Supporting Information

Alkane Elimination Preparation of Heterobimetallic MoAl Tetranuclear and Binuclear Complexes

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Content

A. NMR spectroscopic data

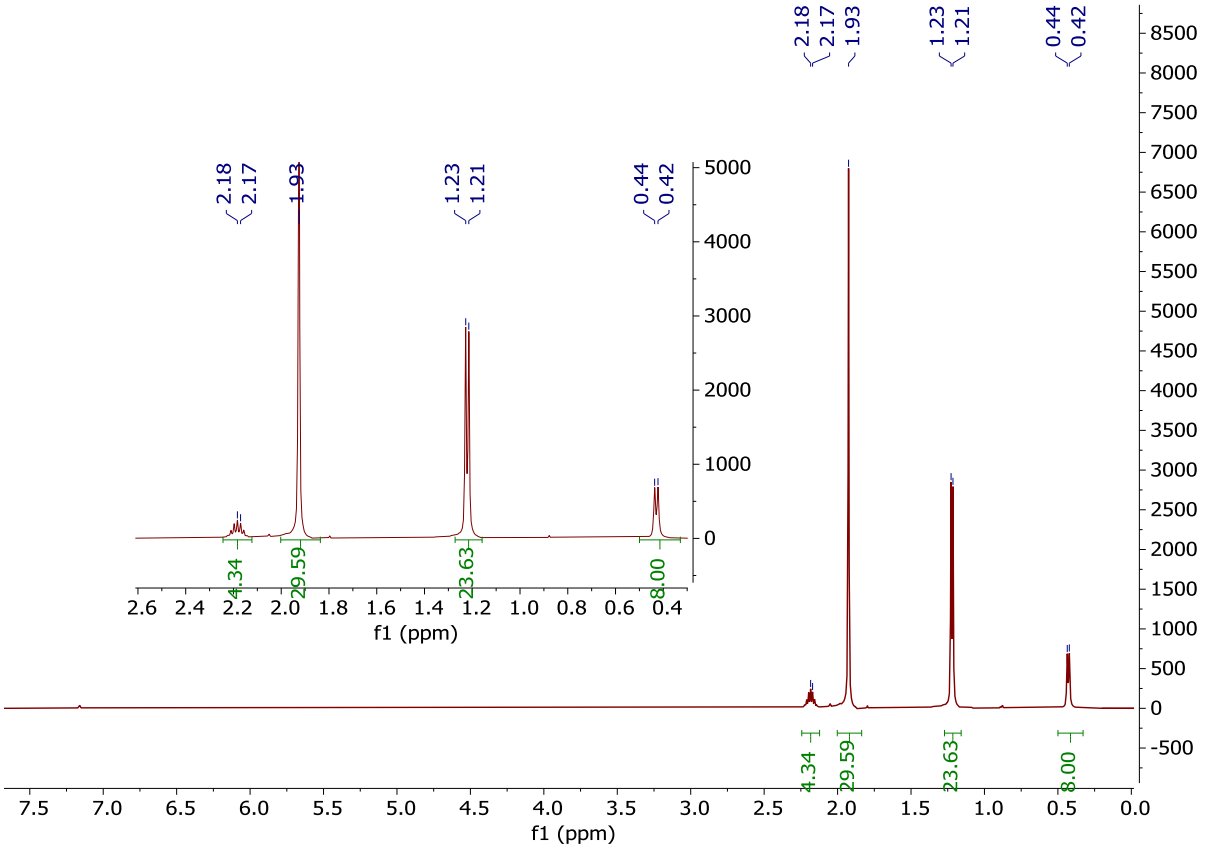

Figure S1. *^{1}H NMR spectrum (293K, 500 MHz, C_6D_6) of compound **1**.*

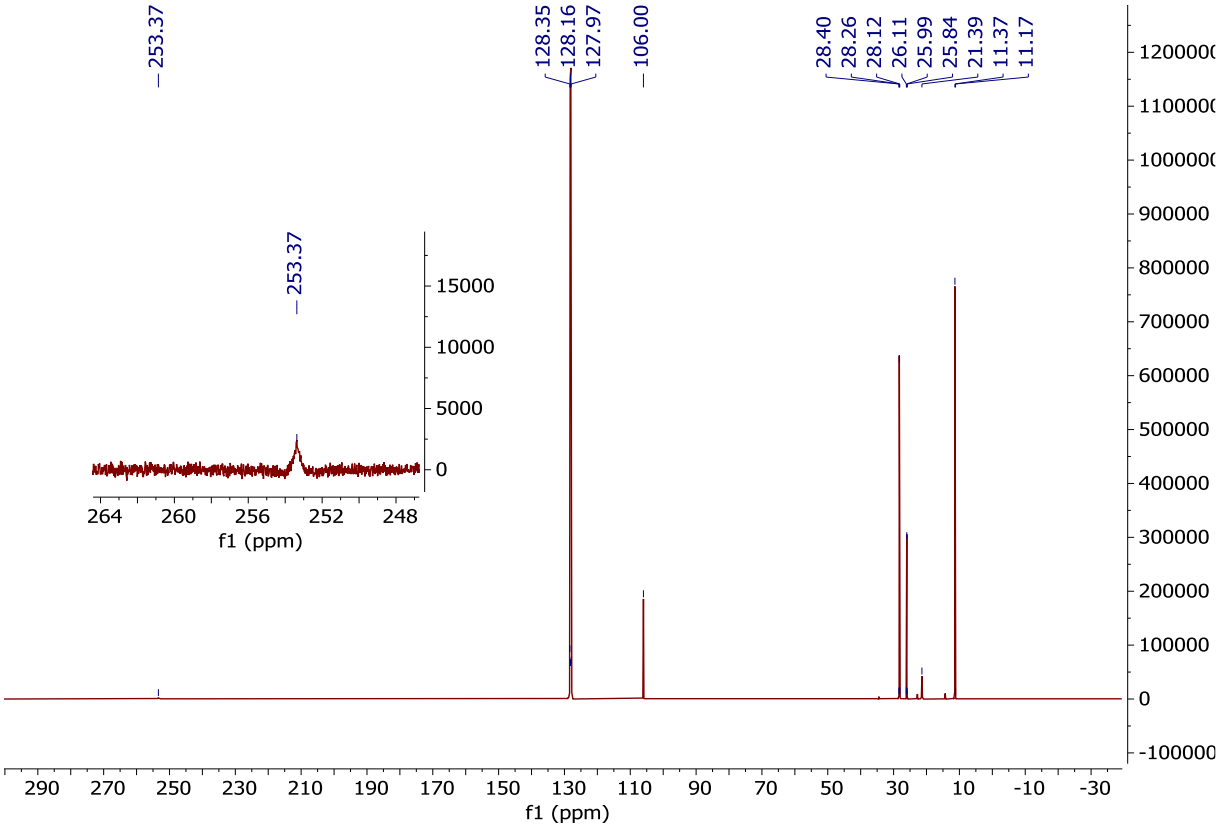

Figure S2. *$^{13}C\{^{1}H\}$-NMR (125 MHz, C_6D_6, RT) of compound **1**.*

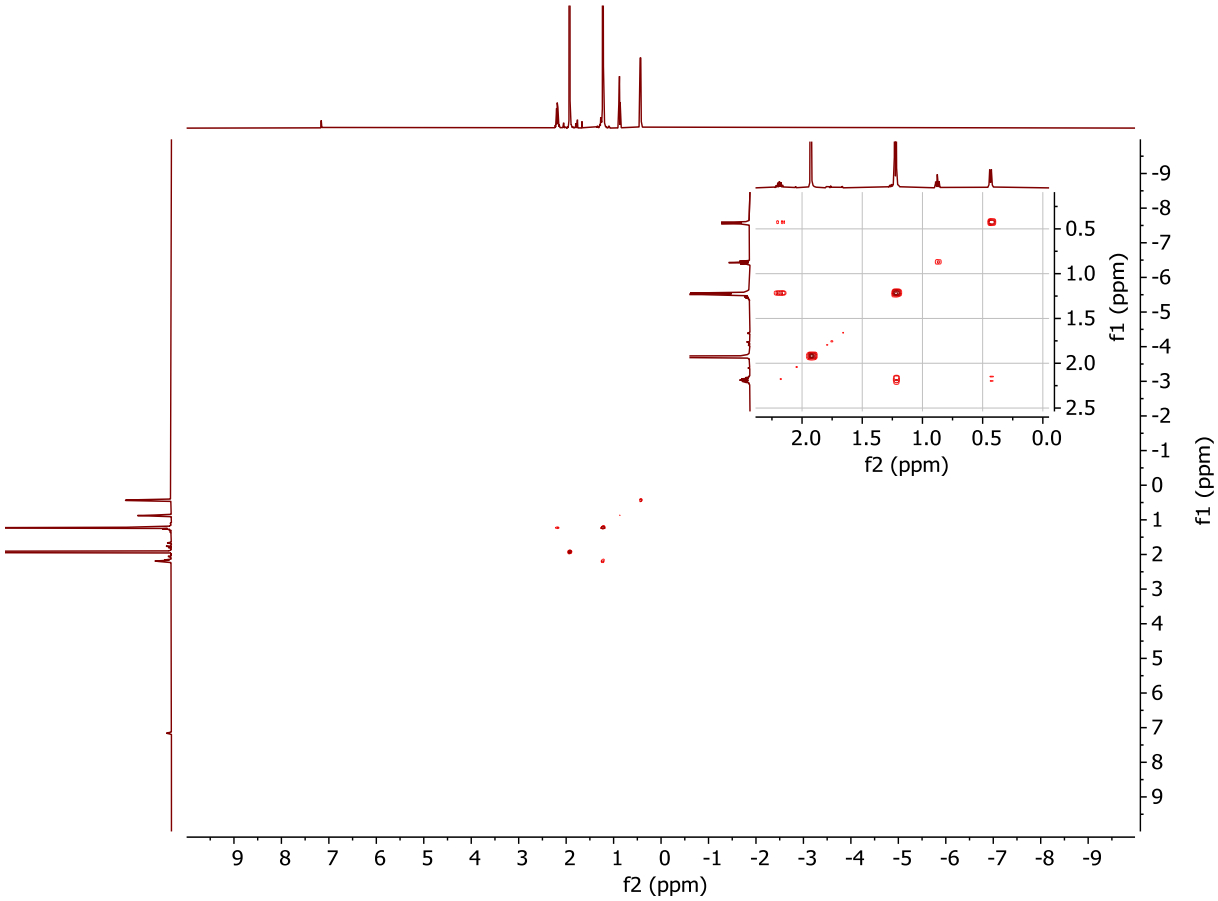

Figure S3. *^{1}H-^{1}H-COSY (500 MHz, C_6D_6, RT) of compound* ***1.***

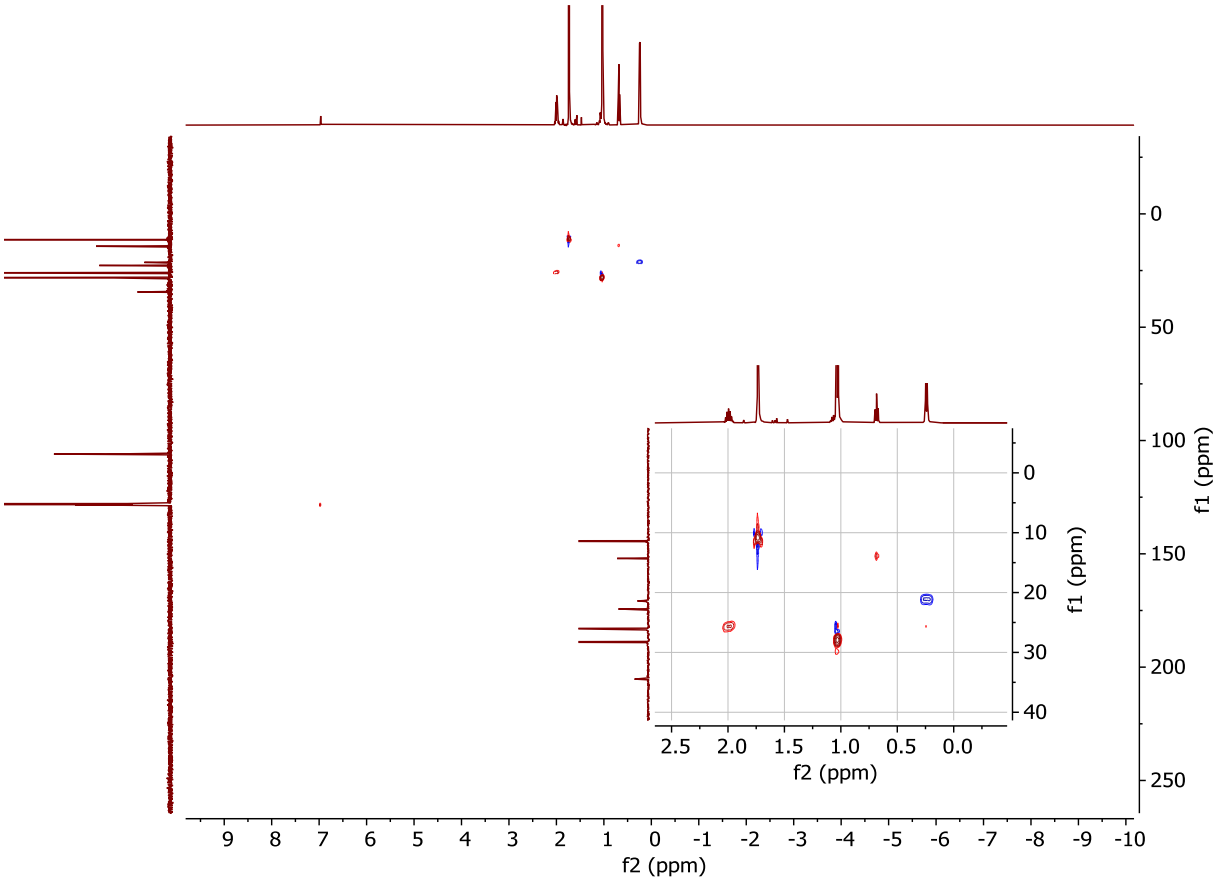

Figure S4. *^{1}H-^{13}C-HSQC (500 MHz, C_6D_6, RT) of compound* ***1.***

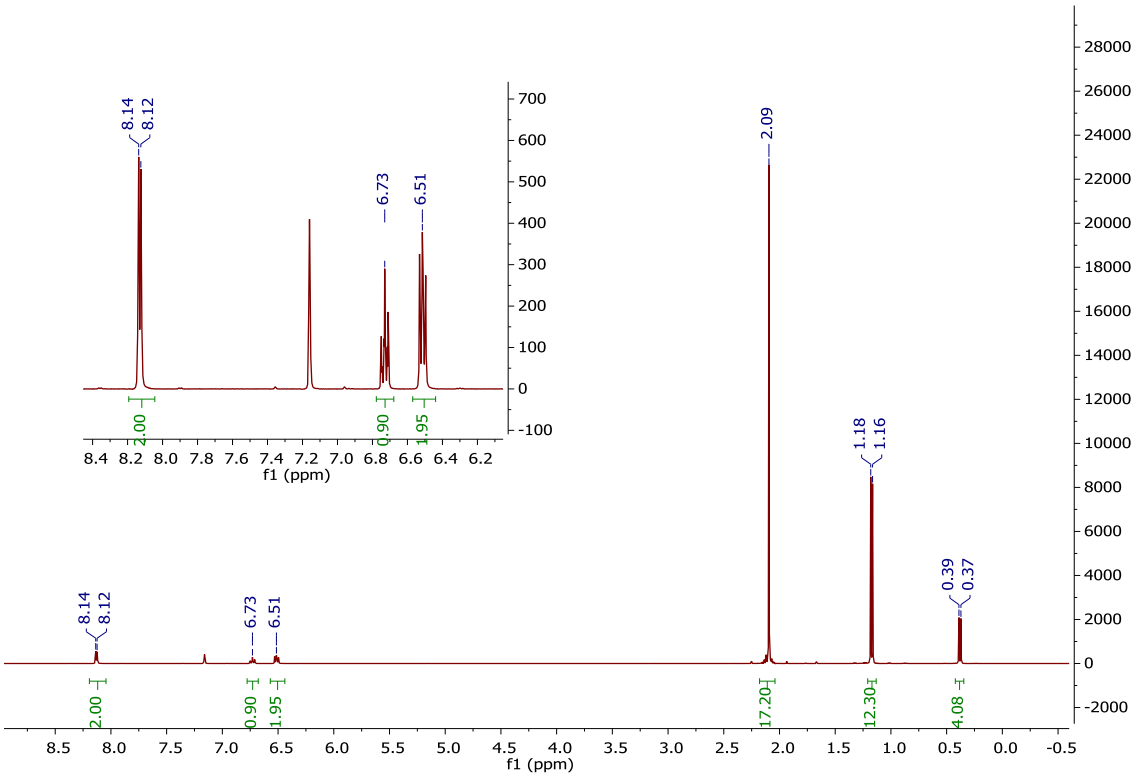

Figure S5. *^{1}H NMR spectrum (293K, 500 MHz, C_6D_6) of compound **2**.*

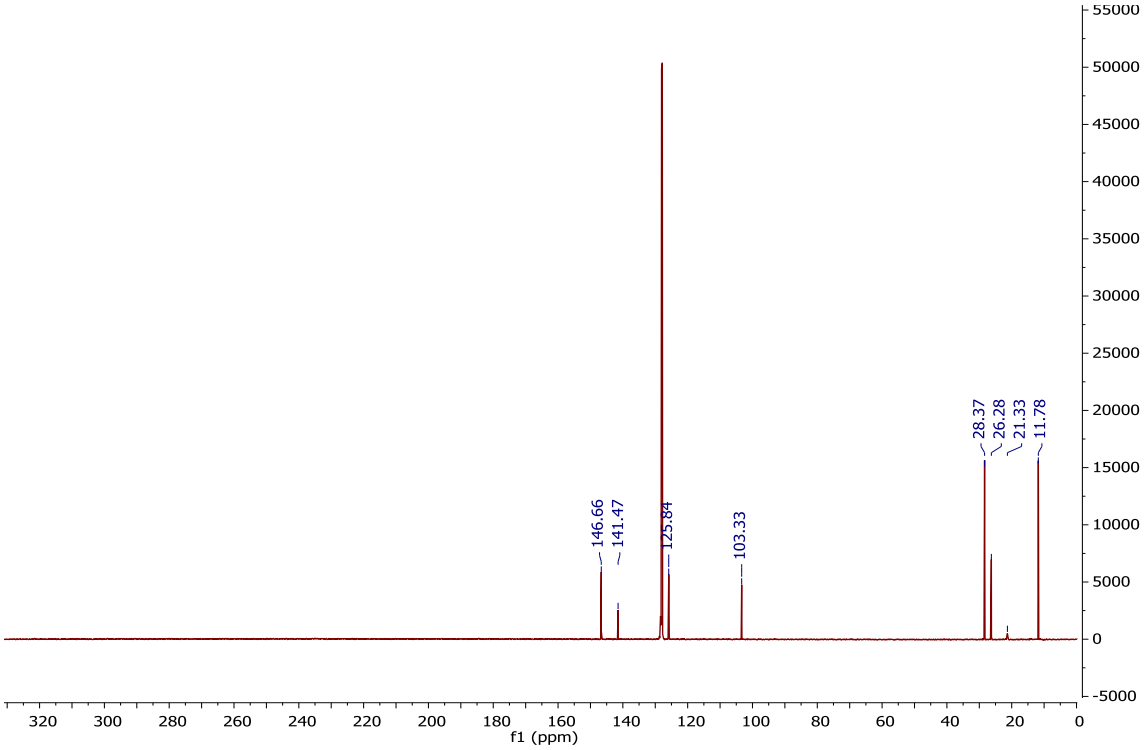

Figure S6. *$^{13}C\{^{1}H\}$-NMR (125 MHz, C_6D_6, RT) of compound* ***2***.

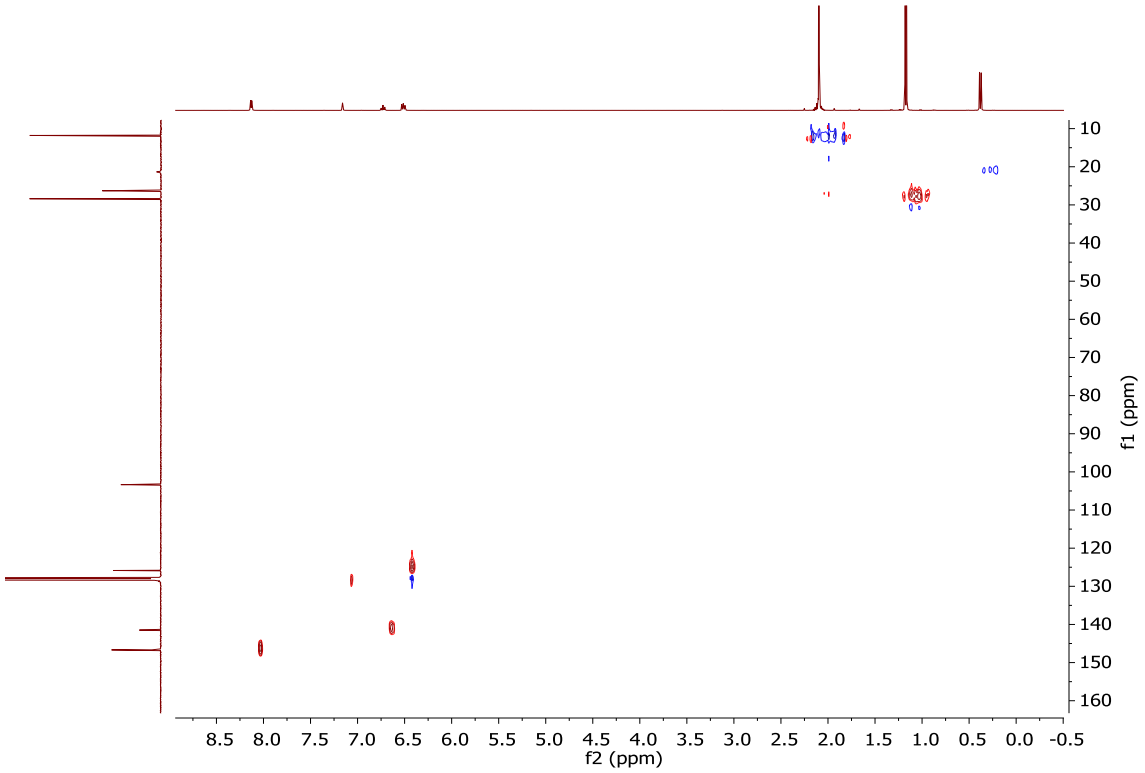

Figure S7. *^{1}H-^{13}C-HSQC (500 MHz, C_6D_6, RT) of compound* ***2.***

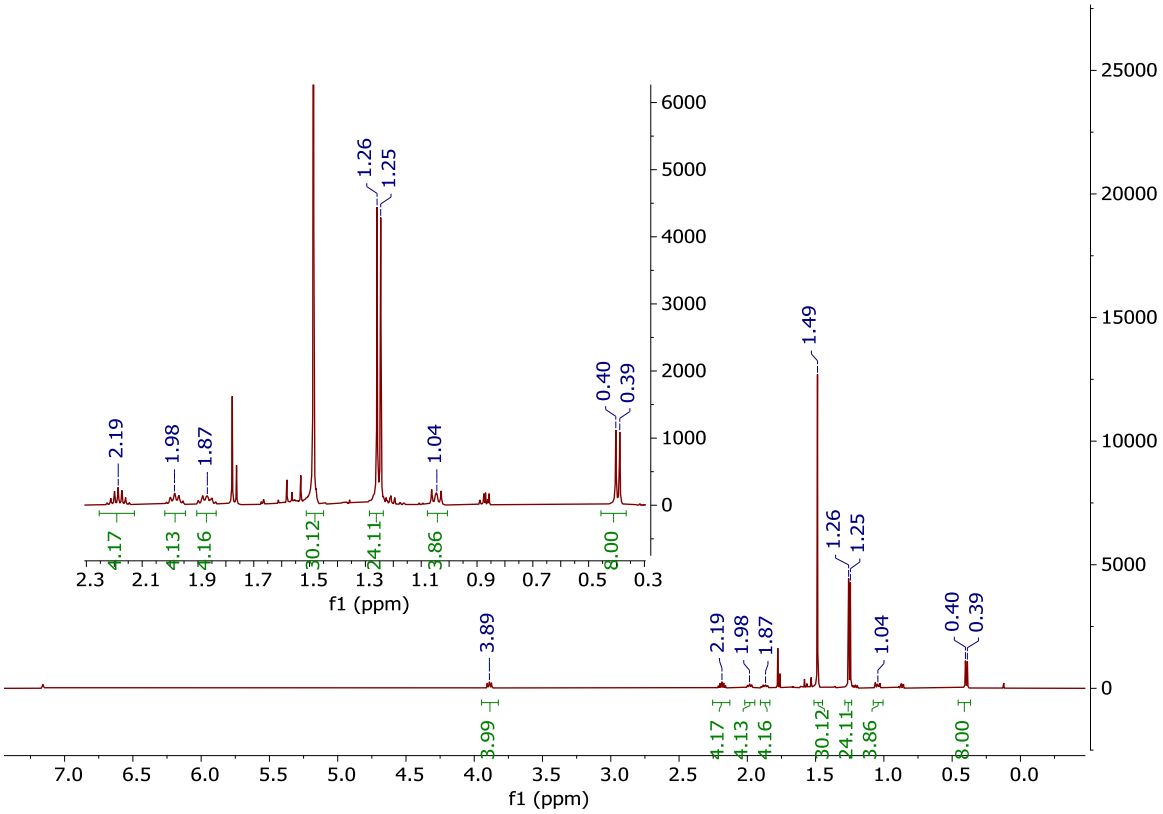

Figure S8. *^{1}H NMR spectrum (293K, 500 MHz, C_6D_6) of compound **3**.*

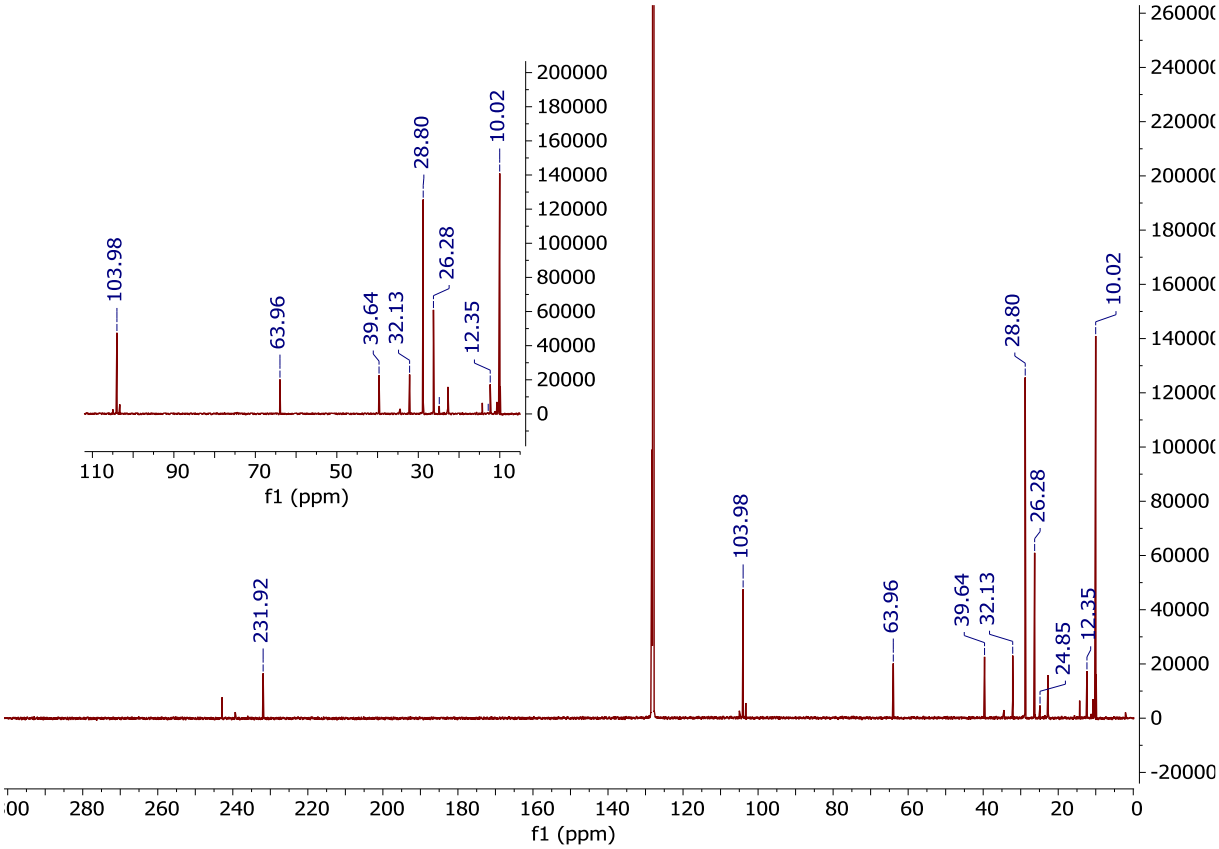

Figure S9. *$^{13}C\{^{1}H\}$-NMR (125 MHz, C_6D_6, RT) of compound **3**.*

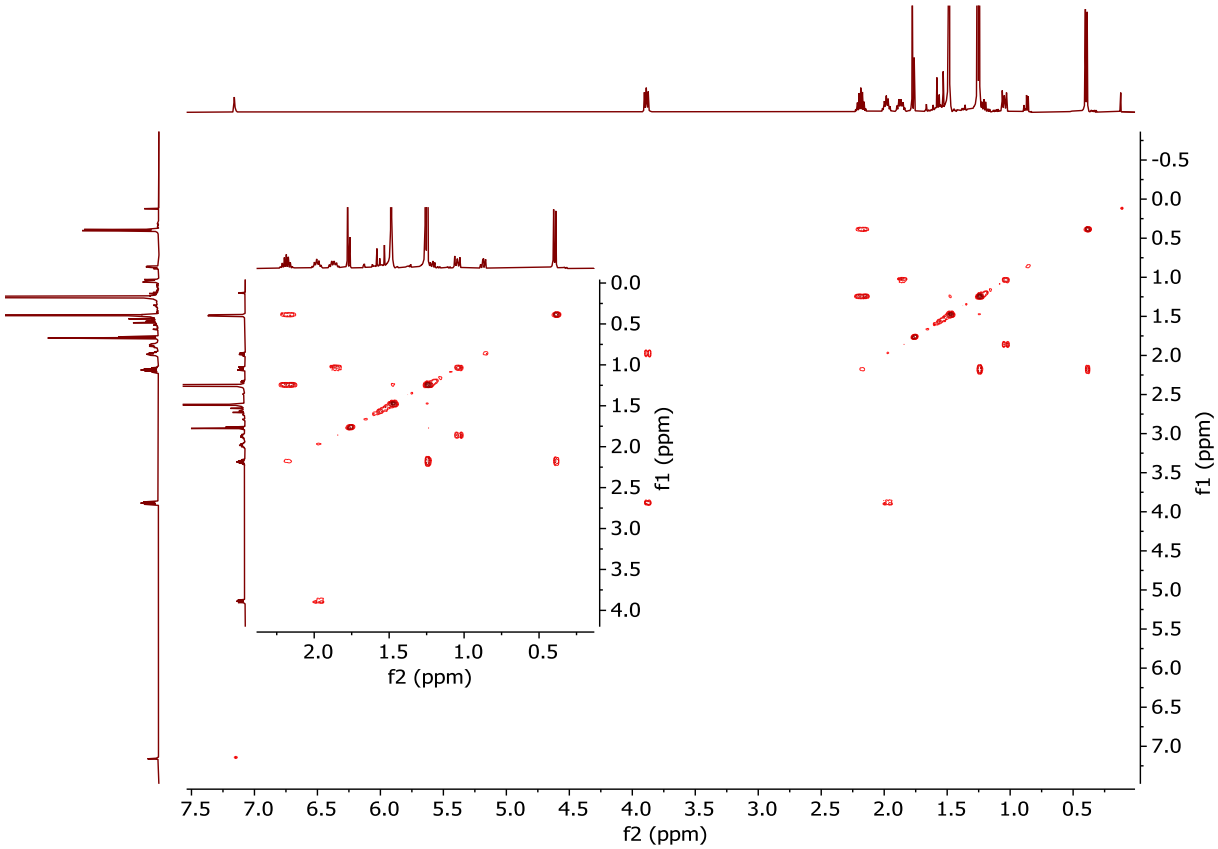

Figure S10. *^{1}H-^{1}H-COSY (500 MHz, C_6D_6, RT) of compound* ***3.***

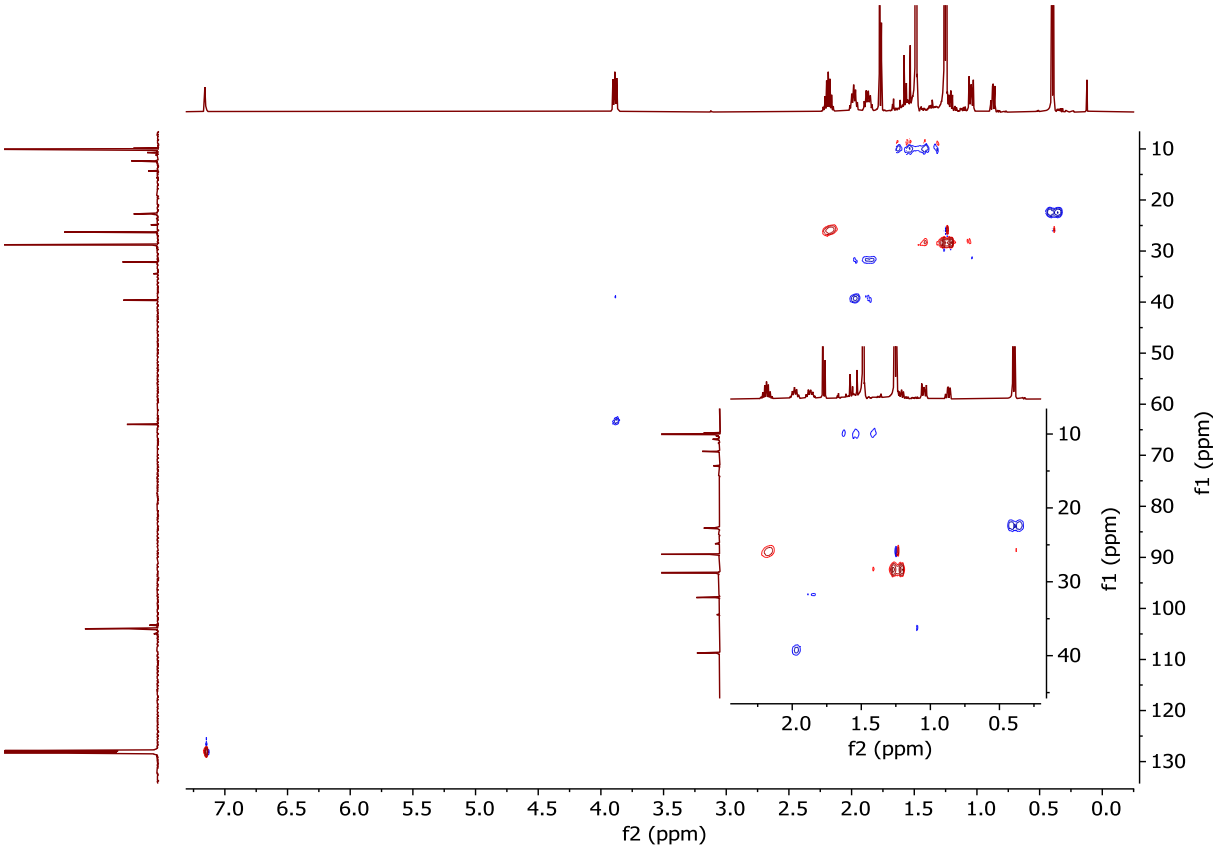

Figure S11. *^{1}H-^{13}C-HSQC (500 MHz, C_6D_6, RT) of compound* ***3***

B. IR spectroscopic data

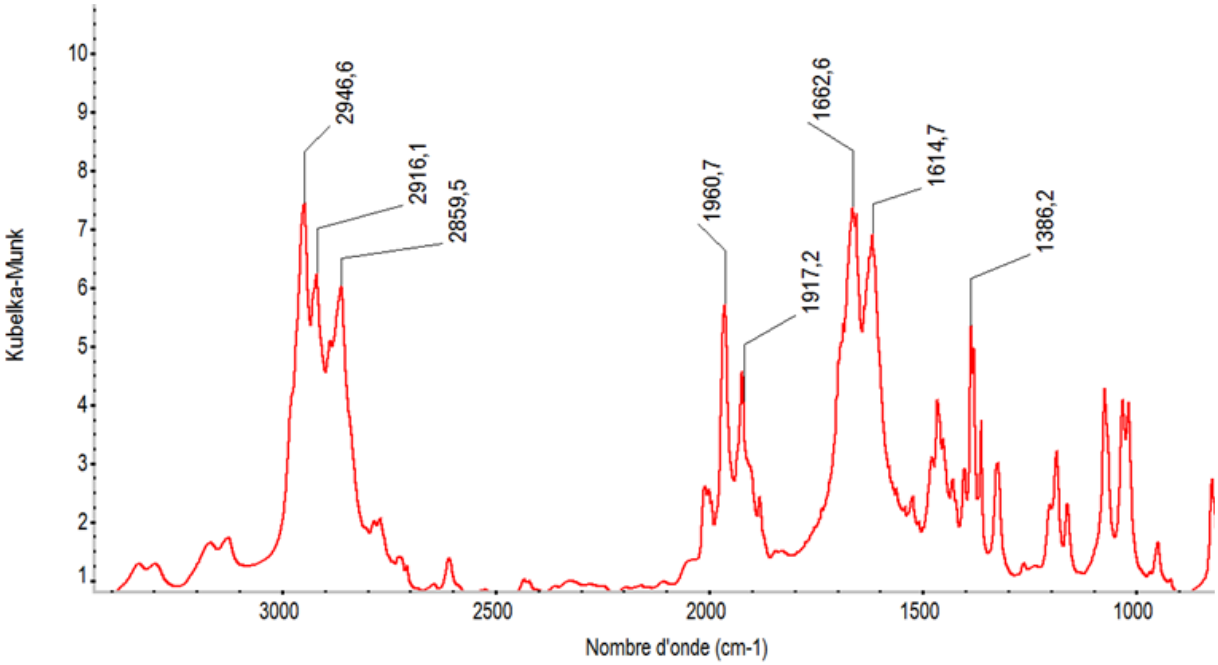

***Figure S12**. DRIFT spectrum (25°C, KBr dilution under argon) for compound **1**.*

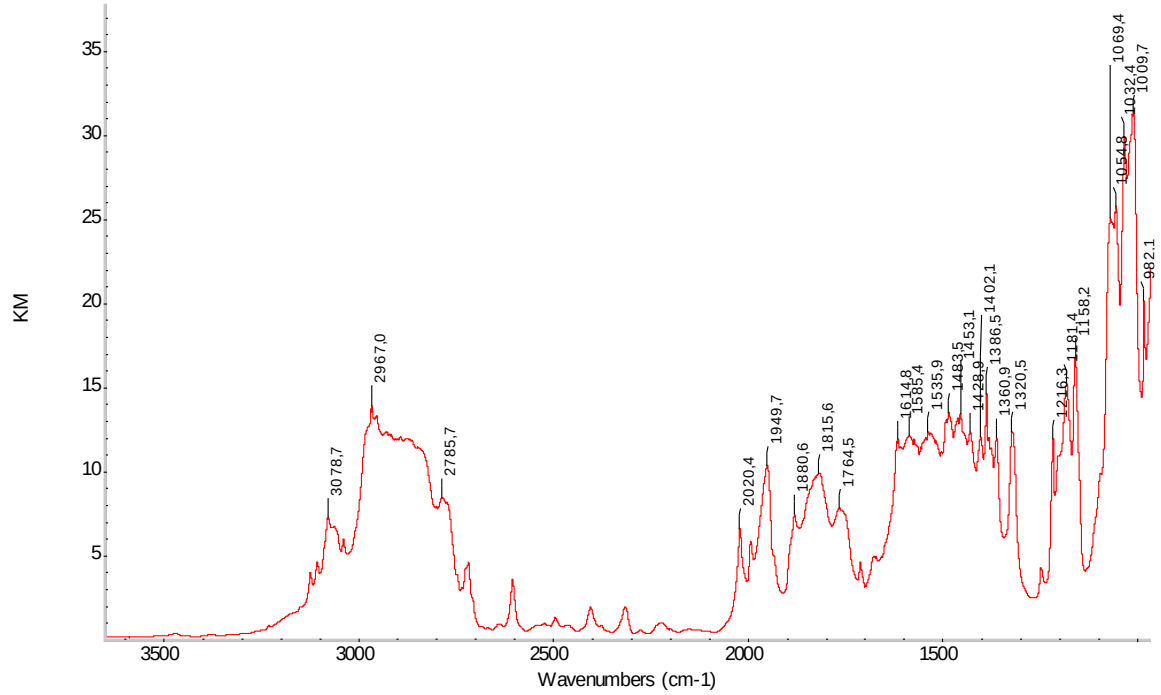

***Figure S13**. DRIFT spectrum (25°C, KBr dilution under argon) for compound **2**.*

C. X-ray crystallography

*Table S1. Crystallographic parameters for compounds **1**, **2** and **3**.*

Compound	**1**	**2**	**3**
Formula	$C_{42}H_{66}Al_2Mo_2O_6$	$C_{26}H_{38}AlMoNO_3$	$C_{50}H_{82}Al_2Mo_2O_8$
cryst syst	Triclinic	Monoclinic	Monoclinic
space group	*P*-1	$P2_1/c$	$P\ 2_1/n$
volume (Å^3)	1144.79(5)	2734.6(7)	2774.0(6)
a (Å)	8.9496(2)	11.9297(18)	9.2045(15)
b (Å)	11.9141(3)	14.9777(17)	8.6863(13)
c (Å)	11.9303(3)	15.841(3)	34.746(5)
α (deg)	76.824(2)	90	90
β (deg)	68.147(2)	104.963(15)	93.083(13)
γ (deg)	89.867(2)	90	90
Z	1 (Z'=0.5)	4	2 (Z'=0.5)
formula weight (g/mol)	912.78	535.49	1057.04
density (g cm^{-3})	1.324	1.301	1.265
absorption coefficient (mm^{-1})	0.627	0.537	0.529
F(000)	476.00	1120	1112
θ_{max} (°)	29.540	29.496	29.607
temp (K)	150.00(10)	150.00(10)	150.00(10)
total no. reflections	25257	18783	38093
indepedant reflections [R(int)]	5676 [0.0274]	6362 [0.1006]	6807 [/]
no. refined parameters	244	299	291
Final R indices [I > 2σ(I)]	R1 = 0.0263 wR2 = 0.0652	R1 = 0.0659 wR2 = 0.0976	R1 = 0.1265 wR2 = 0.2619
GoF	1.144	1.065	1.094

CCDC 2330941 to 2330943 contain the supplementary crystallographic data for this paper. These data are provided free of charge by the Cambridge Crystallographic Data Centre.