Supporting Information
For
Quadruply Bonded Dimolybdenum Complexes with Highly Unusual Geometries and Vacant Coordination Sites

Mario Carrasco,[a] Michelle Faust,[b] Riccardo Peloso,[a] Amor Rodríguez,[a] Joaquín López Serrano,[a] Eleuterio Álvarez,[a] Celia Maya,[a] Philip P. Power*[b] and Ernesto Carmona*[a]

[a] Instituto de Investigaciones Químicas-Departamento de Química Inorgánica. Universidad de Sevilla-Consejo Superior de Investigaciones Científicas. Avenida Américo Vespucio 49, 41092 Sevilla, Spain. Fax: (+) 34-954460565. [b] Department of Chemistry, University of California, Davis, One Shields Avenue, Davis, Califonia 95616, United States.

E-mail: guzman@us.es; pppower@ucdavis.edu.

Materials and Methods

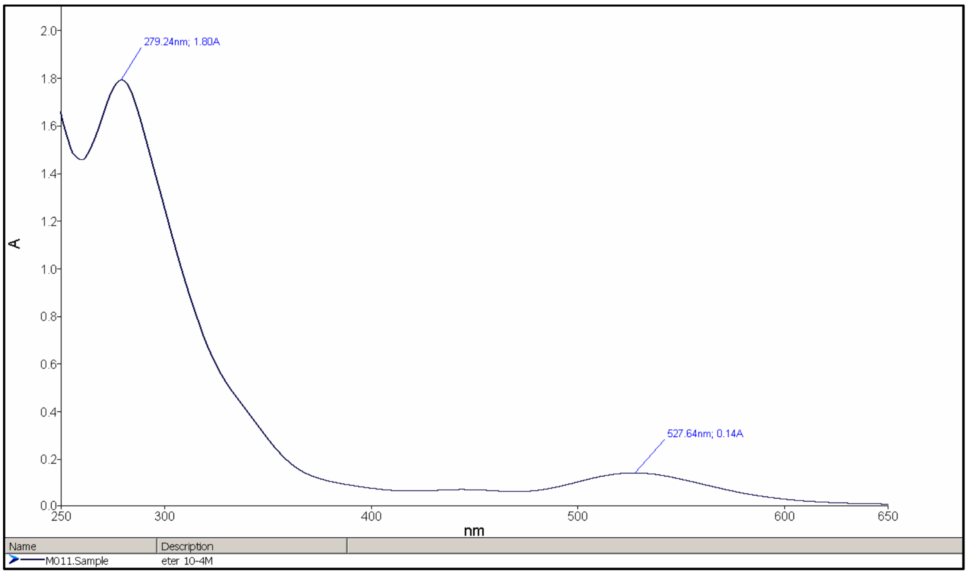
General considerations. All manipulations were carried out using standard Schlenk and glove box techniques under an atmosphere of argon and of high purity nitrogen, respectively. All solvents were dried and degassed prior to use. Toluene, n-hexane and n-pentane were distilled over sodium. Diethyl ether (Et_2O) and tetrahydrofuran (THF) were distilled under nitrogen over sodium/benzophenone. Quadruply bonded dimolybdenum complexes $Mo_2(O_2CR)_4$ (R= H, Me),[1] terphenyl ligand Ar'I (where Ar' = Ar^{Xyl2}),[2] and the corresponding lithium salt (LiAr')[3] were prepared according to literature methods. Dimolybdenum tetracarboxylates were washed with toluene at 100 ºC in order to remove any acidic residue. Benzene-d_6 (C_6D_6) was distilled under argon over sodium/benzophenone and toluene-d_8 (C_7D_8) was distilled under argon over sodium. Both were then degassed and dried over 4 Å molecular sieves. All other compounds were commercially available and were used as received. Solution NMR spectra were recorded on Bruker AMX-300, DRX-400 and DRX-500 spectrometers. The resonances of the solvents were used as the internal standard and the chemical shifts are reported relative to TMS. UV-visible spectra were recorded on a PerkinElmer Lambda 750 spectrometer and elemental analysis was carried out with a LECO TruSpec CHN elementary analyzer.

Preparation of $Mo_2(Ar^{Xyl}{}_2)(O_2CMe)_3$ (2)

Solid samples of $Mo_2(O_2CCH_3)_4$ (1.46 g, 3.42 mmol) and $LiAr^{Xyl}{}_2$ (1.0 g, 3.42 mmol) were mixed and cooled to -40 ºC. 20 ml of THF were added and the mixture was stirred for 12 hours, allowing to reach slowly the room temperature. The solvent was then removed under vacuum and the solid residue was extracted with 20 ml of toluene. The resulting red-wine suspension was centrifuged and the clear solution was transferred to a Schlenk tube, concentrated to ca. 10 mL and stored in the refrigerator at -23 ºC overnight. A bright red crystalline compound separated out, which was isolated by filtration and dried under vacuum for 3 hours. Yield: 1.41 g (63%).

^{1}H NMR (400 MHz, C_6D_6, 25 ºC): δ 2.00 (s, 3 H, trans-Me_{OAc}), 2.18 (s, 6 H, $Me_{Xyl'}$), 2.35 (s, 6 H, Me_{Xyl}), 2.51 (s, 6 H, Me_{OAc}), 6.14 (t, 1 H, $^3J_{HH}$ = 7.6 Hz, *p*-Xyl'), 6.49 (d, 2 H, $^3J_{HH}$ = 7.6 Hz, *m*-Xyl'), 6.78-6.86 (m, 3 H, system AB_2, *m*-Xyl and *p*-Xyl), 6.89 (d, 1 H, $^3J_{HH}$ = 7.6 Hz, *m*'-C_6H_3), 7.06 (d, 1 H, $^3J_{HH}$ = 7.6 Hz, *m*-C_6H_3), 7.31 (t, 1 H, $^3J_{HH}$ = 7.6 Hz, *p*-C_6H_3) ppm. $^{13}C\{^1H\}$ NMR (100 MHz, C_6D_6, 25 ºC): δ 20.9 (Me_{Xyl}), 22.1 ($Me_{Xyl'}$), 22.7 (trans-Me_{OAc}), 23.5 (Me_{OAc}), 123.5 (*m*'-C_6H_3), 125.7 (*m*-C_6H_3), 126.6 (*p*-C_6H_3), 126.9 (*p*-Xyl), 127.4 (*m*-Xyl), 128.5 (*p*-Xyl'), 129.2 (*m*-Xyl'), 135.5 (*o*-Xyl'), 136.3 (*o*-Xyl), 143.3 (*i*-Xyl), 145.7 (*i*-Xyl'), 147.4 (*o*-C_6H_3), 148.0 (*o*'-C_6H_3), 180.1 (Mo-C_{Ar}), 183.7 (O_2CMe), 183.8 (*trans*-O_2CMe). Anal. Calcd. for $C_{28}H_{30}Mo_2O_6$: C, 51.4; H, 4.6; Found: C, 51.3; H, 4.6. UV-Visible (ether solution 10^{-4}M, λ = 279 and 528 nm, ε = 13200 and 1030 mol^{-1} L cm^{-1}, respectively).

UV-Visible spectrum of $Mo_2(Ar^{Xyl}{}_2)(O_2CMe)_3$ (2)

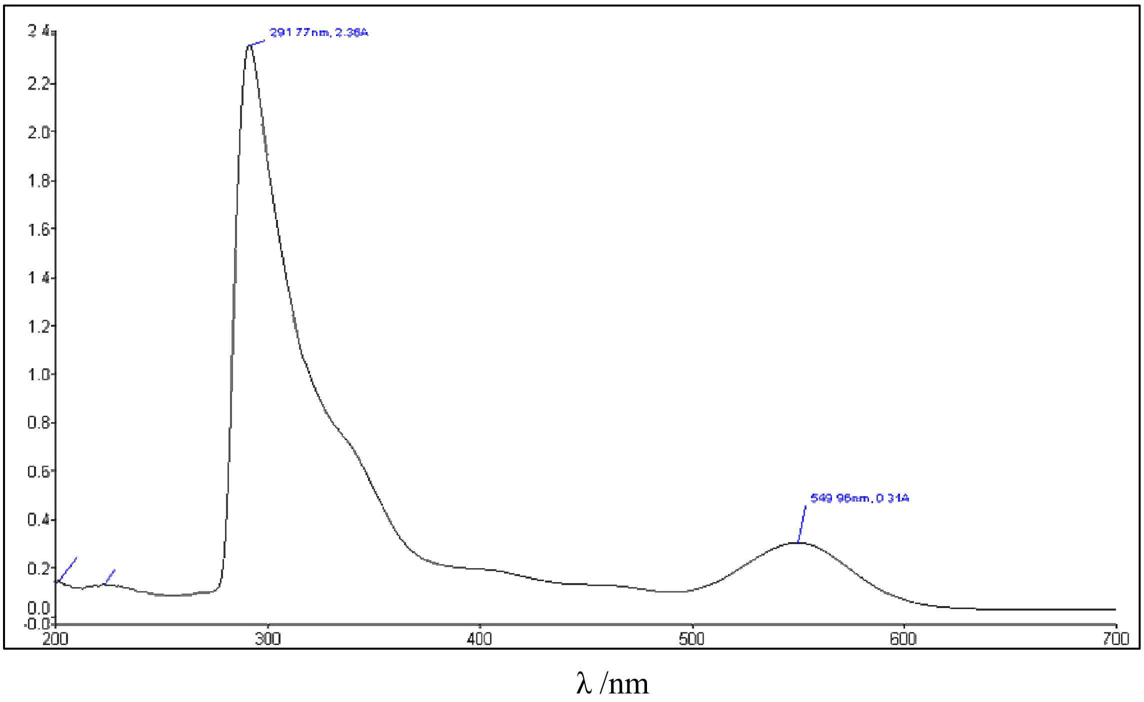


Preparation of $Mo_2(Ar^{Xyl}{}_2)_2(O_2CH)_2$ (3)

$Mo_2(O_2CH)_4$ (372 mg, 1mmol) and $LiAr^{Xyl}{}_2$ (585 mg, 2 mmol) were mixed and cooled to -50 ºC. Then, 50 ml of THF cooled at the same temperature, were added. The mixture was stirred for 24 hour, and the temperature allowed to reach slowly the room temperature. The violet solution was centrifuged and transferred to a Schlenk tube. It was concentrated and stored in the refrigerator at -23°C for two days. Violet crystals separated out, and were isolated by filtration and dried under vacuum for 3 hours, to obtain 260 mg of the desired compound (yield 30%).

^{1}H NMR (400 MHz, C_6D_6, 25 ºC): δ 1.94 (s, 12 H, $Me_{Xyl'}$), 2.17 (s, 12 H, Me_{Xyl}), 6.10 (d, 4 H, $^3J_{HH}$ = 7.6 Hz, *m*-Xyl′), 6.28 (t, 2 H, $^3J_{HH}$ = 7.6 Hz, *p*-Xyl′), 6.58 (dd, 2 H, $^3J_{HH}$ = 7.5 Hz, $^5J_{HH}$ = 1.3 Hz, *m′*-C_6H_3), 6.74 (dd, 2 H, $^3J_{HH}$ = 7.5 Hz, $^5J_{HH}$ = 1.3 Hz, *m*-C_6H_3), 6.89-6.96 (m, 6 H, system AB_2, *m*-Xyl, *p*-Xyl), 7.13 (t, 2 H, $^3J_{HH}$ = 7.5 Hz, *p*-C_6H_3), 8.97 (s, 2 H, *H*CO_2). $^{13}C\{^1H\}$ NMR (100 MHz, C_6D_6, 25 ºC): δ 21.5 (Me_{Xyl}), 22.6 ($Me_{Xyl'}$), 124.8 (*m′*-C_6H_3), 126.4 (*p*-C_6H_3), 126.7 (*m*-C_6H_3), 126.8 (*p*-Xyl), 127.3 (*m*-Xyl), 128.5 (*m*-Xyl′), 129.2 (*p*-Xyl′), 135.5 (*o*-Xyl′), 137.7 (*o*-Xyl), 143.7 (*i*-Xyl), 144.2 (*i*-Xyl′), 146.6, 147.1 (2 C each, *o*-C_6H_3, *o′*-C_6H_3), 171.7 (H*C*O_2), 174.0 (Mo-C_{Ar}). Anal. Calcd. for $C_{46}H_{44}Mo_2O_4$: C, 64.8; H, 5.2; Found: C, 65.4; H, 5.8. UV-Visible (ether solution 10^{-4}M, λ = 292 and 550 nm, ε = 23500 and 3100 mol^{-1} L cm^{-1}, respectively).

UV-Visible spectrum of $Mo_2(Ar^{Xyl}{}_2)_2(O_2CH)_2$ (3)



References:

[1] (a) Cotton, F. A., Norman, J.G, Jr., Stults, B.R., Webb, T.R., *J. Coord. Chemistry*, **1976**, *5*, 217. (b) *Inorganic Sytheses*, **1972**, *XIII,* 87.

[2] (a) Schiemenz B., Power P. P., *Organometallics*, **1996**, *15*, 958; (b) Simons, R. S., Haubrich, S. T., Mork, B. V., Niemeyer, M., Power, P. P., *Main Group Chemistry*, 1998, *2*, 275.

[3] Hino, S., Olmstead, M. M., Fettinger J. C., Power P.P., *J. Organomet. Chem*. **2005**, *690*, 1638.

X-Ray Structural Characterization of New Compounds

A single crystal of suitable size, coated with dry perfluoropolyether, was mounted on a glass fiber and fixed in a cold nitrogen stream [T = 173(2) K for compounds **2** and **3**] to the goniometer head. Data collection was performed on Bruker-Nonius X8APEX-II CCD diffractometer, using monochromatic radiation λ(Mo Kα1) = 0.71073 Å, by means of ω and φ scans. The data were reduced (SAINT)[1] and corrected for Lorentz polarisation effects and absorption by multiscan method applied by SADABS [2] . The structures were solved by direct methods (SIR-2002)[3] and refined against all F2 data by full-matrix least-squares techniques (SHELXTL-6.12)[4]. All the non-hydrogen atoms were refined with anisotropic displacement parameters. The hydrogen atoms were included from calculated positions and refined riding on their respective carbon atoms with isotropic displacement parameters.

References:

[1] SAINT 6.02, BRUKER-AXS, Inc., Madison, WI 53711-5373 USA, 1997–1999.

[2] SADABS George Sheldrick, Bruker AXS, Inc., Madison,Wisconsin, USA, 1999.

[3] M.C.Burla, M. Camalli, B. Carrozzini, G.L. Cascarano, C. Giacovazzo, G. Polidori, R. Spagna SIR2002: the program; *J. Appl. Cryst*. **2003**, *36*, 1103.

[4] SHELXTL 6.14, Bruker AXS, Inc., Madison, Wisconsin, USA, 2000–2003

X-ray Crystal structure of $\mathbf{Mo_2(Ar^{Xyl}{}_2)(O_2CMe)_3}$ (2)

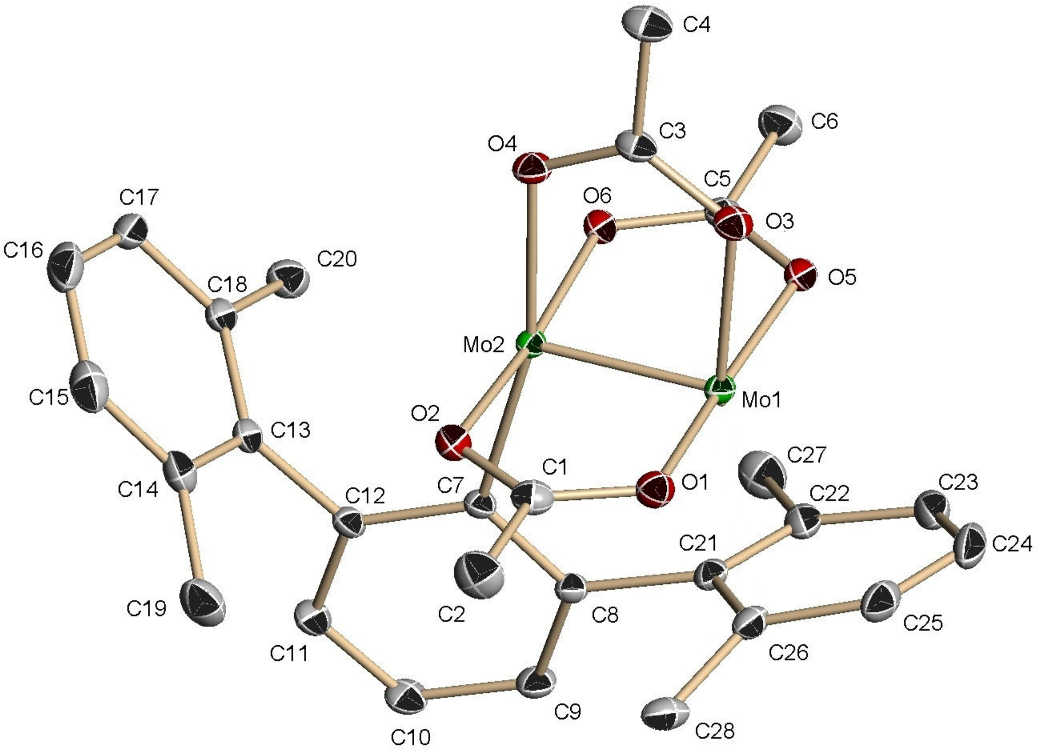


Figure *S*1. The solid state molecular structure of $\mathbf{Mo_2(Ar^{Xyl}{}_2)(O_2CMe)_3}$, **2**, with thermal ellipsoids set at 30% probability and all hydrogen atoms omitted for clarity. Selected bond lengths (Å) : Mo(1)-Mo(2), 2.086(1); Mo(1)-C(7), 2.192(1); Mo(1)-O(1), 2.101(1); Mo(1)-O(2), 2.099(1); Mo(1)-O(3), 2.088(1); Mo(2)-O(4), 2.161(1); Mo(1)-O(5), 2.087 (1); Mo(2)-O(6), 2.117(1); Mo(1)···C(26), 2.57(1).

Table 1S. Crystal data and structure refinement for $\mathbf{Mo_2(Ar^{Xyl}{}_2)(O_2CMe)_3}$, **2**.

Empirical formula	C28 H30 Mo2 O6	
Formula weight	654.40	
Temperature	273(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 8.3595(4) Å	α = 104.220(2)°.
	b = 9.8309(4) Å	β = 96.024(2)°.
	c = 16.4231(7) Å	γ = 91.870(2)°.
Volume	1298.70(10) Å^3	
Z	2	
Density (calculated)	1.673 Mg/m^3	
Absorption coefficient	1.006 mm^{-1}	
F(000)	660	
Crystal size	0.26 × 0.19 × 0.18 mm^3	
Theta range for data collection	2.14 to 36.44°	
Index ranges	-13<=h<=13, -16<=k<=16, -26<=l<=27	
Reflections collected	38302	
Independent reflections	12143 [R(int) = 0.0798]	
Completeness to theta = 36.44°	95.7 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	12143 / 0 / 445	
Goodness-of-fit on F^2	1.030	
Final R indices [I>2sigma(I)]	R1 = 0.0352, wR2 = 0.0984	
R indices (all data)	R1 = 0.0400, wR2 = 0.1010	
Largest diff. peak and hole	2.292 and -1.437 e.Å^{-3}	

X-ray Crystal structure of $Mo_2(Ar^{Xyl}{}_2)_2(O_2CH)_2$ (3)

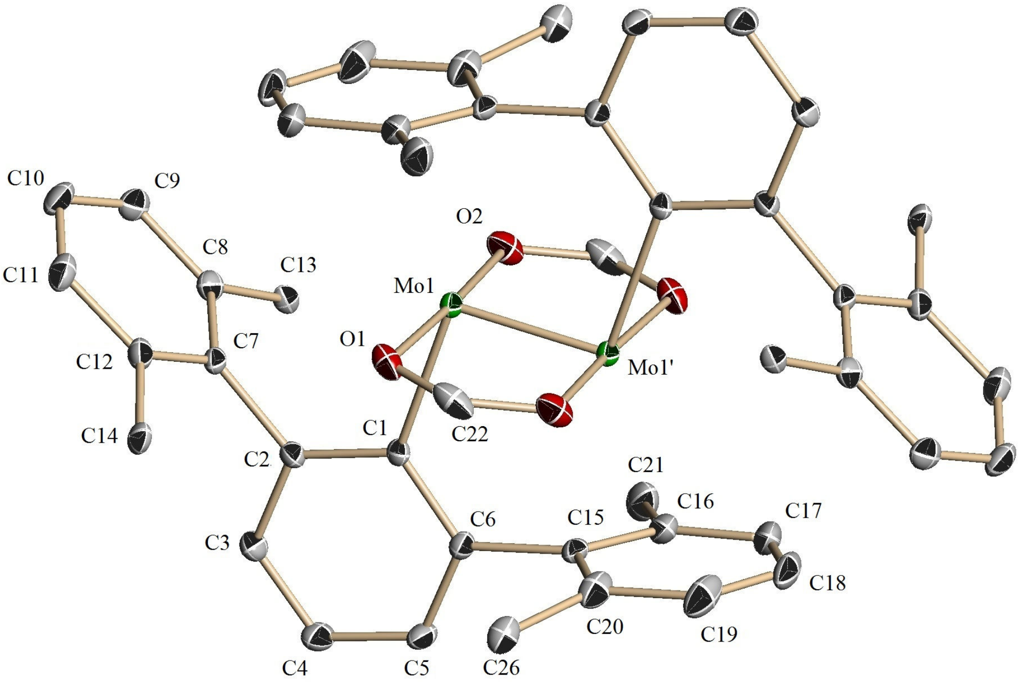


Figure S2. The solid state molecular structure of $\mathbf{Mo_2(Ar^{Xyl}{}_2)_2(O_2CH)_2}$, **3**, with thermal ellipsoids set at 30% probability and all hydrogen atoms omitted for clarity. Selected bond lengths (Å) : Mo(1)-Mo(2), 2.095(1); Mo(1)-C(1), 2.187(3); Mo(1)-O(1), 2.106(3); Mo(1)-O(2), 2.110(3); Mo(2)···C(15), 2.78(1).

Table 2S. Crystal data and structure refinement for **$Mo_2(Ar^{Xyl}{}_2)_2(O_2CH)_2$, 3**.

Empirical formula	$C_{46}H_{44}Mo_2O_4$	
Formula weight	852.69	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 8.3268(4) Å	α = 90°.
	b = 20.3348(9) Å	β = 98.516(2)°.
	c = 11.1270(4) Å	γ = 90°.
Volume	1863.29(14) $Å^3$	
Z	2	
Density (calculated)	1.520 Mg/m^3	
Absorption coefficient	0.718 mm^{-1}	
F(000)	872	
Crystal size	0.25 × 0.12 × 0.05 mm^3	
Theta range for data collection	2.00 to 30.66°	
Index ranges	-8<=h<=11, -29<=k<=22, -14<=l<=15	
Reflections collected	32923	
Independent reflections	5654 [R(int) = 0.0756]	
Completeness to theta = 30.66°	98.2 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9650 and 0.8410	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5654 / 0 / 239	
Goodness-of-fit on F^2	1.012	
Final R indices [I>2sigma(I)]	R1 = 0.0437, wR2 = 0.0972	
R indices (all data)	R1 = 0.0703, wR2 = 0.1281	
Largest diff. peak and hole	0.927 and -0.806 e.$Å^{-3}$	

Computational Details

DFT calculations were performed with the Gaussian 09 package.[1] The Mo atoms were represented by the Stuttgart/Dresden Effective Core Potential and the associated basis set[2] as implemented in Gaussian 09 (SDD). The remaining H, C and O atoms were represented by means of the 6-31G(d,p) basis set in geometry optimizations.[3-5] The geometries for all species described were optimized in the gas phase without symmetry restrictions. Frequency calculations were performed on the optimized structures at the same level of theory to characterize the stationary points. Topological analysis of the charge density, $\rho(\mathbf{r})$, using the "Atom In Molecules" (AIM) approach[6,7], was performed with the AIM2000 program[8]. Wavefunctions suitable for analysis with the AIM2000 program were generated with Gaussian09 from the corresponding optimized molecular structures at the DFT SDD/6311G(d,p) level of theory. Natural Bonding Orbital analysis[9] was made with the NBO 3.1 program as implemented in Gaussian 09[10].

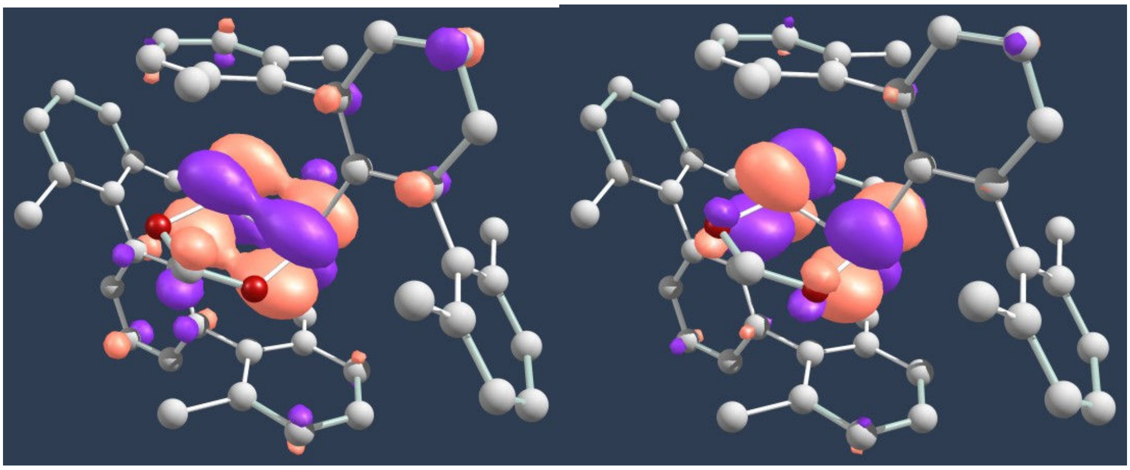
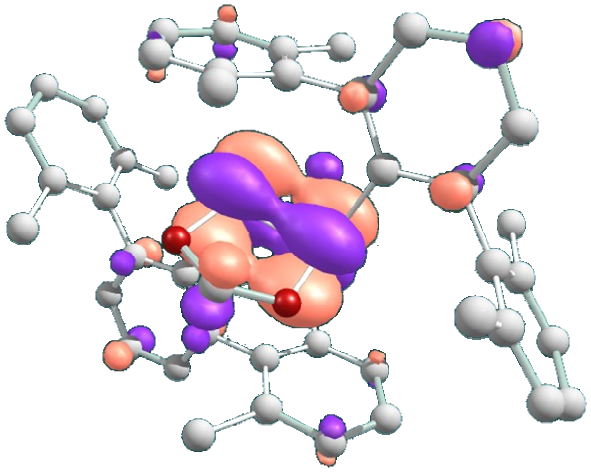
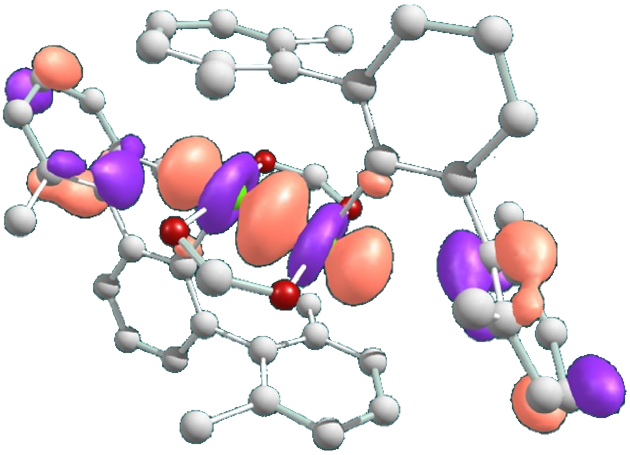
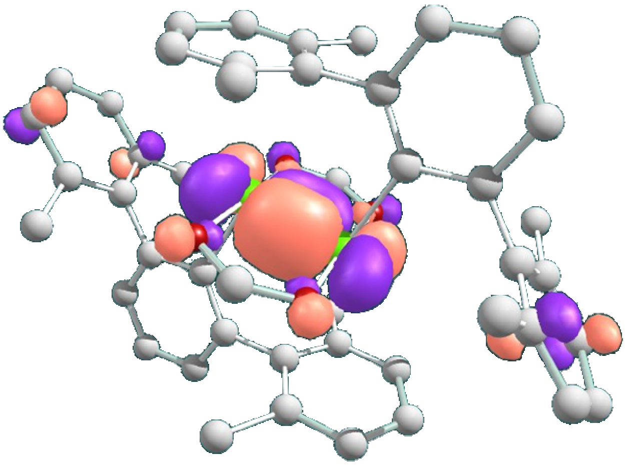
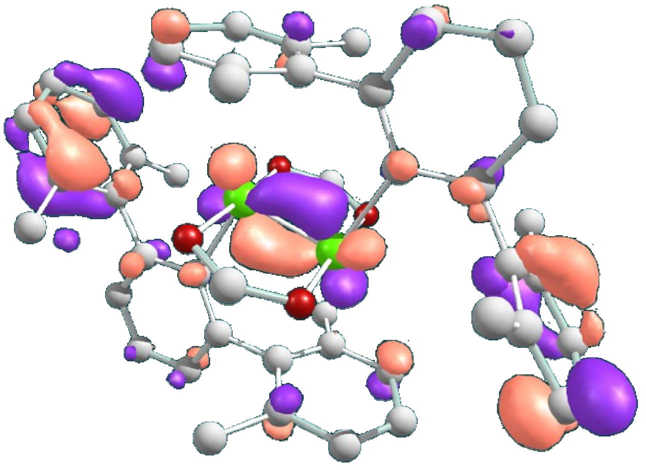
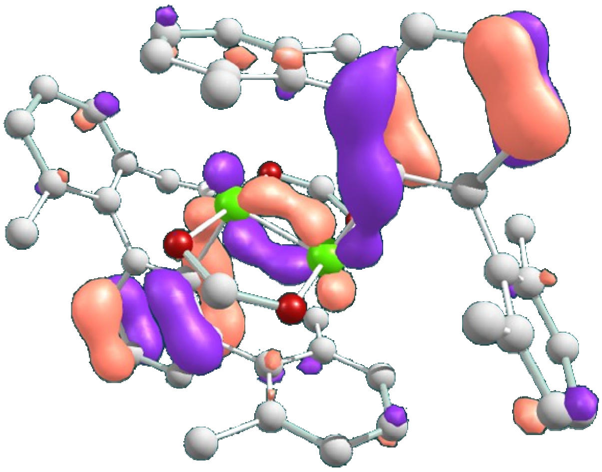
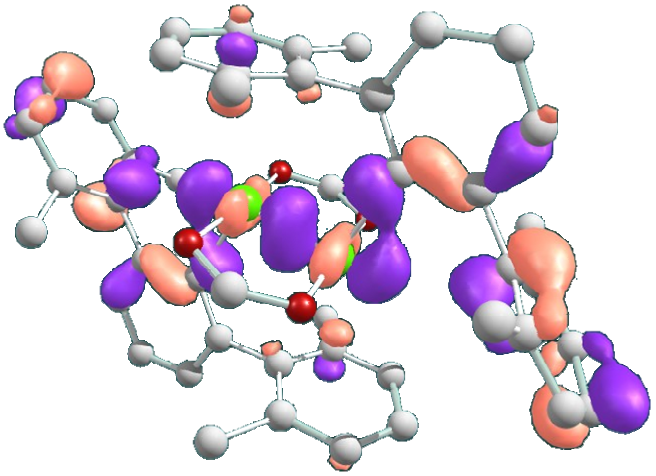
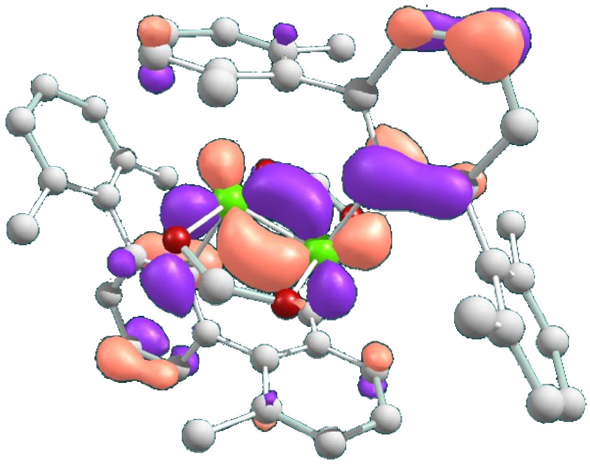
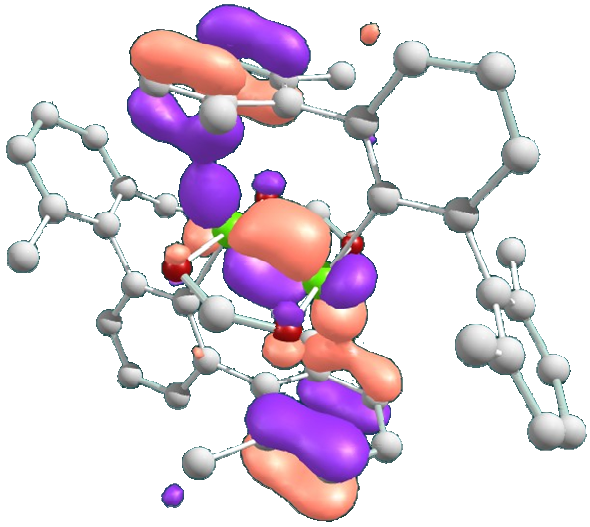


Fig Sx. Contour plots of Kohn-Sham HOMO (left) and LUMO (right) of complex **3b**. The calculated energies are -4.646 and -1.825 eV respectively ($\Delta E_{\mathrm{HOMO\text{-}LUMO}}$ = 2.820 eV or 439 nm).

Table Sx. Relevant Kohn-Sham bonding molecular orbitals involved in the Mo-Mo interaction. The first three MOs are almost pure metal-metal orbitals. The following show a varying degree of mixing with ligand based orbitals. The HOMO -14 show overlapping between Mo-Mo and flanking aryl orbitals.

MO		**Energy (eV)**
HOMO		**-4.65**
HOMO -1		**-6.17**
HOMO -2		**-6.38**

HOMO -3		**-6.42**
HOMO -6		**-6.53**
HOMO -9		**-6.70**

HOMO -10		**-6.72**
HOMO -14		**-7.08**

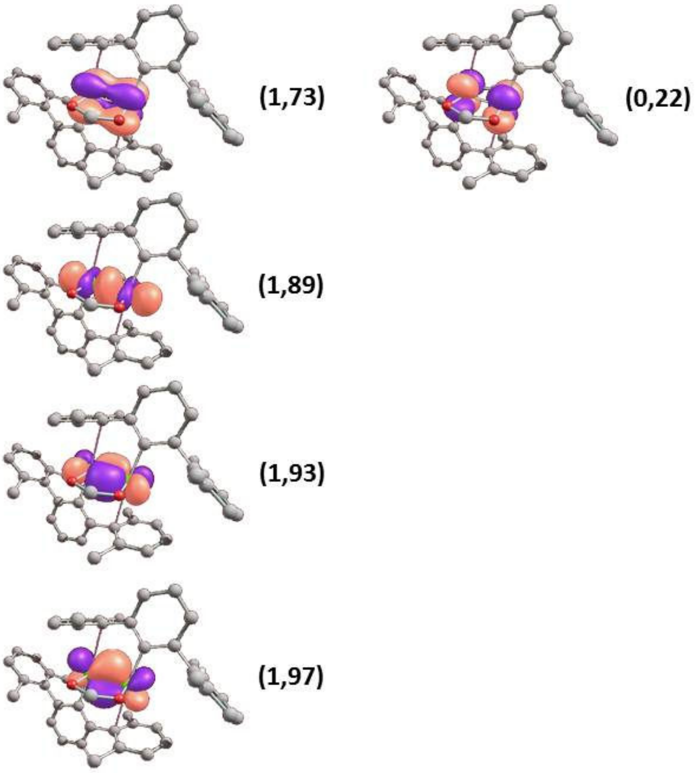


Fig. Sx. Contour plots of the four bonding NBOs and δ^* NBO localized on the Mo-Mo bond of **3b** (orbital occupancy is shown in parenthesis). The NBO analysis failed to find significant second order perturbation energy delocalizations (E > 5 kcal/mol) between Mo related orbitals and their flanking aryl.

Tables of the optimized geometries (Cartesian coordinates, in Angstroms) for the calculated species.

Gas phase Energies (in Hartrees) in parenthesis:

Table S1. 3b (-2215.35672303)

42	-1.015470000	-0.259074000	0.137509000
8	-1.295673000	-0.488608000	-1.966790000
8	-0.850335000	-0.039712000	2.259015000
6	-1.881514000	1.733921000	-0.014917000
6	-3.291138000	1.830742000	-0.047422000
6	-3.930866000	3.073359000	-0.131396000
1	-5.021439000	3.099054000	-0.151629000
6	-3.203070000	4.253726000	-0.189510000
1	-3.709785000	5.213968000	-0.256792000
6	-1.816252000	4.186389000	-0.164209000
1	-1.216678000	5.097000000	-0.214086000
6	-1.170088000	2.951304000	-0.077660000
6	-4.189447000	0.637891000	0.008215000
6	-4.626859000	0.152508000	1.255119000
6	-5.570881000	-0.875896000	1.290371000

1	-5.917123000	-1.242632000	2.256605000
6	-6.087217000	-1.410144000	0.116580000
1	-6.834341000	-2.200827000	0.159072000
6	-5.655023000	-0.924160000	-1.111747000
1	-6.065677000	-1.330049000	-2.035956000
6	-4.715526000	0.105320000	-1.184429000
6	-4.129262000	0.759544000	2.534595000
1	-4.341289000	1.835811000	2.570869000
1	-3.042984000	0.648617000	2.643477000
1	-4.608012000	0.289738000	3.400780000
6	-4.317082000	0.667591000	-2.516955000
1	-4.593818000	1.726135000	-2.600972000
1	-4.805017000	0.123663000	-3.332916000
1	-3.232175000	0.606318000	-2.661804000
6	0.320910000	2.964620000	-0.076841000
6	1.022864000	2.850909000	-1.299411000
6	2.426489000	2.911507000	-1.285044000
1	2.968828000	2.782056000	-2.221833000
6	3.113400000	3.174331000	-0.108273000
1	4.199320000	3.212863000	-0.114331000
6	2.413516000	3.366934000	1.079684000
1	2.954807000	3.570927000	2.002568000
6	1.026139000	3.255303000	1.115126000
6	0.296769000	2.874432000	-2.612431000
1	0.092330000	3.918883000	-2.885984000
1	-0.675429000	2.372285000	-2.573898000
1	0.902877000	2.428730000	-3.407173000
6	-0.289605000	-0.281018000	-2.700481000
1	-0.412245000	-0.383745000	-3.789198000
6	0.282269000	3.473474000	2.397283000
1	0.949856000	3.367306000	3.259373000
1	-0.556197000	2.775057000	2.505087000
1	-0.155180000	4.479970000	2.429237000
42	1.015730000	0.259028000	-0.137756000
8	1.295996000	0.488819000	1.966496000
8	0.850763000	0.039552000	-2.259247000
6	1.881495000	-1.734056000	0.014917000
6	3.291109000	-1.830903000	0.047562000
6	3.930808000	-3.073509000	0.131725000
1	5.021381000	-3.099227000	0.151993000
6	3.202977000	-4.253853000	0.189994000
1	3.709667000	-5.214094000	0.257483000
6	1.816168000	-4.186489000	0.164633000
1	1.216573000	-5.097076000	0.214700000
6	1.170022000	-2.951409000	0.077840000
6	4.189392000	-0.638040000	-0.008083000
6	4.626802000	-0.152659000	-1.254980000
6	5.570810000	0.875753000	-1.290247000
1	5.917027000	1.242487000	-2.256488000
6	6.087158000	1.409983000	-0.116451000
1	6.834272000	2.200677000	-0.158934000
6	5.654854000	0.924100000	1.111879000
1	6.065339000	1.330159000	2.036089000
6	4.715287000	-0.105319000	1.184580000
6	4.128987000	-0.759596000	-2.534419000
1	4.341370000	-1.835785000	-2.570972000
1	3.042632000	-0.648979000	-2.642865000
1	4.607278000	-0.289463000	-3.400679000
6	4.316507000	-0.667175000	2.517185000
1	4.594036000	-1.725456000	2.601924000
1	4.803655000	-0.122467000	3.333097000

1	3.231489000	-0.606610000	2.661545000
6	-0.320982000	-2.964680000	0.076912000
6	-1.023058000	-2.850987000	1.299419000
6	-2.426695000	-2.911288000	1.284855000
1	-2.969140000	-2.781945000	2.221597000
6	-3.113522000	-3.173821000	0.107954000
1	-4.199455000	-3.212063000	0.113862000
6	-2.413510000	-3.366544000	-1.079906000
1	-2.954688000	-3.570422000	-2.002878000
6	-1.026104000	-3.255206000	-1.115148000
6	-0.297108000	-2.874834000	2.612516000
1	-0.092696000	-3.919347000	2.885834000
1	0.675110000	-2.372694000	2.574219000
1	-0.903291000	-2.429330000	3.407312000
6	0.289978000	0.281119000	2.700216000
1	0.412608000	0.383957000	3.788920000
6	-0.282069000	-3.473252000	-2.397234000
1	-0.949601000	-3.367216000	-3.259387000
1	0.556232000	-2.774615000	-2.504962000
1	0.155661000	-4.479617000	-2.429122000

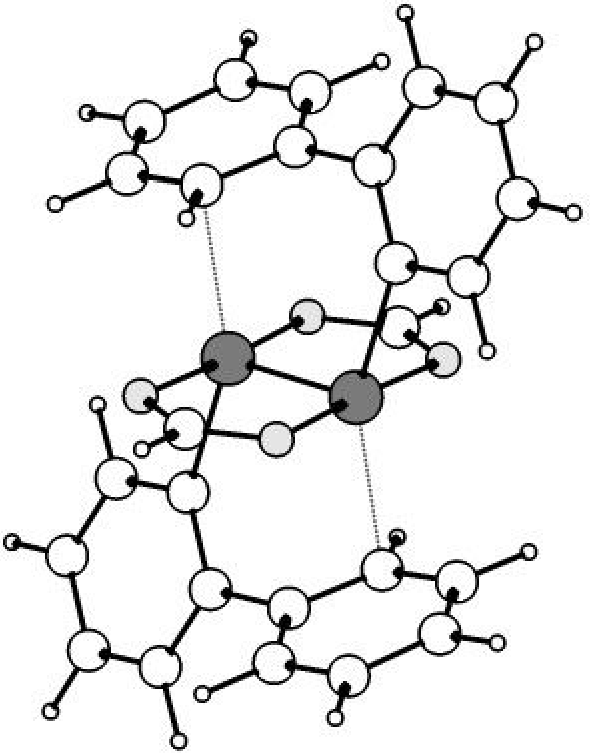


Table S1. 3calc (-1439.29742636)

42	0.153955000	-1.009807000	-0.263773000
8	-0.294768000	-1.670849000	1.704553000
8	0.587072000	-0.466945000	-2.282912000
6	2.253273000	-1.277890000	0.124285000
6	2.623664000	-2.632003000	0.116654000
6	3.957510000	-3.037157000	0.109487000
1	4.206687000	-4.096925000	0.101866000
6	4.969370000	-2.082928000	0.107079000
1	6.013530000	-2.387505000	0.097311000
6	4.637591000	-0.731851000	0.131126000
1	5.423432000	0.023828000	0.153600000
6	3.299413000	-0.332145000	0.157679000
6	2.962557000	1.106862000	0.232722000

6	2.140376000	1.569079000	1.278465000
6	1.739878000	2.912037000	1.336596000
1	1.109183000	3.245733000	2.160216000
6	2.183211000	3.812920000	0.369554000
1	1.870408000	4.853070000	0.405928000
6	3.048597000	3.371893000	-0.628360000
1	3.412557000	4.074969000	-1.374263000
6	3.432218000	2.035685000	-0.699423000
6	-0.563584000	-0.771251000	2.550408000
1	-0.791265000	-1.080201000	3.579987000
42	-0.153773000	1.009226000	0.263745000
8	0.294776000	1.670212000	-1.704709000
8	-0.587042000	0.466284000	2.282855000
6	-2.252922000	1.277986000	-0.124448000
6	-2.622765000	2.632246000	-0.116854000
6	-3.956442000	3.037941000	-0.109908000
1	-4.205184000	4.097812000	-0.102317000
6	-4.968695000	2.084126000	-0.107705000
1	-6.012732000	2.389129000	-0.098151000
6	-4.637462000	0.732913000	-0.131674000
1	-5.423604000	-0.022445000	-0.154326000
6	-3.299443000	0.332661000	-0.157971000
6	-2.963060000	-1.106466000	-0.232754000
6	-2.140574000	-1.569108000	-1.278071000
6	-1.740251000	-2.912117000	-1.335684000
1	-1.109409000	-3.246172000	-2.159049000
6	-2.184111000	-3.812706000	-0.368577000
1	-1.871415000	-4.852902000	-0.404554000
6	-3.049843000	-3.371293000	0.628839000
1	-3.414218000	-4.074126000	1.374770000
6	-3.433236000	-2.034968000	0.699424000
6	0.563543000	0.770593000	-2.550528000
1	0.791039000	1.079480000	-3.580167000
1	1.899374000	0.887303000	2.093535000
1	4.082068000	1.692036000	-1.502878000
1	1.847054000	-3.404031000	0.112794000
1	-1.845847000	3.403969000	-0.112882000
1	-1.899167000	-0.887606000	-2.093247000
1	-4.083311000	-1.691000000	1.502558000

Literature.

(1) Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J.; Gaussian 09, Revision A.1. Gaussian, Inc. Wallingford CT ed. 2009.

(2) Andrae, D.; U., H.; Dolg, M.; Stoll, H.; Preul, H. **1990**, *Theor. Chim. Acc.*, 123.

(3) Hehre, W. J.; Ditchfield, R.; Pople, J. A. *J. Phys. Chem.* **1972**, *56*, 2257.

(4) Hariharan, P. C.; Pople, J. A. *Theor. Chim. Acta.* **1973**, *28*, 213.

(5) Francl, M. M.; Pietro, W. J.; Hehre, W. J.; Binkley, J. S.; Gordon, M. S.; DeFrees, D. J.; Pople, J. A. *J. Chem. Phys.* **1982**, *77*, 3654.

(6) Bader, R. F. *Atom in Molecules: A Quantum Theory*; Oxford University Press: Oxford, UK, 1995.

(7) Bader, R. F. W. *Chem. Rev.* **1991**, *91*, 893.

(8) Biegler-König, F.; Schönbohm, J.; 2.0 ed. 2002, p AIM2000.

(9) Reed, A. E.; Curtis, L. A.; Weinhold, F. *Chem. Rev.* **1988**, *88*, 899.

(10) Glendening, E. D.; Reed, A. E.; Carpenter, J. E.; Weinhold, F. In *NBO*; Version 3.1 ed.