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SUPPORTING INFORMATION

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"Spectroscopic Properties, Electrochemistry and Reactivity of Mo(0), Mo(I) and Mo(II) Complexes with the Mo(bpa)$(CO)_3$ Unit (bpa = di(2-picolyl)amine) and Their Application for the Labelling of Peptides"

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Figure S1. Selected regions from the ^{1}H NMR spectra of **1** (left) and **2** (right) (400 MHz; [D_6]DMSO).

Figure S2. Selected parts from both crystallographically independent molecules (left: A; right: B) of the X-ray crystal structure of **1**, visualising the HNCH torsion angles (see Table S1).

Table S3. HNCH torsion angles [°] for both independent molecules of **1**[a, b]

Figure S1

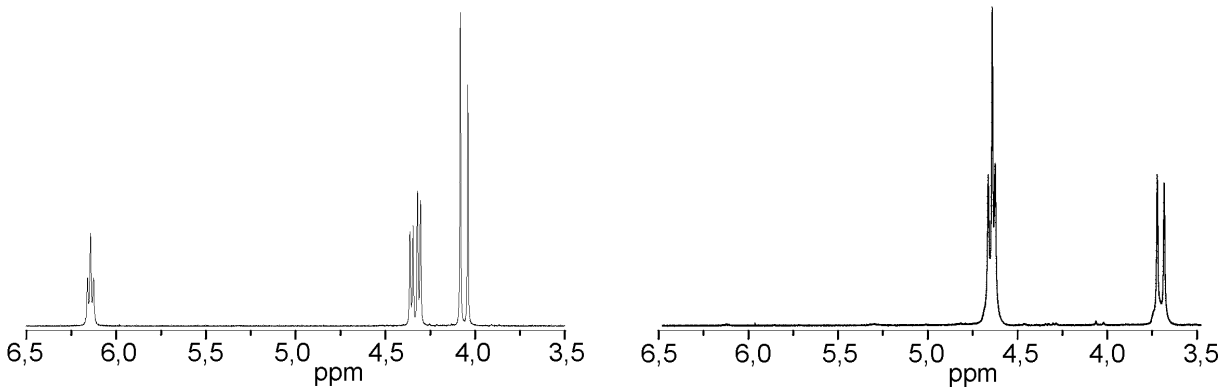

Figure S2

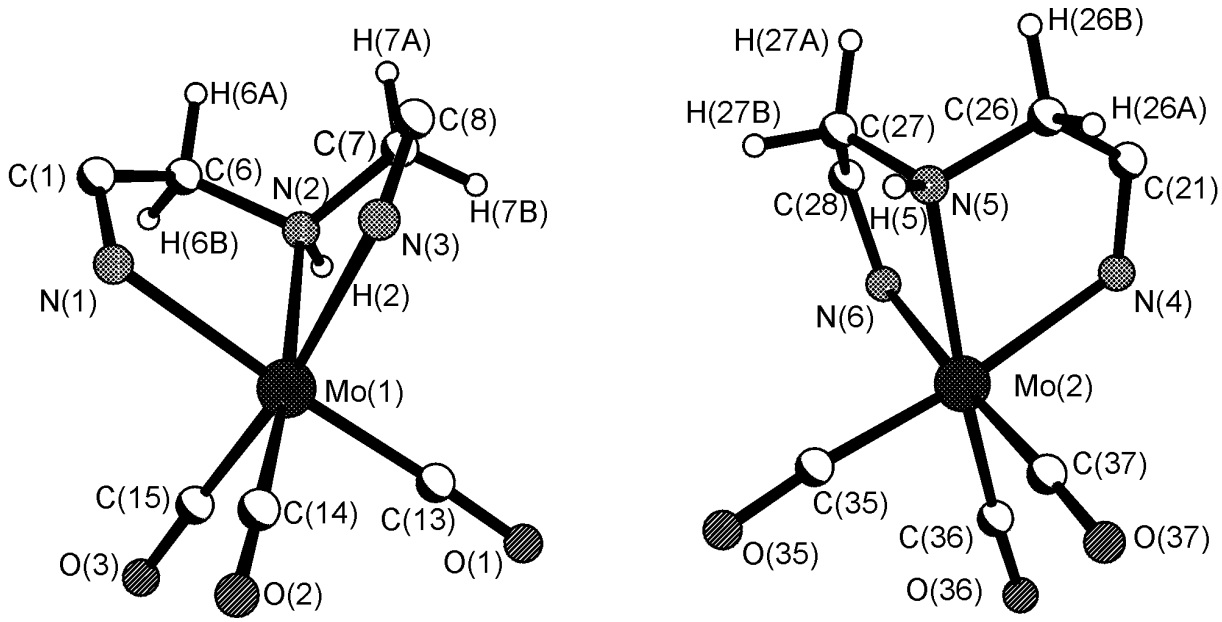

Table S3. HNCH torsion angles [°] for both independent molecules of **1**[a, b]

Molecule A		*Molecule B*	
H(2)-N(2)-C(6)-H(6A)	-94[c]	H(5)-N(5)-C(26)-H(26A)	+30[d]
H(2)-N(2)-C(6)-H(6B)	+33[d]	H(5)-N(5)-C(26)-H(26B)	-88[c]
H(2)-N(2)-C(7)-H(7A)	+85[c]	H(5)-N(5)-C(27)-H(27A)	+89[c]
H(2)-N(2)-C(7)-H(7B)	-32[d]	H(5)-N(5)-C(27)-H(27B)	-32[d]

[a] Torsion angles are visualized in Figure S2. – [b] IUPAC nomenclature used. Angles that increase clockwise and counterclockwise have a positive and negative sign, respectively. – [c] The Karplus equation ($^3J_{HH} = 4.22 - 0.5\cos\varphi + 4.5\cos 2\varphi$)[40] yields a value of 0.2-0.3 Hz for these angles. – [d] The Karplus equation yields a value of 5.8-6.0 Hz for these angles.