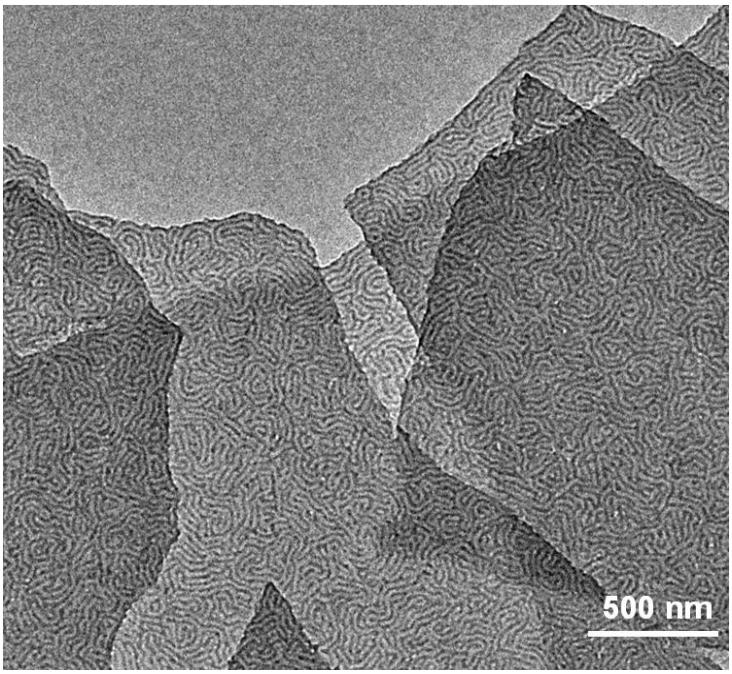
Supplementary Information

Efficient Electrocatalytic Upgrading of Furan-Based Biomass: Key Roles of Two-Dimensional Mesoporous Heterostructure and Ternary Electrolyte

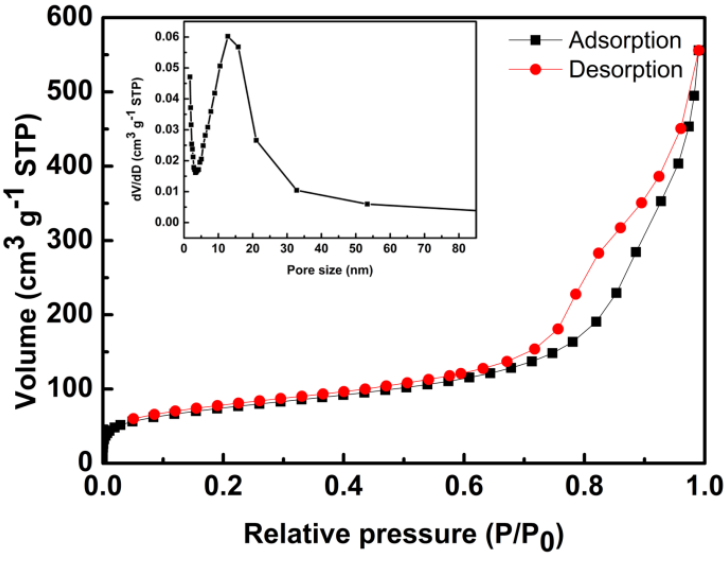
Haoran Wu,[1] Yashi Zou,[1] Haishan Xu,[1] Jianming Yang,[2] Qinye Bao,[2] Liang Wu,[1] and Yiyong Mai [1]*

[1]School of Chemistry and Chemical Engineering, Frontiers Science Center for Transformative Molecules, Shanghai Key Laboratory of Electrical Insulation and Thermal Ageing, Shanghai Jiao Tong University, 800 Dongchuan Road, Shanghai 200240, P. R. China.
*E-mail: mai@sjtu.edu.cn
[2]Key Laboratory of Polar Materials and Devices, School of Physics and Electronic Science, East China Normal University, Shanghai 200241, P. R. China.

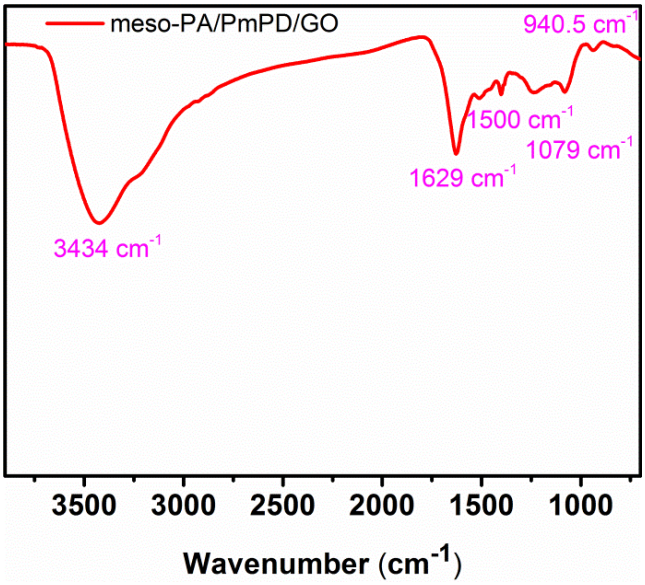
Supplementary Figures and Tables



Supplementary Fig. S1 TEM image of the meso-PA/PmPD/GO nanosheets.

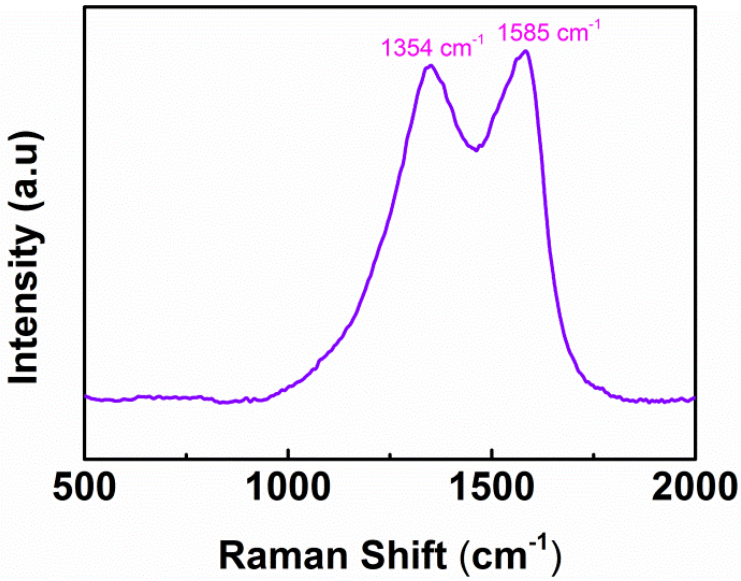


Supplementary Fig. S2 N_2 adsorption-desorption isotherm of the meso-PA/PmPD/GO nanosheets



Supplementary Fig. S3 A FTIR spectrum of the meso-PA/PmPD/GO nanosheets.

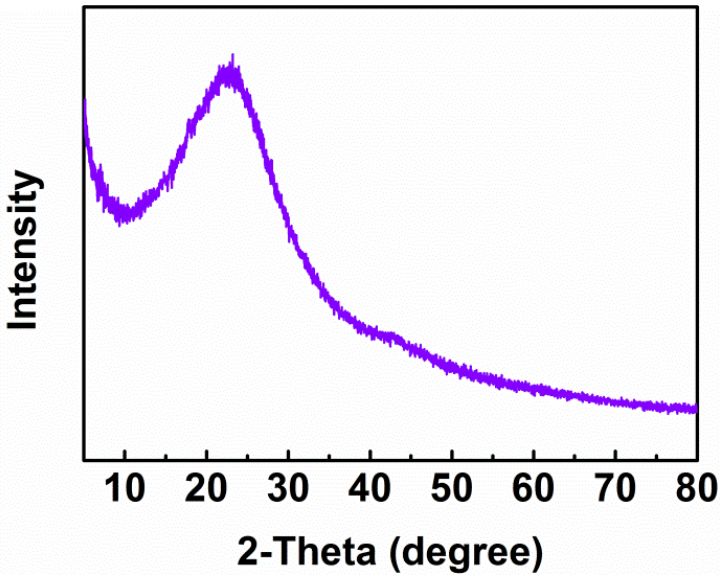
In the FTIR spectrum, the broad peak at 3434cm^{-1} is ascribed to the stretching vibration of -NH- and -OH. The sharp peaks located at 1629 cm^{-1} and 1500 cm^{-1} are assigned to the stretching vibrations of quinoid imine and benzenoid amine, respectively.[1] The peaks at 940.5 cm^{-1} and 1079 cm^{-1} are attributed to the stretching vibrations of the phosphate group.[2,3] Meanwhile, the FTIR spectrum does not show typical signals attributed to P123, indicating the removal of P123.[4]



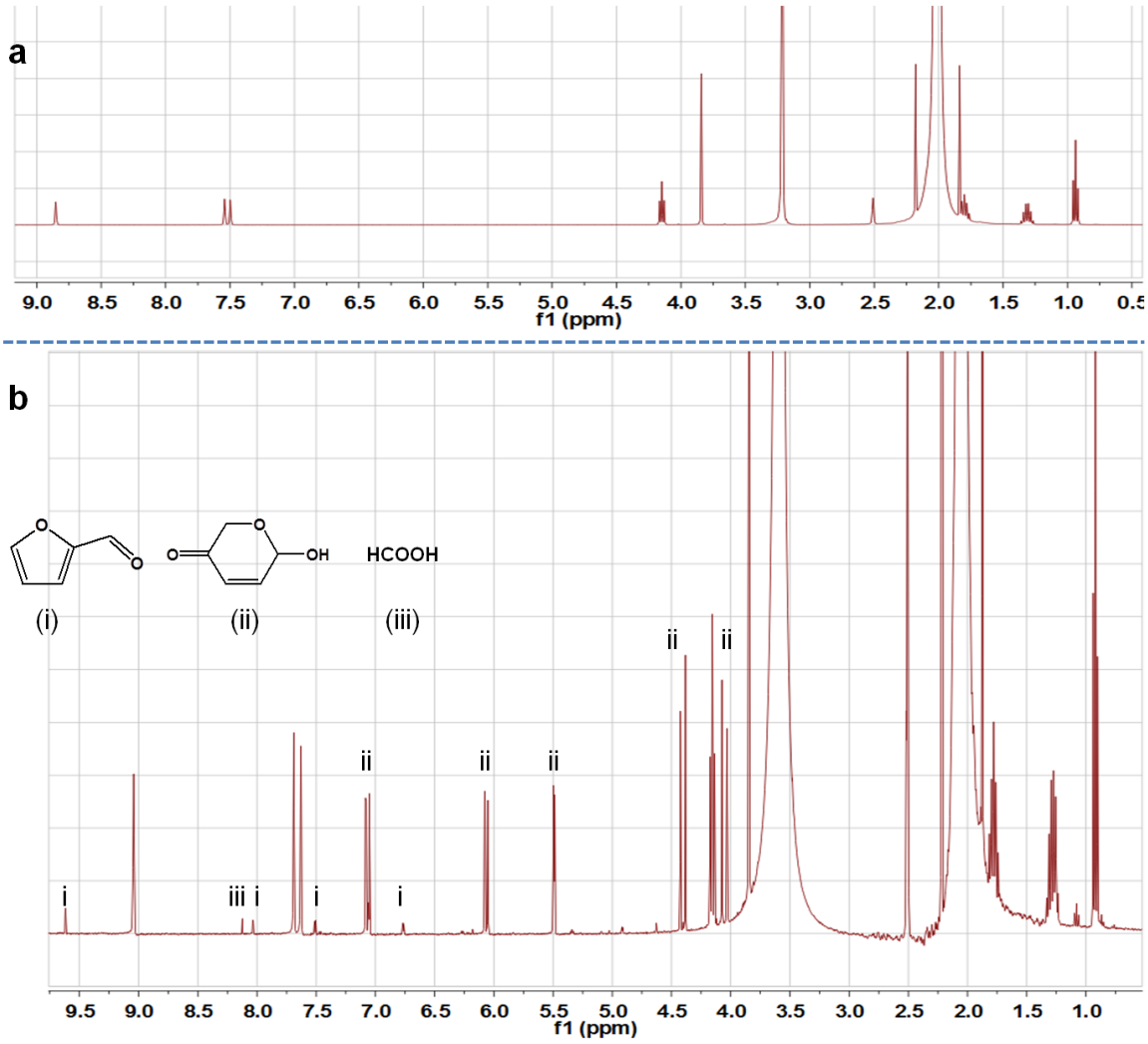
Supplementary Fig. S4 A Raman spectrum of the meso-PA/PmPD/GO nanosheets.

In the Raman spectrum, the two peaks at 1354 cm^{-1} and 1585 cm^{-1} are assigned to the D and G

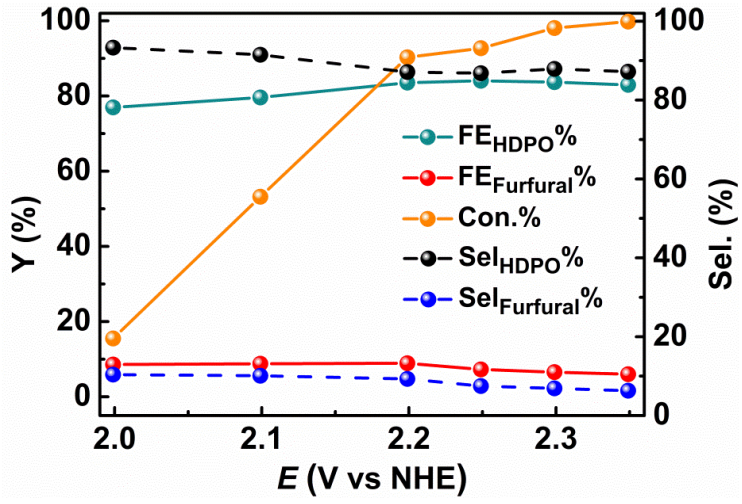
bands of GO, respectively. The D band corresponds to the carbon atoms with a stretching vibration of sp^3 hybridization, which reflects defects and disorders. The G band corresponds to the stretching vibration of sp^2-carbon atoms.



Supplementary Fig. S5 The XRD pattern of the meso-PA/PmPD/GO nanosheets.

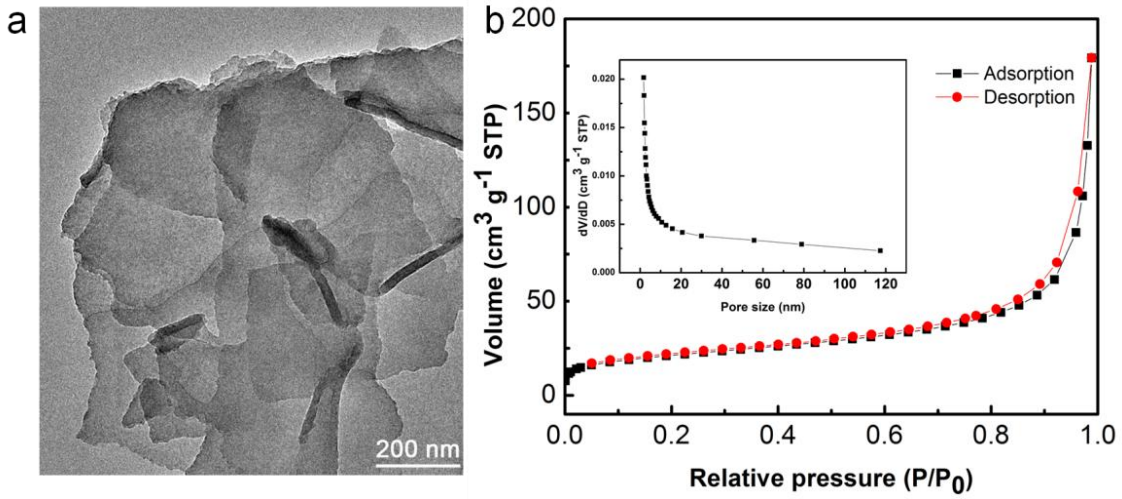


Supplementary Fig. S6 ^{1}H NMR spectra of the ternary electrolyte **(a)** and after the electrochemical oxidation of furfuryl alcohol over the meso-PA/PmPD/GO electrocatalyst in the ternary electrolyte **(b)** using DMSO-d_6 as solvent.

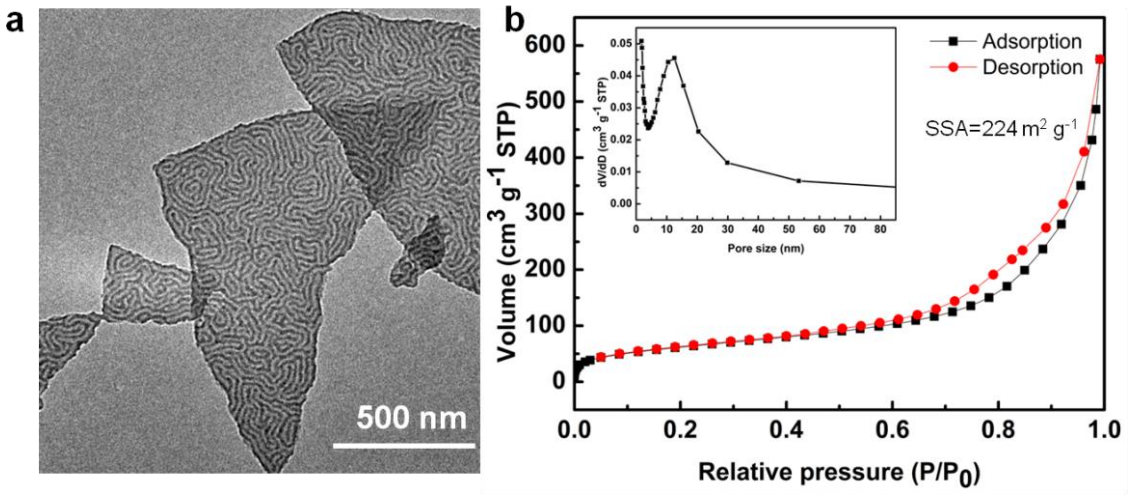


Supplementary Fig. S7 Effect of the potential on the electrochemical oxidation of furfuryl alcohol.

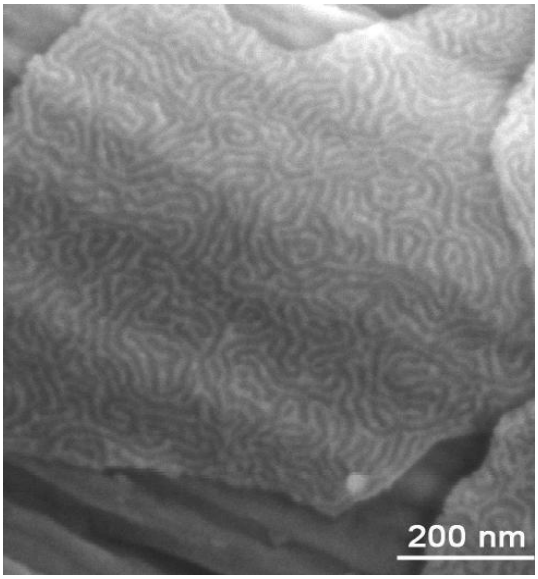
The effect of the potential on the electrochemical oxidation of furfuryl alcohol is presented in Supplementary Fig. S7. At a lower potential (2.0 V vs NHE), a low conversion (15.5%) of furfuryl acohol is obtained because of the low power. With an increase in the potential, the conversion of furfuryl acohol increases, whereas the selectivity of HDPO decreases due to the conversion of partial furfuryl acohol to furfural. In the range of 2.0-2.2 V, the oxidation of furfuryl acohol to HDPO is dominant. As the potential increases to the range of 2.2-2.35 V, the FE of HDPO starts to reduce, whereas both the selectivity and FE of furfural also decrease. The reason is that the resultant furfural can be partly oxidized to produce HCOOH through the cleavage of the aldehyde group of furfural. Meanwhile, the competitive oxygen evolution reaction *via* the electrolysis of H_2O is accompanied at higher potentials. Considering the balance of the conversion, FE and selectivity, 2.3 V is selected as the optimal potential for the subsequent investigations.



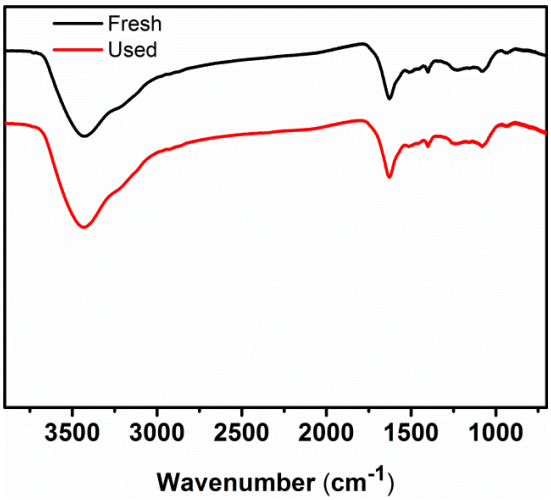
Supplementary Fig. S8 TEM image **(a)** and N_2 adsorption-desorption isotherm **(b)** of non-PA/PmPD/GO.



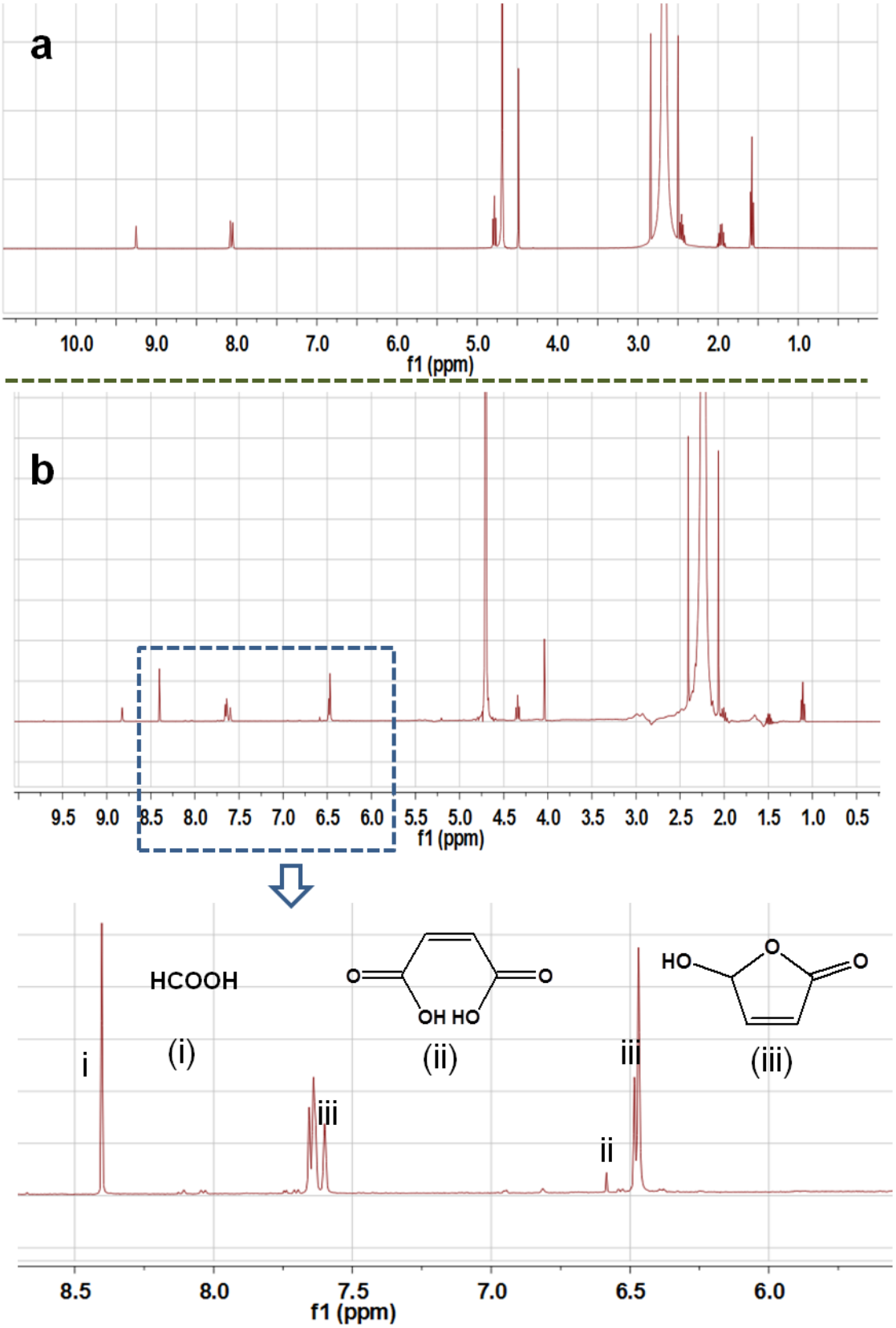
Supplementary Fig. S9 TEM image **(a)** and N_2 adsorption-desorption isotherm **(b)** of meso-PmPD/GO.



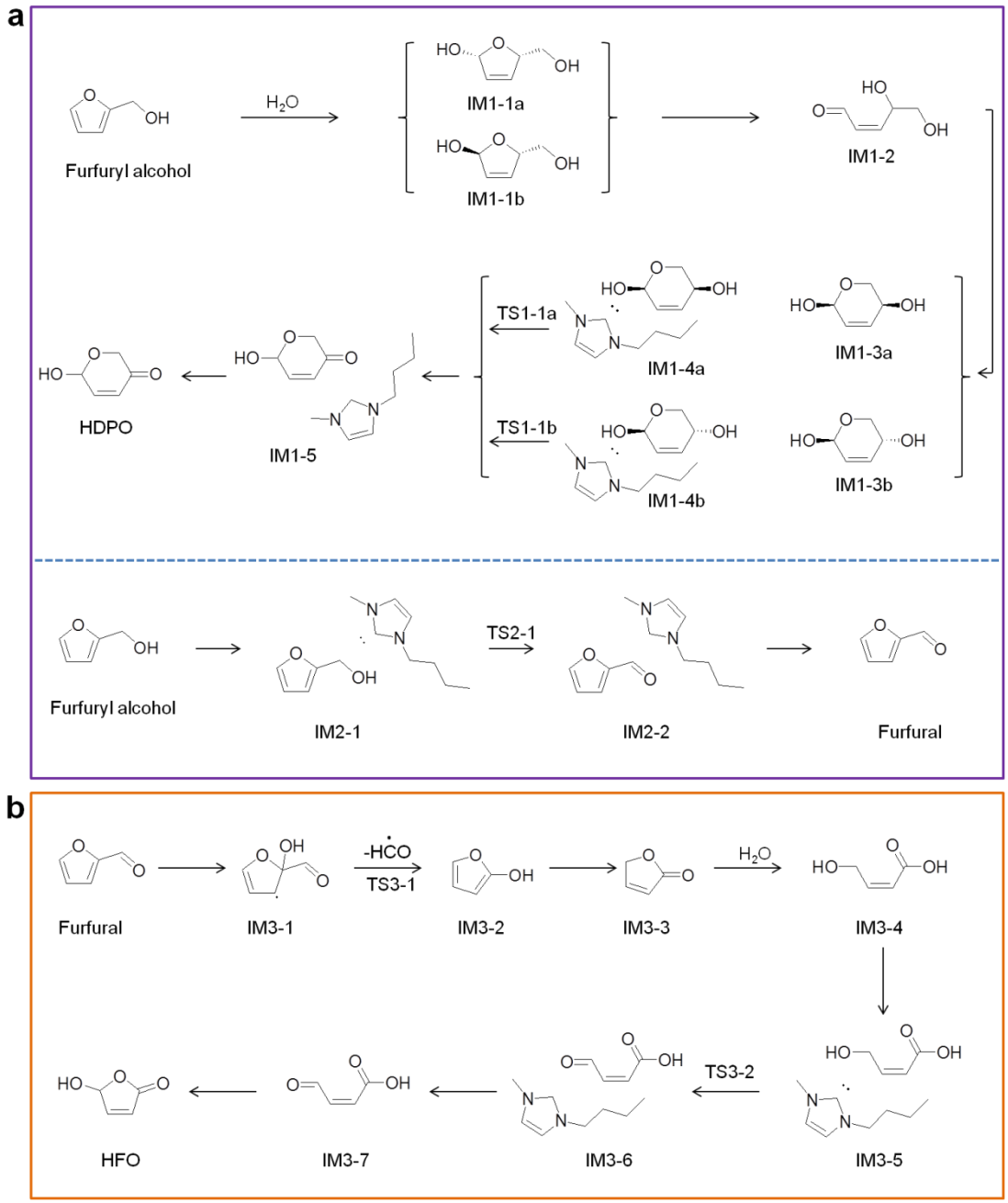
Supplementary Fig. S10 SEM image of the used meso-PA/PmPD/GO nanosheets after the electrochemical oxidation of furfuryl alcohol.



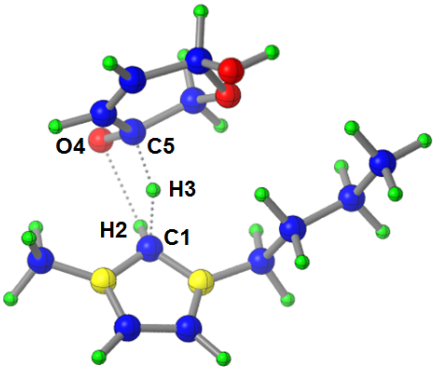
Supplementary Fig. S11 FTIR spectra of the fresh and used meso-PA/PmPD/GO



Supplementary Fig. S12 ^{1}H NMR spectra of the ternary electrolyte **(a)** and after the electrochemical oxidation of furfural over the meso-PA/PmPD/GO electrocatalyst in the ternary electrolyte **(b)** using D_2O as solvent.

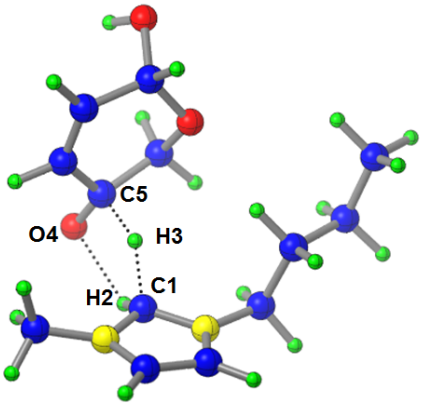


Supplementary Fig. S13 The microscopic mechanism of the electrochemical oxidation of furfuryl alcohol **(a)** and furfural **(b)**.



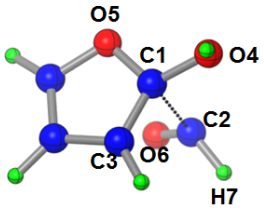
C1-H2 1.10
C1-H3 1.41
O4-H2 2.14
C5-H3 1.42
O4-C5 1.28

TS1-1a



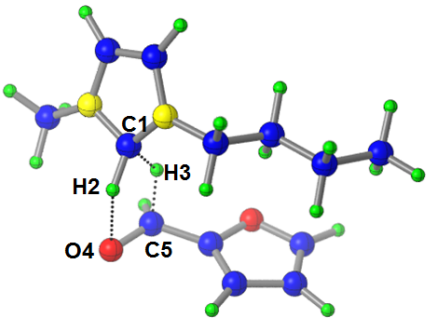
C1-H2 1.11
C1-H3 1.42
O4-H2 2.03
C5-H3 1.44
O4-C5 1.28

TS1-1b



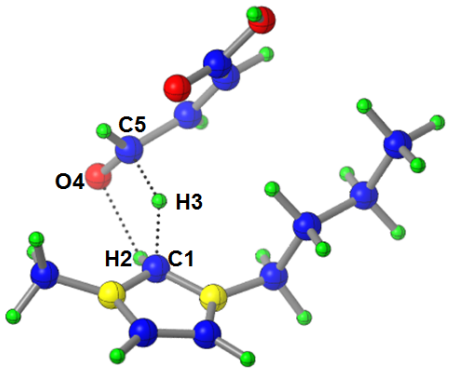
C1-C2 2.15
C1-C3 1.39
C1-O4 1.35
C1-O5 1.38
O6-C2-H7 125.60
C1-O5-C3-O4 10.81

TS3-1



C1-H2 1.11
C1-H3 1.42
O4-H2 2.00
C5-H3 1.45
O4-C5 1.28

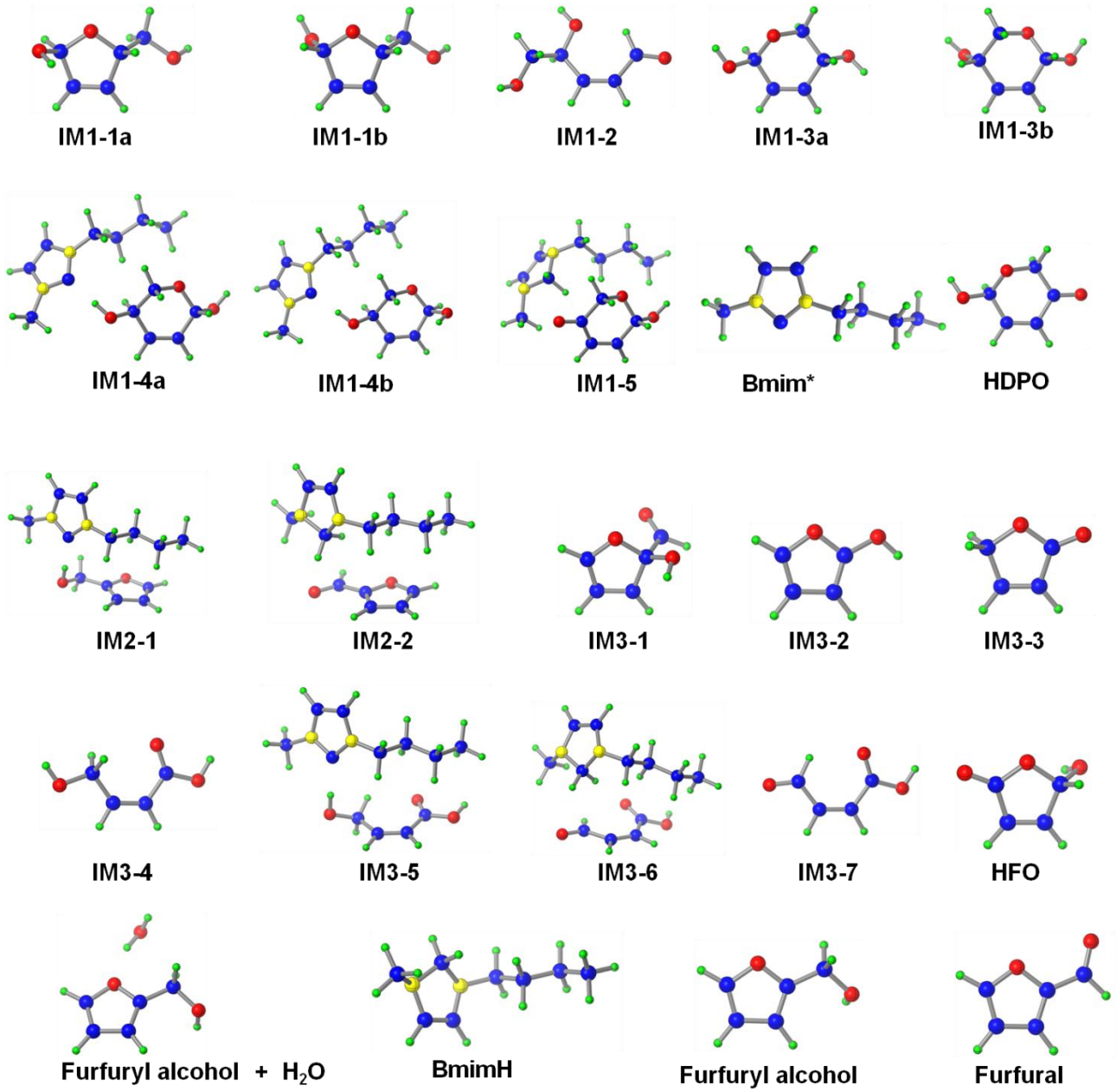
TS2-1



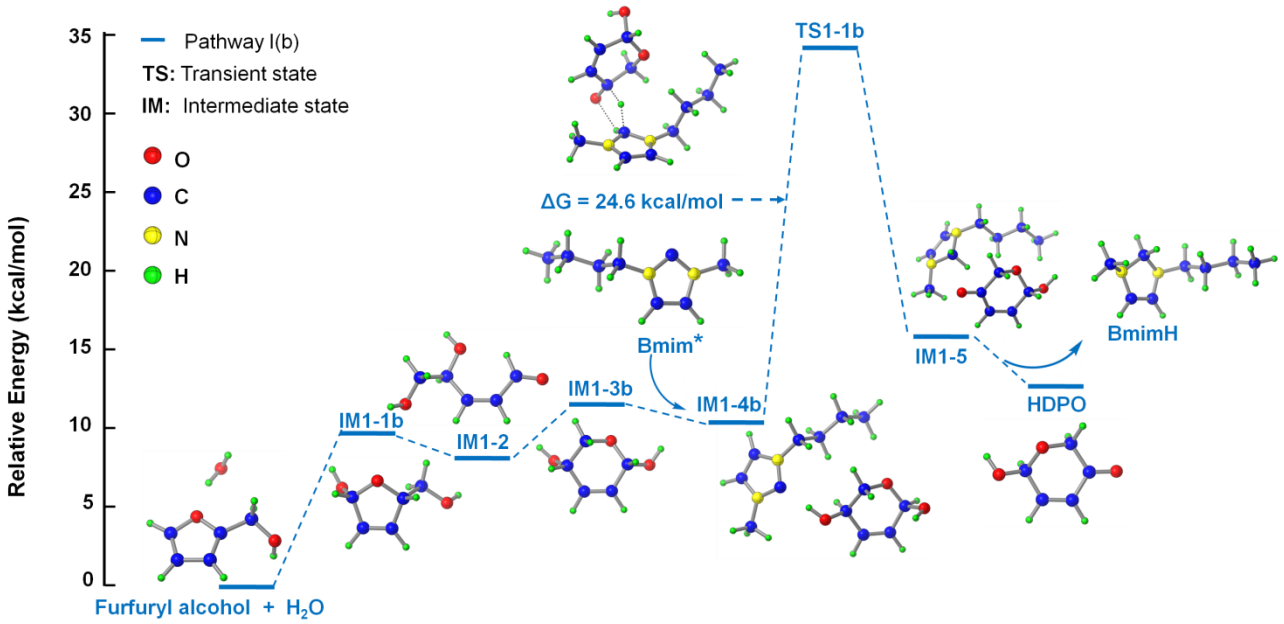
C1-H2 1.11
C1-H3 1.43
O4-H2 2.01
C5-H3 1.44
O4-C5 1.28

TS3-2

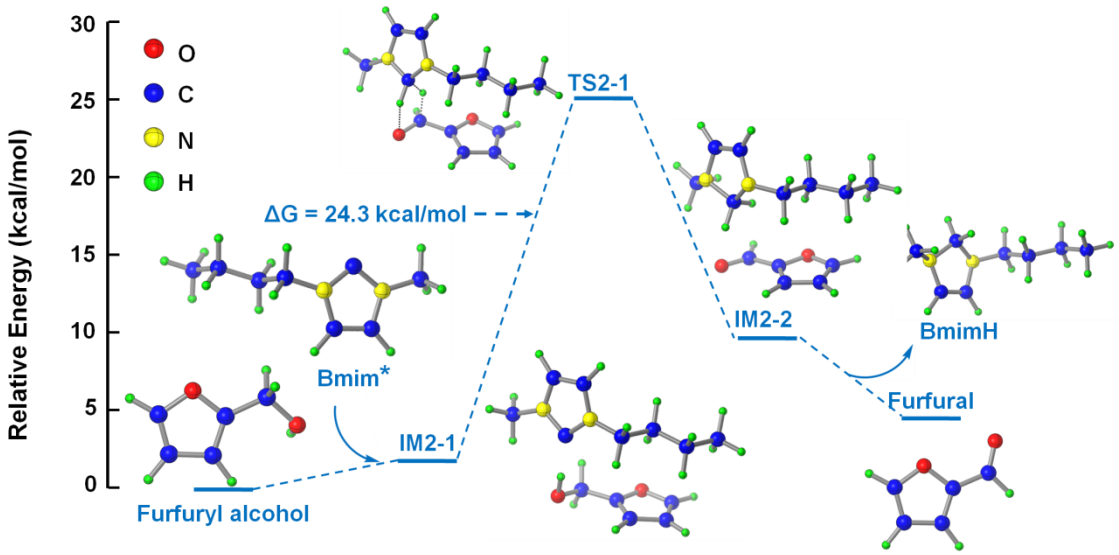
Supplementary Fig. S14 3D structure of transition states (TS) in the process of electrochemical oxidation furfuryl alcohol and furfural. The bond distances are given in Å.



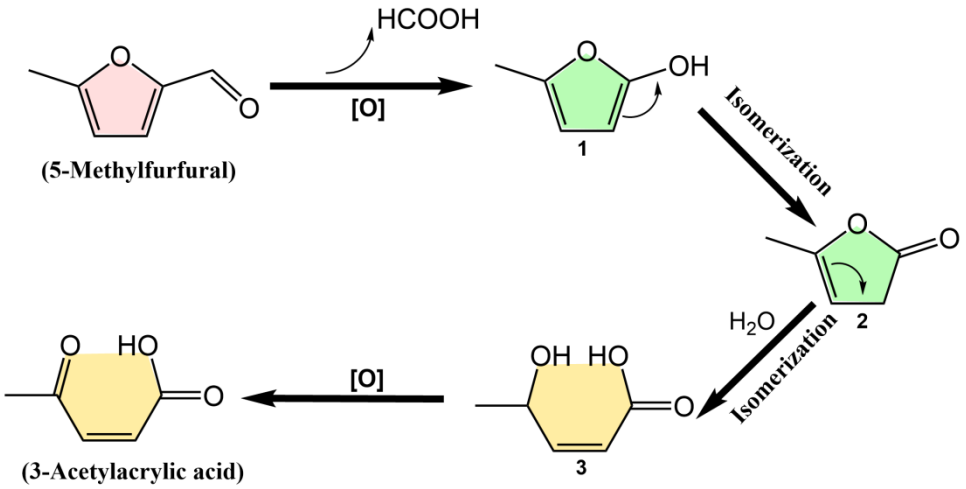
Supplementary Fig. S15 DFT Optimized geometries of the species involved in the catalytic process.



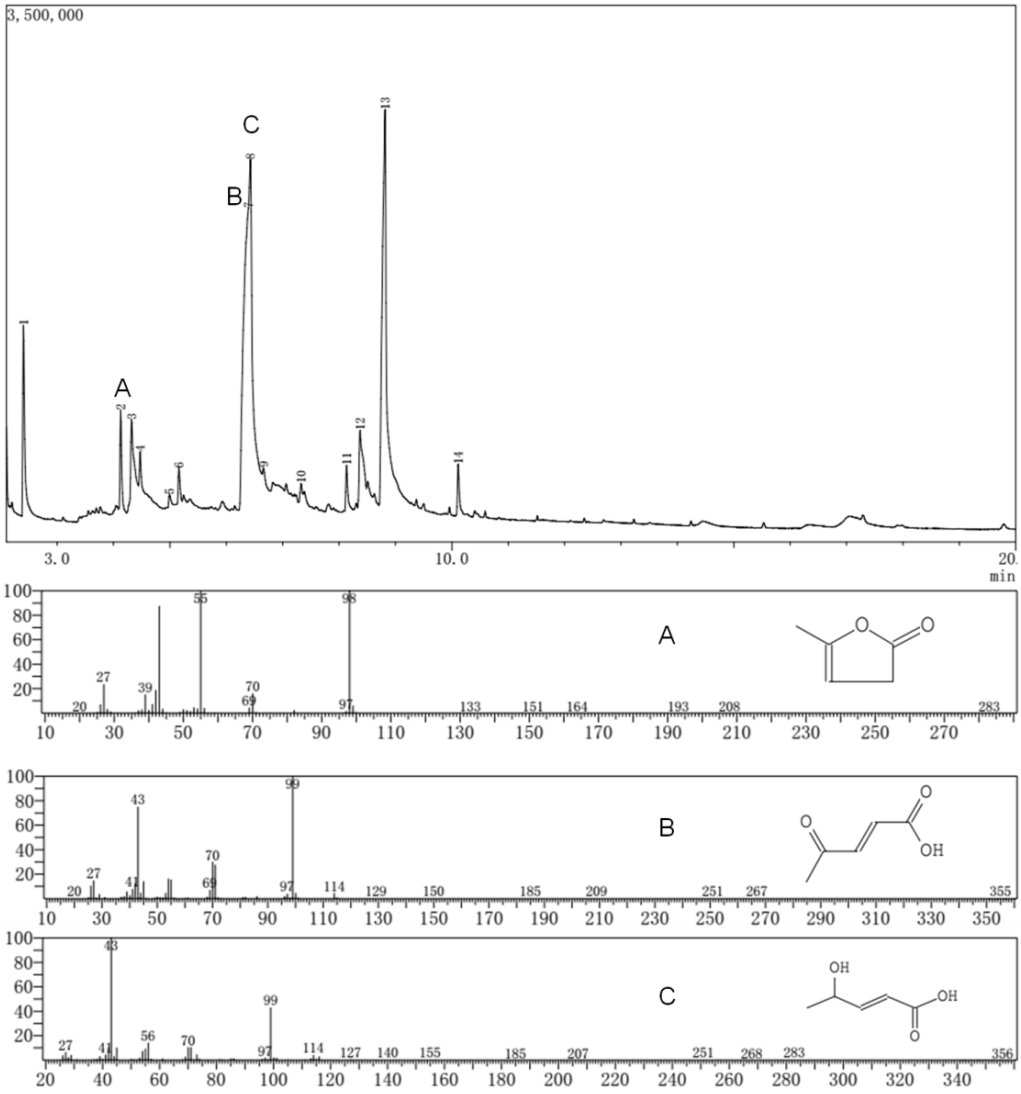
Supplementary Fig. S16 DFT calculation result for the electrochemical oxidation of furfuryl alcohol to HDPO in the ternary electrolyte.



Supplementary Fig. S17 DFT calculation result for the electrochemical oxidation of furfuryl alcohol to furfural in the ternary electrolyte.

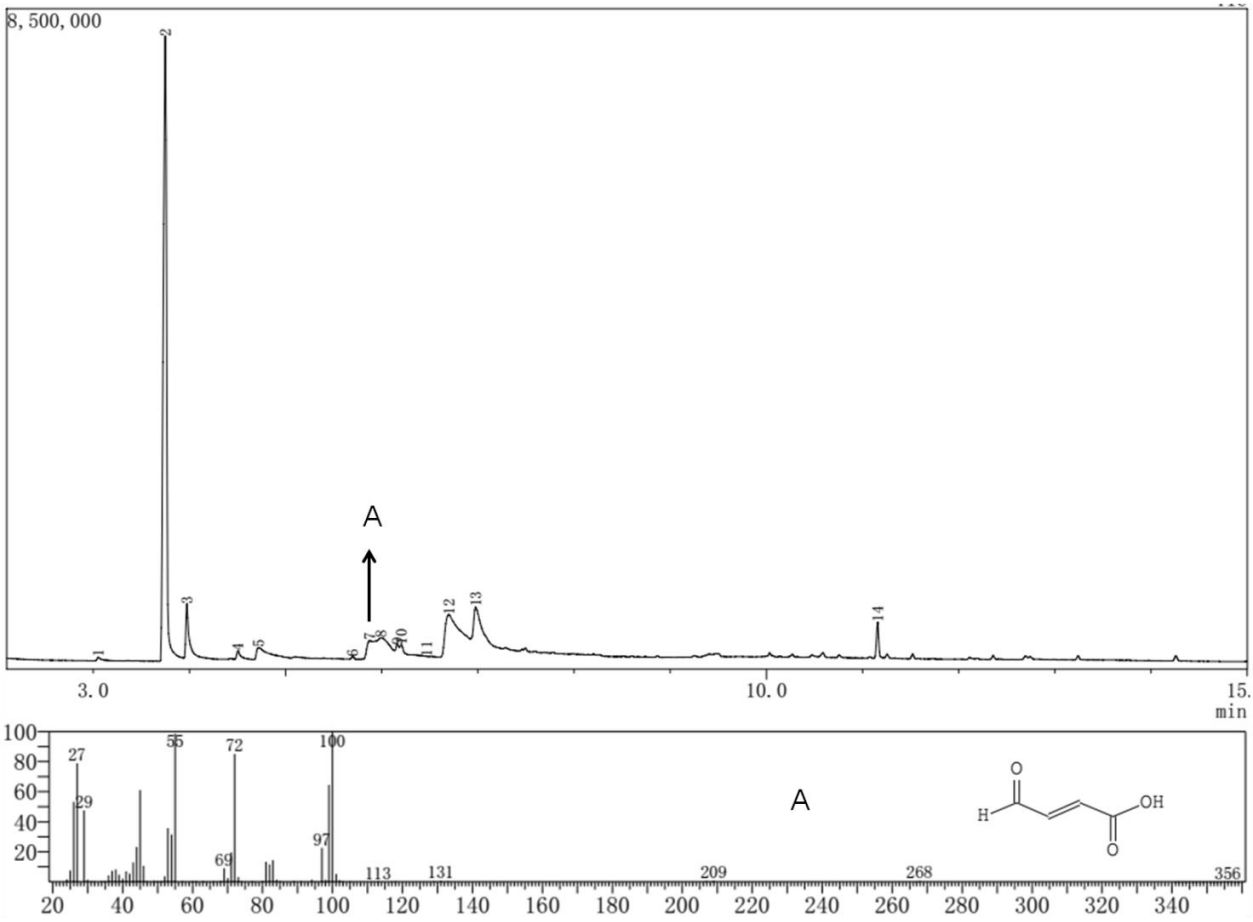


Supplementary Fig. S18 The reaction pathway for the electrochemical oxidation of 5-methylfurfural over the meso-PA/PmPD/GO electrocatalyst in the ternary electrolyte.

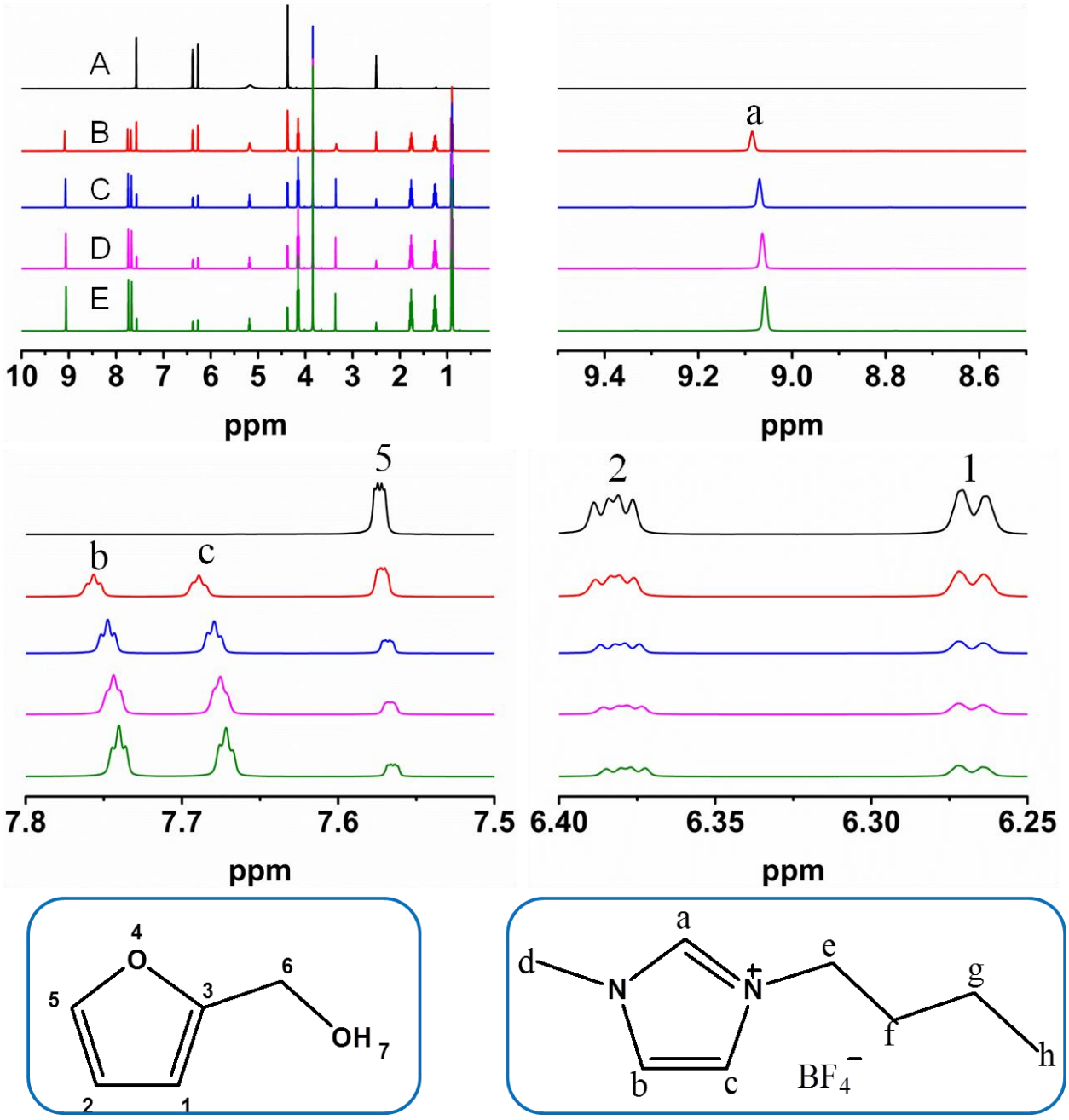


Supplementary Fig. S19 GC-MS spectra of the electrolyte after the electrochemical oxidation of 5-methylfurfural over the meso-PA/PmPD/GO electrocatalyst in the ternary electrolyte.

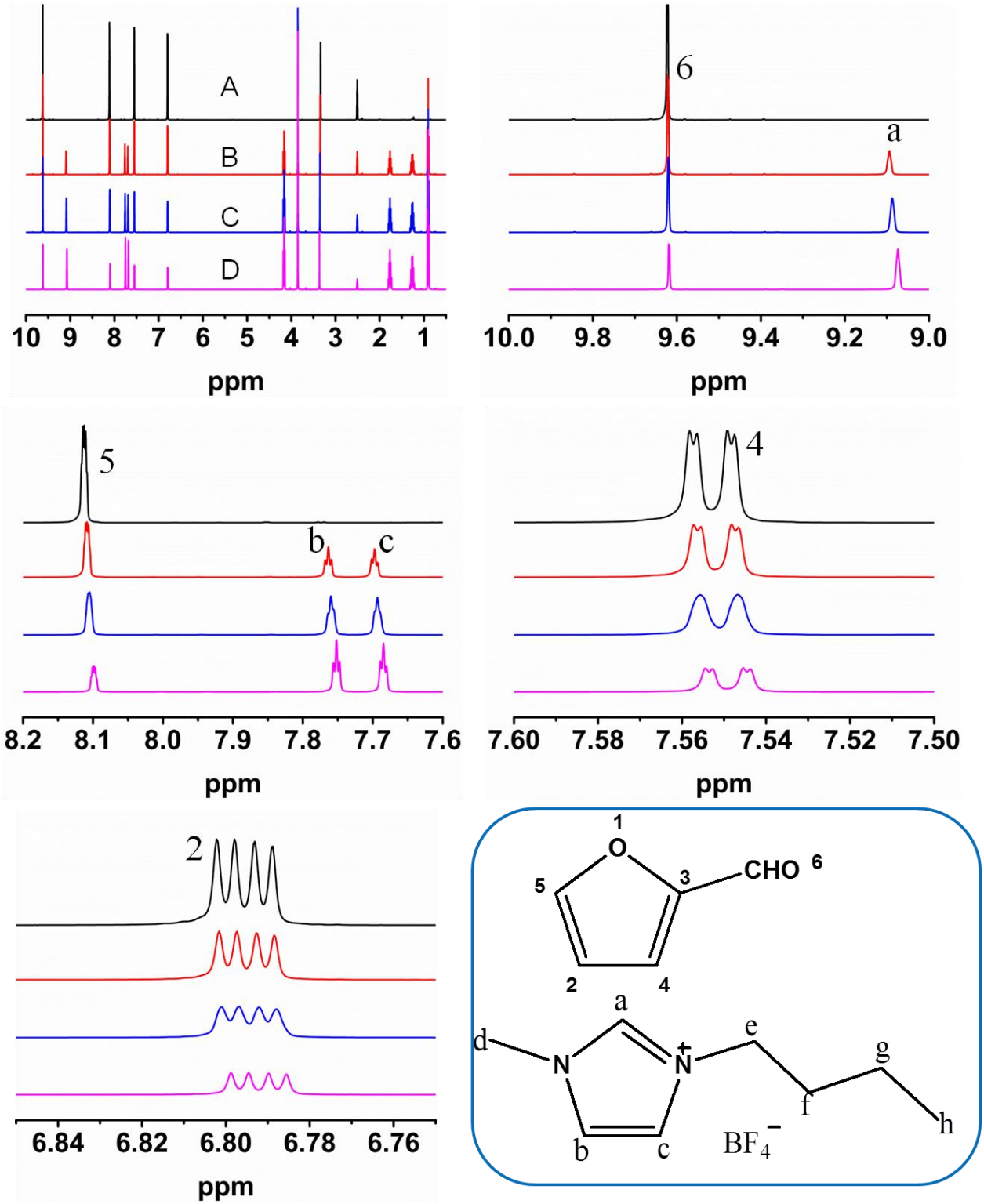
As shown in Supplementary Figs. S18 and S19, intermediates **2**, **3**, and 3-acetylacrylic acid were detected during the oxidation of 5-methylfurfural on the basis of GC-MS analyses. The results indicated that the aldehyde group in 5-methylfurfural could cleave to generate an intermediate **1** and HCOOH. Then, the unstable **1** rearranged to **2**. Afterwards, compound **3** was formed by ring opening and isomerization of **2**. Finally, 3-acetylacrylic acid was formed *via* the oxidation of **3**.



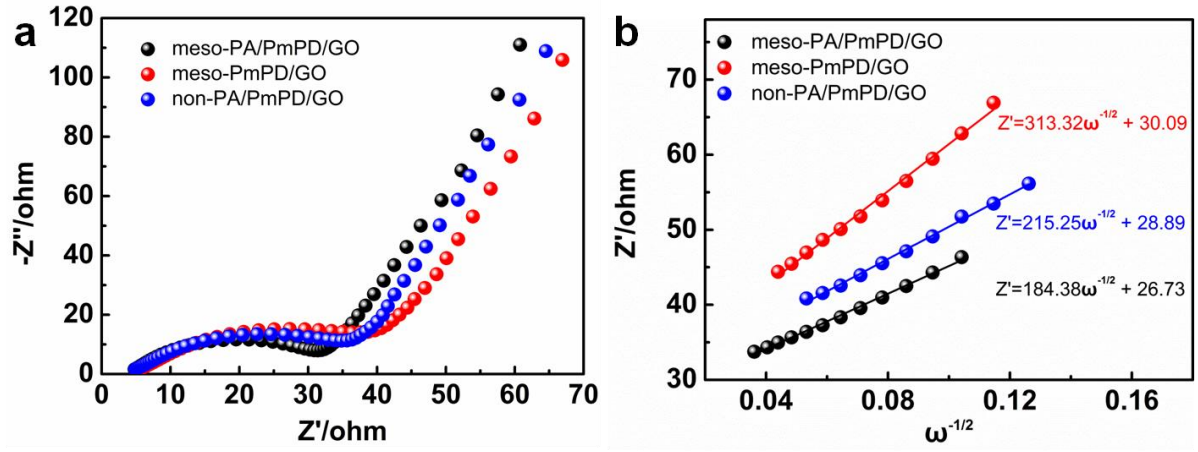
Supplementary Fig. S20 GC-MS spectra of the electrolyte after the electrochemical oxidation of furfural over the meso-PA/PmPD/GO electrocatalyst in the ternary electrolyte.



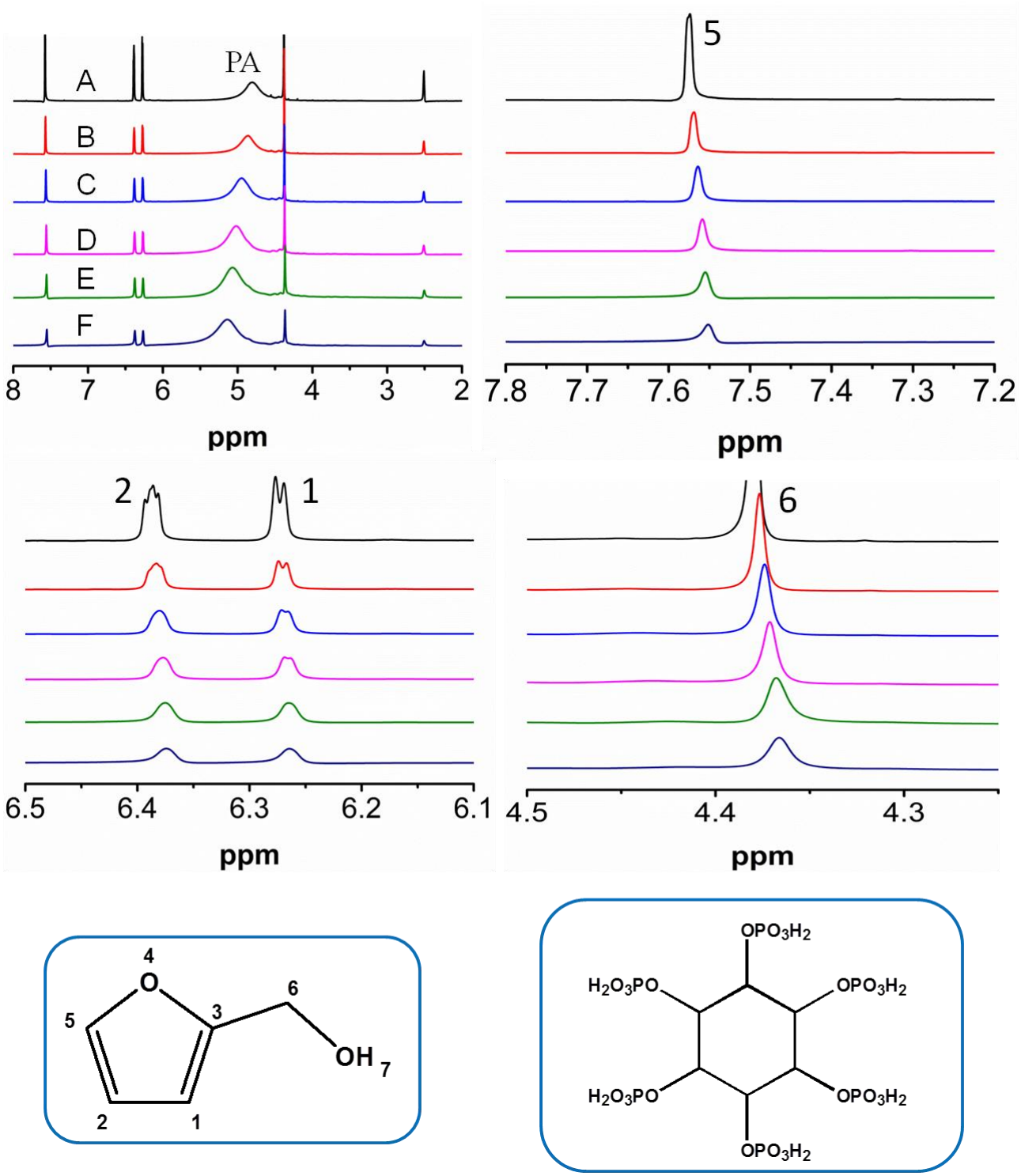
Supplementary Fig. S21 ^{1}H NMR spectra of the mixture of $BmimBF_4$ and furfuryl alcohol (The amount of furfuryl alcohol was 7 uL in all samples, and the amount of $BmimBF_4$ was 0, 7 μL, 21 μL, 28 μL, and 35 μL in A, B, C, D, and E, respectively. DMSO-d_6 was used as solvent).



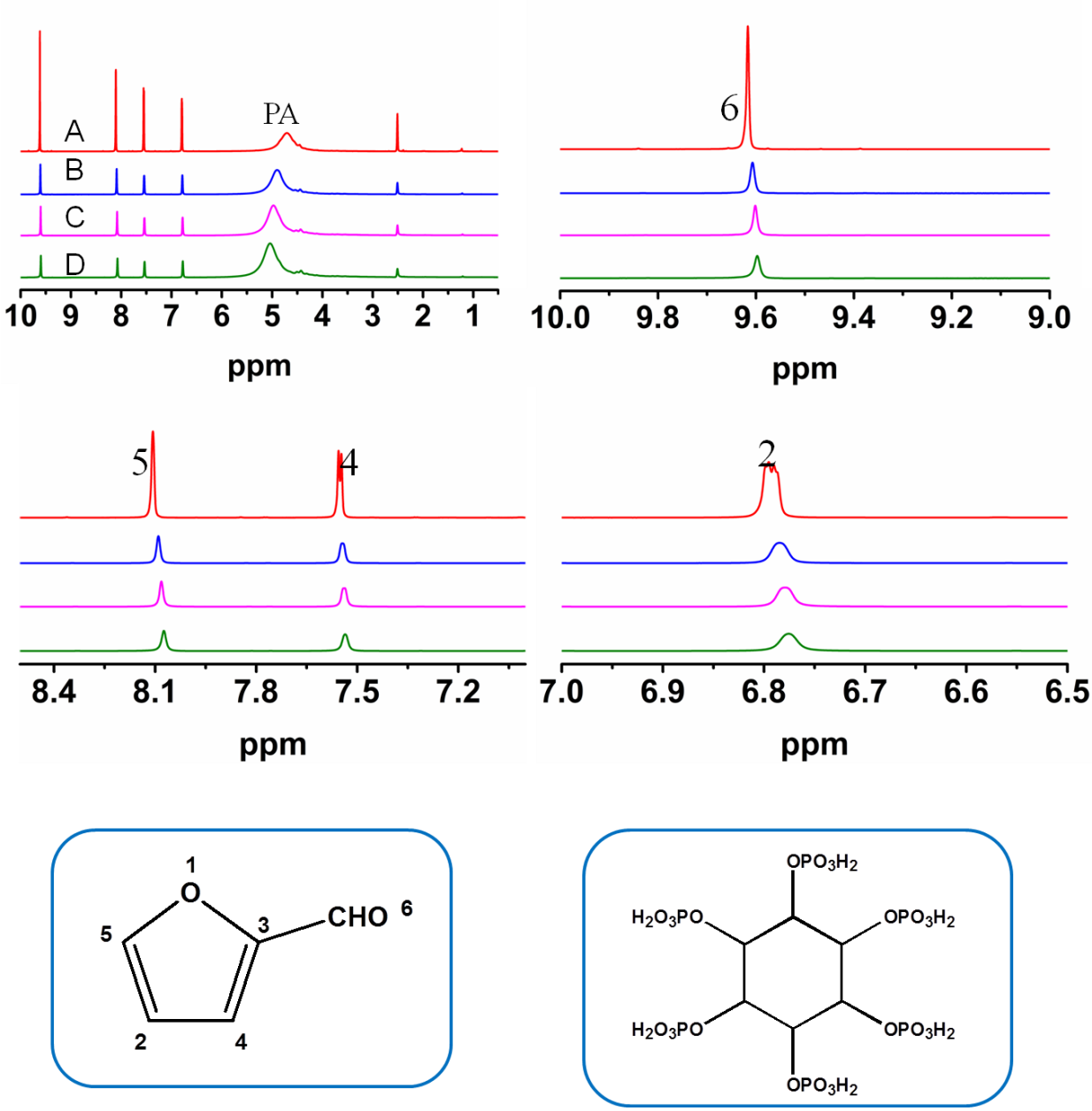
Supplementary Fig. S22 ^{1}H NMR spectra of the mixture of $BmimBF_4$ and furfural (The amount of furfural was 7 uL in all samples, and the amount of $BmimBF_4$ was 0, 7 μL, 14 μL, and 28 μL in A, B, C, and D, respectively. DMSO-d_6 was used as solvent).



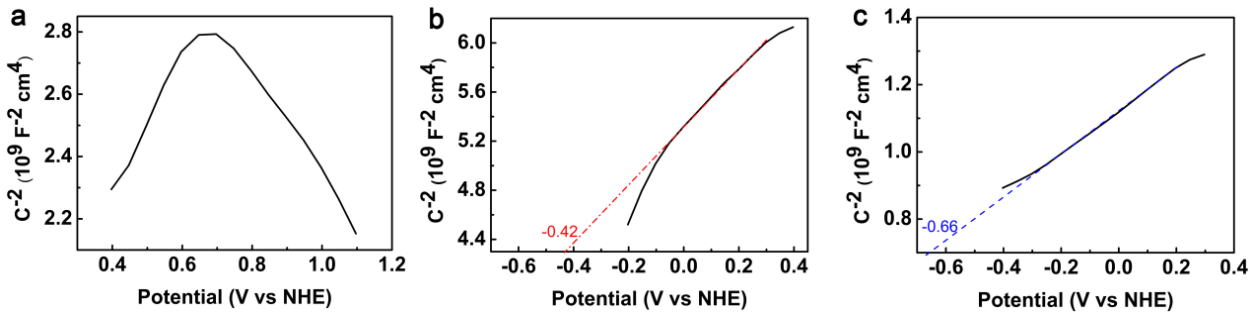
Supplementary Fig. S23 (a) EIS spectra. **(b)** Variations and fittings between Z' and the reciprocal square root of the angular frequency (ω) in the low frequency region of meso-PA/PmPD/GO, meso-PmPD/GO, and non-PA/PmPD/GO in the mixture of furfural and the ternary electrolyte, respectively.



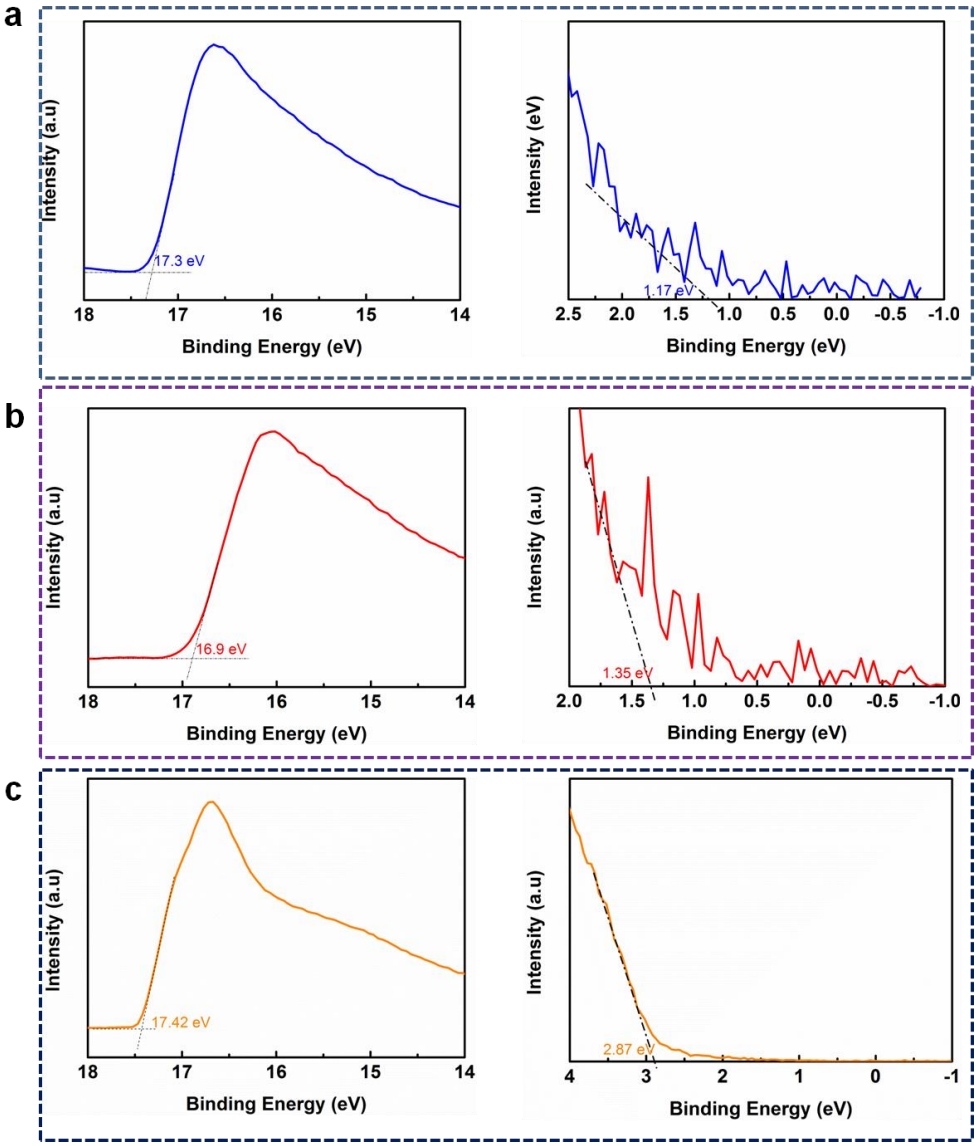
Supplementary Fig. S24 ^{1}H NMR spectra of the mixture of furfuryl alcohol and PA (The amount of furfuryl alcohol was 7 uL in all samples, and the amount of PA was 7 µL, 14 µL, 21 uL, 28uL, 35uL, and 42 µL in A, B, C, D, E, and F, respectively. DMSO-d_6 was used as solvent).



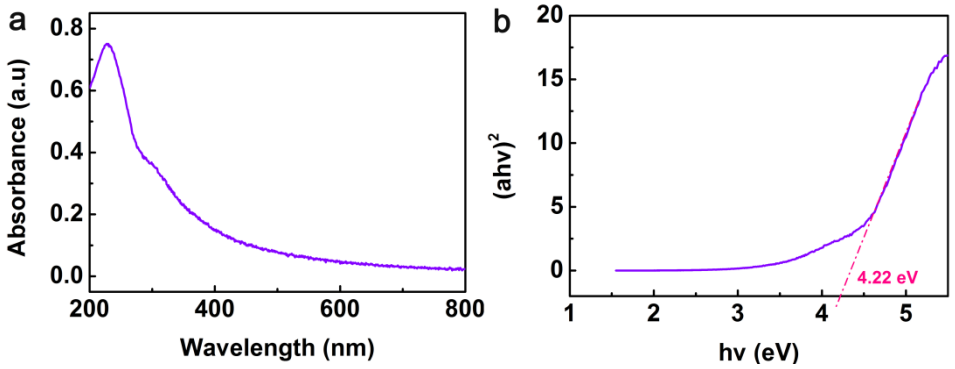
Supplementary Fig. S25 ^{1}H NMR spectra of the mixture of furfural and PA (The amount of furfural was 7 uL in all samples, and the amount of PA was 7 μL, 21 uL, 28uL, and 35uL in A, B, C, and D, respectively. DMSO-d_6 was used as solvent).



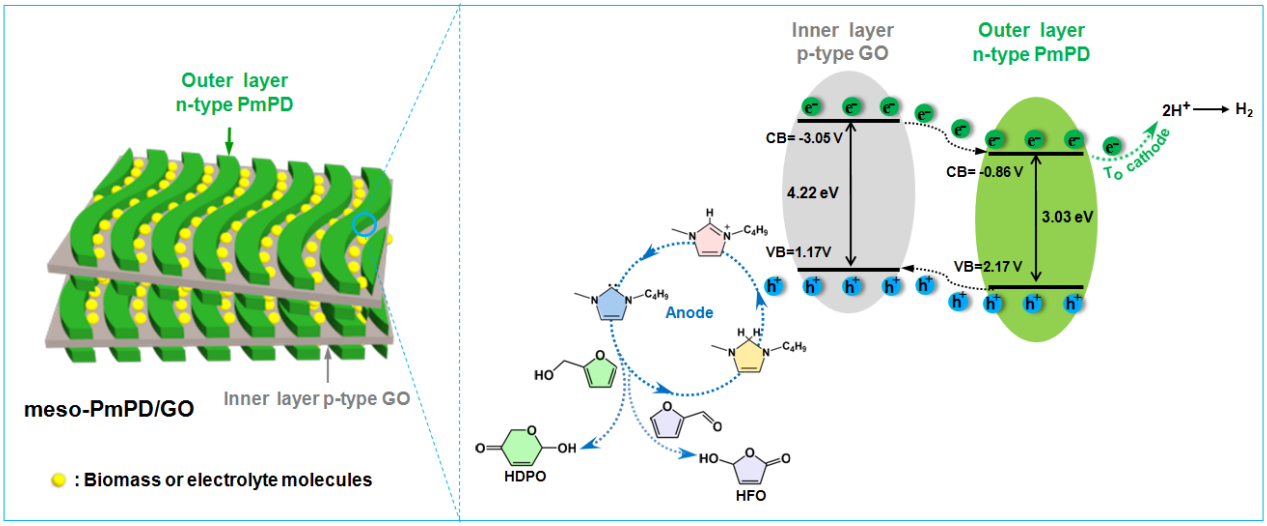
Supplementary Fig. S26 Mott-Schottky curve of meso-PA/PmPD/GO **(a)**, PA/PmPD **(b)**, and PmPD **(c)**.



Supplementary Fig. S27 UPS spectra of PA/PmPD **(a)**, GO **(b)** and PmPD **(c)**.



Supplementary Fig. S**28** UV-Vis absorption spectra of GO **(a)** and the corresponding Tauc plot **(b)**.



Supplementary Fig. S29 Schematic diagram of the charge transfer and separation at the p-n heterojunction interface of the meso-PmPD/GO nanosheets without the PA doping. The generated holes on the outer PmPD layers move to the inner GO layers and thus are shielded by the PmPD layers. This situation is not beneficial to the transform of BmimH back to $Bmim^{+}$.

Supplementary Table S1. Electrochemical oxidation of furfuryl alcohol over the meso-PA/PmPD/GO electrocatalyst in different aqueous inorganic salt electrolytes.

Electrolytes	Potential (V vs NHE)	Con. (%)	$HDPO_{FE\%}$	$HDPO_{Sel.\%}$	$furfural_{FE\%}$	$furfural_{Sel.\%}$
0.5M KH_2PO_4	1.7	8.4	<2	<2	3.3	12.6
	1.8	26.3	17.1	58.6	2.8	9.8
	1.9	34.0	17.6	52.9	7.2	21.6
0.5M $NaNO_3$	1.7	27.5	14.4	31.7	13.5	29.8
	1.8	42.8	50.5	22.9	8.5	18.7
	1.9	56.3	21.6	41.7	4.5	8.8
0.5M $(NH_4)_2SO_4$	1.7	15.5	6.3	12.4	16.0	31.3
	1.8	39.6	23.5	38.2	13.8	22.5
	1.9	52.5	39.2	73.3	2.5	4.6

Supplementary Table S2. Electrochemical oxidation of furfural to HFO over the meso-PA/PmPD/GO electrocatalyst in different aqueous inorganic salt electrolytes.

Electrolytes	Potential (V vs NHE)	Con. (%)	$HFO_{FE\%}$	$HFO_{Sel.\%}$
0.5M KH_2PO_4	1.8	9.7	26.9	70.1
	1.9	25.5	48.5	69.3
	2.0	37.1	59.9	74.6
0.5M $NaNO_3$	1.8	21.3	33.2	55.4
	1.9	36.7	51.7	66.1
	2.0	43.5	43.1	65.2
0.5M $(NH_4)_2SO_4$	1.8	10.3	15.2	51.7
	1.9	18.8	27.9	63.6
	2.0	30.1	36.8	69.7

Supplementary Table S3. DFT calculated energy profile

Intermediate State	Single Point Energy	Gibbs Free Energy
Furfuryl alcohol + H_2O	-421.138305	-421.047486
IM1-1a	-421.129794	-421.032758
IM1-1b	-421.128649	-421.031785
IM1-2	-421.125216	-421.032828
IM1-3a	-421.128453	-421.029736
IM1-3b	-421.127503	-421.028986
IM1-4a	-844.059415	-843.765464
IM1-4b	-844.061872	-843.768541
TS1-1a	-843.727455	-843.727455
TS1-1b	-844.019225	-843.729259
IM1-5	-844.047158	-843.757655
HDPO	-419.924024	-419.848284
Furfuryl alcohol	-344.673569	-344.60157
IM2-1	-767.605132	-767.33702
TS2-1	-767.560907	-767.298356
IM2-2	-767.323393	-767.323393
Furfural	-343.465932	-343.416087
IM3-1	-419.272939	-419.213052
TS3-1	-419.235793	-419.179509
IM3-2	-305.348028	-305.302082
IM3-3	-305.375375	-305.328934
IM3-4	-381.83429	-381.766736
IM3-5	-804.767409	-804.504955
TS3-2	-804.721414	-804.462933
IM3-6	-804.741592	-804.479246
IM3-7	-380.61911	-380.574461
HFO	-380.623552	-380.574094

Coordinates of DFT-computed stationary points

Furfuryl alcohol+H_2O:

C	0.98756600	1.16555500	-0.24460500
H	1.32657600	1.16069600	-1.28523000
C	-0.27626800	0.37717800	-0.11312800
C	-1.58258700	0.72466100	0.02082900
O	-0.16189400	-0.99016500	-0.12809600
C	-2.32931500	-0.50362100	0.09186600
H	-1.96865800	1.73045800	0.05918200
C	-1.42814200	-1.51061000	-0.00405600
H	-3.39731600	-0.61148900	0.20109500
H	-1.49603500	-2.58572100	-0.00239500
H	1.77575100	0.68998800	0.35089200
O	0.79100400	2.52854200	0.10422600
H	0.56103600	2.55437900	1.04173100
O	2.65941200	-1.70168600	0.22920900
H	2.96590900	-1.45975300	-0.65280800
H	1.69703500	-1.69105400	0.13937500

IM1-1a:

C	-1.58320600	-0.73748900	-0.16926600
H	-1.77979400	-1.67248200	0.36985500
C	-0.63688000	0.12007100	0.66686800
C	-0.15402900	1.35447400	-0.03948200
O	0.56197900	-0.61859400	0.95752300
C	1.15395400	1.27081100	-0.25025600
H	-0.81757700	2.15415300	-0.33841300
C	1.66606400	-0.04847800	0.25465000
H	1.79071100	1.98209200	-0.75835600
H	-1.09502100	-0.98031300	-1.12138800
O	-2.77901400	0.01488600	-0.36377500
H	-3.37980400	-0.52261300	-0.89144100
H	-1.12767400	0.35961200	1.61687000
H	2.49782800	0.02490200	0.96341600
O	2.05620500	-0.83312900	-0.85623200
H	2.52255500	-1.60699100	-0.51575600

IM1-1b:

C	1.84834900	-0.58917700	0.33573700
H	2.02669300	-1.66320400	0.20149200
C	0.59381600	-0.19672500	-0.43671900
C	0.14709400	1.21528900	-0.19394000
O	-0.49557700	-1.00906800	0.03135700
C	-1.06415300	1.21800100	0.35033900
H	0.76304100	2.07043600	-0.43601800
C	-1.58940500	-0.18870500	0.45191300
H	-1.65547400	2.07404100	0.64681600
H	1.68407100	-0.39274700	1.40295400
O	2.92401000	0.18851100	-0.18528300
H	3.72012900	-0.04913100	0.30252800
H	0.77109500	-0.38411900	-1.50371300
O	-2.73916200	-0.41146100	-0.33384300
H	-1.88218600	-0.49140800	1.46027000
H	-2.55573300	-0.05983000	-1.21615800

IM1-2:

C	-2.15228200	0.27493900	0.43692400
H	-2.71858200	1.21004800	0.33473600
C	-0.86736500	0.40513900	-0.39500400
C	-0.01317200	-0.80928000	-0.23317300
O	-0.17874900	1.59373700	-0.02786000
C	1.30924700	-0.94057000	-0.03852200
H	-0.60247800	-1.72007700	-0.29033300
C	2.32046000	0.12141400	0.03062600
H	1.71822600	-1.94314400	0.06088900
H	-1.88421500	0.14366400	1.49187800
O	-2.89492600	-0.83186700	-0.06439000
H	-3.60334300	-1.01996000	0.56108300
H	-1.17181900	0.44212500	-1.45284400
H	1.96777000	1.15506200	-0.08892700
O	3.50372100	-0.12689800	0.20109100
H	-0.72726800	2.34266700	-0.29230400

IM1-3a:

C	-0.66035900	-1.13028500	-0.61754100
C	-0.65939900	1.33177100	-0.25541900
C	0.66867500	1.26347000	-0.24019000
C	1.39692500	-0.05237300	-0.26478200
H	-1.17241100	2.28719200	-0.21099400
H	-0.43670900	-1.16059900	-1.69428900
H	1.29002900	2.15299000	-0.22549800
O	0.55149400	-1.12433100	0.13483200
H	-1.19315800	-2.04391200	-0.35016800
H	1.75944000	-0.26217000	-1.28727400
O	2.46851000	0.02049500	0.62965500
H	2.99155300	-0.78352800	0.51797400
C	-1.51788200	0.09784800	-0.31393100
O	-2.19911800	-0.00019600	0.94697600
H	-2.25291200	0.20985100	-1.12219100
H	-2.92068200	-0.63016400	0.83191300

IM1-3b:

C	0.62619300	-1.20608500	0.16229000
C	0.64931400	1.25187400	-0.16014300
C	-0.63051600	1.25724000	0.20322400
C	-1.40977400	-0.01785600	0.36571600
H	1.20142700	2.18049300	-0.27994600
H	0.72264000	-1.19217000	1.25697600
H	-1.16642500	2.17542200	0.42021400
O	-0.74055900	-1.12659400	-0.23073600
H	1.01104400	-2.15544400	-0.21016100
H	-1.54741000	-0.23742800	1.43843900
O	-2.64860800	0.13405100	-0.26440600
H	-3.18463700	-0.63599000	-0.03551900
C	1.40871700	-0.02690300	-0.40718300
O	2.67648800	-0.02233900	0.25947400
H	1.55336900	-0.16847500	-1.48645200
H	3.24782400	0.60303600	-0.20163000

IM1-4a:

C	1.82807300	-0.10915300	0.76099000
C	2.15404100	-2.11368900	-0.63166100
C	3.41387700	-1.71974600	-0.81067800
C	3.89254300	-0.34864000	-0.40924900
H	1.82645200	-3.10839100	-0.92022300
H	2.27264600	-0.54484800	1.66508200
H	4.16552100	-2.37824200	-1.23394700
O	2.82891700	0.51691600	-0.05138100
H	1.13774500	0.67720300	1.06221300
H	4.39232500	0.15257700	-1.23967400
O	4.87653400	-0.43687900	0.61193300
H	4.57245000	-1.08948200	1.25592900
C	1.11690700	-1.21550000	-0.01535500
O	0.26754500	-1.96107200	0.83684200
C	-4.31742100	-0.53171500	-0.51411700
C	-3.90286000	0.71014200	-0.15844200
C	-2.25756500	-0.74951600	0.43670300
N	-3.29927800	-1.39945800	-0.14497800
H	-5.22774800	-0.86962500	-0.98047400
H	-4.37731100	1.67185300	-0.26060600
N	-2.65248100	0.55167300	0.42168500
C	-1.80410200	1.66012300	0.86140100
H	-2.45123200	2.43987100	1.26867000
H	-1.17611900	1.28658100	1.67104200
C	-3.34527000	-2.84297400	-0.34014500
H	-2.36714500	-3.24917900	-0.09022600
H	-4.10265500	-3.29422000	0.30421600
H	-3.57673400	-3.07286800	-1.38148300
C	-0.93559300	2.20782200	-0.26955400
H	-1.57858000	2.57462300	-1.07728600
H	-0.34586400	1.38320100	-0.68159800
C	-0.00005700	3.32242100	0.20148400
H	-0.59247300	4.19062000	0.51246600
H	0.54344500	2.98313900	1.09092700
C	1.00441300	3.73228200	-0.87579800
H	0.49531000	4.06270000	-1.78708600
H	1.64387400	4.55190700	-0.53514200
H	1.65155500	2.88944900	-1.13662500
H	0.52851400	-0.75528000	-0.82451800
H	-0.63754000	-1.52995900	0.78877700

IM1-4b:

C	1.68640200	-0.40640200	1.11982000
C	1.96042800	-2.27028500	-0.46973100
C	3.25557700	-1.96496000	-0.51972700
C	3.80206300	-0.69551100	0.07401600
H	1.58146400	-3.19383100	-0.89819600
H	2.03961600	-0.97298300	1.99256400
H	3.98732000	-2.62807400	-0.96964700
O	2.77663200	0.22078700	0.44361600
H	1.03224300	0.39278300	1.46603300
H	4.39214300	-0.93090200	0.97646200
O	4.61345800	-0.07013100	-0.88278000
H	5.05905700	0.66563700	-0.44348900
C	0.95162200	-1.36569600	0.18232100
O	-0.01287300	-2.11963300	0.89441600
C	-4.30659000	-0.11266300	-0.69768900
C	-3.75141500	1.06768500	-0.32524000
C	-2.36299200	-0.59079100	0.39399100
N	-3.44220500	-1.10334200	-0.25326300
H	-5.22067300	-0.33145300	-1.22414000
H	-4.08195500	2.08285200	-0.46890200
N	-2.57539500	0.75220400	0.34025500
C	-1.61791500	1.74689100	0.82732700
H	-2.18189800	2.60886600	1.19050500
H	-1.09587200	1.30457600	1.67630900
C	-3.66972200	-2.53053600	-0.44110300
H	-2.76095200	-3.05867100	-0.15919500
H	-4.49860600	-2.87420800	0.18142200
H	-3.89760400	-2.73764800	-1.48790400
C	-0.61681100	2.16425600	-0.24926600
H	-1.15399900	2.61192200	-1.09274100
H	-0.12442200	1.26462800	-0.62899900
C	0.43901800	3.13918000	0.27481300
H	-0.03707800	4.09337300	0.52835100
H	0.86115100	2.74532800	1.20638900
C	1.56979200	3.36566400	-0.73008300
H	1.18393500	3.74093200	-1.68374900
H	2.29544500	4.09385600	-0.35512300
H	2.10238400	2.42951600	-0.92001100
H	0.45277500	-0.77834400	-0.60224200
H	-0.86575400	-1.59936800	0.82864900

TS1-1a:

C	1.54752100	-0.46999300	1.08480000
C	0.73922500	-2.49468000	-0.13481300
C	1.75494000	-2.32739300	-0.98952600
C	2.62972200	-1.10442800	-0.95890100
H	0.12250600	-3.38836900	-0.15991900
H	2.34334000	-0.90079000	1.71033500
H	2.01150700	-3.07703900	-1.73143300
O	2.07501300	-0.05637100	-0.18174300
H	1.17995000	0.42880400	1.58057700
H	2.74065100	-0.67411400	-1.95551800
O	3.95169000	-1.43181700	-0.55075400
H	3.88278900	-2.05629200	0.18294400
C	0.43180200	-1.50547100	0.94315000
O	-0.17393600	-1.88032600	2.00714400
C	-3.33056700	-0.12583200	-1.19117600
C	-2.90888700	1.13301400	-0.92614700
C	-1.84662300	-0.25272600	0.51247000
N	-2.74972400	-0.96788800	-0.25155300
H	-4.00956400	-0.49761400	-1.93954300
H	-3.14973500	2.06897600	-1.40048400
N	-2.06371000	1.06915300	0.17753500
C	-1.26977700	2.17370100	0.70107100
H	-1.92958300	3.03519200	0.83134400
H	-0.91798500	1.87351400	1.69041400
C	-2.82166500	-2.41587800	-0.23811600
H	-2.50389500	-2.76892000	0.74263800
H	-3.84654600	-2.73426200	-0.43085400
H	-2.16034800	-2.84869000	-0.99468800
C	-0.08531100	2.52658400	-0.20042800
H	-0.46343000	2.91215600	-1.15402600
H	0.47898900	1.61744300	-0.42142300
C	0.84516500	3.55573000	0.44375200
H	0.29872400	4.48969900	0.62101600
H	1.15771600	3.18784900	1.42840300
C	2.08395900	3.83173400	-0.40845900
H	1.80687200	4.21339800	-1.39652000
H	2.73779800	4.57094500	0.06345900
H	2.66248600	2.91459800	-0.55480800
H	-0.52964800	-0.69933700	0.23002600
H	-1.65770700	-0.57406400	1.55295300

TS1-1b:

C	0.92733200	-1.29602700	1.43728600
C	-0.40380900	-2.52705600	-0.28938300
C	0.74341800	-2.76096600	-0.93446700
C	2.03851700	-2.12876000	-0.50733400
H	-1.33147000	-2.99853900	-0.60087600
H	1.29286700	-2.12426100	2.06453500
H	0.80366900	-3.43762200	-1.78117000
O	1.84258100	-1.02853800	0.37545200
H	0.88768900	-0.39594100	2.05231200
H	2.67400300	-2.87252000	0.00347700
O	2.69252000	-1.64153400	-1.64911500
H	3.57815000	-1.36688400	-1.37895600
C	-0.47155900	-1.66752000	0.93509200
O	-1.37272200	-1.87240300	1.82266600
C	-2.89029500	1.36233700	-1.31135400
C	-1.95518700	2.27322300	-0.95569600
C	-1.80971700	0.55050900	0.50306300
N	-2.86442200	0.34406200	-0.36711200
H	-3.58966200	1.35446600	-2.13010200
H	-1.67751500	3.20871100	-1.41023500
N	-1.34989000	1.82283100	0.21489500
C	-0.13163800	2.38096700	0.79153200
H	-0.28391900	3.45264400	0.94299800
H	-0.00431500	1.92243500	1.77430000
C	-3.62939300	-0.88790600	-0.41642000
H	-3.48887400	-1.41211200	0.52814900
H	-4.68565500	-0.66377600	-0.57380400
H	-3.27466200	-1.53454500	-1.22455300
C	1.09426400	2.11932700	-0.08670600
H	0.98601900	2.67756400	-1.02349000
H	1.12924400	1.05699800	-0.33793400
C	2.40380100	2.50613800	0.60064300
H	2.39126400	3.57281300	0.85552200
H	2.48279100	1.96093900	1.54829100
C	3.62423700	2.19369500	-0.26618100
H	3.59085100	2.74695400	-1.21051400
H	4.55600200	2.45857000	0.24235300
H	3.65997900	1.12688200	-0.50523900
H	-0.82615400	-0.44429000	0.30466200
H	-1.90896500	0.17528700	1.53331100

IM1-5:

C	1.47569800	-1.30920100	1.48945400
C	1.33698300	-2.39228900	-0.79771600
C	2.38398000	-1.63923200	-1.15357900
C	3.00340200	-0.66328100	-0.19323700
H	0.87829700	-3.10453400	-1.47429600
H	2.23712300	-1.83144200	2.09044400
H	2.84575000	-1.71985800	-2.13173400
O	2.05187800	-0.22517300	0.77031700
H	0.73029400	-0.89334300	2.16583100
H	3.83981500	-1.14916600	0.33915800
O	3.44617800	0.44531000	-0.91251700
H	3.90929200	1.02972500	-0.29773400
C	0.82119600	-2.33754900	0.57989300
O	-0.02902600	-3.10286400	1.00426700
C	-3.64617100	0.18961400	-0.84444400
C	-3.22053000	1.30726500	-0.24059400
C	-1.88994600	-0.39932300	0.50265000
N	-3.02410900	-0.94639100	-0.25824600
H	-4.43198100	0.06438600	-1.57380000
H	-3.57125000	2.32121200	-0.36053800
N	-2.29282600	0.98575400	0.77830800
C	-1.21949800	1.93173600	1.08654300
H	-1.68802500	2.85417200	1.44491900
H	-0.65369200	1.51939200	1.92808100
C	-2.66881300	-2.04887800	-1.13941500
H	-2.28652800	-2.88383500	-0.54895400
H	-3.55433100	-2.38430500	-1.68279100
H	-1.89270800	-1.76257200	-1.86913200
C	-0.26459600	2.25900800	-0.06763100
H	-0.83669800	2.70874800	-0.88771000
H	0.18161300	1.33752500	-0.45060000
C	0.85739200	3.20486300	0.36418200
H	0.42462600	4.10923900	0.80957500
H	1.44390300	2.71813300	1.15148500
C	1.78167200	3.59300600	-0.79041100
H	1.23034200	4.11910800	-1.57678800
H	2.58864500	4.25121400	-0.45343700
H	2.23631100	2.70428900	-1.23646500
H	-0.96820500	-0.43610900	-0.11726800
H	-1.70090100	-0.96013200	1.42060900

HDPO:

C	0.70484300	-1.22937400	0.17274700
C	0.73828600	1.29038200	-0.07608300
C	-0.58364800	1.26883000	0.12669500
C	-1.32363400	-0.02508900	0.32312700
H	1.28856800	2.21416800	-0.21796900
H	0.72651600	-1.46869100	1.24831500
H	-1.17145600	2.17869600	0.18724400
O	-0.63270000	-1.10491800	-0.29611800
H	1.16904700	-2.04987200	-0.37314200
H	-1.40821300	-0.23591900	1.40418000
O	-2.57886600	0.08918800	-0.26791000
H	-3.08945000	-0.69263700	-0.02096100
C	1.51623500	0.04054300	-0.03425800
O	2.73312800	0.01354400	-0.09860100

Bmim*

C	-2.30993900	1.06856200	-0.43867100
C	-1.04549900	1.37008000	-0.05571700
C	-1.40533900	-0.83081500	0.46824100
N	-2.50316300	-0.26769100	-0.11358200
H	-3.07536500	1.67291700	-0.89677700
H	-0.48715300	2.28925300	-0.11858300
N	-0.52003000	0.20721100	0.49246000
C	0.85759300	0.09476100	0.96889800
H	1.08890100	0.98223400	1.56403500
H	0.89696900	-0.77309300	1.62783000
C	-3.75038900	-0.97518700	-0.36883500
H	-3.63191300	-2.00880700	-0.05089500
H	-4.57095000	-0.51843300	0.18888200
H	-3.98850500	-0.95183100	-1.43440000
C	1.86040800	-0.05476200	-0.17449400
H	1.76232600	0.79947100	-0.85381200
H	1.60495800	-0.95107300	-0.75073200
C	3.30276500	-0.15039300	0.32523100
H	3.54647900	0.75075900	0.90026500
H	3.38907800	-0.99391500	1.02011600
C	4.31021200	-0.31957500	-0.81207200
H	4.26508100	0.52411000	-1.50841800
H	5.33384000	-0.38271400	-0.43164700
H	4.10973600	-1.23154900	-1.38350400

BmimH

C	-2.19464400	0.59882400	-0.99944700
C	-1.03134300	1.22720200	-0.78353400
C	-1.30208500	-0.27553900	0.91879400
N	-2.55094700	-0.16369400	0.14729000
H	-2.88739500	0.70553800	-1.82010300
H	-0.53676800	1.97122600	-1.38956500
H	-1.48327300	-0.28778600	1.99593700
N	-0.54754300	0.91751000	0.50944500
C	0.89545900	0.91833500	0.74525900
H	1.25700400	1.92960000	0.53227700
H	1.05542800	0.74693400	1.81456600
C	-3.23227200	-1.42885100	-0.07464300
H	-3.56998100	-1.84135700	0.87930300
H	-4.11023600	-1.26533100	-0.70260400
H	-2.58228900	-2.17460500	-0.56342300
C	1.71452800	-0.09183000	-0.06916300
H	1.52518300	0.07231200	-1.13642900
H	1.38332900	-1.11118300	0.15538500
C	3.21444000	0.02415500	0.20995000
H	3.54631400	1.04383900	-0.01972700
H	3.39551300	-0.12442800	1.28128600
C	4.04873100	-0.97615900	-0.59109000
H	3.90517700	-0.83538900	-1.66735000
H	5.11668900	-0.86588200	-0.38036200
H	3.76691600	-2.00651000	-0.35088500
H	-0.76906200	-1.21052100	0.63778800

Furfuryl alcohol:

C	1.59839500	-0.62030400	-0.12840800
H	1.81969700	-1.03023800	-1.11854800
C	0.18138800	-0.14958900	-0.06692500
C	-0.38780300	1.08558500	-0.10068800
O	-0.78623000	-1.10766000	0.04470200
C	-1.80795800	0.87915100	-0.00502400
H	0.13505400	2.02449400	-0.18744400
C	-1.99425900	-0.46215900	0.07719100
H	-2.57880500	1.63431700	0.00124300
H	-2.86287100	-1.09397200	0.16277600
H	1.74397200	-1.43164600	0.59716400
O	2.51563000	0.44669600	0.07103200
H	2.36917200	0.78866300	0.96207100

IM2-1:

C	0.09774300	-2.66549200	-0.29467700
O	-0.74074800	-2.60887800	0.83507800
C	-3.57176900	1.13960400	-0.60740500
C	-2.59336000	1.99085200	-0.20993300
C	-1.98989400	-0.09799000	0.47113700
N	-3.18065100	-0.12263100	-0.18478700
H	-4.49365600	1.31604900	-1.13625700
H	-2.49100200	3.05655900	-0.32909100
N	-1.64515800	1.21682100	0.44497700
C	-0.38188700	1.74368900	0.96269400
H	-0.59391700	2.67906200	1.48646000
H	-0.00894800	1.02409900	1.69156700
C	-3.94972200	-1.33881300	-0.41707500
H	-3.36122800	-2.18254100	-0.06219900
H	-4.89763900	-1.30252100	0.12360300
H	-4.14951200	-1.45977000	-1.48319100
C	0.64985400	1.97298000	-0.14073400
H	0.22109400	2.63527300	-0.90100200
H	0.86442000	1.01710500	-0.63024700
C	1.94548000	2.58076700	0.39860700
H	1.71702500	3.52072700	0.91478800
H	2.37178600	1.90834100	1.15085100
C	2.97533400	2.83891300	-0.70070900
H	2.58963300	3.54468000	-1.44370600
H	3.89874800	3.25828400	-0.29054200
H	3.23250100	1.91254900	-1.22297700
H	-0.38317800	-2.24127300	-1.18917300
H	-1.15093500	-1.69335300	0.83127100
H	0.29820700	-3.72000700	-0.51976600
C	1.39497000	-1.95189200	-0.06601900
C	1.99563000	-1.44694600	1.04558700
O	2.19271600	-1.74664000	-1.15848800
C	3.25110500	-0.89225900	0.61452700
H	1.59255800	-1.46561600	2.04477800
C	3.32054900	-1.09898900	-0.72468900
H	3.99344200	-0.40144400	1.22451500
H	4.05132400	-0.86793200	-1.48159300

TS2-1:

C	-0.56124700	-2.16395000	-0.07584900
O	-1.13695500	-2.53078100	1.00474500
C	-3.24088300	1.44632400	-0.66799500
C	-2.18867600	2.19233500	-0.25643700
C	-1.82967800	0.07213900	0.44541500
N	-3.06853700	0.16432800	-0.16221400
H	-4.10755300	1.71268100	-1.24884900
H	-1.96489400	3.23467500	-0.40595900
N	-1.35953200	1.36813100	0.49868200
C	-0.05061300	1.73762500	1.02195800
H	-0.15071400	2.69812300	1.53420100
H	0.22354000	0.98860100	1.76750100
C	-3.85349900	-1.00553100	-0.50671200
H	-3.62838400	-1.79454600	0.21083700
H	-4.91554300	-0.76210200	-0.47036300
H	-3.59972200	-1.36403900	-1.50975600
C	1.01997300	1.82518100	-0.06658200
H	0.71693500	2.57969000	-0.80108200
H	1.07527400	0.86926900	-0.59504100
C	2.39290400	2.18306800	0.50430400
H	2.31448400	3.11177200	1.08202500
H	2.70364900	1.40292800	1.20794100
C	3.45497900	2.34613300	-0.58252300
H	3.18986500	3.15398000	-1.27214500
H	4.43243600	2.58202900	-0.15183300
H	3.56058900	1.42792400	-1.16763300
H	-1.00561000	-0.80622800	-0.29658700
H	-1.69968700	-0.63661900	1.28587700
H	-0.91013500	-2.54506600	-1.05624700
C	0.89600200	-1.90535600	-0.05892300
C	1.80458600	-1.82522700	0.95855900
O	1.52563000	-1.67133800	-1.25560200
C	3.07048300	-1.52278300	0.35446300
H	1.59064100	-1.97399200	2.00456900
C	2.84668000	-1.43934600	-0.98341200
H	4.01844100	-1.38652700	0.85185800
H	3.47741200	-1.24648500	-1.83531700

IM2-2

C	0.07152400	-2.74293300	-0.52273400
O	-0.75904300	-3.26023300	0.20706300
C	-3.41095500	1.17975000	-0.30302300
C	-2.52328300	2.00662300	0.26668100
C	-1.68944800	-0.10986800	0.47417400
N	-3.08099400	-0.16803200	0.00464500
H	-4.33237200	1.41302000	-0.81437000
H	-2.54002100	3.08414600	0.33094000
N	-1.55691900	1.26012700	0.98135500
C	-0.20206300	1.79571200	1.11358200
H	-0.28750800	2.76926100	1.60674300
H	0.34823200	1.14146500	1.79711100
C	-3.31825800	-1.17379100	-1.01899300
H	-3.11719300	-2.16697900	-0.61292100
H	-4.36117700	-1.13323100	-1.33906600
H	-2.67063700	-1.02833700	-1.90069400
C	0.58491300	1.95587300	-0.19299300
H	-0.00802600	2.55434600	-0.89475200
H	0.73378300	0.97859800	-0.66259900
C	1.94570300	2.61933000	0.02655700
H	1.79886600	3.60518200	0.48377100
H	2.52273700	2.02828700	0.74628000
C	2.74550100	2.77015900	-1.26759200
H	2.21345400	3.40061900	-1.98750300
H	3.72312500	3.22614000	-1.08452500
H	2.91322100	1.79771900	-1.74132500
H	-1.00064100	-0.29163100	-0.37974500
H	-1.47681300	-0.85906500	1.24028100
H	-0.01516200	-2.78150900	-1.62402700
C	1.23469200	-2.03428000	-0.03610800
C	1.70606000	-1.75158200	1.22138400
O	2.08523700	-1.49915400	-0.97641400
C	2.90335300	-1.00645700	1.04674200
H	1.24155000	-2.04530500	2.14919900
C	3.08257500	-0.88270600	-0.30279900
H	3.54784700	-0.60909000	1.81452700
H	3.84068800	-0.40819100	-0.90379300

Furfural:

C	-0.25802600	0.26994900	0.00001900
C	0.77434600	1.17464000	-0.00003900
O	0.24714400	-1.00603000	0.00000300
C	1.97763400	0.41692500	0.00012000
H	0.67112000	2.24890100	-0.00004200
C	1.59514200	-0.89434200	-0.00010500
H	2.99013100	0.78794000	0.00022000
H	2.14691200	-1.82074100	-0.00013600
C	-1.69042700	0.47047500	-0.00010800
H	-1.97475200	1.53966400	-0.00018500
O	-2.52532200	-0.41667600	0.00009900

IM3-1:

C	0.29103000	-0.48084000	0.03967800
C	-0.70241400	-0.49962100	-1.08292800
O	-0.38876400	0.25428400	1.09680800
C	-1.79744000	0.25444100	-0.69131800
H	-0.51588200	-0.99205800	-2.02470900
C	-1.57402800	0.69057300	0.60295400
H	-2.68603500	0.46285300	-1.26872500
H	-2.18501300	1.27805200	1.27080700
C	1.52446500	0.32005500	-0.40489100
H	2.18944500	-0.25832900	-1.07434700
O	1.72525400	1.47173900	-0.11751100
O	0.75568400	-1.70967500	0.49847300
H	0.01042400	-2.32895800	0.49384600

TS3-1

C	0.17154100	0.80563700	0.00460500
C	-0.53218600	0.45137900	1.15136800
O	-0.50364400	0.34768400	-1.10336700
C	-1.59657800	-0.38515100	0.71589400
H	-0.26158100	0.72287400	2.15928900
C	-1.52267000	-0.43538100	-0.64463100
H	-2.31180800	-0.90659300	1.33256300
H	-2.09013200	-0.95997000	-1.39542000
C	1.51245100	-0.86113300	0.22701400
H	2.04830500	-0.70135800	1.19122800
O	1.14472800	-1.91188700	-0.19586800
O	1.07167500	1.78624800	-0.21920600
H	0.71779400	2.61658000	0.13437000

IM3-2:

C	-0.67588600	0.06781000	-0.00003300
C	0.12919200	1.16709800	0.00006600
O	0.04338700	-1.07362400	0.00003700
C	1.47368400	0.64786700	-0.00009900
H	-0.18762200	2.19765700	0.00002700
C	1.37603000	-0.70288300	0.00008100
H	2.38824600	1.22083400	-0.00006300
H	2.08392800	-1.51376400	-0.00006800
O	-2.00038200	-0.13941700	-0.00010300
H	-2.44672200	0.72024900	0.00054500

IM3-3:

C	-0.83719200	0.02674500	-0.00016300
C	0.05520500	1.20242500	-0.00003000
O	-0.05386600	-1.09758000	0.00006500
C	1.31867700	0.77745000	-0.00003500
H	-0.31958000	2.21482400	0.00002900
C	1.33422900	-0.71480700	0.00011100
H	2.22141500	1.37292200	-0.00005300
H	1.81739100	-1.13124300	-0.88837600
O	-2.04139200	-0.03695800	-0.00001700
H	1.81732400	-1.13107300	0.88871700

IM3-4:

C	0.50184900	1.01587300	0.02994000
C	-0.82967600	0.87804700	0.03709200
C	-1.61524700	-0.39377700	0.02529800
H	0.94919400	2.00189600	0.03657300
H	-1.43836100	1.77835300	0.05524700
H	-1.40463700	-0.96784200	0.93771100
O	-2.99663500	-0.04202700	-0.06370500
H	-3.50211300	-0.86239900	-0.06122500
O	2.71249700	0.26708100	-0.05858300
H	3.26112200	-0.53568600	-0.07014300
H	-1.30382000	-1.02193700	-0.81854300
C	1.42166700	-0.12926700	0.00621400
O	1.10502000	-1.30225900	0.03842800

IM3-5:

C	3.80081300	1.20311400	0.39974400
C	2.78802300	1.94664200	-0.11182400
C	2.17467100	-0.24114800	-0.28211500
N	3.40230000	-0.12128800	0.28832800
H	4.75038900	1.49130100	0.81911000
H	2.67692700	3.01277200	-0.21850200
N	1.81357500	1.04718200	-0.52267200
C	0.50920500	1.44243400	-1.05484300
H	0.66644700	2.22506600	-1.80120500
H	0.09362000	0.57025900	-1.55989800
C	4.20853100	-1.25804800	0.71461600
H	3.59012300	-2.15164800	0.65671300
H	5.08087000	-1.37559600	0.06831300
H	4.54175700	-1.11554200	1.74385900
C	-0.43783000	1.92842400	0.04120900
H	0.01999200	2.77703900	0.56144500
H	-0.56247500	1.12877400	0.77866200
C	-1.80449800	2.33721000	-0.50952600
H	-1.67350000	3.11675700	-1.26916900
H	-2.25785800	1.48126600	-1.01957500
C	-2.74845900	2.84175100	0.58197200
H	-2.35642000	3.74950600	1.05185200
H	-3.73745000	3.07484600	0.17770500
H	-2.87525500	2.09380900	1.37058800
H	-0.32134800	-1.80710300	0.92285400
H	1.38743100	-1.90191800	-0.44974600
C	-1.32758000	-2.27579100	-0.91435100
H	-1.06582000	-2.69566900	-1.88300400
C	-2.46739200	-1.57495100	-0.83207700
H	-3.08364900	-1.44152600	-1.71315300
C	-2.96170700	-0.93605900	0.39596600
O	-2.45480700	-0.97722600	1.49968700
C	-0.32507100	-2.59056200	0.16019300
H	-0.64604400	-3.51332900	0.66276400
O	0.96228100	-2.80566100	-0.38591400
O	-4.10987900	-0.25525500	0.16236900
H	-4.37185400	0.16671700	0.99786200

TS3-2:

C	-2.95472400	1.08158700	-1.33611600
C	-2.08402400	2.02687100	-0.90635100
C	-1.89619200	0.25342300	0.47858700
N	-2.89751900	0.02415300	-0.44165700
H	-3.62575600	1.07426300	-2.17822100
H	-1.84690500	2.99720200	-1.30778700
N	-1.49010900	1.55377000	0.25800600
C	-0.29779600	2.11972300	0.88047700
H	-0.47835000	3.17968400	1.07269800
H	-0.17299300	1.62349200	1.84467500
C	-3.56005800	-1.26071300	-0.58244800
H	-3.42085400	-1.81402500	0.34607400
H	-4.62229400	-1.11265100	-0.78044700
H	-3.11591100	-1.83432200	-1.40118100
C	0.94860500	1.92723800	0.01174300
H	0.84740700	2.52704700	-0.89903200
H	0.99912700	0.88038200	-0.29868400
C	2.23522400	2.30375300	0.74559200
H	2.17903300	3.34829700	1.07397200
H	2.31651600	1.69599800	1.65404700
C	3.47991100	2.10084100	-0.11870800
H	3.44481400	2.72928400	-1.01464100
H	4.39181000	2.35383100	0.43002700
H	3.56293200	1.06082700	-0.44788200
H	-0.82977900	-0.67624400	0.30068000
H	-2.00306600	-0.19300100	1.48540800
C	0.86840200	-1.57521900	1.35857200
H	0.94166400	-1.34970900	2.42091000
C	2.00557500	-1.51076500	0.63383800
H	2.93952800	-1.25983000	1.12179500
C	2.06995400	-1.71404300	-0.81096100
O	1.13458900	-1.89894100	-1.56811600
C	-0.51474500	-1.92541100	0.94997400
H	-0.58141300	-2.50793700	0.01704700
O	-1.39912800	-2.07254600	1.86817900
O	3.34892100	-1.64887600	-1.26844100
H	3.31204000	-1.76886200	-2.23206600

IM3-6:

C	3.21126800	0.88709700	1.11290300
C	2.57391400	1.89974300	0.50804000
C	1.90613600	-0.02508100	-0.53062900
N	3.03221000	-0.30751200	0.36771500
H	3.88500500	0.90914500	1.95576100
H	2.59563500	2.95370000	0.73976900
N	1.93248900	1.43428000	-0.66315000
C	0.69774300	2.07765900	-1.10969600
H	0.93849900	3.11346200	-1.36957900
H	0.39102100	1.58402000	-2.03732600
C	2.92245700	-1.56123600	1.09586300
H	2.88889800	-2.39330300	0.38956800
H	3.79424400	-1.68869300	1.74026200
H	2.01276900	-1.60229500	1.71765000
C	-0.46334200	2.06271200	-0.10699000
H	-0.16930500	2.61960000	0.79006300
H	-0.66409800	1.03635200	0.21434200
C	-1.73674100	2.66987200	-0.69803700
H	-1.52195300	3.68551300	-1.05195600
H	-2.03198400	2.09235100	-1.58221400
C	-2.89806700	2.71189100	0.29498600
H	-2.64101200	3.30739300	1.17706600
H	-3.79215100	3.15407200	-0.15498700
H	-3.16138500	1.70719600	0.63747500
H	0.95494400	-0.36861400	-0.06312100
H	2.00666000	-0.53142700	-1.49366700
C	-1.19520400	-1.86808900	-1.34446500
H	-1.17292600	-1.81226000	-2.42879500
C	-2.21483900	-1.29408600	-0.68866700
H	-3.00507800	-0.81022000	-1.25029600
C	-2.36836600	-1.24836500	0.78497600
O	-1.51490200	-1.47977000	1.61309400
C	-0.07686000	-2.62856500	-0.74980900
H	-0.11484800	-2.81943700	0.33050700
O	0.83648700	-3.04717200	-1.43955000
O	-3.62357000	-0.88287100	1.11524000
H	-3.67854600	-0.84674500	2.08639100

IM3-7:

C	-0.96680200	0.90372900	-0.04041200
H	-1.55084700	1.81864400	-0.08086200
C	0.37077600	0.99179100	-0.06187800
H	0.83546000	1.96969400	-0.10711400
C	1.31893200	-0.15098200	-0.02424400
O	1.04692200	-1.32812800	-0.10456100
C	-1.77594400	-0.32971200	0.05468200
H	-1.23575300	-1.28197300	0.14337600
O	-2.99117000	-0.28415900	0.03969700
O	2.58167500	0.29756200	0.10799600
H	3.16994700	-0.47751600	0.13066000

HFO:

C	0.68992200	1.25191400	-0.12142000
O	0.10724100	-0.94502000	0.28381000
C	-0.61499200	1.26638000	0.13148500
H	1.34470200	2.07328800	-0.37219900
C	-1.09199200	-0.13330800	0.41908600
H	-1.29247800	2.10919600	0.13781100
O	-2.10196200	-0.59347700	-0.41149400
H	-1.86568900	-0.38298600	-1.32750900
C	1.17348500	-0.14557600	-0.02093300
O	2.28495200	-0.58394500	-0.16366400
H	-1.44691800	-0.25643000	1.44336500

Supplementary References

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