ESI

Synthesis, properties and structural features of molybdenum(V) oxide trichloride complexes with neutral chalcogenoether ligands

Table S1[a]

Compound	$[MoOCl_3\{MeS(CH_2)_3SMe\}]$	$[MoOCl_3\{^iPrS(CH_2)_2S^iPr\}]$	$[MoOCl_3\{PhS(CH_2)_2SPh\}]$
Formula	$C_5H_{12}Cl_3MoOS_2$	$C_8H_{18}Cl_3MoOS_2$	$C_{14}H_{14}Cl_3MoOS_2$
M	354.56	396.63	464.66
Crystal system	Orthorhombic	Orthorhombic	Monoclinic
Space group (no)	Pnma (62)	Pbca (62)	$P2_1/c$ (14)
a /Å	12.2610(2)	12.4629(2)	19.6139(2)
b /Å	12.7705(2)	13.7536(2)	6.80640(10)
c /Å	7.6085(1)	17.5032(6)	12.9677(2)
α /°	90	90	90
β /°	90	90	96.1600(1)
γ /°	90	90	90
U /Å^3	1191.33(3)	3000.00(1)	1721.19(4)
Z	4	8	4
μ(Mo-K_α)/mm^{-1}	2.080	1.756	1.464
F(000)	700.0	1592.0	924.0
Total number reflns	18361	24043	64024
R_{int}	0.036	0.059	0.052
Unique reflns	1948	4429	5833
No. of params, restraints	62/0	140/0	217/2
GOF	1.105	1.072	0.795
R_1, wR_2 [I > 2σ(I)] [b]	0.040, 0.102	0.046, 0.100	0.054, 0.125
R_1, wR_2 (all data) [b]	0.018, 0.043	0.060, 0.108	0.058, 0.127

[a] common data: T = 100 K; wavelength (Mo-K_α) = 0.71073 Å; θ(max) = 27.5°;

[b] $R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$; $wR_2 = [\Sigma w(F_o^2 - F_c^2)^2 / \Sigma wF_o^4]^{1/2}$.

Compound	$[\{MoOCl_2(SMe_2)\}_2(\mu\text{-}Cl)_2]$	$[\{MoOCl_2(SeMe_2)\}_2(\mu\text{-}Cl)_2]$	$[MoOCl_3\{MeSe(CH_2)_2SeMe\}]$
Formula	$C_4H_{12}Cl_3Mo_2O_2S_2$	$C_4H_{12}Cl_3Mo_2O_2Se_2$	$C_4H_{10}Cl_3MoOSe_2$
M	560.84	654.64	434.33
Crystal system	Monoclinic	Monoclinic	Monoclinic
Space group (no)	$P2_1/c$ (14)	$P2_1/c$ (14)	$P2_1/n$ (14)
a /Å	7.81110(10)	7.8374(2)	7.45509(5)
b /Å	9.50630(10)	9.6744(2)	12.18741(7)
c /Å	11.2487(2)	11.2666(3)	12.5333(8)
α /°	90	90	90
β /°	105.1720(1)	105.647(3)	96.6596(6)
γ /°	90	90	90
U /Å^3	806.15(2)	822.60(4)	1131.074(1)
Z	2	2	4
μ(Mo-K_α) /mm^{-1}	2.791	6.907	8.254
F(000)	540.0	612.0	812.0
Total number reflns	21532	11835	36105
R_{int}	0.018	0.026	0.059
Unique reflns	2693	2616	3593
No. of params, restraints	75/0	75/0	102/0
GOF	1.208	1.035	1.162
R_1, wR_2 [$I > 2\sigma(I)$][b]	0.012, 0.029	0.017, 0.035	0.020, 0.046
R_1, wR_2 (all data)[b]	0.012, 0.028	0.019, 0.035	0.021, 1.047

Compound	$[\{MoOCl(dmpe)_2\}(\mu\text{-}$	$[MoCl\{o\text{-}C_6H_4(TeMe)_2\}_2(\mu\text{-}O)$	$[MoOCl_3\{Me_2PCH_2CH_2PMe_2\}]$

	O)($MoOCl_4$)]	$MoOCl_4$]·CH_2Cl_2	
Formula	$C_{12}H_{32}Cl_5Mo_2O_2P_4$	$C_{17}H_{22}Cl_7Mo_2O_2Te_4$	$C_6H_{16}Cl_3MoOP_2$
M	701.38	1208.77	368.42
Crystal system	Orthorhombic	Monoclinic	Monoclinic
Space group (no)	$Cmc2_1$ (36)	$P2_1/n$ (14)	$P2_1/n$ (14)
a /Å	14.8497(1)	13.4459(2)	7.3716(1)
b /Å	12.54652(1)	16.6158(2)	29.8674(6)
c /Å	13.80599(1)	14.2219(2)	12.4489(2)
α /°	90	90	90
β /°	90	93.570(1)	93.989(2)
γ /°	90	90	90
U /Å^3	2572.22(4)	3171.21(8)	2734.24(8)
Z	4	4	8
μ(Mo-K_α) /mm^{-1}	1.621	5.003	1.745
F(000)	2196.0	2204	1464.0
Total number reflns	48483	82962	24936
R_{int}	0.022	0.035	0.053
Unique reflns	4447	10357	8018
No. of params, restraints	128/1	321/3	253/15
GOF	1.122	1.045	1.035
R_1, wR_2 [I > 2σ(I)][b]	0.010, 0.025	0.025, 0.051	0.040, 0.102
R_1, wR_2 (all data) [b]	0.010, 0.026	0.032, 0.054	0.047, 0.107

IR Spectra (Nujol)

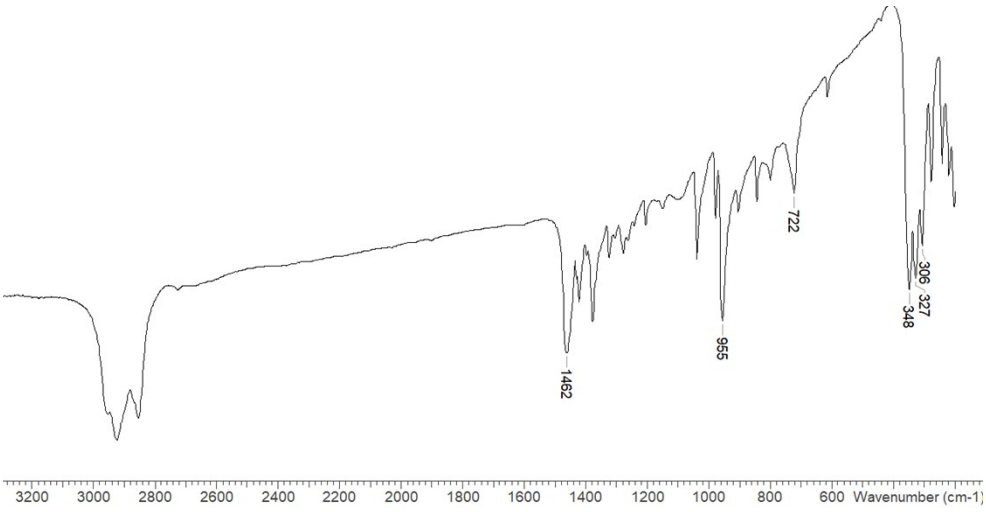

Fig. S1. IR spectrum of $[MoOCl_3\{MeS(CH_2)_3SMe\}]$

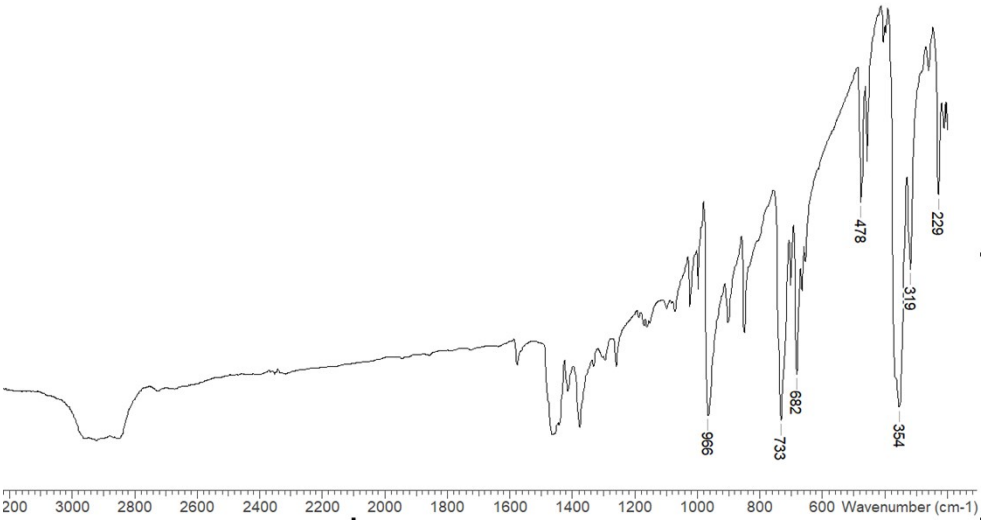

Fig. S2. IR spectrum of $[MoOCl_3\{PhS(CH_2)_2SPh\}]$

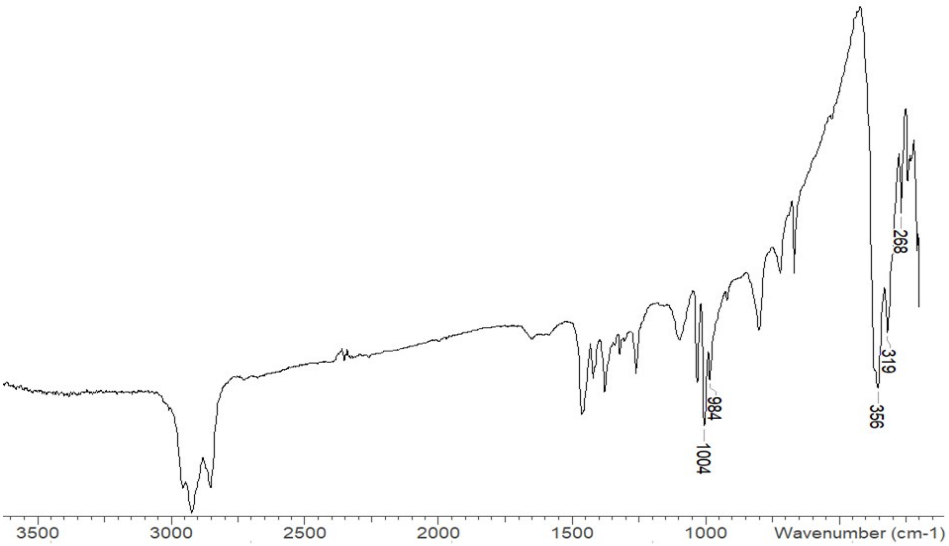

Fig. S3. IR spectrum of $[\{MoOCl_2(SMe_2)\}_2(\mu\text{-}Cl)_2]$

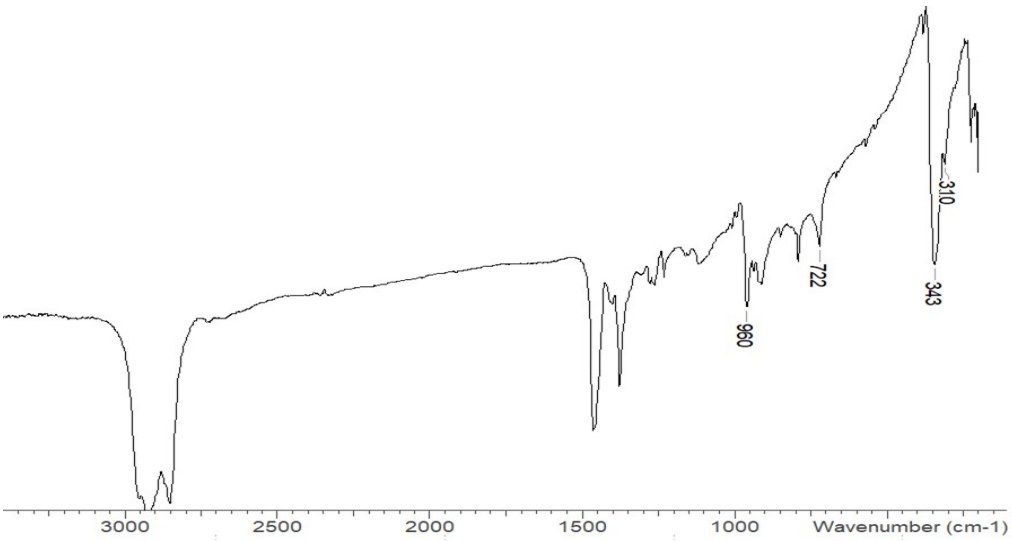

Fig. S4. IR spectrum of $[MoOCl_3\{MeSe(CH_2)_2SeMe\}]$

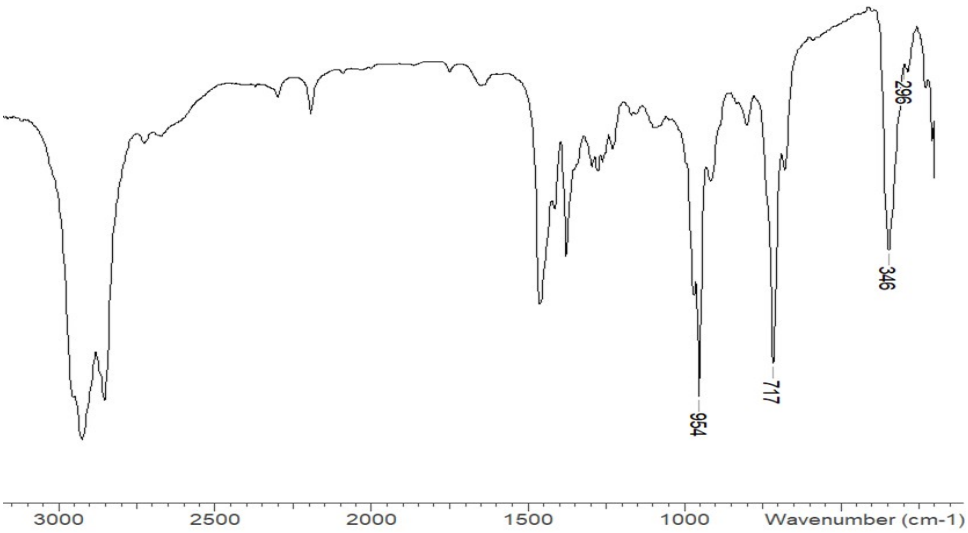

Fig. S5. IR spectrum of $[MoOCl_3\{MeSe(CH_2)_3SeMe\}]$

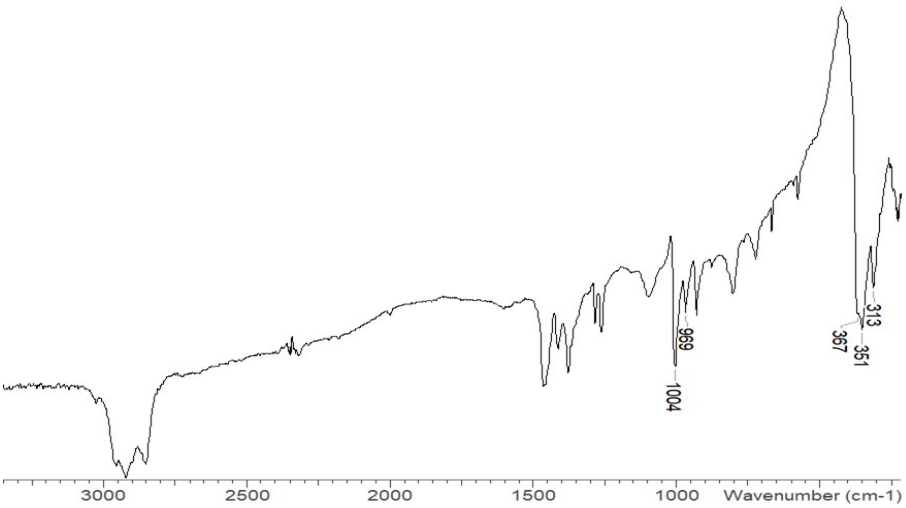

Fig. S6. IR spectrum of $[\{MoOCl_2(SeMe_2)\}_2(\mu\text{-}Cl)_2]$

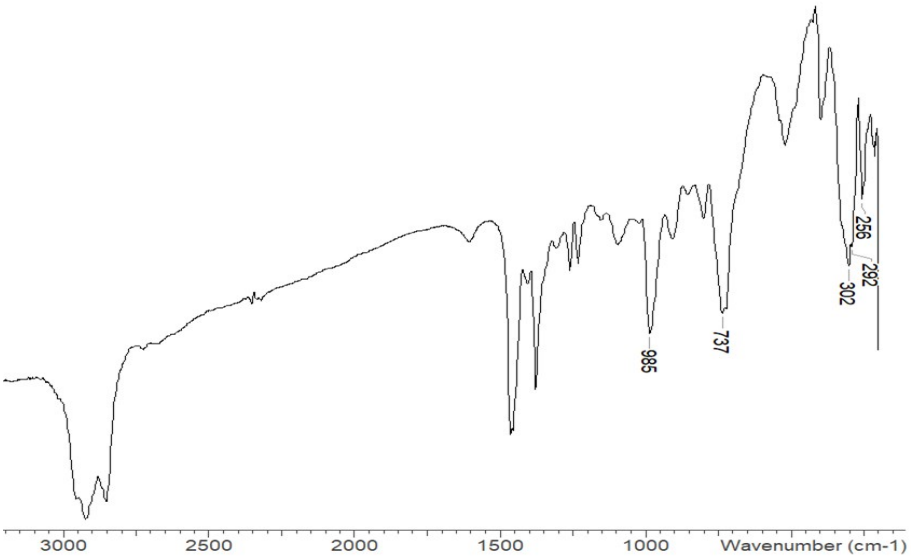

Fig. S7. IR spectrum of $[\{MoOCl_2(TeMe_2)\}_2(\mu\text{-}Cl)_2]$

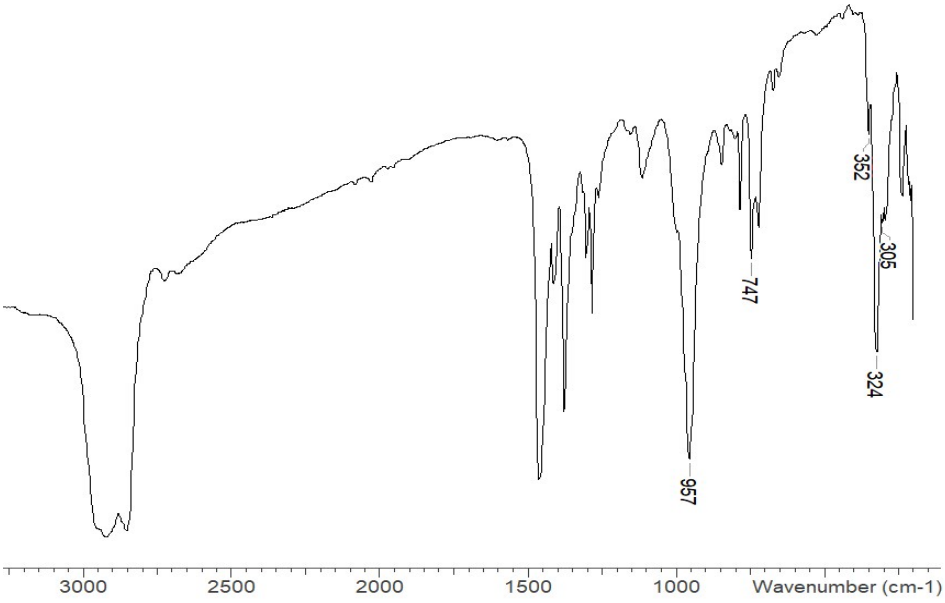

Fig. S8. IR spectrum of $[MoOCl_3(PMe_3)_2]$

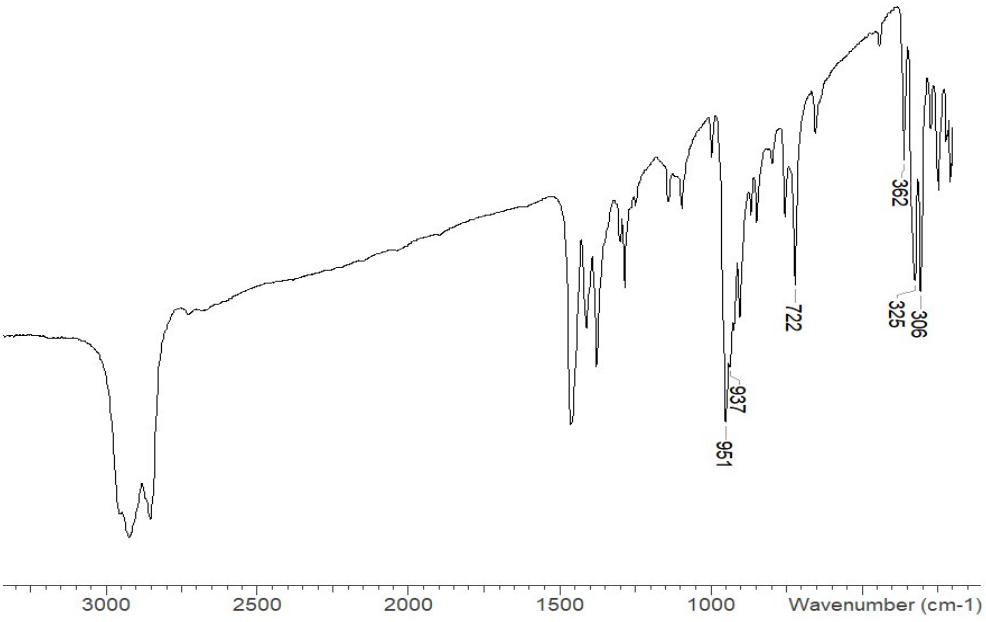

Fig. S9. IR spectrum of $[MoOCl_3\{Me_2PCH_2CH_2PMe_2\}]$

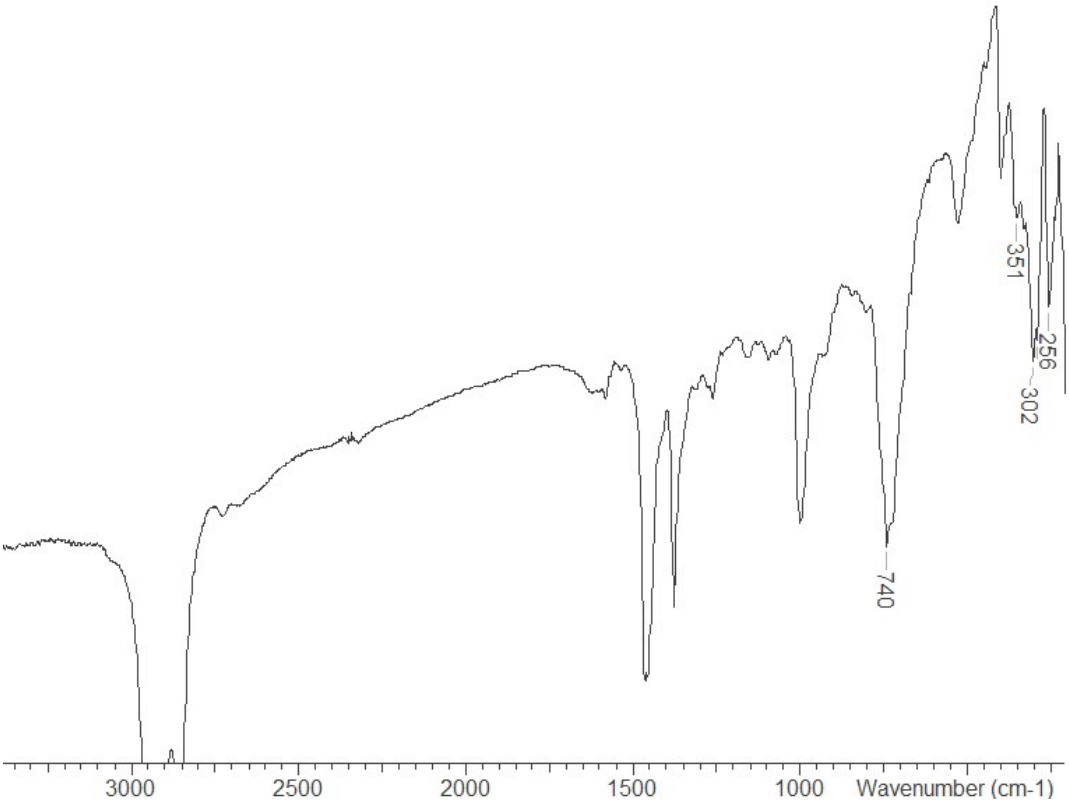

Fig. S10 IR spectrum of $[(MoOCl_3)_2\{o\text{-}C_6H_4(SeMe)_2\}]_n$

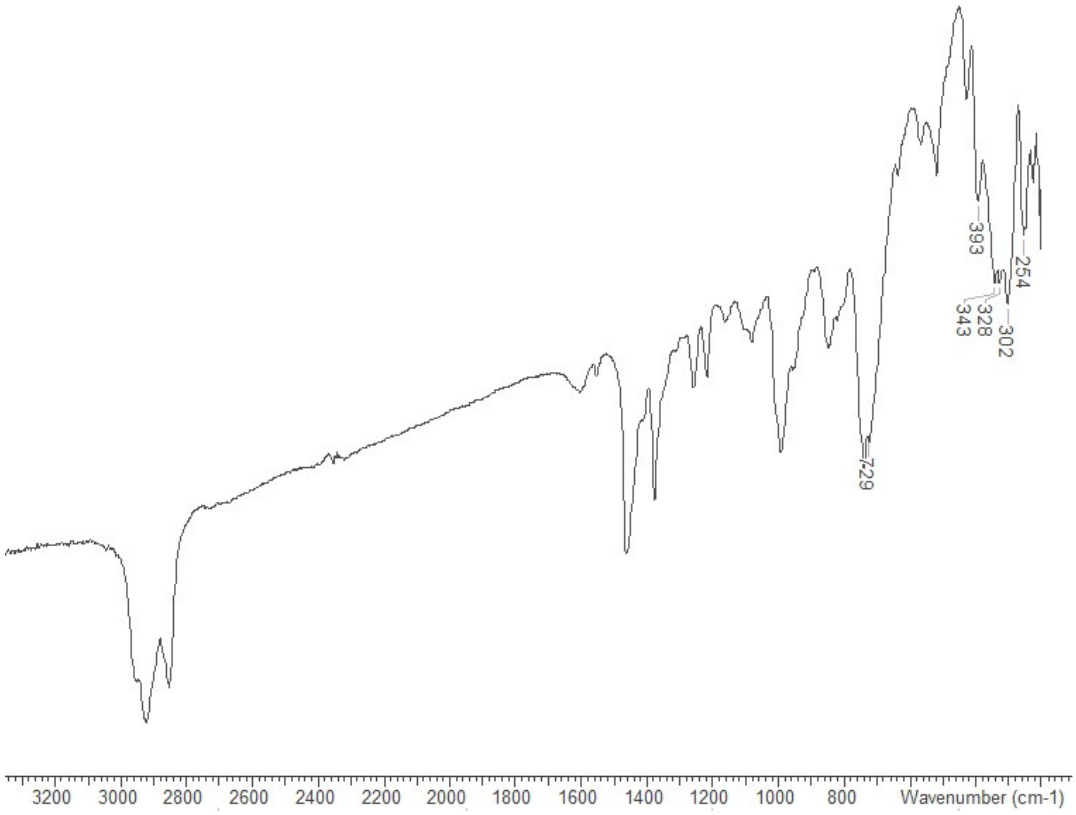

Fig. S11 IR spectrum of $[(MoOCl_3)_2\{o\text{-}C_6H_4(TeMe)_2\}]_n$

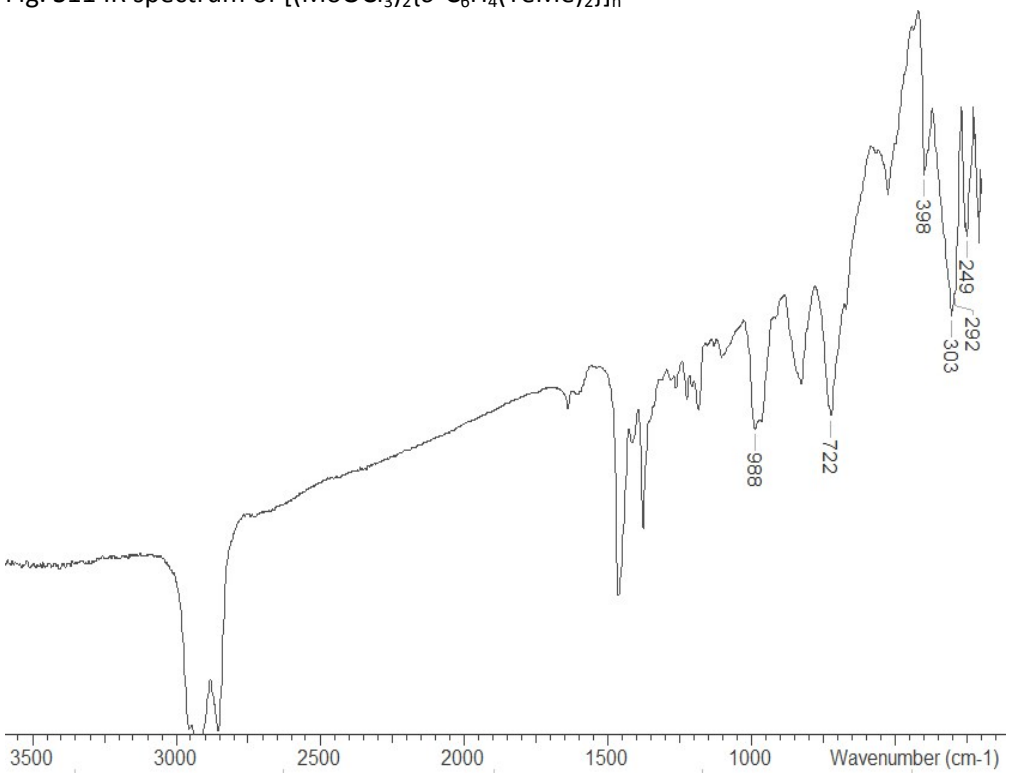

Fig. S12 IR spectrum of $[(MoOCl_3)_2\{MeTe(CH_2)_3TeMe\}]_n$

UV/Visible spectra (diffuse reflectance)

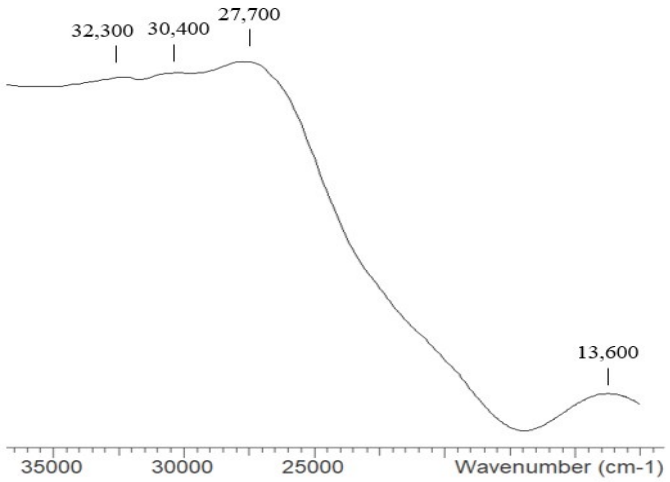

Fig. S13. UV-Vis spectrum of $[MoOCl_3\{^iPrS(CH_2)_2S^iPr\}]$

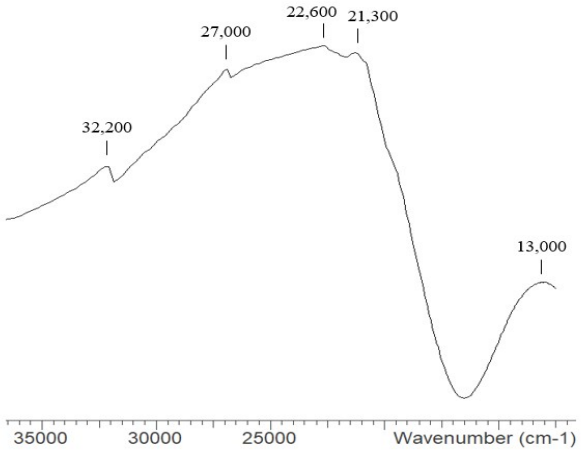

Fig. S14. UV-Vis spectrum of $[MoOCl_3\{PhS(CH_2)_2SPh\}]$

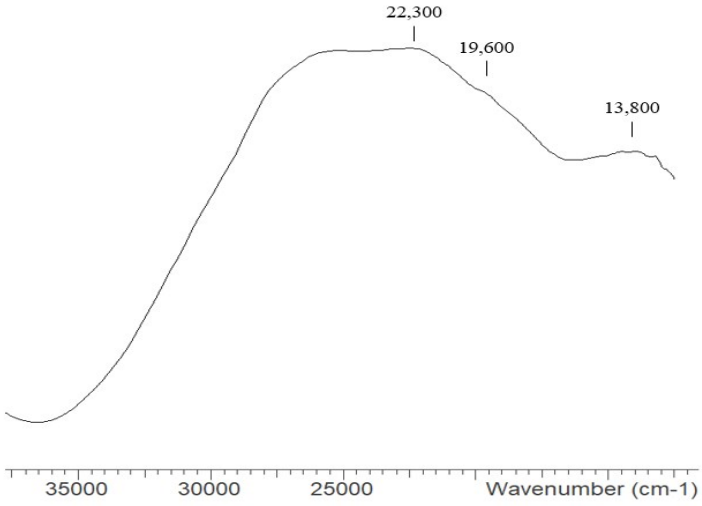

Fig. S15. UV-Vis spectrum of $[\{MoOCl_2(SMe_2)\}_2(\mu\text{-}Cl)_2]$

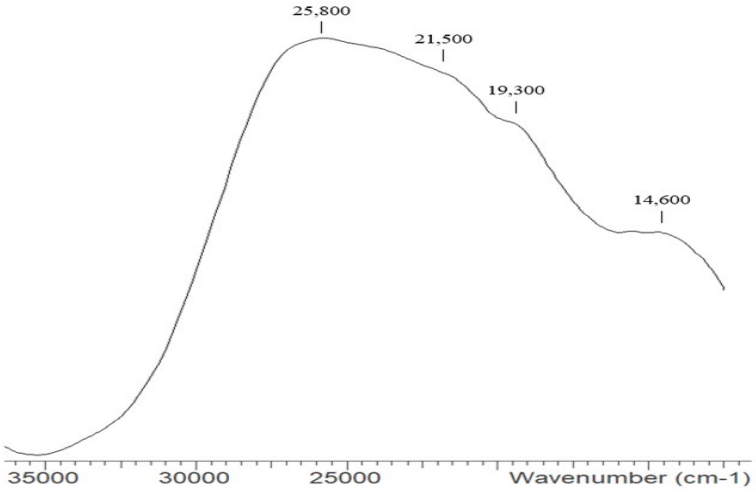

Fig. S16. UV-Vis spectrum of $[MoOCl_3\{MeSe(CH_2)_2SeMe\}]$

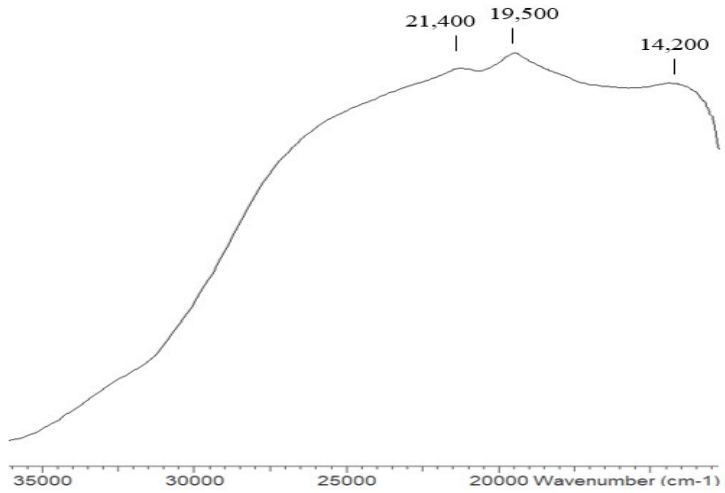

Fig. S17 UV-Vis spectrum of [$MoOCl_3${$MeSe(CH_2)_3SeMe$}]

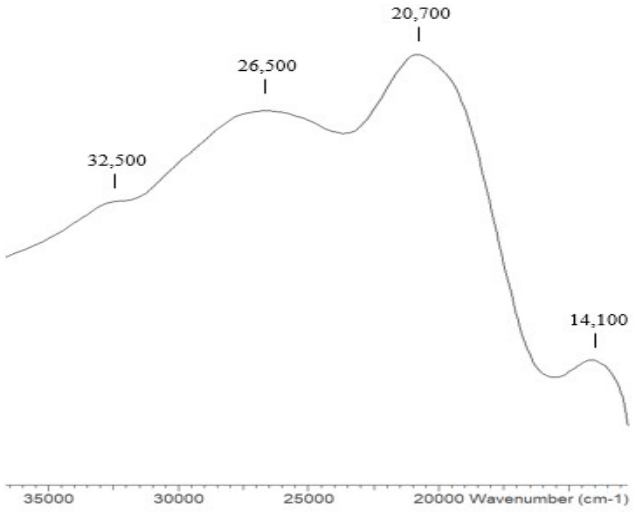

Fig. S18. UV-Vis spectrum of [{$MoOCl_2(SeMe_2)$}$_2$(μ-Cl)$_2$]

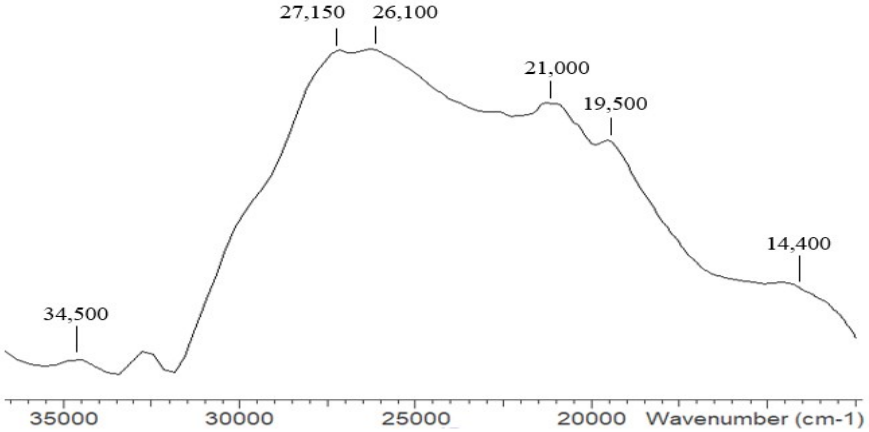

Fig. S19. UV-Vis spectrum of [{$MoOCl_2(TeMe_2)$}$_2$(μ-Cl)$_2$]

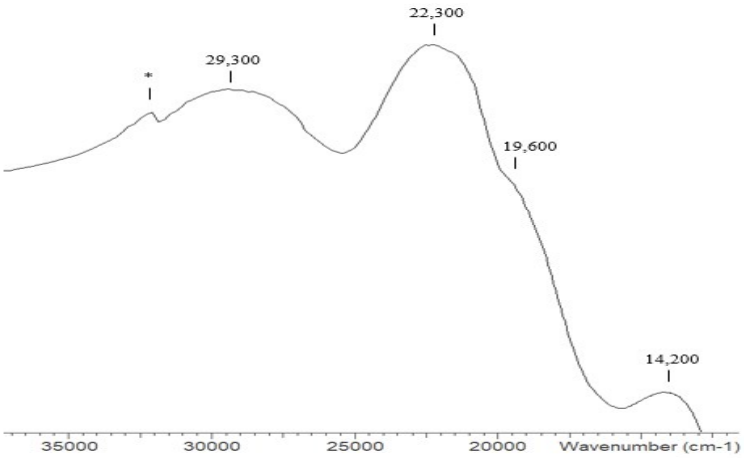

Fig. S20. UV-Vis spectrum of $[MoOCl_3(PMe_3)_2]$

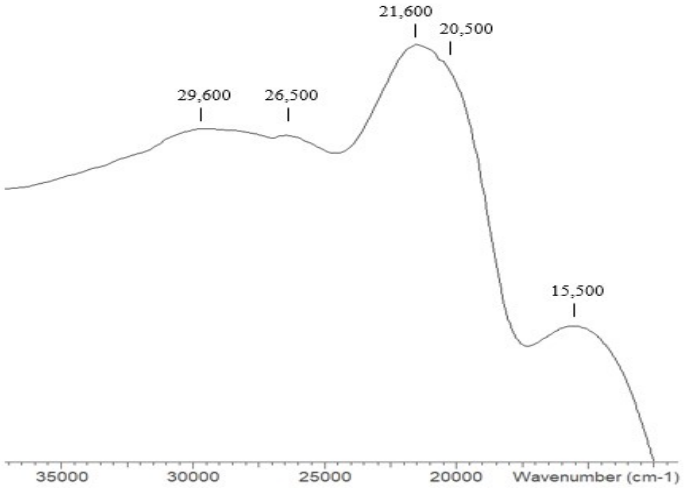

Fig. S21. UV-Vis spectrum of $[MoOCl_3\{Me_2PCH_2CH_2PMe_2\}]$

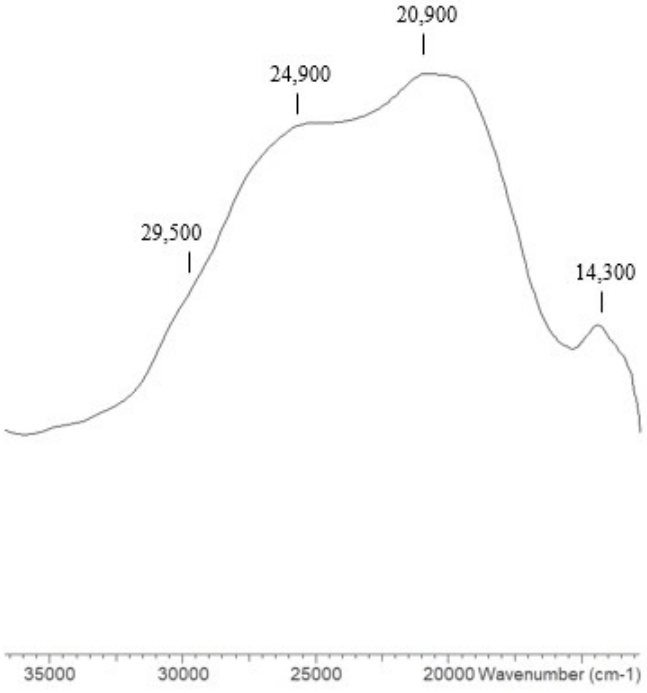

Fig. S22. UV-Vis spectrum of $[\{MoOCl_3\}_2\{o\text{-}C_6H_4(SeMe)_2\}]_n$.

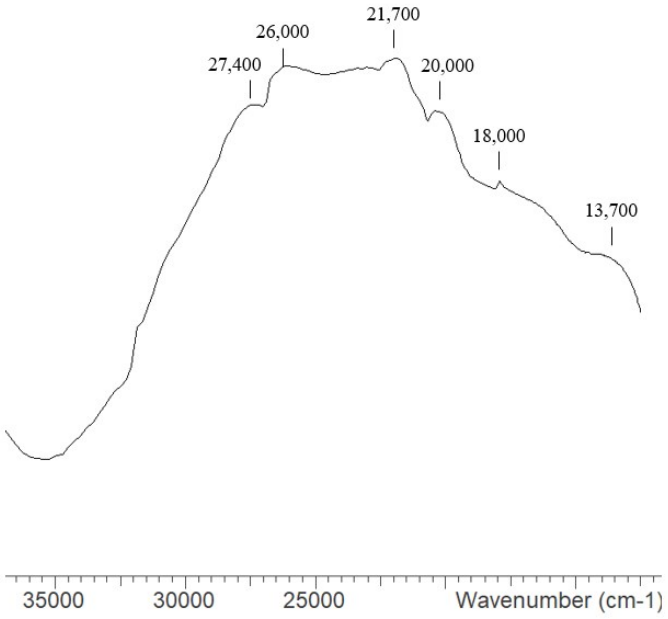

Fig. S23. UV-Vis spectrum of $[MoOCl_3\{MeS(CH_2)_3SMe\}]$.

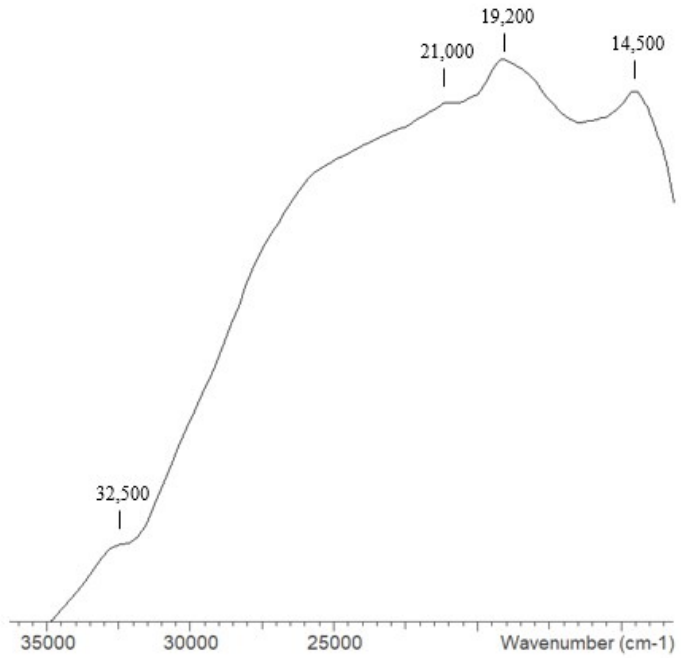

Fig. S24. UV-Vis spectrum of $[\{MoOCl_3\}_2\{o\text{-}C_6H_4(TeMe)_2\}]_n$.

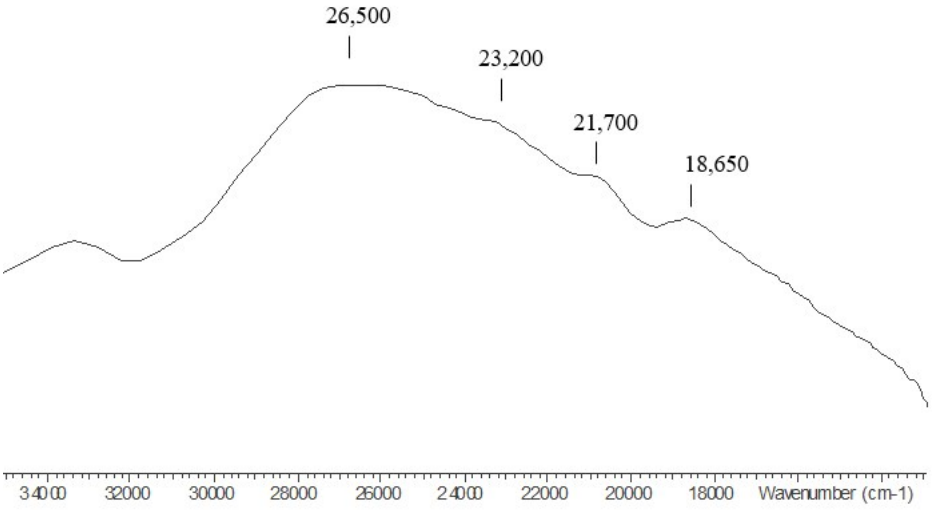

Fig. S25 UV-Vis spectrum of $[MoOCl_3\{MeTe(CH_2)_3TeMe\}]_n$.