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Rare earth transition metal-based coordination compounds of Schiff base derived from sulpha drug molecules: Synthesis, spectroscopic and *in vitro* biological screening

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In order to create novel transition metal-based coordination compounds, Schiff bases based on the sulpha drugs have been reacted with various 2-hydroxy-benzaldehyde derivatives. The antibacterial properties and spectroscopic attributes of the synthesized ligands and their heterochelates have been extensively examined. The structural characterization of the ligands has been accomplished through ^{1}H NMR, IR, mass spectrometry, UV-Vis spectroscopy and elemental analysis, while the heterochelates' structures have been validated using IR spectroscopy. *In vitro* evaluations have been conducted to assess the activity of the ligands and heterochelates against Gram +ve bacteria (*S. aureus*, *B. subtilis*), Gram –ve bacteria (*E. coli*, *P. aeruginosa*), and against the fungus *A. niger*. The findings underscore the promising nature of coordination compounds based on transition metals and highlight the necessity for further exploration in this field.

Keywords: Sulpha drug, Schiff base, Transition metal complexes, Antimicrobial study, Antifungal study

Many of the drugs we rely on to fight infections caused by bacteria, fungi, and parasites come with unwanted side effects that can take a toll on our health. People often experience issues like allergies, nerve problems, or complications with their breathing, digestion, liver, blood, or kidneys[1,2]. On top of that, these treatments are becoming less effective as pathogens develop resistance, and some drugs have toxic ingredients that make things even harder[3]. To find better solutions, we need to look beyond traditional treatments and explore metal complexes in bioinorganic chemistry. These compounds have unique and exciting properties that could lead to ground-breaking medical advances and new materials.

A practical and affordable way to develop new treatments is by tweaking existing drugs to make them more effective or give them new capabilities. Sulfonamides are a well-known type of synthetic drug that slows bacterial growth. They are analogous *para*-aminobenzoic acid and block an enzyme called dihydropteroate synthetase (DHPTS), which is crucial in the folic acid metabolism of bacterial cells[4,5]. These drugs exhibit significant efficacy beside a wide range of microbes, including both Gram +ve and Gram –ve bacteria. Additionally, they demonstrate notable activity against pathogens such as Nocardia, Actinomyces, and protozoan parasites responsible for diseases like malaria and toxoplasmosis[6].

Imine compounds, also known as Schiff bases, are organic molecules featuring the azomethine group (C=N). They are widely studied due to their simple synthesis, versatile DNA-binding modes, strong affinity for metals, and significant biological activities. These compounds are highly adaptable and biologically active, forming strong interactions with transition metals. Schiff bases exhibit antibacterial, antifungal, anti-inflammatory, herbicidal, and anticancer properties[7,8]. Their catalytic properties also make them valuable in chemical and photochemical reactions[9,10]. Additionally, their electronic properties can vary depending on the substituents attached[11]. Compounds containing nitrogen, oxygen, and sulphur are recognized for their broad biological activities[12-14], which are often enhanced when incorporated into metal complexes[15,16]. Notably, Schiff base complexes with transition metals derived from sulfa drugs have been extensively studied for their remarkable medicinal properties[16-19].

Most sulfa drugs work by preventing bacteria from reproducing, as they inhibit a key enzyme required for producing proteins and nucleic acids within bacterial cells[20,21]. Organic molecules with π-conjugated systems are incredibly versatile, allowing for a variety of substitutions and functions, making them important in biochemistry[22,23] and organometallic chemistry. Sulfonamides with a free amino group are especially easy to modify because of free amine group is there, which opens the door to many biomedical uses[24] sulfonamides that include imino or hydrazino-modified groups have also shown to be effective at inhibiting CA isozymes[25].

Schiff bases derived from substituted 2-hydroxybenzaldehydes are widely recognized for their antimicrobial properties, either as a separate compound or as ligands in metal complexes[26–29]. Similar effects have been seen with Schiff bases derived from different sulphonamides[26,30,31]. Additionally, drugs like cotrimoxazole, sulfamethoxazole and sulfadiazine have proven effective against *Mycobacterium tuberculosis*[32] as well as non-tuberculous (atypical) mycobacteria (NTM)[33] at doses that can be easily achieved through oral administration.

When Schiff base ligands react with metals like molybdenum (IV), tungsten (IV), zirconium (IV), or vanadium (IV), they form either mono- or binuclear complexes, depending on the ratio of metal to ligand. Incorporating different elements, such as heteroatoms, halogens, and metal ions, into a single structure is essential, as each contributes a specific function. This combination creates an uneven electron distribution, resulting in distinct electrophilic and nucleophilic regions on the molecule's surface. These features improve its ability to bind with proteins and expand its chemical and biological applications.

By altering the carbonyl group by creating aromatic imines, we have created five sulfonamide derivatives in this work. Molybdenum, tungsten, zirconium, and vanadium metal salts were used to synthesise the metal complexes of sulphonamide derivatives, and their antibacterial properties were assessed. The outcomes show that these compounds have strong antibacterial properties. In addition to advancing the creation of novel medications, this research sheds light on the chemistry of metal coordination with heterocyclic ligands.

Experimental Section

All solvents, reagents, and starting materials utilized in the experimental procedures were of superior purity, sourced from a local vendor, and employed directly without further refinement. The advancement of the reaction was assessed through thin-layer chromatography (TLC) showed on Merck pre-coated aluminium sheets integrated with 60 F-254 silica gel plates, utilizing an optimized solvent system as the mobile phase and visualizing outcomes under iodine vapor and ultraviolet illumination. Infrared (IR) spectra were captured using a Perkin-Elmer spectrometer operating within the 4000–400 cm^{-1} range, while ^{1}H NMR spectra were recorded in DMSO-d_6 solution with an AvanceNeo Ascend 400 MHz instrument at a proximate research facility. Additionally, FT-IR spectra were measured using a Nicolet-400D spectrophotometer with KBr pellet methodology. UV spectra were collected using UV-Vis spectrophotometer V-750.

Common process for the synthesis of ligands L$_1$-L$_5$

The synthesis of all the ligand (L$_1$-L$_5$) was achieved by reacting 10 mmol of 4-Amino-N-(6-methoxypyrimidine-4-yl)benzenesulfonamide with an equimolar amount of different derivatives of 2-hydroxybenzaldehyde in methanol under continuous stirring at 35°C. Using a hexane/ethyl acetate (7:3) combination as the mobile phase, thin-layer chromatography (TLC) was used to track the reaction's progress and verify that all of the starting ingredients had been consumed within 30 minutes. After everything was finished, the solid product was separated by filtering, completely cleaned with ethanol, dried at 60°C, and then stored for later use.

L$_1$: Mol. Formula $C_{18}H_{16}N_4O_4S$. Yield 89%. Mol. Wt. 384.41. Yellow colour. FT-IR (KBr): 3358 (-OH), 1570 (C=N), 1143 (SO$_2$) 1215 cm^{-1}; ^{1}H NMR (400 MHz, DMSO-d_6): δ 3.85 (3H$_a$,s, -OCH$_3$), 5.94 (1H$_b$,s,-OH), 6.96-8.95 (10H,c,Ar-H); FAB-MS: *m/z* 382.95. Anal. Calcd for $C_{18}H_{16}N_4O_4S$: C, 56.24; H, 4.20; N, 14.57. Found: C, 56.22; H, 4.19; N, 14.55%.

L$_2$: Mol. Formula $C_{19}H_{18}N_4O_5S$. Yield 79%. Mol. Wt. 414.44. Orange colour. FT-IR (KBr): 3313 (-OH), 1587 (C=N), 1138 cm^{-1} (SO$_2$); ^{1}H NMR (400 MHz, DMSO-d_6): δ 3.82 (1H$_a$,s,,-OCH$_3$), 3.85 (3H$_b$,s,,-OCH$_3$), 6.37 (1H$_c$,s,-OH), 6.91-8.96 (9H,c,Ar-H); FAB-MS: *m/z* 414.10. Anal. Calcd for $C_{19}H_{18}N_4O_5S$: C, 55.06; H, 4.38; N, 13.52. Found: C, 55.04; H, 4.36; N, 13.51%.

L$_3$: Mol. Formula $C_{18}H_{15}N_5O_6S$. Yield 74%. Mol. Wt. 429.41. Orange colour. FT-IR (KBr): 3238 (-OH), 1585 (C=N), 1141 cm^{-1} (SO$_2$); ^{1}H NMR (400

MHz, DMSO-d_6): δ 3.85 ($3H_a$,s,-OCH_3), 6.31 ($1H_b$,s,-OH), 6.58-8.69 (9H,c,Ar-H); FAB-MS: *m/z* 429.07. Anal. Calcd for $C_{18}H_{15}N_5O_6S$: C, 50.35; H, 3.52; N, 16.31. Found: C, 50.32; H, 3.52; N, 16.28%.

L_4: Mol. Formula $C_{22}H_{25}N_5O_4S$. Yield 89%. Mol. Wt. 455.53. Yellow colour. FT-IR (KBr): 3318 (-OH), 1573 (C=N), 1155 cm^{-1} (SO_2); ^1H NMR (400 MHz, DMSO-d_6): δ 1.11 ($6H_{a, b}$,t,-CH_3), 3.40 (4H,m,-CH_2), 3.84 (3H,s,-OCH_3), 6.07 (1H,s,-OH), 6.34-8.72 (9H,c,Ar-H); FAB-MS: *m/z* 454.10. Anal. Calcd for $C_{22}H_{25}N_5O_4S$: C, 58.01; H, 5.53; N, 15.37. Found: C, 57.99; H, 5.51; N, 15.35%.

L_5: Mol. Formula $C_{17}H_{16}N_4O_4S_2$. Yield 89%. Mol. Wt. 372.40. FT-IR (KBr): 3360 (–OH), 1593 (C=N), 1153 cm^{-1} (SO_2); ^1H NMR (400MHz, DMSO-d_6): δ 2.39 ($3H_a$,s,-CH_3), 3.85 ($3H_b$,s,-OCH_3), 6.38-8.33 (8H,c,Ar-H); FAB-MS: *m/z* 371.00. Anal. Calcd for $C_{17}H_{16}N_4O_4S_2$: C, 54.83; H, 4.33; N, 15.04. Found: C, 54.81; H, 4.31; N, 15.01%.

Common process for the synthesis of co-ordination compound

All heterochelates were synthesised and isolated using a general method. With constant stirring and drop by drop addition of warm metal salt solution prepared in DMF was added to the respective ligand solution in 1:2 Metal to Ligand molar ratios. After heating at 70°C for four hours, the mixture taken at RT to cool overnight. After cooling at RT densely coloured product appeared and allowed to dry in desiccators. Physical and analytical data for all coordination compounds are represented in Table 1.

In vitro Biological Screening

The antibacterial potential of the recently made compounds was assessed *in vitro* against four bacterial strains: B. subtilis and S. aureus as agents of Gram +ve bacteria, and E. coli and P. aeruginosa as Gram –ve counterparts. Mueller Hinton agar (Hi Media, India) was used as the culture medium in this evaluation, which used the agar well diffusion method. The compounds were applied at a concentration of 50 μg and compared with the standard antibiotic, Streptomycin. After dissolving the compounds in DMSO (10 mg/mL), they were placed onto the solidified agar in Petri dishes, and the bacterial strains were added to the surface. This section exhibits textual redundancy and necessitates rephrasing through the incorporation of intricate vocabulary and advanced linguistic structures to eliminate any traces of duplication.

For the antifungal activity, the compounds were tested against Aspergillus niger using the same diffusion method on Sabouraud's dextrose agar (Merck, Germany), with Nystatin as the standard antifungal control. The findings of these antibacterial and antifungal study shown the antimicrobial and antifungal effectiveness of the compounds.

Result and Discussion

The experimental section discusses the overall process for ligand synthesis, and the structure of the synthesised ligands (L_1-L_5) is displayed in Fig. 1. The overall approach for the synthesis of the complex is given in the experimental section and the proposed structure of the complex is represented in Fig. 2. The complexes that were synthesised are solid. These complexes are soluble in solvents such as DMF and DMSO, but not in typical organic solvents.

^{1}H NMR

The ^1H NMR data of synthesized ligands were carried out in DMSO-d6 solvent at RT. All the obtained data is represented in the experimental section, in the case of ^1H NMR spectra of the ligand peak obtained in the range of 3.82-3.85 δppm for –OCH_3 group in each ligands remaining L_5. In ligand L_2 an additional peak of –OCH_3 group is found. The peak for –OH group is found in the range of 5.94-6.37 δppm in ligands L_1-L_4. In ligand $_{L4}$ two additional peak at 1.11 and 3.40 δppm for two –CH_3 and –CH_2 group respectively, while the aromatic protons are found as multiplate in the range of 6.38-8.96 δppm in all ligands. If the –NH proton signal mixes in the upper region, it can be difficult to tell them apart. The chemical formula of the molecules and the number of protons align perfectly. Furthermore, the mass spectra of each ligand provide confirmation.

IR

The comparative IR data of rare earth transition metals with Schiff base ligands are shown in Table 2. For identification purpose of binding mode of metal complexes and Schiff base ligands the IR data were compared. The azomethine group's ν(C=N) is clearly observed as prominent band between 1570 cm^{-1} and 1595 cm^{-1} for Schiff base ligands. This band arise between 1510 cm^{-1} and 1570 cm^{-1} in coordination compounds, its lower energy shift depicts azomethine

Table 1 — Analytical and physical data of Heterochelates

Compd	Mol. Wt.	Colour and Yield (%)	Analysis (%) Found (Calcd)			
			C	H	N	M
$[(L_1)_2MoO_2]$	894.76	Orange (79)	48.27 (48.32)	3.34 (3.38)	12.48 (12.52)	10.78 (10.72)
$[(L_1)_2WO_2]$	982.64	Brown (81)	43.97 (44.00)	3.04 (3.08)	11.37(11.40)	18.79 (18.71)
$[(L_1)_2VO]$	833.74	Green (83)	51.83 (51.86)	3.59 (3.63)	13.37(13.44)	6.17 (6.11)
$[(L_1)_2ZrO]$	874.03	Yellow (77)	49.44 (49.47)	3.44 (3.46)	12.80 (12.82)	14.51 (14.44)
$[(L_2)_2MoO_2]$	954.81	Red (78)	47.76 (47.80)	3.57 (3.59)	11.69 (11.74)	10.11 (10.05)
$[(L_2)_2WO_2]$	1042.69	Brown (73)	43.73(43.77)	3.27 (3.29)	10.71 (10.75)	17.69 (17.63)
$[(L_2)_2VO]$	893.80	Buff (86)	51.01(51.06)	3.80 (3.83)	12.51 (12.54)	5.77 (5.70)
$[(L_2)_2ZrO]$	934.08	Red (81)	48.82 (48.86)	3.63 (3.67)	12.96 (12.00)	9.81 (9.77)
$[(L_3)_2MoO_2]$	984.76	Brown (74)	43.88 (43.91)	2.85 (2.87)	14.20 (14.22)	9.81 (9.74)
$[(L_3)_2WO_2]$	1072.64	Brown (73)	40.29 40.31	2.59 (2.63)	13.04 (13.06)	17.19 (17.14)
$[(L_3)_2VO]$	923.74	Black (87)	46.77 (46.81)	3.02 (3.06)	15.13 (15.16)	5.54 (5.51)
$[(L_3)_2ZrO]$	964.02	Brown (79)	44.83 (44.85)	2.89 (2.93)	14.51 (14.53)	9.51 (9.46)
$[(L_4)_2MoO_2]$	1037	Brown (73)	50.92 (50.96)	4.64 (4.67)	13.49 (13.51)	9.31 (9.25)
$[(L_4)_2WO_2]$	1124.88	Dark Brown (78)	46.45 (46.98)	4.28 (4.30)	12.43 (12.45)	16.37 (16.34)
$[(L_4)_2VO]$	975.99	Brown (87)	54.13 (54.15)	4.93 (4.96)	14.31 (14.35)	5.29 (5.22)
$[(L_4)_2ZrO]$	1016.27	Brown (79)	51.97 (52.00)	4.73 (4.76)	13.75 (13.78)	9.01 (8.98)
$[(L_5)_2MoO_2(NH_4)_2]$	908.83	Orange (72)	44.91 (44.93)	4.42 (4.44)	15.39 (15.41)	10.61 (10.56)
$[(L_5)_2WO_2(Na)_2]$	1006.61	Brown (77)	40.53 (40.57)	3.18 (3.20)	11.10 (11.13)	18.31 (18.26)
$[(L_5)_2VOSO_4]$	907.80	Brown (84)	45.02 (44.98)	3.52 (3.55)	12.31 (12.34)	5.65 (5.61)
$[(L_5)_2ZrO(NO_3)_2]$	976. 003	Brown (73)	41.82 (41.84)	3.27 (3.30)	14.31 (14.35)	9.39 (9.35)

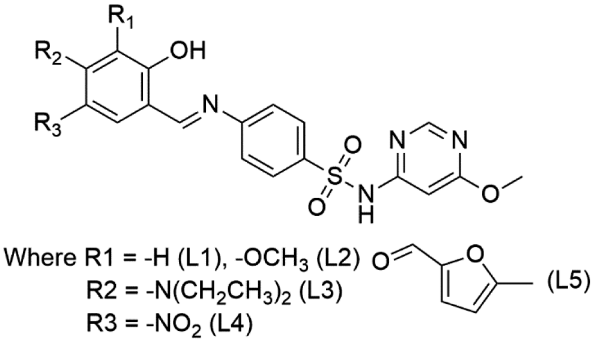

Fig. 1 — Proposed structure of Ligands (L_1-L_5)

N coordination. The band for ν(SO_2) arise between 1130 cm^{-1} and 1155 cm^{-1} for ligands and band arise in between 1130 cm^{-1} and 1160 cm^{-1} for heterochelates. It is clear from the description above that complexes are formed as a result of the coupling process between the ligands and the metal ion.

UV-Vis

The UV-Vis spectrum of the synthesized compound was recorded to analyse its electronic transitions and assess its optical properties as shown in Fig. 3. The absorption spectrum exhibited

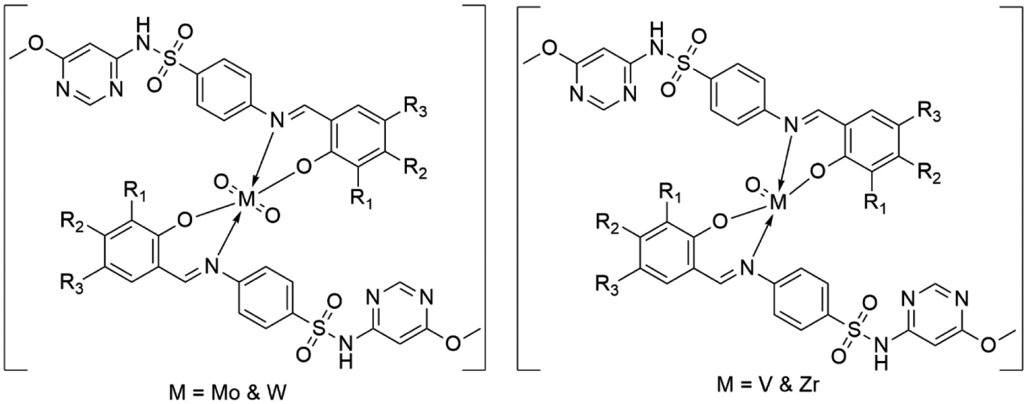

Fig. 2 — Proposed structure of heterochelates

Table 2 — IR Data of Ligands and its Heterochelates

S. No.	Compd	C=N	OH	S=O	M-O	M-N
1	L_1	1570	3358	1143	–	–
2	$[(L_1)_2MoO_2]$	1547	–	1142	574	624
3	$[(L_1)_2WO_2]$	1549	–	1153	470	680
4	$[(L_1)_2VO]$	1542	–	1143	574	624
5	$[(L_1)_2ZrO]$	1546	–	1143	464	626
6	L_2	1587	3313	1138	–	–
7	$[(L_2)_2MoO_2]$	1570	–	1143	576	609
8	$[(L_2)_2WO_2]$	1570	–	1141	576	611
9	$[(L_2)_2VO]$	1570	–	1151	574	609
10	$[(L_2)_2ZrO]$	1570	–	1143	576	611
11	L_3	1585	3238	1141	–	–
12	$[(L_3)_2MoO_2]$	1570	–	1145	578	634
13	$[(L_3)_2WO_2]$	1570	–	1139	580	641
14	$[(L_3)_2VO]$	1568	–	1141	578	653
15	$[(L_3)_2ZrO]$	1570	–	1145	576	651
16	L_4	1573	3318	1155	–	–
17	$[(L_4)_2MoO_2]$	1525	–	1139	567	603
18	$[(L_4)_2WO_2]$	1517	–	1134	572	601
19	$[(L_4)_2VO]$	1525	–	1151	567	607
20	$[(L_4)_2ZrO]$	1525	–	1151	570	609
21	L_5	1597	–	1141	–	–
22	$[(L_5)_2MoO_2(NH_4)_2]$	1563	–	1157	572	680
23	$[(L_5)_2WO_2Na_2]$	1557	–	1159	572	644
24	$[(L_5)_2VOSO_4]$	1549	–	1151	570	646
25	$[(L_5)_2ZrO(NO_3)_2]$	1544	–	1155	570	678

characteristic peaks at specific wavelengths mentioned in Table 3, corresponding to π→π*, n→π* or d-d transitions, indicating the presence of conjugated systems and lone pair interactions. The intensity and position of these peaks suggest Metal-ligand charge transfer (MLCT) or other relevant effects. Shifts between the heterochelate and the matching ligand in the table indicate potential ligand coordination or an electrical environment. These results confirm the successful synthesis and structural integrity of the compound, providing insight into its electronic structure.

FAB-MS

The molecular formula of the coordination molecule $[(L_1)_2ZrO]$ has been verified and the

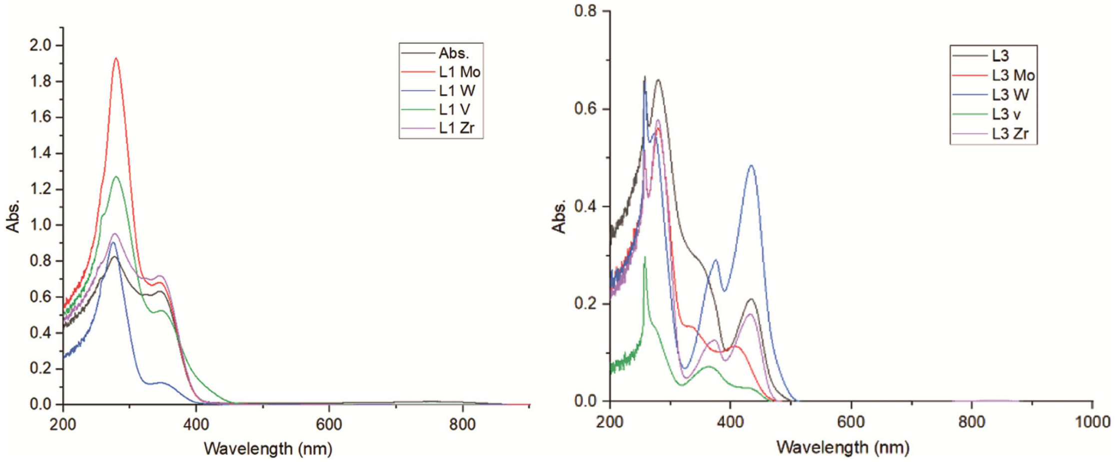

Fig. 3 — UV-Visible overlay spectrum of ligands (L_1, L_3) and their heterochelates

Table 3 — Ligands and metals electronic spectra and magnetic moments

Compd	π→π* λ_{max} (nm)	LMCT λ_{max} (nm)	n→ π* λ_{max} (nm)	d-d transition λ_{max} (nm)	μ (B.M.)	Chemical Shift
L_1	256.2	277.2	345	–	–	–
$[(L_1)_2MoO_2]$	259.4	280	345	–	–	Hyperchromic
$[(L_1)_2WO_2]$	259.2	274	347.8	–	–	Hyperchromic
$[(L_1)_2VO]$	260.4	279	348.4	458.2	1.69	Hyperchromic
$[(L_1)_2ZrO]$	277.2	345.4	–	–	–	Hyperchromic
L_2	257.6	291.6	317.6	–	–	–
$[(L_2)_2MoO_2]$	257	291.6	317.6	–	–	Hyperchromic
$[(L_2)_2WO_2]$	259.8	285.2	323.4	–	–	Hyperchromic & Hypsochromic
$[(L_2)_2VO]$	257.6	285.2	331	458	1.71	Hypochromic & Hypsochromic
$[(L_2)_2ZrO]$	257.8	287.2	314	–	–	Hyperchromic
L_3	257	279.7	353	433.5	–	–
$[(L_3)_2MoO_2]$	257.4	281.2	335.6	410.6	–	Hypochromic
$[(L_3)_2WO_2]$	257	273.2	373.2	435	–	–
$[(L_3)_2VO]$	257.8	274.8	366	433.8	1.69	Hypochromic
$[(L_3)_2ZrO]$	257.4	277.8	372.8	431	–	Hypochromic & Bathochromic
L_4	258.8	396	–	–	–	–
$[(L_4)_2MoO_2]$	260.2	274.2	404.6	–	–	Hyperchromic
$[(L_4)_2WO_2]$	256.8	395.6	–	–	–	Hypochromic
$[(L_4)_2VO]$	283.6	352.8	–	458.8	1.73	Hypsochromic & Hyperchromic
$[(L_4)_2ZrO]$	257.8	277.8	356	399	–	Bathochromic & Hypochromic
L_5	304.4	333.8	471.4	–	–	–
$[(L_5)_2MoO_2(NH_4)_2]$	256.8	280.6	406.6	–	–	Hypsochromic & Hyperchromic
$[(L_5)_2WO_2Na_2]$	257.4	276	407	–	–	Hypsochromic & Hyperchromic
$[(L_5)_2VOSO_4]$	256	285	371.6	493.8	–	Hypsochromic & Hyperchromic
$[(L_5)_2ZrO(NO_3)_2]$	280.6	392.2	473	–	–	Hyperchromic & Hypsochromic

molecular ion peak shown in Fig. 4. At *m/z*=875, the molecular ion peak first emerges. Fig. 5 depicts the compound's likely fragmentation process. The loss of two $C_5H_6N_2O$ groups from species **(a)** causes the compound's primary fragmentation, giving rise to species **(b)**, which has a noticeable base peak at *m/z*=655. By losing a portion of the ligand molecule (H_2NO_2S), more fragmentation results in species **(c)**. After that, species **(c)** breaks down further to create a stable species **(d)**, most likely as a result of losing the ZrO_2 and the remaining ligand molecule. The computed molecular weights for all observed degradation step were consistent with the expected values reported in previous studies[34,35].

Biological Screening

The synthesised Schiff base Ligands L_1-L_5 and their heterochelates based on rare earth metals screened against four bacterial stains *Bacillus subtilus, Staphylococcus aureus*, *E. Coli, Pseudomonas aerugenosa* bacteria and fungi *Aspergillus Niger*. Heterochelates exhibit a stronger inhibitory effect than their parent Schiff base ligands, as demonstrated in the antimicrobial screening results

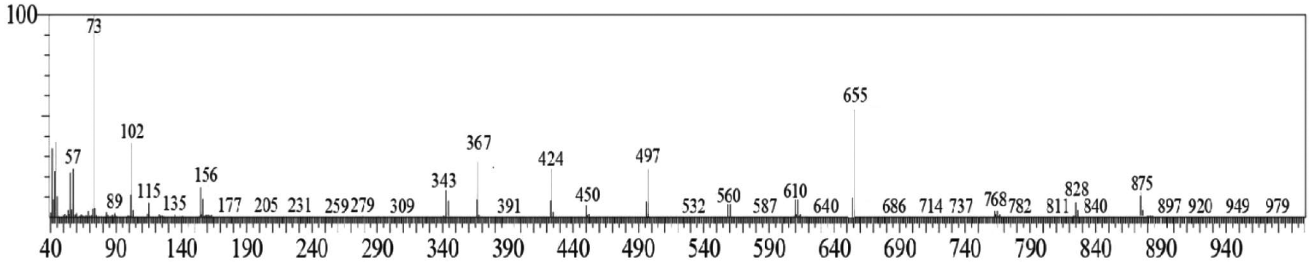

Fig. 4 — FAB mass spectrum of heterochelate $[(L_1)_2ZrO]$

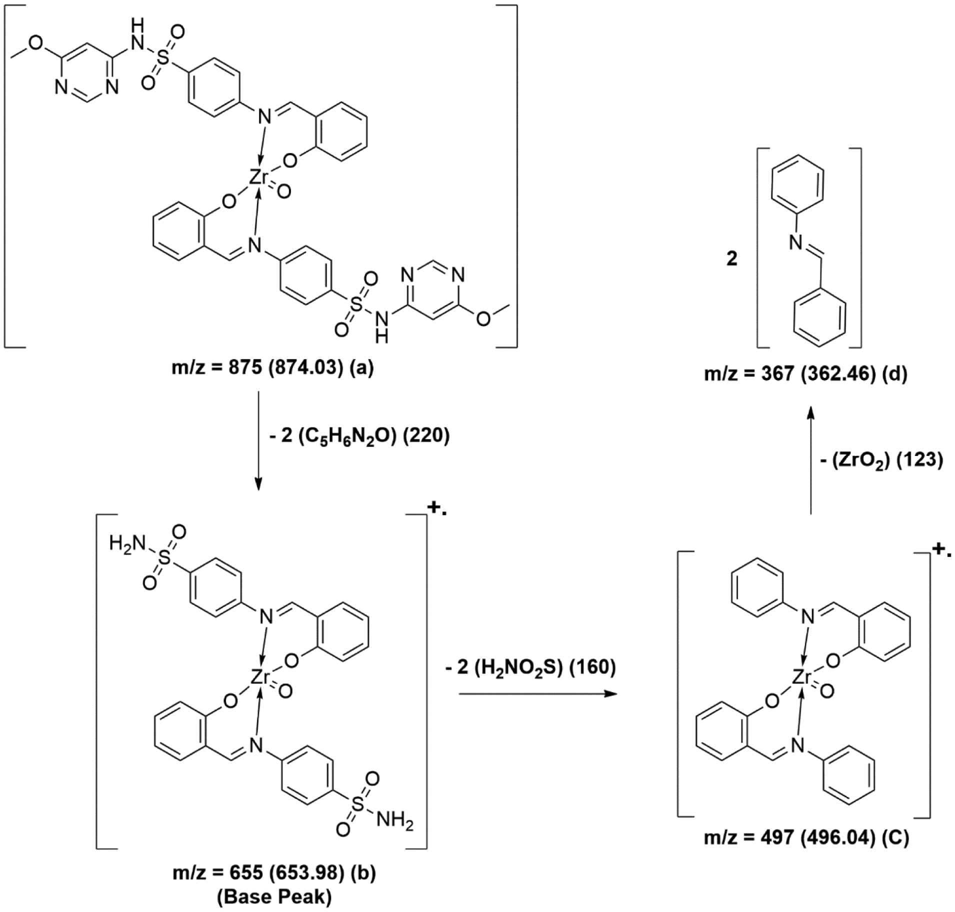

Fig. 5 — Suggested fragmentation pattern of heterochelate $[(L_1)_2ZrO]$

Table 4 — Antibacterial properties of Ligand and it's Heterochelates

S. No.	Compd	Bacteria				Fungi
		Gram +ve		Gram –ve		
		B. subtilis	*S. aureus*	*E. coli*	*P. aeruginosa*	*A. niger*
Ref. Drug 1	Nystatin	NA	NA	NA	NA	22
Ref. Drug 2	Streptomycin	28	29	24	22	NA
Solvent	DMSO	0	0	0	0	0
1	L_1	2	4	12	0	2
2	$[(L_1)_2MoO_2]$	5	16	17	5	2
3	$[(L_1)_2WO_2]$	4	24	22	14	4
4	$[(L_1)_2VO]$	8	20	28	13	10
5	$[(L_1)_2ZrO]$	4	18	19	6	3
6	L_2	9	3	20	4	10
7	$[(L_2)_2MoO_2]$	8	8	17	4	11
8	$[(L_2)_2WO_2]$	2	15	19	4	3
9	$[(L_2)_2VO]$	8	14	20	9	3
10	$[(L_2)_2ZrO]$	10	14	18	6	9
11	L_3	4	8	16	5	0
12	$[(L_3)_2MoO_2]$	12	10	17	8	0
13	$[(L_3)_2WO_2]$	14	11	16	12	5
14	$[(L_3)_2VO]$	2	10	13	10	0
15	$[(L_3)_2ZrO]$	2	8	14	14	2
16	L_4	5	13	18	5	16
17	$[(L_4)_2MoO_2]$	2	20	17	9	2
18	$[(L_4)_2WO_2]$	12	12	14	12	2
19	$[(L_4)_2VO]$	2	18	16	10	2
20	$[(L_4)_2ZrO]$	2	18	19	4	3
21	L_5	0	12	14	0	0
22	$[(L_5)_2MoO_2(NH_4)_2]$	4	18	15	0	0
23	$[(L_5)_2WO_2Na_2]$	16	18	22	13	4
24	$[(L_5)_2VOSO_4]$	2	18	16	2	0
25	$[(L_5)_2ZrO(NO_3)_2]$	4	19	14	3	0

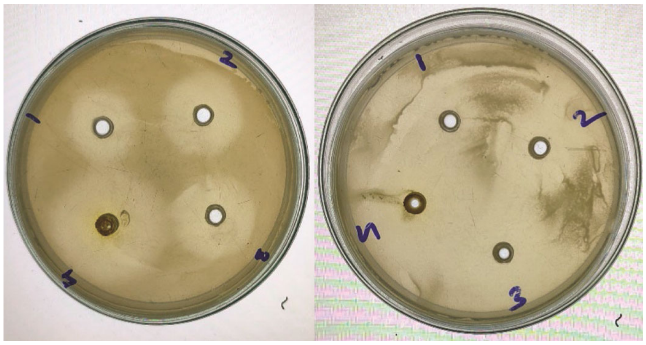

Fig. 6 — Zone of inhibition (mm) of Ligand and heterochelates

presented in Table 4 and Fig. 6. Heterochelate L_5W is considerably affect against *Bacillus subtilis* and L_1W is effective against *Staphylococcus aureus*.

Heterochelate L_1V considerably effective against *E. Coli* and L_1W and L_3Zr is effective against *Pseudomonas aeruginosa*. Ligand L_4 and L_4Zr heterochelate considerably effective against fungi *Aspergillus Niger*. The overtone notion[36,37] and chelation theory[38] can be used to describe the higher activity of heterochelates than the Ligands. Antibiotic Streptomycin used for the antibacterial activity study, in fact heterochelate L_1V (28 mm) found more effective than reference antibiotic (24 mm).

Conclusion

We are exploring the development of unique Schiff base ligands made from sulfa drug molecules and their corresponding heterochelates. To ensure the quality and structure of these compounds, we used advanced techniques like ^1H NMR, IR, UV, and mass spectrometry for verification and characterization. Following the synthesis of these compounds, their efficacy in addressing bacterial and fungal infections was meticulously evaluated. Notably, the coordination compounds exhibited remarkable antibacterial properties, demonstrating pronounced activity compared to Gram +ve bacterial strains, including B. subtilis and S. aureus, as well as Gram –ve strains such as E. coli and P. aeruginosa.

In fact, their antibacterial effects were noticeably stronger than those of their individual ligands. These findings are exciting because they suggest that these compounds could be further researched and developed into a new generation of transition metal-based antibacterial drugs with the potential to fight a wide range of harmful microbes.

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