Supporting information

Epimerization of glucose over ionic liquid/phosphomolybdate hybrids: structure-activity relationship

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Table of contents

Table S1.

	[C2mim]PMo	[C4mim]PMo	[C6mim]PMo
Formula	$C_{18}H_{33}Mo_{12}N_6O_{40}P$	$C_{24}H_{45}Mo_{12}N_6O_{40}P$	$C_{30}H_{57}Mo_{12}N_6O_4P$
M	2155.75	2239.91	2324.07
T [K]	193(2)	193(2)	193(2)
Wavelength [Å]	0.71073	0.71073	0.71073
Crystal system	triclinic	triclinic	orthorhombic
Space group	$P\bar{1}$	$P\bar{1}$	*P*bca
a [Å]	14.9687(5)	12.9158(5)	22.3846(3)
b [Å]	15.0798(5)	21.2163(8)	20.9690(4)
c [Å]	21.8498(8)	21.6946(8)	26.0718(5)
α [°]	86.944(2)	95.876(2)	90.0
β [°]	88.681(2)	105.285(2)	90.0
γ [°]	85.622(2)	101.080(2)	90.0
V	4909.8(3)	5553.7(4)	12237.7(4)
Z	4	4	8
D_{calc}, Mgm^{-3}	2.916	2.679	2.523
μ, mm^{-1}	3.100	2.746	2.498
F(000)	4088	4280	8944
θ_{max}, deg	25.242	25.242	25.242
no. refins collected	65355	78335	118207
no.reflns used	17678	20090	11069
no. of param.	1399	1546	808
$R_1(F)$ $[F^2>2\sigma(F^2)]$[a]	0.0800	0.0538	0.0352
$wR_2(F^2)$[b] (all data)	0.2023	0.1156	0.0817
S[c] (all data)	1080	1.170	1.051

[a] $R_1(F) = \sum(|Fo| - |Fc|)/\sum|Fo|$ for the observed reflections $[F^2>2\sigma(F^2)]$. [b] $wR_2(F^2) = \{\sum [w(F_o^2 - F_c^2)^2]/ \sum w(F_o^2)^2\}^{1/2}$. [c] $S = \{\sum [w(F_o^2 - F_c^2)^2]/(n-p)\}^{1/2}$; (n = number of reflections, p = number of parameters).

Figure S1.

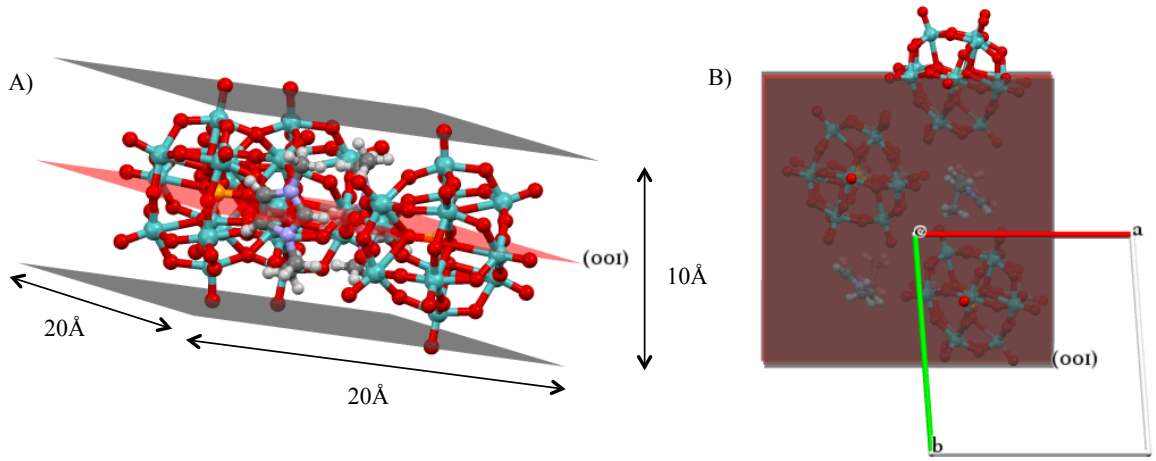


Table S2

Entry	Temperature (ºC)	Conversion (%) over [C2mim]PMo [a]	Equilibrium conversion (ref.)
1	70	18	-
2	80	21	26 [1]
3	90	27	30 [2]
4	100	34	32 [3]
5	110	43	-
6	120	49	-

[a] Reaction conditions: 5 mL of 0.2 M glucose solution, Glucose:hybrid 256:1 molar ratio (1:0.05 Glucose:Metal ratio), 60 min and 600 rpm.

Figure S2.

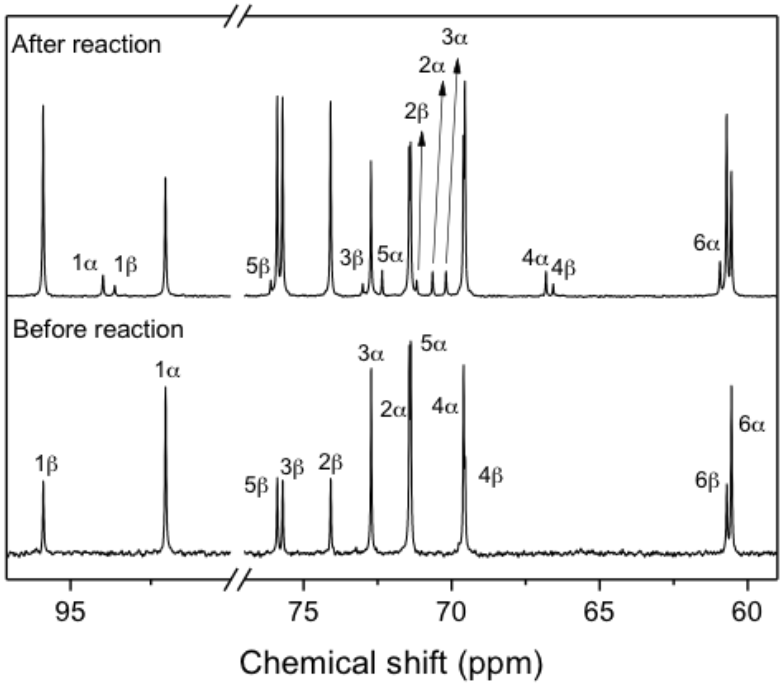
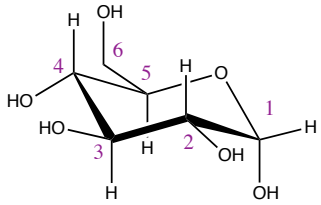
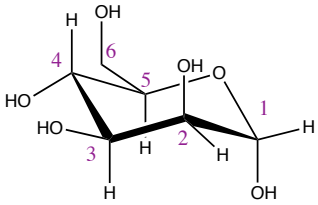

After reaction
1α
1β
5β
3β
5α
3α
2α
2β
4α
4β
6α
Before reaction
1β
1α
5β
3β
2β
3α
2α
5α
4α
4β
6β
6α
95
75
70
65
60
Chemical shift (ppm)

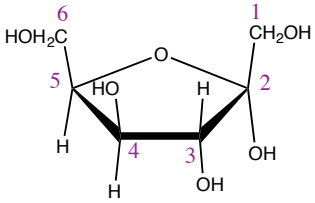
Table S3



α-glucose



α-mannose

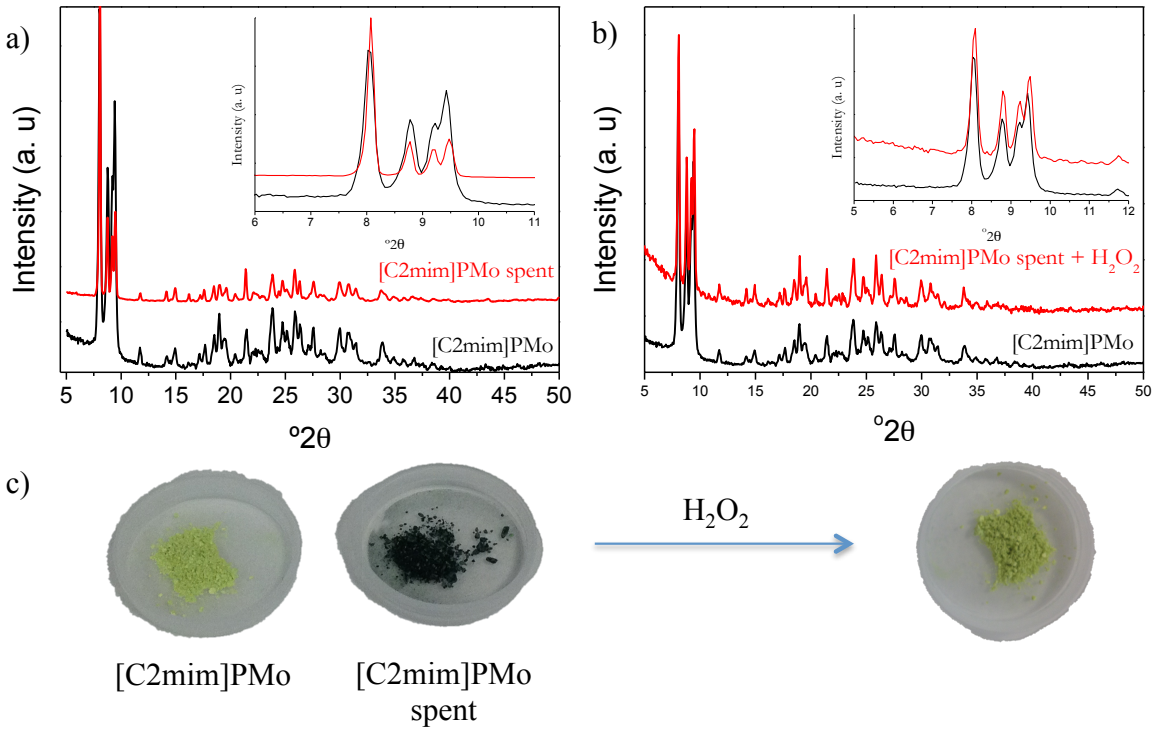


α-fructose

Entry	**Literature** [4]	C1	C2	C3	C4	C5	C6
1	α-glucose	92.9	72.5	73.8	70.6	72.3	61.6
2	β-glucose	96.7	75.1	76.7	70.6	76.8	61.7
3	α-mannose	95.0	71.7	71.3	68.0	73.4	62.1
4	β-mannose	94.6	72.3	74.1	67.8	77.2	62.1
5	α-fructose	63.8	105.5	82.9	77.0	82.2	61.9
6	β-fructose	63.6	102.6	76.4	75.4	81.6	63.2
	Experimental	C1	C2	C3	C4	C5	C6
7	α-glucose	92.1	71.4	72.7	69.6	71.4	60.55
8	β-glucose	95.9	74.1	75.7	69.55	75.9	60.7
9	α-mannose	94.0	70.6	70.2	66.8	72.3	60.9
10	β-mannose	93.6	71.2	73.0	66.6	76.1	*

* Overlaps with C6 of glucose

Figure S3.



References

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