New Journal of Chemistry

Electronic Supplementary Information (ESI)

Supramolecular framework of binuclear dioxomolybdenum(VI) complexes with ONS donor ligands using 4,4′-azopyridine as pillar: Crystal Structure, DFT calculations and Biological Study

Debanjana Biswal[a], Nikhil Ranjan Pramanik[*b], Syamal Chakrabarti[*a], Michael G.B Drew[c], Payel Mitra[d], Krishnendu Acharya[d], Sujan Biswas [e] and Tapan Kumar Mondal[e]

[a]*Department of Chemistry, University College of Science, 92, Acharya Prafulla Chandra Road, Kolkata:700009, West Bengal, India.*

[b]*Department of Chemistry, Bidhannagar College, EB-2,Sector-1, Salt Lake, Kolkata: 700064, India.*

[c]*Department of Chemistry, The University of Reading, Whiteknights, Reading RG66AD, UK.*

[d]*Molecular and Applied Mycology and Plant Pathology Laboratory, Department of Botany, University of Calcutta, Kolkata 700019, West Bengal, India.*

[e]*Department of Chemistry (Inorganic section), Jadavpur University, Kolkata 700032 , India.*

Table of Contents:

Fig. S6 Staircase architecture of complex **1** along the b-axis

Fig. S7 Chain architecture of complex **2** along the b-axis

Fig. S8 Chain architecture of complex **3** along the b-axis

Table S1 Energy and composition of selected molecular orbitals of complex **1**

Table S2 Energy and composition of selected molecular orbitals of complex **2**

Table S3 Energy and composition of selected molecular orbitals of complex **3**

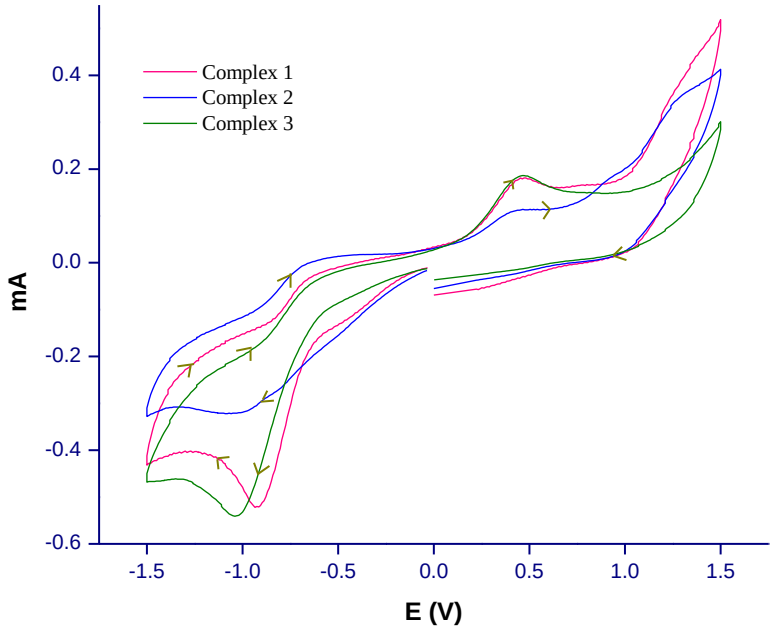

Fig. S1 Cyclic voltammogram of complexes **1-3** in DMF at 298K

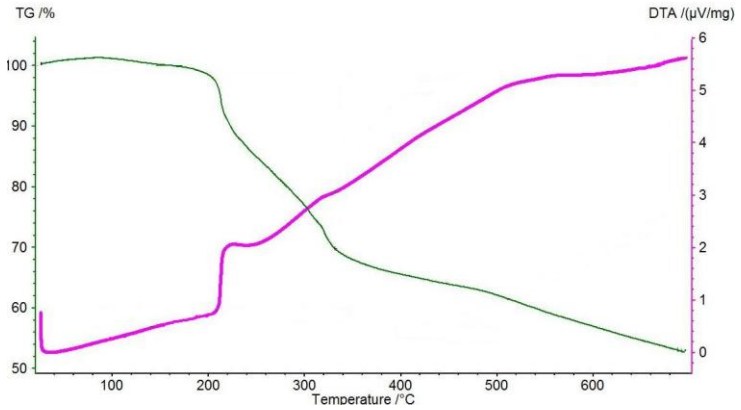

Fig. S2 TG-DT curve of complex **1** under N_2 atmosphere.

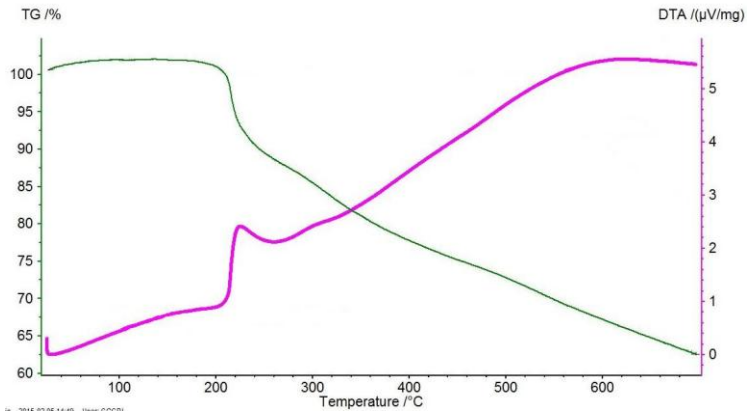

Fig. S3 TG-DT curve of complex **2** under N_2 atmosphere.

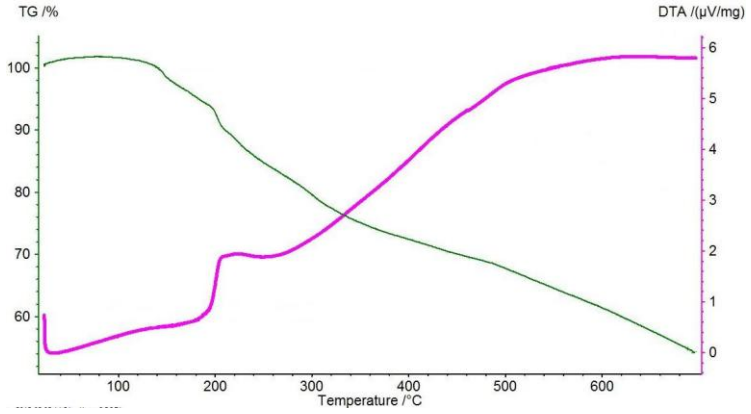

Fig. S4 TG-DT curve of complex **3** under N_2 atmosphere.

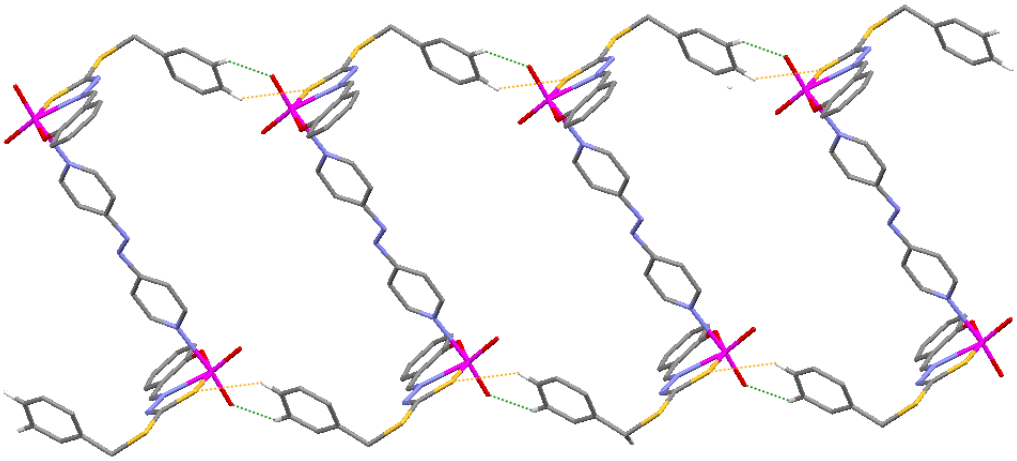

Fig. S5 Chain architecture of complex **1** along the a-axis.

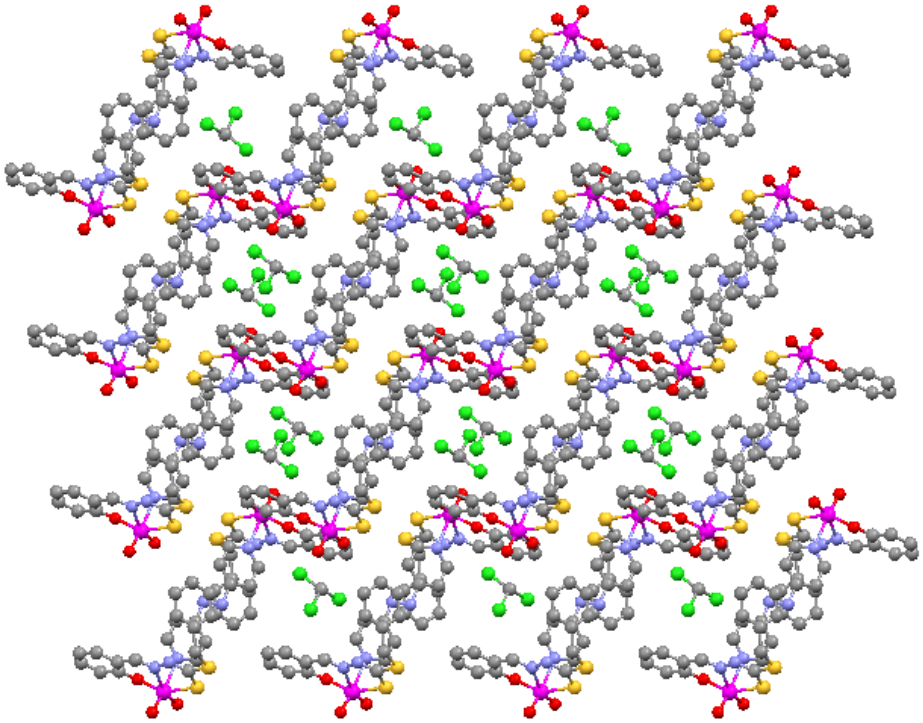

Fig. S6 Staircase architecture of complex **1** along the b-axis.

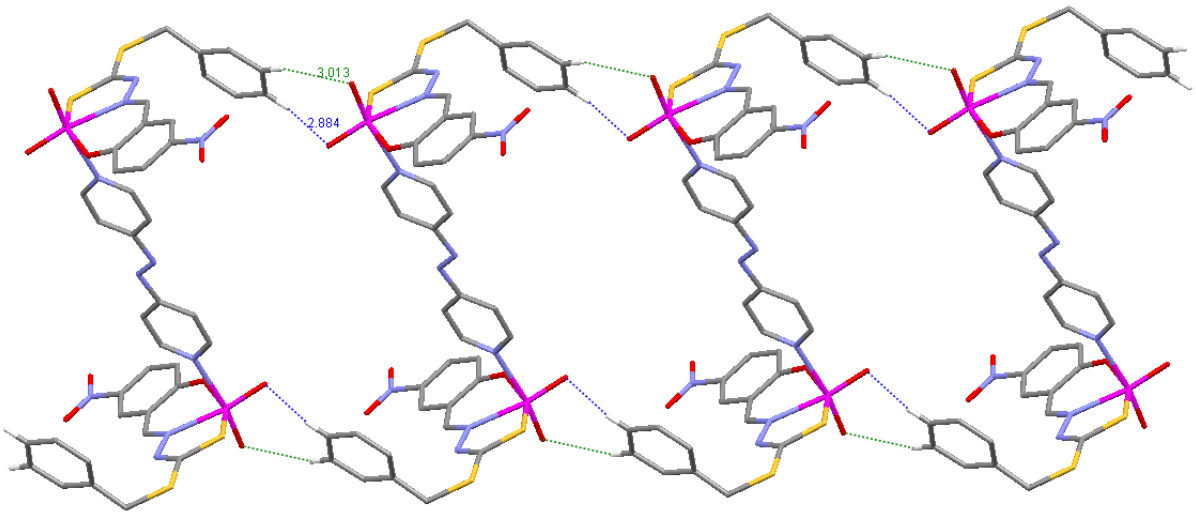

Fig. S7 Chain architecture of complex **2** along the b-axis.

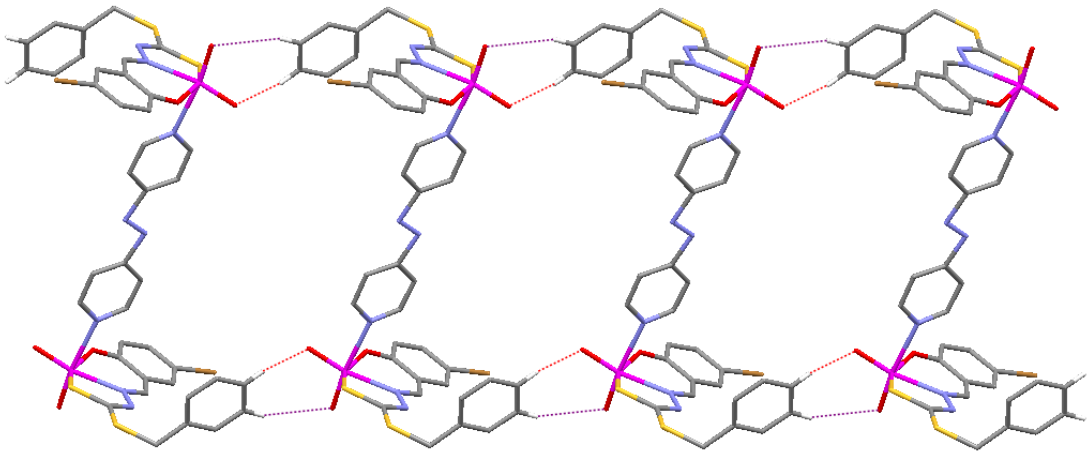

Fig. S8 Chain architecture of complex **3** along the b-axis.

Table S1 Energy and composition of selected molecular orbitals of complex **1**

MO	Energy (eV)	% of composition			
		Mo	Σoxo	L^1	azpy
LUMO+10	-1.09	02	0	03	95
LUMO+9	-1.19	04	01	0	95
LUMO+8	-1.72	61	22	14	03
LUMO+7	-1.72	60	23	14	03
LUMO+6	-1.96	35	13	51	01
LUMO+5	-1.97	32	12	53	03
LUMO+4	-2.33	60	20	20	0
LUMO+3	-2.33	60	20	20	0
LUMO+2	-2.59	29	17	52	02
LUMO+1	-2.61	31	17	50	02
LUMO	-3.58	01	0	01	98
HOMO	-6.14	01	01	97	01
HOMO-1	-6.15	01	01	97	01
HOMO-2	-6.58	01	02	95	02
HOMO-3	-6.59	01	02	95	02
HOMO-4	-6.70	01	03	95	01
HOMO-5	-6.71	01	03	95	01
HOMO-6	-6.93	01	0	98	01
HOMO-7	-6.93	01	0	98	01
HOMO-8	-6.98	0	0	100	0
HOMO-9	-6.98	0	0	100	0
HOMO-10	-7.29	0	01	01	98

Table S2 Energy and composition of selected molecular orbitals of complex **2**

MO	Energy (eV)	% of composition			
		Mo	Σoxo	L^2	azpy
LUMO+10	-2.08	54	21	23	02
LUMO+9	-2.08	54	21	23	02
LUMO+8	-2.42	36	14	49	01
LUMO+7	-2.43	33	13	51	03
LUMO+6	-2.59	21	06	72	01
LUMO+5	-2.60	20	06	73	01
LUMO+4	-2.80	49	17	33	01
LUMO+3	-2.81	49	17	33	01
LUMO+2	-3.04	26	15	56	03
LUMO+1	-3.07	28	16	55	01
LUMO	-3.89	01	01	01	97
HOMO	-6.59	01	01	97	01
HOMO-1	-6.59	01	01	97	01
HOMO-2	-6.88	01	02	95	02
HOMO-3	-6.89	01	02	96	01
HOMO-4	-7.16	01	02	96	01
HOMO-5	-7.17	01	01	97	01
HOMO-6	-7.20	00	02	97	01
HOMO-7	-7.21	00	02	97	01
HOMO-8	-7.37	01	0	98	01
HOMO-9	-7.37	01	01	97	01
HOMO-10	-7.59	0	0	01	99

Table S3 Energy and composition of selected molecular orbitals of complex **3**

MO	Energy (eV)	% of composition			
		Mo	Σoxo	L^3	azpy
LUMO+10	-1.21	02	0	03	95
LUMO+9	-1.31	04	01	0	95
LUMO+8	-1.89	60	22	15	03
LUMO+7	-1.90	60	22	15	03
LUMO+6	-2.15	37	15	47	01
LUMO+5	-2.17	35	13	49	03
LUMO+4	-2.48	59	20	19	02
LUMO+3	-2.48	59	20	19	02
LUMO+2	-2.77	15	26	56	03
LUMO+1	-2.80	28	16	55	01
LUMO	-3.69	01	01	01	97
HOMO	-6.25	01	01	97	01
HOMO-1	-6.26	01	01	97	01
HOMO-2	-6.68	01	0	98	01
HOMO-3	-6.68	01	0	98	01
HOMO-4	-6.76	04	01	93	02
HOMO-5	-6.77	01	04	94	01
HOMO-6	-7.02	01	0	98	01
HOMO-7	-7.02	01	0	98	01
HOMO-8	-7.06	0	0	99	01
HOMO-9	-7.08	0	0	99	01
HOMO-10	-7.40	01	0	01	98