Supporting Information to

Assembling novel Cd(II) complexes with the ligands with multidentate nitrogen donors obtained in situ from the system: zerovalent copper, cadmium oxide, 1-hydroxymethyl-3,5-dimethylpyrazole and ammonia salt

Barbara Barszcz,*[a] Joanna Masternak,[a] Wanda Sawka-Dobrowolska,[b]

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Table 1 Selected angels (°) for **1**, **2**.

1		**2**	
S(1)-Cd(1)-S(1)^{I}	180.0	N(4)-Cd-N(13)	107.63(1)
N(4)-Cd(1)-N(4)^{I}	180.0	N(4)-Cd-N(5)	99.78(1)
N(1)-Cd(1)-N(1)^{I}	180.00(5)	N(13)-Cd-N(5)	86.34(9)
N(4)-Cd(1)-N(1)	87.44(4)	N(4)-Cd-N(1)	111.75(1)
N(4)-Cd(1)-N(1)^{I}	92.56(4)	N(13)-Cd-N(1)	140.62(9)
N(4)-Cd(1)-S(1)^{I}	86.12(3)	N(5)-Cd-N(1)	86.88(9)
N(4)-Cd(1)-S(1)	93.88(3)	N(4)-Cd-N(11)	102.87(1)
N(1)-Cd(1)-S(1)^{I}	89.87(3)	N(13)-Cd-N(11)	91.10(9)
N(1)-Cd(1)-S(1)	90.13(3)	N(5)-Cd-N(11)	156.89(1)
N(3)-Cd(2)-N(3)^{II}	169.25(7)	N(1)-Cd-N(11)	80.59(9)
N(3)-Cd(2)-O(1)^{II}	89.87(4)	N(4)-Cd-N(3)	175.89(9)
N(3)-Cd(2)-O(1)	82.25(4)	N(13)-Cd-N(3)	69.91(8)
O(1)-Cd(2)-O(1)^{II}	85.83(7)	N(5)-Cd-N(3)	83.46(9)
N(3)-Cd(2)-S(2)^{II}	92.30(4)	N(1)-Cd-N(3)	70.79(8)
N(3)-Cd(2)-S(2)	95.35(3)	N(11)-Cd-N(3)	74.12(8)
O(1)-Cd(2)-S(2)	177.08(3)		
O(1)-Cd(2)-S(2)^{II}	92.52(3)		
S(2)-Cd(2)-S(2)^{II}	89.227(2)		

Symmetry transformations used to generate equivalent atoms: (**1**) ^{I}-x-1,- y+2, -z, ^{II} -x, y, -z+1/2;

Table 2 Selected short contacts and C-H···π type interactions in the crystal structure of complexes **1**, **2** (Å and °).

Compound	D-H···A	d(D-H) (Å)	d(H···A) (Å)	d(D···A) (Å)	<(DH···A) (°)
1	O(1)-H(1)···N(2)^{I}	0.74	2.09	2.818	169.6
	C(1)-H(11)···S(1)^{II}	0.92	2.84	3.580	137.4
	C(2)-H(2)···S(1)^{II}	0.92	2.99	3.842	154.8
2	C(13)-H(133)···N(1)^{I}	0.96	2.68	3.592	172.3
	C(13)-H(133)···N(2)^{I}	0.96	2.68	3.534	147.8
	C(16)-H(161)···S(2)^{II}	0.97	2.99	3.693	106.4
	C(17)-H(172)···S(2)^{III}	0.97	2.94	3.416	111.5
	C(18)-H(182)···S(2)^{II}	0.97	2.79	3.610	142.8
	C(25)-H(253)···S(1)^{II}	0.96	2.99	3.947	174.5
	D-H···A	$d_{\pi, H}$ (Å)	θ (°)	α (°)	d (Å)
2	C(33)-H(133)···C(5)^{I}	2.61	93	147	0.13
	C(35)-H(351)···C(33)^{III}	2.58	69	143	0.92

Symmetry transformations used to generate equivalent atoms: (**1**) ^{I}-x, y-1, -z+1/2; ^{II}x, -y+2, z-1/2;
(**2**) ^{I}x, y+1, z; ^{II}x+1, y, z; ^{III}-x, -y, -z+1;

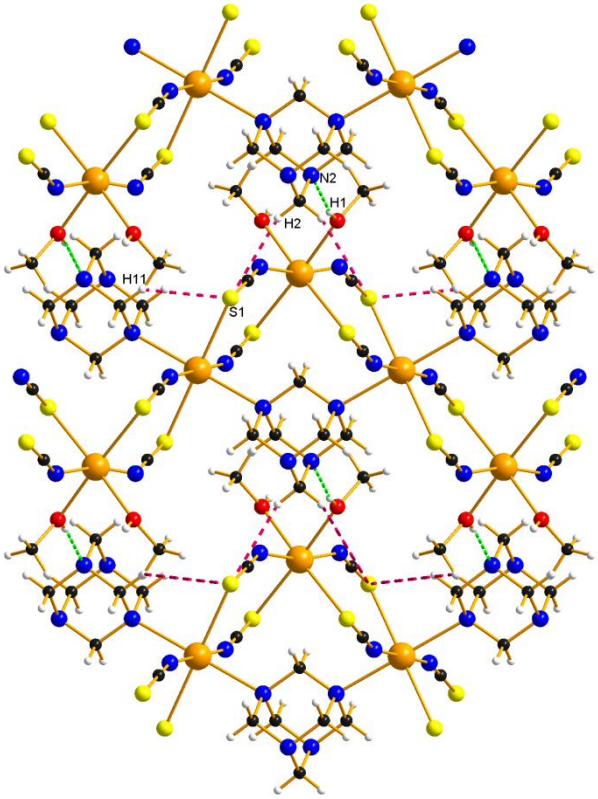

Fig. S1 Perspective view of the 3D network (**4**) with hydrogen bonding interactions O-H···N (green) and C-H···S (wine-cloured) types.

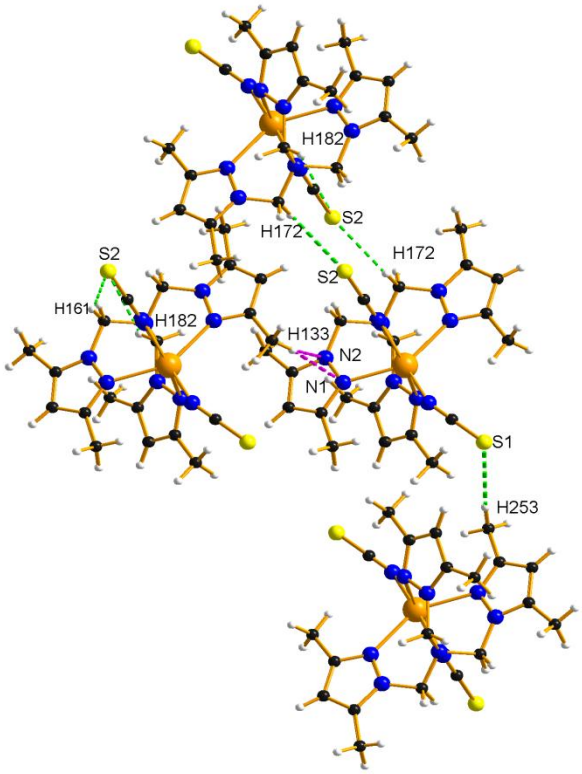

Fig. S2 Perspective view (along c axis) of **5** that emphasizes the intramolecular hydrogen-bonding interaction, C-H···S (green), C-H···N (wine-coloured) type.