

**Neutral Ni(II), Pd(II) and Pt(II) ONS-pincer complexes of 5-acetylbarbituric-4N-dimethylthiosemicarbazone. Synthesis, characterization and properties.**

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***Supplementary Information***

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**Table SM1.** Selected bond distances (Å) and angles (°) for the thiosemicarbazone in [Ni(HAc4DM)<sub>2</sub>] $\cdot$ 2H<sub>2</sub>O, **1a**, [Pd(Acb4DM)(DMSO)] $\cdot$ DMSO, **2a**, and [Pt(Acb4DM)(DMSO)] $\cdot$ DMSO, **3a**.

Compound	<b>1a</b> <sup>a</sup>	<b>2a</b>	<b>3a</b>	
<i>Distances</i>				
S(1)–C(18)	1.704(3)	1.699(3)	1.769(5)	1.758(7)
C(17)–N(12)	1.289(3)	1.290(3)	1.294(5)	1.292(7)
N(12)–N(13)	1.397(3)	1.404(3)	1.410(5)	1.436(7)
N(13)–C(18)	1.357(4)	1.362(3)	1.287(6)	1.297(8)
C(18)–N(14)	1.326(4)	1.331(3)	1.350(6)	1.358(8)
C(16)–C(17)	1.461(4)	1.468(3)	1.458(6)	1.448(8)
C(11)–C(16)	1.413(4)	1.413(3)	1.410(6)	1.409(8)
C(11)–O(11)	1.252(3)	1.254(3)	1.276(5)	1.281(7)
C(13)–O(13)	1.233(4)	1.234(3)	1.222(5)	1.221(7)
C(15)–O(15)	1.231(4)	1.254(3)	1.232(5)	1.232(7)
<i>Angles</i>				
O(11)–C(11)–N(11)	115.3(2)	115.7(2)	112.1(4)	112.2(5)
O(11)–C(11)–C(16)	127.3(2)	126.7(2)	128.2(4)	127.1(5)
N(11)–C(11)–C(16)	117.4(2)	117.6(2)	119.7(4)	120.8(5)
C(11)–C(16)–C(17)	120.7(2)	120.7(2)	123.2(4)	124.9(5)
C(16)–C(17)–N(12)	118.4(2)	118.4(2)	123.3(4)	121.5(5)
C(17)–N(12)–N(13)	116.6(2)	116.7(2)	115.1(3)	113.6(5)
N(12)–N(13)–C(18)	118.6(2)	117.2(2)	116.5(4)	115.9(5)
N(13)–C(18)–N(14)	116.1(3)	116.0(2)	118.5(5)	117.7(6)
N(13)–C(18)–S(1)	120.7(2)	121.6(2)	123.5(4)	124.0(5)
N(14)–C(18)–S(1)	123.2(2)	122.4(2)	117.9(4)	118.3(5)

<sup>a</sup>) The two columns correspond to the values of molecules of ligand 1 and 2.