

Molecular Routes to Two Dimensional Metal Dichalcogenides MX₂ (M = Mo, W; X = S, Se)

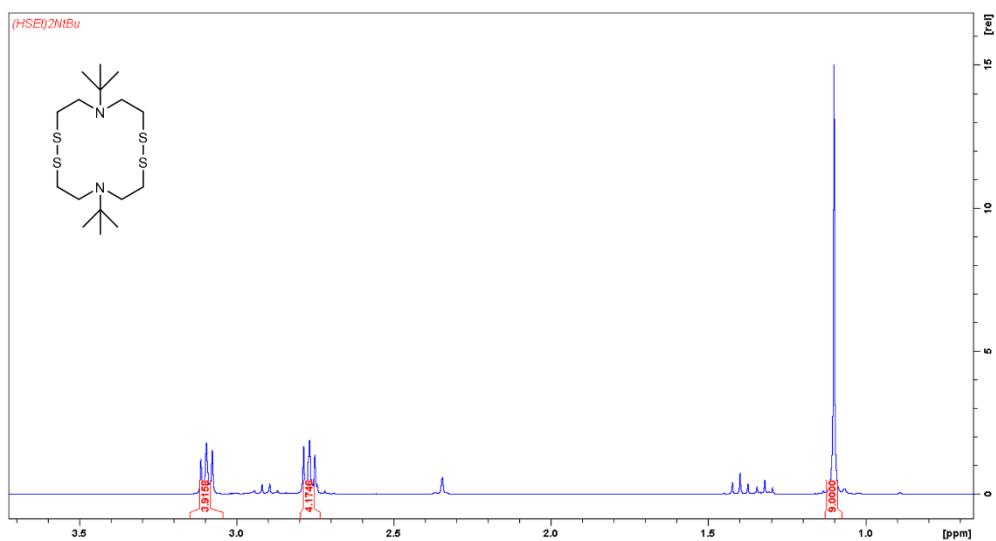
Veronika Brune¹, Corinna Hegemann¹ and Sanjay Mathur^{1,*}

¹Institute of Inorganic Chemistry
University of Cologne, Greinstraße 6, D-50939 Cologne, Germany

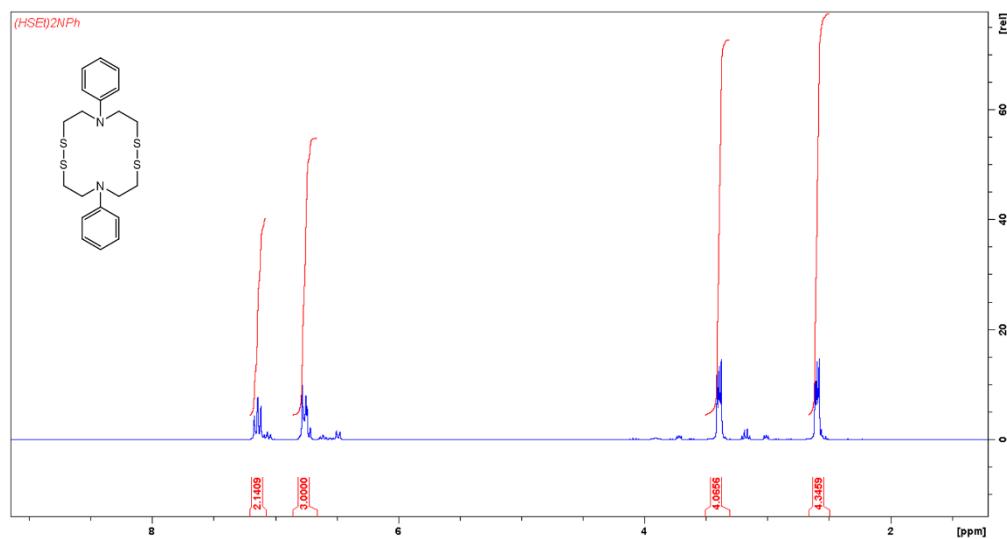
*Author to whom correspondence should be addressed; E-Mail: sanjay.mathur@uni-koeln.de

Supporting Information

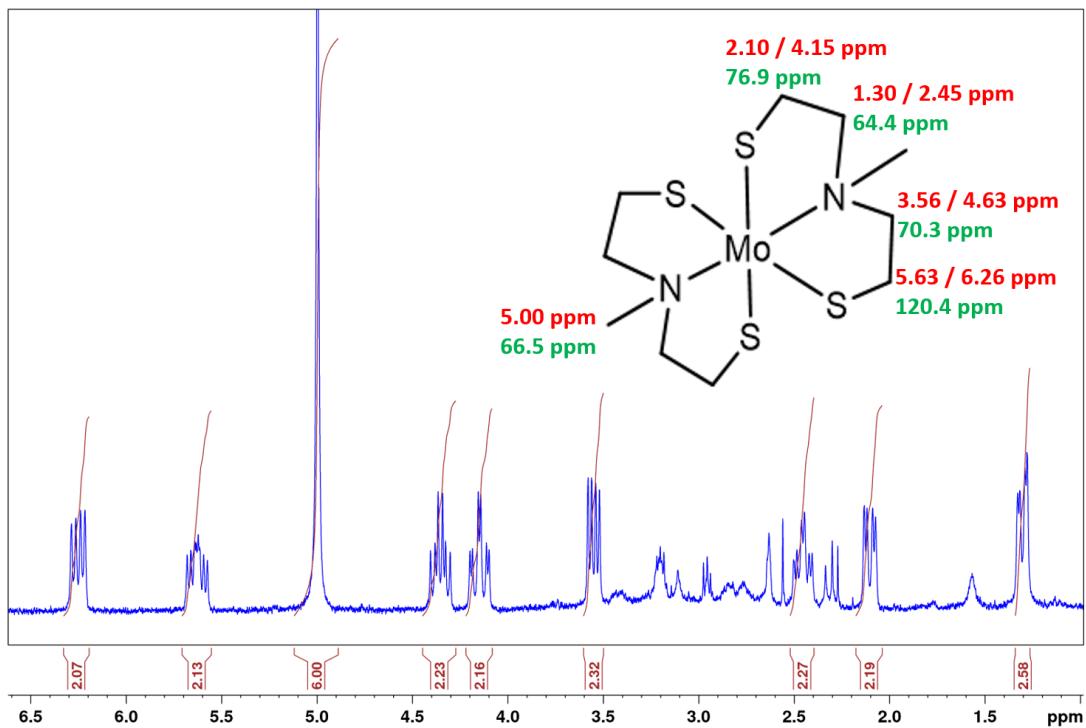
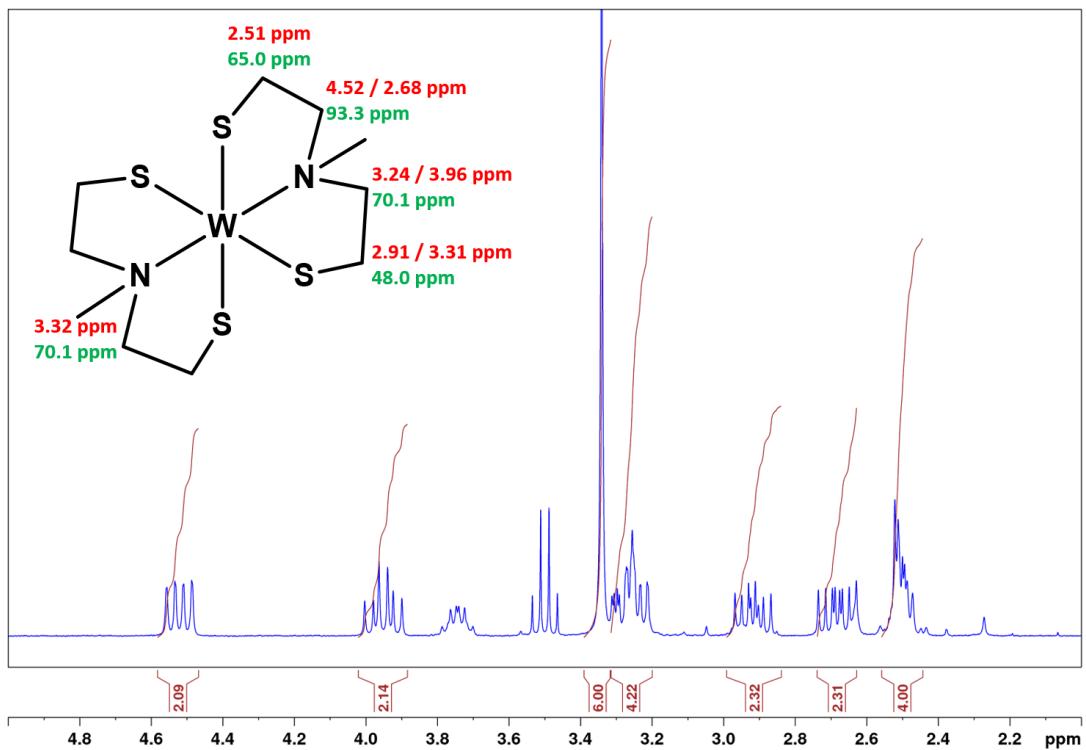
SI Figure S1: ¹ H NMR spectrum: Ring structure of the ligand ((SEt) ₂ N'Bu) ₂ 3b-1	S2
SI Figure S2: ¹ H NMR spectrum: Ring structure of the ligand ((SEt) ₂ NPh) ₂ 3c-1	S2
SI Figure S3: Comparison of the ¹ H NMR spectra of 1a [W(SEtN(Me)EtS) ₂] (top) and 2a [Mo(SEtN(Me)EtS) ₂] (bottem). Molecular structures displayed with related chemical shifts (¹ H (red) and ¹³ C (green))	S3
SI Table S1: Selected bond length and angles for 1a and 2a (M1=W, Mo)	S4



SI-Figure S1: 1H NMR spectrum: Ring structure of the ligand $((SEt)_2N^tBu)_2 3b\text{-I}$.



SI-Figure S2: 1H NMR spectrum: Ring structure of the ligand $((SEt)_2NPh)_2 3c\text{-I}$.



SI-Figure S3: Comparison of the ^1H NMR spectra of **1a** [W(SEt $\text{N}(\text{Me})$)EtS] $_2$ (top) and **2a** [Mo(SEt $\text{N}(\text{Me})$)EtS] $_2$ (bottom). Molecular structures displayed with related chemical shifts (^1H (red) and ^{13}C (green)).

*SI-Table 1: Selected bond length and angles for **1a** and **2a** ($M1=W, Mo$).*

complexes angles and distances	[W(SEtN(Me)EtS) ₂] 1a	[Mo(SEtN(Me)EtS) ₂] 2a
M1-S1	2.38(1) Å	2.37(1) Å
M1-S2	2.28(1) Å	2.28(1) Å
M1-S3	2.28(1) Å	2.38(1) Å
M1-S4	2.36(1) Å	2.27(1) Å
M1-N1	2.38(1) Å	2.40(1) Å
M1-N2	2.38(1) Å	2.39(1) Å
S2-M1-S3	91.24(9)°	91.95(7)°
S2-M1-S4	92.70(9)°	90.80(8)°
S2-M1-S1	107.80(8)°	108.87(8)°
S3-M1-S4	108.40(8)°	108.37(8)°
S3-M1-S1	92.31(9)°	150.55(1)°
S4-M1-S1	150.65(9)°	92.37(8)°
S3-M1-N2	78.71(2)°	78.60(2)°
S1-M1-N1	85.20(2)°	78.85(2)°
S2-M1-N2	164.70(2)°	163.70(2)°
S4-M1-N2	78.70(2)°	79.83(2)°
S2-M1-N1	79.72(2)°	79.85(2)°
S3-M1-N1	164.2(2)°	84.85(2)°
N1-M1-N2	111.8(2)°	112.1(2)°

S3

S4