

Supporting information for

Enhanced aminolysis of cyclic carbonates by β -hydroxyamines for fully biobased polyhydroxyurethanes

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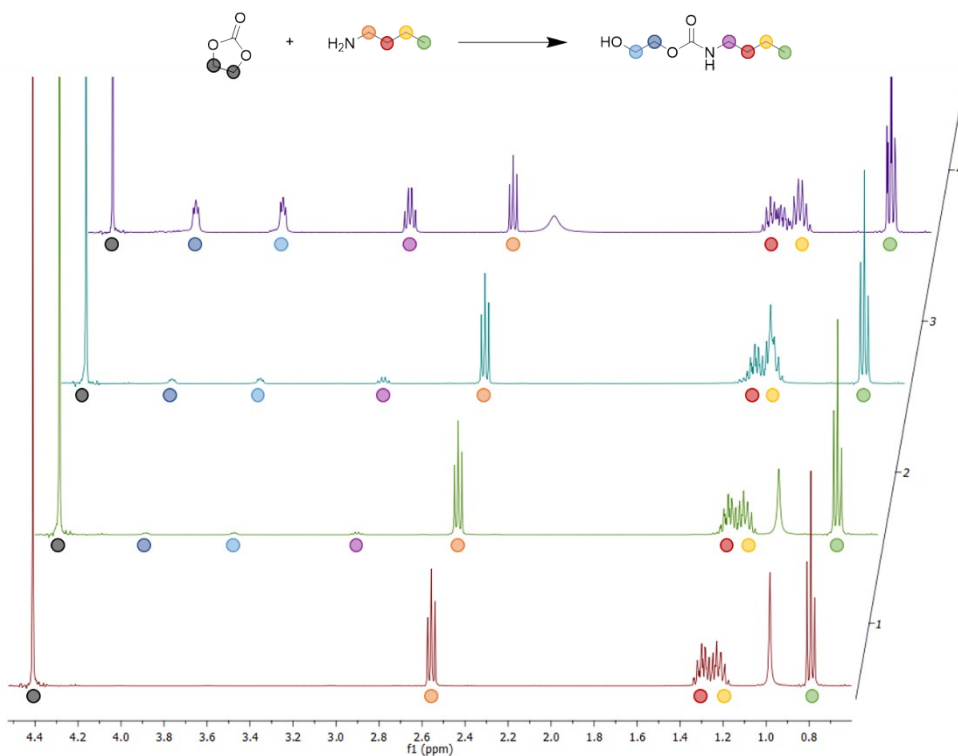


Figure S1: ^1H NMR monitoring of the aminolysis of ethylene carbonate (1 mol/L) with butylamine (1 mol/L) over the time in CDCl_3 at 25°C. **Spectrum 1:** t = 9 min; **spectrum 2:** t = 1 h; **spectrum 3:** t = 2 h; **spectrum 4:** t = 14 h

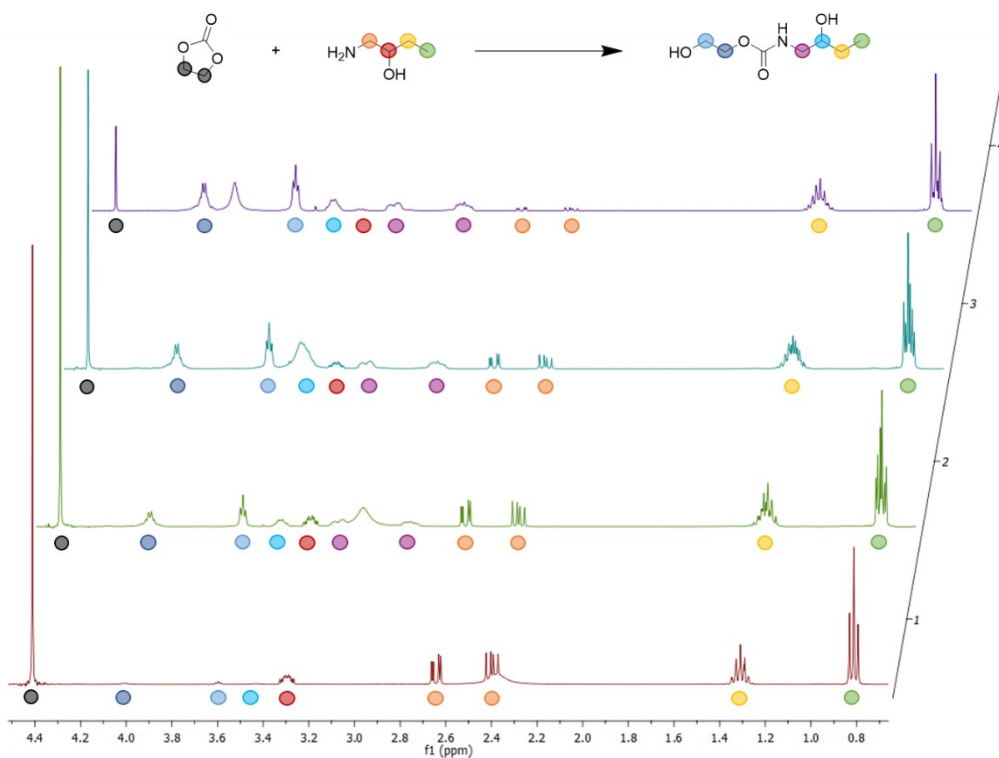


Figure S2: ^1H NMR monitoring of the aminolysis of ethylene carbonate (1 mol/L) with 1-amino-2-butanol (1 mol/L) over the time in CDCl_3 at 25°C. **Spectrum 1:** t = 5 min; **spectrum 2:** t = 1 h; **spectrum 3:** t = 2 h; **spectrum 4:** t = 14 h

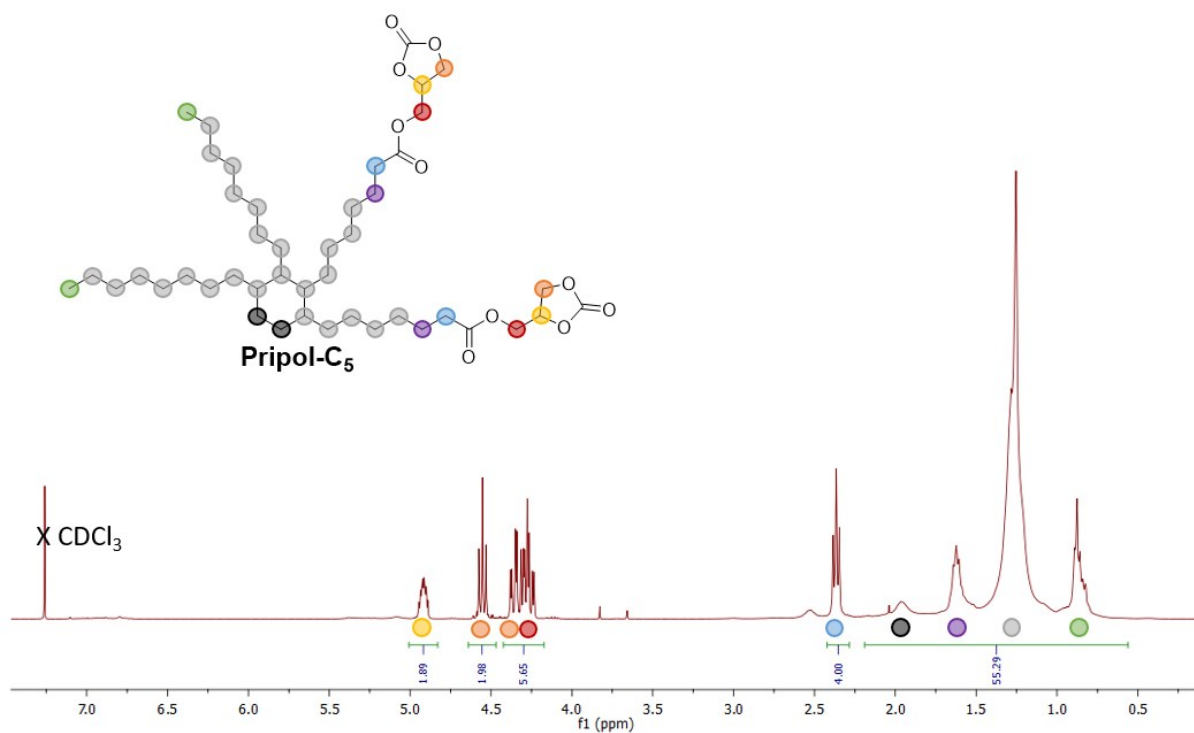


Figure S5: ¹H NMR spectrum of Pripol-C₅ in CDCl₃. Pripol is represented as an ideal structure.

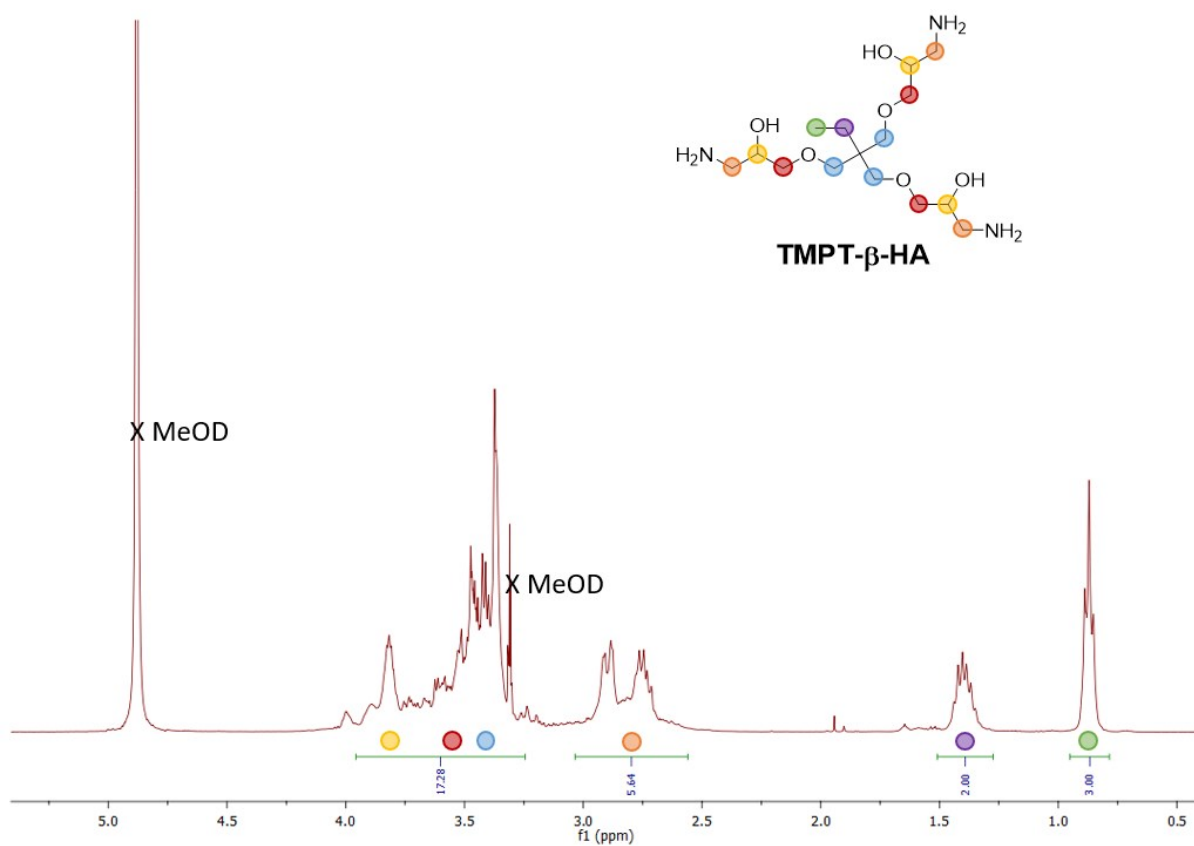


Figure S6: ¹H NMR spectrum of TMPT-β-HA in MeOD

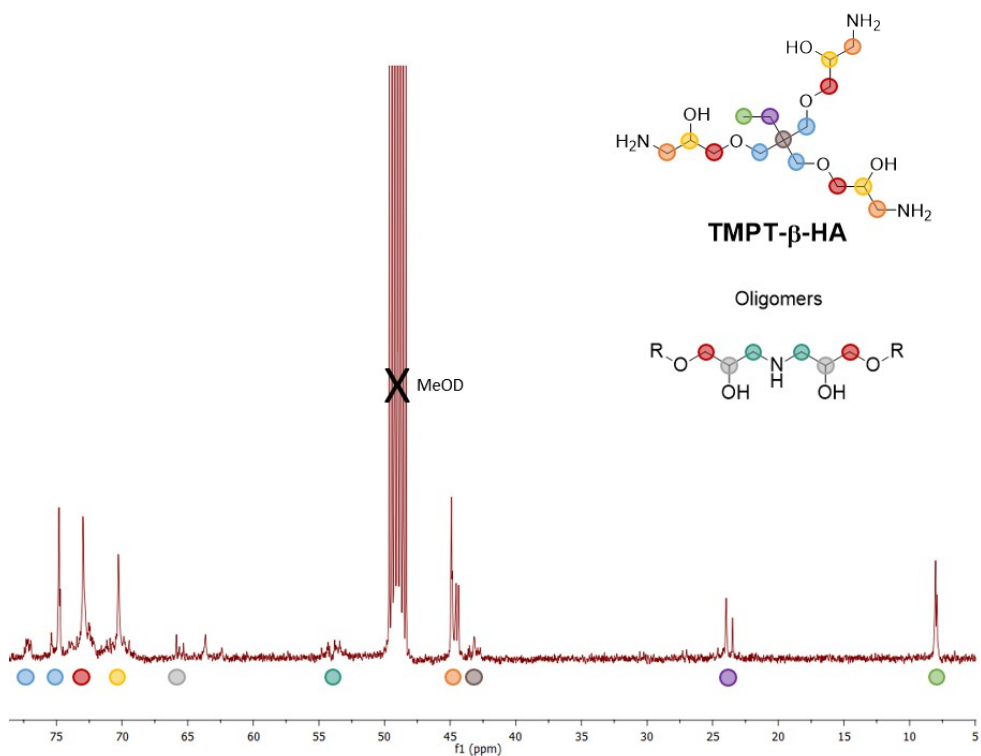


Figure S7: ^{13}C NMR spectrum of TMPT-β-HA in MeOD

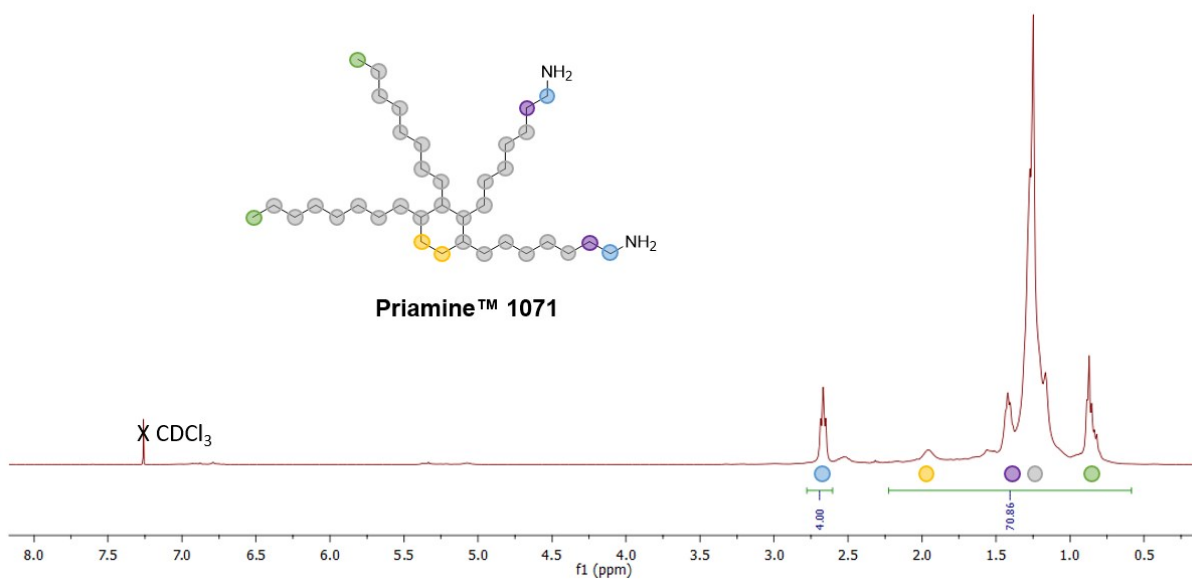


Figure S8: ^1H NMR spectrum of Priamine™ 1071 in CDCl_3 . Priamine™ 1071 is represented with an ideal structure.

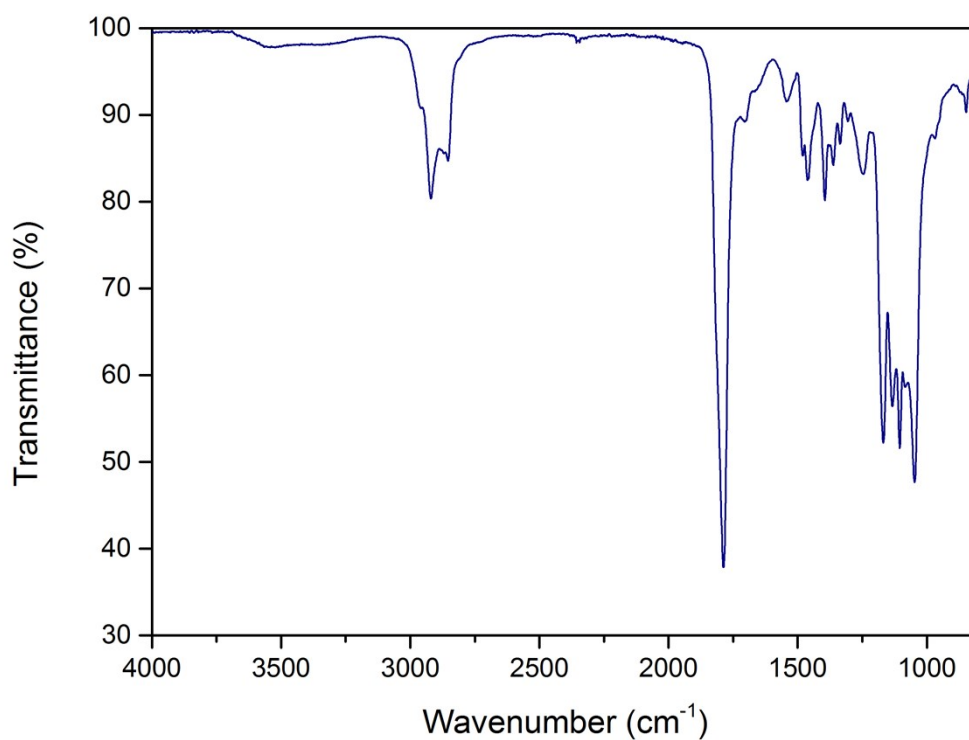


Figure S9: FTIR spectrum of PHU1

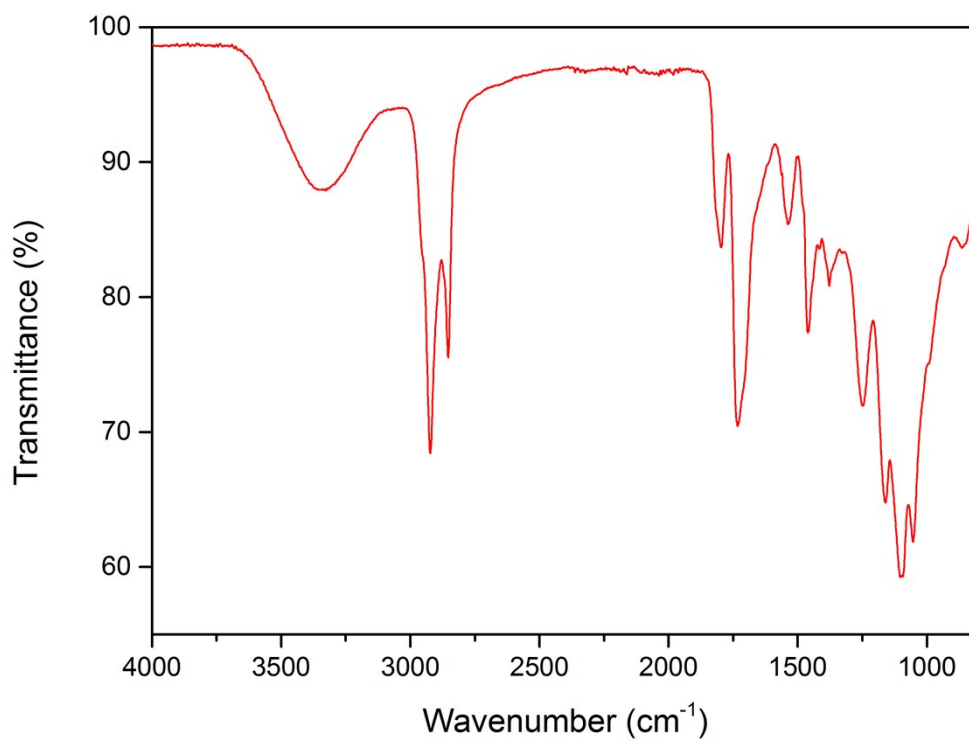


Figure S10: FTIR spectrum of PHU2

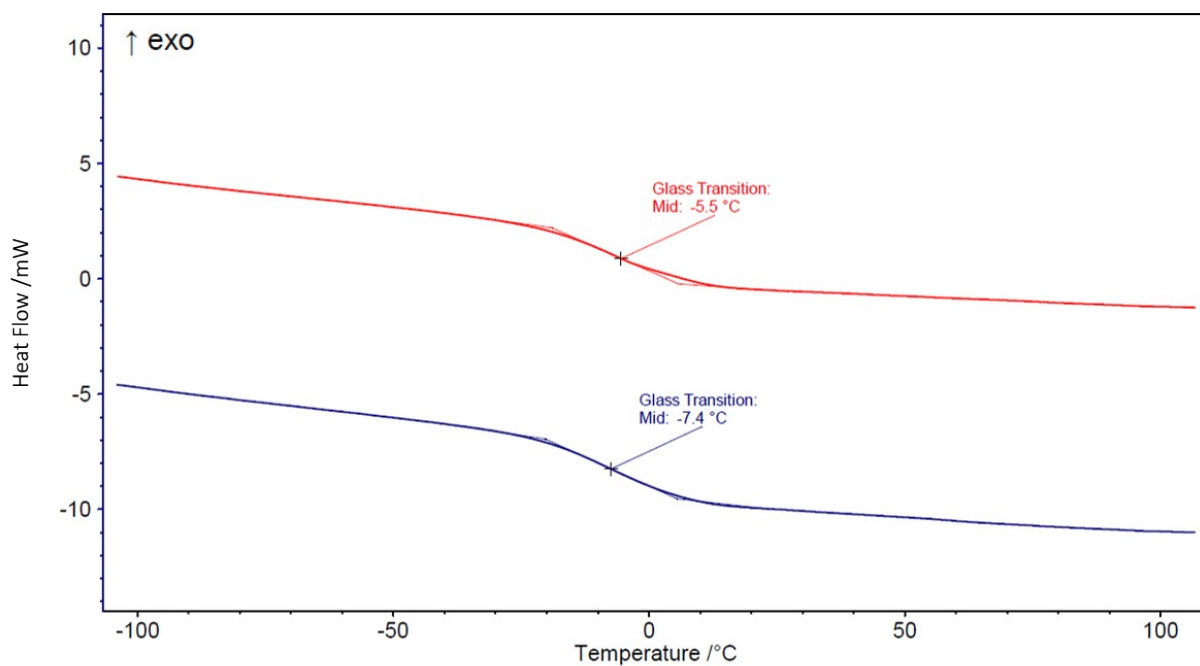


Figure S11: DSC thermograms of PHU1 (blue) and PHU2 (red)

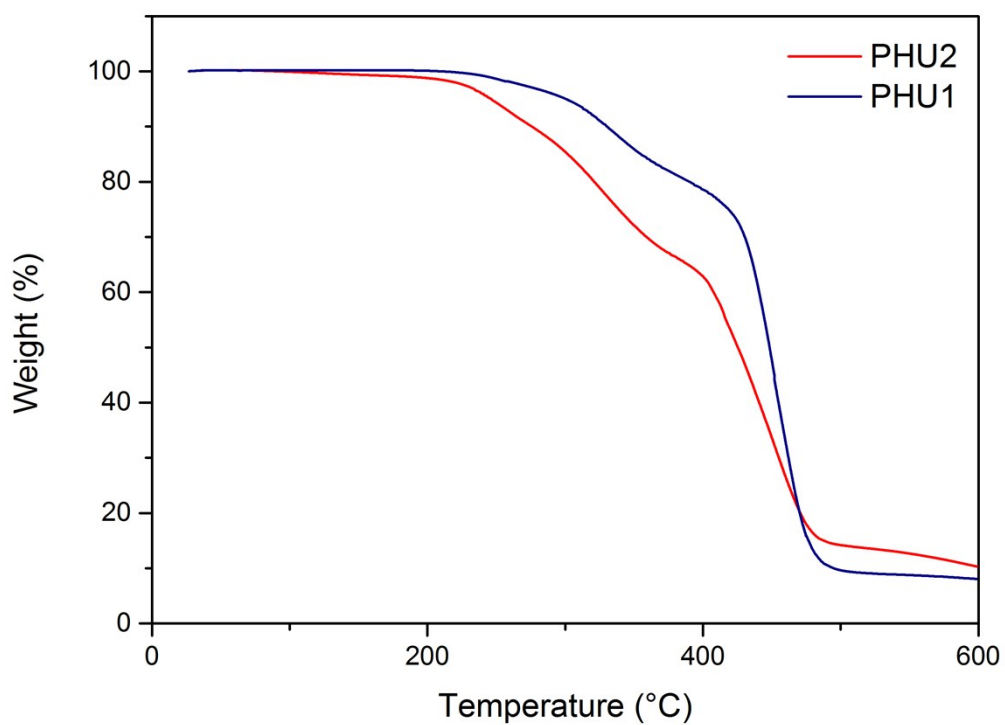


Figure S12: TGA curves of PHU thermosets

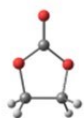
Table S1. Calculated energies (E-D₃_{CHCl₃} and G-D₃_{CHCl₃,298K,1M} in hartrees), views and atomic Cartesian coordinates (in Å) for all optimized structures.

A. Reagents

Ethylene carbonate (EC)

E = -342.516350959

G = -342.469392

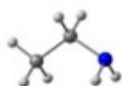


6	0.848373000	-0.000068000	0.000028000
8	0.077144000	1.120014000	0.116006000
8	0.076776000	-1.120042000	-0.115824000
6	-1.312055000	0.754014000	-0.131042000
6	-1.312216000	-0.753847000	0.130930000
1	-1.553416000	1.004374000	-1.176229000
1	-1.951187000	1.323537000	0.555319000
1	-1.951428000	-1.323249000	-0.555469000
1	-1.553927000	-1.004026000	1.176096000
8	2.054247000	-0.000126000	-0.000084000

EtNH₂

E = -135.219854975

G = -135.152756

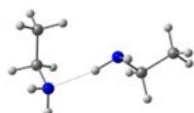


6	-1.239983000	-0.265520000	-0.000011000
1	-1.282083000	-0.914900000	0.891910000
1	-1.282149000	-0.914810000	-0.891978000
1	-2.145597000	0.366979000	0.000079000
6	0.043466000	0.579728000	0.000080000
1	0.051032000	1.243061000	-0.882967000
1	0.051024000	1.243027000	0.883002000
7	1.309026000	-0.183891000	0.000011000
1	1.311854000	-0.810597000	-0.813772000
1	1.311836000	-0.810769000	0.813666000

CH₃CH₂NH₂...NH₂CH₂CH₃

E = -270.44841612

G = -270.299933



7	1.738936000	1.155209000	0.216861000
1	2.308104000	1.279521000	1.061789000
6	2.318900000	0.068645000	-0.606566000
1	1.729205000	0.009308000	-1.537705000
1	3.370141000	0.265699000	-0.904628000
6	2.234154000	-1.265000000	0.137936000
1	1.188024000	-1.489090000	0.402172000
1	2.825189000	-1.234938000	1.070378000
1	2.628599000	-2.087685000	-0.480665000
6	-1.996416000	0.405677000	-0.302423000
1	-1.518433000	0.250174000	-1.286352000
1	-2.240058000	1.490577000	-0.242883000
7	-1.047340000	-0.047815000	0.731115000
1	-0.152636000	0.469741000	0.633773000
1	-1.421549000	0.192648000	1.656343000
6	-3.298240000	-0.397056000	-0.239771000
1	-3.815571000	-0.233877000	0.722431000
1	-3.992591000	-0.105798000	-1.045952000
1	-3.090222000	-1.476222000	-0.328964000
1	1.790240000	2.044592000	-0.290623000

HOCH₂CH₂NH₂

E = -210.459640109



G = -210.389818

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1	-0.490775000	-1.143050000	0.896546000
1	-0.490633000	-1.143034000	-0.896577000
6	0.557041000	0.529142000	0.000061000
1	0.449776000	1.178702000	-0.885668000
1	0.449841000	1.178567000	0.885891000
7	1.909887000	-0.053171000	-0.000031000
1	2.013096000	-0.666482000	-0.816651000
1	2.013203000	-0.666389000	0.816641000
8	-1.826412000	0.230508000	-0.000113000
1	-2.544201000	-0.426686000	0.000620000

HOCH₂CH₂NH₂...NH₂CH₂CH₂OH

E = -420.953641688

G = -420.794179



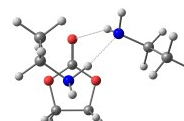
7	-1.361962000	1.493574000	0.237795000
1	-2.004601000	1.841369000	-0.483249000
6	-1.920523000	0.271757000	0.854164000
1	-1.179937000	-0.098251000	1.583805000
1	-2.864253000	0.451858000	1.409937000
6	-2.189883000	-0.809073000	-0.204498000
1	-3.053728000	-0.499293000	-0.823661000
1	-2.501952000	-1.733290000	0.333963000
6	2.334517000	-0.627090000	0.161361000
1	2.654062000	-0.918390000	-0.852982000
1	3.184004000	-0.813424000	0.851773000
7	1.136330000	-1.427494000	0.505812000
1	1.351829000	-2.427941000	0.440875000
1	0.885655000	-1.257664000	1.486739000
6	2.023751000	0.875289000	0.152111000
1	1.619166000	1.166749000	1.147726000
1	2.982807000	1.415292000	0.030563000
1	-1.283483000	2.239065000	0.936586000
8	-1.109164000	-1.036069000	-1.095635000
1	-0.277421000	-1.145705000	-0.539915000
8	1.154763000	1.263005000	-0.899766000
1	0.215315000	1.236285000	-0.543023000

B. Amine two-molecule pathway

EC... CH₃CH₂NH₂...NH₂CH₂CH₃

E = -612.981768028

G = -612.770246

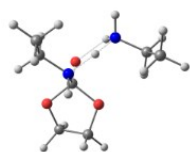


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6	1.494684000	-1.528812000	-1.203727000
1	3.654132000	-1.044045000	-0.999863000
1	2.628037000	0.316385000	-1.610879000
1	1.812923000	-2.542426000	-1.484176000
1	0.775747000	-1.121567000	-1.926199000
8	0.918422000	-0.456349000	2.035523000
1	-1.251252000	-0.446143000	1.502754000
7	-0.006757000	1.258539000	-0.991824000
1	-0.407415000	1.588322000	-1.877761000
6	0.374377000	2.428583000	-0.175687000

1	0.756683000	2.049218000	0.787399000
1	1.224077000	2.939519000	-0.664274000
6	-0.758939000	3.434961000	0.081411000
1	-1.601795000	2.942009000	0.594667000
1	-1.140064000	3.849321000	-0.868791000
1	-0.422200000	4.279851000	0.708488000
1	-0.773380000	0.762303000	-0.494659000
6	-2.557586000	-1.442294000	0.242862000
1	-1.722075000	-2.015022000	-0.192240000
7	-1.984003000	-0.211234000	0.822638000
6	-3.577547000	-1.097015000	-0.843653000
1	-4.423436000	-0.523986000	-0.425240000
1	-3.113716000	-0.483414000	-1.633989000
1	-3.989149000	-2.008513000	-1.307914000
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(EC+2EtNH₂) TS1

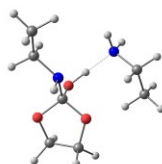
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1	3.369613000	-1.370369000	0.641700000
1	3.874729000	-0.521523000	-0.868379000
1	2.142480000	-2.676202000	-1.036132000
1	1.816075000	-1.203910000	-2.022858000
8	0.625988000	-0.053501000	1.737632000
1	-1.272843000	-0.348282000	1.640543000
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1	0.228104000	0.759450000	-1.324977000
6	0.109361000	2.310673000	0.044466000
1	-0.051975000	2.352776000	1.133596000
1	1.131831000	2.680218000	-0.149081000
6	-0.928219000	3.150530000	-0.700075000
1	-1.951864000	2.795082000	-0.494170000
1	-0.768269000	3.110102000	-1.791163000
1	-0.866464000	4.207007000	-0.392379000
1	-1.227234000	0.352334000	0.128039000
6	-2.463529000	-1.525711000	0.342076000
1	-1.556010000	-2.100430000	0.104961000
7	-1.986895000	-0.224235000	0.884535000
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1	-4.214065000	-0.709723000	-0.681490000
1	-2.742765000	-0.801667000	-1.692524000
1	-3.656921000	-2.282510000	-1.304612000
1	-3.023085000	-2.067405000	1.122350000
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(EC+2EtNH₂) tetrahedral intermediate

E = -612.973651845
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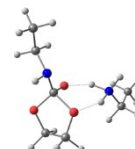


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6	0.336974000	-2.807469000	0.427270000
6	-0.624548000	-2.442790000	-0.717940000
1	-0.182673000	-2.831815000	1.402141000
1	0.875502000	-3.752752000	0.269001000

1	-1.669656000	-2.715022000	-0.496213000
1	-0.322513000	-2.908872000	-1.672513000
8	-0.070244000	-0.140612000	1.301943000
1	-0.620071000	0.708745000	1.094912000
7	1.246966000	0.472176000	-0.536325000
1	1.600513000	0.089466000	-1.418939000
6	2.355628000	1.040496000	0.255680000
1	1.929373000	1.397630000	1.205698000
1	3.116049000	0.274744000	0.511565000
6	3.009936000	2.194089000	-0.504215000
1	2.270973000	2.977417000	-0.740219000
1	3.449858000	1.846297000	-1.454896000
1	3.819172000	2.645187000	0.092695000
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1	-2.880231000	2.525859000	-0.917523000
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1	-0.793968000	2.753937000	0.362878000
1	-2.048838000	2.470984000	1.391214000
6	-3.305283000	0.558162000	-0.085199000
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(EC+2EtNH₂) TS2

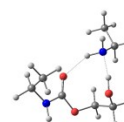
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6	0.012314000	2.492851000	-0.696612000
6	-0.440506000	2.327482000	0.770641000
1	-0.772073000	2.155330000	-1.401035000
1	0.321156000	3.517571000	-0.950826000
1	-1.521412000	2.545611000	0.881573000
1	0.121587000	3.031159000	1.419781000
8	-0.016911000	-0.348477000	-1.006110000
1	-1.110941000	-0.983593000	-0.126104000
7	1.844574000	-0.298450000	0.385113000
1	2.446318000	0.401221000	0.827059000
6	2.622050000	-1.232040000	-0.449110000
1	1.899576000	-1.900889000	-0.940709000
1	3.177378000	-0.708957000	-1.256972000
6	3.595912000	-2.036661000	0.412422000
1	3.055517000	-2.584057000	1.202407000
1	4.334931000	-1.378949000	0.901937000
1	4.152515000	-2.764793000	-0.200709000
6	-3.197756000	-0.626342000	0.269494000
1	-3.125004000	0.325942000	-0.277075000
1	-3.820935000	-0.459708000	1.161755000
7	-1.815206000	-0.958824000	0.714598000
1	-1.328419000	-0.142424000	1.213696000
1	-1.773290000	-1.820894000	1.270212000
6	-3.775407000	-1.722723000	-0.619916000
1	-3.837009000	-2.682948000	-0.081104000
1	-4.791853000	-1.451260000	-0.944878000
1	-3.154954000	-1.866515000	-1.518914000

(EC+2EtNH₂) product

E = -613.00529134
G = -612.731899



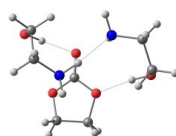
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6	-0.636718000	2.327671000	0.756962000
1	-1.015606000	1.219792000	-1.100179000
1	-0.472891000	2.913050000	-1.338894000
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8	0.414748000	-0.623006000	-1.054600000
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6	3.023588000	-1.358217000	-0.234327000
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1	3.225645000	-1.109217000	1.927704000
1	3.065676000	-2.807720000	1.397232000
6	-3.188548000	-0.585154000	0.143279000
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1	-3.913770000	-0.360512000	0.944026000
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1	-0.983439000	0.489416000	1.398740000
1	-1.949254000	-1.686270000	1.376657000
6	-3.714761000	-1.717530000	-0.747907000
1	-3.842489000	-2.647436000	-0.167370000
1	-4.690726000	-1.458245000	-1.193368000
1	-3.008299000	-1.924292000	-1.569569000

C. Hydroxylamine two-molecule pathway

EC...HOCH₂CH₂NH₂...NH₂CH₂CH₂OH

E = -763.474846537

G = -763.252799



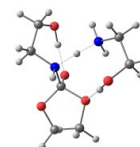
6	0.582272000	1.066738000	-0.843582000
8	1.690559000	1.767158000	-0.537667000
8	-0.511900000	1.542039000	-0.182578000
6	1.422879000	2.543581000	0.665457000
6	-0.108216000	2.652335000	0.673825000
1	1.932224000	3.510057000	0.568725000
1	1.811363000	1.975257000	1.521679000
1	-0.480563000	3.581994000	0.218818000
1	-0.555017000	2.504039000	1.664877000
8	0.518355000	0.203720000	-1.697872000
7	0.891433000	-0.586672000	1.252730000
1	0.019840000	-1.027137000	0.897538000
1	0.673943000	-0.222418000	2.185405000
6	1.950446000	-1.607669000	1.355899000
1	2.887166000	-1.122216000	1.684208000
1	1.719788000	-2.411073000	2.092177000
6	2.209887000	-2.289722000	0.007421000
1	1.267291000	-2.757123000	-0.348945000
1	2.937549000	-3.105250000	0.163388000
8	2.769679000	-1.430337000	-0.988396000
1	2.050399000	-0.834247000	-1.286067000
7	-1.497860000	-1.757939000	-0.274402000
1	-1.284322000	-1.110616000	-1.043072000
1	-1.240306000	-2.686599000	-0.622583000
6	-2.941105000	-1.716500000	0.032773000
1	-3.151757000	-2.459368000	0.822825000
1	-3.581770000	-1.964265000	-0.839538000

6	-3.344965000	-0.333271000	0.543334000
1	-2.748159000	-0.083577000	1.444108000
1	-4.408668000	-0.353565000	0.837256000
8	-3.211415000	0.683165000	-0.462734000
1	-2.273424000	0.959478000	-0.465881000

(EC+2HOCH₂CH₂NH₂) TS1

E = -763.467416152

G = -763.240831

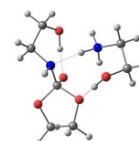


6	-1.107542000	0.287860000	-0.235338000
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8	-0.934309000	-1.241136000	-0.399065000
6	-3.185115000	-0.695842000	-0.162025000
6	-2.200115000	-1.865126000	-0.112364000
1	-3.478192000	-0.460081000	-1.203164000
1	-4.083699000	-0.846667000	0.452973000
1	-2.406463000	-2.642488000	-0.865424000
1	-2.182075000	-2.323593000	0.895036000
8	-0.914689000	0.935169000	-1.311179000
7	-0.089923000	0.611135000	0.853681000
1	-0.277816000	0.027795000	1.675180000
1	0.988656000	0.245309000	0.230783000
6	-0.087493000	2.064027000	1.220344000
1	-1.062987000	2.497709000	0.950167000
1	0.036085000	2.148141000	2.310838000
6	1.045276000	2.821030000	0.524121000
1	2.017746000	2.445055000	0.907242000
1	0.976052000	3.885706000	0.820769000
8	1.020667000	2.708715000	-0.901506000
1	0.247751000	2.107227000	-1.144435000
7	1.919049000	-0.052561000	-0.655445000
1	1.386704000	-0.354736000	-1.482543000
1	2.347030000	0.848132000	-0.907343000
6	2.898782000	-1.080116000	-0.224643000
1	3.353509000	-0.728577000	0.715500000
1	3.699177000	-1.206174000	-0.975261000
6	2.188502000	-2.416953000	0.009603000
1	1.796181000	-2.796160000	-0.956553000
1	2.931113000	-3.147974000	0.372459000
8	1.149614000	-2.319283000	0.985041000
1	0.352253000	-1.972174000	0.504421000

(EC+2EtNH₂) charge-separated intermediate

E = -763.470559589

G = -763.241019

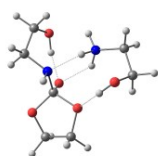


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8	-0.581382000	-1.395588000	-0.143825000
6	-2.899626000	-1.352053000	-0.383707000
6	-1.711818000	-2.278854000	-0.099015000
1	-3.024536000	-1.182475000	-1.470625000
1	-3.847484000	-1.700294000	0.051143000
1	-1.598381000	-3.077943000	-0.850659000
1	-1.802312000	-2.733385000	0.906616000
8	-0.951006000	0.652635000	-1.283811000
7	-0.389809000	0.699251000	0.980066000
1	-0.627887000	0.196047000	1.838589000
1	1.170084000	0.368997000	0.211366000
6	-0.667942000	2.154795000	1.131309000
1	-1.655285000	2.402275000	0.702709000
1	-0.700250000	2.394030000	2.206509000

6	0.414939000	3.015882000	0.476016000
1	1.378928000	2.832483000	0.995141000
1	0.160658000	4.082908000	0.628970000
8	0.578794000	2.756005000	-0.927655000
1	-0.086850000	2.026004000	-1.163916000
7	1.831162000	0.281041000	-0.639685000
1	1.211689000	-0.113206000	-1.369238000
1	2.011932000	1.263173000	-0.921493000
6	3.029966000	-0.561844000	-0.364970000
1	3.577634000	-0.086856000	0.462165000
1	3.668494000	-0.579642000	-1.261481000
6	2.578621000	-1.973775000	0.026214000
1	2.098118000	-2.458805000	-0.847140000
1	3.476377000	-2.562223000	0.281256000
8	1.709934000	-1.956859000	1.155574000
1	0.796395000	-1.788109000	0.793642000

(EC+2HOCH₂CH₂NH₂) TS1'

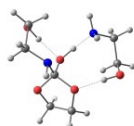
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G = -763.239275



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6	2.711443000	1.637048000	-0.488879000
6	1.500555000	2.453975000	-0.021655000
1	2.729569000	1.543883000	-1.591746000
1	3.674429000	2.029830000	-0.132038000
1	1.239185000	3.272880000	-0.712093000
1	1.666958000	2.866276000	0.991769000
8	0.802091000	-0.439028000	-1.302211000
1	-1.134579000	-0.173805000	-1.226445000
7	0.514382000	-0.665567000	1.008187000
1	0.769453000	-0.160143000	1.860615000
6	0.997759000	-2.071899000	1.084076000
1	1.978679000	-2.171516000	0.584985000
1	1.138671000	-2.331290000	2.145927000
6	0.002671000	-3.062185000	0.475961000
1	-0.950229000	-3.002982000	1.043618000
1	0.398251000	-4.088030000	0.607297000
8	-0.258548000	-2.828223000	-0.917242000
1	0.252205000	-1.991474000	-1.167710000
7	-1.838106000	-0.538758000	-0.539819000
1	-1.968657000	-1.532572000	-0.795736000
1	-1.246620000	-0.550247000	0.348638000
6	-3.083693000	0.269800000	-0.416006000
1	-3.704790000	-0.201077000	0.360334000
1	-3.619981000	0.242469000	-1.376792000
6	-2.721472000	1.704815000	-0.019329000
1	-2.174885000	2.189067000	-0.851720000
1	-3.658843000	2.265028000	0.139856000
8	-1.956382000	1.732662000	1.183935000
1	-1.004956000	1.683833000	0.895696000

(EC+2EtNH₂) tetrahedral intermediate 1

E = -763.473196518
G = -763.245871

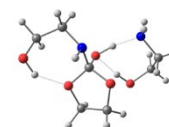


6	0.598697000	0.735794000	0.143087000
8	1.305074000	1.842712000	-0.403874000
8	-0.614270000	1.326232000	0.716587000
6	0.284729000	2.685682000	-0.974514000
6	-0.830382000	2.612465000	0.078722000
1	-0.044477000	2.283701000	-1.948491000

1	0.701903000	3.693382000	-1.104394000
1	-1.841314000	2.644072000	-0.355570000
1	-0.731046000	3.399557000	0.844454000
8	0.283587000	-0.140917000	-0.881106000
1	-0.278017000	-0.947399000	-0.464751000
7	1.281401000	0.104618000	1.233315000
1	1.331714000	0.787412000	1.993926000
6	2.636353000	-0.433610000	0.957980000
1	3.269057000	0.288383000	0.404602000
1	3.096969000	-0.593902000	1.946495000
6	2.648443000	-1.768271000	0.200199000
1	1.853919000	-2.418684000	0.628138000
1	3.617106000	-2.264408000	0.382719000
1	-1.178887000	-1.804306000	1.155781000
6	-2.520456000	-2.051854000	-0.392617000
1	-2.485823000	-2.458626000	-1.416904000
7	-1.142757000	-2.054040000	0.160640000
6	-3.047668000	-0.613246000	-0.426998000
1	-2.450375000	-0.023326000	-1.149092000
1	-4.095698000	-0.619311000	-0.773678000
1	-3.199138000	-2.684733000	0.208878000
1	-0.722660000	-2.986740000	0.105614000
8	-3.007481000	-0.011573000	0.873495000
1	-2.128113000	0.432901000	0.935155000
8	2.528993000	-1.641957000	-1.218939000
1	1.728854000	-1.079750000	-1.355026000

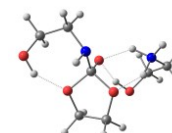
(EC+2EtNH₂) tetrahedral intermediate 2

E = -763.471154873
G = -763.243197



6	-0.547896000	0.096002000	-0.259149000
8	-1.296922000	1.224130000	0.253126000
8	0.327572000	0.666113000	-1.244967000
6	-0.359276000	2.315756000	0.306029000
6	0.544573000	2.059376000	-0.917084000
1	0.210095000	2.285038000	1.251175000
1	-0.923263000	3.256856000	0.247364000
1	1.605587000	2.223105000	-0.676022000
1	0.250213000	2.663735000	-1.790708000
8	0.146308000	-0.475283000	0.800522000
1	0.843267000	-1.140997000	0.367714000
7	-1.373829000	-0.857652000	-0.928468000
1	-1.908116000	-0.370944000	-1.652968000
6	-2.265116000	-1.688637000	-0.093546000
1	-2.858290000	-2.294950000	-0.797424000
1	-1.650791000	-2.378256000	0.508504000
6	-3.208520000	-0.901202000	0.836154000
1	-2.629713000	-0.486912000	1.682615000
1	-3.972012000	-1.584649000	1.245877000
1	1.661659000	-2.272874000	-1.192328000
6	3.147613000	-0.950615000	-0.583255000
1	4.027215000	-1.467470000	-1.011862000
7	2.033139000	-1.898270000	-0.313098000
6	3.571774000	-0.212853000	0.690486000
1	3.757161000	-0.956696000	1.496957000
1	4.529295000	0.299153000	0.498512000
1	2.780468000	-0.217703000	-1.317605000
1	2.372497000	-2.698369000	0.232131000
8	2.656989000	0.800531000	1.122482000
1	1.755238000	0.402689000	1.160659000
8	-3.901165000	0.144109000	0.135154000
1	-3.226853000	0.846925000	0.030021000

(EC+2HOCH₂CH₂NH₂) TS2



E = -763.464017632

G = -763.234609

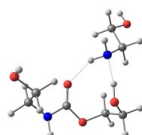
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8	-1.313084000	1.226960000	0.261733000
8	0.354124000	0.760164000	-1.271982000
6	-0.370084000	2.294827000	0.374798000
6	0.494853000	2.141589000	-0.895040000
1	0.234684000	2.188597000	1.294516000
1	-0.918484000	3.247171000	0.412435000
1	1.551966000	2.380585000	-0.694382000
1	0.117634000	2.772025000	-1.719682000
8	0.149110000	-0.551140000	0.709472000
1	1.349184000	-1.473424000	-0.237116000
7	-1.394363000	-0.801925000	-1.004427000
1	-1.984238000	-0.213319000	-1.599327000
6	-2.236035000	-1.734821000	-0.228218000
1	-2.879821000	-2.254406000	-0.957572000
1	-1.586813000	-2.487609000	0.248855000
6	-3.107569000	-1.061930000	0.850113000
1	-2.459091000	-0.735095000	1.684695000
1	-3.837960000	-1.789244000	1.245466000
1	1.689819000	-0.345333000	-1.319771000
6	3.446754000	-1.047657000	-0.309059000
1	3.977786000	-2.011377000	-0.298876000
7	2.103600000	-1.251075000	-0.953673000
6	3.269294000	-0.516540000	1.119515000
1	2.842011000	-1.322635000	1.751125000
1	4.270840000	-0.281418000	1.518580000
1	4.005823000	-0.333967000	-0.931437000
1	2.121055000	-1.947257000	-1.707364000
8	2.469348000	0.656610000	1.170458000
1	1.519304000	0.324881000	1.095374000
8	-3.850529000	0.049154000	0.321721000
1	-3.181283000	0.762576000	0.241021000

(EC+2HOCH₂CH₂NH₂) product

E = -763.506326919

G = -763.283924

6	0.981009000	0.514872000	-0.183730000
8	0.638675000	1.619452000	-0.902524000
8	-1.286091000	1.816276000	1.196568000
6	-0.776815000	1.802577000	-1.201229000
6	-1.458189000	2.507917000	-0.029883000
1	-1.251637000	0.833646000	-1.413106000
1	-0.801739000	2.420933000	-2.111395000
1	-2.527995000	2.648992000	-0.302944000
1	-1.014491000	3.511139000	0.097555000
8	0.323962000	-0.530977000	-0.095122000
7	2.204456000	0.678425000	0.386107000
1	2.619221000	1.606033000	0.357415000
6	2.839965000	-0.380934000	1.172997000
1	3.604115000	0.097909000	1.803011000
1	2.089024000	-0.855883000	1.826610000
6	3.495771000	-1.434030000	0.272370000
1	2.712499000	-1.945235000	-0.320761000
1	3.999862000	-2.189370000	0.896671000
1	-1.742455000	0.919446000	1.120551000
6	-3.515409000	-1.262113000	0.410222000
1	-4.249980000	-1.925715000	0.911087000
7	-2.615542000	-0.592052000	1.380138000
1	-1.931289000	-1.271075000	1.733953000
6	-2.741986000	-2.113840000	-0.598147000



1	-2.174822000	-2.896712000	-0.047975000
1	-3.473248000	-2.636355000	-1.238804000
1	-4.082132000	-0.484517000	-0.130330000
1	-3.161478000	-0.292780000	2.195289000
8	-1.882989000	-1.376186000	-1.466112000
1	-1.095079000	-1.086659000	-0.941245000
8	4.502923000	-0.861159000	-0.573682000
1	4.041320000	-0.204350000	-1.127922000

D. Hydroxylamine one-molecule pathway

EC...HOCH₂CH₂NH₂

E = -552.993393881

G = -552.858955

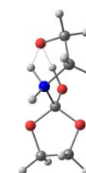


6	0.921777000	0.833506000	-0.312068000
8	1.773676000	0.103759000	-1.073387000
8	1.120614000	0.631680000	1.011471000
6	2.649791000	-0.657501000	-0.189714000
6	1.942546000	-0.557534000	1.167766000
1	3.640037000	-0.176448000	-0.194448000
1	2.723300000	-1.683366000	-0.572985000
1	2.624793000	-0.397711000	2.011897000
1	1.271445000	-1.406940000	1.360880000
8	0.132149000	1.639279000	-0.765772000
7	-0.792304000	-1.314492000	-0.495765000
6	-2.169416000	-1.302329000	0.039438000
1	-2.841274000	-2.040205000	-0.452930000
1	-2.122998000	-1.560008000	1.111818000
6	-2.819220000	0.079325000	-0.095301000
1	-3.874528000	-0.004174000	0.218984000
1	-2.821773000	0.376066000	-1.166817000
1	-0.810962000	-1.059120000	-1.489753000
8	-2.225790000	1.088150000	0.722180000
1	-1.382823000	1.344960000	0.288432000
1	-0.417145000	-2.267356000	-0.461381000

EC...HOCH₂CH₂NH₂ TS1

E = -552.953868467

G = -552.819458



6	-0.406067000	-0.272125000	0.187452000
8	-1.333221000	-0.969001000	-0.662379000
8	-1.130760000	0.727335000	0.874175000
6	-2.658680000	-0.479111000	-0.356886000
6	-2.372538000	0.925873000	0.160309000
1	-3.125396000	-1.110043000	0.420767000
1	-3.264086000	-0.504872000	-1.274245000
1	-3.116687000	1.309761000	0.871094000
1	-2.236284000	1.649950000	-0.665680000
8	0.290683000	-1.031510000	1.033872000
1	1.291244000	-1.205490000	0.568424000
7	0.577156000	0.372593000	-0.825540000
1	0.075995000	0.752869000	-1.632513000
6	1.584199000	1.280621000	-0.208462000
1	1.876200000	2.029613000	-0.956832000
1	1.146710000	1.784181000	0.662844000
6	2.773249000	0.297053000	0.173400000
1	2.951028000	0.351368000	1.263053000
1	3.698353000	0.614845000	-0.341683000
8	2.399175000	-1.012689000	-0.229473000
1	1.334842000	-0.507277000	-1.000887000



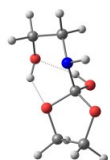
EC...HOCH₂CH₂NH₂ tetrahedral intermediate 1

E = -552.975956137
G = -552.838390

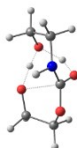
6	-0.451631000	-0.070099000	0.074636000
8	-1.265171000	-0.862335000	-0.794870000
8	-1.332266000	0.914413000	0.663301000
6	-2.618372000	-0.733947000	-0.313657000
6	-2.649598000	0.728707000	0.111599000
1	-2.791000000	-1.409590000	0.544729000
1	-3.302796000	-0.985593000	-1.135698000
1	-3.394879000	0.953397000	0.889358000
1	-2.806947000	1.396596000	-0.757759000
8	0.071757000	-0.777351000	1.151859000
1	0.973583000	-1.097080000	0.890706000
7	0.592014000	0.476467000	-0.757216000
1	0.171840000	1.043290000	-1.493790000
6	1.686877000	1.165398000	-0.046367000
1	1.880292000	2.147454000	-0.506336000
1	1.410565000	1.339346000	1.006243000
6	2.957638000	0.294226000	-0.122811000
1	3.674658000	0.569843000	0.665188000
1	3.451785000	0.416727000	-1.104043000
8	2.638464000	-1.106826000	0.080198000
1	2.137048000	-1.358576000	-0.722396000

EC...HOCH₂CH₂NH₂ tetrahedral intermediate 2

E = -552.976377031
G = -552.837235

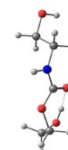


6	-0.403120000	0.413290000	0.136480000
8	-0.616564000	-0.815982000	-0.606645000
8	-1.623550000	1.103566000	0.109017000
6	-1.960408000	-1.203125000	-0.245374000
6	-2.678382000	0.153618000	-0.205765000
1	-1.967974000	-1.702290000	0.738864000
1	-2.342329000	-1.883183000	-1.018391000
1	-3.458745000	0.203650000	0.568436000
1	-3.103588000	0.426975000	-1.185443000
8	-0.120456000	0.098704000	1.487938000
1	0.674134000	-0.488938000	1.460233000
7	0.598665000	1.190365000	-0.552125000
1	0.302767000	2.167698000	-0.514801000
6	1.991369000	1.046958000	-0.091269000
1	2.585264000	1.811079000	-0.618690000
1	2.103009000	1.228305000	0.997555000
6	2.576501000	-0.325428000	-0.431104000
1	3.640037000	-0.345568000	-0.143958000
1	2.502718000	-0.506537000	-1.518875000
8	1.936695000	-1.404166000	0.298731000
1	1.109283000	-1.612597000	-0.190189000

EC...HOCH₂CH₂NH₂ TS2

E = -552.963022742
G = -552.827695

6	0.229394000	-0.876885000	0.142515000
8	0.639017000	1.205893000	-0.615221000
8	1.468836000	-1.209486000	-0.216960000
6	2.025818000	1.141755000	-0.437025000
6	2.430526000	-0.195854000	0.250028000
1	2.443512000	1.962283000	0.188521000
1	2.541167000	1.190252000	-1.421232000
1	2.374476000	-0.139223000	1.346249000
1	3.415870000	-0.568447000	-0.057843000
8	-0.008030000	-0.567584000	1.399285000
1	-0.739520000	0.230220000	1.356160000
7	-0.778551000	-1.237211000	-
0.674469000			
1	-0.531641000	-1.237919000	-
1.665844000			
6	-2.147836000	-0.798423000	-
0.332842000			
1	-2.825828000	-1.201941000	-1.097928000
1	-2.421296000	-1.249903000	0.634000000
6	-2.290960000	0.730825000	-0.266228000
1	-3.331341000	0.975770000	0.004942000
1	-2.068861000	1.176064000	-1.251169000
8	-1.404218000	1.325883000	0.725169000
1	-0.453172000	1.477164000	0.208550000

**EC...HOCH₂CH₂NH₂ product**

E = -553.006586716
G = -552.872099

7	0.954344000	-1.196934000	-0.070507000
1	0.946632000	-1.989682000	0.568141000
6	2.232460000	-0.594709000	-0.439004000
1	2.969620000	-1.397041000	-0.593299000
1	2.097040000	-0.064046000	-1.394672000
6	2.749903000	0.387954000	0.626418000
1	2.887087000	-0.139414000	1.584682000
1	1.998423000	1.186965000	0.782254000
6	-0.224715000	-0.557403000	-0.288011000
8	-0.348976000	0.465185000	-0.974873000
8	-1.247507000	-1.206239000	0.336210000
6	-2.612571000	-0.784074000	0.005834000
1	-2.733748000	-0.758211000	-1.090165000
1	-3.224509000	-1.597132000	0.421863000
6	-3.016185000	0.555158000	0.619621000
1	-4.116139000	0.561357000	0.719917000
1	-2.592650000	0.603952000	1.646799000
8	-2.663465000	1.693373000	-0.165151000
1	-1.769079000	1.487356000	-0.525126000
8	4.033044000	0.917543000	0.270659000
1	3.898788000	1.483990000	-0.510748000