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Synthesis of some transition metal complexes of novel 1-methylpyrazole-3-aldehyde-4-(2-pyridyl) thiosemicarbazone: Spectroscopic and in vitro biological activity studies

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ABSTRACT

Four new mixed ligand metal(II) complexes with 1-methylpyrazole-3-aldehyde-4-(2-pyridyl)thiosemicarbazone (MPAPT) and 1,10-phenanthroline are reported. These complexes namely Cu(MPAPT)(1,10-phen)(Cl)] (**1**), [Ni(MPAPT)(1,10-phen)(Cl)] (**2**), [Mn(MPAPT)(1,10-phen)(Cl)].H_2O (**3**) and [Co(MPAPT)(1,10-phen)(Cl)].H_2O (**4**), were characterized by elemental analysis, spectral (IR, ^1H NMR and UV-Vis) and magnetic moment measurements. The magnetic and spectral data indicates octahedral structure for all complexes. Metal complexes have been modeled using parameterized PM3 semi-empirical method. The free ligand and its M(II) chelates have been screened for their antimicrobial activities. The antimicrobial screening demonstrated that, the Cu(II) complex have the maximum and broad activities among the investigated complexes.

Supplementary material

Table S1. Bond distances (Å) and angles (°) for [Co(MPAPT)(1,10-phen)Cl] complex.

Atoms	Bond distances (Å)	Atoms	Angle (°)	Atoms	Angle (°)
C(34)-H(53)	1.101	C(34)-N(35)-C(30)	117.2772	Co(20)-N(17)-C(18)	135.2391
C(34)-N(35)	1.3811	C(34)-N(35)-Co(20)	136.7981	Co(20)-N(17)-N(15)	101.9061
C(33)-H(52)	1.0942	C(30)-N(35)-Co(20)	105.7442	C(18)-N(17)-N(15)	122.8027
C(33)-C(34)	1.3805	H(53)-C(34)-N(35)	118.335	Co(20)-S(16)-C(14)	76.816
C(32)-H(51)	1.0946	H(53)-C(34)-C(33)	119.8108	N(17)-N(15)-C(14)	111.5762
C(32)-C(33)	1.4081	N(35)-C(34)-C(33)	121.8542	S(16)-C(14)-N(15)	124.8698
C(31)-C(32)	1.385	H(52)-C(33)-C(34)	119.6171	S(16)-C(14)-N(7)	119.2454
C(30)-N(35)	1.4101	H(52)-C(33)-C(32)	119.4509	N(15)-C(14)-N(7)	111.8506
C(30)-C(31)	1.421	C(34)-C(33)-C(32)	120.9314	Co(20)-N(13)-C(12)	112.171
C(29)-H(50)	1.0955	H(51)-C(32)-C(33)	119.9768	Co(20)-N(13)-C(8)	132.8817
C(28)-H(49)	1.0943	H(51)-C(32)-C(31)	120.8384	C(12)-N(13)-C(8)	114.8765
C(28)-C(29)	1.3955	C(33)-C(32)-C(31)	119.1843	H(44)-C(12)-N(13)	118.0116
C(27)-H(48)	1.1082	C(32)-C(31)-C(30)	118.857	H(44)-C(12)-C(11)	117.8647
C(27)-C(28)	1.3949	C(32)-C(31)-C(23)	123.0785	N(13)-C(12)-C(11)	124.1193
N(26)-C(27)	1.3619	C(30)-C(31)-C(23)	118.0592	H(43)-C(11)-C(12)	119.1998
C(25)-N(26)	1.4063	N(35)-C(30)-C(31)	121.8296	H(43)-C(11)-C(10)	120.785
C(25)-C(30)	1.4073	N(35)-C(30)-C(25)	117.807	C(12)-C(11)-C(10)	120.0151
C(24)-C(29)	1.3917	C(31)-C(30)-C(25)	120.3459	H(42)-C(10)-C(11)	120.8462
C(24)-C(25)	1.4204	H(50)-C(29)-C(28)	120.1914	H(42)-C(10)-C(9)	120.4967
C(23)-H(47)	1.096	H(50)-C(29)-C(24)	120.2534	C(11)-C(10)-C(9)	118.6565
C(23)-C(31)	1.4437	C(28)-C(29)-C(24)	119.555	H(41)-C(9)-C(10)	120.1161
C(22)-H(46)	1.0962	H(49)-C(28)-C(29)	120.1614	H(41)-C(9)-C(8)	120.1093

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Table S1. (Continued).

Atoms	Bond distances (Å)	Atoms	Angle (°)	Atoms	Angle (°)
C(22)-C(24)	1.4391	H(49)-C(28)-C(27)	119.0894	C(10)-C(9)-C(8)	119.7735
C(22)-C(23)	1.3539	C(29)-C(28)-C(27)	120.7409	N(13)-C(8)-C(9)	122.5317
Co(20)-N(26)	1.906	H(48)-C(27)-C(28)	120.7723	N(13)-C(8)-N(7)	118.9358
Co(20)-N(35)	1.9262	H(48)-C(27)-N(26)	117.9591	C(9)-C(8)-N(7)	118.4535
Co(20)-Cl(21)	2.2349	C(28)-C(27)-N(26)	121.2608	H(19)-N(7)-C(14)	117.8339
C(18)-H(45)	1.118	C(27)-N(26)-C(25)	118.6267	H(19)-N(7)-C(8)	114.4391
N(17)-Co(20)	1.9472	C(27)-N(26)-Co(20)	134.5134	C(14)-N(7)-C(8)	103.3805
N(17)-C(18)	1.3136	C(25)-N(26)-Co(20)	106.4311	H(40)-C(6)-H(39)	108.8056
S(16)-Co(20)	2.297	C(30)-C(25)-N(26)	117.9672	H(40)-C(6)-H(38)	108.1669
N(15)-N(17)	1.4123	C(30)-C(25)-C(24)	120.8153	H(40)-C(6)-N(2)	110.9487
C(14)-S(16)	1.7631	N(26)-C(25)-C(24)	121.2156	H(39)-C(6)-H(38)	108.5526
C(14)-N(15)	1.3259	C(29)-C(24)-C(25)	118.5838	H(39)-C(6)-N(2)	109.2362
N(13)-Co(20)	1.9966	C(29)-C(24)-C(22)	123.352	H(38)-C(6)-N(2)	111.0685
C(12)-H(44)	1.1048	C(25)-C(24)-C(22)	118.0642	H(37)-C(5)-C(4)	129.0625
C(12)-N(13)	1.3645	H(47)-C(23)-C(31)	117.6087	H(37)-C(5)-N(1)	121.5682
C(11)-H(43)	1.096	H(47)-C(23)-C(22)	121.0115	C(4)-C(5)-N(1)	109.3693
C(11)-C(12)	1.3923	C(31)-C(23)-C(22)	121.3797	H(36)-C(4)-C(5)	126.0252
C(10)-H(42)	1.0956	H(46)-C(22)-C(24)	117.7719	H(36)-C(4)-C(3)	127.2709
C(10)-C(11)	1.3867	H(46)-C(22)-C(23)	120.9504	C(5)-C(4)-C(3)	106.7037
C(9)-H(41)	1.0976	C(24)-C(22)-C(23)	121.2777	C(18)-C(3)-C(4)	132.7494
C(9)-C(10)	1.3891	N(35)-Co(20)-N(26)	90.627	C(18)-C(3)-N(2)	121.6613
C(8)-C(9)	1.3969	N(35)-Co(20)-Cl(21)	85.6496	C(4)-C(3)-N(2)	105.5817
C(8)-N(13)	1.4231	N(35)-Co(20)-N(17)	92.2677	C(6)-N(2)-C(3)	126.0618
N(7)-H(19)	0.9953	N(35)-Co(20)-S(16)	174.0398	C(6)-N(2)-N(1)	123.3397
N(7)-C(14)	1.4675	N(35)-Co(20)-N(13)	95.5768	C(3)-N(2)-N(1)	110.5875
N(7)-C(8)	1.4547	N(26)-Co(20)-Cl(21)	86.4626	C(5)-N(1)-N(2)	107.7574
C(6)-H(40)	1.099	N(26)-Co(20)-N(17)	170.072		
C(6)-H(39)	1.1042	N(26)-Co(20)-S(16)	91.0014		
C(6)-H(38)	1.0993	N(26)-Co(20)-N(13)	91.2435		
C(5)-H(37)	1.0893	Cl(21)-Co(20)-N(17)	84.2916		
C(4)-H(36)	1.0883	Cl(21)-Co(20)-S(16)	88.7287		
C(4)-C(5)	1.4142	Cl(21)-Co(20)-N(13)	177.4144		
C(3)-C(18)	1.4406	N(17)-Co(20)-S(16)	85.1943		
C(3)-C(4)	1.4024	N(17)-Co(20)-N(13)	97.9199		
N(2)-C(6)	1.469	S(16)-Co(20)-N(13)	90.1198		
N(2)-C(3)	1.4126	H(45)-C(18)-N(17)	116.6279		
N(1)-C(5)	1.3613	H(45)-C(18)-C(3)	115.932		
N(1)-N(2)	1.3478	N(17)-C(18)-C(3)	127.4082		