Syntheses, Luminescence Switching and Electrochemical Studies of Photochromic

Dithienyl-1,10-Phenanthroline Zinc(II) Bis(thiolate) Complexes

Tung-Wan Ngan, Chi-Chiu Ko, Nianyong Zhu, Vivian Wing-Wah Yam*

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Supporting Information
Table S1  Crystal data and structure refinement for complex 4.

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Table S3  Bond lengths [Å] and angles [°] for complex 4

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Symmetry transformations used to generate equivalent atoms:

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N(1)-C(1)-C(2) 122.9(4) C(18)-C(19)-C(20) 110.7(4)
C(3)-C(2)-C(1) 119.9(4) C(21)-C(20)-C(19) 112.3(4)
C(2)-C(3)-C(4) 119.4(4) C(21)-C(20)-C(12) 123.1(4)
C(5)-C(4)-C(3) 117.0(4) C(19)-C(20)-C(12) 124.6(4)
C(5)-C(4)-C(11) 119.6(3) C(20)-C(21)-C(22) 129.4(4)
C(3)-C(4)-C(11) 123.4(4) C(20)-C(21)-S(4) 110.9(4)
N(1)-C(5)-C(4) 123.5(3) C(22)-C(21)-S(4) 119.6(4)
N(1)-C(5)-C(6) 116.8(4) C(24)-C(23)-C(28) 115.7(4)
C(4)-C(5)-C(6) 119.6(4) C(24)-C(23)-S(1) 122.2(4)
N(2)-C(6)-C(7) 123.3(3) C(28)-C(23)-S(1) 122.1(4)
N(2)-C(6)-C(5) 116.6(3) C(23)-C(24)-C(25) 122.6(4)
C(7)-C(6)-C(5) 120.0(4) C(26)-C(25)-C(24) 121.0(4)
C(6)-C(7)-C(8) 116.0(4) C(27)-C(26)-C(25) 116.6(5)
C(6)-C(7)-C(12) 119.8(3) C(27)-C(26)-C(29) 122.8(5)
C(8)-C(7)-C(12) 124.1(4) C(25)-C(26)-C(29) 120.7(5)
C(9)-C(8)-C(7) 118.8(4) C(27)-C(28)-C(23) 120.3(5)
N(2)-C(10)-C(9) 122.2(4) C(35)-C(30)-C(31) 116.3(4)
C(12)-C(11)-C(4) 121.0(4) C(35)-C(30)-S(2) 121.4(4)
C(12)-C(11)-C(15) 122.6(4) C(31)-C(30)-S(2) 122.3(4)
C(4)-C(11)-C(15) 116.4(4) C(32)-C(31)-C(30) 120.9(4)
C(11)-C(12)-C(7) 119.9(4) C(33)-C(32)-C(31) 122.0(4)
C(11)-C(12)-C(20) 121.4(4) C(34)-C(33)-C(32) 117.2(4)
C(7)-C(12)-C(20) 118.8(3) C(34)-C(33)-C(36) 121.7(5)
C(14)-C(13)-S(3) 113.2(5) C(32)-C(33)-C(36) 121.1(5)
C(13)-C(14)-C(15) 109.9(6) C(33)-C(34)-C(35) 121.3(5)
C(16)-C(15)-C(14) 114.1(6) C(30)-C(35)-C(34) 122.2(4)
C(16)-C(15)-C(11) 124.5(6) Cl(1)-C(37)-Cl(2) 113.6(3)
C(14)-C(15)-C(11) 121.2(5)
C(15)-C(16)-C(17) 128.7(6)
C(15)-C(16)-S(3) 113.1(5)
C(17)-C(16)-S(3) 118.2(5)
Table S4  Anisotropic displacement parameters (Å$^2$×10$^3$) for complex 4. The anisotropic displacement factor exponent takes the form: -2π$^2$[h^2α^2U$^{11}$ + ... + 2hka*b*U$^{12}$]

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Table S5  Hydrogen coordinates ($\times10^4$) and isotropic displacement parameters ($\AA^2\times10^3$) for complex 4.

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**Table S6**  Crystal data and structure refinement for complex 6(1)

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Symmetry transformations used to generate equivalent atoms:
Table S9  Anisotropic displacement parameters (Å²×10³) for complex 6. The anisotropic displacement factor exponent takes the form: -2π²[h²a*²U₁₁ + ... + 2hka*b*U₁₂]

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