

Supporting information

Regulating the Hydrodeoxygenation Activity of Molybdenum Carbide with Different Diamines as Carbon Sources

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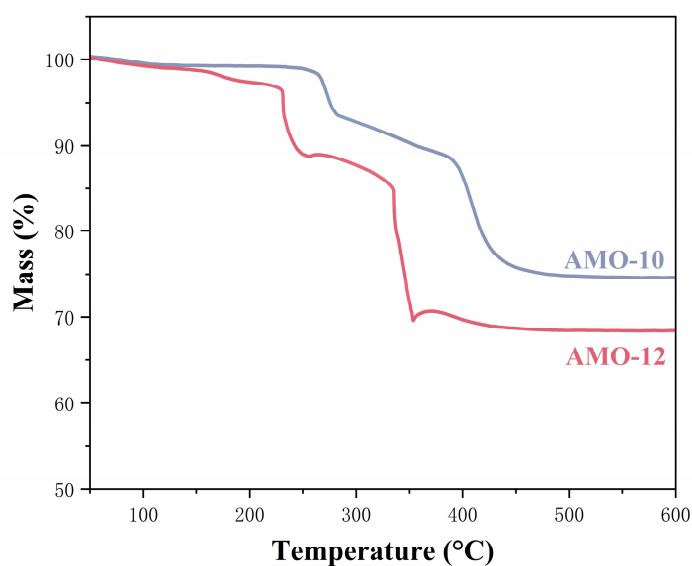


Figure S1. TG curves for AMO-10 and AMO-12 in 20% O₂/N₂ atmosphere.

Table S1. Element contents of AMO-10 and AMO-12.

Catalyst	Mo ^a (wt%)	C ^b (wt%)	N ^b (wt%)	H ^b
Mo ₂ C-10	50.07	15.79	3.74	3.19
Mo ₂ C-12	46.07	18.88	3.69	3.78

^a Calculated by TG results;^b Obtained by elemental analysis.

In order to calculate the possible chemical formula of AMO-10 and AMO-12, TG of AMO-10 and AMO-12 were conducted under 20% O₂/N₂ atmosphere, as shown in Figure S1. Weight loss before 150 °C was considered as water. AMO precursors were ultimately completely oxidized to MoO₃, with the remaining masses of AMO-10 and AMO-12 being 74.63% and 68.45%. Based on the element contents shown in Table S1, the simplest chemical composition of AMO-10 and AMO-12 were calculated, which are (NH₃C₁₀H₂₀NH₃)·Mo₄O₁₃ and (NH₃C₁₂H₂₄NH₃)·Mo₄O₁₃, respectively.

Table S2. Surface contents on Mo₂C catalysts calculated from XPS.

Catalyst	Mo (at%)	C (at%)	O (at%)
Mo ₂ C-6	36.9	15.5	47.6
Mo ₂ C-8	37.2	18.9	43.9
Mo ₂ C-10	33.9	27.3	38.8
Mo ₂ C-12	24.6	52.1	23.2

Table S3. Surface contents of C and Mo in different chemical states in catalysts.

Catalyst	C 1s (%)			Mo 3d (%)	
	C-Mo	C-C	C-O/C=O	Mo ₂ C	Mo ^{b+} /Mo ⁴⁺ /Mo ⁶⁺
Mo₂C-6	9.7	34.8	55.5	25.3	74.7
Mo ₂ C-8	18.2	39.9	41.9	22.8	77.2
Mo ₂ C-10	15.0	49.9	35.1	29.3	70.7
Mo ₂ C-12	14.2	48.0	37.8	29.7	70.3

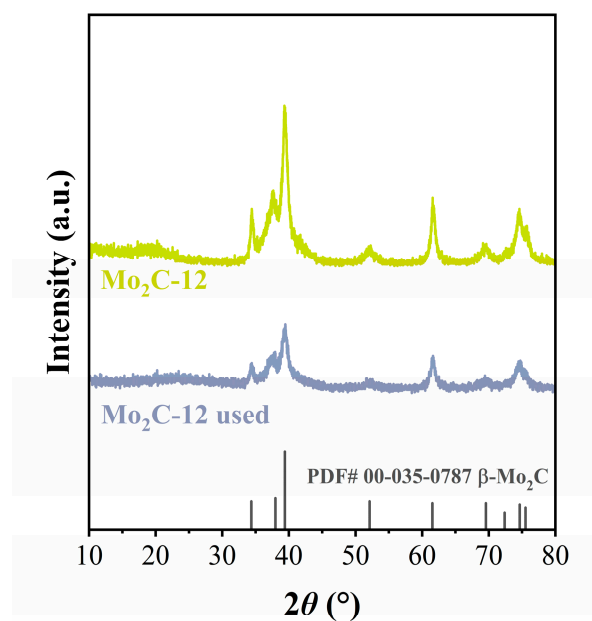


Figure S2. XRD patterns of fresh and used Mo₂C-12 catalyst.

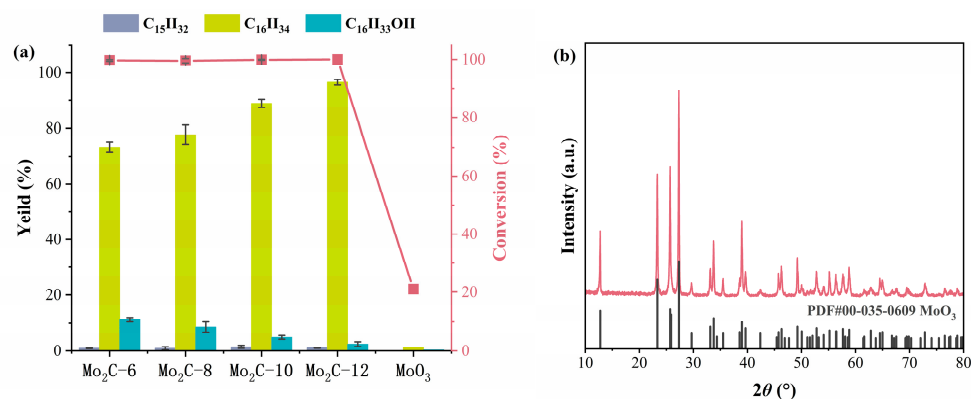


Figure S3. (a) The reactivity results for converting palmitic acid over different Mo₂C catalysts and MoO₃. (b) XRD pattern of MoO₃.

AHM powder was calcined in a muffle oven at 500°C for 4 hours to synthesize MoO₃. The catalytic activity was tested under the same reaction conditions as other catalysts. The results were shown in Figure S3 (a). The conversion rate of palmitic acid on pure MoO₃ is only 21.0%, almost no other corresponding products have been detected. There might be undetected products palmityl palmitate. Figure S3 (b) shows the XRD pattern of MoO₃. This indicated that MoO₃ has poor activity for the hydrodeoxygenation of palmitic acid.