Supporting information

for

Molybdenum(II) complexes with *p*-substituted BIAN ligands: synthesis, characterization, biological activity and computational study

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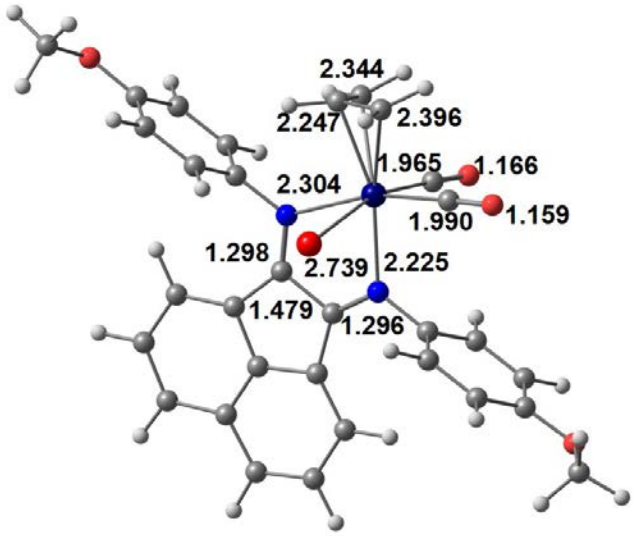

Figure S1. DFT optimized structures of the axial isomer of complex **3a** with some relevant distances (Å).

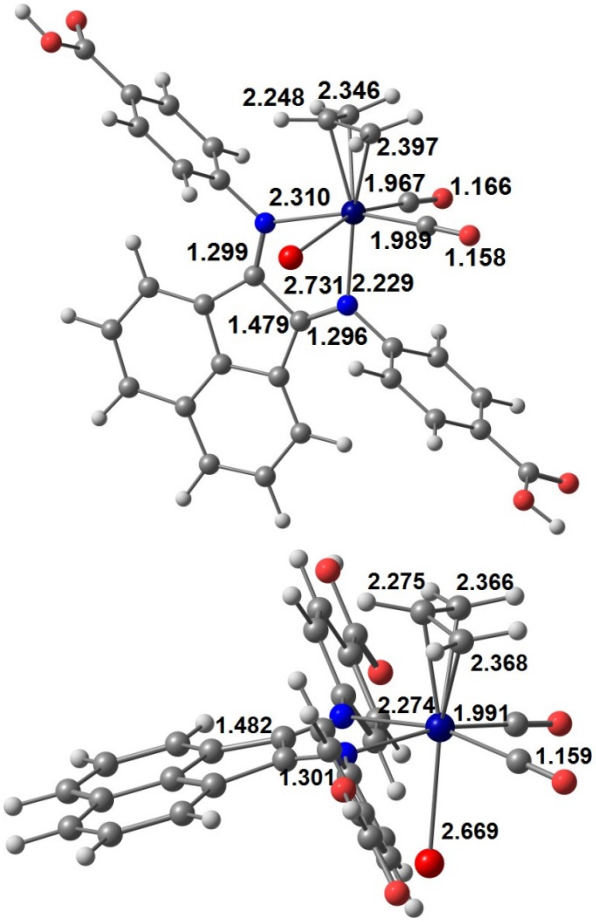

Figure S2. DFT optimized structures of the two isomers of isomer **4** (axial, top; equatorial, bottom) with some relevant distances (Å).

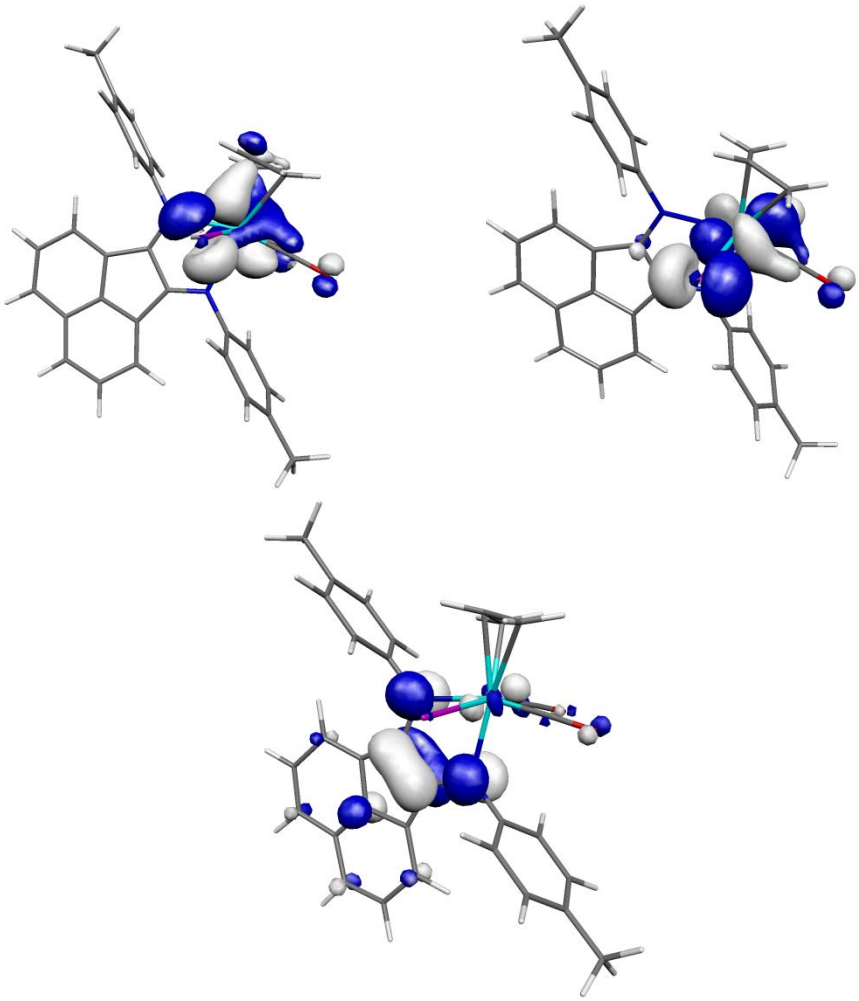

Figure S3. HOMO-1 (top, left), HOMO (top, right) and LUMO (bottom) of complex [Mo(η^3-C_3H_5)Br(CO)$_2$(L2)] (**2**).

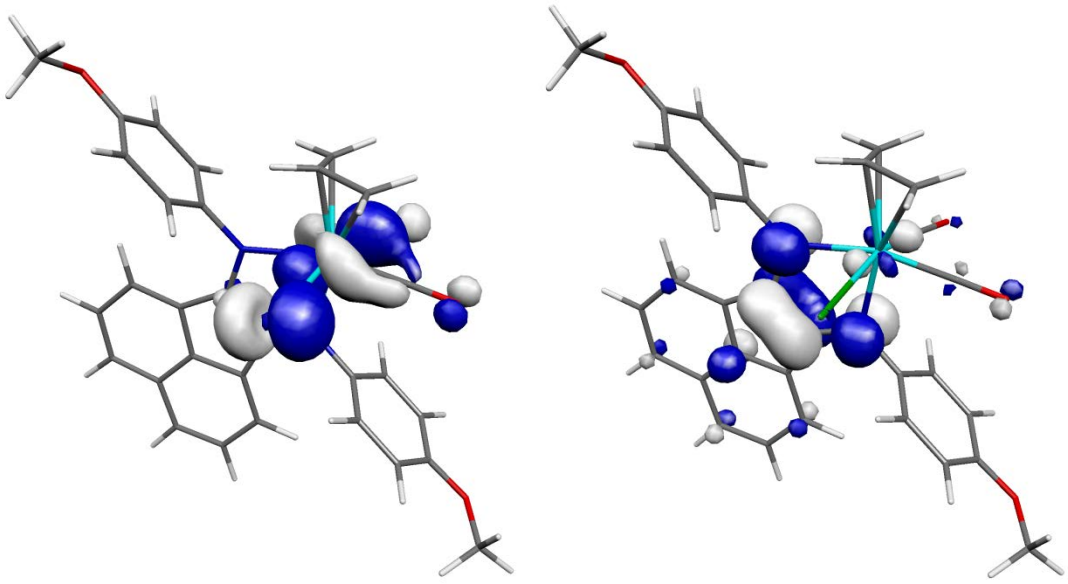

Figure S4. HOMO (left) and LUMO (right) of complex [Mo(η^3-C_3H_5)Br(CO)$_2$(L3)] (**3a**).

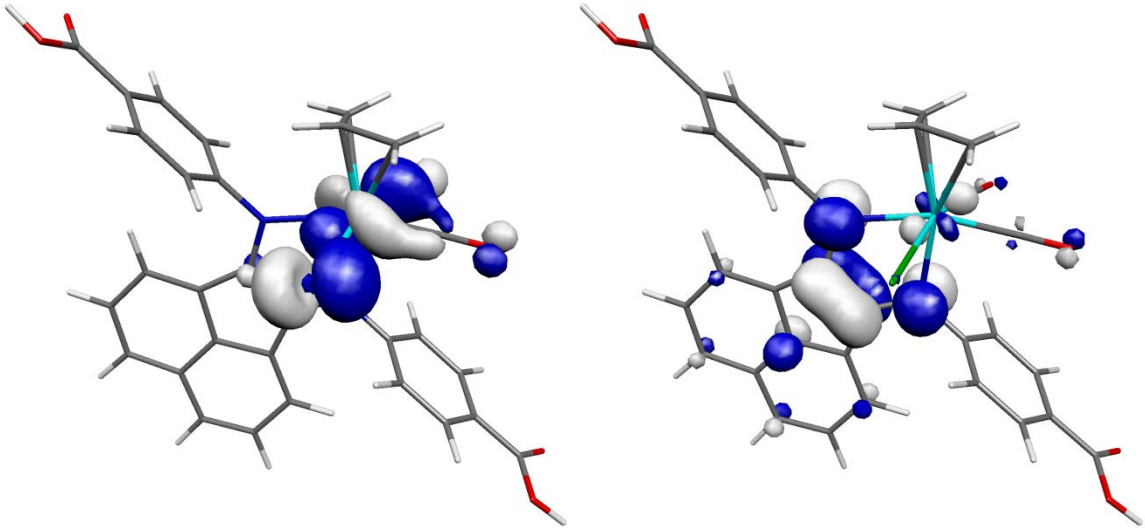

Figure S5. HOMO (left) and LUMO (right) of complex [Mo(η^3-C_3H_5)Br(CO)$_2$(L4)] (**4**).

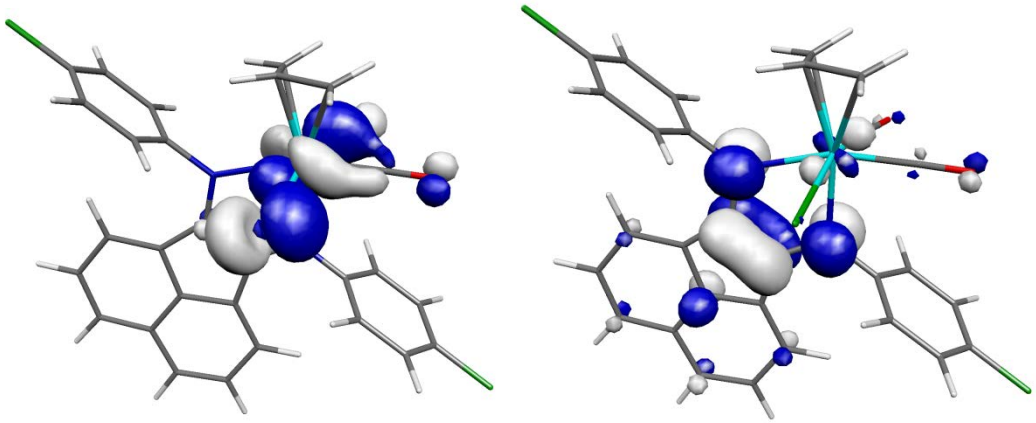

Figure S6. HOMO (left) and LUMO (right) of complex [Mo(η^3-C_3H_5)Br(CO)$_2$(L5)] (**5**).

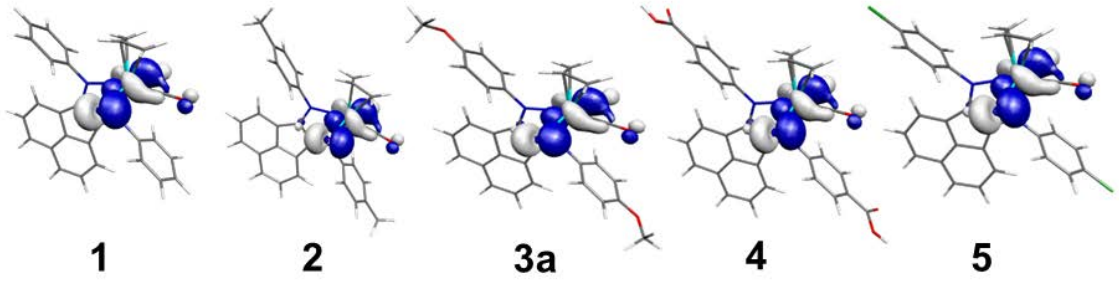

Figure S7. The HOMOs of complexes **1**, **2**, **3a**, **4** and **5**.

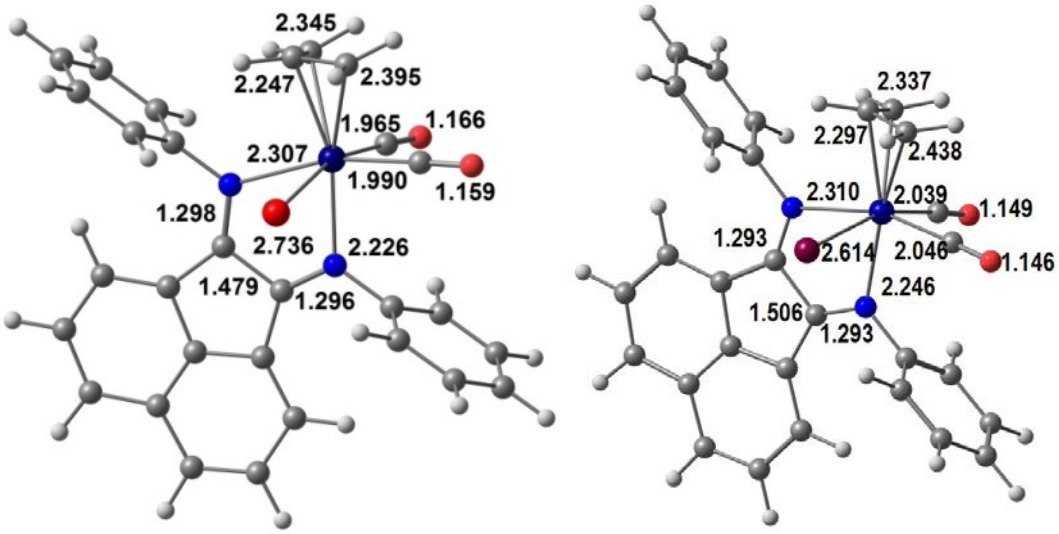

Figure S8. DFT optimized structures of the axial isomers of **1** and $\mathbf{1}^{+}$ with some relevant distances (Å).

Table S1. Crystal data and selected refinement details for **2** and **3c.**

Compound	**2**	**3c**
Empirical formula	$C_{31}H_{25}N_2O_2BrMo$	$C_{34}H_{28}F_3MoN_3O_7S$
Formula weight	633.38	775.59
Temperature	150(2)	293(2)
Crystal system	Triclinic	Triclinic
Space group	$P\bar{1}$	$P\bar{1}$
a/Å	10.2544(17)	9.9182(6)
b/Å	11.748(2)	13.4256(8)
c/Å	12.826(2)	14.5907(8)
α/°	78.519(9)	66.621(6)
β/°	68.136(8)	71.534(5)
γ/°	68.329(8)	72.517(5)
Volume/Å^3	1329.24(4)	1657.12(19)
Z	2	2
ρ_{calc}g/cm^3	1.582	1.554
μ/mm^{-1}	2.028	0.529
F(000)	636.0	788.0
2θ range for data collection/°	6.516 to 49.998	5.306 to 49.996
Index ranges	$-11 \le h \le 12$, $-13 \le k \le 13$, $-15 \le l \le 15$	$-11 \le h \le 9$, $-15 \le k \le 10$, $-17 \le l \le 14$
Reflections collected	12965	8078
Independent reflections, R_{int}, R_{sigma}	4601, 0.0194, 0.0228	5726, 0.0134, 0.0183
Data/restraints/parameters	4601/12/379	5726/60/533
Goodness-of-fit on F^2	1.036	1.060
Final *R* indexes [I≥2*σ* (I)]		
R_1, wR_2	0.0203, 0.0512	0.0248, 0.0605
Final R indexes [all data]		
R_1, wR_2	0.0245, 0.0529	0.0278, 0.0616
Largest diff. peak/hole / eÅ^{-3}	0.30/-0.34	0.36/-0.28