

Supporting Information for

**Intermolecular Anagostic Interactions in Group 10 Metal
Dithiocarbamates**

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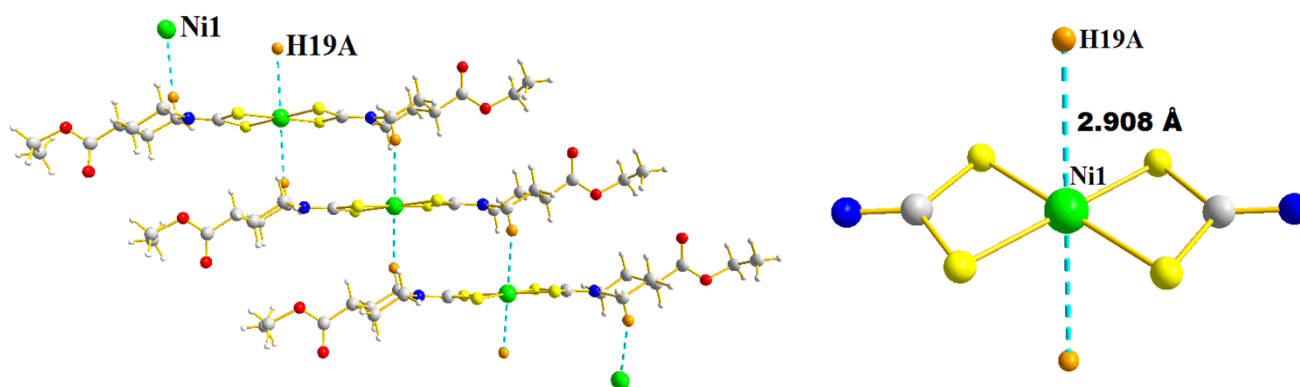
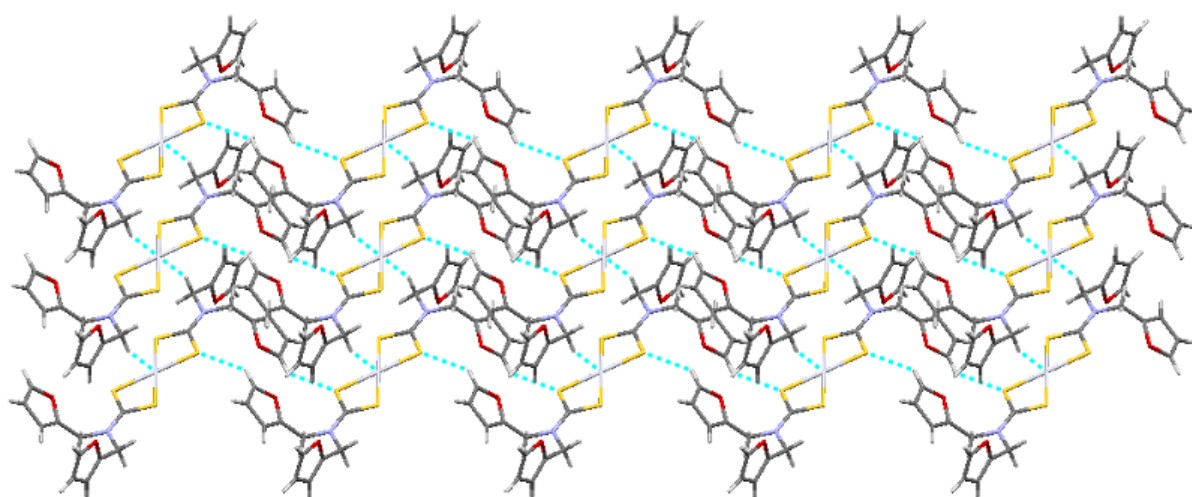
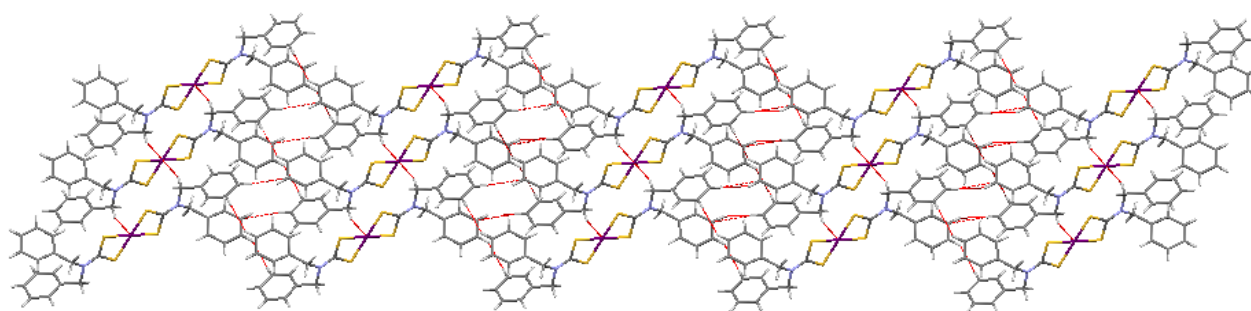


Fig. S1 Intermolecular M...H-C anagostic interactions in **2** presenting 1-D polymeric chain motifs along with their core. Colour code: Ni, Bright green; S, Yellow; N, Ink blue; C, Grey; O, Red; H, Light orange.



(a)



(b)

Figure S2. The supramolecular architecture (a) via Pt...H and S...H interactions in **4** along the b axis (b) via Pd...H and H...H interactions in **5** along the b axis.

Table S1

Compound	1	2	3	4	5
Chemical formula	C20H22NiO4S4	C18H28N2NiO4S4	C22H20N2NiO4S4	C22H20N2O4PtS4	C28H26N4PdS4
Formula weight	513.32	523.37	563.35	699.73	653.17
Crystal system	monoclinic	triclinic	monoclinic	monoclinic	triclinic
Space group	P2 ₁ /n	P-1	P2 ₁ /c	P2 ₁ /c	P-1
<i>a</i> (Å)	4.7556(2)	6.2640(13)	5.6942(9)	5.7453(3)	6.503(6)
<i>b</i> (Å)	5.8030(4)	6.4556(14)	18.8463(14)	19.0518(10)	10.171(9)
<i>c</i> (Å)	39.1558(19)	14.969(3)	10.8100(7)	11.0760(7)	11.709(10)
α (°)	90	78.985(17)	90	90	75.41(8)
β (°)	90.537(4)	86.378(16)	90.696(9)	91.441(4)	80.37(8)
γ (°)	90	86.602(17)	90	90	72.19(8)
<i>V</i> (Å ³)	1080.53(10)	592.3(2)	1160.0(2)	1211.98(12)	710.2(11)
<i>Z</i>	2	1	2	2	1
ρ_{calc} (g cm ⁻³)	1.578	1.467	1.613	1.156	1.527
<i>T</i> (K)	150(2)	293(2)	150(2)	150(2)	293(2)
μ (Mo <i>K</i> α) (mm ⁻¹)	1.309	1.197	1.230	6.166	0.972
<i>F</i> (000)	532	274	580	680	332
Reflections collected	7232	4224	5412	4254	5245
Independent reflections	3156	2600	3292	2128	3100
Reflections with <i>I</i> > 2 σ (<i>I</i>)	2500	1576	2213	1440	1479
Final indices [<i>I</i> > 2 σ (<i>I</i>)] R ₁ ^a , wR ₂ ^b	0.0583, 0.1021	0.0564, 0.1313	0.0588, 0.0977	0.0378, 0.0590	0.0763, 0.1631
R ₁ [_a], wR ₂ [_b] [all data]	0.0791, 0.1096	0.1038, 0.1591	0.1001, 0.1114	0.0660, 0.0671	0.1376, 0.2144
GOF ^c	1.092	0.963	0.982	0.927	0.930
Residual electron Density, e/Å ⁻³	0.669, -0.547	0.515, -0.341	0.569, -0.422	1.156, -0.795	1.266, -1.391

^aR₁ = $\sum \|F_0\| - \|F_c\| / \sum \|F_0\|$, ^bwR₂ = $\{[\sum w (F_0^2 - F_c^2) / \sum w (F_0^2)^2]\}^{1/2}$, ^cGOF = $S = \{ \sum [w(F_0^2 - F_c^2)^2] / (n-p) \}^{1/2}$, where *n* is the number of reflections, and *p* is the number of the refined parameters.