

# Inorganic Chemistry

including bioinorganic chemistry

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Table 1. Crystal data and structure refinement for 1.

|                                   |                                                                                                                     |
|-----------------------------------|---------------------------------------------------------------------------------------------------------------------|
| Identification code               | ts1                                                                                                                 |
| Empirical formula                 | C <sub>20</sub> H <sub>19</sub> B Co F <sub>6</sub> Fe P                                                            |
| Formula weight                    | 529.91                                                                                                              |
| Temperature                       | 293(2) K                                                                                                            |
| Wavelength                        | 0.71073 Å                                                                                                           |
| Crystal system                    | monoclin                                                                                                            |
| Space group                       | P(2) <sub>1</sub> /c                                                                                                |
| Unit cell dimensions              | a = 10.541(3) Å    alpha = 90 deg.<br>b = 17.647(5) Å    beta = 96.38(2) deg.<br>c = 10.965(3) Å    gamma = 90 deg. |
| Volume                            | 2027.0(10) Å <sup>3</sup>                                                                                           |
| Z                                 | 4                                                                                                                   |
| Density (calculated)              | 1.736 Mg/m <sup>3</sup>                                                                                             |
| Absorption coefficient            | 1.671 mm <sup>-1</sup>                                                                                              |
| F(000)                            | 1064                                                                                                                |
| Crystal size                      | 0.3 x 0.35 x 0.35 mm                                                                                                |
| Theta range for data collection   | 2.26 to 30.08 deg.                                                                                                  |
| Index ranges                      | -2 ≤ h ≤ 14, -2 ≤ k ≤ 24, -15 ≤ l ≤ 15                                                                              |
| Reflections collected             | 8543                                                                                                                |
| Independent reflections           | 5942 [R(int) = 0.0435]                                                                                              |
| Refinement method                 | Full-matrix least-squares on F <sup>2</sup>                                                                         |
| Data / restraints / parameters    | 5942 / 36 / 339                                                                                                     |
| Goodness-of-fit on F <sup>2</sup> | 1.111                                                                                                               |
| Final R indices [I > 2sigma(I)]   | R1 = 0.0588, wR2 = 0.1394                                                                                           |
| R indices (all data)              | R1 = 0.0805, wR2 = 0.1576                                                                                           |
| Largest diff. peak and hole       | 0.484 and -0.659 e.Å <sup>-3</sup>                                                                                  |

Table 2. Atomic coordinates ( $\times 10^4$ ) and equivalent isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for 1.  $U(\text{eq})$  is defined as one third of the trace of the orthogonalized  $U_{ij}$  tensor.

|       | x         | y        | z        | $U(\text{eq})$ |
|-------|-----------|----------|----------|----------------|
| Fe(1) | 2158(1)   | 2214(1)  | 4516(1)  | 36(1)          |
| C(1)  | 2963(3)   | 1176(2)  | 4248(3)  | 40(1)          |
| C(2)  | 2806(4)   | 1291(2)  | 5515(3)  | 47(1)          |
| C(3)  | 3511(4)   | 1947(2)  | 5938(4)  | 59(1)          |
| C(4)  | 4097(4)   | 2239(2)  | 4971(5)  | 60(1)          |
| C(5)  | 3781(3)   | 1775(2)  | 3933(4)  | 49(1)          |
| C(6)  | 1210(4)   | 2822(2)  | 3113(3)  | 53(1)          |
| C(7)  | 400(4)    | 2267(2)  | 3504(4)  | 53(1)          |
| C(8)  | 287(4)    | 2402(2)  | 4762(4)  | 54(1)          |
| C(9)  | 1046(4)   | 3040(2)  | 5139(3)  | 51(1)          |
| C(10) | 1618(4)   | 3302(2)  | 4122(4)  | 52(1)          |
| Co(1) | 2473(1)   | -594(1)  | 2673(1)  | 41(1)          |
| C(11) | 2472(4)   | 530(2)   | 2014(4)  | 52(1)          |
| C(12) | 1727(5)   | 49(3)    | 1202(4)  | 69(1)          |
| C(13) | 789(5)    | -403(3)  | 1601(5)  | 75(2)          |
| C(14) | 565(4)    | -417(3)  | 2833(6)  | 74(2)          |
| C(15) | 1266(4)   | 34(2)    | 3707(4)  | 57(1)          |
| C(16) | 4237(6)   | -784(3)  | 3465(8)  | 97(2)          |
| C(17) | 4172(6)   | -956(4)  | 2271(8)  | 94(2)          |
| C(18) | 3297(7)   | -1525(3) | 2015(6)  | 91(2)          |
| C(19) | 2790(6)   | -1704(3) | 3074(8)  | 94(2)          |
| C(20) | 3420(8)   | -1227(4) | 3988(5)  | 106(3)         |
| B(1)  | 2214(4)   | 627(2)   | 3351(4)  | 42(1)          |
| P(1)  | -3010(5)  | 912(3)   | 2058(4)  | 57(2)          |
| P(2)  | -2918(4)  | 856(2)   | 2171(4)  | 57(2)          |
| F(1)  | -3779(10) | 522(5)   | 2989(7)  | 159(7)         |
| F(2)  | -2377(14) | 1424(8)  | 3081(7)  | 159(7)         |
| F(3)  | -3645(13) | 400(8)   | 1038(8)  | 156(6)         |
| F(4)  | -1939(10) | 328(7)   | 2335(15) | 287(13)        |
| F(5)  | -4082(11) | 1495(7)  | 1783(14) | 227(10)        |
| F(6)  | -2241(11) | 1302(6)  | 1130(7)  | 213(9)         |
| F(11) | -3985(6)  | 624(5)   | 2941(8)  | 134(7)         |
| F(12) | -1851(8)  | 1088(5)  | 1404(7)  | 139(5)         |
| F(13) | -2966(12) | 1666(3)  | 2670(11) | 151(6)         |
| F(14) | -2872(11) | 45(3)    | 1675(10) | 137(5)         |
| F(15) | -3920(8)  | 1066(8)  | 1102(8)  | 215(9)         |
| F(16) | -1917(7)  | 646(8)   | 3241(6)  | 142(5)         |

Table 3. Bond lengths [Å] and angles [deg] for 1.

---

|             |           |
|-------------|-----------|
| Fe(1)-C(10) | 2.035(3)  |
| Fe(1)-C(9)  | 2.036(4)  |
| Fe(1)-C(2)  | 2.038(3)  |
| Fe(1)-C(5)  | 2.043(4)  |
| Fe(1)-C(6)  | 2.043(4)  |
| Fe(1)-C(3)  | 2.047(4)  |
| Fe(1)-C(8)  | 2.048(4)  |
| Fe(1)-C(4)  | 2.049(4)  |
| Fe(1)-C(1)  | 2.053(3)  |
| Fe(1)-C(7)  | 2.054(4)  |
| C(1)-C(5)   | 1.429(5)  |
| C(1)-C(2)   | 1.431(5)  |
| C(1)-B(1)   | 1.535(5)  |
| C(2)-C(3)   | 1.425(6)  |
| C(3)-C(4)   | 1.384(7)  |
| C(4)-C(5)   | 1.412(6)  |
| C(6)-C(7)   | 1.397(6)  |
| C(6)-C(10)  | 1.421(5)  |
| C(7)-C(8)   | 1.418(6)  |
| C(8)-C(9)   | 1.417(6)  |
| C(9)-C(10)  | 1.403(6)  |
| Co(1)-C(16) | 1.992(5)  |
| Co(1)-C(17) | 1.997(5)  |
| Co(1)-C(20) | 2.001(5)  |
| Co(1)-C(19) | 2.026(4)  |
| Co(1)-C(18) | 2.028(5)  |
| Co(1)-C(13) | 2.044(4)  |
| Co(1)-C(12) | 2.055(4)  |
| Co(1)-C(14) | 2.062(4)  |
| Co(1)-C(15) | 2.111(4)  |
| Co(1)-C(11) | 2.112(4)  |
| Co(1)-B(1)  | 2.307(4)  |
| C(11)-C(12) | 1.405(6)  |
| C(11)-B(1)  | 1.531(6)  |
| C(12)-C(13) | 1.379(8)  |
| C(13)-C(14) | 1.397(8)  |
| C(14)-C(15) | 1.393(6)  |
| C(15)-B(1)  | 1.528(6)  |
| C(16)-C(17) | 1.338(10) |
| C(16)-C(20) | 1.339(10) |
| C(17)-C(18) | 1.372(9)  |
| C(18)-C(19) | 1.368(9)  |
| C(19)-C(20) | 1.416(10) |
| P(1)-F(15)  | 1.367(8)  |
| P(1)-F(13)  | 1.489(8)  |
| P(1)-F(12)  | 1.517(10) |
| P(1)-F(4)   | 1.533(2)  |
| P(1)-F(6)   | 1.533(2)  |

|            |           |
|------------|-----------|
| P(1)-F(3)  | 1.533(2)  |
| P(1)-F(5)  | 1.533(2)  |
| P(1)-F(2)  | 1.534(2)  |
| P(1)-F(1)  | 1.535(2)  |
| P(1)-F(11) | 1.572(10) |
| P(1)-F(14) | 1.597(8)  |
| P(1)-F(16) | 1.702(8)  |
| P(2)-F(4)  | 1.386(8)  |
| P(2)-F(1)  | 1.468(10) |
| P(2)-F(2)  | 1.483(9)  |
| P(2)-F(14) | 1.533(2)  |
| P(2)-F(15) | 1.533(2)  |
| P(2)-F(12) | 1.533(2)  |
| P(2)-F(13) | 1.533(2)  |
| P(2)-F(16) | 1.534(2)  |
| P(2)-F(11) | 1.535(2)  |
| P(2)-F(3)  | 1.603(9)  |
| P(2)-F(6)  | 1.616(10) |
| P(2)-F(5)  | 1.686(8)  |
| F(2)-F(13) | 0.841(14) |
| F(2)-F(16) | 1.461(13) |
| F(3)-F(14) | 1.190(12) |
| F(3)-F(15) | 1.215(12) |
| F(4)-F(16) | 1.139(14) |
| F(4)-F(14) | 1.258(13) |
| F(4)-F(12) | 1.69(2)   |
| F(5)-F(15) | 1.091(12) |
| F(5)-F(13) | 1.472(14) |
| F(6)-F(12) | 0.61(2)   |

|                  |          |
|------------------|----------|
| C(10)-Fe(1)-C(9) | 40.3(2)  |
| C(10)-Fe(1)-C(2) | 159.6(2) |
| C(9)-Fe(1)-C(2)  | 124.3(2) |
| C(10)-Fe(1)-C(5) | 121.0(2) |
| C(9)-Fe(1)-C(5)  | 155.4(2) |
| C(2)-Fe(1)-C(5)  | 67.8(2)  |
| C(10)-Fe(1)-C(6) | 40.8(2)  |
| C(9)-Fe(1)-C(6)  | 68.0(2)  |
| C(2)-Fe(1)-C(6)  | 158.6(2) |
| C(5)-Fe(1)-C(6)  | 108.7(2) |
| C(10)-Fe(1)-C(3) | 122.3(2) |
| C(9)-Fe(1)-C(3)  | 106.7(2) |
| C(2)-Fe(1)-C(3)  | 40.8(2)  |
| C(5)-Fe(1)-C(3)  | 67.3(2)  |
| C(6)-Fe(1)-C(3)  | 159.3(2) |
| C(10)-Fe(1)-C(8) | 67.9(2)  |
| C(9)-Fe(1)-C(8)  | 40.6(2)  |
| C(2)-Fe(1)-C(8)  | 109.2(2) |
| C(5)-Fe(1)-C(8)  | 162.7(2) |
| C(6)-Fe(1)-C(8)  | 67.4(2)  |
| C(3)-Fe(1)-C(8)  | 122.4(2) |
| C(10)-Fe(1)-C(4) | 106.2(2) |

|                  |            |
|------------------|------------|
| C(9)-Fe(1)-C(4)  | 119.9(2)   |
| C(2)-Fe(1)-C(4)  | 67.7(2)    |
| C(5)-Fe(1)-C(4)  | 40.4(2)    |
| C(6)-Fe(1)-C(4)  | 124.3(2)   |
| C(3)-Fe(1)-C(4)  | 39.5(2)    |
| C(8)-Fe(1)-C(4)  | 156.0(2)   |
| C(10)-Fe(1)-C(1) | 157.1(2)   |
| C(9)-Fe(1)-C(1)  | 161.7(2)   |
| C(2)-Fe(1)-C(1)  | 40.95(14)  |
| C(5)-Fe(1)-C(1)  | 40.83(14)  |
| C(6)-Fe(1)-C(1)  | 122.41(14) |
| C(3)-Fe(1)-C(1)  | 68.87(14)  |
| C(8)-Fe(1)-C(1)  | 125.7(2)   |
| C(4)-Fe(1)-C(1)  | 68.7(2)    |
| C(10)-Fe(1)-C(7) | 68.1(2)    |
| C(9)-Fe(1)-C(7)  | 68.3(2)    |
| C(2)-Fe(1)-C(7)  | 123.7(2)   |
| C(5)-Fe(1)-C(7)  | 125.8(2)   |
| C(6)-Fe(1)-C(7)  | 39.9(2)    |
| C(3)-Fe(1)-C(7)  | 158.8(2)   |
| C(8)-Fe(1)-C(7)  | 40.5(2)    |
| C(4)-Fe(1)-C(7)  | 161.1(2)   |
| C(1)-Fe(1)-C(7)  | 109.0(2)   |
| C(5)-C(1)-C(2)   | 105.5(3)   |
| C(5)-C(1)-B(1)   | 126.4(3)   |
| C(2)-C(1)-B(1)   | 127.1(3)   |
| C(5)-C(1)-Fe(1)  | 69.2(2)    |
| C(2)-C(1)-Fe(1)  | 69.0(2)    |
| B(1)-C(1)-Fe(1)  | 117.6(2)   |
| C(3)-C(2)-C(1)   | 108.6(4)   |
| C(3)-C(2)-Fe(1)  | 69.9(2)    |
| C(1)-C(2)-Fe(1)  | 70.1(2)    |
| C(4)-C(3)-C(2)   | 108.3(3)   |
| C(4)-C(3)-Fe(1)  | 70.3(2)    |
| C(2)-C(3)-Fe(1)  | 69.2(2)    |
| C(3)-C(4)-C(5)   | 108.4(4)   |
| C(3)-C(4)-Fe(1)  | 70.2(2)    |
| C(5)-C(4)-Fe(1)  | 69.6(2)    |
| C(4)-C(5)-C(1)   | 109.2(4)   |
| C(4)-C(5)-Fe(1)  | 70.0(2)    |
| C(1)-C(5)-Fe(1)  | 69.9(2)    |
| C(7)-C(6)-C(10)  | 108.7(3)   |
| C(7)-C(6)-Fe(1)  | 70.5(2)    |
| C(10)-C(6)-Fe(1) | 69.3(2)    |
| C(6)-C(7)-C(8)   | 107.5(3)   |
| C(6)-C(7)-Fe(1)  | 69.7(2)    |
| C(8)-C(7)-Fe(1)  | 69.5(2)    |
| C(9)-C(8)-C(7)   | 108.1(4)   |
| C(9)-C(8)-Fe(1)  | 69.3(2)    |
| C(7)-C(8)-Fe(1)  | 70.0(2)    |
| C(10)-C(9)-C(8)  | 108.0(3)   |
| C(10)-C(9)-Fe(1) | 69.8(2)    |

|                   |          |
|-------------------|----------|
| C(8)-C(9)-Fe(1)   | 70.1(2)  |
| C(9)-C(10)-C(6)   | 107.6(4) |
| C(9)-C(10)-Fe(1)  | 69.9(2)  |
| C(6)-C(10)-Fe(1)  | 69.9(2)  |
| C(16)-Co(1)-C(17) | 39.2(3)  |
| C(16)-Co(1)-C(20) | 39.2(3)  |
| C(17)-Co(1)-C(20) | 65.9(3)  |
| C(16)-Co(1)-C(19) | 67.6(3)  |
| C(17)-Co(1)-C(19) | 67.0(2)  |
| C(20)-Co(1)-C(19) | 41.2(3)  |
| C(16)-Co(1)-C(18) | 66.6(3)  |
| C(17)-Co(1)-C(18) | 39.9(3)  |
| C(20)-Co(1)-C(18) | 66.7(3)  |
| C(19)-Co(1)-C(18) | 39.4(3)  |
| C(16)-Co(1)-C(13) | 170.8(3) |
| C(17)-Co(1)-C(13) | 132.0(3) |
| C(20)-Co(1)-C(13) | 146.9(3) |
| C(19)-Co(1)-C(13) | 113.3(3) |
| C(18)-Co(1)-C(13) | 107.9(2) |
| C(16)-Co(1)-C(12) | 133.8(3) |
| C(17)-Co(1)-C(12) | 106.1(3) |
| C(20)-Co(1)-C(12) | 172.0(3) |
| C(19)-Co(1)-C(12) | 138.0(3) |
| C(18)-Co(1)-C(12) | 108.1(2) |
| C(13)-Co(1)-C(12) | 39.3(2)  |
| C(16)-Co(1)-C(14) | 149.4(3) |
| C(17)-Co(1)-C(14) | 167.1(3) |
| C(20)-Co(1)-C(14) | 115.9(3) |
| C(19)-Co(1)-C(14) | 105.5(2) |
| C(18)-Co(1)-C(14) | 127.8(3) |
| C(13)-Co(1)-C(14) | 39.8(2)  |
| C(12)-Co(1)-C(14) | 72.0(2)  |
| C(16)-Co(1)-C(15) | 116.3(3) |
| C(17)-Co(1)-C(15) | 153.6(3) |
| C(20)-Co(1)-C(15) | 100.9(2) |
| C(19)-Co(1)-C(15) | 119.1(2) |
| C(18)-Co(1)-C(15) | 157.5(3) |
| C(13)-Co(1)-C(15) | 71.7(2)  |
| C(12)-Co(1)-C(15) | 86.0(2)  |
| C(14)-Co(1)-C(15) | 39.0(2)  |
| C(16)-Co(1)-C(11) | 105.8(2) |
| C(17)-Co(1)-C(11) | 101.0(2) |
| C(20)-Co(1)-C(11) | 138.8(3) |
| C(19)-Co(1)-C(11) | 167.4(2) |
| C(18)-Co(1)-C(11) | 128.6(3) |
| C(13)-Co(1)-C(11) | 71.4(2)  |
| C(12)-Co(1)-C(11) | 39.4(2)  |
| C(14)-Co(1)-C(11) | 85.6(2)  |
| C(15)-Co(1)-C(11) | 73.3(2)  |
| C(16)-Co(1)-B(1)  | 98.9(2)  |
| C(17)-Co(1)-B(1)  | 120.7(3) |
| C(20)-Co(1)-B(1)  | 110.9(2) |

|                   |          |
|-------------------|----------|
| C(19)-Co(1)-B(1)  | 148.8(3) |
| C(18)-Co(1)-B(1)  | 160.5(2) |
| C(13)-Co(1)-B(1)  | 84.6(2)  |
| C(12)-Co(1)-B(1)  | 71.9(2)  |
| C(14)-Co(1)-B(1)  | 71.3(2)  |
| C(15)-Co(1)-B(1)  | 40.2(2)  |
| C(11)-Co(1)-B(1)  | 40.2(2)  |
| C(12)-C(11)-B(1)  | 121.9(4) |
| C(12)-C(11)-Co(1) | 68.1(2)  |
| B(1)-C(11)-Co(1)  | 76.8(2)  |
| C(13)-C(12)-C(11) | 121.2(4) |
| C(13)-C(12)-Co(1) | 69.9(3)  |
| C(11)-C(12)-Co(1) | 72.5(2)  |
| C(12)-C(13)-C(14) | 121.4(4) |
| C(12)-C(13)-Co(1) | 70.8(3)  |
| C(14)-C(13)-Co(1) | 70.8(3)  |
| C(15)-C(14)-C(13) | 121.4(5) |
| C(15)-C(14)-Co(1) | 72.4(2)  |
| C(13)-C(14)-Co(1) | 69.4(3)  |
| C(14)-C(15)-B(1)  | 121.9(4) |
| C(14)-C(15)-Co(1) | 68.6(2)  |
| B(1)-C(15)-Co(1)  | 76.8(2)  |
| C(17)-C(16)-C(20) | 108.7(6) |
| C(17)-C(16)-Co(1) | 70.6(3)  |
| C(20)-C(16)-Co(1) | 70.8(3)  |
| C(16)-C(17)-C(18) | 109.1(6) |
| C(16)-C(17)-Co(1) | 70.2(3)  |
| C(18)-C(17)-Co(1) | 71.3(3)  |
| C(19)-C(18)-C(17) | 108.2(6) |
| C(19)-C(18)-Co(1) | 70.2(3)  |
| C(17)-C(18)-Co(1) | 68.8(3)  |
| C(18)-C(19)-C(20) | 105.5(6) |
| C(18)-C(19)-Co(1) | 70.4(3)  |
| C(20)-C(19)-Co(1) | 68.5(3)  |
| C(16)-C(20)-C(19) | 108.5(6) |
| C(16)-C(20)-Co(1) | 70.0(3)  |
| C(19)-C(20)-Co(1) | 70.4(3)  |
| C(15)-B(1)-C(11)  | 111.0(3) |
| C(15)-B(1)-C(1)   | 125.0(4) |
| C(11)-B(1)-C(1)   | 123.4(3) |
| C(15)-B(1)-Co(1)  | 63.0(2)  |
| C(11)-B(1)-Co(1)  | 63.0(2)  |
| C(1)-B(1)-Co(1)   | 136.5(2) |
| F(15)-P(1)-F(13)  | 98.8(5)  |
| F(15)-P(1)-F(12)  | 97.5(6)  |
| F(13)-P(1)-F(12)  | 92.5(5)  |
| F(15)-P(1)-F(4)   | 136.3(5) |
| F(13)-P(1)-F(4)   | 121.7(6) |
| F(12)-P(1)-F(4)   | 67.5(7)  |
| F(15)-P(1)-F(6)   | 77.2(8)  |
| F(13)-P(1)-F(6)   | 84.6(7)  |
| F(12)-P(1)-F(6)   | 23.1(7)  |

|                  |           |
|------------------|-----------|
| F(4)-P(1)-F(6)   | 90.04(10) |
| F(15)-P(1)-F(3)  | 49.1(5)   |
| F(13)-P(1)-F(3)  | 147.7(5)  |
| F(12)-P(1)-F(3)  | 94.9(6)   |
| F(4)-P(1)-F(3)   | 90.03(10) |
| F(6)-P(1)-F(3)   | 90.03(10) |
| F(15)-P(1)-F(5)  | 43.7(5)   |
| F(13)-P(1)-F(5)  | 58.3(6)   |
| F(12)-P(1)-F(5)  | 112.6(7)  |
| F(4)-P(1)-F(5)   | 179.9(6)  |
| F(6)-P(1)-F(5)   | 90.03(10) |
| F(3)-P(1)-F(5)   | 89.99(10) |
| F(15)-P(1)-F(2)  | 130.9(5)  |
| F(13)-P(1)-F(2)  | 32.3(5)   |
| F(12)-P(1)-F(2)  | 85.2(6)   |
| F(4)-P(1)-F(2)   | 90.01(10) |
| F(6)-P(1)-F(2)   | 90.06(10) |
| F(3)-P(1)-F(2)   | 179.9(4)  |
| F(5)-P(1)-F(2)   | 89.98(10) |
| F(15)-P(1)-F(1)  | 102.8(8)  |
| F(13)-P(1)-F(1)  | 95.3(7)   |
| F(12)-P(1)-F(1)  | 156.9(7)  |
| F(4)-P(1)-F(1)   | 89.96(10) |
| F(6)-P(1)-F(1)   | 179.9(5)  |
| F(3)-P(1)-F(1)   | 90.07(10) |
| F(5)-P(1)-F(1)   | 89.97(10) |
| F(2)-P(1)-F(1)   | 89.84(10) |
| F(15)-P(1)-F(11) | 94.9(5)   |
| F(13)-P(1)-F(11) | 90.1(5)   |
| F(12)-P(1)-F(11) | 166.9(6)  |
| F(4)-P(1)-F(11)  | 100.3(6)  |
| F(6)-P(1)-F(11)  | 169.6(6)  |
| F(3)-P(1)-F(11)  | 89.8(5)   |
| F(5)-P(1)-F(11)  | 79.6(6)   |
| F(2)-P(1)-F(11)  | 90.1(5)   |
| F(1)-P(1)-F(11)  | 10.4(6)   |
| F(15)-P(1)-F(14) | 93.7(5)   |
| F(13)-P(1)-F(14) | 167.3(6)  |
| F(12)-P(1)-F(14) | 88.3(4)   |
| F(4)-P(1)-F(14)  | 47.3(5)   |
| F(6)-P(1)-F(14)  | 100.6(6)  |
| F(3)-P(1)-F(14)  | 44.6(5)   |
| F(5)-P(1)-F(14)  | 132.7(5)  |
| F(2)-P(1)-F(14)  | 135.4(5)  |
| F(1)-P(1)-F(14)  | 79.4(6)   |
| F(11)-P(1)-F(14) | 86.5(5)   |
| F(15)-P(1)-F(16) | 175.4(7)  |
| F(13)-P(1)-F(16) | 85.3(4)   |
| F(12)-P(1)-F(16) | 84.5(4)   |
| F(4)-P(1)-F(16)  | 40.8(5)   |
| F(6)-P(1)-F(16)  | 105.5(6)  |
| F(3)-P(1)-F(16)  | 126.7(5)  |

|                  |           |
|------------------|-----------|
| F(5)-P(1)-F(16)  | 139.2(5)  |
| F(2)-P(1)-F(16)  | 53.4(5)   |
| F(1)-P(1)-F(16)  | 74.5(6)   |
| F(11)-P(1)-F(16) | 82.9(4)   |
| F(14)-P(1)-F(16) | 82.1(4)   |
| F(4)-P(2)-F(1)   | 98.8(5)   |
| F(4)-P(2)-F(2)   | 98.2(5)   |
| F(1)-P(2)-F(2)   | 94.5(5)   |
| F(4)-P(2)-F(14)  | 50.7(6)   |
| F(1)-P(2)-F(14)  | 83.6(6)   |
| F(2)-P(2)-F(14)  | 147.6(5)  |
| F(4)-P(2)-F(15)  | 134.5(6)  |
| F(1)-P(2)-F(15)  | 98.3(6)   |
| F(2)-P(2)-F(15)  | 122.1(5)  |
| F(14)-P(2)-F(15) | 90.01(10) |
| F(4)-P(2)-F(12)  | 70.7(7)   |
| F(1)-P(2)-F(12)  | 169.5(7)  |
| F(2)-P(2)-F(12)  | 86.4(6)   |
| F(14)-P(2)-F(12) | 90.05(10) |
| F(15)-P(2)-F(12) | 90.06(10) |
| F(4)-P(2)-F(13)  | 129.3(6)  |
| F(1)-P(2)-F(13)  | 96.2(6)   |
| F(2)-P(2)-F(13)  | 32.3(5)   |
| F(14)-P(2)-F(13) | 179.9(3)  |
| F(15)-P(2)-F(13) | 90.03(10) |
| F(12)-P(2)-F(13) | 90.09(10) |
| F(4)-P(2)-F(16)  | 45.6(6)   |
| F(1)-P(2)-F(16)  | 81.7(6)   |
| F(2)-P(2)-F(16)  | 57.9(5)   |
| F(14)-P(2)-F(16) | 89.99(10) |
| F(15)-P(2)-F(16) | 179.9(5)  |
| F(12)-P(2)-F(16) | 90.02(10) |
| F(13)-P(2)-F(16) | 89.97(10) |
| F(4)-P(2)-F(11)  | 109.3(7)  |
| F(1)-P(2)-F(11)  | 10.5(7)   |
| F(2)-P(2)-F(11)  | 93.5(6)   |
| F(14)-P(2)-F(11) | 90.05(10) |
| F(15)-P(2)-F(11) | 89.99(10) |
| F(12)-P(2)-F(11) | 179.9(5)  |
| F(13)-P(2)-F(11) | 89.81(10) |
| F(16)-P(2)-F(11) | 89.94(10) |
| F(4)-P(2)-F(3)   | 92.8(5)   |
| F(1)-P(2)-F(3)   | 89.8(5)   |
| F(2)-P(2)-F(3)   | 167.5(6)  |
| F(14)-P(2)-F(3)  | 44.5(4)   |
| F(15)-P(2)-F(3)  | 45.5(5)   |
| F(12)-P(2)-F(3)  | 91.5(6)   |
| F(13)-P(2)-F(3)  | 135.5(5)  |
| F(16)-P(2)-F(3)  | 134.5(5)  |
| F(11)-P(2)-F(3)  | 88.6(6)   |
| F(4)-P(2)-F(6)   | 92.2(5)   |
| F(1)-P(2)-F(6)   | 168.0(6)  |

|                  |           |
|------------------|-----------|
| F(2)-P(2)-F(6)   | 88.8(5)   |
| F(14)-P(2)-F(6)  | 99.8(6)   |
| F(15)-P(2)-F(6)  | 70.3(6)   |
| F(12)-P(2)-F(6)  | 22.2(7)   |
| F(13)-P(2)-F(6)  | 80.4(6)   |
| F(16)-P(2)-F(6)  | 109.8(6)  |
| F(11)-P(2)-F(6)  | 157.8(7)  |
| F(3)-P(2)-F(6)   | 84.7(4)   |
| F(4)-P(2)-F(5)   | 172.8(7)  |
| F(1)-P(2)-F(5)   | 86.6(4)   |
| F(2)-P(2)-F(5)   | 86.1(4)   |
| F(14)-P(2)-F(5)  | 125.8(5)  |
| F(15)-P(2)-F(5)  | 39.2(5)   |
| F(12)-P(2)-F(5)  | 103.9(7)  |
| F(13)-P(2)-F(5)  | 54.2(5)   |
| F(16)-P(2)-F(5)  | 140.7(5)  |
| F(11)-P(2)-F(5)  | 76.1(7)   |
| F(3)-P(2)-F(5)   | 82.4(4)   |
| F(6)-P(2)-F(5)   | 82.1(4)   |
| P(2)-F(1)-P(1)   | 6.3(3)    |
| F(13)-F(2)-F(16) | 139.2(9)  |
| F(13)-F(2)-P(2)  | 77.1(6)   |
| F(16)-F(2)-P(2)  | 62.8(4)   |
| F(13)-F(2)-P(1)  | 70.9(6)   |
| F(16)-F(2)-P(1)  | 69.3(4)   |
| P(2)-F(2)-P(1)   | 6.5(3)    |
| F(14)-F(3)-F(15) | 128.8(7)  |
| F(14)-F(3)-P(1)  | 70.5(5)   |
| F(15)-F(3)-P(1)  | 58.3(4)   |
| F(14)-F(3)-P(2)  | 64.6(4)   |
| F(15)-F(3)-P(2)  | 64.2(4)   |
| P(1)-F(3)-P(2)   | 6.0(3)    |
| F(16)-F(4)-F(14) | 129.5(11) |
| F(16)-F(4)-P(2)  | 74.1(6)   |
| F(14)-F(4)-P(2)  | 70.7(5)   |
| F(16)-F(4)-P(1)  | 77.6(5)   |
| F(14)-F(4)-P(1)  | 69.0(4)   |
| P(2)-F(4)-P(1)   | 4.0(4)    |
| F(16)-F(4)-F(12) | 98.0(9)   |
| F(14)-F(4)-F(12) | 93.4(7)   |
| P(2)-F(4)-F(12)  | 58.7(5)   |
| P(1)-F(4)-F(12)  | 55.8(5)   |
| F(15)-F(5)-F(13) | 114.8(9)  |
| F(15)-F(5)-P(1)  | 60.0(4)   |
| F(13)-F(5)-P(1)  | 59.3(4)   |
| F(15)-F(5)-P(2)  | 62.8(4)   |
| F(13)-F(5)-P(2)  | 57.6(3)   |
| P(1)-F(5)-P(2)   | 3.3(3)    |
| F(12)-F(6)-P(1)  | 76.9(9)   |
| F(12)-F(6)-P(2)  | 71.2(8)   |
| P(1)-F(6)-P(2)   | 5.7(3)    |
| P(2)-F(11)-P(1)  | 6.4(3)    |

|                 |           |
|-----------------|-----------|
| F(6)-F(12)-P(1) | 80.0(10)  |
| F(6)-F(12)-P(2) | 86.6(10)  |
| P(1)-F(12)-P(2) | 6.7(3)    |
| F(6)-F(12)-F(4) | 134.8(12) |
| P(1)-F(12)-F(4) | 56.7(4)   |
| P(2)-F(12)-F(4) | 50.6(4)   |
| F(2)-F(13)-F(5) | 137.5(9)  |
| F(2)-F(13)-P(1) | 76.8(6)   |
| F(5)-F(13)-P(1) | 62.4(4)   |
| F(2)-F(13)-P(2) | 70.5(6)   |
| F(5)-F(13)-P(2) | 68.2(4)   |
| P(1)-F(13)-P(2) | 6.6(3)    |
| F(3)-F(14)-F(4) | 124.7(9)  |
| F(3)-F(14)-P(2) | 70.8(4)   |
| F(4)-F(14)-P(2) | 58.6(4)   |
| F(3)-F(14)-P(1) | 64.8(4)   |
| F(4)-F(14)-P(1) | 63.7(4)   |
| P(2)-F(14)-P(1) | 6.1(3)    |
| F(5)-F(15)-F(3) | 140.2(12) |
| F(5)-F(15)-P(1) | 76.3(6)   |
| F(3)-F(15)-P(1) | 72.6(5)   |
| F(5)-F(15)-P(2) | 78.0(5)   |
| F(3)-F(15)-P(2) | 70.3(5)   |
| P(1)-F(15)-P(2) | 2.6(4)    |
| F(4)-F(16)-F(2) | 112.5(8)  |
| F(4)-F(16)-P(2) | 60.4(4)   |
| F(2)-F(16)-P(2) | 59.3(4)   |
| F(4)-F(16)-P(1) | 61.6(4)   |
| F(2)-F(16)-P(1) | 57.4(3)   |
| P(2)-F(16)-P(1) | 2.1(3)    |

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Table 4. Anisotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for 1.

The anisotropic displacement factor exponent takes the form:

$$-2\pi^2 [h^2 a^{*2} U_{11} + \dots + 2hk a^* b^* U_{12}]$$

|       | U11     | U22     | U33     | U23    | U13     | U12      |
|-------|---------|---------|---------|--------|---------|----------|
| Fe(1) | 39(1)   | 28(1)   | 40(1)   | -4(1)  | -2(1)   | 5(1)     |
| C(1)  | 44(2)   | 29(1)   | 46(2)   | -3(1)  | 4(1)    | 9(1)     |
| C(2)  | 54(2)   | 39(2)   | 47(2)   | 1(1)   | 0(2)    | 15(2)    |
| C(3)  | 58(2)   | 57(2)   | 56(2)   | -19(2) | -17(2)  | 19(2)    |
| C(4)  | 41(2)   | 46(2)   | 91(3)   | -18(2) | -9(2)   | 0(2)     |
| C(5)  | 41(2)   | 38(2)   | 67(2)   | -5(2)  | 7(2)    | 4(1)     |
| C(6)  | 65(2)   | 50(2)   | 43(2)   | 4(2)   | 1(2)    | 18(2)    |
| C(7)  | 44(2)   | 53(2)   | 58(2)   | -9(2)  | -10(2)  | 9(2)     |
| C(8)  | 45(2)   | 55(2)   | 61(2)   | 5(2)   | 9(2)    | 11(2)    |
| C(9)  | 61(2)   | 44(2)   | 47(2)   | -4(2)  | 5(2)    | 16(2)    |
| C(10) | 64(2)   | 31(2)   | 59(2)   | 4(1)   | 4(2)    | 11(2)    |
| Co(1) | 41(1)   | 28(1)   | 52(1)   | -5(1)  | -3(1)   | 3(1)     |
| C(11) | 71(2)   | 32(2)   | 50(2)   | 2(1)   | -3(2)   | 7(2)     |
| C(12) | 97(4)   | 51(2)   | 52(2)   | -2(2)  | -22(2)  | 20(2)    |
| C(13) | 62(3)   | 57(3)   | 97(4)   | -15(2) | -31(3)  | 4(2)     |
| C(14) | 38(2)   | 53(2)   | 130(5)  | -19(3) | 1(2)    | -3(2)    |
| C(15) | 47(2)   | 43(2)   | 83(3)   | -10(2) | 16(2)   | 1(2)     |
| C(16) | 66(3)   | 59(3)   | 153(6)  | -15(4) | -40(4)  | 23(3)    |
| C(17) | 71(3)   | 77(4)   | 141(6)  | 30(4)  | 48(4)   | 32(3)    |
| C(18) | 110(5)  | 71(3)   | 88(4)   | -30(3) | -4(3)   | 45(3)    |
| C(19) | 81(4)   | 36(2)   | 169(7)  | 26(3)  | 34(4)   | 14(2)    |
| C(20) | 149(6)  | 104(5)  | 66(3)   | 24(3)  | 11(4)   | 86(5)    |
| B(1)  | 44(2)   | 28(2)   | 53(2)   | 2(1)   | 4(2)    | 7(1)     |
| P(1)  | 61(3)   | 49(2)   | 63(3)   | 1(2)   | 8(2)    | -5(2)    |
| P(2)  | 56(3)   | 46(2)   | 69(3)   | 3(2)   | 13(2)   | -1(2)    |
| F(1)  | 256(18) | 112(9)  | 116(10) | 23(7)  | 51(10)  | -79(10)  |
| F(2)  | 211(13) | 189(14) | 76(5)   | -32(7) | 13(7)   | -137(12) |
| F(3)  | 165(12) | 188(14) | 113(8)  | -57(9) | 10(8)   | -92(10)  |
| F(4)  | 190(17) | 293(25) | 376(31) | 30(24) | 25(19)  | 188(18)  |
| F(5)  | 179(14) | 241(19) | 265(21) | 72(16) | 43(14)  | 132(14)  |
| F(6)  | 340(24) | 206(15) | 107(8)  | 2(10)  | 87(13)  | -144(16) |
| F(11) | 83(5)   | 138(10) | 200(14) | -86(9) | 99(8)   | -48(6)   |
| F(12) | 138(8)  | 186(11) | 107(7)  | -17(7) | 74(6)   | -86(8)   |
| F(13) | 242(17) | 26(3)   | 195(14) | -19(5) | 64(12)  | -7(5)    |
| F(14) | 181(12) | 70(5)   | 177(11) | -55(6) | 93(10)  | -10(6)   |
| F(15) | 196(14) | 283(22) | 144(11) | 20(14) | -85(11) | 113(15)  |
| F(16) | 112(7)  | 207(14) | 104(7)  | 56(8)  | 2(5)    | 47(8)    |

Table 5. Hydrogen coordinates ( $\times 10^4$ ) and isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for 1.

|       | x       | y        | z       | U(eq)   |
|-------|---------|----------|---------|---------|
| H(2)  | 2325(4) | 988(2)   | 5983(3) | 59(6)   |
| H(3)  | 3567(4) | 2144(2)  | 6728(4) | 59(6)   |
| H(4)  | 4611(4) | 2668(2)  | 5000(5) | 59(6)   |
| H(5)  | 4060(3) | 1847(2)  | 3167(4) | 59(6)   |
| H(6)  | 1443(4) | 2869(2)  | 2323(3) | 65(6)   |
| H(7)  | 6(4)    | 1880(2)  | 3026(4) | 65(6)   |
| H(8)  | -201(4) | 2120(2)  | 5255(4) | 65(6)   |
| H(9)  | 1148(4) | 3249(2)  | 5922(3) | 65(6)   |
| H(10) | 2166(4) | 3714(2)  | 4110(4) | 65(6)   |
| H(11) | 3141(4) | 797(2)   | 1730(4) | 78(7)   |
| H(12) | 1869(5) | 35(3)    | 380(4)  | 78(7)   |
| H(13) | 296(5)  | -706(3)  | 1038(5) | 78(7)   |
| H(14) | -67(4)  | -734(3)  | 3075(6) | 78(7)   |
| H(15) | 1153(4) | -28(2)   | 4530(4) | 78(7)   |
| H(16) | 4763(6) | -417(3)  | 3865(8) | 126(11) |
| H(17) | 4645(6) | -727(4)  | 1706(8) | 126(11) |
| H(18) | 3085(7) | -1751(3) | 1253(6) | 126(11) |
| H(19) | 2162(6) | -2062(3) | 3173(8) | 126(11) |
| H(20) | 3289(8) | -1223(4) | 4813(5) | 126(11) |

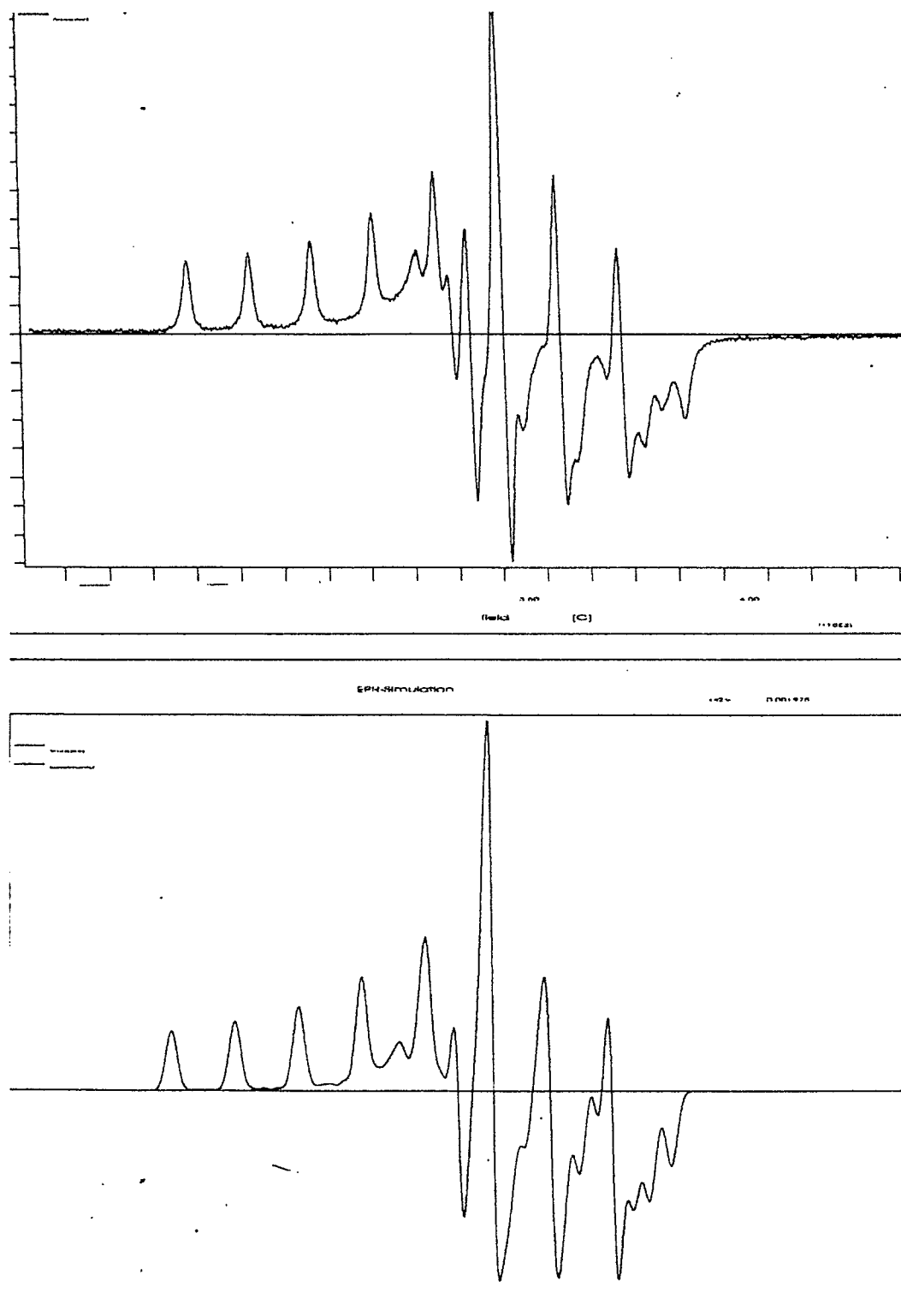


Figure S 1: Experimental (top) and simulated (bottom) ESR spectra of 1