

SUPPLEMENTARY INFORMATION

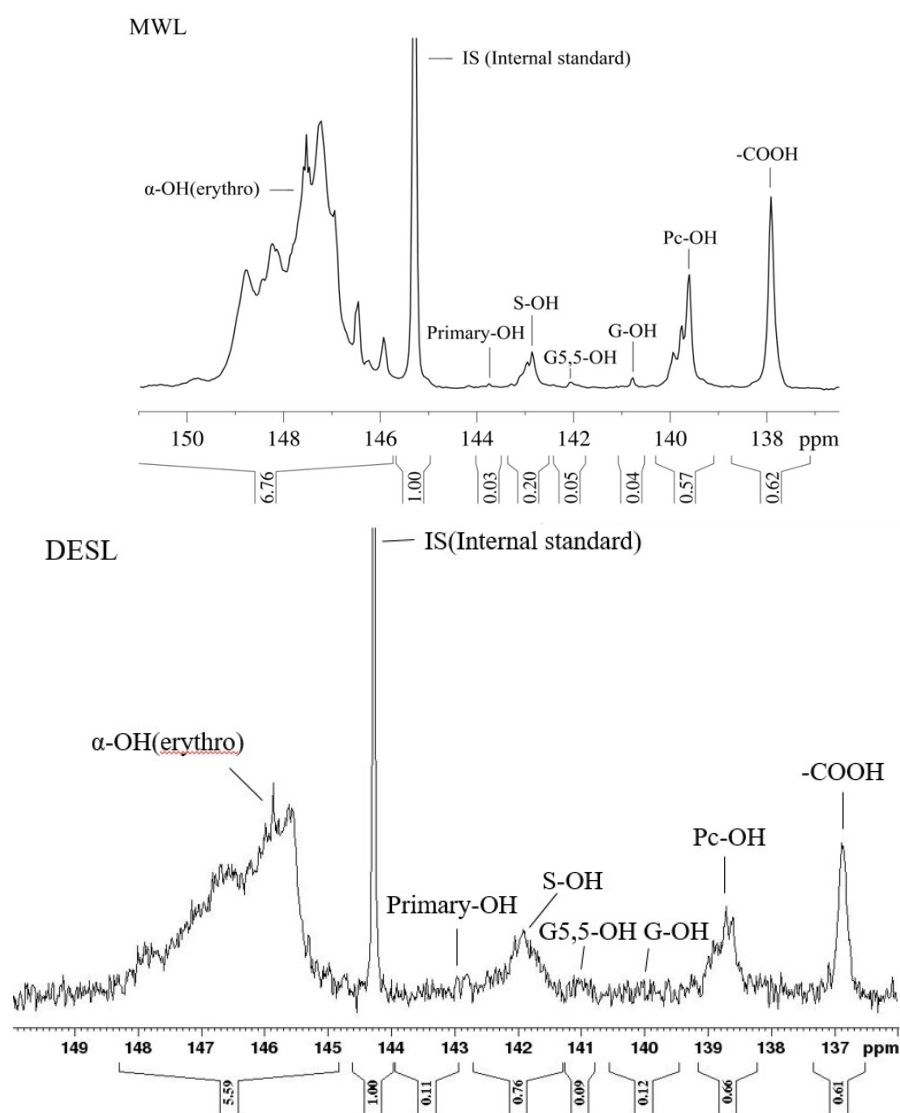
Mechanistic insights into lignin dissolution behaviors of recyclable acid hydrotrope, deep eutectic solvent (DES), and ionic liquid (IL)

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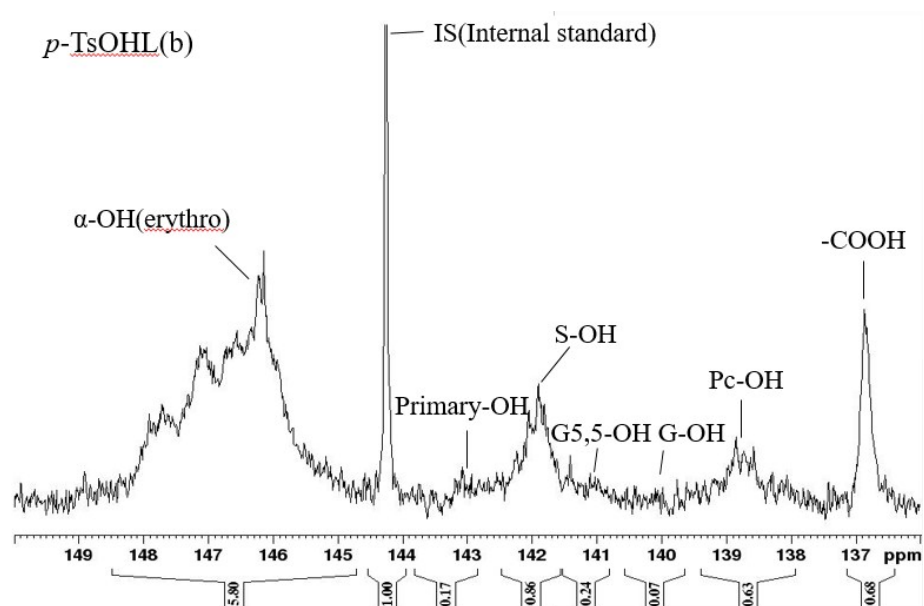


Fig.S1. The ^{31}P NMR spectra of the MWL and the lignin extracted by DES and *p*-TsOH aqueous solution.

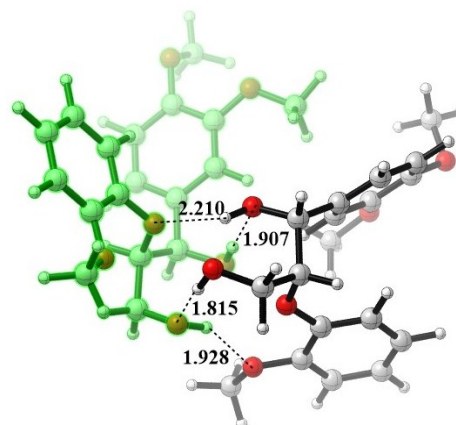
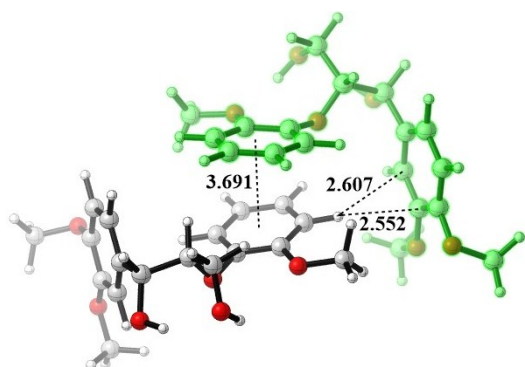
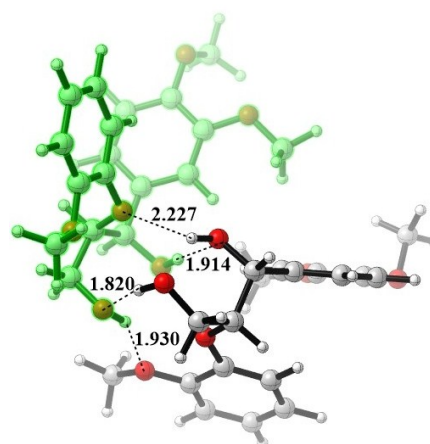
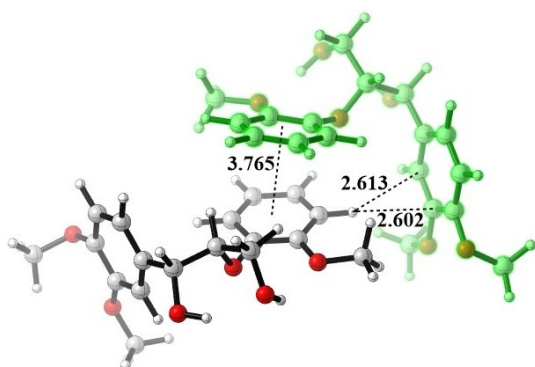
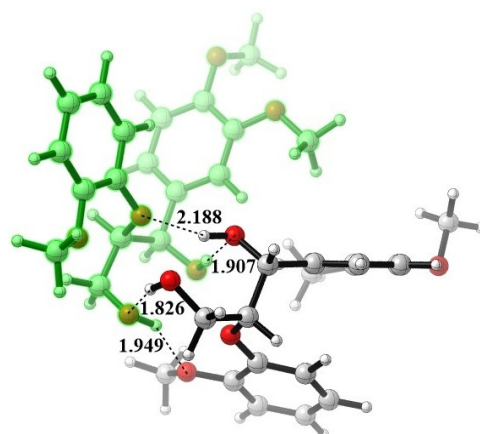
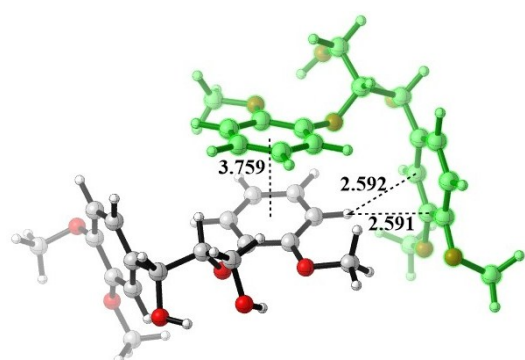


Figure S2. The main noncovalent interactions between two VG dimers in solvent and the interaction energies (kcal/mol) as shown in parentheses.

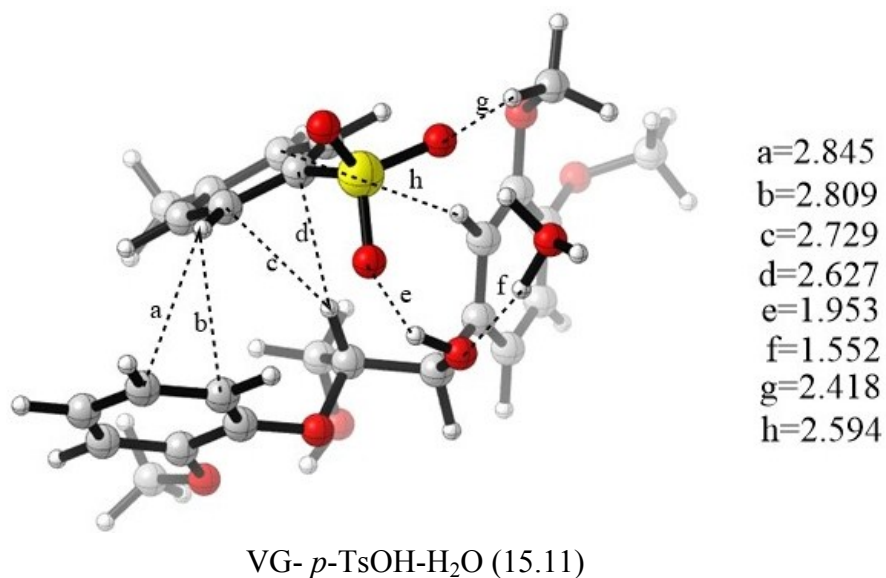
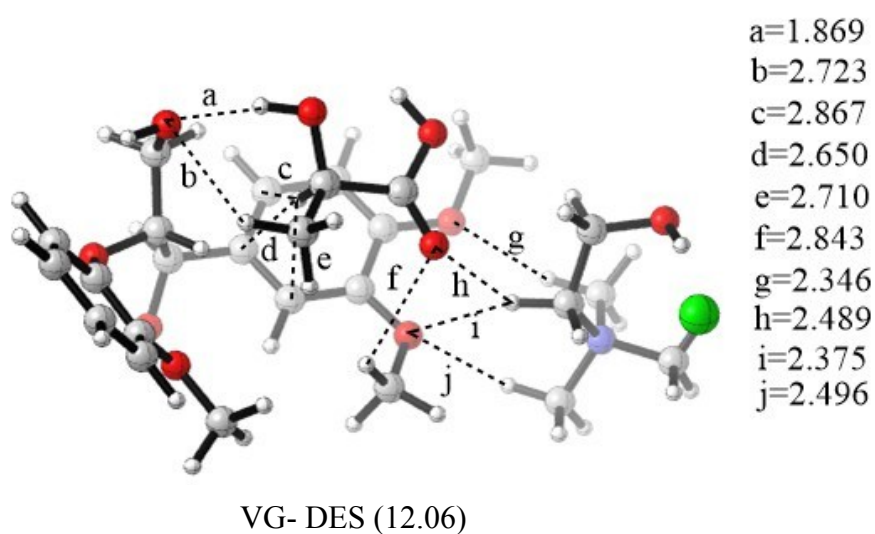
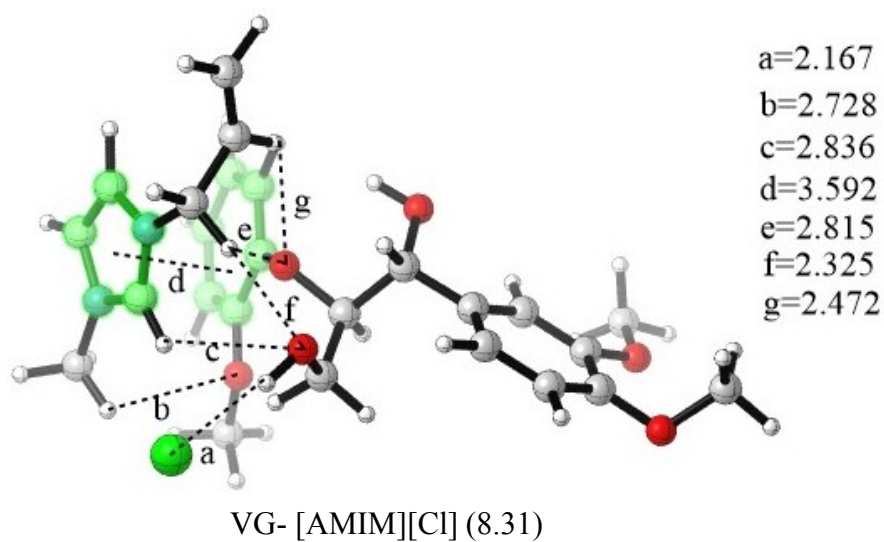


Figure S3. The key structures for VG-solvent and the interaction energies (kcal/mol) as shown in parentheses.

Table S1. The zero-point energy (ZPE) corrections at the M06-2X/6-311G(d,p)-SMD level, electronic energies (E) and the basis set superposition error (BSSE) at the M06-2X/6-311+G(d,p)-SMD level for the key structures.^a

Structure	ZPE	E	BSSE
[AMIM][Cl]	0.175346	-843.0130618	
Lignin ([AMIM][Cl])	0.382056	-1150.338775	
VG1 ([AMIM][Cl])	0.766363	-2300.699021	0.004244696
VG2 ([AMIM][Cl])	0.76779	-2300.707188	0.006428035
VG- [AMIM][Cl]	0.560119	-1993.372384	0.004592789
Lacticacid	0.095857	-343.6035668	
Choline chloride	0.199712	-789.1136802	
Lignin (DES)	0.382076	-1150.348243	
VG1 (DES)	0.765193	-2300.717358	0.004213919
VG2 (DES)	0.767447	-2300.723932	0.006332155
VG- DES	0.683422	-2283.097234	0.006750292
<i>p</i> -TsOH	0.143171	-895.3140259	
H ₂ O	0.021381	-76.43464715	
Lignin (<i>p</i> -TsOH -H ₂ O)	0.381937	-1150.340501	
VG1 (<i>p</i> -TsOH -H ₂ O)	0.765759	-2300.706461	0.004494129
VG2 (<i>p</i> -TsOH -H ₂ O)	0.766719	-2300.712151	0.006495879
VG- <i>p</i> -TsOH -H ₂ O	0.551588	-2122.128413	0.010057438

^aAll energies are given in Hartree.

Cartesian coordinates of the structures

[AMIM][Cl]				C	-3.21263900	0.93289500	0.20438800
C	2.60762800	-0.72218100	-0.08939400	C	-1.27546100	1.79703000	-0.96040400
C	1.60377000	-1.53938600	-0.49979800	C	-3.91657200	2.08993700	-0.11613000
C	0.72961000	0.42986700	-0.03146400	C	-1.98214100	2.95396700	-1.28479100
H	3.66539000	-0.89339900	0.02027600	C	-3.29600000	3.09364600	-0.86067900
H	1.60911100	-2.56815600	-0.81909200	H	-4.94161800	2.21691200	0.20629400
H	-0.00001000	1.22427100	0.08801000	H	-1.50267500	3.73786700	-1.85798500
N	2.03773300	0.49916700	0.19608000	H	-3.85471900	3.98975900	-1.10356700
N	0.44470100	-0.79713100	-0.46010000	H	-0.24321900	1.65914900	-1.26658200
C	-0.91189700	-1.28377700	-0.76578000	O	-3.71949200	-0.10846200	0.91821200
H	-0.81739900	-1.94611500	-1.62786800	C	-5.09779600	-0.06263500	1.27174600
H	-1.50949100	-0.41305500	-1.03830000	H	-5.72497300	0.02173500	0.38051800
C	-1.50725700	-1.99563000	0.41492100	H	-5.30620000	-1.00380800	1.77676300
H	-0.97707700	-2.87744000	0.76694500	H	-5.29911600	0.76866700	1.95175900
C	-2.62567100	-1.58873000	1.00021600	VG1 ([AMIM][Cl])			
H	-3.04877200	-2.12698700	1.84126000	C	4.54906000	-1.47466400	-1.32355100
H	-3.14808900	-0.70148000	0.65362200	C	5.04688900	-2.07935700	-0.15690000
C	2.75963600	1.68521300	0.65159800	C	5.56468200	-1.29098500	0.85800500
H	2.03776700	2.47615900	0.84011300	C	5.55689200	0.09802200	0.74935700
H	3.29495600	1.44624700	1.56887100	C	5.02767000	0.70179300	-0.38636700
H	3.45938900	1.99836000	-0.12144200	C	4.54427800	-0.08615400	-1.42977500
Cl	-2.22810100	2.15029900	-0.25917900	H	5.95221100	-1.78400700	1.74261300
Lignin ([AMIM][Cl])				H	5.94656800	0.70537400	1.55968500
C	2.91029200	0.25028100	0.61521000	H	4.12900200	0.40385400	-2.29961400
C	3.66542900	0.37081800	-0.56705200	O	4.95994900	-3.43720500	0.00807800
C	3.30560400	-0.35040400	-1.69193000	O	4.03854100	-2.31642800	-2.25753600
C	2.19380700	-1.19269300	-1.66716700	C	3.58944100	-1.74782600	-3.48173100
C	1.44780900	-1.31713300	-0.50311700	H	4.40051400	-1.21291400	-3.98346900
C	1.80745800	-0.59617400	0.63872500	H	3.26886800	-2.58543800	-4.09772200
H	3.90646600	-0.23739800	-2.58745400	H	2.74466500	-1.07267400	-3.31976500
H	1.91739800	-1.75416600	-2.55343300	C	5.90022200	-4.17943100	-0.77092500
H	1.20406600	-0.70617900	1.52886400	H	6.92259400	-3.91939900	-0.48027700
O	4.73768100	1.22389600	-0.60961700	H	5.71767700	-5.23206800	-0.55880700
O	3.32671100	1.00235200	1.66362000	H	5.75960700	-3.99225900	-1.83742500
C	2.52844000	0.97750700	2.83904500	C	4.85752700	2.20749400	-0.43011100
H	2.50179300	-0.02343300	3.27862300	H	5.79032700	2.68458900	-0.09828100
H	2.99947900	1.66783800	3.53569000	O	4.54167400	2.61724900	-1.74659700
H	1.50921700	1.31249000	2.62514200	H	3.97567500	3.40136400	-1.68490400
C	5.89841300	0.70782200	0.04293300	C	3.77681100	2.61687900	0.57840800
H	6.24259500	-0.20219300	-0.45838500	H	4.11691400	2.32420900	1.57759800
H	6.66685700	1.47652700	-0.03034400	C	3.45549300	4.10853800	0.57150100
H	5.69462800	0.49536900	1.09506300	H	2.80718200	4.34635600	1.42232000
C	0.19728100	-2.16652700	-0.48784300	H	4.37444400	4.69060400	0.66749500
H	0.29568500	-2.94006600	-1.26193100	O	2.82992200	4.48934200	-0.64833600
O	0.04694400	-2.75722000	0.78959900	H	1.96531500	4.04909800	-0.65322000
H	-0.88624200	-2.99826400	0.88385600	O	2.59049500	1.89706300	0.22908700
C	-1.02603700	-1.32451500	-0.87237800	C	1.68219300	1.69908800	1.23378400
H	-0.82145200	-0.84678100	-1.83756900	C	0.46259800	2.39215700	1.17450200
C	-2.31024500	-2.14020900	-0.97967200	C	1.92916300	0.80055900	2.25918000
H	-3.11256200	-1.51269600	-1.38446300	C	-0.50661200	2.15375000	2.14561400
H	-2.15638400	-2.97895000	-1.66180700	C	0.96557800	0.57564500	3.24121500
O	-2.68817900	-2.67424000	0.28317200	C	-0.24658000	1.24934400	3.17646700
H	-2.95428800	-1.90877700	0.81525900	H	-1.45596800	2.67255200	2.11259000
O	-1.18734600	-0.32898300	0.14656400	H	1.16151300	-0.12732300	4.04181700
C	-1.88185400	0.79432800	-0.22200200	H	-1.00709300	1.07729100	3.93001300
				H	2.87958700	0.27523300	2.26786600

O	0.33004700	3.27724800	0.15132900	H	3.52581700	4.11894000	2.56588400
C	-0.92892600	3.92149200	0.00117300	H	3.08241800	1.73569400	3.16490300
H	-1.13532900	4.57811900	0.85080600	H	0.06192300	1.56994200	0.13093200
H	-0.85580200	4.51462500	-0.90828800	O	2.32400600	5.47330900	0.70679700
H	-1.73096500	3.18577500	-0.10374100	O	0.38142400	4.14590300	-0.61120200
C	-5.77777500	-0.36325100	-1.12147200	C	-0.71251100	3.47918800	-1.23085500
C	-5.98659300	0.99610800	-0.82358200	H	-1.46793300	3.20168200	-0.48820700
C	-5.55832300	1.50952500	0.38909300	H	-1.13756200	4.19017500	-1.93666200
C	-4.91299900	0.69166200	1.31552600	H	-0.37996100	2.58588800	-1.76754800
C	-4.70634800	-0.65173900	1.02628900	C	1.35929300	6.40203200	1.20293700
C	-5.13835300	-1.17789200	-0.19179700	H	1.33516300	6.37761500	2.29694600
H	-5.73709900	2.55982800	0.59122500	H	1.67570100	7.38936700	0.86877800
H	-4.57566200	1.10270800	2.26187700	H	0.36498900	6.18428500	0.80626900
H	-4.94985600	-2.22242800	-0.39715000	C	1.31357700	0.03315600	1.99455600
O	-6.59234900	1.81758000	-1.73851300	H	1.27690600	-0.09861000	3.08107100
O	-6.21891600	-0.77852800	-2.33382300	O	0.08993000	-0.45830400	1.49100800
C	-5.96698600	-2.13130000	-2.68887100	H	0.15797400	-0.55271200	0.52241300
H	-6.46137300	-2.81982000	-1.99788400	C	2.49105200	-0.79961700	1.47374700
H	-6.37963400	-2.26049900	-3.68727400	H	3.41478200	-0.40002300	1.90545200
H	-4.89282500	-2.33637500	-2.70726600	C	2.40207300	-2.28564400	1.81457900
C	-8.00259900	1.61453200	-1.84075500	H	3.36396700	-2.75099300	1.60116800
H	-8.48316500	1.78791100	-0.87285500	H	2.20590400	-2.38689500	2.88862400
H	-8.37187200	2.34014200	-2.56451700	O	1.44167300	-2.98992600	1.04916100
H	-8.22831900	0.60436700	-2.18950100	H	0.54400500	-2.72155700	1.30998600
C	-3.90211900	-1.50948500	1.97771800	O	2.50980500	-0.63476000	0.04979500
H	-4.11205600	-1.18576600	3.00670800	C	3.71536800	-0.35804300	-0.54334600
O	-4.24163800	-2.87335300	1.81157700	C	4.49621000	-1.42496700	-1.01786200
H	-3.45881500	-3.39852200	2.03380200	C	4.11953300	0.95300600	-0.73548200
C	-2.41027400	-1.26475700	1.73412900	C	5.67278600	-1.14823400	-1.71078600
H	-2.21726400	-0.19366900	1.84566300	C	5.30555800	1.22536300	-1.41610700
C	-1.50027400	-2.04755200	2.67717100	C	6.07166900	0.17481800	-1.90201000
H	-0.47832600	-1.66733600	2.60234300	H	6.28209800	-1.95496300	-2.09779500
H	-1.84386000	-1.93511500	3.70839900	H	5.61658400	2.25128400	-1.57035200
O	-1.53099800	-3.43511500	2.36248500	H	6.99076100	0.37524300	-2.44018900
H	-1.12612900	-3.50307600	1.48579400	H	3.48117800	1.74903400	-0.36455300
O	-2.13133100	-1.67473100	0.38928800	O	4.02830100	-2.66589800	-0.74945300
C	-1.23578200	-0.89477800	-0.29771200	C	4.53544600	-3.74350700	-1.52084900
C	0.11306800	-1.27929900	-0.32197800	H	5.58292900	-3.94724800	-1.28087500
C	-1.66337600	0.22528000	-0.99321300	H	3.93215800	-4.61024500	-1.25738900
C	1.02150000	-0.51436700	-1.04599500	H	4.43266100	-3.53662200	-2.58977300
C	-0.75116000	0.98057600	-1.72989200	C	-3.54763800	1.14090300	-0.62618100
C	0.58577300	0.60941800	-1.74637100	C	-4.44318000	1.25931300	-1.70512900
H	2.07324300	-0.76537000	-1.04038900	C	-4.16649200	0.61929100	-2.90167800
H	-1.08414500	1.85863700	-2.27053100	C	-3.00433300	-0.13838200	-3.05105900
H	1.31580800	1.20589800	-2.28169800	C	-2.11101700	-0.24259800	-1.99409000
H	-2.71756900	0.48607300	-0.95006600	C	-2.38438800	0.40064200	-0.78519000
O	0.43085300	-2.39852000	0.38084100	H	-4.87712100	0.72681100	-3.71347100
C	1.81303900	-2.73086000	0.48111700	H	-2.79627200	-0.63442000	-3.99293400
H	2.36823700	-1.92005500	0.96367400	H	-1.70076500	0.28184600	0.04429900
H	1.86066000	-3.62712200	1.09681100	O	-5.59794100	1.98278800	-1.56681400
H	2.24174900	-2.93918100	-0.50301200	O	-3.89772900	1.76570700	0.52482700
VG2 ([AMIM][Cl])				C	-3.11485700	1.47035700	1.67691100
C	1.04797300	3.46420900	0.35217000	H	-2.09195700	1.84563900	1.57135100
C	2.04833500	4.17275600	1.04028400	H	-3.60306100	1.97785100	2.50640600
C	2.76534400	3.54589900	2.04697800	H	-3.09391900	0.39131400	1.86454300
C	2.51344300	2.21565300	2.37508700	C	-5.38318300	3.39515100	-1.54107500
C	1.53406000	1.50500700	1.68936000	H	-4.91356100	3.72423500	-2.47340000
C	0.80525800	2.13206100	0.67893200	H	-6.36420900	3.85838900	-1.44383800

H	-4.75972300	3.68265600	-0.69145600	O	0.00730600	-2.36000400	-0.15505100
C	-0.87071600	-1.09390800	-2.10743300	H	-0.48642900	-2.97023400	-0.73320100
H	-0.59738500	-1.17490300	-3.16710900	O	-0.93243900	0.26212800	0.53907700
O	0.15939300	-0.44419300	-1.38100900	C	-1.55899300	1.45361400	0.28365100
H	0.96294100	-0.98433200	-1.45768900	C	-1.87742800	1.84702900	-1.03003900
C	-1.07406500	-2.53686900	-1.59485800	C	-1.97027000	2.23831900	1.35179000
H	-1.97153000	-2.96415900	-2.05162200	C	-2.57586100	3.03254200	-1.24209200
C	0.10048600	-3.43696900	-1.96992500	C	-2.68706900	3.41403100	1.13858300
H	-0.00985800	-4.38923500	-1.44009900	C	-2.98143500	3.81049000	-0.15744200
H	0.04348900	-3.63289400	-3.04338000	H	-2.81674900	3.34621200	-2.25000600
O	1.37183700	-2.86073500	-1.72693300	H	-2.99968200	4.01457600	1.98403900
H	1.56974400	-2.90065700	-0.76968200	H	-3.52753200	4.72837300	-0.33962800
O	-1.17838400	-2.55071100	-0.16932200	H	-1.73290200	1.91133600	2.35832800
C	-2.38476900	-2.55047000	0.46575100	O	-1.50325500	0.99362200	-2.01449800
C	-2.31002500	-2.70706000	1.86509600	C	-1.51549200	1.47024300	-3.35485200
C	-3.62536100	-2.38564300	-0.13378700	H	-0.91020200	2.37626000	-3.44619900
C	-3.46050000	-2.61584400	2.63646900	H	-1.07955100	0.67447100	-3.95626300
C	-4.78161300	-2.31909000	0.64702600	H	-2.53200000	1.66961700	-3.70340800
C	-4.70046300	-2.41739200	2.02559500	C	-4.88901300	0.33702000	0.24693500
H	-3.39851700	-2.71122300	3.71296400	C	-4.40054700	-0.20325100	1.39352000
H	-5.73821800	-2.17009200	0.16057800	C	-3.33597400	-1.12717100	-0.29995600
H	-5.59223000	-2.34838800	2.63670200	H	-5.64283600	1.08797900	0.07865800
H	-3.70471600	-2.25536200	-1.20472900	H	-4.64261000	-0.01562100	2.42627500
O	-1.07346600	-2.96172900	2.36965500	H	-2.66578700	-1.75105900	-0.88022400
C	-0.85945800	-2.66856200	3.74222200	N	-4.21173100	-0.25832800	-0.79505100
H	-1.42633900	-3.34544500	4.38675900	N	-3.43570800	-1.11475700	1.02582200
H	0.20290800	-2.82282700	3.92336900	C	-2.62425300	-1.95015000	1.92787900
H	-1.13031700	-1.63174800	3.96127800	H	-1.78398400	-2.30324200	1.32583200
VG-[AMIM][Cl]				H	-3.23233900	-2.79790700	2.24780600
Cl	-1.87513300	-3.72544100	-2.21493100	C	-2.13193100	-1.16507900	3.10621200
C	4.83934400	0.61630600	-0.07075900	H	-1.46177900	-0.34186600	2.87705900
C	5.33924500	-0.67821000	-0.30557600	C	-2.45484000	-1.46442500	4.35783800
C	4.54371200	-1.78169400	-0.05133400	H	-2.05437500	-0.90111700	5.19340800
C	3.24501800	-1.62431200	0.43080000	H	-3.12063600	-2.29129400	4.58750600
C	2.74703300	-0.34903600	0.66395300	C	-4.43037400	0.01066700	-2.21287000
C	3.54368800	0.77159600	0.41152700	H	-3.65523400	-0.49532500	-2.78481900
H	4.95675000	-2.76564600	-0.24392100	H	-5.41190600	-0.36218700	-2.50259400
H	2.61688000	-2.48956500	0.61303300	H	-4.37667200	1.08678000	-2.37688400
H	3.13812900	1.75599700	0.60356500	Lacticacid			
O	6.60089900	-0.84196000	-0.81489600	C	-0.78649600	-0.16144700	-0.02694300
O	5.68567200	1.63691100	-0.35122400	C	0.66303300	0.07457400	-0.39272000
C	5.21071100	2.95856100	-0.13813200	H	0.68040000	0.35316400	-1.45321800
H	4.96062500	3.12267400	0.91396200	C	1.24149500	1.20816500	0.44855700
H	6.02817900	3.61795500	-0.42229300	H	2.28948200	1.35830500	0.18106600
H	4.33818200	3.16900800	-0.76299500	H	0.70287400	2.14072600	0.27570900
C	7.63357500	-0.64380800	0.15141100	H	1.18384000	0.94995800	1.50860700
H	7.55939400	-1.39288100	0.94592900	O	-1.53770800	0.90020100	-0.33011700
H	8.58064100	-0.76386400	-0.37326600	H	-2.45437800	0.72147200	-0.06667600
H	7.57953700	0.35885900	0.58165700	O	-1.22374900	-1.16064700	0.48065900
C	1.32649900	-0.15917700	1.13673600	O	1.33992800	-1.14469900	-0.17533400
H	1.01436900	-1.04569000	1.69985900	H	2.26182200	-1.01023000	-0.42052300
O	1.27253700	0.99176700	1.96573800	Choline chloride			
H	0.36741100	1.06684400	2.28625400	N	1.39741600	-0.30647600	0.01681800
C	0.36361500	0.01199000	-0.04716200	C	1.20175900	1.16247400	-0.28298200
H	0.67199800	0.88189100	-0.63580600	H	1.61160800	1.70074400	0.57400000
C	0.29345900	-1.21254500	-0.93772100	H	1.81526300	1.36985100	-1.16190800
H	-0.48349200	-1.05563300	-1.68752100	C	-0.21934800	1.62325000	-0.55361100
H	1.25367500	-1.32261300	-1.45628000	H	-0.11774800	2.64530300	-0.93279400

H	-0.68523800	1.03364500	-1.34837100	O	-3.69513500	-0.13538400	0.96328100
O	-1.02769600	1.64549100	0.60531700	C	-5.06734700	-0.12255500	1.34672600
H	-1.70073700	0.94547300	0.50475800	H	-5.71534200	-0.07643900	0.46763600
C	2.86749400	-0.54576900	0.13378400	H	-5.23560700	-1.05818300	1.87647200
H	3.02774600	-1.59528500	0.37536000	H	-5.27790800	0.71748700	2.01287600
H	3.33709600	-0.29998500	-0.81756200	VG1 (DES)			
H	3.25908600	0.09048500	0.92623000	C	4.54559600	-1.51280300	-1.31696400
C	0.85351300	-1.15790200	-1.08271900	C	5.03829400	-2.11119300	-0.14632800
H	-0.23323900	-1.08510500	-1.08851900	C	5.55904900	-1.32073500	0.86500400
H	1.27307700	-0.81578400	-2.02805100	C	5.55963100	0.06717600	0.74639400
H	1.14903200	-2.18797200	-0.88708300	C	5.03519300	0.66698500	-0.39428000
C	0.74936100	-0.69814500	1.30679800	C	4.54647900	-0.12476700	-1.43285300
H	1.11146700	-0.03414700	2.09010000	H	5.94331500	-1.80899700	1.75393200
H	-0.32944300	-0.62039600	1.20292800	H	5.95207700	0.67768500	1.55295600
H	1.03181000	-1.72851500	1.52114000	H	4.13401600	0.35611700	-2.30899700
Cl	-2.87216500	-0.74943300	-0.05988900	O	4.94719700	-3.47172100	0.01844800
Lignin (DES)				O	4.03595400	-2.35960000	-2.24811300
C	2.93175300	0.26354000	0.61972100	C	3.60106900	-1.79857300	-3.48275200
C	3.68549300	0.38135300	-0.56218900	H	4.42036500	-1.27219400	-3.97978200
C	3.32334700	-0.33571800	-1.68856900	H	3.28309000	-2.64047900	-4.09436700
C	2.20757000	-1.17214600	-1.66430100	H	2.75852100	-1.11802300	-3.33331600
C	1.46019000	-1.29356200	-0.50034000	C	5.93547300	-4.20774400	-0.70933400
C	1.82290300	-0.57524500	0.64264500	H	6.93741100	-3.94196600	-0.35973900
H	3.92447800	-0.22514100	-2.58446000	H	5.74630300	-5.26204500	-0.51172100
H	1.92831600	-1.73125800	-2.55115900	H	5.85506800	-4.01569700	-1.78167600
H	1.22297900	-0.68035800	1.53596700	C	4.88277600	2.17453200	-0.44595700
O	4.76517100	1.23009200	-0.59800900	H	5.82352500	2.64376200	-0.12756700
O	3.35627900	1.01107700	1.66991600	O	4.55623800	2.57686700	-1.76468000
C	2.56210800	0.98715200	2.85055500	H	4.04528900	3.39846500	-1.70487000
H	2.53039500	-0.01603700	3.28411800	C	3.81297800	2.60413700	0.56476500
H	3.04306700	1.67017100	3.54765400	H	4.14641500	2.29907200	1.56228500
H	1.54542500	1.33230700	2.64174600	C	3.52452500	4.10157100	0.57242900
C	5.93441000	0.68050500	0.01621600	H	2.87390700	4.34254300	1.42050100
H	6.25705200	-0.21764800	-0.51880300	H	4.45621100	4.65986900	0.68512400
H	6.70953600	1.44330400	-0.04829000	O	2.91867600	4.51710300	-0.64727100
H	5.74627700	0.43881600	1.06521500	H	2.04011100	4.10585000	-0.66775900
C	0.20804200	-2.14100100	-0.48943400	O	2.61237100	1.90749000	0.20927300
H	0.31115400	-2.92295300	-1.25330500	C	1.69488800	1.72982200	1.21156800
O	0.04724200	-2.71881800	0.79534600	C	0.48593500	2.43860400	1.13674400
H	-0.87919700	-2.99290900	0.87074200	C	1.92576800	0.83867100	2.24669000
C	-1.01268000	-1.30203700	-0.88720500	C	-0.49218400	2.22324800	2.10484300
H	-0.79861800	-0.82300500	-1.84966100	C	0.95375800	0.63736900	3.22542000
C	-2.29288900	-2.11920000	-1.01525300	C	-0.24926600	1.32645800	3.14640700
H	-3.09693600	-1.48635600	-1.40779500	H	-1.43463200	2.75402200	2.06207200
H	-2.13172500	-2.93939400	-1.71783900	H	1.13641200	-0.05904800	4.03496700
O	-2.67653600	-2.68870700	0.23160300	H	-1.01597200	1.17249000	3.89769700
H	-2.96970300	-1.94510800	0.78032200	H	2.86988700	0.30221400	2.26710500
O	-1.18165300	-0.30602900	0.13226700	O	0.37219700	3.31034200	0.09945700
C	-1.91044800	0.79971800	-0.23158300	C	-0.87519500	3.97679800	-0.06245400
C	-3.23361400	0.90994400	0.22446700	H	-1.07128400	4.64655600	0.77914600
C	-1.34502900	1.80783900	-0.99425500	H	-0.78740900	4.55643800	-0.97930500
C	-3.97401100	2.04493000	-0.09290800	H	-1.68997900	3.25429500	-0.16102100
C	-2.08793300	2.94299400	-1.31497300	C	-5.78489700	-0.38631100	-1.13274200
C	-3.39539000	3.05463700	-0.86271900	C	-6.03091700	0.96636700	-0.83679000
H	-4.99471700	2.15006500	0.25090000	C	-5.64032200	1.49005100	0.38324500
H	-1.64159900	3.73136000	-1.90872100	C	-4.99225000	0.68604200	1.31995300
H	-3.98176800	3.93368000	-1.10388600	C	-4.74342900	-0.65072600	1.03149500
H	-0.31736200	1.69287200	-1.32456400	C	-5.14009900	-1.18680100	-0.19512600

H	-5.84680000	2.53579500	0.58403900	H	1.75374000	7.39769200	0.94656700
H	-4.68209400	1.10381300	2.27247600	H	0.42267700	6.21230800	0.92447100
H	-4.92189100	-2.22487600	-0.40500000	C	1.31876800	0.02943300	1.97693300
O	-6.63655200	1.76746900	-1.77396400	H	1.27555300	-0.11250800	3.06147000
O	-6.19734200	-0.80799800	-2.35445800	O	0.08901500	-0.44262500	1.46422600
C	-5.90671100	-2.15421000	-2.71161700	H	0.15530100	-0.53043500	0.49442500
H	-6.39437800	-2.85638800	-2.02991500	C	2.48734600	-0.81237600	1.45319700
H	-6.30234100	-2.28853500	-3.71618200	H	3.41284400	-0.42358600	1.89037700
H	-4.82757800	-2.33170200	-2.71560900	C	2.38639500	-2.29713800	1.79377700
C	-8.05328400	1.58305000	-1.84726900	H	3.34688900	-2.77026800	1.59000200
H	-8.52366400	1.87705700	-0.90409700	H	2.17871100	-2.39547100	2.86546500
H	-8.41105000	2.22744800	-2.64942400	O	1.42393800	-2.99945000	1.02330700
H	-8.30067300	0.54366000	-2.07618000	H	0.52751400	-2.73697400	1.29310500
C	-3.92993200	-1.48491900	1.99585200	O	2.51519900	-0.64157300	0.02786000
H	-4.15064400	-1.15772500	3.02066200	C	3.73245600	-0.37608300	-0.55016600
O	-4.24666000	-2.85789900	1.83706200	C	4.49983900	-1.44865900	-1.03456900
H	-3.47313200	-3.36982000	2.11710400	C	4.16435500	0.93010600	-0.71165500
C	-2.44017700	-1.22121400	1.75685500	C	5.69577100	-1.18256900	-1.69744700
H	-2.26604000	-0.14477200	1.84811400	C	5.36780500	1.19228800	-1.36555700
C	-1.52071900	-1.96642300	2.71908200	C	6.12357300	0.13608300	-1.85517700
H	-0.50225900	-1.58113400	2.62675100	H	6.29808900	-1.99275400	-2.08806700
H	-1.85960700	-1.82142800	3.74759800	H	5.70160700	2.21471300	-1.49428700
O	-1.53907100	-3.36563900	2.45318600	H	7.05747000	0.32756400	-2.37095500
H	-1.12346200	-3.46815100	1.58485900	H	3.53659100	1.73240100	-0.33563500
O	-2.14867000	-1.65292800	0.42024100	O	3.99655400	-2.68508300	-0.80777600
C	-1.24854300	-0.88377500	-0.27551100	C	4.56841700	-3.77488700	-1.51795200
C	0.09542400	-1.28376200	-0.30573400	H	5.59750600	-3.96028200	-1.19818400
C	-1.66975400	0.23437500	-0.97774100	H	3.95480700	-4.64133300	-1.27789300
C	1.00521800	-0.54202400	-1.05263400	H	4.54071000	-3.59150900	-2.59581600
C	-0.75591200	0.96949900	-1.73262800	C	-3.53130400	1.19854200	-0.58850800
C	0.57541500	0.57823900	-1.76285700	C	-4.42714300	1.35877000	-1.66002000
H	2.05235400	-0.81196400	-1.06260900	C	-4.16967400	0.74352300	-2.87311200
H	-1.08408000	1.84454100	-2.28118400	C	-3.02372100	-0.03352400	-3.04437500
H	1.30489500	1.15570300	-2.32018100	C	-2.12949300	-0.18243200	-1.99264500
H	-2.71988900	0.50996800	-0.92799600	C	-2.38594500	0.43555600	-0.76676800
O	0.40739500	-2.39606100	0.41134700	H	-4.88059300	0.88389800	-3.67989600
C	1.78946300	-2.73108400	0.51649400	H	-2.82932400	-0.51144200	-3.99852600
H	2.34657700	-1.91253900	0.98341000	H	-1.70231700	0.28689300	0.05711700
H	1.83487500	-3.61622500	1.14839600	O	-5.56493600	2.10863200	-1.49166200
H	2.21431800	-2.95863800	-0.46493900	O	-3.86430500	1.81075200	0.57597300
VG2 (DES)				C	-3.07828500	1.48446600	1.71926000
C	1.06018400	3.48274900	0.38270900	H	-2.04903300	1.83916600	1.60813600
C	2.08456200	4.16963500	1.05495200	H	-3.54957800	1.99217500	2.55836500
C	2.81644600	3.52332100	2.03833100	H	-3.07984000	0.40296200	1.89303900
C	2.55591400	2.19232700	2.35596400	C	-5.32074300	3.51774500	-1.54352000
C	1.55289100	1.50152000	1.68335900	H	-4.89615500	3.79318200	-2.51363200
C	0.80775400	2.15037800	0.69925100	H	-6.28544300	4.00678200	-1.41418300
H	3.59547300	4.08004500	2.54794700	H	-4.64391500	3.82682200	-0.74293200
H	3.13687200	1.69651800	3.12701300	C	-0.90684600	-1.05469600	-2.13601800
H	0.03498100	1.60993800	0.17130900	H	-0.65031900	-1.12557900	-3.20023800
O	2.36569900	5.47352900	0.72702300	O	0.15070700	-0.43541600	-1.41699500
O	0.37712400	4.18447600	-0.55667800	H	0.93546400	-1.00156800	-1.49955700
C	-0.75368800	3.54431200	-1.14195200	C	-1.13437000	-2.49914900	-1.64189000
H	-1.48201500	3.26990300	-0.37178100	H	-2.04528200	-2.89886000	-2.09626300
H	-1.19335900	4.27262100	-1.82072400	C	0.01250700	-3.42262300	-2.03852400
H	-0.45595600	2.65389600	-1.70336500	H	-0.13130400	-4.38905300	-1.54408600
C	1.43655700	6.41045100	1.28016200	H	-0.03534300	-3.57808000	-3.11864800
H	1.46050300	6.36761200	2.37329400	O	1.30031500	-2.89498100	-1.75765400

H	1.46940800	-2.94683400	-0.79561800	H	6.59046900	0.83871400	1.20493100
O	-1.22548500	-2.52944000	-0.21449500	O	3.41011900	0.79505100	-1.93923500
C	-2.42745500	-2.55954400	0.43058600	C	2.57403500	1.50177400	-2.85336800
C	-2.33935200	-2.78401300	1.82008700	H	2.00762800	0.74165000	-3.38858900
C	-3.67257200	-2.36276700	-0.14839400	H	1.89356900	2.16817500	-2.31714300
C	-3.48233300	-2.74300300	2.60635300	H	3.17706200	2.07324000	-3.56325400
C	-4.82193200	-2.34311400	0.64585000	N	-5.15896100	-0.05090100	-1.35811600
C	-4.72811900	-2.51773000	2.01614600	C	-4.20721800	0.65798900	-0.41635100
H	-3.41189000	-2.89805900	3.67531000	H	-3.20604000	0.30284000	-0.66666800
H	-5.78383800	-2.17392800	0.17631000	H	-4.28947900	1.72014200	-0.65432200
H	-5.61513300	-2.48818600	2.63761700	C	-4.43928200	0.40737100	1.06653800
H	-3.76196600	-2.18268000	-1.21143700	H	-4.19983900	-0.62746900	1.31789300
O	-1.09171100	-3.04757000	2.29555300	H	-3.71393400	1.04043500	1.58780600
C	-0.88234500	-2.93746100	3.69802100	O	-5.75658200	0.65581600	1.51473900
H	-1.42611000	-3.71468900	4.24086700	H	-5.91380600	1.61725700	1.41810700
H	0.18596600	-3.08014300	3.85280100	C	-5.36084800	-1.47060900	-0.94773600
H	-1.18417900	-1.94949000	4.05713300	H	-5.95814700	-1.96109800	-1.71536900
VG-DES				H	-4.38315500	-1.94419500	-0.86285700
C	-0.47233400	-1.59014700	-0.99002300	H	-5.88869100	-1.48935700	0.00390500
C	-1.00522800	-2.41220200	0.02932700	C	-4.54766700	-0.02721900	-2.72048200
C	-0.15967900	-3.25269700	0.73689400	H	-4.33558000	1.00838300	-2.98443000
C	1.21316900	-3.26471800	0.46399100	H	-3.63025100	-0.61358200	-2.69762600
C	1.74811900	-2.42386700	-0.49547900	H	-5.25801300	-0.45758100	-3.42482100
C	0.89145900	-1.59201100	-1.23075300	C	-6.48066200	0.64656300	-1.42381600
H	-0.55282900	-3.90087900	1.50854700	H	-6.94192400	0.61718200	-0.44213300
H	1.85983600	-3.92347100	1.03403600	H	-6.30814000	1.67638500	-1.73337700
H	1.31045200	-0.94389100	-1.99059500	C	-0.65161700	0.40619100	1.67246400
O	-2.34273400	-2.30000200	0.23789300	C	0.86399200	0.41347000	1.76150500
O	-1.36900900	-0.82590900	-1.66238600	H	1.16475500	-0.50347300	1.23565500
C	-0.84382600	0.23319100	-2.45394800	C	1.46775800	1.63264400	1.08674000
H	-0.30931200	-0.15479100	-3.32548800	H	1.03779900	2.55081800	1.49270700
H	-1.70082100	0.81819800	-2.78464600	H	2.54598100	1.63819900	1.26287100
H	-0.17980300	0.86452700	-1.85666600	H	1.29153600	1.60186600	0.00780700
C	-2.90329800	-3.10588400	1.26817700	O	-1.27724500	-0.24547500	2.65147000
H	-3.97208000	-2.89883500	1.27064500	H	-0.61722700	-0.51519000	3.31422400
H	-2.74296200	-4.16814100	1.06428900	O	1.21114700	0.30874800	3.13151600
H	-2.47811400	-2.84414800	2.24099500	H	2.16329000	0.11271000	3.16141700
C	3.24851500	-2.26666800	-0.67379800	Cl	-5.93590300	3.70349200	1.00293900
H	3.75273200	-3.18460200	-0.35353100	H	-7.09697300	0.12842600	-2.15796800
O	3.60533600	-2.04511800	-2.02339800	O	-1.26782700	0.91422400	0.76980800
H	3.62912300	-1.08849600	-2.17435500	P-TSOH			
C	3.69523600	-1.09421600	0.22630700	C	1.93223800	-1.20008100	-0.00437700
H	2.96068800	-0.29423700	0.12793100	C	0.54861800	-1.20980800	-0.05589000
C	3.81092800	-1.49849100	1.68545400	C	-0.12191000	0.01085400	-0.09399500
H	2.93114300	-2.06481800	1.99378800	C	0.55311700	1.22445600	-0.07498300
H	4.69665200	-2.12940500	1.81488200	C	1.94161100	1.20838600	-0.02321100
O	3.86221100	-0.36856000	2.54998600	C	2.64598400	0.00438100	0.01387500
H	4.67813800	0.12332500	2.39922700	H	2.47233600	-2.13988200	0.02128600
O	4.96558700	-0.58662800	-0.22222900	H	0.00026900	-2.14392300	-0.07401500
C	5.05977900	0.78505900	-0.26803800	H	0.01022600	2.16093500	-0.10743400
C	4.25749700	1.52164800	-1.15839000	H	2.48482000	2.14615900	-0.01178200
C	5.97346400	1.43739300	0.54232900	C	4.14720400	-0.01368000	0.05954500
C	4.36178700	2.90749100	-1.18943800	H	4.55028500	0.99125800	0.18406800
C	6.09045200	2.82646500	0.49825300	H	4.49874800	-0.63833300	0.88347200
C	5.27859400	3.55372200	-0.35917300	H	4.54966900	-0.43518400	-0.86513400
H	3.74283900	3.48959700	-1.85965300	S	-1.88326600	0.00628500	-0.11285600
H	6.80764000	3.32779100	1.13650700	O	-2.36682100	1.30894000	-0.52620000
H	5.35211400	4.63412700	-0.39627200	O	-2.37066300	-1.18088800	-0.78102600

O	-2.29014500	-0.22194300	1.41826500	C	-4.94172900	0.95125100	0.36125300
H	-2.09424100	0.56249000	1.96113600	C	-4.45022900	0.23888600	1.45514400
H2O				H	-6.14091400	-1.66091600	-1.45772800
O	0.00000000	0.00000000	0.11923300	H	-5.95897200	0.82746800	-1.52995900
H	0.00000000	0.75493200	-0.47693200	H	-3.95231600	0.77313700	2.25280700
H	0.00000000	-0.75493200	-0.47693200	O	-5.18027300	-3.20518100	0.41362200
Lignin (<i>p</i>-TsOH-H2O)				O	-4.05747000	-1.93174100	2.48721000
C	2.94662400	0.26862200	0.62196100	C	-3.51960400	-1.27347900	3.63182500
C	3.70053600	0.38977200	-0.55808900	H	-4.27199400	-0.63095100	4.09600400
C	3.33663900	-0.31720100	-1.68972700	H	-3.23478200	-2.06433300	4.32164700
C	2.21655400	-1.14755600	-1.67071300	H	-2.63862100	-0.68245600	3.36900500
C	1.46782000	-1.27307800	-0.50783600	C	-6.21913500	-3.74922900	1.23637300
C	1.83338300	-0.56411700	0.63990900	H	-7.19810300	-3.47027700	0.83749000
H	3.93899700	-0.20501800	-2.58400100	H	-6.10541500	-4.83151000	1.20935500
H	1.93409900	-1.69981600	-2.56030400	H	-6.12449000	-3.39509900	2.26506700
H	1.23460200	-0.66890000	1.53383700	C	-4.67419500	2.43717000	0.22611200
O	4.78882300	1.23697200	-0.58591600	H	-5.58413000	2.93849000	-0.12765500
O	3.37347300	1.01071300	1.67942600	O	-4.27227300	2.97613800	1.47558300
C	2.57771600	0.97401600	2.86040300	H	-3.67070400	3.71460800	1.29487700
H	2.54744700	-0.03380600	3.28155000	C	-3.60449500	2.64783100	-0.85076400
H	3.05681600	1.65037600	3.56422700	H	-3.98599800	2.24410000	-1.79354400
H	1.56140000	1.31855200	2.65226100	C	-3.19319700	4.10086700	-1.05735800
C	5.95826400	0.66161800	0.00783500	H	-2.56382500	4.17304300	-1.95071200
H	6.25747600	-0.23608300	-0.53989500	H	-4.07764600	4.72330600	-1.20351400
H	6.74451500	1.41168100	-0.05994200	O	-2.49351400	4.60309500	0.07845300
H	5.77853000	0.41320600	1.05629800	H	-1.66154800	4.10601600	0.12308200
C	0.21509700	-2.11943800	-0.50656200	O	-2.45206800	1.91129800	-0.42324200
H	0.31893500	-2.89343200	-1.27741700	C	-1.60520400	1.46564800	-1.40409000
O	0.04721300	-2.71240900	0.77290700	C	-0.31821700	2.02100600	-1.46056200
H	-0.88416800	-2.97334400	0.84026200	C	-1.97272900	0.44140300	-2.25974500
C	-1.00561900	-1.27905600	-0.89656900	C	0.59787900	1.52208200	-2.38258400
H	-0.79255800	-0.79179700	-1.85463500	C	-1.05615400	-0.05563900	-3.18549800
C	-2.28440500	-2.09693400	-1.03195500	C	0.22019600	0.48761400	-3.24133000
H	-3.08958800	-1.46112600	-1.41548200	H	1.59942900	1.92960500	-2.44067700
H	-2.12104400	-2.90832400	-1.74309700	H	-1.33908900	-0.86413000	-3.84831200
O	-2.66865200	-2.68125900	0.21010300	H	0.94396700	0.10316800	-3.95148400
H	-2.96149300	-1.94204700	0.76548200	H	-2.97352800	0.02806700	-2.17401400
O	-1.17455100	-0.28949700	0.13110800	O	-0.06902500	3.02939300	-0.58054900
C	-1.92713600	0.80585800	-0.22769600	C	1.26537500	3.52576000	-0.51993700
C	-3.24431100	0.89695700	0.24679700	H	1.54175800	4.01240100	-1.45868500
C	-1.38871100	1.81459300	-1.00813000	H	1.27616700	4.25380100	0.28812300
C	-4.00966500	2.01483200	-0.07132700	H	1.96761600	2.71645900	-0.29917400
C	-2.15609900	2.93317000	-1.32883200	C	5.61162000	-0.07815900	1.23916900
C	-3.45903000	3.02638900	-0.85883900	C	5.53649700	1.27191600	0.86002600
H	-5.02700000	2.10462600	0.28580900	C	5.02006200	1.61744900	-0.37760300
H	-1.73354900	3.72246100	-1.93769000	C	4.55589000	0.63168900	-1.24521900
H	-4.06390700	3.89184700	-1.10139700	C	4.61622700	-0.70685600	-0.87028900
H	-0.36553500	1.71043600	-1.35459200	C	5.14571900	-1.06201600	0.37031600
O	-3.67656500	-0.14982400	1.00456700	H	4.97914400	2.66764000	-0.64457200
C	-5.05483600	-0.17573600	1.36976000	H	4.14274400	0.90783800	-2.21010000
H	-5.68962500	-0.14750600	0.48098400	H	5.17348900	-2.10547000	0.65083400
H	-5.20251300	-1.11533700	1.89743900	O	5.96236800	2.24934100	1.73498300
H	-5.29670700	0.65952100	2.03039500	O	6.13226700	-0.32165000	2.47123400
VG1 (<i>p</i>-TsOH-H2O)				C	6.17980000	-1.67932000	2.90031800
C	-4.55580200	-1.14945300	1.49182800	H	6.81273000	-2.27764400	2.24043500
C	-5.15364800	-1.82717200	0.41856300	H	6.60735000	-1.65942400	3.89990700
C	-5.67281200	-1.11265200	-0.64792600	H	5.17513900	-2.10788600	2.94043000
C	-5.56993600	0.27582500	-0.68065800	C	7.38485200	2.41592000	1.73505500

H	7.72736000	2.73649700	0.74747100	H	2.27390400	-2.29496300	2.89413500
H	7.60810100	3.18861900	2.46881000	O	1.58544900	-2.95338900	1.04568200
H	7.88494500	1.48677900	2.01748800	H	0.67237400	-2.74345100	1.30517000
C	3.98804900	-1.74983800	-1.76677200	O	2.55127300	-0.53882100	0.05131300
H	4.23744700	-1.51504400	-2.81001200	C	3.75490600	-0.18307500	-0.50931600
O	4.46716000	-3.03988300	-1.42395600	C	4.61296300	-1.19499700	-0.96944700
H	3.80916900	-3.67981300	-1.73372700	C	4.08283400	1.15175800	-0.68201200
C	2.46171500	-1.66451400	-1.65573800	C	5.79852700	-0.84231400	-1.60932700
H	2.16754600	-0.63853900	-1.88468800	C	5.27463700	1.50190100	-1.31549600
C	1.73300600	-2.61370400	-2.59641900	C	6.12354900	0.50418000	-1.77446100
H	0.66674400	-2.37570400	-2.60620200	H	6.46998500	-1.60647800	-1.97854700
H	2.12848800	-2.50658500	-3.60837500	H	5.52648900	2.54596000	-1.45326300
O	1.93307000	-3.97188400	-2.20609900	H	7.04923200	0.76409500	-2.27381700
H	1.56175500	-4.05599300	-1.31781900	H	3.38633000	1.90585800	-0.32859300
O	2.09017300	-1.99129300	-0.30445800	O	4.20290300	-2.46877700	-0.74789600
C	1.22184300	-1.11711900	0.31602000	C	4.88004800	-3.51004500	-1.44244100
C	-0.15190000	-1.40773100	0.32010300	H	5.91036300	-3.61215500	-1.09351900
C	1.70228400	0.00500300	0.97444300	H	4.33036200	-4.42189300	-1.21916600
C	-1.01864400	-0.56220200	1.00642200	H	4.86788400	-3.32502100	-2.51968900
C	0.82864000	0.84971900	1.65831500	C	-3.52252200	1.00697000	-0.58235400
C	-0.52839300	0.56033900	1.67122900	C	-4.31217800	1.32835100	-1.69972400
H	-2.08271400	-0.75347100	0.99997200	C	-3.97371800	0.84277100	-2.95001600
H	1.21219700	1.72780200	2.16399400	C	-2.84243500	0.04193400	-3.11492300
H	-1.22827800	1.21476300	2.17948200	C	-2.04439000	-0.25548500	-2.01908500
H	2.76921800	0.19986500	0.95780800	C	-2.38871300	0.22864200	-0.75470800
O	-0.54391800	-2.52519400	-0.34922800	H	-4.60274700	1.10663000	-3.79256700
C	-1.94082100	-2.81584600	-0.36002900	H	-2.57632800	-0.32714700	-4.09888400
H	-2.50005800	-2.01546300	-0.85387200	H	-1.77481300	-0.02397800	0.09747900
H	-2.04726000	-3.74018100	-0.92345500	O	-5.42844800	2.12148000	-1.53840600
H	-2.32094900	-2.95679000	0.65579200	O	-3.93698600	1.49741700	0.61691700
VG2 (p-TsOH-H2O)				C	-3.18512400	1.10117400	1.76240100
C	0.70210500	3.49841300	0.42756300	H	-2.15482300	1.46341300	1.69936100
C	1.72243800	4.24107400	1.03988500	H	-3.68266300	1.55614600	2.61569900
C	2.55316000	3.63949600	1.97123500	H	-3.18961100	0.01093800	1.86952300
C	2.39646400	2.29371900	2.29096800	C	-5.10040400	3.51278400	-1.43622000
C	1.40237400	1.54317400	1.67003500	H	-4.60621700	3.85026200	-2.35153900
C	0.55782300	2.14837100	0.73900400	H	-6.04101300	4.04581700	-1.30876100
H	3.32344700	4.24226600	2.43908300	H	-4.45343500	3.69858900	-0.57566900
H	3.05233100	1.83195600	3.02140000	C	-0.80170300	-1.09845400	-2.16699300
H	-0.21414400	1.56551800	0.25666300	H	-0.53113700	-1.13442200	-3.22872300
O	1.88935800	5.57041400	0.70963500	O	0.22670900	-0.45614000	-1.42081000
O	-0.09072300	4.17090200	-0.45082700	H	1.02341200	-1.00897000	-1.47418800
C	-1.24724300	3.48674000	-0.93246800	C	-0.97730600	-2.56195600	-1.71463400
H	-1.87086800	3.15861600	-0.09517500	H	-1.86003400	-2.98751000	-2.19921700
H	-1.79029500	4.20950300	-1.53805200	C	0.21288400	-3.42756600	-2.11237400
H	-0.96889000	2.62673800	-1.54812800	H	0.07878700	-4.42280200	-1.67752000
C	0.99195200	6.43237500	1.41853300	H	0.21818400	-3.52221600	-3.19963100
H	1.17274000	6.36341400	2.49468600	O	1.47168600	-2.88015000	-1.74049300
H	1.19585900	7.44577700	1.07671300	H	1.57353500	-2.93471100	-0.76894100
H	-0.04705700	6.17444700	1.20027800	O	-1.08947300	-2.64213300	-0.28967600
C	1.27693900	0.06004300	1.97688300	C	-2.30069600	-2.73831200	0.33384100
H	1.22922300	-0.07561100	3.06168100	C	-2.22501300	-2.96492000	1.72256300
O	0.09047000	-0.50637200	1.45348400	C	-3.54367200	-2.59631900	-0.26587800
H	0.16895500	-0.56742800	0.48169100	C	-3.38086300	-2.98958400	2.49006600
C	2.50804100	-0.70250400	1.47827500	C	-4.70485500	-2.63875000	0.50945900
H	3.39830200	-0.25349400	1.92895900	C	-4.62570000	-2.82178600	1.88023900
C	2.49420000	-2.18853500	1.82656800	H	-3.31801600	-3.14804400	3.55880600
H	3.48388900	-2.60332100	1.64013400	H	-5.66587600	-2.51039400	0.02644800

H	-5.52315200	-2.83971000	2.48626700	O	0.80157100	-3.32468400	-0.57449100
H	-3.62339600	-2.40730300	-1.32832200	H	1.68008000	-3.35559300	-0.97853000
O	-0.97155100	-3.16142500	2.22555600	O	1.90474200	-0.94988400	-1.72370900
C	-0.79207600	-3.00298900	3.62663900	C	3.08044400	-0.51303900	-1.14449400
H	-1.28729600	-3.80523100	4.17803600	C	3.92756300	-1.44038600	-0.51919300
H	0.28150700	-3.05819000	3.79792600	C	3.43335900	0.82339400	-1.21019500
H	-1.17402400	-2.03321700	3.95625700	C	5.09743200	-0.99574400	0.09036800
VG- <i>p</i> -TsOH-H2O				C	4.61701700	1.26502000	-0.62195900
C	-0.11503100	0.40183700	2.63071300	C	5.43455500	0.35664600	0.03699500
C	-0.53325600	1.45049600	1.81860300	H	5.75120200	-1.69784600	0.59142700
C	0.42248500	2.19943400	1.14371000	H	4.88474100	2.31357500	-0.66800800
C	1.78186200	1.95965800	1.32285400	H	6.35045900	0.69050600	0.50967900
C	2.18332300	0.91020900	2.13656300	H	2.75397100	1.51124900	-1.70169800
C	1.24103900	0.10000700	2.77817300	O	3.53901700	-2.74435300	-0.56829300
H	-0.85763400	-0.20690300	3.13597200	C	4.08559300	-3.62869600	0.40845300
H	-1.58819900	1.66267700	1.69602900	H	3.97451500	-3.20509900	1.41021900
H	2.52033400	2.55777700	0.80164900	H	3.51105700	-4.54952900	0.33041200
H	3.24221400	0.69660900	2.24854000	H	5.13821400	-3.83575000	0.20499000
C	1.67833500	-1.07340100	3.60966700				
H	2.65484700	-1.43810400	3.28581600				
H	1.75805700	-0.78949300	4.66292600				
H	0.95563800	-1.88840500	3.53983000				
S	-0.02747700	3.33547700	-0.14691400				
O	0.45638000	4.67202900	0.21098200				
O	0.58824700	2.78629800	-1.37758500				
O	-1.52691400	3.27998400	-0.25425000				
H	-2.09086600	2.64345300	-1.45621500				
O	-2.43938500	2.09662300	-2.27412900				
H	-1.76691900	1.34088400	-2.43426600				
H	-2.46931000	2.66675700	-3.05878400				
C	-3.51920500	-0.65103500	0.36543500				
C	-4.04563600	-1.94350200	0.24529400				
C	-3.42486900	-2.86955000	-0.58108400				
C	-2.27706600	-2.52357700	-1.28763500				
C	-1.74409500	-1.24411900	-1.16235100				
C	-2.36940700	-0.31427700	-0.33635800				
H	-3.85906200	-3.85901400	-0.66671100				
H	-1.79381100	-3.25023500	-1.93040000				
H	-1.93954400	0.67149200	-0.21733600				
O	-5.17065500	-2.29650200	0.95582900				
O	-4.15159400	0.21940700	1.21302700				
C	-4.40762200	1.51875300	0.66671400				
H	-4.95932900	1.42716800	-0.27288100				
H	-5.01549400	2.04191300	1.40232600				
H	-3.48339100	2.07460900	0.49949100				
C	-6.37580100	-1.77398600	0.38381200				
H	-6.52765400	-2.18821900	-0.61649500				
H	-7.19050200	-2.08226600	1.03663400				
H	-6.34117500	-0.68313300	0.33176500				
C	-0.44425500	-0.88910300	-1.84047000				
H	-0.24620500	-1.61805700	-2.62926100				
O	-0.52664500	0.40782300	-2.46033800				
H	0.12743500	1.02322300	-2.07993400				
C	0.74145800	-0.91105900	-0.87056800				
H	0.74125600	0.02311200	-0.29375300				
C	0.74741700	-2.08112200	0.10314900				
H	1.59603000	-1.97222400	0.78882000				
H	-0.16326000	-2.06383400	0.70484700				