

Supporting Information

Belonging to the manuscript

**High Yield of Ethyl Valerate from the Esterification of  
Renewable Valeric Acid Catalyzed by Amino Acid Ionic  
Liquids**

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### **Geometry Coordinates**

B3LYP/6-311++G(d,p) optimized geometries (Å)

#### **GlyHSO<sub>4</sub>**

N	-1.52247900	1.72958000	0.25264200
C	-1.91715600	0.73077800	-0.79333300
C	-2.29208900	-0.56884700	-0.05214800
O	-1.57726200	-1.64251300	-0.31310400
O	-3.22054100	-0.53806500	0.72044800
H	-0.49196700	1.49784400	0.54392400
H	-1.54624500	2.68501600	-0.10190500
H	-2.15961000	1.65617600	1.05066300
H	-1.08178000	0.61781500	-1.48034500
H	-2.80755000	1.08337200	-1.31324700
H	-0.68067200	-1.39705800	-0.67915800
S	1.68524800	0.04534900	-0.05159500
O	0.78264000	-0.67801000	-0.99598800
O	0.93555200	1.11976100	0.67915300
O	2.96043900	0.44967300	-0.61538500
O	1.99251400	-1.00758700	1.17556900
H	2.72994400	-1.57345600	0.90443100

#### **AlaHSO<sub>4</sub>**

N	1.35594300	-1.27419300	0.92668000
C	1.80015000	-0.57436600	-0.33642200
C	1.95443900	0.91765200	0.05496100
O	1.12920200	1.77659800	-0.50527700
O	2.82023800	1.22434800	0.84048200
H	0.28903800	-1.08717200	1.05840100
H	1.49409800	-2.28296800	0.86016500
H	1.89527300	-0.92246100	1.72246800
H	0.99284000	-0.71261700	-1.05401200
H	0.30649700	1.32617300	-0.85363900
S	-1.96060600	-0.15791800	-0.08675000
O	-1.03507200	0.40811100	-1.11362800
O	-1.19101200	-0.87274300	0.98236300
O	-3.09894600	-0.88007000	-0.62678500
O	-2.54318700	1.13113500	0.75507700
H	-3.30065000	1.48559400	0.26720600
C	3.11558000	-1.14563400	-0.84944300
H	3.01380200	-2.21063600	-1.07758700
H	3.39983000	-0.63564300	-1.77177900
H	3.91655800	-0.99918500	-0.12240300

**ProHSO<sub>4</sub>**

C	1.44208400	1.68995500	0.04335300
O	0.37904200	2.37307100	-0.33258100
O	2.34527800	2.16016600	0.69445100
H	-0.35919200	1.78054800	-0.65502700
S	-2.25715000	-0.29838000	-0.12378000
O	-1.50513300	0.65183000	-0.99780100
O	-1.32119600	-1.09189600	0.73152800
O	-3.28603900	-1.06353000	-0.80581800
O	-3.00266500	0.63890600	1.01297700
H	-3.80424800	1.00821300	0.61499000
C	1.49199800	0.20341500	-0.36744500
C	2.84548700	-0.29307200	-0.86864000
H	0.69201200	-0.04143000	-1.06498400
C	2.77266400	-1.80540800	-0.60439500
H	3.64431100	0.17926100	-0.29127000
H	2.99351200	-0.05161400	-1.92159400
C	2.05024700	-1.91795400	0.74766200
H	2.19050200	-2.30143200	-1.38451500
H	3.75545500	-2.27696800	-0.57104600
H	1.36645700	-2.76228700	0.81465500
H	2.74544700	-1.95539700	1.58575500
N	1.24069900	-0.63894200	0.87197900
H	1.53110200	-0.11297700	1.69713000
H	0.18497700	-0.82922900	0.92727500

**Deprotoned GlyHSO<sub>4</sub>**

N	-1.05339500	1.56381000	0.43950100
C	-1.77416700	0.85495600	-0.63519900
C	-2.49843300	-0.37398800	-0.07610200
O	-1.75125800	-1.44260900	0.16750900
O	-3.69407000	-0.36540700	0.14230100
H	0.41341900	0.60865800	1.39272700
H	-0.29966200	2.11108700	0.02969700
H	-1.67767500	2.17322300	0.95614300
H	-1.02881600	0.53999700	-1.36689200
H	-2.52716700	1.47679900	-1.13079600
H	-0.78670300	-1.31077600	-0.08425900
S	1.75998300	-0.11720800	-0.10620900
O	0.74922500	-1.13415000	-0.55702000
O	1.31447800	0.22118700	1.45876100

O	1.60707600	1.16274100	-0.84057700
O	3.11907900	-0.63628100	0.01578000

#### Deprotoned AlaHSO<sub>4</sub>

N	-0.96535800	1.03511500	1.01794700
C	-1.64615100	0.60895800	-0.22413300
C	-2.15702200	-0.82977400	-0.00805100
O	-1.26892300	-1.79850500	-0.18248700
O	-3.30273300	-1.06547400	0.32007800
H	0.68254300	0.06026700	1.53726600
H	-0.34555900	1.81372200	0.80403100
H	-1.64368300	1.32297700	1.71722700
H	-0.86850400	0.58109700	-0.98910100
H	-0.35602000	-1.45785600	-0.43413300
S	2.00578600	0.02115200	-0.14954800
O	1.11090500	-0.94436700	-0.87652800
O	1.62502500	-0.20830600	1.45176300
O	1.63668600	1.42802800	-0.43989200
O	3.42639100	-0.30754000	-0.22730200
C	-2.77310300	1.54321000	-0.66658000
H	-2.38018500	2.55446200	-0.80759700
H	-3.21224200	1.20956800	-1.61150300
H	-3.57256500	1.56648200	0.07847000

#### Deprotoned ProHSO<sub>4</sub>

C	1.60523100	1.55948700	0.02462100
O	0.49107700	2.26389100	0.16641800
O	2.68489200	2.00205000	0.36415600
H	-0.33925200	1.77932700	-0.14786000
S	-2.37077200	-0.07522900	0.00277900
O	-1.63997300	1.04323900	-0.69422300
O	-1.72236000	-1.45591400	-0.65437400
O	-3.78738300	-0.15825700	-0.33933400
O	-2.01779900	-0.12593700	1.44059900
C	1.41951100	0.14412800	-0.56883100
C	2.75324300	-0.51119100	-0.99502800
H	0.71452000	0.22924000	-1.39924400
C	2.83705700	-1.83266800	-0.19959700
H	3.57249000	0.15657800	-0.72465100
H	2.78918700	-0.67616700	-2.07382400
C	1.95237600	-1.55981400	1.01904000
H	2.41544300	-2.66086500	-0.77698700
H	3.86240900	-2.09550200	0.07257000

H	1.57406300	-2.46881100	1.49463300
H	2.51035000	-0.98380300	1.77348200
N	0.84258200	-0.79974500	0.43149700
H	0.24549800	-0.34882200	1.12407100
H	-0.78256000	-1.48150500	-0.35431500