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A series of 2-D and 3-D silver(I) coordination polymers constructed from a new angular-shaped di-2-pyrazinylsulfide: role of anions in molecular construction

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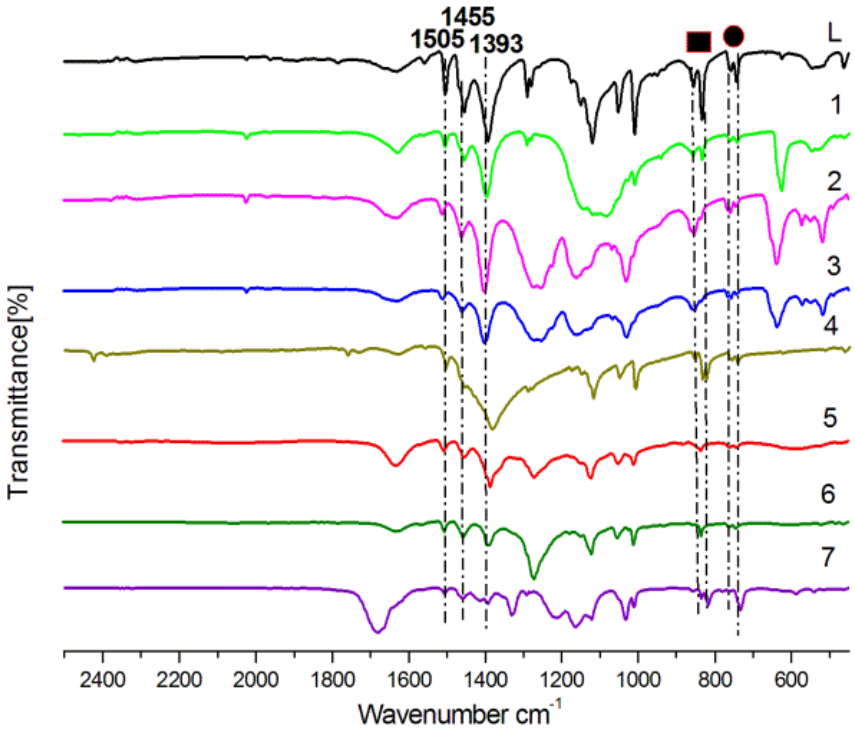
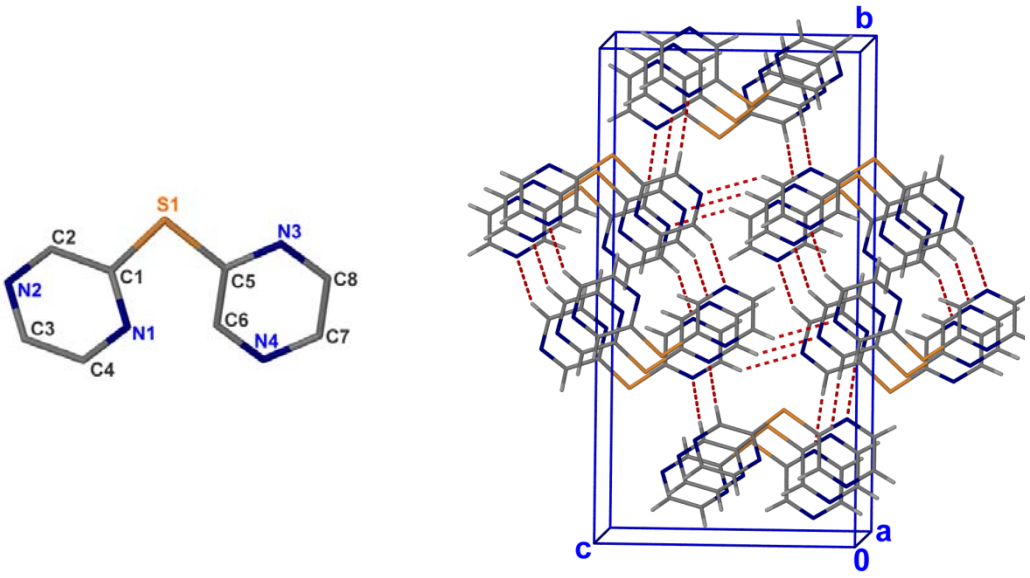


Fig. S1 FTIR spectra of DpzS (L) and complexes **1-7**. and denote double bands around 841~861 cm^{-1} and 730~756 cm^{-1}, respectively.



(a) (b)

Fig. S2 (a) Structure of DpzS. Selected bond lengths: S1–C5 1.763(2) Å, S1–C1 1.765(2) Å; C5–S1–C1 angle 104.28(8)°. (b) Intermolecular C-H···N interactions of DpzS, with $\pi\cdots\pi$ interactions omitted for clarity.

Di-2-pyrazinylsulfide (DpzS) was found reported very recently in Z. Kristallogr. New Cryst.Struct. (2013), 228(3), 325-326, doi: 10.1524/ncrs.2013.0158 by Dr. Jia *et al*, the crystallographic data of which exhibit slightly different from that in this study. The selected crystallographic data of the DpzS Ligand herein are listed as following: Empirical formula, $C_8H_6N_4S$, M = 190.23, Monoclinic, space group $P2_1/n$, a = 3.90610(1) Å, b = 20.4757(3) Å, c = 10.6097(2) Å, α = 90°, β = 98.4360(1) °, γ = 90°, V =839.38 Å^3, Z = 4, D_c = 1.505 g mm^{-3}, μ(Mo-Ka) = 0.337 mm^{-1}, 2017 unique (R_{int} = 0.0387) and 1469 observed ($I > 2\sigma(I)$) reflections, $R1$ = 0.0405, $wR2$ = 0.1178, S = 1.091. Herein, the value of the C–S–C bond angle of DpzS is 104.28(8)° with the dihedral angle between the pair of pyrazinyl rings equaling 48.54(3)°, a typical angular configuration (Fig. S2). Such angular-shaped molecules are arranged along the a axis through intermolecular π(pyrazinyl)···π(pyrazinyl) interactions (centroid···centroid = 3.906(2) Å) to form a column arrangement, which are parallel and stacked to form a three-dimensional (3-D) framework through intermolecular C-H···N hydrogen bonding interactions (C2-H···N3a: D···A 3.515(2) Å, D-H···A 171.9°; C3-H···N4b: D···A 3.511(3) Å, D-H···A 114.2°; C8-H···N2c: D···A 3.364(2) Å, D-H···A 137.7°. Symmetry codes: a $x - {}^1/_2, -y + {}^1/_2, z + {}^1/_2$; b $-x, -y, -z+1$; c $x, y, z - 1$), as shown in Fig. S2b.

Table S1. Selected bond lengths and bond angles in DpzS and complexes **1-7**.

	Bond	d, Å	Angle	ω, deg
DpzS	S(1)-C(5)	1.7626(2)	C(5)-S(1)-C(1)	104.28(8)
	S(1)-C(1)	1.7648(2)	C(5)-N(3)-C(8)	115.82(2)
	C(2)-N(2)	1.320(2)	C(6)-N(4)-C(7)	116.15(2)
	C(4)-N(1)	1.331(2)	N(1)-C(1)-C(2)	121.53(2)
	N(3)-C(5)	1.332(2)	N(1)-C(1)-S(1)	121.47(1)
	N(3)-C(8)	1.332(2)	C(2)-C(1)-S(1)	116.97(1)
	N(4)-C(6)	1.319(2)	C(4)-N(1)-C(1)	115.78(1)
	N(4)-C(7)	1.336(2)	C(2)-N(2)-C(3)	116.05(2)
	C(1)-N(1)	1.331(2)	N(3)-C(5)-C(6)	121.51(2)
	C(3)-N(2)	1.337(3)	N(3)-C(5)-S(1)	114.33(1)
			C(6)-C(5)-S(1)	124.03(1)
	Bond	d, Å	Angle	ω, deg
1	Ag(1)-N(2)	2.411(5)	N(2)-Ag(1)-N(2)a	99.1(2)

	Ag(2)-N(1)	2.426(4)	N(1)-Ag(2)-N(1)b	159.7(2)
	Ag(2)-Ag(3)	2.9918(1)	N(1)-Ag(2)-Ag(3)	79.85(1)
	Ag(3)-O(6)	2.464(7)	O(6)bAg(3)-O(6)	112.0(4)
	Ag(3)-S(1)	2.507(2)	O(6)bAg(3)-S(1)b	96.52(4)
	N(1)-C(1)	1.321(7)	S(1)bAg(3)-S(1)	156.56(1)
	N(1)-C(4)	1.340(7)	O(6)Ag(3)-Ag(2)	124.01(2)
	N(2)-C(3)	1.321(7)	S(1)-Ag(3)-Ag(2)	78.28(5)
	N(2)-C(2)	1.328(7)	C(1)-N(1)-Ag(2)	121.1(4)
	S(1)-C(1)	1.790(5)	C(4)-N(1)-Ag(2)	122.6(4)
			C(3)-N(2)-Ag(1)	120.9(4)
			C(2)-N(2)-Ag(1)	122.5(4)
			C(1)-S(1)-Ag(3)	104.37(2)
	Symmetry codes: a $x, -y + {}^{3}/_{2}, z$; b $-x + 1, -y + {}^{1}/_{2}, z$			
	Bond	d, Å	Angle	ω, deg
2	Ag(1)-N(2)	2.2661(2)	N(2)a-Ag(1)-N(2)	141.29(1)
	Ag(2)-N(1)	2.2229(2)	N(1)-Ag(2)-N(4)b	144.60(7)
	Ag(2)-N(4)b	2.2981(2)	N(1)-Ag(2)-N(3)c	131.74(7)
	Ag(2)-N(3)c	2.4352(2)	N(4)b-Ag(2)-N(3)c	83.48(6)
	S(1)-C(1)	1.755(2)	C(1)-S(1)-C(5)	105.41(1)
	S(1)-C(5)	1.771(2)	C(4)-N(1)-Ag(2)	121.18(1)
			C(1)-N(1)-Ag(2)	120.45(1)
			C(3)-N(2)-Ag(1)	115.67(2)
			C(2)-N(2)-Ag(1)	126.97(1)
			C(5)-N(3)-Ag(2)c	112.89(1)
			C(8)-N(3)-Ag(2)c	131.06(2)
			C(7)-N(4)-Ag(2)e	122.46(2)
			C(6)-N(4)-Ag(2)e	119.08(2)
	Symmetry codes: a $-x + 1, y, -z + {}^{1}/_{2}$; b $x, -y, z + {}^{1}/_{2}$; c $-x + {}^{1}/_{2}, -y + {}^{1}/_{2}, -z + 1$; d $-x + 1, y, -z + {}^{3}/_{2}$; e $x, -y, z - {}^{1}/_{2}$			
	Bond	d, Å	Angle	ω, deg
3	Ag(1)-N(7)c	2.254(5)	N(7)a-Ag(1)-O(1W)	132.4(2)
	Ag(1)-O(1W)	2.352(6)	N(7)a-Ag(1)-N(1)	120.0(2)
	Ag(1)-N(1)	2.376(6)	O(1W)-Ag(1)-N(1)	96.1(2)
	Ag(1)-O(2W)	2.419(6)	N(7)a-Ag(1)-O(2W)	125.52(2)

	Ag(2)-N(8)b	2.242(5)	O(1W)-Ag(1)-O(2W)	82.0(2)
	Ag(2)-N(3)	2.265(5)	N(1)-Ag(1)-O(2W)	88.1(2)
	Ag(2)-O(9)	2.401(17)	N(8)b-Ag(2)-N(3)	146.5(2)
	Ag(2)-N(6)	2.403(6)	N(8)b-Ag(2)-O(9)	94.7(6)
	Ag(3)-N(2)c	2.274(6)	N(3)-Ag(2)-O(9)	105.1(7)
	Ag(3)-N(5)	2.302(6)	N(3)-Ag(2)-N(6)	104.3(2)
	Ag(3)-N(4)d	2.402(5)	O(9)-Ag(2)-N(6)	89.4(6)
			N(2)c-Ag(3)-N(5)	152.94(2)
			N(2)c-Ag(3)-N(4)d	105.9(2)
			N(5)-Ag(3)-N(4)d	95.93(2)
			C(5)-S(1)-C(1)	102.3(3)
			C(13)-S(2)-C(9)	102.0(3)
			C(2)-N(2)-Ag(3)c	123.5(4)
			C(3)-N(2)-Ag(3)c	119.1(5)
			C(7)-N(4)-Ag(3)e	120.8(4)
			C(6)-N(4)-Ag(3)e	122.3(4)
			C(13)-N(7)-Ag(1)f	120.0(4)
			C(16)-N(7)-Ag(1)f	123.3(4)
			C(14)-N(8)-Ag(2)b	120.8(4)
			C(15)-N(8)-Ag(2)b	123.2(4)
	Symmetry codes: a $x+1,y-1,z$; b $-x+1,-y+1,-z+2$; c $-x+1,-y+1,-z+1$; d $x-1,y,z$; e $x+1,y,z$; f $x-1,y+1,z$			
	Bond	d, Å	Angle	ω, deg
4	Ag(1)-N(4)a	2.280(4)	N(4)a-Ag(1)-N(1)	117.83(1)
	Ag(1)-N(1)	2.358(4)	N(4)a-Ag(1)-O(1W)	107.01(2)
	Ag(1)-O(1W)	2.363(4)	N(1)-Ag(1)-O(1W)	113.00(2)
	Ag(1)-N(3)b	2.392(4)	N(4)a-Ag(1)-N(3)b	126.68(1)
	Ag(2)-N(2)	2.244(4)	N(1)-Ag(1)-N(3)b	101.21(1)
	Ag(2)-O(2)	2.429(4)	O(1W)-Ag(1)-N(3)b	87.29(2)
	Ag(2)-O(3)	2.536(4)	N(2)-Ag(2)-O(2)	157.99(1)
	Ag(2)-O(4)	2.538(4)	N(2)-Ag(2)-O(3)	143.41(1)
	S(1)-C(1)	1.765(4)	O(2)-Ag(2)-O(3)	51.08(1)
	S(1)-C(5)	1.772(5)	N(2)-Ag(2)-O(4)	106.05(2)
			O(2)-Ag(2)-O(4)	87.11(2)

			O(3)-Ag(2)-O(4)	90.55(2)
			C(1)-S(1)-C(5)	102.6(2)
			C(4)-N(1)-Ag(1)	128.0(3)
			C(1)-N(1)-Ag(1)	114.2(3)
			C(5)-N(3)-Ag(1)c	120.3(3)
			C(8)-N(3)-Ag(1)c	123.9(3)
			C(6)-N(4)-Ag(1)d	122.9(3)
			C(7)-N(4)-Ag(1)d	120.5(3)
			N(5)-O(2)-Ag(2)	96.6(3)
			N(5)-O(3)-Ag(2)	92.4(3)
			N(6)-O(4)-Ag(2)	100.7(4)
	Symmetry codes: a $x,y,z+1$; b $x+{}^1/_2, -y+{}^1/_2, z+{}^1/_2$; c $x-{}^1/_2, -y+{}^1/_2, z-{}^1/_2$; d $x,y,z-1$			
	Bond	d, Å	Angle	ω, deg
5	Ag(1)-N(3)	2.214(4)	N(3)-Ag(1)-N(1)a	127.43(7)
	Ag(1)-N(1)	2.3996(2)	N(3)-Ag(1)-N(1)	127.43(7)
	S(1)-C(1)	1.783(2)	N(1)a-Ag(1)-N(1)	82.90(9)
	O(1)-N(3)	1.207(3)	C(1)b-S(1)-C(1	100.67(1)
	N(1)-C(1)	1.332(3)	C(1)-N(1)-C(4)	116.31(2)
	N(1)-C(4)	1.338(3)	C(1)-N(1)-Ag(1)	121.55(1)
	N(2)-C(3)	1.329(3)	C(4)-N(1)-Ag(1)	121.57(2)
	N(2)-C(2)	1.336(4)	C(3)-N(2)-C(2)	116.3(2)
			O(1)-N(3)-Ag(1)	119.7(2)
	Symmetry codes: a $x, -y+{}^1/_2, z$			
	Bond	d, Å	Angle	ω, deg
6	Ag(1)-N(2)	2.274(3)	N(2)-Ag(1)-N(4)a	123.72(1)
	Ag(1)-N(4)a	2.349(4)	N(2)-Ag(1)-O(1)b	140.15(2)
	Ag(1)-O(1)b	2.380(5)	N(4)a-Ag(1)-O(1)b	95.64(2)
	Ag(1)-N(5)	2.635(4)	N(2)-Ag(1)-N(5)	89.27(1)
	Ag(2)-O(2)c	2.353(5)	N(4)a-Ag(1)-N(5)	86.65(1)
	Ag(2)-O(4)d	2.374(4)	O(1)b-Ag(1)-N(5)	86.92(2)
	Ag(2)-N(3)	2.461(4)	O(2)c-Ag(2)-O(4)d	127.07(2)
	Ag(2)-N(1)b	2.557(4)	O(2)c-Ag(2)-N(3)	138.05(2)
	S(1)-C(1)	1.760(4)	O(4)d-Ag(2)-N(3)	93.21(2)

	S(1)-C(5)	1.773(4)	O(2)c-Ag(2)-N(1)b	100.51(1)
			O(4)d-Ag(2)-N(1)b	89.78(1)
			N(3)-Ag(2)-N(1)b	89.55(1)
			C(1)-S(1)-C(5)	100.19(2)
	Symmetry codes: a $-x+{}^{3}/_{2}, -y+{}^{3}/_{2}, -z+1$; b $-x+1, y, -z+{}^{1}/_{2}$; c $-x+1, y-1, -z+{}^{1}/_{2}$; d $-x+{}^{3}/_{2}, y-{}^{1}/_{2}, -z+{}^{1}/_{2}$			
	Bond	d, Å	Angle	ω, deg
7	Ag(1)-O(2)a	2.275(7)	O(2)a-Ag(1)-N(1)	124.8(3)
	Ag(1)-N(1)	2.318(5)	O(2)a-Ag(1)-N(3)b	102.2(2)
	Ag(1)-N(3)b	2.397(6)	N(1)-Ag(1)-N(3)b	113.9(2)
	Ag(1)-O(1)	2.453(6)	O(2)a-Ag(1)-O(1)	139.1(3)
	Ag(1)-Ag(1)a	3.3126(1)	N(1)-Ag(1)-O(1)	88.4(2)
	Ag(2)-N(2)	2.294(6)	N(3)b-Ag(1)-O(1)	81.1(2)
	Ag(2)-O(3)	2.403(9)	O(2)a-Ag(1)-Ag(1)a	92.8(2)
	S(1)-C(1)	1.753(6)	N(1)-Ag(1)-Ag(1)a	95.37(1)
	S(1)-C(5)	1.782(7)	N(3)b-Ag(1)-Ag(1)a	128.65(2)
			O(1)-Ag(1)-Ag(1)a	57.5(2)
			N(4)c-Ag(2)-N(2)	118.9(2)
			N(4)c-Ag(2)-O(3)	131.8(2)
			N(2)-Ag(2)-O(3)	109.2(2)
			C(1)-S(1)-C(5)	101.1(3)
	Symmetry codes: a $-x+1, y, -z+{}^{3}/_{2}$; b $-x+1, -y+1, -z+1$			