

Supporting Information

Article for *Molecules*

A comparative study of molybdenum carbonyl and oxomolybdenum derivatives bearing 1,2,3-triazole or 1,2,4-triazole in catalytic olefin epoxidation

Lucie S. Nogueira, Patrícia Neves, Ana C. Gomes, Tatiana A. Amarante, Filipe A. Almeida Paz, Anabela A. Valente *, Isabel S. Gonçalves, Martyn Pillinger *

Department of Chemistry, CICECO – Aveiro Institute of Materials, University of Aveiro, Campus Universitário de Santiago, 3810-193 Aveiro, Portugal;

lucienogueira@ua.pt (L.S.N.); pneves@ua.pt (P.N.); agomes1@ua.pt (A.C.G.);
tatiana.amarante@ua.pt (T.A.A.); filipe.paz@ua.pt (F.A.A.P.); atav@ua.pt (A.A.V.);
igoncalves@ua.pt (I.S.G.); mpillinger@ua.pt (M.P.)

* Correspondence: atav@ua.pt (A.A.V.), mpillinger@ua.pt (M.P.); Tel.: +351-234-370603

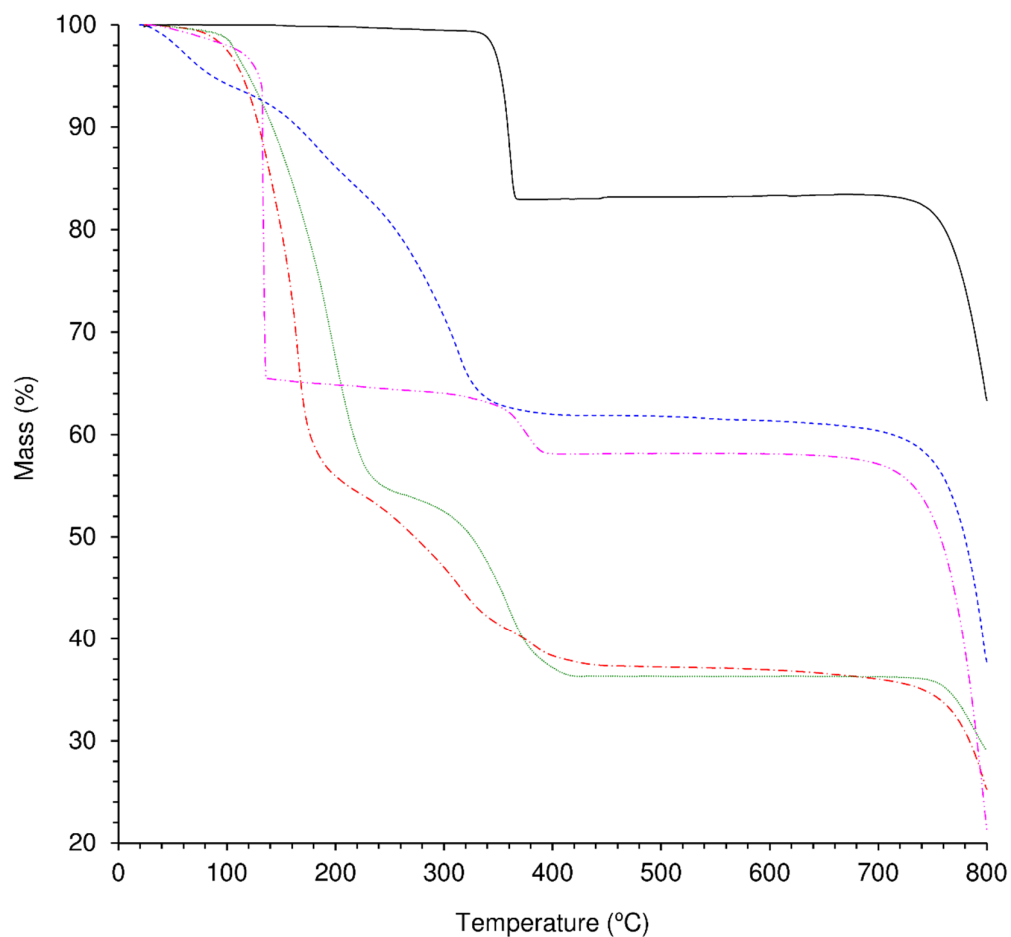


Figure S1. TGA curves for $[\text{Mo}(\text{CO})_3(1,2,3\text{-trz})_3]$ (**1**) ($\cdot - \cdot - \cdot$), $[\text{Mo}(\text{CO})_3(1,2,4\text{-trz})_3]$ (**2**) (\cdots), **1^{OD}** ($- - -$), $[\text{MoO}_3(1,2,3\text{-trz})_{0.5}]$ (**3**) (—), and $(\text{NH}_4)_{1.8}(\text{H}_3\text{O})_{0.2}[\text{Mo}_2\text{O}_2(\mu_2\text{-O})(\text{O}_2)_4(1,2,4\text{-trz})]\cdot\text{H}_2\text{O}$ (**5**) ($\cdot \cdots \cdot$).

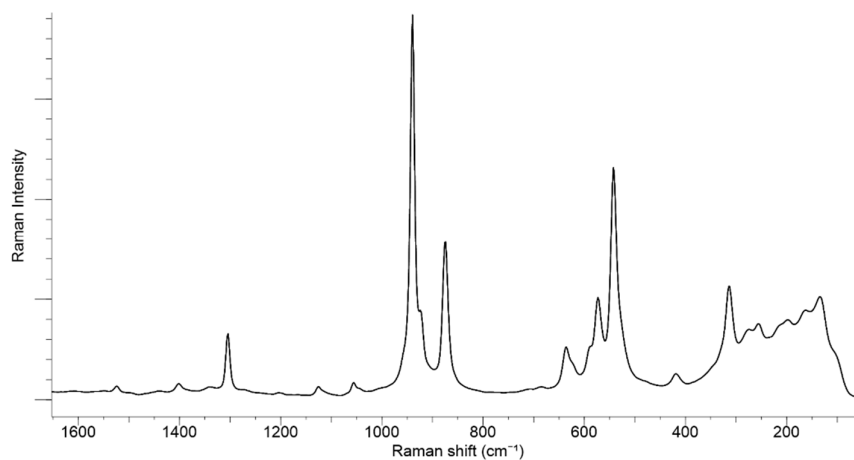


Figure S2. Raman spectrum in the range of 100-1600 cm^{-1} of $(\text{NH}_4)_{1.8}(\text{H}_3\text{O})_{0.2}[\text{Mo}_2\text{O}_2(\mu_2\text{-O})(\text{O}_2)_4(1,2,4\text{-trz})]\cdot\text{H}_2\text{O}$ (**5**).

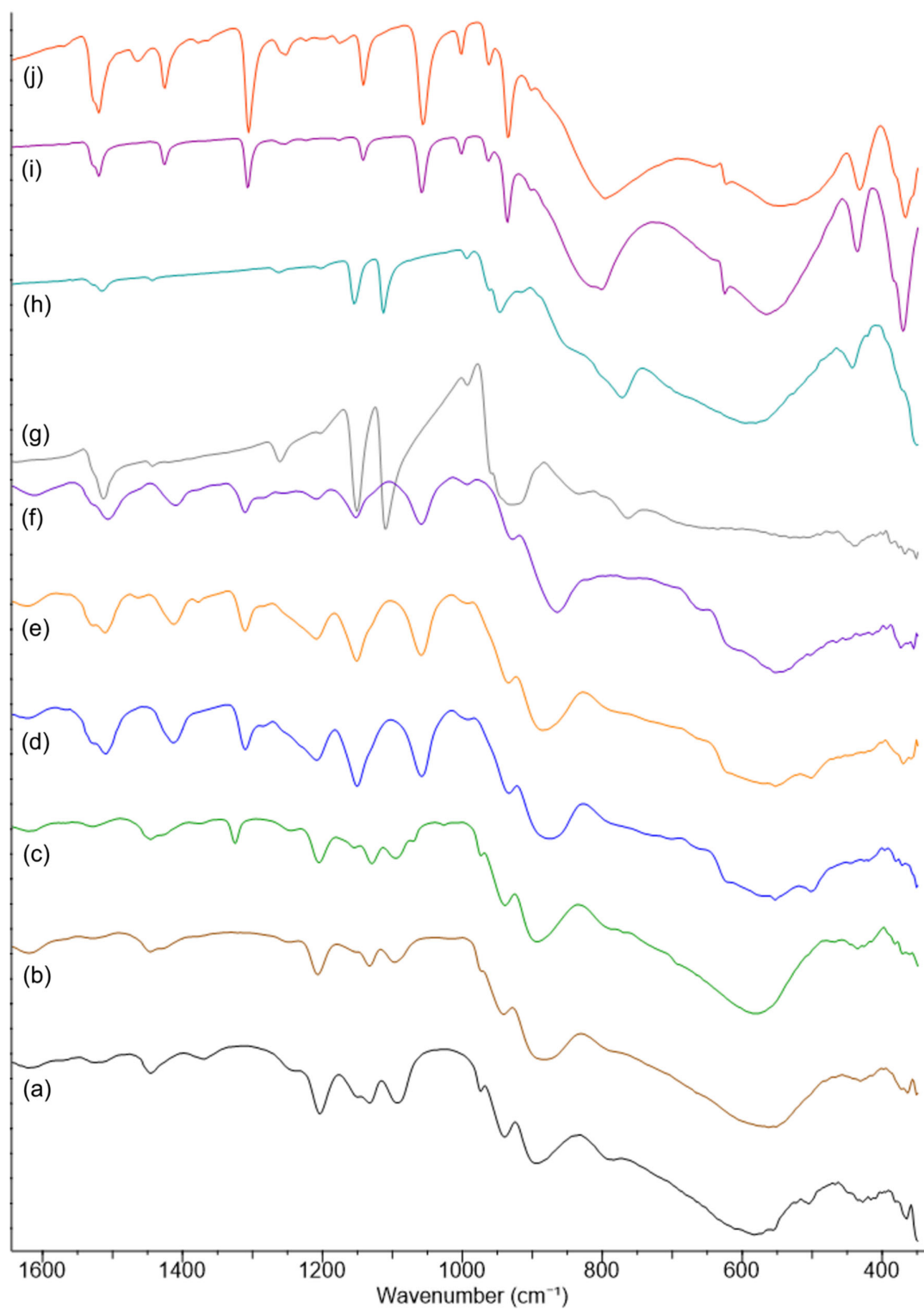


Figure S3. ATR FT-IR spectra in the range of 350-1600 cm⁻¹ of (a) **1**^{OD}, (b) recovered solid **1**^{ODr}, (c) recovered solid **1**^r, (d) **2**^{OD}, (e) recovered solid **2**^{ODr}, (f) recovered solid **2**^r, (g) hybrid **3**, (h) recovered solid **3**^r, (i) hybrid **4**, and (j) recovered solid **4**^r.

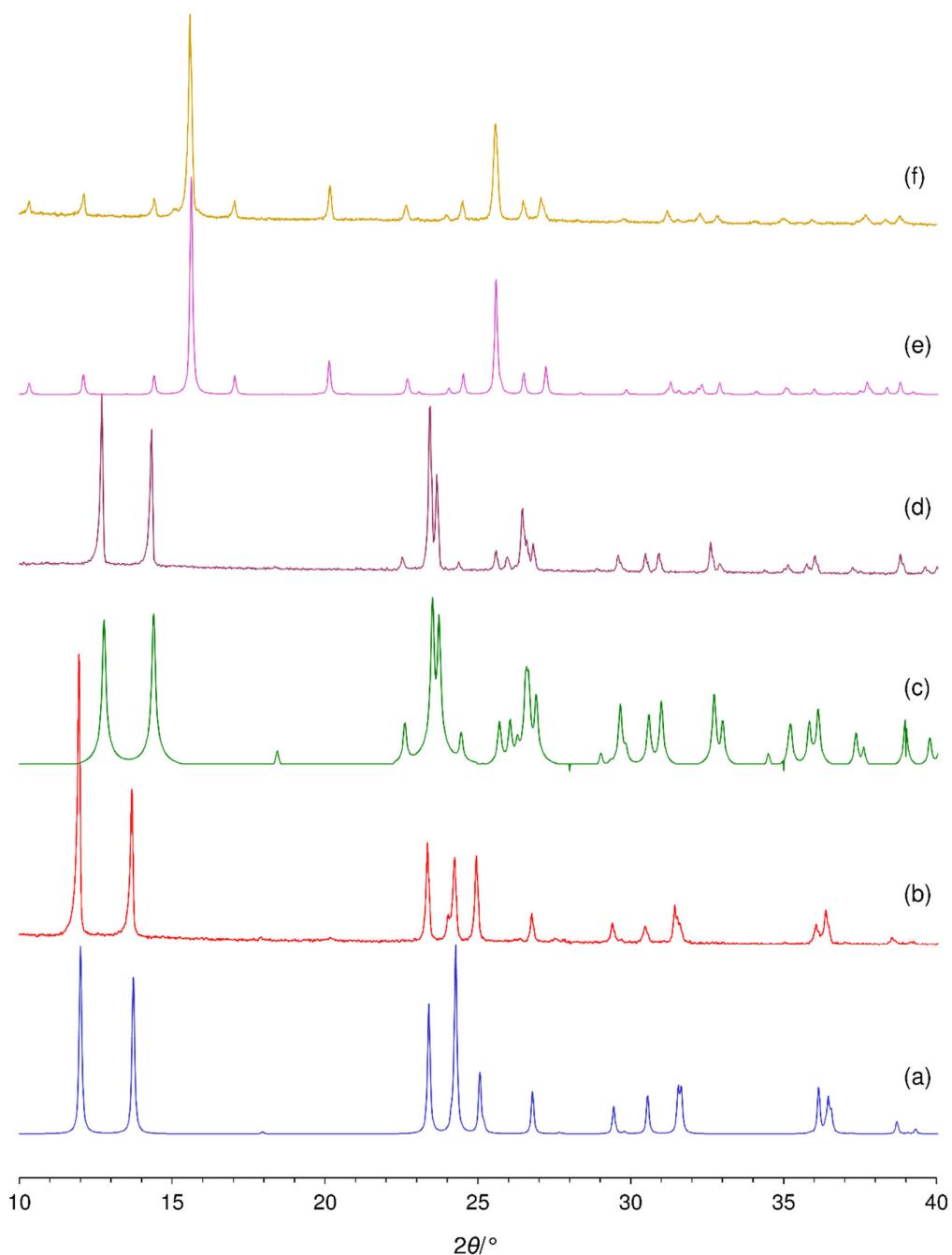


Figure S4. Computed (a,c,e) and experimental (b,d,f) PXRd patterns of (a,b) $[\text{MoO}_3(1,2,3\text{-trz})_{0.5}]$ (**3**), (c,d) $[\text{MoO}_3(1,2,4\text{-trz})_{0.5}]$ (**4**), and (e,f) $(\text{NH}_4)_{1.8}(\text{H}_3\text{O})_{0.2}[\text{Mo}_2\text{O}_2(\mu_2\text{-O})(\text{O}_2)_4(1,2,4\text{-trz})] \cdot \text{H}_2\text{O}$ (**5**). The program Mercury (copyright CCDC, ver. 3.9) [S1] was used to generate the computed patterns from the crystal structure data published for **3** [S2] and **4** [S3], and the data reported in this paper for **5**.

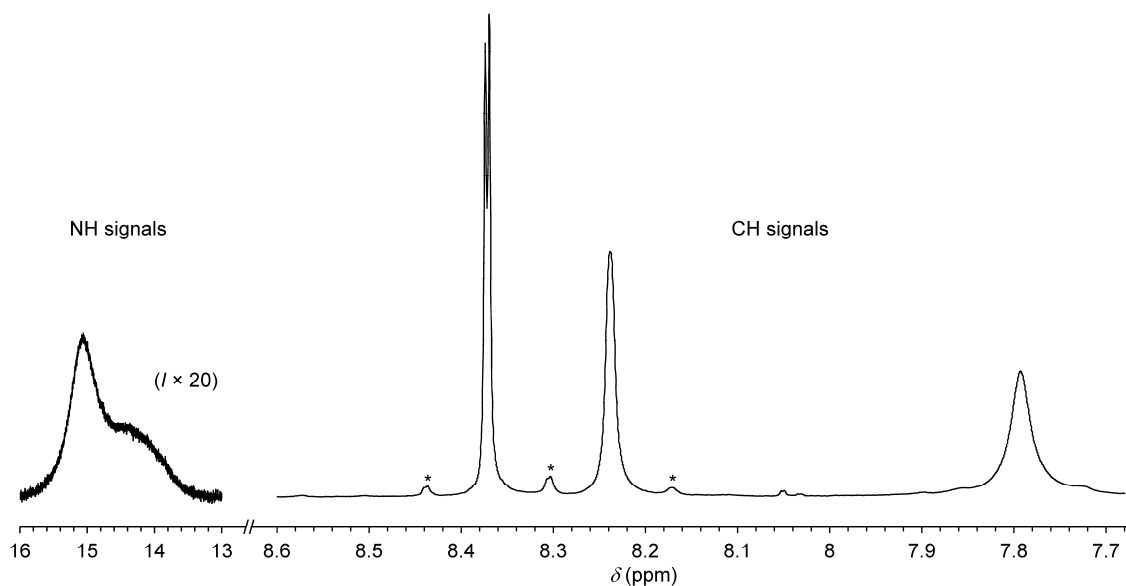


Figure S5. Regions of the ^1H NMR spectrum of **1** in $(\text{CD}_3)_2\text{CO}$ containing signals due to 1,2,3-trz NH and CH protons. The asterisks denote spinning sidebands.

Table S1. Bond distances (\AA) and angles ($^\circ$) for the crystallographically independent Mo^{VI} center present in $(\text{NH}_4)_{1.8}[(\text{H}_3\text{O})_{0.2}[\text{Mo}_2\text{O}_2(\mu_2\text{-O})(\text{O}_2)_4(1,2,4\text{-trz})] \cdot \text{H}_2\text{O}$ (**5**).

Mo1–O1	1.944(3)	O1–Mo1–O3	86.9(4)
Mo1–O2	1.700(6)	O1–Mo1–O6	88.3(3)
Mo1–O3	1.951(6)	O1–Mo1–N1	80.0(3)
Mo1–O4	1.933(7)	O2–Mo1–O1	98.1(3)
Mo1–O5	1.941(6)	O2–Mo1–O3	101.5(3)
Mo1–O6	1.958(6)	O2–Mo1–O4	101.1(3)
Mo1–N1	2.398(9)	O2–Mo1–O5	100.5(3)
		O2–Mo1–O6	101.2(3)
		O2–Mo1–N1	178.0(3)
		O3–Mo1–O6	157.3(3)
		O3–Mo1–N1	78.8(3)
		O4–Mo1–O1	130.2(4)
		O4–Mo1–O3	44.4(3)
		O4–Mo1–O5	89.2(3)
		O4–Mo1–O6	131.1(3)
		O4–Mo1–N1	80.4(3)
		O5–Mo1–O1	131.4(4)
		O5–Mo1–O3	131.6(3)
		O5–Mo1–O6	44.1(3)
		O5–Mo1–N1	80.7(3)
		O6–Mo1–N1	78.6(3)

References

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- [S3] J. Chuang, W. Oullette, J. Zubieta, *Inorg. Chim. Acta* **2008**, *361*, 2357-2364.