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SUPPLEMENTARY MATERIAL TO

Synthesis and characterization of *cis*-dioxomolybdenum(VI) complexes having furil as a precursor molecule

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PHYSICAL AND ANALYTICAL DATA OF THE MOLYBDENUM COMPLEXES

$[MoO_2(L^1)](acac)_2$ ***(1)***. Yield: 62 %; m.p. 306 °C; Anal. Calcd. for $C_{32}H_{32}MoN_4O_8$ (FW 696.57): C, 55.2; H, 4.6; N, 8.1; Mo, 13.8 %. Found: C, 55.1; H, 4.5; N, 8.0; Mo, 13.7 %.

$[MoO_2(L^2)](acac)_2$ ***(2)***. Yield: 64 %; m.p. 304 °C; Anal. Calcd. for $C_{30}H_{30}MoN_6O_8$ (FW 698.54): C, 51.6; H, 4.3; N, 12.0; Mo, 13.7 %. Found: C, 51.5; H, 4.2; N, 12.0; Mo, 13.7 %.

$[MoO_2(mac^1)](acac)_2$ ***(3)***. Yield 65 %; m.p. 305 °C; Anal. Calcd. for $C_{37}H_{36}MoN_4O_8$ (FW 760.66): C, 58.4; H, 4.7; N, 7.4; Mo, 12.6 %. Found: C, 58.3; H, 4.6; N, 7.3; Mo, 12.5 %.

$[MoO_2(mac^2)](acac)_2$ ***(4)***. Yield 62 %; m.p. 308 °C; Anal. Calcd. for $C_{42}H_{38}MoN_4O_8$ (FW 822.73): C, 61.3; H, 4.6; N, 6.8; Mo, 11.7 % . Found: C, 61.2; H, 4.5; N, 6.7; Mo, 11.6 %.

$[MoO_2(mac^3)](acac)_2$ ***(5)***. Yield: 65 %; m.p. 306 °C; Anal. Calcd. for $C_{40}H_{33}F_3MoN_4O_8S$ (FW 882.73): C, 54.4; H, 3.7; N, 6.3; Mo, 10.9; S, 3.7 %. Found: C, 54.3; H, 3.6; N, 6.2; Mo, 10.8; S, 3.6 %.

$[MoO_2(mac^4)](acac)_2$ ***(6)***. Yield 67 %; m.p. 305 °C; Anal. Calcd. for $C_{47}H_{40}MoN_4O_8$ (FW 884.80): C, 63.8; H, 4.6; N, 6.3; Mo, 10.8 %. Found: C, 63.7; H, 4.5; N, 6.2; Mo, 10.8 %.

$[MoO_2(mac^5)](acac)_2$ ***(7)***. Yield: 65 %; m.p. 304 °C; Anal. Calcd. for $C_{35}H_{34}MoN_6O_8$ (FW 762.63): C, 55.1; H, 4.5; N, 11.0; Mo, 12.6 %. Found: C, 55.0; H, 4.4; N, 11.0; Mo, 12.5 %.

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[$MoO_2(mac^6)$](acac)$_2$ ***(8)***. Yield: 67 %; m.p. 306 °C; Anal. Calcd. for $C_{40}H_{36}MoN_6O_8$ (FW 824.70): C, 58.3; H, 4.4; N, 10.2; Mo, 11.6 %. Found: C, 58.2; H, 4.3; N, 10.1; Mo, 11.5 %.

[$MoO_2(mac^7)$](acac)$_2$ ***(9)***. Yield: 62 %; m.p. 308 °C; Anal. Calcd. for $C_{38}H_{31}F_3MoN_6O_8S$ (FW 884.70): C, 51.6; H, 3.5; N, 9.5; Mo, 10.8; S, 3.6 %. Found: C, 51.5; H, 3.4; N, 9.4; Mo, 10.7; S, 3.5 %.

[$MoO_2(mac^8)$](acac)$_2$ ***(10)***. Yield: 65 %; m.p. 304 °C; Anal. Calcd. for $C_{45}H_{38}MoN_6O_8$ (FW 886.77): C, 61.0; H, 4.3; N, 9.5; Mo, 10.8 %. Found: C, 60.9; H, 4.2, N, 9.5; Mo, 10.7 %.

L^1 = ligand derived by condensation of furil with 1,2-diaminobenzene (1:2); L^2 = ligand derived by condensation of furil with 2,3-diaminopyridine(1:2); mac^1 = macrocyclic ligand derived by condensation of L^1 with acetylacetone; mac^2 = macrocyclic ligand derived by condensation of L^1 with benzoylacetone; mac^3 = macrocyclic ligand derived by condensation of L^1 with thenoyltrifluoroacetone; mac^4 = macrocyclic ligand derived by condensation of L^1 with dibenzoylmethane; mac^5 = macrocyclic ligand derived by condensation of L^2 with acetylacetone; mac^6 = macrocyclic ligand derived by condensation of L^2 with benzoylacetone; mac^7 = macrocyclic ligand derived by condensation of L^2 with thenoyltrifluoroacetone; mac^8 = macrocyclic ligand derived by condensation of L^2 with dibenzoylmethane.

INFRARED DATA

TABLE S-I. Infrared spectral bands (ν / cm^{-1}) of the molybdenum complexes. All spectra were recorded in KBr pellets in the range 4000–200 cm^{-1}

Complex	>C=N	Mo–N	>C=O	>C=C<	ν_{asym}	ν_{sym}	ν_{asym}	ν_{sym}
			of acetylacetonate		O=Mo=O		N–H	
$[MoO_2(L^1)](acac)_2$	1622	302	1560	1517	906	938	3352	3182
$[MoO_2(L^2)](acac)_2$	1620	300	1564	1515	904	936	3350	3180
$[MoO_2(mac^1)](acac)_2$	1622	301	1562	1513	903	943	–	–
$[MoO_2(mac^2)](acac)_2$	1616	304	1560	1517	904	940	–	–
$[MoO_2(mac^3)](acac)_2$	1618	304	1562	1513	905	942	–	–
$[MoO_2(mac^4)](acac)_2$	1622	303	1560	1515	904	943	–	–
$[MoO_2(mac^5)](acac)_2$	1624	301	1564	1517	908	940	–	–
$[MoO_2(mac^6)](acac)_2$	1616	302	1562	1513	906	942	–	–
$[MoO_2(mac^7)](acac)_2$	1618	300	1560	1515	904	936	–	–
$[MoO_2(mac^8)](acac)_2$	1622	303	1564	1517	905	944	–	–