Electronic Supplementary Information for Dalton Transactions

Solvent Effects in the Geometric Reorganization of an Oxo-Molybdenum (V) System.

Supporting information

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Table S1. Solvatochromic shifts in the *cis* and *trans*-(L1O) isomers

Solvent	*cis*-(L1O)$MoOCl_2$, λ max, nm		*trans*-(L1O)$MoOCl_2$, λ max, nm
Acetonitrile	506	326	349
Dimethylformamide	513	318	351
Dimethysulfoxide	496	325	345
Tetrahydrofuran	495	305	348
Ethylacetate	494	308	347
Benzene	477	314	342

Table S2. First order rate constants for the isomerization reaction.

compound	Solvent	Temperature, K	Rate, sec^{-1}
cis-(L1O)$MoOCl_2$	DMSO	313.15	0.000446
		322.65	0.000776
		328.15	0.000977
		333.65	0.001437
	THF	308.15	0.000115
		313.15	0.000322
		319.15	0.00049
		330.15	0.001283
	EtOAc	313.15	0.000206
		322.65	0.000496
		328.15	0.001163
		333.65	0.002302
	DMF	313.15	4.85E-05
		318.15	8.95E-05
		325.15	0.000201
		330.15	0.000341
	Benzene	313.15	0.000281
		318.15	0.000871
		327.15	0.001214
		334.15	0.004483
	Acetonitrile	298.15	9.23E-06
		303.15	1.88E-05
		308.15	3.36E-05
		313.15	6.10E-05
		313.15	5.64E-05
		318.15	0.000103

		323.15	0.00017
		328.15	0.000336
		333.65	0.000839
cis-(LO)$MoOCl_2$		289.15	4.14E-05
		308.15	0.000208
		313.15	0.000476
		318.15	0.000758
		323.15	0.001389

Table S3. Electrochemical data in acetonitrile.

	$E_{1/2}$ ($Mo^{VI/V}$)mV; (ΔE_p, mV)	$E_{1/2}$ ($Mo^{V/IV}$),mV, (ΔE_p, mV)
cis-(LO)$MoOCl_2$	864 (89)	-1031 (72)
trans-(LO)$MoOCl_2$		-841 (-85)
cis-(L1O)$MoOCl_2$	726 (70)	-1150 (83)
trans-(L1O)$MoOCl_2$	861 (65)	-934 (62)

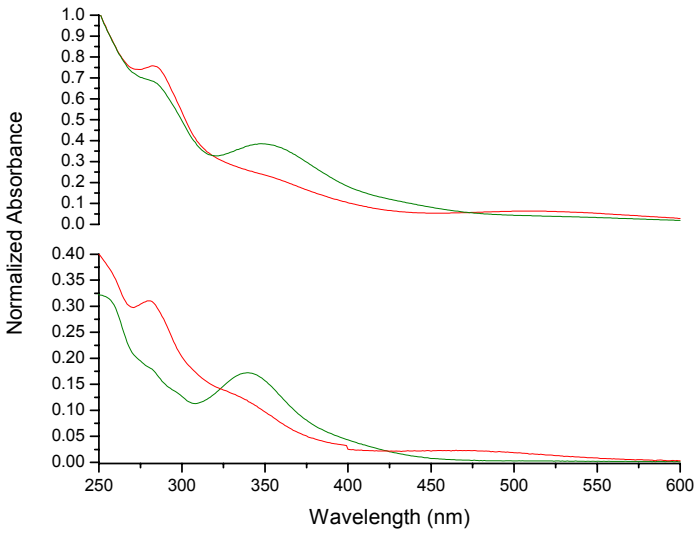

Figure S1. UV-Vis spectra of *cis* and *trans*-(LO)$MoOCl_2$

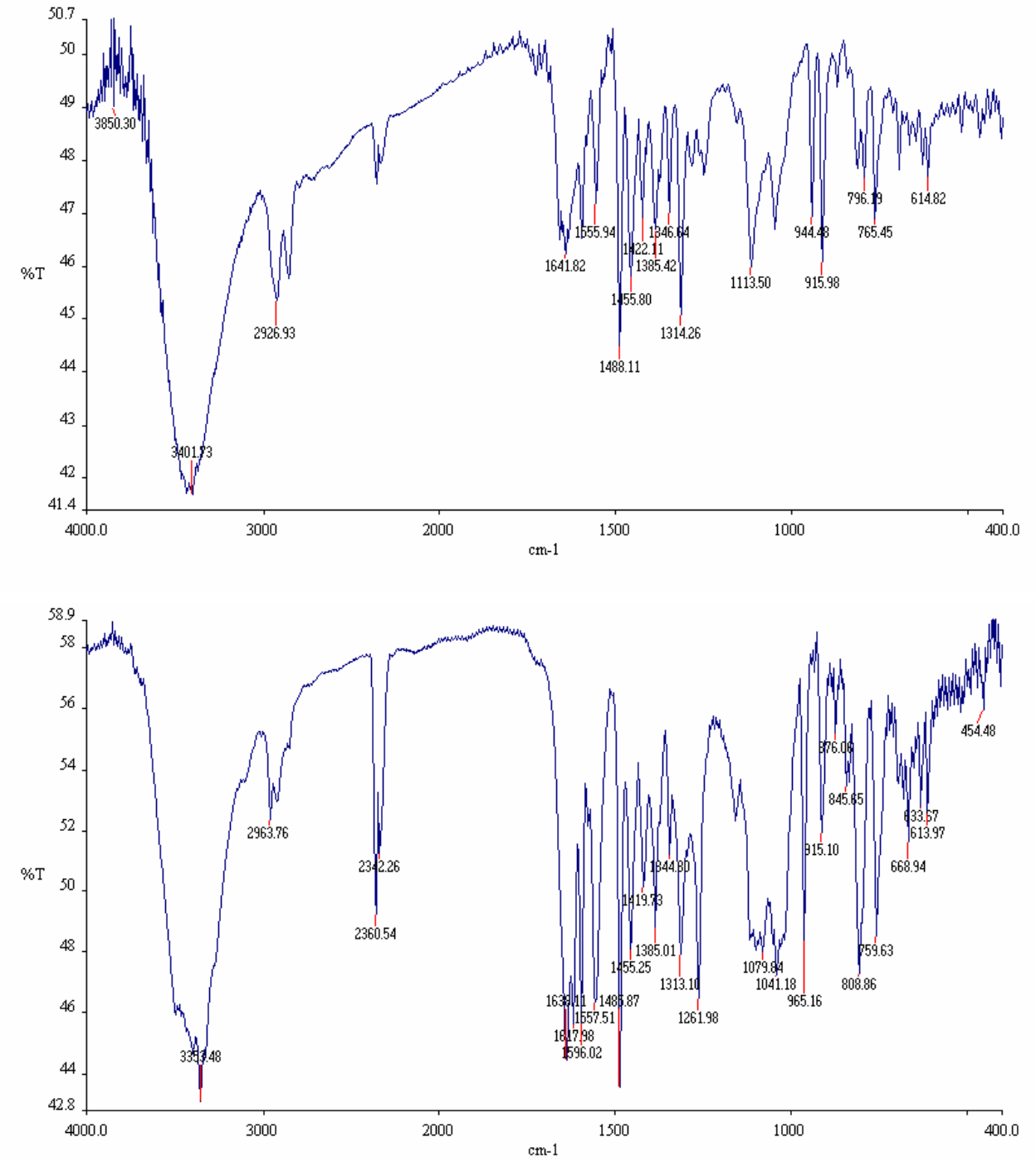

Figure S2. IR spectra of *cis*-(LO)$MoOCl_2$ (bottom) and *trans*-(LO)$MoOCl_2$ (top).