

Supporting information

Photoreduction of CO₂ to methanol with hexanuclear molybdenum [Mo₆Br₁₄]²⁻ cluster units under visible light irradiation

Pawan Kumar^a, Subodh Kumar^a, Stéphane Cordier^b, Serge Paofai^b, Rabah Boukherroub^{c*} and Suman L. Jain^{a*}

^a Chemical Sciences Division, CSIR-Indian Institute of Petroleum, Dehradun-248005, India; Tel.: +91-135-2525788; Fax: +91-135-2660202; Email: suman@iip.res.in

^b Université de Rennes 1, Institut Sciences Chimiques de Rennes, URI-CNRS 6226, Equipe Chimie du Solide et Matériaux, Campus de Beaulieu, CS 74205, 35042 Rennes Cedex, France

^c Institut de Recherche Interdisciplinaire (IRI, USR CNRS 3078), Université Lille 1, Parc de la Haute Borne, 50 Avenue de Halley, BP 70478, 59658 Villeneuve d'Ascq, France

Fig. S1: GC chromatogram of reaction product after 12 h of photoreduction of CO₂ using Cs₂[Mo₆Br₈] cluster as catalyst, and DMF/H₂O/TEA (3:1:1) as reaction medium.

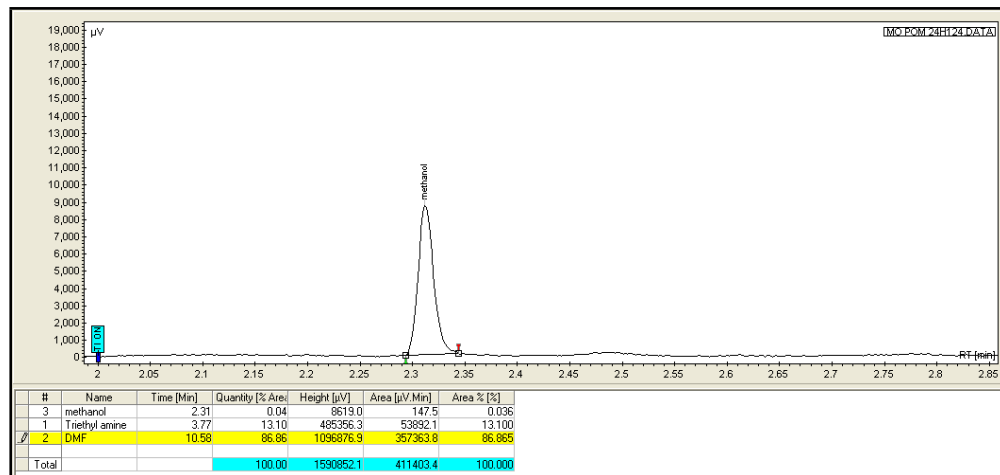


Fig. S2: GC-MS spectra of the reaction product after 12 h of photoreduction of CO₂ using Cs₂[Mo₆Br₈] cluster as catalyst and DMF/H₂O/TEA (3:1:1) as reaction medium.

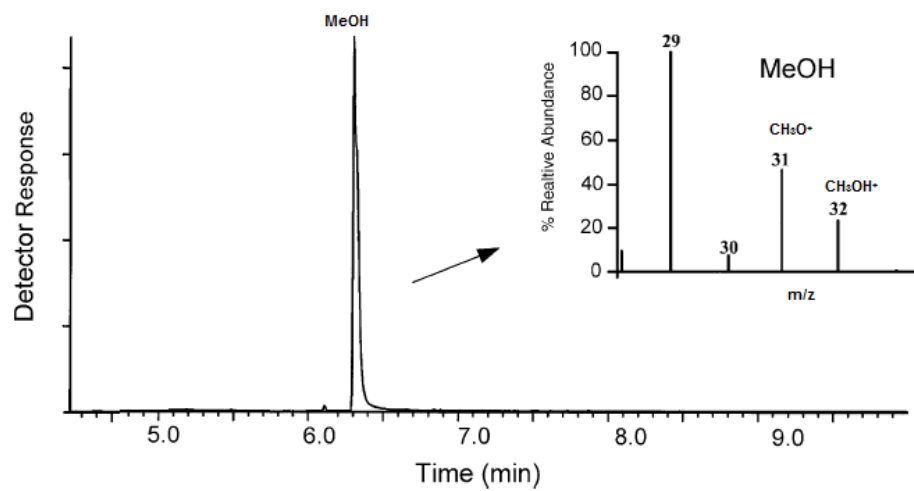
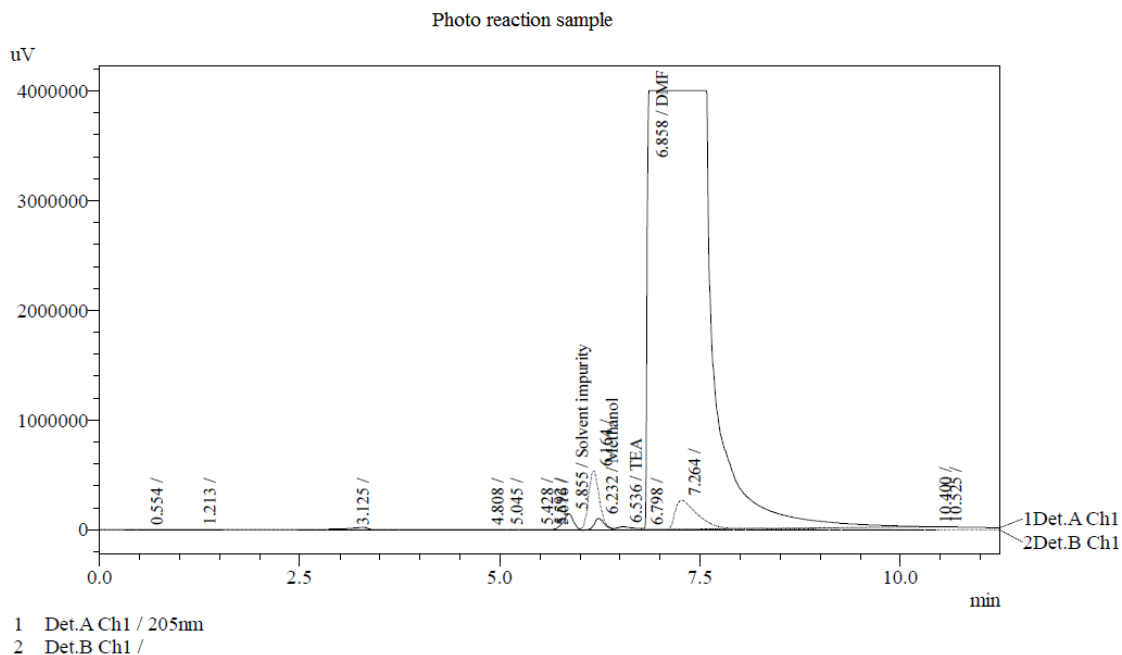


Fig. S3: HPLC chromatogram of the reaction product after 12 h of photoreduction of CO₂ using Cs₂[Mo₆Br₈] cluster as catalyst and DMF/H₂O/TEA (3:1:1) as reaction medium.



Results

PeakTable

Detector A Ch1 205nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	5.592	-16409	-30	-0.008	-0.001
2	5.855	1259415	146155	0.577	3.419
3	6.232	894177	104106	0.409	2.435
4	6.536	338454	26659	0.155	0.624
5	6.858	216059897	3996108	98.936	93.472
6	10.400	7003	2213	0.003	0.052
7	10.525	-159525	-28	-0.073	-0.001
8	17.558	0	0	0.000	0.000
9	23.867	0	0	0.000	0.000
10	25.500	0	0	0.000	0.000
11	31.775	0	0	0.000	0.000
12	34.267	0	0	0.000	0.000
13	36.950	0	0	0.000	0.000
Total		218383013	4275182	100.000	100.000

Solvent Impurity
Methanol
TEA
DMF

Fig. S4: Calibration curve for methanol analysis

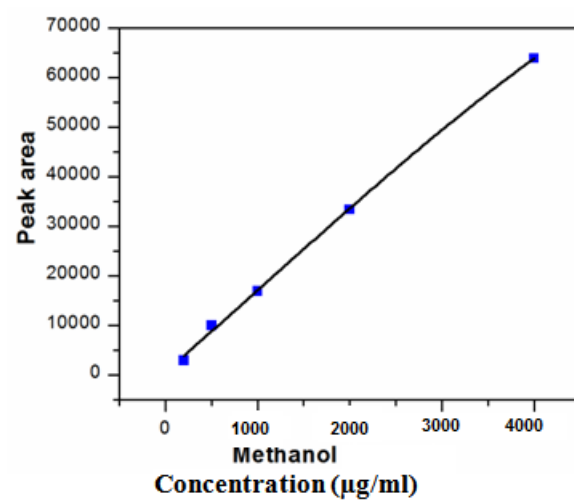


Fig. S5: Methanol yield after 24 h of the photoreduction of CO₂ using Cs₂[Mo₆Br₈] cluster as catalyst and CH₃CN/H₂O/TEA (3:1:1) as reaction medium.

