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Lewis base controlled supramolecular architectures via non-covalent interactions of dioxomolybdenum(VI) complexes with an ONS donor ligand: DFT Calculations and Biological Study

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Table S1

Energy and composition of selected molecular orbitals of complex **1.**

MOs	Energy (eV)	% of composition			
		Mo	L	THF	Oxo
LUMO+5	-0.30	13	83	0	04
LUMO+4	-0.62	16	78	0	06
LUMO+3	-1.71	59	17	01	23
LUMO+2	-1.82	22	68	0	10
LUMO+1	-2.30	58	22	0	20
LUMO	-2.41	43	33	0	24
HOMO	-6.00	02	96 (S, 26)	01	01
HOMO-1	-6.48	01	94 (S, 42)	01	04
HOMO-2	-6.53	01	97 (S, 56)	01	01
HOMO-3	-6.58	01	97	01	01
HOMO-4	-7.01	0	100	0	0
HOMO-5	-7.10	02	69	21	08
HOMO-6	-7.31	01	20	73	06
HOMO-7	-7.46	0	98	0	01
HOMO-8	-7.81	09	77 (S, 49)	03	11
HOMO-9	-7.93	03	08	04	85
HOMO-10	-8.29	05	62	01	32

Table S2

Energy and composition of selected molecular orbitals of complex **2.**

MOs	Energy (eV)	% of composition			
		Mo	L	imz	Oxo
LUMO+5	-0.18	02	98	0	0
LUMO+4	-0.52	10	86	0	04
LUMO+3	-1.44	60	14	02	24
LUMO+2	-1.61	19	73	0	08
LUMO+1	-2.06	54	24	0	22
LUMO	-2.25	49	27	01	23
HOMO	-5.80	01	96 (S, 25)	02	01
HOMO-1	-6.29	0	96 (S, 24)	01	03
HOMO-2	-6.38	01	90 (S, 71)	07	02
HOMO-3	-6.69	0	07	92	01
HOMO-4	-6.72	01	93	01	05
HOMO-5	-6.95	03	87	01	09
HOMO-6	-6.97	0	100	0	0
HOMO-7	-7.27	0	97	01	02
HOMO-8	-7.55	02	11	19	68
HOMO-9	-7.59	07	75 (S, 41)	04	14
HOMO-10	-8.00	03	26	59	12

Table S3

Energy and composition of selected molecular orbitals of complex **3.**

MOs	Energy (eV)	% of composition			
		Mo	L	allylimz	Oxo
LUMO+5	-0.33	0	01	99	0
LUMO+4	-0.51	09	87	0	04
LUMO+3	-1.41	60	14	02	24
LUMO+2	-1.59	20	72	0	08
LUMO+1	-2.04	54	24	0	22
LUMO	-2.23	49	27	01	23
HOMO	-5.77	01	96 (S, 25)	02	01
HOMO-1	-6.27	01	94 (S, 25)	02	03
HOMO-2	-6.36	01	88 (S, 68)	09	02
HOMO-3	-6.63	0	09	90	01
HOMO-4	-6.72	01	93	01	05
HOMO-5	-6.93	02	88	01	09
HOMO-6	-6.97	0	100	0	0
HOMO-7	-7.25	0	97	01	02
HOMO-8	-7.53	03	14	22	61
HOMO-9	-7.56	06	66 (S, 32)	08	20
HOMO-10	-7.78	02	10	83	05

Table S4

Energy and composition of selected molecular orbitals of complex **4.**

MOs	Energy (eV)	% of composition			
		Mo	L	pic	Oxo
LUMO+5	-0.60	06	33	59	02
LUMO+4	-1.05	04	01	94	01
LUMO+3	-1.63	58	15	03	24
LUMO+2	-1.75	19	72	02	07
LUMO+1	-2.18	57	23	0	20
LUMO	-2.36	44	31	02	23
HOMO	-5.90	01	96 (S, 25)	02	01
HOMO-1	-6.39	01	95 (S, 32)	01	03
HOMO-2	-6.44	01	95 (S, 66)	02	02
HOMO-3	-6.77	01	97	0	02
HOMO-4	-6.98	0	100	0	0
HOMO-5	-7.05	03	84	02	11
HOMO-6	-7.36	0	79	18	03
HOMO-7	-7.48	0	98	02	0
HOMO-8	-7.64	04	43	21	32
HOMO-9	-7.68	05	35 (S, 27)	21	39
HOMO-10	-7.97	01	07	76	16

Table S5

Energy and composition of selected molecular orbitals of complex **5.**

MOs	Energy (eV)	% of composition			
		Mo	L	py	Oxo
LUMO+5	-0.65	01	06	93	0
LUMO+4	-1.16	05	01	93	01
LUMO+3	-1.64	58	14	04	24
LUMO+2	-1.78	19	72	02	07
LUMO+1	-2.21	57	23	0	20
LUMO	-2.39	44	31	02	23
HOMO	-5.95	02	94 (S, 25)	02	02
HOMO-1	-6.41	01	95 (S, 26)	01	03
HOMO-2	-6.50	01	97 (S, 59)	01	01
HOMO-3	-6.75	0	97	01	02
HOMO-4	-6.89	0	100	0	0
HOMO-5	-7.07	03	83	02	12
HOMO-6	-7.39	0	86	11	03
HOMO-7	-7.55	0	13	86	01
HOMO-8	-7.68	05	53 (S, 23)	17	25
HOMO-9	-7.75	05	30 (S, 23)	11	54
HOMO-10	-8.19	06	42	13	39