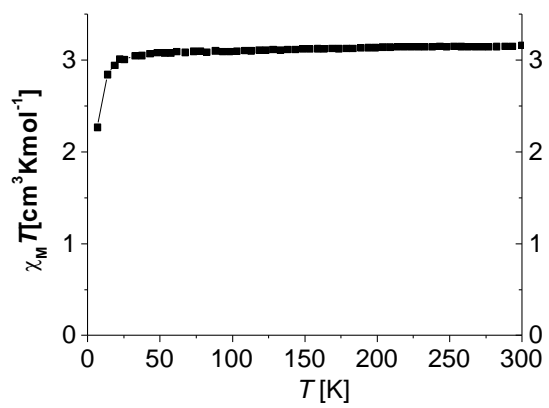
**Table S3:** Short contacts observed in the crystal structure of [Fe7(py)2] with relevant distances (Å) and angles (°) at 170 K.

| Donor–H...acceptor  | D–H  | H...A | D...A    | D–H...A |
|---|------|-------|----------|---------|
| C(4)–H(4)···O(4)  | 0.93 | 2.17  | 2.577(6) | 105     |
| C(8)–H(8)···O(12) <sup>[a]</sup>  | 0.93 | 2.58  | 3.356(8) | 142     |
| C(11)–H(11)···O(6)  | 0.93 | 2.23  | 2.637(7) | 106     |
| C(14)–H(14B)···O(5)   | 0.96 | 2.29  | 2.723(7) | 106     |
| C(16)–H(16B)···O(1) <sup>[b]</sup>  | 0.96 | 2.41  | 3.190(6) | 138     |
| C(21)–H(21)···O(8) <sup>[b]</sup>   | 0.93 | 2.32  | 3.126(7) | 145     |
| C(22)–H(22)···O(10) <sup>[c]</sup>  | 0.93 | 2.58  | 3.414(7) | 150     |
| C(23)–H(23)···O(1)  | 0.93 | 2.51  | 2.860(7) | 103     |
| C(23)–H(23)···O(2)  | 0.93 | 2.51  | 2.876(7) | 104     |
| C(28)–H(28)···O(3) <sup>[d]</sup>   | 0.93 | 2.53  | 3.293(7) | 139     |
| C(29)–H(29B)···O(9)   | 0.96 | 2.37  | 2.743(8) | 102     |
| C(32)–H(32)···O(10)   | 0.93 | 2.28  | 2.670(7) | 104     |
| C(39)–H(39)···O(12)   | 0.93 | 2.27  | 2.675(7) | 105     |
| C(49)–H(49)···O(12) <sup>[e]</sup>  | 0.93 | 2.60  | 3.413(7) | 147     |
| C(54)–H(54)···O(3) <sup>[f]</sup>   | 0.93 | 2.50  | 3.365(8) | 156     |
| [a]: -1+x,1+y,z; [b]: -1+x,y,z; [c]: x, y, z; [d]: -x,2-y,-z; [e]: 1-x,1-y,1-z; [f]: 1-x,1-y,-z |      |       |          |         |

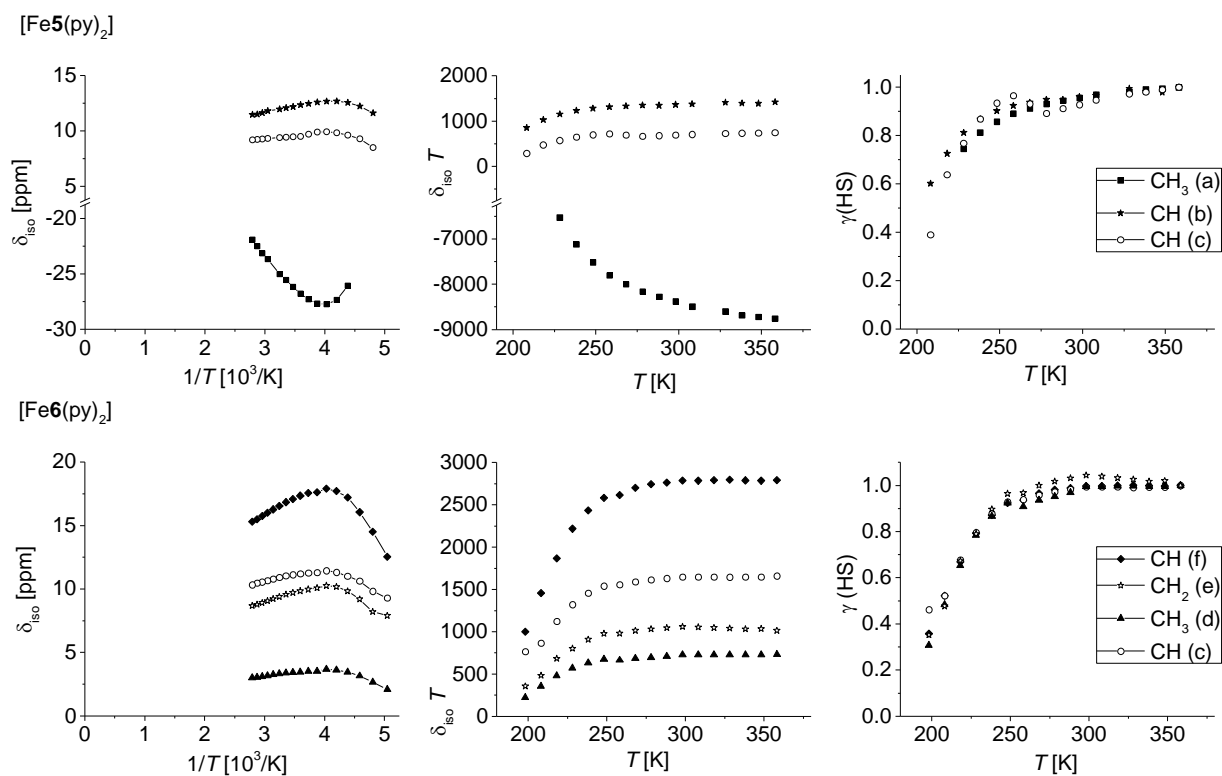
**Table S4:** Short contacts observed in the crystal structure of [Fe7(py)2] with relevant distances (Å) and angles (°) at 220 K.

| Donor–H...acceptor   | D–H  | H...A | D...A     | D–H...A |
|--|------|-------|-----------|---------|
| C(4)–H(3)···O(13)  | 0.94 | 2.41  | 2.782(3)  | 103     |
| C(11)–H(6)···O(22)   | 0.94 | 2.18  | 2.601(3)  | 106     |
| C(18)–H(10)···O(15)  | 0.97 | 2.45  | 3.302(3)  | 147     |
| C(21)–H(33)···O(24) <sup>[a]</sup>                               | 0.94 | 2.46  | 3.210(4)  | 137     |
| C(24)–H(36)···O(11) <sup>[b]</sup>                               | 0.94 | 2.59  | 3.398(3)  | 144     |
| C(29)–H(43)···O(25) <sup>[c]</sup>                               | 0.97 | 2.48  | 2.812(17) | 100     |
| C(29)–H(46)···O(11)  | 0.97 | 2.20  | 2.695(17) | 110     |
| C(32)–H(50)···O(23)  | 0.94 | 2.24  | 2.651(3)  | 106     |
| C(39)–H(72)···O(25)  | 0.94 | 2.22  | 2.629(3)  | 106     |
| C(49)–H(74)···O(23) <sup>[d]</sup>                               | 0.94 | 2.42  | 3.336(4)  | 165     |
| [a]: 1+x,y,z; [b]: 1+x,1+y,z; [c]: 3-x,1-y,1-z; [d]: 2-x,1-y,1-z |      |       |           |         |

**Figure S4:** Plot of the  $\chi_M T$  product vs.  $T$  for  $[\text{Fe6}(\text{py})_2] \times \text{py}$  illustrating the pure HS state.

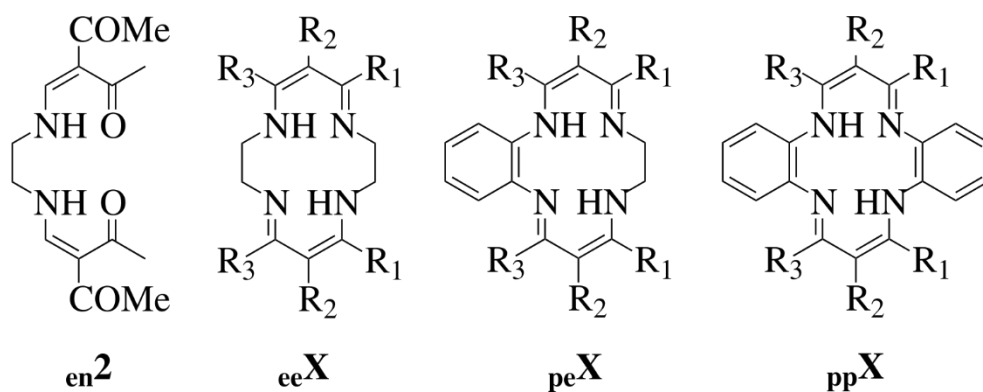


**Figure S5:** Left: Curie plot of  $^1\text{H}$  NMR chemical shifts ( $\delta_{\text{obs}}$ ) recorded for  $[\text{Fe5}(\text{py})_2]$  and  $[\text{Fe6}(\text{py})_2]$  in a mixture of pyridine- $d_5$  and toluene- $d_8$  (1 : 1) in the temperature range between 200 K and 360 K (400 MHz) with the signal assignment given in the manuscript, Figure 2. Middle: product of the paramagnetic chemical shift ( $\delta_{\text{para}} = \delta_{\text{obs}} - \delta_{\text{dia}}$ ) and temperature ( $\delta_{\text{para}} \times T$ ) plotted vs. temperature for both complexes. Right: HS fractions ( $\gamma_{\text{HS}}$ ) of  $[\text{Fe5}(\text{py})_2]$  and  $[\text{Fe6}(\text{py})_2]$  computed from chemical shift data according to  $\gamma_{\text{HS}} = (\delta_{\text{para}} \times T) / (\delta_{\text{para}} \times T)_{\text{HS}}$ , the average  $\gamma_{\text{HS}}$  is given in the manuscript, Figure 6.





**Figure S6:** Structure plots of the reference compounds (X = 1–8) discussed in Figure 8 of the main manuscript.



## Cartesian Coordinates of the optimized structures

**Table S5:** Cartesian coordinates of DFT-optimized LS-[Fe1(py)<sub>2</sub>] (BP86-D3/TZVP)

|    |           |          |           |
|----|-----------|----------|-----------|
| Fe | 5.960783  | 4.122667 | 7.261591  |
| O  | 7.474669  | 5.128147 | 6.586378  |
| O  | 6.330105  | 4.915833 | 8.990562  |
| N  | 4.486085  | 3.120425 | 7.896894  |
| O  | 7.099793  | 4.191042 | 1.917603  |
| O  | 2.591527  | 3.294994 | 11.481093 |
| N  | 5.579084  | 3.331676 | 5.584505  |
| C  | 4.006015  | 2.189545 | 6.948906  |
| C  | 5.590434  | 4.896049 | 10.037690 |
| C  | 3.920427  | 3.280723 | 9.075124  |
| H  | 3.020115  | 2.705691 | 9.311689  |
| C  | 4.609876  | 2.307633 | 5.669295  |
| C  | 7.808027  | 5.314300 | 5.362449  |
| C  | 6.107322  | 3.708514 | 4.438685  |
| H  | 5.750132  | 3.245131 | 3.514184  |
| C  | 7.128809  | 4.685349 | 4.266407  |
| C  | 4.367327  | 4.149420 | 10.111118 |
| C  | 3.034908  | 1.201540 | 7.172611  |
| H  | 2.584094  | 1.083959 | 8.157995  |
| C  | 3.469918  | 4.143526 | 11.281674 |
| C  | 2.657530  | 0.347999 | 6.133448  |
| C  | 4.228478  | 1.437864 | 4.635804  |
| H  | 4.701280  | 1.503884 | 3.655963  |
| C  | 7.446824  | 4.929562 | 2.847683  |
| C  | 3.252047  | 0.466718 | 4.867365  |
| C  | 9.014548  | 6.206126 | 5.191330  |
| C  | 6.158577  | 5.678722 | 11.197491 |
| O  | 3.652235  | 5.188469 | 12.131882 |
| C  | 2.815242  | 5.203080 | 13.327868 |
| O  | 8.132812  | 6.081537 | 2.620292  |
| C  | 8.519727  | 6.342466 | 1.237433  |
| H  | 2.979591  | 4.268922 | 13.884228 |
| H  | 1.760789  | 5.238134 | 13.018661 |
| C  | 3.209788  | 6.422307 | 14.136014 |
| H  | 4.263898  | 6.371528 | 14.440894 |
| H  | 2.591441  | 6.473650 | 15.042792 |
| H  | 3.053163  | 7.345079 | 13.559572 |
| H  | 7.609401  | 6.418654 | 0.626317  |
| H  | 9.109377  | 5.490199 | 0.870349  |
| C  | 9.318431  | 7.630430 | 1.229926  |
| H  | 8.718930  | 8.469337 | 1.610394  |
| H  | 9.621966  | 7.864460 | 0.199777  |
| H  | 10.224875 | 7.537597 | 1.842932  |
| H  | 7.193932  | 5.942202 | 10.952260 |
| H  | 6.124914  | 5.111843 | 12.135733 |
| H  | 5.581951  | 6.598876 | 11.362853 |
| H  | 9.736739  | 5.795354 | 4.474986  |
| H  | 9.485303  | 6.330472 | 6.173848  |
| H  | 8.714409  | 7.191794 | 4.809660  |
| N  | 7.164813  | 2.609992 | 7.697147  |
| C  | 7.090161  | 1.983915 | 8.897418  |
| H  | 6.352988  | 2.369089 | 9.599070  |
| C  | 8.067562  | 2.151053 | 6.795941  |

|   |          |           |           |
|---|----------|-----------|-----------|
| H | 8.101742 | 2.668327  | 5.839053  |
| C | 7.899385 | 0.901835  | 9.229610  |
| C | 8.907494 | 1.072872  | 7.059299  |
| C | 8.826534 | 0.428351  | 8.296987  |
| H | 7.792406 | 0.437578  | 10.209900 |
| H | 9.610711 | 0.745117  | 6.293380  |
| H | 9.469052 | -0.422231 | 8.527584  |
| N | 4.816857 | 5.648789  | 6.854689  |
| C | 3.601220 | 5.515332  | 6.264513  |
| H | 3.286552 | 4.500724  | 6.028920  |
| C | 5.239728 | 6.902884  | 7.162635  |
| H | 6.217337 | 6.963679  | 7.634561  |
| C | 2.788942 | 6.604224  | 5.967937  |
| C | 4.477766 | 8.034571  | 6.893573  |
| C | 3.226576 | 7.893922  | 6.284483  |
| H | 1.823004 | 6.433032  | 5.492986  |
| H | 4.868999 | 9.015706  | 7.163271  |
| H | 2.610183 | 8.765426  | 6.062324  |
| H | 1.907441 | -0.423396 | 6.315564  |
| H | 2.964558 | -0.211082 | 4.062105  |

**Table S6:** Cartesian coordinates of DFT-optimized HS-[Fe1(py)<sub>2</sub>] (BP86-D3/TZVP)

|    |          |          |           |
|----|----------|----------|-----------|
| Fe | 6.480590 | 3.866097 | 7.485337  |
| O  | 7.979892 | 4.700373 | 6.432236  |
| O  | 6.559258 | 4.451838 | 9.407215  |
| N  | 4.717053 | 2.906959 | 8.023252  |
| O  | 6.488328 | 4.589630 | 1.912747  |
| O  | 2.171376 | 3.716482 | 11.098670 |
| N  | 5.849218 | 3.110330 | 5.653778  |
| C  | 4.295218 | 1.968316 | 7.068551  |
| C  | 5.617749 | 4.695623 | 10.248868 |
| C  | 3.956227 | 3.248607 | 9.039175  |
| H  | 2.933251 | 2.855276 | 9.093155  |
| C  | 4.906670 | 2.079191 | 5.787280  |
| C  | 7.998409 | 5.147552 | 5.226304  |
| C  | 6.114697 | 3.656427 | 4.487957  |
| H  | 5.526156 | 3.354267 | 3.612572  |
| C  | 7.081699 | 4.676729 | 4.237125  |
| C  | 4.309101 | 4.144454 | 10.093533 |
| C  | 3.378946 | 0.933341 | 7.309488  |
| H  | 2.942166 | 0.820253 | 8.302605  |
| C  | 3.185989 | 4.418001 | 11.010751 |
| C  | 3.049142 | 0.031878 | 6.292869  |
| C  | 4.581060 | 1.154699 | 4.782854  |
| H  | 5.077667 | 1.214937 | 3.813478  |
| C  | 7.031665 | 5.182431 | 2.852153  |
| C  | 3.648122 | 0.143377 | 5.030394  |
| C  | 9.085264 | 6.159763 | 4.951854  |
| C  | 6.034253 | 5.558450 | 11.416935 |
| O  | 3.330657 | 5.552172 | 11.744931 |
| C  | 2.276203 | 5.832871 | 12.715188 |
| O  | 7.602351 | 6.403628 | 2.686113  |
| C  | 7.617603 | 6.931828 | 1.325174  |
| H  | 2.184915 | 4.973554 | 13.394831 |

|   |          |           |           |
|---|----------|-----------|-----------|
| H | 1.324424 | 5.947418  | 12.177071 |
| C | 2.667934 | 7.098306  | 13.449804 |
| H | 3.622100 | 6.969533  | 13.979728 |
| H | 1.893115 | 7.343347  | 14.190505 |
| H | 2.761201 | 7.945561  | 12.755876 |
| H | 6.580357 | 7.026683  | 0.973567  |
| H | 8.136564 | 6.214267  | 0.673770  |
| C | 8.324778 | 8.271002  | 1.373041  |
| H | 7.797718 | 8.971810  | 2.035574  |
| H | 8.350409 | 8.704622  | 0.362772  |
| H | 9.358895 | 8.160234  | 1.726966  |
| H | 7.130345 | 5.601041  | 11.432655 |
| H | 5.655337 | 5.184007  | 12.375039 |
| H | 5.639394 | 6.577956  | 11.298873 |
| H | 9.602572 | 5.979580  | 4.002397  |
| H | 9.798340 | 6.125620  | 5.785227  |
| H | 8.655620 | 7.170275  | 4.889197  |
| N | 7.622043 | 2.062193  | 7.880749  |
| C | 7.385002 | 1.335684  | 8.994601  |
| H | 6.753833 | 1.810790  | 9.746715  |
| C | 8.393296 | 1.516631  | 6.915266  |
| H | 8.554804 | 2.134991  | 6.031319  |
| C | 7.901919 | 0.056031  | 9.182242  |
| C | 8.948435 | 0.243856  | 7.025570  |
| C | 8.696437 | -0.506889 | 8.178369  |
| H | 7.677762 | -0.488588 | 10.099855 |
| H | 9.562828 | -0.149995 | 6.215438  |
| H | 9.111667 | -1.508687 | 8.292574  |
| N | 5.345394 | 5.779802  | 7.089479  |
| C | 4.139014 | 5.763841  | 6.494260  |
| H | 3.742260 | 4.779294  | 6.243326  |
| C | 5.882421 | 6.968945  | 7.421789  |
| H | 6.861155 | 6.932527  | 7.902288  |
| C | 3.425865 | 6.927011  | 6.206458  |
| C | 5.239289 | 8.180949  | 7.171097  |
| C | 3.987166 | 8.159814  | 6.550440  |
| H | 2.451499 | 6.862526  | 5.722563  |
| H | 5.713926 | 9.119517  | 7.457276  |
| H | 3.457673 | 9.089674  | 6.338507  |
| H | 2.339766 | -0.773284 | 6.493508  |
| H | 3.406206 | -0.574087 | 4.244036  |

**Table S7:** Cartesian coordinates of DFT-optimized LS-[Fe2(py)<sub>2</sub>] (BP86-D3/TZVP)

|    |           |          |           |
|----|-----------|----------|-----------|
| Fe | 6.318793  | 4.066529 | 7.610843  |
| O  | 7.855442  | 5.058132 | 6.981708  |
| O  | 6.793248  | 4.636468 | 9.400489  |
| N  | 4.808678  | 3.088759 | 8.196537  |
| O  | 8.578166  | 6.230219 | 3.032167  |
| O  | 2.971946  | 3.120713 | 11.781509 |
| N  | 5.839785  | 3.482848 | 5.878427  |
| N  | 5.246624  | 5.687828 | 7.418392  |
| C  | 4.256205  | 2.279853 | 7.177940  |
| C  | 6.060609  | 4.582836 | 10.451176 |
| C  | 4.268832  | 3.186518 | 9.392169  |
| H  | 3.335206  | 2.654562 | 9.599611  |
| C  | 4.826627  | 2.496801 | 5.896713  |
| C  | 8.157577  | 5.357458 | 5.775026  |
| C  | 6.344645  | 3.951231 | 4.754499  |
| H  | 5.900489  | 3.589838 | 3.825156  |
| C  | 7.415971  | 4.884314 | 4.631060  |
| C  | 4.771514  | 3.956684 | 10.483090 |
| C  | 3.248420  | 1.317888 | 7.339684  |
| H  | 2.823539  | 1.124916 | 8.324742  |
| C  | 3.862360  | 3.986626 | 11.644271 |
| C  | 2.801619  | 0.586322 | 6.237147  |
| C  | 4.378140  | 1.746138 | 4.799377  |
| H  | 4.826819  | 1.880158 | 3.814916  |
| C  | 7.755668  | 5.323306 | 3.270698  |
| C  | 3.365219  | 0.799830 | 4.969914  |
| C  | 9.384498  | 6.222889 | 5.649993  |
| H  | 10.084958 | 5.835398 | 4.899042  |
| H  | 9.109264  | 7.234138 | 5.317809  |
| H  | 9.863779  | 6.277850 | 6.635753  |
| C  | 6.733060  | 5.155556 | 11.677896 |
| H  | 6.455136  | 4.639992 | 12.603045 |
| H  | 7.818538  | 5.080814 | 11.532312 |
| H  | 6.486842  | 6.222839 | 11.792366 |
| C  | 3.900880  | 5.118960 | 12.654998 |
| H  | 4.332495  | 6.045975 | 12.262247 |
| H  | 2.869662  | 5.304970 | 12.981513 |
| H  | 4.475024  | 4.818764 | 13.545651 |
| C  | 7.071300  | 4.655604 | 2.080298  |
| H  | 7.197893  | 3.562737 | 2.087713  |
| H  | 5.991002  | 4.867355 | 2.066387  |
| H  | 7.515947  | 5.060830 | 1.164617  |
| C  | 3.753727  | 8.055352 | 7.185603  |
| C  | 5.032726  | 8.064978 | 7.751128  |
| H  | 5.483742  | 8.987990 | 8.115788  |
| H  | 6.742579  | 6.834945 | 8.283308  |
| C  | 5.745275  | 6.874868 | 7.851548  |
| C  | 4.005856  | 5.682106 | 6.868265  |
| C  | 3.239202  | 6.835067 | 6.737686  |
| H  | 2.248997  | 6.767113 | 6.287645  |
| H  | 3.631811  | 4.718793 | 6.528265  |
| N  | 7.448209  | 2.453593 | 7.835701  |
| C  | 8.289573  | 2.046266 | 6.854043  |
| C  | 7.383149  | 1.710015 | 8.967127  |
| H  | 6.694289  | 2.056775 | 9.734548  |

|   |          |           |           |
|---|----------|-----------|-----------|
| C | 8.144735 | 0.560098  | 9.152585  |
| H | 8.048923 | 0.001685  | 10.083766 |
| H | 8.315382 | 2.657125  | 5.954010  |
| C | 9.080045 | 0.906654  | 6.970292  |
| H | 9.735943 | 0.626758  | 6.145761  |
| C | 9.011010 | 0.141986  | 8.138309  |
| H | 9.615944 | -0.757691 | 8.254497  |
| H | 3.174460 | 8.974802  | 7.095343  |
| H | 2.022890 | -0.166700 | 6.370003  |
| H | 3.026086 | 0.213986  | 4.114240  |

**Table S8:** Cartesian coordinates of DFT-optimized HS-[Fe2(py)<sub>2</sub>] (BP86-D3/TZVP)

|    |          |          |           |
|----|----------|----------|-----------|
| Fe | 6.714265 | 3.944944 | 7.753431  |
| O  | 8.179332 | 4.861002 | 6.724175  |
| O  | 6.840469 | 4.341317 | 9.730182  |
| N  | 4.953223 | 2.953667 | 8.258937  |
| O  | 7.995950 | 6.569726 | 2.905633  |
| O  | 2.426586 | 3.682872 | 11.326816 |
| N  | 6.030670 | 3.342040 | 5.888063  |
| N  | 5.575333 | 5.884672 | 7.596866  |
| C  | 4.511630 | 2.089156 | 7.245254  |
| C  | 5.908785 | 4.539962 | 10.592123 |
| C  | 4.199094 | 3.251271 | 9.291353  |
| H  | 3.165280 | 2.884050 | 9.321991  |
| C  | 5.099986 | 2.293460 | 5.965634  |
| C  | 8.183138 | 5.384736 | 5.553315  |
| C  | 6.290043 | 3.946930 | 4.749259  |
| H  | 5.676452 | 3.665855 | 3.886802  |
| C  | 7.261969 | 4.972058 | 4.528688  |
| C  | 4.570321 | 4.083752 | 10.394448 |
| C  | 3.601078 | 1.038296 | 7.429786  |
| H  | 3.180067 | 0.856286 | 8.419570  |
| C  | 3.442643 | 4.406365 | 11.291681 |
| C  | 3.259615 | 0.206466 | 6.359243  |
| C  | 4.766693 | 1.434767 | 4.906773  |
| H  | 5.249723 | 1.556396 | 3.936281  |
| C  | 7.273647 | 5.596271 | 3.197109  |
| C  | 3.841695 | 0.404525 | 5.099629  |
| C  | 9.236137 | 6.440722 | 5.338526  |
| H  | 9.843240 | 6.238265 | 4.446698  |
| H  | 8.771024 | 7.422286 | 5.168392  |
| H  | 9.868380 | 6.479978 | 6.234920  |
| C  | 6.381164 | 5.210906 | 11.861777 |
| H  | 5.810390 | 4.922257 | 12.749846 |
| H  | 7.436211 | 4.946647 | 12.007547 |
| H  | 6.328614 | 6.306958 | 11.757943 |
| C  | 3.427774 | 5.680300 | 12.119714 |
| H  | 4.085425 | 6.465837 | 11.731160 |
| H  | 2.392966 | 6.046323 | 12.143269 |
| H  | 3.720621 | 5.464287 | 13.158950 |
| C  | 6.357229 | 5.046576 | 2.106119  |
| H  | 6.516284 | 3.972117 | 1.932132  |
| H  | 5.295856 | 5.187457 | 2.362498  |
| H  | 6.569088 | 5.593328 | 1.180504  |
| C  | 4.100638 | 8.256488 | 7.583742  |
| C  | 5.379049 | 8.217683 | 8.147530  |

|   |          |           |          |
|---|----------|-----------|----------|
| H | 5.828203 | 9.104540  | 8.594579 |
| H | 7.080058 | 6.931127  | 8.561905 |
| C | 6.080497 | 7.012520  | 8.132511 |
| C | 4.346275 | 5.927776  | 7.050548 |
| C | 3.576027 | 7.089787  | 7.021104 |
| H | 2.584646 | 7.074479  | 6.568851 |
| H | 3.977961 | 4.992146  | 6.628199 |
| N | 7.858961 | 2.112110  | 7.954011 |
| C | 8.602900 | 1.658473  | 6.921390 |
| C | 7.642199 | 1.281202  | 8.997241 |
| H | 7.033812 | 1.685086  | 9.807299 |
| C | 8.151074 | -0.014657 | 9.045539 |
| H | 7.943061 | -0.645698 | 9.910022 |
| H | 8.749693 | 2.358958  | 6.098301 |
| C | 9.148630 | 0.377175  | 6.892732 |
| H | 9.740370 | 0.060342  | 6.033531 |
| C | 8.916416 | -0.481651 | 7.972054 |
| H | 9.324505 | -1.492911 | 7.976881 |
| H | 3.523636 | 9.182452  | 7.581189 |
| H | 2.556130 | -0.613334 | 6.515160 |
| H | 3.594139 | -0.261168 | 4.271003 |

**Table S9:** Cartesian coordinates of DFT-optimized LS-[Fe3(py)<sub>2</sub>] (BP86-D3/TZVP)

|    |           |          |           |
|----|-----------|----------|-----------|
| Fe | 6.431723  | 3.704500 | 7.396927  |
| O  | 7.753102  | 5.932465 | 2.557689  |
| O  | 3.351527  | 3.016529 | 11.876265 |
| N  | 4.935576  | 2.806155 | 8.135170  |
| O  | 7.967405  | 4.649059 | 6.611407  |
| O  | 7.067658  | 4.313059 | 9.147261  |
| N  | 5.784056  | 3.083667 | 5.724046  |
| C  | 4.257756  | 2.006002 | 7.189898  |
| C  | 4.328426  | 3.744221 | 11.650439 |
| C  | 4.496954  | 2.951726 | 9.371532  |
| H  | 3.554945  | 2.473364 | 9.654394  |
| C  | 4.723076  | 2.163277 | 5.857317  |
| C  | 7.559521  | 4.776686 | 2.924376  |
| C  | 6.230248  | 3.476660 | 4.542845  |
| H  | 5.695536  | 3.129397 | 3.653633  |
| C  | 7.317391  | 4.349718 | 4.314706  |
| C  | 5.119076  | 3.689192 | 10.410288 |
| C  | 3.217615  | 1.104033 | 7.462039  |
| H  | 2.871584  | 0.953562 | 8.485026  |
| C  | 6.421712  | 4.277932 | 10.233494 |
| C  | 2.631111  | 0.378922 | 6.422486  |
| C  | 4.133276  | 1.419276 | 4.823431  |
| H  | 4.493311  | 1.511608 | 3.798339  |
| C  | 8.125482  | 4.874872 | 5.379371  |
| C  | 3.088714  | 0.535855 | 5.105021  |
| O  | 7.501355  | 3.818499 | 1.934898  |
| C  | 7.840005  | 2.419300 | 2.211213  |
| O  | 4.717302  | 4.702856 | 12.531643 |
| C  | 3.958414  | 4.773116 | 13.775329 |
| O  | 7.024536  | 4.777956 | 11.333265 |
| C  | 8.355458  | 5.349552 | 11.138588 |
| O  | 9.189920  | 5.614596 | 4.992508  |
| C  | 10.042114 | 6.131215 | 6.061091  |
| H  | 8.291478  | 6.144518 | 10.382160 |
| H  | 9.022979  | 4.566225 | 10.752064 |
| C  | 8.807920  | 5.878073 | 12.483518 |
| H  | 8.126602  | 6.658559 | 12.849955 |
| H  | 9.812130  | 6.313877 | 12.382373 |
| H  | 8.855547  | 5.072290 | 13.229465 |
| H  | 10.445133 | 5.282038 | 6.631100  |
| H  | 9.425453  | 6.736524 | 6.740979  |
| C  | 11.131895 | 6.950301 | 5.403301  |
| H  | 11.736576 | 6.332628 | 4.724150  |
| H  | 11.794855 | 7.358805 | 6.179250  |
| H  | 10.707403 | 7.789894 | 4.835448  |
| H  | 4.001862  | 3.793104 | 14.272930 |
| H  | 2.906651  | 4.989930 | 13.537621 |
| C  | 4.584737  | 5.864937 | 14.619165 |
| H  | 5.634009  | 5.633738 | 14.846806 |
| H  | 4.036604  | 5.953116 | 15.567510 |
| H  | 4.541559  | 6.835344 | 14.104580 |
| C  | 8.639217  | 1.893134 | 1.035850  |
| H  | 6.906983  | 1.852609 | 2.341623  |
| H  | 8.412745  | 2.371695 | 3.147212  |
| H  | 8.061916  | 1.964881 | 0.103271  |

|   |          |           |          |
|---|----------|-----------|----------|
| H | 8.884784 | 0.834960  | 1.207612 |
| H | 9.577218 | 2.452038  | 0.917948 |
| N | 7.518637 | 2.073888  | 7.578753 |
| C | 7.514378 | 1.350968  | 8.725824 |
| H | 6.882113 | 1.722507  | 9.529353 |
| C | 8.286066 | 1.630072  | 6.552437 |
| H | 8.263981 | 2.226579  | 5.643021 |
| C | 8.263456 | 0.188352  | 8.881862 |
| C | 9.059782 | 0.476740  | 6.637468 |
| C | 9.053341 | -0.266317 | 7.821782 |
| H | 8.217324 | -0.352145 | 9.827440 |
| H | 9.655606 | 0.168213  | 5.778178 |
| H | 9.646206 | -1.176832 | 7.914939 |
| N | 5.414385 | 5.359301  | 7.239634 |
| C | 4.138260 | 5.396091  | 6.778202 |
| H | 3.701429 | 4.442211  | 6.491360 |
| C | 5.992327 | 6.533907  | 7.606073 |
| H | 7.014219 | 6.457560  | 7.969918 |
| C | 3.415100 | 6.579211  | 6.670100 |
| C | 5.326664 | 7.751911  | 7.523765 |
| C | 4.011830 | 7.786034  | 7.047778 |
| H | 2.393818 | 6.545309  | 6.291303 |
| H | 5.841046 | 8.662344  | 7.832098 |
| H | 3.467675 | 8.728063  | 6.972884 |
| H | 1.826260 | -0.324023 | 6.642805 |
| H | 2.640228 | -0.042545 | 4.296349 |

**Table S10:** Cartesian coordinates of DFT-optimized HS-[Fe3(py)<sub>2</sub>] (BP86-D3/TZVP)

|    |          |          |           |
|----|----------|----------|-----------|
| Fe | 6.858136 | 3.563254 | 7.557289  |
| O  | 7.242896 | 6.101924 | 2.572913  |
| O  | 2.941466 | 3.467876 | 11.614455 |
| N  | 5.123737 | 2.649985 | 8.270253  |
| O  | 8.278636 | 4.476663 | 6.390152  |
| O  | 7.218953 | 3.978867 | 9.537584  |
| N  | 5.981166 | 2.929499 | 5.775405  |
| C  | 4.531347 | 1.805638 | 7.318889  |
| C  | 4.032809 | 4.043633 | 11.507686 |
| C  | 4.497648 | 2.973365 | 9.382594  |
| H  | 3.454794 | 2.658910 | 9.516287  |
| C  | 4.996367 | 1.949755 | 5.979379  |
| C  | 7.194497 | 4.912566 | 2.870179  |
| C  | 6.218599 | 3.426649 | 4.576823  |
| H  | 5.547622 | 3.141581 | 3.756205  |
| C  | 7.222413 | 4.367669 | 4.242322  |
| C  | 5.019252 | 3.741936 | 10.457615 |
| C  | 3.576483 | 0.820155 | 7.616060  |
| H  | 3.252277 | 0.679306 | 8.648276  |
| C  | 6.400424 | 4.139510 | 10.490287 |
| C  | 3.062965 | 0.000975 | 6.606734  |
| C  | 4.491602 | 1.098265 | 4.982945  |
| H  | 4.873911 | 1.168622 | 3.964034  |
| C  | 8.181438 | 4.854191 | 5.186706  |
| C  | 3.522303 | 0.139195 | 5.290025  |
| O  | 7.040864 | 4.025676 | 1.827663  |
| C  | 7.461426 | 2.625845 | 1.940286  |
| O  | 4.384600 | 5.054596 | 12.342774 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 3.443207  | 5.354558  | 13.415085 |
| O | 6.861070  | 4.665896  | 11.645353 |
| C | 8.267487  | 5.058150  | 11.668787 |
| O | 9.084975  | 5.738281  | 4.702148  |
| C | 10.079909 | 6.233094  | 5.649866  |
| H | 8.448061  | 5.779559  | 10.859323 |
| H | 8.886506  | 4.169527  | 11.479989 |
| C | 8.534608  | 5.657490  | 13.033709 |
| H | 7.906583  | 6.541966  | 13.205749 |
| H | 9.588463  | 5.963938  | 13.095532 |
| H | 8.339883  | 4.926206  | 13.830516 |
| H | 10.671955 | 5.382926  | 6.017674  |
| H | 9.557479  | 6.683021  | 6.506134  |
| C | 10.933014 | 7.243380  | 4.913381  |
| H | 11.444350 | 6.780744  | 4.057834  |
| H | 11.696870 | 7.640060  | 5.597636  |
| H | 10.325236 | 8.083218  | 4.550190  |
| H | 3.277594  | 4.442492  | 14.006781 |
| H | 2.481971  | 5.653984  | 12.972769 |
| C | 4.053326  | 6.464450  | 14.246135 |
| H | 5.016108  | 6.151879  | 14.673168 |
| H | 3.374269  | 6.717890  | 15.072849 |
| H | 4.213681  | 7.368334  | 13.642157 |
| C | 8.153491  | 2.240795  | 0.647930  |
| H | 6.565598  | 2.011545  | 2.109712  |
| H | 8.127387  | 2.521630  | 2.807219  |
| H | 7.482430  | 2.370791  | -0.212745 |
| H | 8.450342  | 1.183030  | 0.696772  |
| H | 9.055686  | 2.847304  | 0.490339  |
| N | 7.986883  | 1.732823  | 7.659764  |
| C | 7.856511  | 0.901384  | 8.717668  |
| H | 7.309212  | 1.301400  | 9.571591  |
| C | 8.651299  | 1.280074  | 6.572582  |
| H | 8.731779  | 1.979187  | 5.739402  |
| C | 8.375219  | -0.391335 | 8.727259  |
| C | 9.200062  | 0.002254  | 6.503250  |
| C | 9.058322  | -0.856285 | 7.598663  |
| H | 8.237985  | -1.021770 | 9.606219  |
| H | 9.726040  | -0.312398 | 5.601571  |
| H | 9.471893  | -1.864939 | 7.573277  |
| N | 5.783698  | 5.531381  | 7.487959  |
| C | 4.525671  | 5.619415  | 7.018112  |
| H | 4.088992  | 4.691632  | 6.646646  |
| C | 6.373672  | 6.646185  | 7.960181  |
| H | 7.392958  | 6.525914  | 8.330213  |
| C | 3.811435  | 6.816891  | 7.002929  |
| C | 5.732612  | 7.883945  | 7.984653  |
| C | 4.425367  | 7.970815  | 7.497438  |
| H | 2.794326  | 6.838911  | 6.612463  |
| H | 6.250010  | 8.758627  | 8.378722  |
| H | 3.893941  | 8.923668  | 7.502705  |
| H | 2.324347  | -0.763825 | 6.853703  |
| H | 3.143862  | -0.516762 | 4.504367  |

**Table S11:** Cartesian coordinates of DFT-optimized LS-[Fe4(py)<sub>2</sub>] (BP86-D3/TZVP)

|    |           |           |           |
|----|-----------|-----------|-----------|
| Fe | 6.467825  | 3.749384  | 7.342605  |
| N  | 4.927618  | 2.916481  | 8.088411  |
| O  | 8.050864  | 4.623503  | 6.552665  |
| O  | 7.135018  | 4.424529  | 9.072322  |
| N  | 5.805200  | 3.104392  | 5.679963  |
| C  | 4.241979  | 2.101421  | 7.160145  |
| C  | 4.554899  | 3.935094  | 11.589229 |
| C  | 4.492096  | 3.088190  | 9.321251  |
| H  | 3.542877  | 2.632540  | 9.617790  |
| C  | 4.727143  | 2.203371  | 5.831476  |
| C  | 7.704906  | 4.611578  | 2.931212  |
| C  | 6.250021  | 3.465090  | 4.491499  |
| H  | 5.733575  | 3.101550  | 3.598090  |
| C  | 7.376065  | 4.299024  | 4.268772  |
| C  | 5.173220  | 3.825617  | 10.324125 |
| C  | 3.177911  | 1.233303  | 7.448301  |
| H  | 2.811991  | 1.124452  | 8.469649  |
| C  | 6.465664  | 4.427003  | 10.138078 |
| C  | 2.591951  | 0.485930  | 6.424926  |
| C  | 4.140502  | 1.435776  | 4.814076  |
| H  | 4.523080  | 1.482607  | 3.794300  |
| C  | 8.217511  | 4.807058  | 5.318982  |
| C  | 3.073271  | 0.585586  | 5.110592  |
| O  | 6.970848  | 5.019440  | 11.240852 |
| C  | 8.292638  | 5.636063  | 11.101154 |
| O  | 9.276460  | 5.524542  | 4.887965  |
| C  | 10.163232 | 6.064665  | 5.920570  |
| H  | 8.248687  | 6.373606  | 10.287647 |
| H  | 9.010921  | 4.853576  | 10.819365 |
| C  | 8.629006  | 6.273652  | 12.431352 |
| H  | 7.899927  | 7.053557  | 12.691744 |
| H  | 9.623319  | 6.737957  | 12.366002 |
| H  | 8.651612  | 5.524409  | 13.235050 |
| H  | 10.573925 | 5.225038  | 6.498535  |
| H  | 9.566660  | 6.691522  | 6.598407  |
| C  | 11.239748 | 6.856926  | 5.211876  |
| H  | 11.819058 | 6.217334  | 4.531166  |
| H  | 11.927777 | 7.276771  | 5.959373  |
| H  | 10.806299 | 7.687288  | 4.637254  |
| N  | 4.022896  | 4.016247  | 12.631093 |
| N  | 7.959327  | 4.860348  | 1.813787  |
| N  | 7.497556  | 2.088218  | 7.587216  |
| C  | 7.469805  | 1.414787  | 8.763600  |
| H  | 6.849725  | 1.837280  | 9.551189  |
| C  | 8.249942  | 1.577867  | 6.581298  |
| H  | 8.246412  | 2.129209  | 5.643588  |
| C  | 8.182447  | 0.237848  | 8.970732  |
| C  | 8.987336  | 0.405683  | 6.717514  |
| C  | 8.957984  | -0.285083 | 7.932284  |
| H  | 8.118649  | -0.260069 | 9.938322  |
| H  | 9.570865  | 0.042873  | 5.871411  |
| H  | 9.521930  | -1.208675 | 8.064929  |
| N  | 5.506481  | 5.435772  | 7.122051  |
| C  | 4.234463  | 5.495543  | 6.651756  |
| H  | 3.766698  | 4.546156  | 6.401320  |

|   |          |           |          |
|---|----------|-----------|----------|
| C | 6.120940 | 6.604675  | 7.443639 |
| H | 7.138088 | 6.510758  | 7.816340 |
| C | 3.551570 | 6.696297  | 6.490276 |
| C | 5.496753 | 7.839678  | 7.306716 |
| C | 4.186597 | 7.896955  | 6.821128 |
| H | 2.531671 | 6.680275  | 6.107106 |
| H | 6.039378 | 8.744524  | 7.580357 |
| H | 3.674639 | 8.852419  | 6.703309 |
| H | 1.768351 | -0.191005 | 6.656684 |
| H | 2.625453 | -0.013078 | 4.316376 |

**Table S12:** Cartesian coordinates of DFT-optimized HS-[Fe4(py)<sub>2</sub>] (BP86-D3/TZVP)

|    |           |          |           |
|----|-----------|----------|-----------|
| Fe | 6.761790  | 3.664106 | 7.437647  |
| N  | 4.971415  | 2.846164 | 8.140632  |
| O  | 8.276626  | 4.447894 | 6.272859  |
| O  | 7.146390  | 4.204074 | 9.395332  |
| N  | 5.875465  | 3.036801 | 5.652490  |
| C  | 4.373702  | 1.988381 | 7.201402  |
| C  | 4.117016  | 4.274972 | 11.402773 |
| C  | 4.364156  | 3.171030 | 9.260782  |
| H  | 3.327671  | 2.849165 | 9.426062  |
| C  | 4.859715  | 2.088929 | 5.866923  |
| C  | 7.230515  | 4.930331 | 2.825325  |
| C  | 6.109815  | 3.535834 | 4.458559  |
| H  | 5.438377  | 3.284293 | 3.627141  |
| C  | 7.174522  | 4.425062 | 4.143824  |
| C  | 4.940268  | 3.952243 | 10.300622 |
| C  | 3.391323  | 1.033218 | 7.507628  |
| H  | 3.048302  | 0.920359 | 8.536985  |
| C  | 6.296151  | 4.424133 | 10.299772 |
| C  | 2.872185  | 0.206650 | 6.508131  |
| C  | 4.348436  | 1.231604 | 4.879765  |
| H  | 4.750522  | 1.272661 | 3.866880  |
| C  | 8.187796  | 4.832696 | 5.075675  |
| C  | 3.351161  | 0.305101 | 5.194719  |
| O  | 6.635198  | 5.149308 | 11.387956 |
| C  | 8.009552  | 5.652505 | 11.436644 |
| O  | 9.100159  | 5.689929 | 4.568006  |
| C  | 10.155615 | 6.137252 | 5.479383  |
| H  | 8.185216  | 6.272955 | 10.546691 |
| H  | 8.695653  | 4.794748 | 11.402538 |
| C  | 8.149007  | 6.445157 | 12.717993 |
| H  | 7.450593  | 7.292874 | 12.737282 |
| H  | 9.172305  | 6.840209 | 12.787125 |
| H  | 7.964244  | 5.811267 | 13.596317 |
| H  | 10.721925 | 5.257030 | 5.814202  |
| H  | 9.684659  | 6.600880 | 6.357355  |
| C  | 11.019986 | 7.115812 | 4.715242  |
| H  | 11.476117 | 6.638548 | 3.837245  |
| H  | 11.826504 | 7.472284 | 5.371759  |
| H  | 10.435546 | 7.984785 | 4.383731  |
| N  | 3.415176  | 4.531037 | 12.306387 |
| N  | 7.255920  | 5.336195 | 1.725647  |
| N  | 7.786009  | 1.785031 | 7.670808  |
| C  | 7.623498  | 1.049402 | 8.792743  |
| H  | 7.082655  | 1.532160 | 9.607237  |



|   |          |           |          |
|---|----------|-----------|----------|
| C | 8.444975 | 1.225966  | 6.631759 |
| H | 8.552220 | 1.848776  | 5.742961 |
| C | 8.107261 | -0.250533 | 8.916142 |
| C | 8.959212 | -0.067442 | 6.675511 |
| C | 8.786178 | -0.826049 | 7.837531 |
| H | 7.946743 | -0.800594 | 9.843698 |
| H | 9.481901 | -0.470230 | 5.807747 |
| H | 9.172999 | -1.843471 | 7.901316 |
| N | 5.811785 | 5.681318  | 7.249790 |
| C | 4.553641 | 5.815791  | 6.789659 |
| H | 4.039640 | 4.891128  | 6.525192 |
| C | 6.493814 | 6.792346  | 7.591486 |
| H | 7.509113 | 6.634082  | 7.958200 |
| C | 3.932487 | 7.056574  | 6.653367 |
| C | 5.949638 | 8.071211  | 7.487554 |
| C | 4.643249 | 8.205976  | 7.008585 |
| H | 2.912108 | 7.115052  | 6.275741 |
| H | 6.540529 | 8.940142  | 7.776382 |
| H | 4.186717 | 9.192161  | 6.913833 |
| H | 2.112099 | -0.534145 | 6.761507 |
| H | 2.966094 | -0.357797 | 4.418613 |

**Table S13:** Cartesian coordinates of DFT-optimized LS-[Fe5(py)<sub>2</sub>] (BP86-D3/TZVP)

|    |           |           |           |
|----|-----------|-----------|-----------|
| Fe | 5.815595  | 4.406997  | 7.298228  |
| O  | 7.464189  | 5.302882  | 6.790013  |
| O  | 6.042606  | 5.195692  | 9.048275  |
| N  | 4.214946  | 3.508657  | 7.763740  |
| O  | 8.813911  | 5.721872  | 2.779281  |
| O  | 2.920555  | 5.638908  | 11.830726 |
| N  | 5.548503  | 3.651020  | 5.585750  |
| C  | 3.788851  | 2.596759  | 6.772674  |
| C  | 5.191535  | 5.227068  | 10.003688 |
| C  | 3.535628  | 3.703931  | 8.875346  |
| H  | 2.566957  | 3.207920  | 8.972983  |
| C  | 4.535300  | 2.669476  | 5.568034  |
| C  | 7.890376  | 5.500586  | 5.599005  |
| C  | 6.139474  | 4.075839  | 4.488741  |
| H  | 5.797478  | 3.666866  | 3.533419  |
| C  | 7.221368  | 5.000506  | 4.429802  |
| C  | 3.932866  | 4.530323  | 9.965280  |
| C  | 2.756058  | 1.655956  | 6.895767  |
| H  | 2.193511  | 1.568093  | 7.825965  |
| C  | 2.984258  | 4.643154  | 11.080970 |
| C  | 2.458990  | 0.807006  | 5.826439  |
| C  | 4.236939  | 1.804215  | 4.505446  |
| H  | 4.826257  | 1.832160  | 3.588566  |
| C  | 7.646471  | 5.402957  | 3.083384  |
| C  | 3.195968  | 0.881543  | 4.634287  |
| N  | 6.853868  | 2.817953  | 7.852819  |
| C  | 6.617587  | 2.210009  | 9.040502  |
| H  | 5.849630  | 2.658415  | 9.667923  |
| C  | 7.801791  | 2.287680  | 7.042972  |
| H  | 7.965014  | 2.794693  | 6.093652  |
| C  | 7.308625  | 1.074374  | 9.450372  |
| C  | 8.531253  | 1.154372  | 7.387533  |
| C  | 8.283675  | 0.527578  | 8.611896  |
| H  | 7.076445  | 0.627258  | 10.416789 |
| H  | 9.280518  | 0.771244  | 6.694665  |
| H  | 8.836977  | -0.364875 | 8.905324  |
| N  | 4.838895  | 6.007750  | 6.744239  |
| C  | 3.711291  | 5.948976  | 5.990197  |
| H  | 3.338276  | 4.954825  | 5.752423  |
| C  | 5.323106  | 7.234660  | 7.068600  |
| H  | 6.223669  | 7.236593  | 7.678187  |
| C  | 3.056121  | 7.086754  | 5.532239  |
| C  | 4.717180  | 8.412228  | 6.644679  |
| C  | 3.563706  | 8.348268  | 5.856886  |
| H  | 2.155433  | 6.974742  | 4.928897  |
| H  | 5.153682  | 9.368498  | 6.932911  |
| H  | 3.072178  | 9.256618  | 5.508115  |
| H  | 1.660126  | 0.071062  | 5.930270  |
| H  | 2.971265  | 0.203612  | 3.809386  |
| H  | 7.919832  | 4.768438  | 0.478011  |
| H  | 0.408416  | 4.820223  | 11.823873 |
| H  | -1.180289 | 2.971296  | 12.354821 |
| C  | -0.155866 | 2.742437  | 12.056281 |
| H  | -0.417485 | 0.599899  | 12.223224 |
| C  | 0.271760  | 1.410285  | 11.979781 |

|   |          |          |           |
|---|----------|----------|-----------|
| C | 0.728921 | 3.779310 | 11.754291 |
| C | 1.586568 | 1.120838 | 11.596576 |
| C | 2.042895 | 3.497256 | 11.344537 |
| H | 1.929001 | 0.085575 | 11.550112 |
| C | 2.465006 | 2.157768 | 11.271752 |
| H | 3.490274 | 1.929249 | 10.976982 |
| H | 6.218794 | 4.953231 | -1.340126 |
| C | 5.962150 | 5.241881 | -0.319347 |
| H | 3.938487 | 5.820500 | -0.825401 |
| C | 4.679292 | 5.725384 | -0.029385 |
| C | 6.913891 | 5.130692 | 0.695910  |
| C | 4.350104 | 6.090686 | 1.281237  |
| C | 6.584288 | 5.471652 | 2.018061  |
| H | 3.356932 | 6.482218 | 1.507070  |
| C | 5.293718 | 5.955047 | 2.301826  |
| H | 5.037403 | 6.243279 | 3.322919  |
| C | 5.639601 | 6.005545 | 11.213797 |
| C | 9.138120 | 6.339375 | 5.507692  |
| H | 9.017862 | 7.157822 | 4.785016  |
| H | 9.988757 | 5.739673 | 5.154944  |
| H | 9.358524 | 6.743899 | 6.502649  |
| H | 6.724327 | 6.154635 | 11.145566 |
| H | 5.380571 | 5.500510 | 12.152814 |
| H | 5.143798 | 6.986364 | 11.237249 |

**Table S14:** Cartesian coordinates of DFT-optimized HS-[Fe5(py)<sub>2</sub>] (BP86-D3/TZVP)

|    |          |          |           |
|----|----------|----------|-----------|
| Fe | 6.226544 | 4.358832 | 7.486352  |
| O  | 7.878842 | 5.110767 | 6.596775  |
| O  | 6.085896 | 5.086220 | 9.348682  |
| N  | 4.444031 | 3.366584 | 7.876164  |
| O  | 8.570651 | 5.779943 | 2.459667  |
| O  | 2.539695 | 5.772290 | 11.522676 |
| N  | 5.811004 | 3.525311 | 5.626707  |
| C  | 4.118778 | 2.411376 | 6.897351  |
| C  | 5.088527 | 5.229555 | 10.141513 |
| C  | 3.616459 | 3.636432 | 8.863957  |
| H  | 2.618586 | 3.184608 | 8.833996  |
| C  | 4.851577 | 2.504420 | 5.680831  |
| C  | 8.087423 | 5.448113 | 5.374876  |
| C  | 6.200058 | 4.045652 | 4.484611  |
| H  | 5.682527 | 3.728941 | 3.569478  |
| C  | 7.257410 | 4.988853 | 4.306557  |
| C  | 3.854737 | 4.524976 | 9.954466  |
| C  | 3.185018 | 1.376774 | 7.062113  |
| H  | 2.650864 | 1.270259 | 8.007278  |
| C  | 2.733261 | 4.717325 | 10.887112 |
| C  | 2.956062 | 0.461332 | 6.030982  |
| C  | 4.625932 | 1.565896 | 4.661724  |
| H  | 5.216944 | 1.609514 | 3.745759  |
| C  | 7.456812 | 5.485970 | 2.935744  |
| C  | 3.673043 | 0.557707 | 4.830400  |
| N  | 7.312138 | 2.588432 | 8.130706  |
| C  | 6.978914 | 1.963113 | 9.280184  |
| H  | 6.288194 | 2.499822 | 9.931853  |
| C  | 8.161272 | 1.963538 | 7.287184  |
| H  | 8.399855 | 2.500564 | 6.368408  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 7.475685  | 0.708751  | 9.625740  |
| C | 8.701550  | 0.708353  | 7.557477  |
| C | 8.351489  | 0.063041  | 8.747420  |
| H | 7.175520  | 0.247854  | 10.566825 |
| H | 9.381131  | 0.246264  | 6.840925  |
| H | 8.753756  | -0.921869 | 8.986288  |
| N | 5.112864  | 6.222290  | 6.758286  |
| C | 3.856719  | 6.109241  | 6.284738  |
| H | 3.393020  | 5.127951  | 6.388270  |
| C | 5.732523  | 7.412497  | 6.643185  |
| H | 6.746384  | 7.463813  | 7.041710  |
| C | 3.176065  | 7.169536  | 5.687304  |
| C | 5.131550  | 8.521721  | 6.047212  |
| C | 3.827692  | 8.399368  | 5.560149  |
| H | 2.158572  | 7.025734  | 5.324809  |
| H | 5.679066  | 9.461261  | 5.970340  |
| H | 3.328981  | 9.247339  | 5.089242  |
| H | 2.231666  | -0.342403 | 6.174037  |
| H | 3.509172  | -0.170687 | 4.034145  |
| H | 7.234233  | 5.109067  | 0.267552  |
| H | 0.074369  | 4.896970  | 11.229286 |
| H | -1.559922 | 3.057825  | 11.646779 |
| C | -0.500059 | 2.829264  | 11.520711 |
| H | -0.764555 | 0.697717  | 11.793139 |
| C | -0.053691 | 1.503238  | 11.600800 |
| C | 0.410732  | 3.860188  | 11.282812 |
| C | 1.306436  | 1.213505  | 11.438642 |
| C | 1.773502  | 3.575801  | 11.093848 |
| H | 1.660350  | 0.184114  | 11.515520 |
| C | 2.214385  | 2.242608  | 11.177369 |
| H | 3.274594  | 2.015927  | 11.054622 |
| H | 5.236742  | 5.515077  | -1.175837 |
| C | 5.184116  | 5.705408  | -0.102323 |
| H | 3.127132  | 6.378170  | -0.165143 |
| C | 3.996357  | 6.186467  | 0.466497  |
| C | 6.301023  | 5.470901  | 0.702235  |
| C | 3.927704  | 6.426310  | 1.844068  |
| C | 6.231330  | 5.684619  | 2.088993  |
| H | 3.010045  | 6.816406  | 2.287716  |
| C | 5.035915  | 6.165706  | 2.652525  |
| H | 4.986566  | 6.354678  | 3.725362  |
| C | 5.326919  | 6.149999  | 11.311567 |
| C | 9.235068  | 6.401046  | 5.154355  |
| H | 8.987702  | 7.185740  | 4.428267  |
| H | 10.105960 | 5.865096  | 4.748666  |
| H | 9.508593  | 6.845077  | 6.119435  |
| H | 6.409512  | 6.275149  | 11.438108 |
| H | 4.871722  | 5.778400  | 12.237521 |
| H | 4.877310  | 7.134993  | 11.114724 |

**Table S15:** Cartesian coordinates of DFT-optimized LS-[Fe6(py)<sub>2</sub>] (BP86-D3/TZVP)

|    |          |           |           |
|----|----------|-----------|-----------|
| Fe | 5.943145 | 4.164821  | 7.237531  |
| O  | 7.398420 | 5.240233  | 6.550241  |
| O  | 6.262094 | 5.044866  | 8.931857  |
| N  | 4.522359 | 3.085912  | 7.896184  |
| O  | 7.182524 | 4.289597  | 1.874675  |
| O  | 2.505457 | 3.588171  | 11.499896 |
| N  | 5.624587 | 3.267570  | 5.591422  |
| C  | 4.135777 | 2.070454  | 6.997402  |
| C  | 5.486831 | 5.002351  | 9.954398  |
| C  | 3.883794 | 3.308331  | 9.028111  |
| H  | 2.978367 | 2.733592  | 9.250351  |
| C  | 4.745164 | 2.172499  | 5.719642  |
| C  | 7.716382 | 5.363901  | 5.312447  |
| C  | 6.100945 | 3.658530  | 4.425982  |
| H  | 5.750635 | 3.164198  | 3.514120  |
| C  | 7.037995 | 4.707335  | 4.240047  |
| C  | 4.260366 | 4.269792  | 10.000382 |
| C  | 3.249999 | 1.016383  | 7.266958  |
| H  | 2.803235 | 0.911596  | 8.255636  |
| C  | 3.284715 | 4.453707  | 11.089314 |
| C  | 2.961549 | 0.080658  | 6.270727  |
| C  | 4.456372 | 1.219780  | 4.730554  |
| H  | 4.940012 | 1.272674  | 3.755271  |
| C  | 7.282012 | 5.064026  | 2.831083  |
| C  | 3.561641 | 0.183128  | 5.005651  |
| O  | 3.285435 | 5.722464  | 11.572963 |
| C  | 2.561172 | 5.956038  | 12.816856 |
| O  | 7.581014 | 6.379413  | 2.676336  |
| C  | 8.100696 | 6.790736  | 1.377102  |
| H  | 2.851897 | 5.180252  | 13.540200 |
| H  | 1.482701 | 5.861866  | 12.623977 |
| C  | 2.940538 | 7.344068  | 13.291284 |
| H  | 4.024249 | 7.411397  | 13.459282 |
| H  | 2.423894 | 7.563540  | 14.236401 |
| H  | 2.649470 | 8.105866  | 12.554438 |
| H  | 7.291918 | 6.727516  | 0.634626  |
| H  | 8.895617 | 6.090458  | 1.082214  |
| C  | 8.622413 | 8.203731  | 1.539429  |
| H  | 7.816713 | 8.892372  | 1.830103  |
| H  | 9.044397 | 8.551432  | 0.585554  |
| H  | 9.410879 | 8.237966  | 2.304605  |
| N  | 7.242661 | 2.755771  | 7.748235  |
| C  | 7.194544 | 2.176201  | 8.972059  |
| H  | 6.411733 | 2.525496  | 9.642171  |
| C  | 8.194050 | 2.334699  | 6.880759  |
| H  | 8.199642 | 2.809048  | 5.901231  |
| C  | 8.083560 | 1.180243  | 9.364259  |
| C  | 9.115818 | 1.343249  | 7.203933  |
| C  | 9.065347 | 0.748995  | 8.467926  |
| H  | 7.996254 | 0.748125  | 10.360909 |
| H  | 9.857438 | 1.041471  | 6.464248  |
| H  | 9.772233 | -0.033421 | 8.746405  |
| N  | 4.705030 | 5.593589  | 6.763861  |
| C  | 3.506720 | 5.360700  | 6.171211  |
| H  | 3.264814 | 4.320854  | 5.961316  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 5.040467  | 6.880965  | 7.038099  |
| H | 6.010491  | 7.016902  | 7.510640  |
| C | 2.624244  | 6.384036  | 5.842780  |
| C | 4.205685  | 7.950816  | 6.737575  |
| C | 2.970194  | 7.708053  | 6.128400  |
| H | 1.675423  | 6.135202  | 5.367640  |
| H | 4.527179  | 8.963356  | 6.982443  |
| H | 2.296163  | 8.528853  | 5.881932  |
| H | 2.280133  | -0.743617 | 6.487216  |
| H | 3.346456  | -0.560788 | 4.236895  |
| H | 9.873676  | 4.741426  | 3.750368  |
| H | 5.621908  | 4.070524  | 12.523933 |
| H | 6.590633  | 5.232877  | 14.493748 |
| C | 6.581019  | 5.728287  | 13.521191 |
| H | 7.530476  | 7.530897  | 14.251116 |
| C | 7.113809  | 7.016284  | 13.383688 |
| C | 6.034605  | 5.075044  | 12.415631 |
| C | 7.117130  | 7.638130  | 12.128943 |
| C | 6.021888  | 5.700293  | 11.157509 |
| H | 7.532697  | 8.640731  | 12.016606 |
| C | 6.586983  | 6.977274  | 11.018720 |
| H | 6.588518  | 7.455555  | 10.038244 |
| H | 11.938701 | 6.085233  | 3.434315  |
| C | 11.137999 | 6.461954  | 4.073073  |
| H | 12.176336 | 8.296274  | 4.566192  |
| C | 11.273888 | 7.700277  | 4.713354  |
| C | 9.977457  | 5.706611  | 4.249179  |
| C | 10.251263 | 8.168244  | 5.548050  |
| C | 8.942462  | 6.177862  | 5.074516  |
| H | 10.352957 | 9.131973  | 6.049754  |
| C | 9.097909  | 7.403387  | 5.739923  |
| H | 8.298969  | 7.760917  | 6.390912  |

**Table S16:** Cartesian coordinates of DFT-optimized HS-[Fe6(py)<sub>2</sub>] (BP86-D3/TZVP)

|    |          |           |           |
|----|----------|-----------|-----------|
| Fe | 6.470623 | 3.973660  | 7.475215  |
| O  | 7.938256 | 4.873862  | 6.430483  |
| O  | 6.513140 | 4.632254  | 9.378455  |
| N  | 4.759240 | 2.917561  | 8.031770  |
| O  | 6.618410 | 4.635842  | 1.857059  |
| O  | 2.103695 | 3.978455  | 11.070446 |
| N  | 5.900882 | 3.098395  | 5.671638  |
| C  | 4.412377 | 1.913129  | 7.116504  |
| C  | 5.527759 | 4.820180  | 10.187345 |
| C  | 3.935937 | 3.297727  | 8.985489  |
| H  | 2.916069 | 2.890025  | 9.006869  |
| C  | 5.030882 | 2.010894  | 5.838455  |
| C  | 7.952586 | 5.204207  | 5.185401  |
| C  | 6.122460 | 3.631931  | 4.489361  |
| H  | 5.539045 | 3.283572  | 3.626311  |
| C  | 7.029322 | 4.695612  | 4.228843  |
| C  | 4.232453 | 4.267308  | 9.982226  |
| C  | 3.558079 | 0.835462  | 7.392819  |
| H  | 3.116143 | 0.737877  | 8.385340  |
| C  | 3.068406 | 4.693787  | 10.783903 |
| C  | 3.300995 | -0.126850 | 6.410986  |
| C  | 4.777952 | 1.028674  | 4.869100  |

|   |           |           |           |   |           |          |          |
|---|-----------|-----------|-----------|---|-----------|----------|----------|
| H | 5.280603  | 1.081259  | 3.902411  | C | 9.866893  | 5.811511 | 3.656175 |
| C | 6.923986  | 5.267921  | 2.872353  | C | 10.459593 | 8.039887 | 5.238362 |
| C | 3.908322  | -0.029588 | 5.151435  | C | 9.077722  | 6.094852 | 4.784108 |
| O | 3.136961  | 6.001274  | 11.131762 | H | 10.685918 | 8.912628 | 5.853700 |
| C | 2.176924  | 6.475692  | 12.119701 | C | 9.397362  | 7.202155 | 5.584910 |
| O | 7.143355  | 6.605255  | 2.862984  | H | 8.792784  | 7.412185 | 6.468072 |
| C | 7.321514  | 7.240153  | 1.563206  |   |           |          |          |
| H | 2.166823  | 5.771404  | 12.964702 |   |           |          |          |
| H | 1.175114  | 6.484366  | 11.666852 |   |           |          |          |
| C | 2.629195  | 7.858999  | 12.540774 |   |           |          |          |
| H | 3.640892  | 7.819331  | 12.967519 |   |           |          |          |
| H | 1.941638  | 8.255141  | 13.302055 |   |           |          |          |
| H | 2.635662  | 8.547872  | 11.684614 |   |           |          |          |
| H | 6.356940  | 7.247681  | 1.035407  |   |           |          |          |
| H | 8.031499  | 6.640031  | 0.975376  |   |           |          |          |
| C | 7.842600  | 8.638209  | 1.827669  |   |           |          |          |
| H | 7.123637  | 9.220343  | 2.421006  |   |           |          |          |
| H | 8.005083  | 9.156538  | 0.871951  |   |           |          |          |
| H | 8.796079  | 8.596504  | 2.372006  |   |           |          |          |
| N | 7.733457  | 2.264733  | 7.946729  |   |           |          |          |
| C | 7.544340  | 1.574151  | 9.091632  |   |           |          |          |
| H | 6.868744  | 2.029969  | 9.816276  |   |           |          |          |
| C | 8.557013  | 1.740911  | 7.013677  |   |           |          |          |
| H | 8.678633  | 2.328190  | 6.102580  |   |           |          |          |
| C | 8.161833  | 0.351219  | 9.342956  |   |           |          |          |
| C | 9.212642  | 0.524159  | 7.186980  |   |           |          |          |
| C | 9.009865  | -0.190347 | 8.371874  |   |           |          |          |
| H | 7.973185  | -0.167202 | 10.283289 |   |           |          |          |
| H | 9.865479  | 0.144623  | 6.400561  |   |           |          |          |
| H | 9.503241  | -1.148952 | 8.535361  |   |           |          |          |
| N | 5.228364  | 5.791401  | 7.024876  |   |           |          |          |
| C | 4.016233  | 5.698452  | 6.448767  |   |           |          |          |
| H | 3.687611  | 4.692527  | 6.183639  |   |           |          |          |
| C | 5.683158  | 7.009763  | 7.371704  |   |           |          |          |
| H | 6.670312  | 7.032925  | 7.834327  |   |           |          |          |
| C | 3.215473  | 6.811896  | 6.199134  |   |           |          |          |
| C | 4.949750  | 8.175793  | 7.159749  |   |           |          |          |
| C | 3.690375  | 8.074824  | 6.562739  |   |           |          |          |
| H | 2.239711  | 6.686372  | 5.730187  |   |           |          |          |
| H | 5.359591  | 9.140466  | 7.458677  |   |           |          |          |
| H | 3.089064  | 8.966991  | 6.382748  |   |           |          |          |
| H | 2.641904  | -0.966736 | 6.637493  |   |           |          |          |
| H | 3.722796  | -0.793172 | 4.393923  |   |           |          |          |
| H | 9.641864  | 4.934763  | 3.045704  |   |           |          |          |
| H | 4.889995  | 4.222413  | 12.785625 |   |           |          |          |
| H | 5.528773  | 5.499870  | 14.817567 |   |           |          |          |
| C | 5.833545  | 5.858119  | 13.832887 |   |           |          |          |
| H | 6.856705  | 7.601557  | 14.606722 |   |           |          |          |
| C | 6.584139  | 7.034923  | 13.714918 |   |           |          |          |
| C | 5.472012  | 5.141194  | 12.691585 |   |           |          |          |
| C | 6.991768  | 7.476481  | 12.449798 |   |           |          |          |
| C | 5.864168  | 5.587958  | 11.418362 |   |           |          |          |
| H | 7.579031  | 8.391424  | 12.352777 |   |           |          |          |
| C | 6.647132  | 6.748037  | 11.309595 |   |           |          |          |
| H | 6.964249  | 7.085049  | 10.322305 |   |           |          |          |
| H | 11.549336 | 6.407551  | 2.444874  |   |           |          |          |
| C | 10.939749 | 6.638375  | 3.320357  |   |           |          |          |
| H | 12.065377 | 8.414414  | 3.836217  |   |           |          |          |
| C | 11.232507 | 7.761818  | 4.104061  |   |           |          |          |

**Table S17:** Cartesian coordinates of DFT-optimized LS-[Fe7(py)<sub>2</sub>] (BP86-D3/TZVP)

|    |          |           |           |
|----|----------|-----------|-----------|
| Fe | 5.961535 | 4.122646  | 7.261448  |
| O  | 7.475278 | 5.128521  | 6.586626  |
| O  | 6.329754 | 4.916685  | 8.989930  |
| N  | 4.485470 | 3.122269  | 7.895913  |
| O  | 7.103578 | 4.190485  | 1.918112  |
| O  | 2.583644 | 3.305028  | 11.475075 |
| N  | 5.581659 | 3.330317  | 5.584848  |
| C  | 4.006213 | 2.190301  | 6.948289  |
| C  | 5.589758 | 4.897778  | 10.036594 |
| C  | 3.918057 | 3.284252  | 9.072872  |
| H  | 3.016695 | 2.710602  | 9.308213  |
| C  | 4.612143 | 2.306288  | 5.669584  |
| C  | 7.808177 | 5.315724  | 5.362848  |
| C  | 6.110548 | 3.706163  | 4.439253  |
| H  | 5.754690 | 3.241272  | 3.515198  |
| C  | 7.130851 | 4.684871  | 4.266871  |
| C  | 4.365448 | 4.152747  | 10.109342 |
| C  | 3.034220 | 1.203262  | 7.171907  |
| H  | 2.581724 | 1.087295  | 8.156692  |
| C  | 3.467981 | 4.146559  | 11.277919 |
| C  | 2.658204 | 0.348486  | 6.133282  |
| C  | 4.232247 | 1.435261  | 4.636630  |
| H  | 4.706796 | 1.499503  | 3.657533  |
| C  | 7.448310 | 4.927660  | 2.849128  |
| C  | 3.254923 | 0.465016  | 4.868023  |
| C  | 9.011734 | 6.211369  | 5.191615  |
| C  | 6.158049 | 5.680844  | 11.195990 |
| O  | 3.655672 | 5.186852  | 12.136900 |
| C  | 2.816588 | 5.185434  | 13.318030 |
| O  | 8.134660 | 6.081649  | 2.618744  |
| C  | 8.506901 | 6.327244  | 1.240438  |
| H  | 7.193058 | 5.945386  | 10.949616 |
| H  | 6.126527 | 5.113960  | 12.134532 |
| H  | 5.581279 | 6.601387  | 11.360631 |
| H  | 9.734862 | 5.804572  | 4.473963  |
| H  | 9.483147 | 6.335353  | 6.173779  |
| H  | 8.707446 | 7.197347  | 4.813416  |
| N  | 7.164463 | 2.610138  | 7.699511  |
| C  | 7.085755 | 1.982911  | 8.898934  |
| H  | 6.346515 | 2.367493  | 9.598613  |
| C  | 8.070108 | 2.152248  | 6.800838  |
| H  | 8.107557 | 2.670658  | 5.844639  |
| C  | 7.893185 | 0.899991  | 9.232480  |
| C  | 8.908855 | 1.073802  | 7.065921  |
| C  | 8.823258 | 0.427561  | 8.302408  |
| H  | 7.782665 | 0.434194  | 10.211659 |
| H  | 9.614685 | 0.747202  | 6.302057  |
| H  | 9.464324 | -0.423571 | 8.534323  |
| N  | 4.817873 | 5.649234  | 6.852112  |
| C  | 3.603790 | 5.515281  | 6.259073  |
| H  | 3.290113 | 4.500642  | 6.022245  |
| C  | 5.239470 | 6.903295  | 7.161631  |
| H  | 6.215943 | 6.964480  | 7.635889  |
| C  | 2.791631 | 6.603856  | 5.961008  |
| C  | 4.477518 | 8.034741  | 6.891315  |

|   |          |           |           |
|---|----------|-----------|-----------|
| C | 3.227886 | 7.893591  | 6.279208  |
| H | 1.826912 | 6.432322  | 5.483701  |
| H | 4.867558 | 9.015982  | 7.162385  |
| H | 2.611578 | 8.764879  | 6.055952  |
| H | 1.907367 | -0.422142 | 6.315291  |
| H | 2.968537 | -0.213875 | 4.063328  |
| H | 3.126421 | 6.067180  | 13.887864 |
| H | 2.976850 | 4.271833  | 13.905564 |
| H | 1.757402 | 5.261593  | 13.039093 |
| H | 9.056065 | 7.273742  | 1.258431  |
| H | 7.613662 | 6.413251  | 0.608500  |
| H | 9.146907 | 5.518628  | 0.863348  |

**Table S18:** Cartesian coordinates of DFT-optimized HS-[Fe7(py)<sub>2</sub>] (BP86-D3/TZVP)

|    |          |          |           |
|----|----------|----------|-----------|
| Fe | 6.476489 | 3.870283 | 7.484172  |
| O  | 7.976364 | 4.703864 | 6.430135  |
| O  | 6.556047 | 4.453370 | 9.407453  |
| N  | 4.713853 | 2.911001 | 8.021886  |
| O  | 6.488288 | 4.587684 | 1.910022  |
| O  | 2.169291 | 3.716123 | 11.100262 |
| N  | 5.844288 | 3.116427 | 5.652710  |
| C  | 4.292402 | 1.971769 | 7.067341  |
| C  | 5.615169 | 4.696219 | 10.249725 |
| C  | 3.953537 | 3.249880 | 9.038970  |
| H  | 2.931492 | 2.854331 | 9.092849  |
| C  | 4.902931 | 2.083794 | 5.786015  |
| C  | 7.997761 | 5.148604 | 5.223682  |
| C  | 6.111260 | 3.660032 | 4.486303  |
| H  | 5.523712 | 3.355526 | 3.611171  |
| C  | 7.079961 | 4.679129 | 4.234591  |
| C  | 4.306416 | 4.145242 | 10.094145 |
| C  | 3.377975 | 0.935341 | 7.309129  |
| H  | 2.941594 | 0.820471 | 8.302150  |
| C  | 3.184092 | 4.415737 | 11.011100 |
| C  | 3.049389 | 0.033576 | 6.292348  |
| C  | 4.578838 | 1.158939 | 4.781419  |
| H  | 5.074499 | 1.219000 | 3.811618  |
| C  | 7.033057 | 5.178375 | 2.848692  |
| C  | 3.647588 | 0.146175 | 5.029633  |
| C  | 9.089844 | 6.154737 | 4.947910  |
| C  | 6.031785 | 5.557213 | 11.418897 |
| O  | 3.326017 | 5.551270 | 11.749085 |
| C  | 2.268426 | 5.814971 | 12.704686 |
| O  | 7.613461 | 6.397484 | 2.673890  |
| C  | 7.626392 | 6.897789 | 1.313229  |
| H  | 7.127970 | 5.596786 | 11.436880 |
| H  | 5.650897 | 5.182623 | 12.376275 |
| H  | 5.641183 | 6.578419 | 11.299613 |
| H  | 9.605645 | 5.971040 | 3.998198  |
| H  | 9.803854 | 6.116265 | 5.780291  |
| H  | 8.666691 | 7.168327 | 4.887930  |
| N  | 7.619972 | 2.067047 | 7.878022  |
| C  | 7.385395 | 1.340090 | 8.992122  |
| H  | 6.751860 | 1.812931 | 9.743668  |
| C  | 8.393783 | 1.523915 | 6.913207  |
| H  | 8.553111 | 2.142292 | 6.028878  |

|   |          |           |           |
|---|----------|-----------|-----------|
| C | 7.907603 | 0.062792  | 9.180862  |
| C | 8.954256 | 0.253616  | 7.024545  |
| C | 8.705048 | -0.497415 | 8.177779  |
| H | 7.685299 | -0.482361 | 10.098586 |
| H | 9.570587 | -0.138389 | 6.215003  |
| H | 9.124553 | -1.497320 | 8.292873  |
| N | 5.340780 | 5.784742  | 7.093004  |
| C | 4.133870 | 5.768767  | 6.498667  |
| H | 3.738496 | 4.784300  | 6.245275  |
| C | 5.876053 | 6.973876  | 7.428410  |
| H | 6.855174 | 6.937791  | 7.908182  |
| C | 3.418541 | 6.931572  | 6.215025  |
| C | 5.230721 | 8.185567  | 7.182022  |
| C | 3.978021 | 8.164264  | 6.562419  |
| H | 2.443842 | 6.866995  | 5.731834  |
| H | 5.703974 | 9.124019  | 7.470830  |
| H | 3.446757 | 9.093893  | 6.353927  |
| H | 2.341620 | -0.772620 | 6.493508  |
| H | 3.406787 | -0.571423 | 4.243306  |
| H | 2.566704 | 6.738108  | 13.211156 |
| H | 2.183786 | 4.990569  | 13.424854 |
| H | 1.308912 | 5.952241  | 12.190245 |
| H | 8.149077 | 7.857429  | 1.368364  |
| H | 6.602126 | 7.039065  | 0.945319  |
| H | 8.161899 | 6.204620  | 0.651613  |

**Table S19:** Cartesian coordinates of DFT-optimized LS-[Fe8(py)<sub>2</sub>] (BP86-D3/TZVP)

|    |          |          |           |
|----|----------|----------|-----------|
| Fe | 6.059722 | 3.957514 | 7.231290  |
| O  | 7.582400 | 4.944828 | 6.559456  |
| O  | 6.434440 | 4.759700 | 8.949405  |
| N  | 4.567732 | 2.971503 | 7.864000  |
| O  | 7.378073 | 3.983800 | 1.897485  |
| O  | 2.693288 | 3.315377 | 11.530153 |
| N  | 5.677334 | 3.141860 | 5.562180  |
| C  | 4.100428 | 2.017494 | 6.932579  |
| C  | 5.648897 | 4.748868 | 9.953149  |
| C  | 3.967468 | 3.176018 | 9.017460  |
| H  | 3.047238 | 2.629355 | 9.243792  |
| C  | 4.713955 | 2.112411 | 5.658232  |
| C  | 7.871628 | 5.100728 | 5.327511  |
| C  | 6.195750 | 3.509692 | 4.410016  |
| H  | 5.837993 | 3.038314 | 3.490088  |
| C  | 7.201567 | 4.502305 | 4.233287  |
| C  | 4.404390 | 4.077624 | 10.028783 |
| C  | 3.132331 | 1.031151 | 7.171474  |
| H  | 2.675427 | 0.930410 | 8.155643  |
| C  | 3.445452 | 4.213488 | 11.149846 |
| C  | 2.769769 | 0.155646 | 6.146201  |
| C  | 4.347665 | 1.222029 | 4.637882  |
| H  | 4.828284 | 1.269754 | 3.661121  |
| C  | 7.482804 | 4.803418 | 2.810561  |
| C  | 3.374353 | 0.251843 | 4.882822  |
| C  | 9.153593 | 5.952444 | 5.148090  |
| F  | 9.957698 | 5.505677 | 4.141430  |
| F  | 8.877635 | 7.266066 | 4.914047  |
| F  | 9.905272 | 5.914734 | 6.279378  |
| C  | 6.275713 | 5.473539 | 11.170016 |
| F  | 5.985996 | 4.877408 | 12.361199 |
| F  | 7.631376 | 5.474807 | 11.066327 |
| F  | 5.894458 | 6.779708 | 11.248739 |
| O  | 3.427566 | 5.461481 | 11.668010 |
| C  | 2.580195 | 5.665601 | 12.843743 |
| O  | 7.800963 | 6.100506 | 2.606099  |
| C  | 8.210259 | 6.464750 | 1.248657  |
| H  | 2.890709 | 4.953710 | 13.621786 |
| H  | 1.541303 | 5.441779 | 12.563814 |
| C  | 2.755217 | 7.104263 | 13.281036 |
| H  | 3.799139 | 7.310931 | 13.552838 |
| H  | 2.124212 | 7.293246 | 14.161183 |
| H  | 2.452617 | 7.798810 | 12.484835 |
| H  | 7.370123 | 6.265956 | 0.568834  |
| H  | 9.051994 | 5.820256 | 0.957042  |
| C  | 8.591684 | 7.929133 | 1.270911  |
| H  | 7.742196 | 8.554323 | 1.579506  |
| H  | 8.896225 | 8.238507 | 0.261004  |
| H  | 9.431042 | 8.108737 | 1.956231  |
| N  | 7.254894 | 2.435160 | 7.695159  |
| C  | 7.162711 | 1.823156 | 8.899616  |
| H  | 6.408598 | 2.204993 | 9.584453  |
| C  | 8.174452 | 1.975262 | 6.814439  |
| H  | 8.220712 | 2.478195 | 5.850515  |
| C  | 7.975389 | 0.752739 | 9.259182  |

|   |          |           |           |
|---|----------|-----------|-----------|
| C | 9.020329 | 0.909079  | 7.104833  |
| C | 8.923137 | 0.279505  | 8.348424  |
| H | 7.854774 | 0.298003  | 10.242114 |
| H | 9.739720 | 0.579785  | 6.355260  |
| H | 9.569739 | -0.561496 | 8.600877  |
| N | 4.926552 | 5.497227  | 6.803378  |
| C | 3.715976 | 5.366775  | 6.205465  |
| H | 3.397349 | 4.353576  | 5.968895  |
| C | 5.356911 | 6.747468  | 7.112202  |
| H | 6.332471 | 6.804757  | 7.589790  |
| C | 2.911716 | 6.459696  | 5.902181  |
| C | 4.602684 | 7.882824  | 6.837087  |
| C | 3.355300 | 7.746187  | 6.221113  |
| H | 1.948183 | 6.293611  | 5.421154  |
| H | 4.997213 | 8.862089  | 7.107773  |
| H | 2.744730 | 8.620588  | 5.994584  |
| H | 2.022846 | -0.616303 | 6.337190  |
| H | 3.097263 | -0.444277 | 4.089925  |

**Table S20:** Cartesian coordinates of DFT-optimized HS-[Fe8(py)<sub>2</sub>] (BP86-D3/TZVP)

|    |           |           |           |
|----|-----------|-----------|-----------|
| Fe | 6.534431  | 3.698095  | 7.458458  |
| O  | 8.051704  | 4.532496  | 6.428556  |
| O  | 6.616967  | 4.275547  | 9.393989  |
| N  | 4.756936  | 2.755109  | 7.982273  |
| O  | 6.805503  | 4.380162  | 1.849553  |
| O  | 2.194391  | 3.814393  | 11.087149 |
| N  | 5.920077  | 2.923514  | 5.632070  |
| C  | 4.359830  | 1.789222  | 7.042625  |
| C  | 5.628134  | 4.527793  | 10.166011 |
| C  | 3.958186  | 3.148973  | 8.947390  |
| H  | 2.922485  | 2.787047  | 8.972736  |
| C  | 4.991222  | 1.878012  | 5.772160  |
| C  | 8.032478  | 4.940775  | 5.215001  |
| C  | 6.187504  | 3.454254  | 4.460725  |
| H  | 5.617931  | 3.130985  | 3.580738  |
| C  | 7.136954  | 4.495325  | 4.224161  |
| C  | 4.308104  | 4.077979  | 9.973997  |
| C  | 3.447436  | 0.755070  | 7.295321  |
| H  | 2.994645  | 0.662162  | 8.283048  |
| C  | 3.153171  | 4.526210  | 10.790944 |
| C  | 3.148680  | -0.173015 | 6.293811  |
| C  | 4.695242  | 0.930118  | 4.781797  |
| H  | 5.206602  | 0.973168  | 3.819607  |
| C  | 7.063143  | 5.050856  | 2.848609  |
| C  | 3.769887  | -0.084894 | 5.040204  |
| C  | 9.185239  | 5.930107  | 4.911100  |
| F  | 9.738464  | 5.757365  | 3.677657  |
| F  | 8.796466  | 7.231407  | 5.019244  |
| F  | 10.194458 | 5.755544  | 5.808157  |
| C  | 6.060786  | 5.306443  | 11.433911 |
| F  | 5.353729  | 4.971841  | 12.549039 |
| F  | 7.365220  | 5.035538  | 11.717445 |
| F  | 5.974433  | 6.656109  | 11.269945 |
| O  | 3.233774  | 5.835290  | 11.107700 |
| C  | 2.192936  | 6.360624  | 11.991112 |
| O  | 7.231333  | 6.387855  | 2.822358  |



|   |          |           |           |
|---|----------|-----------|-----------|
| C | 7.245395 | 7.017783  | 1.501844  |
| H | 2.186871 | 5.762371  | 12.913510 |
| H | 1.221606 | 6.238322  | 11.491851 |
| C | 2.519868 | 7.814682  | 12.254679 |
| H | 3.496790 | 7.915927  | 12.746848 |
| H | 1.753000 | 8.244514  | 12.915168 |
| H | 2.533980 | 8.390713  | 11.319571 |
| H | 6.283748 | 6.811731  | 1.010834  |
| H | 8.044981 | 6.554549  | 0.905492  |
| C | 7.472157 | 8.499050  | 1.711935  |
| H | 6.672174 | 8.936566  | 2.324892  |
| H | 7.477861 | 9.005841  | 0.736739  |
| H | 8.436381 | 8.685341  | 2.204246  |
| N | 7.685389 | 1.895880  | 7.873698  |
| C | 7.434260 | 1.163210  | 8.979278  |
| H | 6.755173 | 1.610351  | 9.705972  |
| C | 8.517066 | 1.383929  | 6.941776  |
| H | 8.691673 | 2.006150  | 6.063267  |
| C | 7.998250 | -0.092398 | 9.192335  |
| C | 9.121830 | 0.136616  | 7.078833  |
| C | 8.856012 | -0.621011 | 8.223302  |
| H | 7.761370 | -0.644341 | 10.102014 |
| H | 9.785207 | -0.231457 | 6.295956  |
| H | 9.309784 | -1.603312 | 8.357924  |
| N | 5.432684 | 5.607511  | 7.071966  |
| C | 4.241008 | 5.615481  | 6.445373  |
| H | 3.840831 | 4.641431  | 6.161687  |
| C | 5.971042 | 6.784923  | 7.445055  |
| H | 6.937019 | 6.731232  | 7.948752  |
| C | 3.546301 | 6.790822  | 6.166987  |
| C | 5.343583 | 8.006233  | 7.206958  |
| C | 4.108313 | 8.010050  | 6.554569  |
| H | 2.584524 | 6.745661  | 5.656763  |
| H | 5.818424 | 8.933297  | 7.527258  |
| H | 3.591680 | 8.948838  | 6.351146  |
| H | 2.444466 | -0.980502 | 6.500030  |
| H | 3.550040 | -0.823367 | 4.267671  |

**Table S21:** Cartesian coordinates of DFT-optimized LS-[Fe<sub>en</sub>2(py)<sub>2</sub>] (BP86-D3/TZVP)

|    |           |           |           |
|----|-----------|-----------|-----------|
| Fe | 6.369027  | 3.972292  | 7.621609  |
| O  | 7.925829  | 4.957205  | 6.989975  |
| O  | 6.830155  | 4.530759  | 9.431814  |
| N  | 4.854215  | 3.041554  | 8.198256  |
| O  | 8.439903  | 6.381897  | 3.080840  |
| O  | 2.693848  | 3.494115  | 11.543027 |
| N  | 5.893169  | 3.424725  | 5.900585  |
| N  | 5.335856  | 5.619823  | 7.437489  |
| C  | 4.309147  | 2.068003  | 7.231131  |
| C  | 6.032051  | 4.583630  | 10.438645 |
| C  | 4.254176  | 3.207825  | 9.342068  |
| H  | 3.313057  | 2.676015  | 9.526846  |
| C  | 4.932504  | 2.303495  | 5.840358  |
| C  | 8.154756  | 5.342547  | 5.787333  |
| C  | 6.338607  | 3.933883  | 4.784187  |
| H  | 5.900505  | 3.545101  | 3.859455  |
| C  | 7.367358  | 4.934467  | 4.658134  |
| C  | 4.707325  | 4.049037  | 10.423072 |
| C  | 3.716678  | 4.220347  | 11.489542 |
| C  | 7.605734  | 5.480714  | 3.324304  |
| C  | 9.352124  | 6.250145  | 5.659679  |
| H  | 10.037720 | 5.916714  | 4.870144  |
| H  | 9.036932  | 7.264851  | 5.378025  |
| H  | 9.863441  | 6.278542  | 6.630540  |
| C  | 6.676931  | 5.190943  | 11.665346 |
| H  | 6.353261  | 4.724399  | 12.601380 |
| H  | 7.763657  | 5.079686  | 11.560151 |
| H  | 6.458244  | 6.268107  | 11.728079 |
| C  | 3.822650  | 5.332190  | 12.520856 |
| H  | 4.323403  | 6.231939  | 12.145445 |
| H  | 2.804307  | 5.588036  | 12.838146 |
| H  | 4.367885  | 4.984128  | 13.412000 |
| C  | 6.784232  | 4.949797  | 2.148968  |
| H  | 6.930630  | 3.869166  | 1.998686  |
| H  | 5.706542  | 5.119062  | 2.295185  |
| H  | 7.105858  | 5.479062  | 1.244978  |
| C  | 3.899671  | 8.023980  | 7.219246  |
| C  | 5.176498  | 7.998511  | 7.789769  |
| H  | 5.647512  | 8.907491  | 8.164320  |
| H  | 6.854382  | 6.723075  | 8.317314  |
| C  | 5.860034  | 6.791262  | 7.882535  |
| C  | 4.098677  | 5.649004  | 6.882017  |
| C  | 3.359084  | 6.820218  | 6.757872  |
| H  | 2.369499  | 6.779486  | 6.303146  |
| H  | 3.706037  | 4.697810  | 6.532346  |
| N  | 7.485723  | 2.356868  | 7.848289  |
| C  | 8.338639  | 1.955093  | 6.873204  |
| C  | 7.417721  | 1.614361  | 8.981201  |
| H  | 6.721326  | 1.963268  | 9.740908  |
| C  | 8.183947  | 0.468497  | 9.172273  |
| H  | 8.084887  | -0.090578 | 10.102819 |
| H  | 8.365325  | 2.570150  | 5.975862  |
| C  | 9.133967  | 0.819683  | 6.996205  |
| H  | 9.797876  | 0.542558  | 6.177101  |
| C  | 9.059698  | 0.054353  | 8.164035  |

|   |          |           |          |
|---|----------|-----------|----------|
| H | 9.668331 | -0.842190 | 8.285023 |
| H | 3.342314 | 8.957538  | 7.135015 |
| H | 5.468858 | 1.398511  | 5.517323 |
| H | 4.158180 | 2.513726  | 5.087240 |
| H | 4.555146 | 1.053617  | 7.579778 |
| H | 3.211947 | 2.148326  | 7.195989 |

**Table S22:** Cartesian coordinates of DFT-optimized HS-[Fe<sub>en</sub>2(py)<sub>2</sub>] (BP86-D3/TZVP)

|    |           |          |           |
|----|-----------|----------|-----------|
| Fe | 6.402971  | 4.453770 | 7.667537  |
| O  | 7.936702  | 5.203901 | 6.581142  |
| O  | 6.668575  | 4.879326 | 9.629375  |
| N  | 4.598503  | 3.624299 | 8.280875  |
| O  | 8.680022  | 5.485503 | 2.470440  |
| O  | 3.152535  | 2.650919 | 11.879735 |
| N  | 5.757203  | 3.675600 | 5.851052  |
| N  | 5.316854  | 6.366955 | 7.379912  |
| C  | 3.746911  | 3.262935 | 7.147475  |
| C  | 6.072774  | 4.533207 | 10.715937 |
| C  | 4.144679  | 3.484376 | 9.491687  |
| H  | 3.154710  | 3.028455 | 9.637696  |
| C  | 4.642082  | 2.745094 | 6.019708  |
| C  | 8.205627  | 5.302522 | 5.330012  |
| C  | 6.257396  | 3.862686 | 4.662831  |
| H  | 5.765331  | 3.346390 | 3.828355  |
| C  | 7.399271  | 4.675316 | 4.322000  |
| C  | 4.803558  | 3.881212 | 10.714228 |
| C  | 4.038251  | 3.532528 | 11.923025 |
| C  | 7.713016  | 4.820462 | 2.896039  |
| C  | 9.434914  | 6.116807 | 5.014289  |
| H  | 10.162876 | 5.535173 | 4.432806  |
| H  | 9.181910  | 6.986633 | 4.392375  |
| H  | 9.878305  | 6.447325 | 5.961658  |
| C  | 6.869672  | 4.824143 | 11.968609 |
| H  | 6.754627  | 4.057670 | 12.742872 |
| H  | 7.926643  | 4.895330 | 11.683755 |
| H  | 6.575775  | 5.792539 | 12.402654 |
| C  | 4.220105  | 4.270795 | 13.238355 |
| H  | 4.567667  | 5.302964 | 13.120249 |
| H  | 3.251883  | 4.264831 | 13.755649 |
| H  | 4.938301  | 3.736766 | 13.879865 |
| C  | 6.815259  | 4.142921 | 1.862474  |
| H  | 6.806839  | 3.048786 | 1.982421  |
| H  | 5.774041  | 4.490574 | 1.933718  |
| H  | 7.203844  | 4.386717 | 0.866976  |
| C  | 3.692846  | 8.612830 | 6.952105  |
| C  | 3.753313  | 8.003211 | 8.209209  |
| H  | 3.175177  | 8.382157 | 9.052193  |
| H  | 4.642146  | 6.381131 | 9.341681  |
| C  | 4.571654  | 6.887801 | 8.378999  |
| C  | 5.250942  | 6.957731 | 6.167078  |
| C  | 4.459118  | 8.076542 | 5.913197  |
| H  | 4.445512  | 8.513629 | 4.914453  |
| H  | 5.854998  | 6.508250 | 5.377933  |
| N  | 7.518081  | 2.555271 | 7.974841  |
| C  | 8.350644  | 2.085633 | 7.020291  |
| C  | 7.247325  | 1.752546 | 9.027071  |

|   |          |           |           |
|---|----------|-----------|-----------|
| H | 6.564105 | 2.152794  | 9.777249  |
| C | 7.793061 | 0.477532  | 9.166166  |
| H | 7.537505 | -0.127502 | 10.036509 |
| H | 8.542609 | 2.754560  | 6.180948  |
| C | 8.938250 | 0.823427  | 7.082247  |
| H | 9.603133 | 0.497087  | 6.281975  |
| C | 8.654579 | -0.001877 | 8.174947  |
| H | 9.095262 | -0.996372 | 8.251974  |
| H | 3.063232 | 9.487875  | 6.786245  |
| H | 5.049782 | 1.761583  | 6.309221  |
| H | 4.067471 | 2.617415  | 5.086800  |
| H | 2.987155 | 2.513368  | 7.425613  |
| H | 3.223590 | 4.171061  | 6.801275  |

**Table S23:** Cartesian coordinates of DFT-optimized LS-[Feee(py)<sub>2</sub>] (BP86-D3/TZVP)

|    |           |           |           |
|----|-----------|-----------|-----------|
| Fe | 6.232907  | 4.194131  | 7.591461  |
| N  | 7.763184  | 5.116989  | 6.863315  |
| N  | 6.841445  | 4.693828  | 9.355209  |
| N  | 4.664697  | 3.347836  | 8.261258  |
| O  | 8.382099  | 5.878349  | 2.694860  |
| O  | 3.218521  | 3.035081  | 12.021740 |
| N  | 5.703591  | 3.537135  | 5.895646  |
| N  | 5.190509  | 5.872683  | 7.387862  |
| C  | 3.760150  | 2.919712  | 7.182458  |
| C  | 6.310192  | 4.401464  | 10.530330 |
| C  | 4.264277  | 3.312995  | 9.503659  |
| H  | 3.282164  | 2.879569  | 9.730073  |
| C  | 4.634442  | 2.531829  | 5.993631  |
| C  | 8.139090  | 5.268661  | 5.604072  |
| C  | 6.285638  | 3.761674  | 4.747387  |
| H  | 5.857799  | 3.254945  | 3.877184  |
| C  | 7.400521  | 4.638323  | 4.511406  |
| C  | 4.974582  | 3.838780  | 10.634523 |
| C  | 4.204629  | 3.807180  | 11.869729 |
| C  | 7.675532  | 4.921818  | 3.109131  |
| C  | 9.403274  | 6.050471  | 5.318696  |
| H  | 9.684954  | 5.976223  | 4.268355  |
| H  | 9.266949  | 7.118966  | 5.552133  |
| H  | 10.223018 | 5.681928  | 5.952774  |
| C  | 7.181477  | 4.519598  | 11.765749 |
| H  | 6.750850  | 3.992254  | 12.618930 |
| H  | 8.165091  | 4.071580  | 11.563182 |
| H  | 7.357239  | 5.566375  | 12.057172 |
| C  | 4.462403  | 4.807223  | 12.991302 |
| H  | 5.085713  | 5.659230  | 12.697765 |
| H  | 3.482180  | 5.179414  | 13.320480 |
| H  | 4.925614  | 4.312822  | 13.859634 |
| C  | 7.048616  | 4.034592  | 2.027696  |
| H  | 7.140455  | 2.959484  | 2.238823  |
| H  | 5.978338  | 4.260507  | 1.896487  |
| H  | 7.558401  | 4.259457  | 1.083325  |
| C  | 3.752832  | 8.277640  | 7.122519  |
| C  | 3.789335  | 7.591540  | 8.339749  |
| H  | 3.266706  | 7.969268  | 9.218892  |
| H  | 4.562578  | 5.851652  | 9.370485  |
| C  | 4.511846  | 6.405360  | 8.435991  |
| C  | 5.146590  | 6.538852  | 6.206734  |
| C  | 4.446893  | 7.730933  | 6.040155  |
| H  | 4.453907  | 8.220110  | 5.065663  |
| H  | 5.696389  | 6.092514  | 5.381876  |
| N  | 7.301603  | 2.515751  | 7.807012  |
| C  | 8.189915  | 2.124626  | 6.858973  |
| C  | 7.159997  | 1.724498  | 8.900348  |
| H  | 6.434441  | 2.050941  | 9.641239  |
| C  | 7.890608  | 0.553353  | 9.082643  |
| H  | 7.731756  | -0.037766 | 9.984982  |
| H  | 8.282785  | 2.771560  | 5.990256  |
| C  | 8.949941  | 0.963641  | 6.972180  |
| H  | 9.645751  | 0.703798  | 6.173911  |
| C  | 8.806104  | 0.156384  | 8.104196  |

|   |          |           |           |
|---|----------|-----------|-----------|
| H | 9.388958 | -0.758083 | 8.218915  |
| H | 3.199808 | 9.211821  | 7.020902  |
| C | 8.234501 | 5.148862  | 9.269075  |
| C | 8.446510 | 5.855712  | 7.936304  |
| H | 8.010846 | 6.869719  | 7.984703  |
| H | 9.525319 | 5.972003  | 7.762916  |
| H | 8.503568 | 5.835948  | 10.084499 |
| H | 8.906421 | 4.273687  | 9.335790  |
| H | 3.113828 | 2.086411  | 7.500465  |
| H | 3.116406 | 3.771537  | 6.903143  |
| H | 5.093561 | 1.545679  | 6.181089  |
| H | 4.050254 | 2.468874  | 5.062078  |

**Table S24:** Cartesian coordinates of DFT-optimized HS-[Feee(py)<sub>2</sub>] (BP86-D3/TZVP)

|    |           |          |           |
|----|-----------|----------|-----------|
| Fe | 6.150368  | 4.384987 | 7.602868  |
| N  | 7.778447  | 5.264317 | 6.819385  |
| N  | 6.780482  | 4.898068 | 9.451384  |
| N  | 4.566326  | 3.368444 | 8.306041  |
| O  | 8.330641  | 5.959509 | 2.728621  |
| O  | 3.228688  | 3.087332 | 12.123365 |
| N  | 5.687443  | 3.529969 | 5.854344  |
| N  | 4.926801  | 6.203058 | 7.307371  |
| C  | 3.738543  | 2.876938 | 7.205021  |
| C  | 6.319960  | 4.378174 | 10.575579 |
| C  | 4.200290  | 3.346175 | 9.559308  |
| H  | 3.230567  | 2.906585 | 9.837764  |
| C  | 4.654377  | 2.505787 | 6.012949  |
| C  | 8.180565  | 5.306311 | 5.562519  |
| C  | 6.306483  | 3.748471 | 4.723644  |
| H  | 5.938193  | 3.213876 | 3.838007  |
| C  | 7.410062  | 4.648378 | 4.505140  |
| C  | 4.957081  | 3.859148 | 10.670320 |
| C  | 4.244092  | 3.810068 | 11.939803 |
| C  | 7.683630  | 4.951948 | 3.103037  |
| C  | 9.502188  | 5.969677 | 5.236852  |
| H  | 9.894476  | 5.646178 | 4.271606  |
| H  | 9.395903  | 7.065040 | 5.196376  |
| H  | 10.234492 | 5.737828 | 6.023087  |
| C  | 7.276986  | 4.181369 | 11.733662 |
| H  | 6.832674  | 3.611318 | 12.553728 |
| H  | 8.155163  | 3.620607 | 11.374268 |
| H  | 7.652739  | 5.137938 | 12.129126 |
| C  | 4.628761  | 4.750121 | 13.077074 |
| H  | 5.355519  | 5.520516 | 12.796651 |
| H  | 3.705659  | 5.240936 | 13.418076 |
| H  | 5.022951  | 4.179547 | 13.932106 |
| C  | 7.135287  | 4.042973 | 1.999748  |
| H  | 7.259129  | 2.972599 | 2.216095  |
| H  | 6.063325  | 4.230292 | 1.829125  |
| H  | 7.670282  | 4.289553 | 1.074826  |
| C  | 3.449533  | 8.555127 | 6.978519  |
| C  | 3.475827  | 7.895387 | 8.212158  |
| H  | 2.927651  | 8.281050 | 9.072208  |
| H  | 4.288038  | 6.180526 | 9.278787  |
| C  | 4.227348  | 6.727425 | 8.335371  |
| C  | 4.897154  | 6.838295 | 6.117245  |

|   |          |           |           |
|---|----------|-----------|-----------|
| C | 4.174011 | 8.012608  | 5.911941  |
| H | 4.183480 | 8.491748  | 4.932395  |
| H | 5.478733 | 6.378065  | 5.315734  |
| N | 7.506051 | 2.378020  | 7.948085  |
| C | 8.432276 | 2.015444  | 7.041292  |
| C | 7.242446 | 1.532131  | 8.961981  |
| H | 6.478019 | 1.858718  | 9.670360  |
| C | 7.893257 | 0.306132  | 9.114385  |
| H | 7.645101 | -0.342790 | 9.955124  |
| H | 8.611518 | 2.727687  | 6.232850  |
| C | 9.128589 | 0.807169  | 7.110974  |
| H | 9.869187 | 0.559234  | 6.349572  |
| C | 8.854898 | -0.065239 | 8.169494  |
| H | 9.379823 | -1.017720 | 8.254803  |
| H | 2.877031 | 9.474692  | 6.851441  |
| C | 8.195411 | 5.256735  | 9.287039  |
| C | 8.453649 | 5.952437  | 7.928530  |
| H | 8.062165 | 6.983367  | 7.971681  |
| H | 9.543969 | 6.026687  | 7.796054  |
| H | 8.535042 | 5.936067  | 10.086446 |
| H | 8.816711 | 4.346567  | 9.343999  |
| H | 3.127015 | 2.006576  | 7.498718  |
| H | 3.053937 | 3.683674  | 6.890337  |
| H | 5.148991 | 1.543927  | 6.233448  |
| H | 4.055067 | 2.376147  | 5.095273  |

**Table S25:** Cartesian coordinates of DFT-optimized LS-[Fepe(py)<sub>2</sub>] (BP86-D3/TZVP)

|    |           |          |           |
|----|-----------|----------|-----------|
| Fe | 6.312712  | 4.193139 | 7.614257  |
| N  | 7.800085  | 5.214661 | 6.987877  |
| N  | 6.774421  | 4.789395 | 9.365275  |
| N  | 4.829581  | 3.138437 | 8.211889  |
| O  | 7.917649  | 6.763072 | 3.111131  |
| O  | 2.671271  | 3.745747 | 11.605502 |
| N  | 5.870038  | 3.497509 | 5.890219  |
| N  | 5.109606  | 5.717766 | 7.353418  |
| C  | 4.349063  | 2.258732 | 7.228269  |
| C  | 6.050682  | 4.691866 | 10.461741 |
| C  | 4.220651  | 3.336507 | 9.367655  |
| H  | 3.246583  | 2.867484 | 9.545799  |
| C  | 4.934460  | 2.449207 | 5.943070  |
| C  | 8.105824  | 5.511230 | 5.739509  |
| C  | 6.321794  | 4.001421 | 4.755018  |
| H  | 5.875420  | 3.624858 | 3.831319  |
| C  | 7.294173  | 5.024133 | 4.624923  |
| C  | 4.693689  | 4.163620 | 10.414927 |
| C  | 3.397621  | 1.244039 | 7.416187  |
| H  | 2.970279  | 1.073421 | 8.405114  |
| C  | 3.702475  | 4.446689 | 11.452779 |
| C  | 3.018460  | 0.433171 | 6.342452  |
| C  | 4.555299  | 1.616406 | 4.878188  |
| H  | 5.019954  | 1.731963 | 3.898334  |
| C  | 7.389413  | 5.642989 | 3.305456  |
| C  | 3.596065  | 0.619090 | 5.076269  |
| C  | 9.382615  | 6.272549 | 5.468052  |
| H  | 9.623834  | 6.296671 | 4.405050  |
| H  | 9.305222  | 7.315152 | 5.815734  |
| H  | 10.215242 | 5.809764 | 6.020084  |
| C  | 6.705074  | 4.964091 | 11.801612 |
| H  | 6.071789  | 4.654253 | 12.635933 |
| H  | 7.643638  | 4.394087 | 11.872200 |
| H  | 6.960687  | 6.026774 | 11.934529 |
| C  | 3.824477  | 5.698313 | 12.311894 |
| H  | 4.571912  | 6.414166 | 11.951737 |
| H  | 2.838200  | 6.183862 | 12.319427 |
| H  | 4.060546  | 5.430896 | 13.353542 |
| C  | 6.783465  | 4.938216 | 2.090737  |
| H  | 7.019466  | 3.865684 | 2.051223  |
| H  | 5.687105  | 5.044214 | 2.079381  |
| H  | 7.178107  | 5.426940 | 1.192114  |
| C  | 3.374082  | 7.908924 | 6.996435  |
| C  | 4.613088  | 8.064982 | 7.625350  |
| H  | 4.942752  | 9.035214 | 7.997400  |
| H  | 6.405150  | 7.052986 | 8.280056  |
| C  | 5.443422  | 6.961510 | 7.784393  |
| C  | 3.903294  | 5.572009 | 6.744790  |
| C  | 3.023145  | 6.630854 | 6.551568  |
| H  | 2.070848  | 6.444309 | 6.054779  |
| H  | 3.650925  | 4.570029 | 6.406839  |
| N  | 7.492878  | 2.612575 | 7.865730  |
| C  | 8.378942  | 2.240897 | 6.909401  |
| C  | 7.405748  | 1.847784 | 8.982342  |
| H  | 6.678529  | 2.169439 | 9.725405  |

|   |          |           |           |
|---|----------|-----------|-----------|
| C | 8.188314 | 0.713972  | 9.178224  |
| H | 8.074550 | 0.139588  | 10.097752 |
| H | 8.420938 | 2.871669  | 6.023861  |
| C | 9.191928 | 1.118341  | 7.036709  |
| H | 9.885037 | 0.868438  | 6.233046  |
| C | 9.101976 | 0.333938  | 8.190434  |
| H | 9.725320 | -0.552071 | 8.315019  |
| H | 2.702924 | 8.757229  | 6.857828  |
| H | 2.285673 | -0.360633 | 6.498279  |
| H | 3.313326 | -0.029709 | 4.245566  |
| C | 8.198866 | 5.141958  | 9.428884  |
| C | 8.655683 | 5.712675  | 8.081154  |
| H | 8.614113 | 6.815334  | 8.100786  |
| H | 9.711404 | 5.445248  | 7.920981  |
| H | 8.413481 | 5.872341  | 10.221112 |
| H | 8.772996 | 4.228598  | 9.663234  |

**Table S26:** Cartesian coordinates of DFT-optimized HS-[Fepe(py)<sub>2</sub>] (BP86-D3/TZVP)

|    |           |          |           |
|----|-----------|----------|-----------|
| Fe | 6.181497  | 4.448007 | 7.624000  |
| N  | 7.763938  | 5.414311 | 6.850079  |
| N  | 6.756813  | 5.046210 | 9.462830  |
| N  | 4.717770  | 3.240347 | 8.331199  |
| O  | 8.413609  | 6.024972 | 2.800019  |
| O  | 3.202349  | 3.211802 | 12.100863 |
| N  | 5.753815  | 3.532544 | 5.877152  |
| N  | 4.792622  | 6.119144 | 7.275520  |
| C  | 4.129267  | 2.470603 | 7.314988  |
| C  | 6.285177  | 4.566233 | 10.595641 |
| C  | 4.301016  | 3.295569 | 9.582838  |
| H  | 3.368495  | 2.795660 | 9.875644  |
| C  | 4.689008  | 2.620630 | 5.999265  |
| C  | 8.221677  | 5.388746 | 5.615391  |
| C  | 6.363315  | 3.825905 | 4.741347  |
| H  | 5.970894  | 3.375484 | 3.824092  |
| C  | 7.470160  | 4.707353 | 4.554522  |
| C  | 4.950757  | 3.965942 | 10.660377 |
| C  | 3.079867  | 1.557692 | 7.510608  |
| H  | 2.664579  | 1.419210 | 8.509729  |
| C  | 4.172709  | 3.982123 | 11.902339 |
| C  | 2.561013  | 0.820006 | 6.443369  |
| C  | 4.160847  | 1.856641 | 4.945692  |
| H  | 4.580487  | 1.948047 | 3.942711  |
| C  | 7.781296  | 5.004688 | 3.151777  |
| C  | 3.103435  | 0.968201 | 5.160008  |
| C  | 9.574624  | 5.995334 | 5.311690  |
| H  | 9.984739  | 5.625469 | 4.370823  |
| H  | 9.512112  | 7.091660 | 5.236460  |
| H  | 10.273737 | 5.757355 | 6.126058  |
| C  | 7.193258  | 4.500554 | 11.804676 |
| H  | 6.741299  | 3.959681 | 12.640049 |
| H  | 8.117692  | 3.970184 | 11.523821 |
| H  | 7.495034  | 5.501114 | 12.149915 |
| C  | 4.445580  | 5.042554 | 12.960617 |
| H  | 5.134354  | 5.830794 | 12.637167 |
| H  | 3.480008  | 5.498778 | 13.221308 |
| H  | 4.838454  | 4.576771 | 13.877154 |

|   |          |           |           |
|---|----------|-----------|-----------|
| C | 7.297602 | 4.069223  | 2.043373  |
| H | 7.427830 | 3.005685  | 2.286741  |
| H | 6.231825 | 4.238656  | 1.822394  |
| H | 7.867166 | 4.307084  | 1.137119  |
| C | 3.029229 | 8.243947  | 6.831928  |
| C | 3.100740 | 7.626052  | 8.084937  |
| H | 2.477064 | 7.957198  | 8.915697  |
| H | 4.091821 | 6.060983  | 9.225671  |
| C | 3.995057 | 6.572303  | 8.265755  |
| C | 4.721921 | 6.716755  | 6.067276  |
| C | 3.856310 | 7.777311  | 5.805103  |
| H | 3.836866 | 8.228582  | 4.812827  |
| H | 5.387216 | 6.320595  | 5.297712  |
| N | 7.662929 | 2.537538  | 8.000762  |
| C | 8.534614 | 2.152183  | 7.050362  |
| C | 7.472578 | 1.723427  | 9.055908  |
| H | 6.747670 | 2.062391  | 9.798616  |
| C | 8.143172 | 0.508386  | 9.207175  |
| H | 7.953126 | -0.114181 | 10.082153 |
| H | 8.654209 | 2.833633  | 6.205478  |
| C | 9.246950 | 0.953336  | 7.116124  |
| H | 9.940242 | 0.686656  | 6.317564  |
| C | 9.048491 | 0.114071  | 8.217088  |
| H | 9.586147 | -0.831498 | 8.299636  |
| H | 2.343071 | 9.074250  | 6.659548  |
| H | 1.740968 | 0.120958  | 6.616901  |
| H | 2.707561 | 0.388547  | 4.324606  |
| C | 8.153035 | 5.480402  | 9.322841  |
| C | 8.402785 | 6.149055  | 7.950869  |
| H | 8.434232 | 6.197879  | 10.110446 |
| H | 8.817778 | 4.605141  | 9.420274  |
| H | 7.971679 | 7.164349  | 7.961101  |
| H | 9.489825 | 6.260833  | 7.825273  |

**Table S27:** Cartesian coordinates of DFT-optimized LS-[Fepp(py)<sub>2</sub>] (BP86-D3/TZVP)

|    |           |          |           |
|----|-----------|----------|-----------|
| Fe | 6.138383  | 4.452754 | 7.552289  |
| N  | 7.644135  | 5.516050 | 6.918979  |
| N  | 6.572532  | 5.165716 | 9.314129  |
| N  | 4.728117  | 3.317612 | 8.166442  |
| O  | 8.654041  | 6.166637 | 2.959536  |
| O  | 3.008548  | 3.142034 | 11.806263 |
| N  | 5.754463  | 3.674111 | 5.851908  |
| N  | 4.854557  | 5.903901 | 7.202099  |
| C  | 4.234494  | 2.436827 | 7.183086  |
| C  | 6.035589  | 4.739874 | 10.463331 |
| C  | 4.205904  | 3.374572 | 9.375558  |
| H  | 3.284504  | 2.823399 | 9.588928  |
| C  | 4.805620  | 2.634529 | 5.899309  |
| C  | 8.177394  | 5.424953 | 5.698310  |
| C  | 6.262921  | 4.099204 | 4.709565  |
| H  | 5.801711  | 3.734104 | 3.789445  |
| C  | 7.392162  | 4.939513 | 4.575336  |
| C  | 4.760962  | 4.059217 | 10.481816 |
| C  | 3.299049  | 1.409073 | 7.379053  |
| H  | 2.879232  | 1.227093 | 8.368368  |
| C  | 3.932387  | 3.980118 | 11.698520 |
| C  | 2.917179  | 0.599968 | 6.305256  |
| C  | 4.434422  | 1.797731 | 4.834993  |
| H  | 4.894626  | 1.914166 | 3.853728  |
| C  | 7.778974  | 5.309899 | 3.209671  |
| C  | 3.483070  | 0.794024 | 5.036069  |
| C  | 9.657501  | 5.650318 | 5.465029  |
| H  | 10.012447 | 4.919859 | 4.727624  |
| H  | 9.893367  | 6.638601 | 5.052680  |
| H  | 10.210085 | 5.509915 | 6.402477  |
| C  | 6.843273  | 4.734431 | 11.752195 |
| H  | 6.615086  | 3.818289 | 12.311359 |
| H  | 7.915066  | 4.738546 | 11.518577 |
| H  | 6.647704  | 5.579280 | 12.424232 |
| C  | 4.087921  | 4.995284 | 12.819186 |
| H  | 4.503966  | 5.952088 | 12.481119 |
| H  | 3.095057  | 5.163752 | 13.255362 |
| H  | 4.734782  | 4.597432 | 13.615919 |
| C  | 7.068246  | 4.658704 | 2.024889  |
| H  | 7.107031  | 3.560127 | 2.068935  |
| H  | 6.009602  | 4.954855 | 1.975184  |
| H  | 7.563741  | 4.998507 | 1.108389  |
| C  | 3.004914  | 7.972575 | 6.686050  |
| C  | 4.243884  | 8.240502 | 7.275842  |
| H  | 4.532347  | 9.254436 | 7.554035  |
| H  | 6.097290  | 7.387352 | 7.972562  |
| C  | 5.130849  | 7.196942 | 7.515469  |
| C  | 3.647051  | 5.650889 | 6.629406  |
| C  | 2.712556  | 6.645601 | 6.361202  |
| H  | 1.764680  | 6.369047 | 5.899363  |
| H  | 3.433574  | 4.614503 | 6.382210  |
| N  | 7.402579  | 2.919860 | 7.881273  |
| C  | 8.269134  | 2.503891 | 6.925514  |
| C  | 7.374326  | 2.224085 | 9.044088  |
| H  | 6.649386  | 2.549336 | 9.785553  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 8.207211  | 1.137923  | 9.295838  |
| H | 8.134473  | 0.621992  | 10.253316 |
| H | 8.254583  | 3.050926  | 5.986476  |
| C | 9.132065  | 1.426601  | 7.105001  |
| H | 9.804080  | 1.142803  | 6.294930  |
| C | 9.111085  | 0.725784  | 8.313469  |
| H | 9.772983  | -0.124601 | 8.480729  |
| H | 2.291225  | 8.772323  | 6.486164  |
| H | 2.190152  | -0.198203 | 6.464440  |
| H | 3.198037  | 0.147302  | 4.204771  |
| C | 7.640114  | 6.086304  | 9.254726  |
| C | 8.220739  | 6.275612  | 7.961728  |
| H | 7.476322  | 6.933217  | 11.243430 |
| C | 7.986132  | 6.981240  | 10.287670 |
| H | 9.175054  | 8.662903  | 10.915828 |
| C | 8.926629  | 7.992101  | 10.091884 |
| C | 9.492435  | 8.177162  | 8.827503  |
| H | 10.190475 | 8.995686  | 8.644641  |
| C | 9.113710  | 7.348481  | 7.771346  |
| H | 9.479818  | 7.581149  | 6.777628  |

**Table S28:** Cartesian coordinates of DFT-optimized HS-[Fepp(py)<sub>2</sub>] (BP86-D3/TZVP)

|    |          |          |           |
|----|----------|----------|-----------|
| Fe | 6.566934 | 3.858287 | 7.671501  |
| N  | 8.070510 | 4.909811 | 7.008287  |
| N  | 6.996381 | 4.542704 | 9.449691  |
| N  | 4.972893 | 2.909699 | 8.267343  |
| O  | 8.512840 | 6.259938 | 3.064931  |
| O  | 2.847622 | 3.872275 | 11.669149 |
| N  | 6.005075 | 3.313320 | 5.890177  |
| N  | 5.201082 | 5.822772 | 7.431236  |
| C  | 4.466853 | 2.086728 | 7.252765  |
| C  | 6.079323 | 4.821232 | 10.387574 |
| C  | 4.302297 | 3.293620 | 9.348857  |
| H  | 3.262899 | 2.965523 | 9.463857  |
| C  | 5.034177 | 2.304835 | 5.952504  |
| C  | 8.096624 | 5.541825 | 5.827800  |
| C  | 6.321168 | 4.008889 | 4.804877  |
| H  | 5.753697 | 3.793070 | 3.895661  |
| C  | 7.304485 | 5.036064 | 4.722181  |
| C  | 4.768986 | 4.230930 | 10.311717 |
| C  | 3.496277 | 1.088666 | 7.424778  |
| H  | 3.080197 | 0.906317 | 8.417061  |
| C  | 3.655546 | 4.683762 | 11.187285 |
| C  | 3.077928 | 0.320524 | 6.333415  |
| C  | 4.616541 | 1.509662 | 4.874397  |
| H  | 5.067346 | 1.651955 | 3.891018  |
| C  | 7.499256 | 5.602863 | 3.376429  |
| C  | 3.636846 | 0.529771 | 5.062595  |
| C  | 8.818755 | 6.865414 | 5.725080  |
| H  | 9.812539 | 6.774549 | 5.265477  |
| H  | 8.251105 | 7.568501 | 5.104286  |
| H  | 8.942915 | 7.287064 | 6.731899  |
| C  | 6.450942 | 5.701954 | 11.554565 |
| H  | 5.582856 | 6.175733 | 12.016123 |
| H  | 6.940848 | 5.111926 | 12.344748 |
| H  | 7.156783 | 6.483377 | 11.241847 |



|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 3.366918  | 6.170534  | 11.339754 |
| H | 4.037742  | 6.811828  | 10.758818 |
| H | 2.339147  | 6.323010  | 10.976828 |
| H | 3.380362  | 6.469517  | 12.398323 |
| C | 6.446506  | 5.373650  | 2.294264  |
| H | 6.466558  | 4.333364  | 1.933461  |
| H | 5.426785  | 5.585080  | 2.645270  |
| H | 6.684849  | 6.028758  | 1.448270  |
| C | 3.434324  | 7.968274  | 7.730205  |
| C | 4.771359  | 8.087721  | 8.121734  |
| H | 5.154642  | 9.011379  | 8.556119  |
| H | 6.662514  | 7.030286  | 8.262916  |
| C | 5.615268  | 6.988329  | 7.957518  |
| C | 3.918466  | 5.717561  | 7.044877  |
| C | 3.000234  | 6.761307  | 7.175176  |
| H | 1.967881  | 6.624184  | 6.852695  |
| H | 3.622536  | 4.755420  | 6.621477  |
| N | 7.858335  | 2.088212  | 7.942138  |
| C | 8.665467  | 1.676510  | 6.945492  |
| C | 7.872682  | 1.412784  | 9.107323  |
| H | 7.203860  | 1.788682  | 9.883744  |
| C | 8.689849  | 0.303046  | 9.319967  |
| H | 8.667981  | -0.212658 | 10.280345 |
| H | 8.618455  | 2.259001  | 6.023672  |
| C | 9.512393  | 0.576211  | 7.074067  |
| H | 10.146646 | 0.277776  | 6.238911  |
| C | 9.525903  | -0.125216 | 8.283954  |
| H | 10.176126 | -0.991054 | 8.416684  |
| H | 2.743177  | 8.803381  | 7.854322  |
| H | 2.323413  | -0.454823 | 6.477622  |
| H | 3.317803  | -0.082817 | 4.217864  |
| C | 8.357056  | 4.891043  | 9.419718  |
| C | 8.916859  | 5.119324  | 8.107788  |
| H | 10.728508 | 5.479515  | 6.992067  |
| H | 12.192608 | 5.564785  | 8.990347  |
| C | 10.299269 | 5.352866  | 7.985711  |
| C | 11.123621 | 5.379565  | 9.108985  |
| C | 10.584414 | 5.136035  | 10.382536 |
| H | 11.231689 | 5.126153  | 11.260979 |
| C | 9.221558  | 4.879435  | 10.530444 |
| H | 8.825858  | 4.639243  | 11.515057 |