

Sequential recognition of zinc ion and hydrogen sulfide by a new quinoline derivative with logic gate behavior

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Experimental Sections

1.1 Synthesis of compound 1

Compound 1 was obtained by the procedure of literature.¹ ¹H-NMR (CDCl₃, 400 MHz): δ=2.03 (s, 2H, -NH₂), 3.59 (s, 2H, CH₂NH₂), 7.30-7.46 (m, 3H), 8.01 (m, 1H), 8.76 (m, 2H), 11.22 (s, NHCO, 1H); ¹³C NMR (CDCl₃, 100 MHz): δ 45.73, 115.99, 121.08, 121.30, 126.75, 127.58, 133.82, 135.72, 138.41, 148.05, 171.29. EI (M/z): 201.

1.2 Synthesis of compound 2

4-Methyl-2, 6-Diformyl Phenol was synthesized as reported.² ¹H NMR (CDCl₃, 400 MHz): δ 2.39 (s, 3H), 7.77 (s, 2H), 10.21 (s, 2H), 11.46 (s, 1H) ppm; ¹³C NMR (CDCl₃, 100 MHz): δ 20.17, 122.97, 129.6, 138.07, 161.84, 193.1 ppm; EI: (m/z) 164.

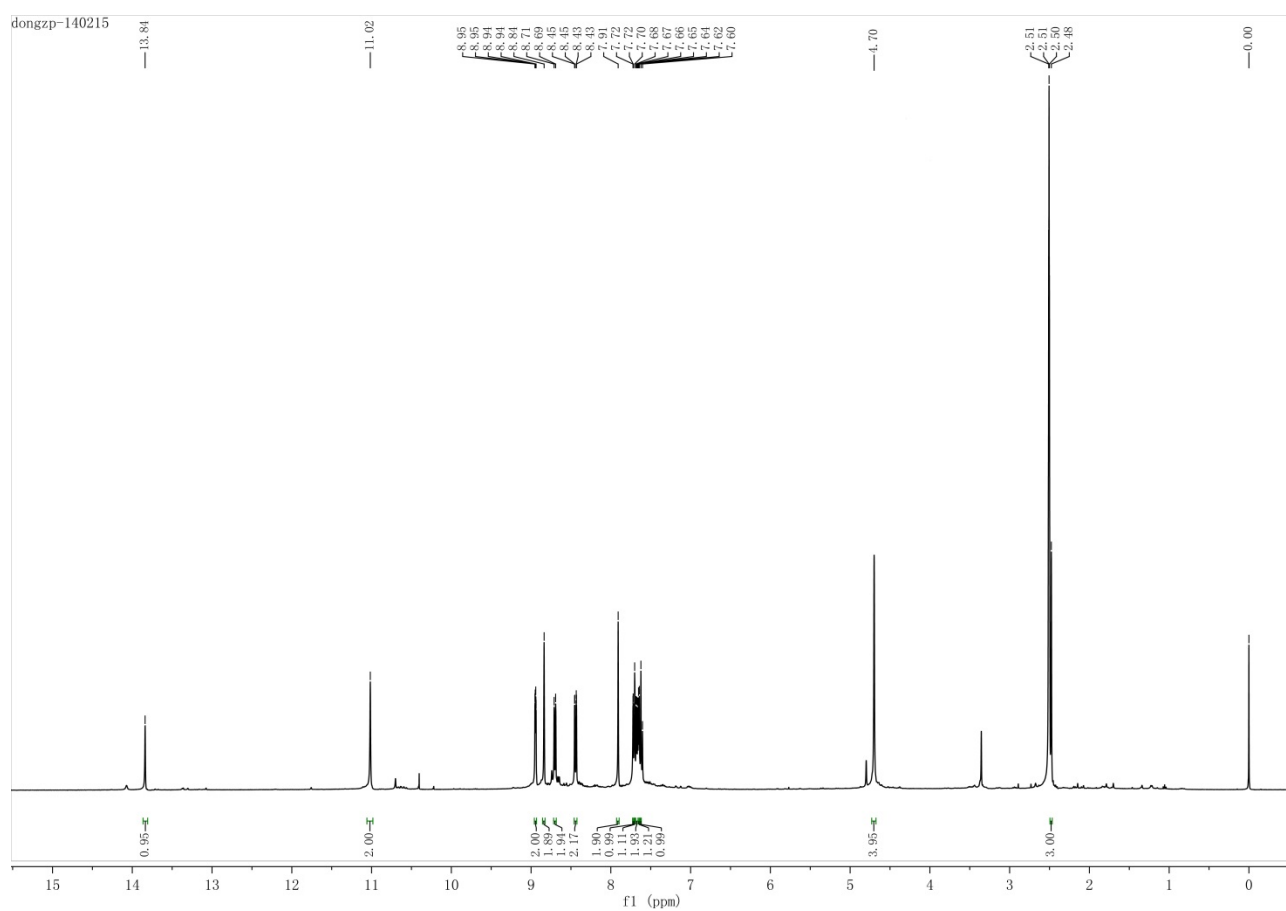
1.3 Synthesis of compound L

A stirred solution of Compound 1 (0.442 g, 2.2 mmol), 4-Methyl-2, 6-Diformyl Phenol (0.164 g, 1.0 mmol) in ethanol (50 mL) was heated under reflux for 5 h under N₂ atmosphere. Then the yellow precipitate was filtered and washed with ethanol several times to give the compound **L** (0.37 g, yield: 70%). Mp.: 138-139°C; ¹H NMR (d⁶-DMSO, 400 MHz): δ 2.48 (s, 3H, Ar-CH₃), 4.70 (s, 4H), 7.60-7.72, 8.43, 8.70, 8.84, 8.94 (14H, Ar-H), 7.91 (s, 2H, Ar-NH), 11.02 (s, 2H, N=CH), 13.84 (s, 1H, Ar-OH) ppm; Solid State ¹³C CP MAS NMR: δ 20.93, 63.24, 114.48, 119.83, 123.55, 127.25, 130.76, 135.29, 138.78, 146.39, 158.95, 169.06, 172.86 ppm; FT-IR (KBr pellet, cm⁻¹): 3300, 2968-2987, 1682, 1529, 1433, 1386, 1317, 1160, 935, 793; ESI: 531.4 [M+H]⁺, calcd C₃₁H₂₆N₆O₃=530.21.

References

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- 2 J. C. Wu, N. Tang, W. S. Liu, M. Y. Tan and A. S. C. Chan, *Chin. Chem. Lett.*, 2001, **12**, 757-760.

¹H NMR of L



Solid State ^{13}C CP MAS NMR of L

