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Unusual Activation Pathways of Amines in the Reactions with Molybdenum Pentachloride

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Supporting Information

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Figure S1. C-PCM/ωB97X calculated structure of $[MoCl_5(C_4H_7N)]$, **1**. Dichloromethane as continuous medium.

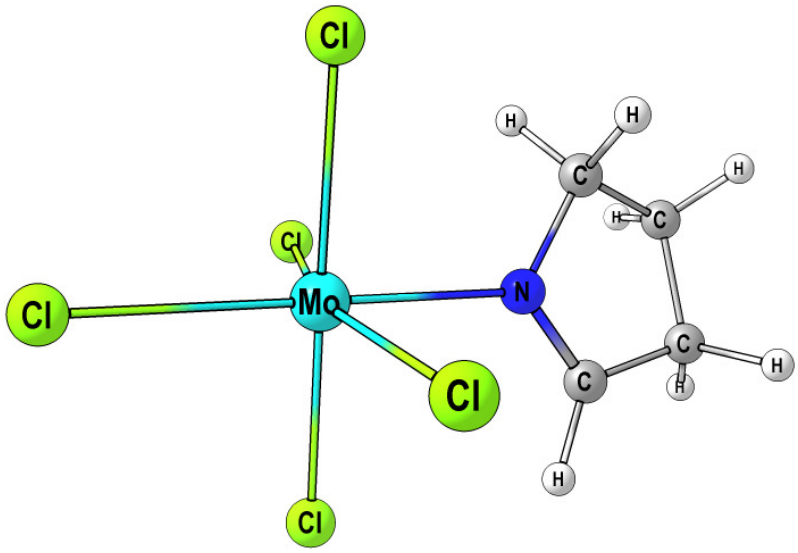

Table S1. Selected computed bond lengths (Å) and angles (°) for $[MoCl_5(C_4H_7N)]$, **1**.

Bond		**Angle**	
Mo–N	2.217	N–Mo–Cl	178.2
Mo–$Cl_{trans\ to\ N}$	2.288		80.3
Mo–$Cl_{cis\ to\ N}$	2.288		82.3
	2.333		89.3
	2.340		90.0
	2.384		
C=N	1.278		

Figure S2. DFT EDF2 calculated structures for $MoCl_4(NEt_2)$, **3**, and relative Gibbs free energy values, referred to the $[MoCl_4(NEt_2)]$ unit (kcal mol^{-1}).