



SUPPLEMENTARY MATERIAL TO
Microwave synthesis and spectral, thermal and antimicrobial activities of some novel transition metal complexes with tridentate Schiff base ligands

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Table S-I. Analytical and molar conductance data of the compounds

Compound Empirical formula (FW)	Elemental analysis, Found (Calcd.), %				$\Lambda_m / \Omega^{-1} \text{ cm}^2 \text{ mol}^{-1}$
	C	H	N	M	
BSAP	49.02	3.07	9.50	–	–
C ₁₂ H ₉ N ₂ O ₂ Br (293.12)	(49.17)	(3.09)	(9.56)		
[Cr(BSAP)(H ₂ O) ₃]Cl	33.29	2.98	6.45	11.97	92.5
C ₁₂ H ₇ N ₂ O ₂ BrClCr (432.60)	(33.32)	(3.03)	(6.48)	(12.01)	
[Co(BSAP)(H ₂ O) ₃]	35.65	3.20	6.87	14.55	17.6
C ₁₂ H ₁₃ N ₂ O ₅ BrCo (404.08)	(35.67)	(3.24)	(6.93)	(14.58)	
[Ni(BSAP)(H ₂ O) ₃]	35.65	3.19	6.90	14.50	11.5
C ₁₂ H ₁₃ N ₂ O ₅ BrNi (403.84)	(35.69)	(3.24)	(6.94)	(14.53)	
[Cu(BSAP)(H ₂ O)]	38.67	2.39	7.49	17.0	12.8
C ₁₂ H ₉ N ₂ O ₃ BrCu (372.66)	(38.68)	(2.43)	(7.52)	(17.05)	
HNAC	74.35	4.11	3.58	–	–
C ₂₄ H ₁₆ NO ₂ Cl (385.84)	(74.41)	(4.18)	(3.63)		
[Cr(HNAC)(H ₂ O)Cl ₂]	54.80	3.07	2.58	9.47	56.6
C ₂₄ H ₁₇ NO ₃ Cl ₃ Cr (525.75)	(54.83)	(3.10)	(2.66)	(9.89)	
[Co(HNAC)Cl]·2H ₂ O	55.86	3.17	2.61	11.29	36.4
C ₂₄ H ₁₉ NO ₄ Cl ₂ Co (515.25)	(55.94)	(3.72)	(2.72)	(11.44)	
[Ni(HNAC)Cl]·3H ₂ O	54.00	3.91	2.55	10.95	30.6
C ₂₄ H ₂₁ NO ₅ Cl ₂ Ni (533.03)	(54.08)	(3.97)	(2.63)	(11.01)	
[Cu(HNAC)Cl]·2H ₂ O	55.36	3.60	2.60	12.02	49.5
C ₂₄ H ₁₉ NO ₄ Cl ₂ Cu (519.86)	(55.45)	(3.68)	(2.69)	(12.22)	

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Table S-II. IR bands (cm^{-1}) of the Schiff base ligands and their complexes

Compound	$\nu(\text{OH})/\delta(\text{OH})$	$\nu(\text{C}=\text{N})$	$\nu(\text{C}-\text{O})$	$\nu(\text{C}=\text{N})$ (pyridine ring)	$\nu(\text{C}=\text{O})$	$\nu(\text{M}-\text{O})$	$\nu(\text{M}-\text{N})$
BSAP	3150/ 1361	1625	1268	1496	–	–	–
[Cr(BSAP)(H ₂ O) ₃]Cl	–	1596	1290	1495	–	522	490
[Co(BSAP)(H ₂ O) ₃]	–	1603	1295	1492	–	538	486
[Ni(BSAP)(H ₂ O) ₃]	–	1607	1288	1494	–	540	495
[Cu(BSAP)(H ₂ O)]	–	1606	1292	1495	–	526	497
HNAC	3230/ 1336	1613	1236	–	1675	–	–
[Cr(HNAC)(H ₂ O)Cl ₂]	–	1589	1260	–	1640	519	488
[Co(HNAC)Cl]·2H ₂ O	–	1594	1255	–	1652	524	492
[Ni(HNAC)Cl]·3H ₂ O	–	1590	1258	–	1647	527	489
[Cu(HNAC)Cl]·2H ₂ O	–	1582	1263	–	1645	529	485

Table S-III. Magnetic moment values, electronic spectral data and ligand field parameters data of the complexes

Complex	μ_{eff} μ_{B}	λ_{max} cm^{-1}	Band assignments	Ligand field parameter				
				$10Dq$ cm^{-1}	B cm^{-1}	β	$\beta\%$	$LFSE$ kJ mol^{-1}
[Cr(BSAP)(H ₂ O) ₃]Cl	3.88	16654 24212 35982	⁴ A _{2g} → ⁴ T _{2g} (F) ⁴ A _{2g} → ⁴ T _{1g} (F) ⁴ A _{2g} → ⁴ T _{1g} (P)	16654	794.97	0.77	22.82	238.77
[Co(BSAP)(H ₂ O) ₃]	5.02	9486 15823 20618	⁴ T _{1g} → ⁴ T _{2g} (F) ⁴ T _{1g} → ⁴ A _{2g} (F) ⁴ T _{1g} → ⁴ T _{1g} (P)	10696	822.75	0.73	26.54	102.23
[Ni(BSAP)(H ₂ O) ₃]	3.04	10691 20360 23838	³ A _{2g} → ³ T _{2g} (F) ³ A _{2g} → ³ T _{1g} (F) ³ A _{2g} → ³ T _{1g} (P)	10691	808.33	0.78	22.35	153.28
[Cu(BSAP)(H ₂ O)]	1.92	15150 19230	² B _{1g} → ² B _{2g} ² B _{1g} → ² E _g	–	–	–	–	–
[Cr(HNAC)(H ₂ O)Cl ₂]	3.84	16871 23837 34942	⁴ A _{2g} → ⁴ T _{2g} (F) ⁴ A _{2g} → ⁴ T _{1g} (F) ⁴ A _{2g} → ⁴ T _{1g} (P)	16871	704.34	0.68	31.62	241.88
[Co(HNAC)Cl]·2H ₂ O	4.32	– 14142 19514	⁴ A ₂ → ⁴ T ₂ (F) ⁴ A ₂ → ⁴ T ₁ (F) ⁴ A ₂ → ⁴ T ₁ (P)	–	–	–	–	–
[Ni(HNAC)Cl]·3H ₂ O	Dia.	12748 20750	¹ A _{1g} → ¹ E _g ¹ A _{1g} → ¹ B _{2g}	–	–	–	–	–
[Cu(HNAC)Cl]·2H ₂ O	1.81	– 15110 19456	¹ A _{1g} → ¹ B _{1g} ² B _{1g} → ² B _{2g} ² B _{1g} → ² E _g	–	–	–	–	–

Table S-IV. Kinetic and thermodynamic parameters of the complexes

Complex	Method ^a	Dec. stage <i>t</i> / °C	<i>E</i> * kJ mol ⁻¹	<i>Z</i> s ⁻¹	ΔS^* J K ⁻¹ mol ⁻¹	ΔH^* kJ mol ⁻¹	ΔG^* kJ mol ⁻¹
[Co(BSAP)(H ₂ O) ₃]	P-N	I st /185	31.39	5.47×10 ⁻⁶	-349.28	22.62	182.59
	C-R		51.64	6.44×10 ¹	-213.88	42.87	140.83
	P-N	II nd /342	59.51	3.78×10 ⁻³	-297.35	47.75	230.32
	C-R		87.86	1.57×10 ⁶	-132.32	76.11	157.35
	P-N	III rd /559	64.43	9.33×10 ⁻⁷	-368.95	48.50	355.47
	C-R		112.79	6.04×10 ³	-181.10	96.86	247.53
[Ni(HNAC)Cl]·3H ₂ O	P-N	I st /98	31.61	3.03×10 ⁻³	-294.99	24.51	133.95
	C-R		49.23	3.90×10 ⁴	-158.86	42.13	101.06
	P-N	II nd /354	49.41	1.22×10 ⁻⁵	-345.22	37.41	253.86
	C-R		71.07	4.23×10 ¹	-219.99	59.07	197.01
	P-N	III rd /537	81.75	1.71×10 ⁻³	-306.27	66.24	314.32
	C-R		123.04	1.87×10 ⁶	-133.16	107.53	215.39

^aP-N: Piloyan–Novikova¹; C-R: Coats–Redfern²

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