

Electronic Supplementary Information

SO₃H-Functionalized Brønsted Acidic Ionic Liquids as Efficient Catalysts for the Synthesis of Isoamyl Salicylate

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1. The fully optimized geometries of BAILs

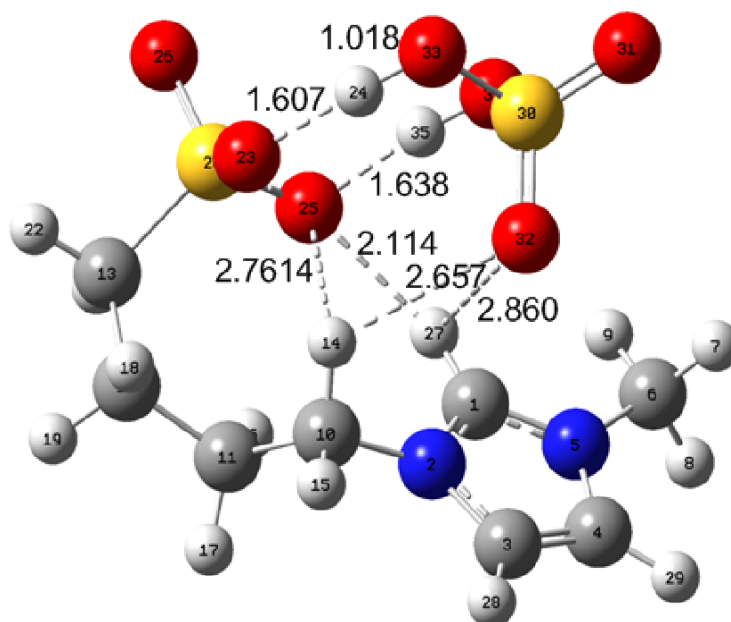


Figure S1. [BSmim][HSO₄]

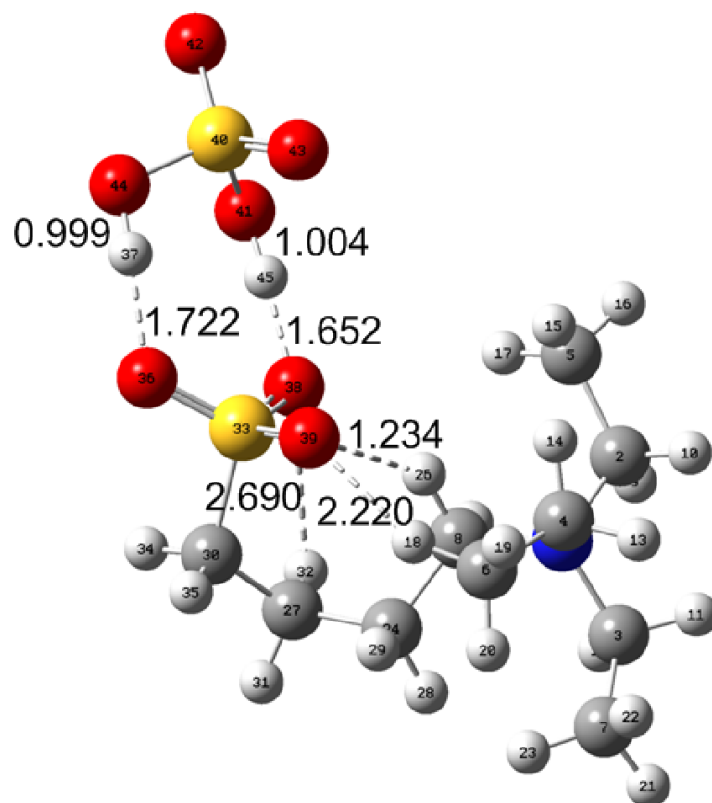


Figure S2. [BSEt₃N][HSO₄]

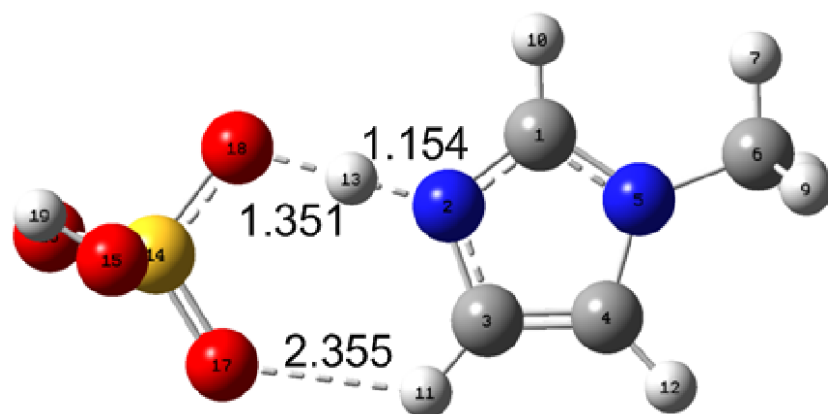


Figure S3. [Hmim][HSO₄]

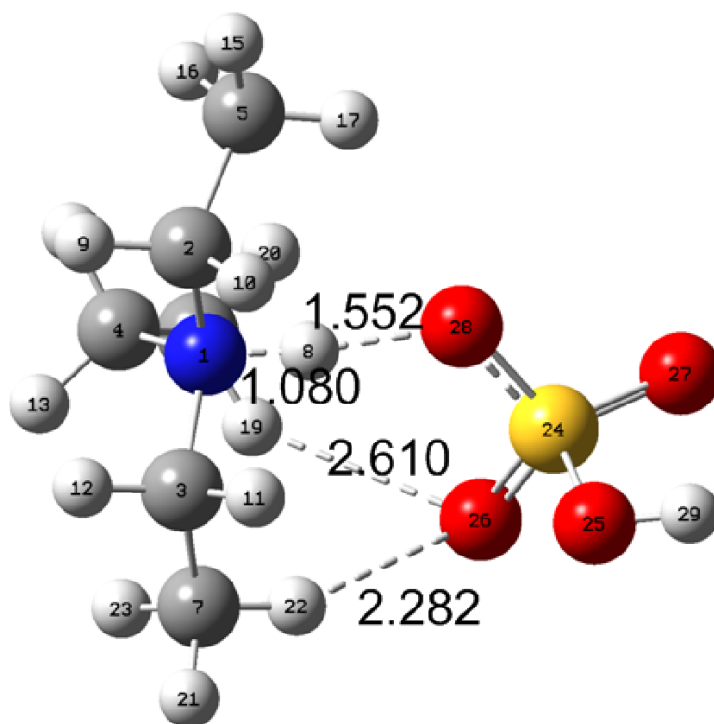


Figure S4. [Et₃NH][HSO₄]

2. Molecular coordinates

[BSmim][HSO₄]:

C	-1.60468300	-1.14581200	0.61359500
N	-1.36446400	-1.83745100	-0.50384600
C	-2.57354400	-2.22366200	-1.04855200
C	-3.55560100	-1.75987500	-0.22275000
N	-2.92551400	-1.09392900	0.81544400
C	-3.58396900	-0.32055000	1.87112800
H	-4.03708800	0.57389800	1.43807300
H	-4.34501900	-0.93539600	2.35496800
H	-2.83600100	-0.02028200	2.60445400
C	-0.02090000	-1.96055700	-1.10797300
C	0.92997700	-2.83223300	-0.27264800
C	2.41134800	-2.54326300	-0.60564500
C	3.12885100	-1.57847000	0.34647600
H	0.36294300	-0.94523600	-1.22122500
H	-0.16692300	-2.37915600	-2.10650400
H	0.75623100	-2.64163900	0.79107000
H	0.69980100	-3.88920900	-0.44907400
H	2.50460600	-2.17021300	-1.63203500
H	2.97590600	-3.48214800	-0.56924700
S	2.48173600	0.12088700	0.48055900
H	3.13591100	-1.95096000	1.37552700

H	4.16554600	-1.43418900	0.03094800
O	2.19465200	0.55837400	-0.93850100
H	1.26480700	1.85187600	-1.15221400
O	1.16335800	0.00933500	1.24319700
O	3.50827900	0.89578200	1.18942700
H	-0.83310500	-0.68500700	1.21467500
H	-2.63384100	-2.78277000	-1.96833800
H	-4.62880900	-1.84022500	-0.28512800
S	-0.73959300	2.38161100	-0.47653800
O	-1.53636600	3.58847600	-0.55255900
O	-1.30190700	1.10986500	-0.96265000
O	0.64407800	2.65673000	-1.20805800
O	-0.33539200	2.18206200	1.06763200
H	0.28807400	1.39189300	1.17883600

[BSEt₃][HSO₄]:

N	-3.09177200	-1.04257000	-0.13220000
C	-2.60223600	-2.42847100	-0.61727400
C	-4.49046000	-0.88648900	-0.72820500
C	-3.11933300	-1.10732500	1.40365100
C	-1.12976300	-2.75768400	-0.39208400
C	-3.10171800	0.19510800	2.19553400
C	-5.44850700	0.11014100	-0.08333300
C	-2.09076400	-0.02214600	-0.69620500
H	-2.83695400	-2.45869100	-1.68461600
H	-3.24472300	-3.15250700	-0.10822600
H	-4.94164800	-1.88134800	-0.68429500
H	-4.33025600	-0.64449600	-1.78210600
H	-3.99782900	-1.71511500	1.64077900
H	-2.23364200	-1.67653000	1.68226800
H	-0.83276900	-2.73577000	0.65872500
H	-0.97799200	-3.78142500	-0.74927000
H	-0.45000800	-2.10730100	-0.94406800
H	-2.15621100	0.72360000	2.06051900
H	-3.16435200	-0.08916100	3.25164600
H	-3.94285500	0.85567800	1.98391000
H	-6.36683300	0.09918400	-0.67943200
H	-5.72084700	-0.17682000	0.93440500
H	-5.07151600	1.13216100	-0.07346400
C	-2.47673200	1.45895400	-0.76994000
H	-1.88039000	-0.37319400	-1.70978700
H	-1.19531700	-0.15107300	-0.09788000
C	-1.32727600	2.29327900	-1.39704500
H	-3.35501600	1.58566000	-1.41259200
H	-2.72450300	1.86449300	0.21297600
C	-0.18134700	2.75350500	-0.48186700
H	-1.77549300	3.20624300	-1.80717000

H	-0.90006900	1.75014700	-2.24735800
S	0.79524500	1.40954700	0.27260200
H	0.53241800	3.34352700	-1.06268700
H	-0.53768200	3.36408000	0.35319800
O	2.08307600	2.02210300	0.70664200
H	3.55695600	1.13155300	0.69001300
O	0.96695200	0.40985400	-0.85012500
O	-0.04833000	0.87637800	1.37974300
S	4.11811500	-0.85767700	0.02250800
O	3.35452800	-0.62627600	-1.37609000
O	5.40504700	-1.44587900	-0.29149400
O	3.19575900	-1.50698900	0.95338900
O	4.41162700	0.64148000	0.52462100
H	2.43573700	-0.26341000	-1.19472700

[Hmim][HSO₄]:

C	-2.17038600	-0.94216100	-0.03981200
N	-1.04817500	-0.23627500	-0.07395700
C	-1.37379000	1.09965000	-0.03771200
C	-2.73798800	1.19217600	0.01951900
N	-3.22675500	-0.10533000	0.01773600
C	-4.63358300	-0.49499500	0.06909200
H	-4.70118300	-1.58325100	0.04929000
H	-5.16613700	-0.08861700	-0.79391000
H	-5.09110900	-0.12548600	0.98981400
H	-2.23973400	-2.01913000	-0.05555400
H	-0.59599900	1.84816100	-0.05651500
H	-3.39428800	2.04691200	0.06116700
H	0.02986700	-0.64603800	-0.12420100
S	2.34519400	-0.00264100	-0.11783300
O	2.93829300	-0.12466500	1.42923100
O	3.48591000	-0.25796100	-1.00065800
O	1.69735100	1.31871600	-0.14085600
O	1.29601400	-1.11362900	-0.19277600
H	3.71393800	-0.70676200	1.38273200

[Et₃NH][HSO₄]:

N	-1.63191600	0.05241400	-0.28665900
C	-2.26104900	-1.12225000	-0.99664400
C	-1.54328400	1.23215900	-1.22889500
C	-2.33130200	0.38285900	1.01839400
C	-2.08665900	-2.44137300	-0.25050200
C	-1.36957600	0.45573800	2.20052900
C	-0.88926500	2.47306400	-0.63136900
H	-0.61628300	-0.26124400	-0.09503400
H	-3.31643200	-0.87684200	-1.15880700

H	-1.77077900	-1.18324200	-1.97113000
H	-0.95806200	0.87979300	-2.08203700
H	-2.56351400	1.43867900	-1.57221300
H	-2.86084400	1.32743900	0.87361500
H	-3.08762400	-0.38587700	1.18745800
H	-2.52097600	-3.24281200	-0.85589200
H	-2.59724800	-2.44983300	0.71701000
H	-1.02741000	-2.65869600	-0.09396700
H	-1.92530500	0.76423600	3.09169300
H	-0.55608600	1.16423000	2.02776000
H	-0.91566500	-0.51909600	2.39816600
H	-0.79534100	3.21941300	-1.42633500
H	0.10981000	2.25439200	-0.24460400
H	-1.48975600	2.92037600	0.16591500
S	2.03746500	-0.19473900	0.14216700
O	2.49313600	0.23884900	-1.41149400
O	1.75619700	1.08561800	0.81836300
O	3.14518500	-1.01594500	0.64626000
O	0.76205100	-0.97516300	-0.09485500
H	3.34974400	-0.19004900	-1.56493200