Supporting Information

Accurate Prediction of Carbon Dioxide Capture by Deep Eutectic Solvents using Quantum Chemistry and a Neural Network

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Cartesian coordinates (in Å) of all the molecules investigated in this study (CO_2, HBA, and HBD). The molecules were optimized at B3LYP/6-311++G(d,p) level of theory and basis set.

Carbon dioxide (CO_2)

C	0.00000	0.00000	0.00000
O	1.17200	0.00000	0.00000
O	-1.17200	0.00000	0.00000

HBA's

[Ach]Cl

N	-1.39600	-0.20000	-0.08200
C	-1.94100	1.19400	-0.26100
C	-2.47000	-1.18400	-0.48000
C	-1.03200	-0.42600	1.36100
H	-1.19400	1.92100	0.07100
H	-2.84100	1.28700	0.35400
H	-2.17800	1.32900	-1.32500
H	-0.28800	0.31400	1.66400
H	-0.62600	-1.43700	1.46500
H	-1.94200	-0.31700	1.96000
H	-2.07900	-2.19900	-0.34700
H	-2.72500	-0.99800	-1.53200
H	-3.33800	-1.02400	0.16700
C	-0.21000	-0.43700	-1.01800
H	0.06100	-1.49500	-0.91400
C	1.00500	0.44200	-0.82400
H	-0.61400	-0.26700	-2.03100
H	0.76100	1.50200	-0.67600
H	1.61600	0.36500	-1.73300
O	1.78100	-0.04300	0.31100
C	2.98200	0.56600	0.51400
O	3.38200	1.48900	-0.18200
C	3.73400	-0.06200	1.65300
H	4.41300	0.67500	2.09700
H	4.33600	-0.89300	1.25700
H	3.05500	-0.46600	2.41300
Cl	-2.25300	0.36200	-3.88300

[Ch]Cl

N	0.01800	-0.73300	-0.10100
C	-0.11100	0.37600	0.94600
C	-0.58400	-1.98600	0.48300
C	1.45900	-1.00000	-0.44100
H	1.49800	-1.88100	-1.09000
H	2.01200	-1.18800	0.48500
H	1.87100	-0.13400	-0.96700
H	-0.56300	-2.77000	-0.28200
H	-1.61600	-1.77200	0.77900
H	0.00700	-2.28800	1.35400
C	0.69900	1.64800	0.70400
H	0.21500	-0.06900	1.89600
H	-1.18400	0.60000	1.01100
H	0.54400	2.25900	1.61200
O	0.36100	2.37200	-0.47500
H	1.77300	1.42300	0.65400
C	-0.73800	-0.37800	-1.35900
H	-0.32600	0.55200	-1.75700
H	-1.79400	-0.24700	-1.10000
H	-0.62200	-1.20300	-2.07000
H	-0.54600	2.78000	-0.32800
Cl	-2.37100	3.64000	0.04700

[TOA]Cl

N	-0.16600	-0.09700	0.28100
C	1.07100	-0.53400	-0.50500
C	-0.22900	-0.79000	1.64300
C	-1.37800	-0.46500	-0.58500
C	2.41500	-0.25800	0.15700
H	0.99900	-0.02500	-1.47400
H	0.94400	-1.60800	-0.69200
H	2.53400	0.81700	0.36600
C	3.56300	-0.71800	-0.75800
H	2.49300	-0.78600	1.11900
H	3.48800	-0.19900	-1.72900
H	3.45300	-1.79600	-0.96900
C	4.94600	-0.45800	-0.14700
H	5.05400	0.62100	0.06000
C	6.10300	-0.91900	-1.04400
H	5.01500	-0.97000	0.82800
H	6.02800	-0.41300	-2.02300
H	5.99800	-2.00000	-1.24600
C	7.48800	-0.65000	-0.44100

H	7.59400	0.43200	-0.24200
C	8.64800	-1.11400	-1.33100
H	7.56100	-1.15100	0.54100
H	8.57200	-0.61500	-2.31300
H	8.54300	-2.19500	-1.52700
C	10.02700	-0.83600	-0.72200
H	10.17300	0.24100	-0.54600
H	10.83700	-1.18000	-1.38200
H	10.14300	-1.35000	0.24600
H	-1.27400	0.09600	-1.52700
C	-2.74900	-0.20500	0.02900
H	-1.25900	-1.53100	-0.81700
H	-2.87000	0.86100	0.27800
H	-2.88500	-0.77500	0.96100
C	-3.84800	-0.60300	-0.97300
H	-3.68700	-0.04400	-1.90900
C	-5.26000	-0.35300	-0.42700
H	-3.74300	-1.67400	-1.22300
H	-5.36700	0.71500	-0.16300
H	-5.38200	-0.91500	0.51500
C	-6.38900	-0.74900	-1.39400
H	-6.24800	-1.79900	-1.70600
C	-6.50600	0.14100	-2.64000
H	-7.34900	-0.71900	-0.85000
H	-5.56300	0.11800	-3.21200
H	-6.64500	1.19000	-2.32000
C	-7.66200	-0.26000	-3.56700
H	-7.51800	-1.30600	-3.89100
C	-7.79300	0.64300	-4.79900
H	-8.60600	-0.24300	-2.99600
H	-8.62700	0.32800	-5.44300
H	-6.87400	0.62100	-5.40600
H	-7.97200	1.68900	-4.50600
H	-1.10500	-0.36700	2.15100
H	0.65800	-0.45200	2.19300
C	-0.30000	-2.31200	1.62100
H	-1.18500	-2.65400	1.06400
C	-0.37000	-2.85700	3.05700
H	0.58300	-2.73600	1.11900
H	-1.25900	-2.44200	3.56200
H	0.50700	-2.50200	3.62600
C	-0.42200	-4.39000	3.11000
H	-1.29300	-4.74400	2.53100
C	-0.50200	-4.94300	4.53800
H	0.47100	-4.80100	2.60800
H	-1.39900	-4.53400	5.03600
H	0.36500	-4.57900	5.11800

C	-0.54300	-6.47500	4.60000
H	-1.40700	-6.84100	4.01700
C	-0.62600	-7.03000	6.02700
H	0.35600	-6.88400	4.10400
H	-1.52600	-6.62300	6.52100
H	0.23600	-6.66300	6.60900
C	-0.66300	-8.56200	6.08000
H	-0.72400	-8.92800	7.11600
H	0.24000	-8.99700	5.62400
H	-1.53500	-8.95700	5.53500
C	-0.13200	1.40800	0.56400
H	-1.08700	1.63700	1.05200
H	0.65700	1.55300	1.31300
C	0.09600	2.31400	-0.64100
C	-0.08200	3.78700	-0.23500
H	-0.59900	2.07600	-1.46300
H	1.11600	2.17700	-1.03200
H	-1.11400	3.94400	0.12400
C	0.20900	4.75500	-1.38900
H	0.58200	4.02200	0.61500
H	-0.44600	4.50700	-2.24300
H	1.24500	4.60100	-1.73800
C	0.01700	6.22900	-1.00900
H	-1.02100	6.38300	-0.66300
C	0.31700	7.20000	-2.15700
H	0.66700	6.47000	-0.14900
H	-0.33300	6.96000	-3.01700
H	1.35500	7.04500	-2.50300
C	0.12800	8.67600	-1.78100
H	0.77700	8.91500	-0.92000
C	0.43400	9.63800	-2.93500
H	-0.90900	8.83100	-1.43600
H	1.47400	9.52800	-3.27800
H	0.29000	10.68700	-2.63400
H	-0.22300	9.44400	-3.79700
Cl	-1.81500	1.27500	-3.79400

[TOA]Br

N	0.00800	0.15300	0.10400
C	1.29400	0.24200	-0.71900
C	0.30700	-0.22800	1.55600
C	-0.86600	-0.90500	-0.57800
C	2.34300	1.22900	-0.22100
H	0.97500	0.49300	-1.73800
H	1.70200	-0.77600	-0.74700
H	1.92200	2.24300	-0.14400
C	3.54400	1.25700	-1.18200
H	2.69700	0.94700	0.78300
H	3.20200	1.56500	-2.18500
H	3.95000	0.23700	-1.28900
C	4.65800	2.20100	-0.71000
H	4.24600	3.21800	-0.59000
C	5.85800	2.24800	-1.66400
H	5.00000	1.88500	0.29100
H	5.51600	2.57400	-2.66200
H	6.25900	1.22700	-1.79400
C	6.98300	3.17400	-1.18600
H	6.58200	4.19500	-1.05200
C	8.18500	3.22700	-2.13900
H	7.32600	2.84500	-0.18900
H	7.84200	3.55900	-3.13400
H	8.58200	2.20600	-2.27600
C	9.30500	4.15100	-1.65000
H	9.69000	3.82300	-0.67100
H	8.94500	5.18600	-1.53600
H	10.15200	4.16700	-2.35300
H	-1.02200	-0.56100	-1.61200
C	-2.20400	-1.20600	0.08600
H	-0.24700	-1.81000	-0.62300
H	-2.84700	-0.31300	0.09200
H	-2.06800	-1.51600	1.13400
C	-2.92400	-2.33100	-0.67900
H	-3.03700	-2.02900	-1.73500
C	-4.29700	-2.66900	-0.08500
H	-2.29200	-3.23500	-0.67500
H	-4.92900	-1.76300	-0.09200
H	-4.17700	-2.95400	0.97500
C	-5.01900	-3.79600	-0.83400
H	-5.14000	-3.50900	-1.89400
C	-6.39200	-4.14300	-0.24400
H	-4.38400	-4.70000	-0.83000
H	-7.02800	-3.24000	-0.24600
H	-6.27100	-4.43100	0.81600

C	-7.11700	-5.27000	-0.99200
H	-7.23900	-4.98100	-2.05000
C	-8.48600	-5.61100	-0.39300
H	-6.48000	-6.17100	-0.99100
H	-8.39100	-5.93600	0.65500
H	-8.98000	-6.42100	-0.95000
H	-9.15500	-4.73600	-0.41000
H	-0.65700	-0.18900	2.07900
H	0.92500	0.58400	1.95600
C	0.98300	-1.57700	1.77200
H	0.35300	-2.39500	1.39100
C	1.24100	-1.80300	3.27200
H	1.94100	-1.62500	1.23300
H	0.28500	-1.74200	3.82000
H	1.87600	-0.98900	3.66000
C	1.90800	-3.15300	3.56300
H	1.27000	-3.96500	3.17200
C	2.17100	-3.38800	5.05600
H	2.86100	-3.21400	3.01000
H	1.21700	-3.32000	5.60800
H	2.81200	-2.57700	5.44400
C	2.83100	-4.74000	5.35500
H	2.19100	-5.55200	4.96700
C	3.09600	-4.97800	6.84800
H	3.78500	-4.81000	4.80200
H	2.14300	-4.90500	7.40000
H	3.73800	-4.16800	7.23500
C	3.75200	-6.33200	7.13800
H	4.72300	-6.42000	6.62600
H	3.11700	-7.16300	6.79200
H	3.92800	-6.47300	8.21500
C	-0.70700	1.50700	0.15600
H	-1.64000	1.32600	0.70400
H	-0.08100	2.15200	0.78500
C	-0.98700	2.17300	-1.18700
C	-1.84900	3.43000	-0.98000
H	-1.50400	1.48700	-1.87800
H	-0.04300	2.46600	-1.67300
H	-2.80500	3.14300	-0.50800
C	-2.13300	4.17500	-2.29100
H	-1.34500	4.11200	-0.27300
H	-2.62400	3.48200	-2.99400
H	-1.17600	4.46600	-2.75900
C	-2.99600	5.42900	-2.09100
H	-3.96400	5.13800	-1.64400
C	-3.25500	6.23700	-3.37400
H	-2.50100	6.08300	-1.35300

H	-2.28800	6.50200	-3.83800
H	-3.73400	7.19300	-3.09900
C	-4.13800	5.53000	-4.41300
H	-5.09300	5.24500	-3.93600
C	-4.42000	6.39700	-5.64500
H	-3.66200	4.58900	-4.73300
H	-3.48600	6.66900	-6.16100
H	-4.92900	7.33300	-5.36400
H	-5.06100	5.87200	-6.37000
Br	-2.14900	-0.25200	-4.24400

[BTEA]Cl

N	0.48600	0.75600	-0.13600
C	-0.44600	1.62400	0.71000
C	-0.14700	0.66100	-1.52700
C	-0.60700	-1.47400	0.60600
C	-0.93200	-2.40500	-0.39800
C	-2.07000	-3.21000	-0.28400
C	-2.89600	-3.10200	0.84100
C	-2.57100	-2.19700	1.85700
C	-1.43200	-1.39400	1.74300
H	-3.19900	-2.12100	2.74600
H	-1.17800	-0.70900	2.55400
H	-2.30700	-3.92700	-1.07200
H	-3.78400	-3.73100	0.93100
H	-0.27400	-2.51600	-1.26100
C	0.72400	0.02700	-2.60000
H	-0.42100	1.68600	-1.80300
H	-1.07800	0.09900	-1.38100
H	-1.39600	1.07700	0.75200
H	-0.61900	2.53600	0.12700
C	0.05500	1.97100	2.10300
C	1.88900	1.35500	-0.20700
H	2.28000	1.32700	0.81700
C	1.95800	2.76100	-0.78000
H	2.48300	0.65100	-0.80300
C	0.65200	-0.65200	0.49000
H	1.09600	-0.47200	1.47700
H	1.39900	-1.17400	-0.12900
H	1.41500	3.49500	-0.17100
H	1.59000	2.81700	-1.81300
H	3.01500	3.06100	-0.79000
H	1.53200	0.69600	-2.92500
H	0.08400	-0.16500	-3.47300
H	1.17600	-0.92700	-2.29000

H	0.27900	1.09000	2.71900
H	-0.74800	2.52600	2.60800
H	0.94100	2.61800	2.08400
Cl	3.05200	-2.66000	-1.32300

[BTMA]Cl

N	0.99000	-0.19000	0.98100
C	1.82700	-0.70700	-0.15900
C	-0.46700	-0.68200	0.87600
C	1.56100	-0.71400	2.27500
C	-1.21000	-0.25200	-0.36100
C	-1.97300	0.92900	-0.35900
C	-2.69100	1.31300	-1.49600
C	-2.66300	0.51400	-2.64500
C	-1.92300	-0.67400	-2.65100
C	-1.20500	-1.05700	-1.51400
H	-1.91100	-1.30800	-3.53800
H	-0.64700	-1.99600	-1.51800
H	-3.28100	2.23100	-1.48000
H	-3.22700	0.81100	-3.53100
H	-2.01600	1.54600	0.54100
H	-0.40200	-1.77600	0.93800
H	-0.95800	-0.30800	1.78200
H	2.59800	-0.36100	2.34700
H	1.52100	-1.80800	2.25600
H	0.95900	-0.32500	3.10400
H	2.85600	-0.35900	0.00700
H	1.43200	-0.30900	-1.09900
H	1.78200	-1.80100	-0.15800
C	1.05900	1.31400	0.99700
H	0.66900	1.69800	0.05000
H	2.11400	1.59100	1.12200
H	0.45900	1.68300	1.83600
Cl	4.74600	0.99500	1.39700

[TBA]Cl

N	-0.08400	0.00400	0.00100
C	-1.47200	0.45200	0.46000
C	-2.07400	-0.32600	1.62600
C	-3.46500	0.23300	1.97300
C	-4.11900	-0.51200	3.14100
C	0.91900	0.01500	1.16300
C	1.01500	1.31600	1.95500
C	2.06900	1.16900	3.06600
C	2.23000	2.44800	3.89300
C	-0.18400	-1.42600	-0.54100
C	1.03600	-1.94500	-1.29500
C	0.91500	-3.46200	-1.52000
C	2.08400	-4.02600	-2.33500
C	0.42200	0.96600	-1.07700
C	-0.40400	1.03400	-2.35900
C	0.27500	1.96900	-3.37400
C	-0.52500	2.10200	-4.67400
H	-2.11900	0.37100	-0.42100
H	-1.37800	1.51700	0.71000
H	-1.43100	-0.25900	2.51600
H	-2.17200	-1.39200	1.37400
H	-4.11400	0.17000	1.08300
H	-3.37600	1.30400	2.21900
H	-3.50600	-0.43700	4.05200
H	-4.24600	-1.58100	2.90900
H	-5.11200	-0.09700	3.36800
H	1.90000	-0.21200	0.71600
H	0.62500	-0.81400	1.81900
H	0.04900	1.58200	2.41100
H	1.30600	2.15200	1.30100
H	3.03300	0.89500	2.60700
H	1.78600	0.33400	3.72800
H	2.54700	3.29200	3.26100
H	2.98500	2.31700	4.68200
H	1.28300	2.73100	4.37900
H	-1.07600	-1.44900	-1.18000
H	-0.38500	-2.05600	0.33500
H	1.97000	-1.72500	-0.75400
H	1.12100	-1.44600	-2.27300
H	-0.03500	-3.68500	-2.03500
H	0.86600	-3.97000	-0.54300
H	2.12900	-3.56500	-3.33400
H	1.98500	-5.11300	-2.47000
H	3.04500	-3.83400	-1.83400
H	1.45800	0.65800	-1.28100

H	0.45400	1.95300	-0.60200
H	-1.41700	1.41200	-2.15200
H	-0.51700	0.03600	-2.81100
H	1.28700	1.59100	-3.59800
H	0.40800	2.96400	-2.91900
H	-0.01800	2.77300	-5.38300
H	-1.52900	2.51200	-4.48300
H	-0.64900	1.12500	-5.16600
Cl	4.20600	-0.06400	-0.33700

[TBA]Br

N	-0.08400	-0.00900	-0.01100
C	-1.56300	0.05200	0.38100
C	-2.02000	1.32200	1.08800
C	-3.52500	1.24200	1.40000
C	-4.03900	2.49600	2.11600
C	0.82100	0.16000	1.21500
C	0.64000	-0.86000	2.33300
C	1.56100	-0.50800	3.51500
C	1.46400	-1.52700	4.65400
C	0.12900	-1.37700	-0.66800
C	1.50800	-1.62900	-1.26500
C	1.62600	-3.09500	-1.71900
C	2.97500	-3.39500	-2.37900
C	0.28100	1.12400	-0.97100
C	-0.50800	1.18000	-2.27500
C	0.00400	2.33400	-3.15500
C	-0.76900	2.45200	-4.47200
H	-1.74100	-0.82900	1.00900
H	-2.12400	-0.09600	-0.55000
H	-1.83200	2.20800	0.46300
H	-1.46900	1.46500	2.03000
H	-3.72000	0.35400	2.02300
H	-4.08300	1.09600	0.46100
H	-3.88400	3.39500	1.50100
H	-3.51800	2.64800	3.07400
H	-5.11500	2.41500	2.32700
H	0.62500	1.17500	1.58400
H	1.85600	0.14100	0.84400
H	0.88900	-1.87300	1.98100
H	-0.40200	-0.88600	2.68700
H	1.30000	0.49500	3.89100
H	2.60000	-0.44700	3.15100
H	0.43700	-1.59100	5.04600
H	2.12500	-1.25100	5.48800

H	1.75600	-2.53300	4.31400
H	-0.64900	-1.46300	-1.43700
H	-0.10200	-2.11500	0.11000
H	2.31000	-1.40600	-0.54200
H	1.67500	-0.97500	-2.13500
H	0.81000	-3.32800	-2.42200
H	1.48500	-3.75600	-0.84700
H	3.12400	-2.77500	-3.27600
H	3.03900	-4.45000	-2.68500
H	3.80800	-3.19200	-1.68900
H	1.35400	1.00900	-1.16900
H	0.15300	2.05200	-0.40100
H	-1.58000	1.33200	-2.07700
H	-0.41200	0.23500	-2.83300
H	1.07600	2.18300	-3.36500
H	-0.07400	3.28000	-2.59400
H	-0.38300	3.28200	-5.08200
H	-1.83800	2.63800	-4.29000
H	-0.68400	1.52900	-5.06600
Br	4.68600	0.07000	0.69000

[TMA]Cl

N	0.22600	0.00700	0.00000
C	-0.25600	-0.98100	-1.03200
C	-0.27300	-0.41600	1.35900
C	1.72900	0.05000	0.00100
C	-0.32400	1.37200	-0.32700
H	0.11000	-0.66200	-2.01400
H	-1.35300	-0.98500	-1.00400
H	0.14500	-1.96900	-0.78000
H	0.07900	0.31100	2.09900
H	-1.37000	-0.43500	1.32000
H	0.12800	-1.41000	1.58200
H	2.10800	-0.94900	0.24000
H	2.05800	0.77200	0.75600
H	2.07100	0.35800	-0.99300
H	0.02900	2.07900	0.43200
H	0.04000	1.66400	-1.31700
H	-1.42000	1.30100	-0.31700
Cl	-3.72600	-0.10600	-0.00500

[TEA]Cl

N	0.05400	-0.01800	0.13400
C	-1.11100	0.80900	-0.42200
C	-1.07700	2.29400	-0.09800
C	-0.21500	-1.46600	-0.27400
C	0.82600	-2.47800	0.17500
C	1.39100	0.47000	-0.42900
C	1.57300	0.29400	-1.92800
C	0.15000	0.11900	1.65500
C	-1.09500	-0.27700	2.43100
H	-2.01800	0.34400	-0.01600
H	-1.11800	0.65300	-1.51100
H	-1.96900	2.74200	-0.55800
H	-0.20400	2.80400	-0.52500
H	-1.12300	2.50600	0.97800
H	-0.30800	-1.45100	-1.36600
H	-1.20300	-1.71400	0.13300
H	0.51500	-3.45900	-0.21000
H	0.89500	-2.56300	1.26700
H	1.82600	-2.26900	-0.22900
H	2.16500	-0.07000	0.12800
H	1.46200	1.52600	-0.14200
H	2.50200	0.81300	-2.20600
H	0.75300	0.72700	-2.52000
H	1.68900	-0.76000	-2.21300
H	0.41500	1.16600	1.84300
H	1.01000	-0.49100	1.95600
H	-1.96100	0.35500	2.19800
H	-0.86900	-0.14300	3.49800
H	-1.37100	-1.32900	2.28600
Cl	-1.58400	0.86500	-4.03700

Guanidinium chloride

C	0.34700	-0.01000	-0.02300
N	-0.34400	-1.10500	0.31600
N	1.68500	-0.04600	-0.11200
N	-0.32200	1.12300	-0.27300
H	2.19800	-0.90000	0.07600
H	2.21500	0.77900	-0.36700
H	0.12400	-1.98200	0.51500
H	-1.37100	-1.04100	0.37600
H	0.16300	1.97500	-0.53400
Cl	-3.34500	0.09100	0.22200
H	-1.35000	1.11600	-0.19500

[TOMA]Cl

N	-0.65800	-0.70000	1.47000
C	0.30100	-1.85400	1.15000
C	-1.05500	-0.77900	2.92200
C	-1.89800	-0.93000	0.59800
C	1.65900	-1.81000	1.84200
H	0.42600	-1.85000	0.06000
H	-0.26000	-2.76000	1.43000
H	2.23000	-0.92200	1.53000
C	2.46800	-3.07100	1.48900
H	1.54300	-1.75700	2.93500
H	2.57000	-3.14600	0.39300
H	1.90800	-3.96500	1.81200
C	3.86200	-3.08100	2.13000
H	4.41900	-2.18600	1.80300
C	4.67500	-4.33700	1.78900
H	3.75800	-2.99900	3.22600
H	4.77100	-4.42200	0.69300
H	4.11800	-5.23200	2.12000
C	6.07300	-4.35100	2.42100
H	6.63100	-3.45600	2.08900
C	6.88800	-5.60600	2.08300
H	5.97800	-4.26400	3.51800
H	6.98000	-5.69400	0.98700
H	6.33100	-6.49900	2.41600
C	8.28500	-5.60900	2.71500
H	8.87600	-4.74500	2.37300
H	8.84400	-6.52100	2.45500
H	8.22300	-5.55600	3.81300
H	-1.52900	-1.03200	-0.43100
C	-2.97900	0.14200	0.67200
H	-2.28300	-1.91000	0.92400
H	-2.59700	1.10900	0.31100
H	-3.31700	0.29000	1.70900
C	-4.18500	-0.26900	-0.19000
H	-3.85000	-0.44500	-1.22700
C	-5.30200	0.78200	-0.18900
H	-4.58400	-1.23000	0.17700
H	-4.89800	1.74200	-0.55500
H	-5.63200	0.96100	0.85000
C	-6.51100	0.38200	-1.04400
H	-6.17800	0.19800	-2.08100
C	-7.62900	1.43400	-1.05300
H	-6.91700	-0.57600	-0.67500
H	-7.22400	2.39300	-1.42200
H	-7.96200	1.62000	-0.01600

C	-8.84000	1.03700	-1.90600
H	-8.50700	0.85000	-2.94200
C	-9.95000	2.09500	-1.91000
H	-9.24600	0.08000	-1.53600
H	-10.80400	1.78200	-2.53000
H	-9.58200	3.05400	-2.30800
H	-10.32500	2.28000	-0.89200
C	-0.02200	0.66200	1.22000
H	-0.77100	1.40300	1.52800
H	0.81600	0.73600	1.92400
C	0.44300	0.92100	-0.20800
C	1.05200	2.32900	-0.32300
H	-0.40000	0.83600	-0.91200
H	1.19500	0.17700	-0.51200
H	0.30000	3.07700	-0.01900
C	1.54700	2.65100	-1.73800
H	1.89100	2.42200	0.38800
H	0.70800	2.54800	-2.44900
H	2.30200	1.90300	-2.03900
C	2.14800	4.05800	-1.86300
H	1.39000	4.80400	-1.56500
C	2.65200	4.38600	-3.27400
H	2.98100	4.16200	-1.14600
H	1.82000	4.27700	-3.99300
H	3.41300	3.64300	-3.57100
C	3.24600	5.79500	-3.40300
H	4.07400	5.90500	-2.68100
C	3.75200	6.11200	-4.81400
H	2.48300	6.53700	-3.11000
H	2.93900	6.04000	-5.55300
H	4.54200	5.40800	-5.11900
H	4.16900	7.12900	-4.87400
H	-0.16300	-0.64900	3.54200
H	-1.51100	-1.76300	3.09300
H	-1.76500	0.02400	3.14000
Cl	-2.34500	-4.20000	2.33600

[TOMA]Br

N	0.79000	-0.70700	-1.41400
C	-0.09800	-1.91500	-1.09000
C	1.25600	-0.80400	-2.84400
C	2.00500	-0.81100	-0.48100
C	-1.42700	-1.98900	-1.83300
H	-0.26400	-1.88600	-0.00600
H	0.53200	-2.79000	-1.31500
H	-2.07000	-1.13600	-1.56700
C	-2.15800	-3.29500	-1.47300
H	-1.27400	-1.95600	-2.92200
H	-2.28400	-3.35500	-0.37800
H	-1.53200	-4.15500	-1.76300
C	-3.53000	-3.41100	-2.14700
H	-4.15700	-2.55300	-1.84700
C	-4.26300	-4.71600	-1.81000
H	-3.40600	-3.33500	-3.24200
H	-4.37300	-4.79800	-0.71400
H	-3.64000	-5.57300	-2.12200
C	-5.64500	-4.82900	-2.46500
H	-6.26900	-3.97500	-2.14800
C	-6.37600	-6.13800	-2.13700
H	-5.53700	-4.74000	-3.56100
H	-6.47800	-6.23000	-1.04200
H	-5.75400	-6.99000	-2.45900
C	-7.75900	-6.23800	-2.78900
H	-8.41500	-5.41800	-2.45700
H	-8.25700	-7.18700	-2.53700
H	-7.68500	-6.18100	-3.88700
H	1.59800	-0.90100	0.53500
C	3.00800	0.33400	-0.55600
H	2.47600	-1.77000	-0.74600
H	2.53800	1.28500	-0.26100
H	3.38500	0.46000	-1.58200
C	4.19600	0.05400	0.38100
H	3.82400	-0.09200	1.41000
C	5.23500	1.18200	0.37200
H	4.67900	-0.89300	0.08600
H	4.74600	2.12900	0.66300
H	5.60400	1.32900	-0.65800
C	6.42400	0.91800	1.30400
H	6.05300	0.76800	2.33300
C	7.46500	2.04600	1.30200
H	6.91300	-0.02800	1.01100
H	6.97600	2.99300	1.59400
H	7.83600	2.19700	0.27200

C	8.65600	1.78600	2.23400
H	8.28400	1.63400	3.26200
C	9.68800	2.91800	2.22600
H	9.14400	0.84000	1.94100
H	10.10200	3.07100	1.21600
H	10.52900	2.70200	2.90200
H	9.23600	3.87000	2.54700
C	0.04600	0.61300	-1.24200
H	0.75500	1.39700	-1.53900
H	-0.75800	0.60200	-1.99000
C	-0.51100	0.88100	0.15000
C	-1.21600	2.24700	0.18800
H	0.29600	0.87200	0.90000
H	-1.22800	0.09600	0.43700
H	-0.49500	3.03700	-0.08200
C	-1.83000	2.56300	1.55700
H	-2.00800	2.27100	-0.58100
H	-1.04100	2.52100	2.32900
H	-2.56100	1.77700	1.81700
C	-2.51900	3.93400	1.60900
H	-1.78300	4.71900	1.36100
C	-3.15600	4.24800	2.96800
H	-3.29500	3.98100	0.82400
H	-2.38300	4.19200	3.75500
H	-3.89900	3.46800	3.21100
C	-3.83400	5.62400	3.02500
H	-4.60100	5.68300	2.23300
C	-4.47800	5.92600	4.38300
H	-3.09000	6.40400	2.78900
H	-5.25200	5.18200	4.62800
H	-4.95200	6.91900	4.39400
H	-3.72900	5.90400	5.19100
H	0.38500	-0.76800	-3.50500
H	1.79500	-1.75300	-2.96300
H	1.91100	0.04300	-3.06400
Br	2.90100	-4.30300	-2.12100

[TEA]Br

N	-0.14600	0.05800	-0.00300
C	-1.67100	0.14100	-0.11600
C	0.47000	-0.55100	-1.26600
C	0.34200	1.49200	0.21500
H	-0.03600	2.06700	-0.63900
C	1.84500	1.65900	0.36400
H	-0.18400	1.85200	1.10600
C	0.22100	0.21500	-2.55400
H	0.06100	-1.56600	-1.33000
H	1.54400	-0.65200	-1.05400
H	-1.87000	0.83600	-0.94000
C	-2.39100	-1.17900	-0.33300
H	-2.01100	0.62600	0.80600
C	0.27500	-0.85200	1.15400
H	-0.11100	-1.84600	0.90100
C	-0.20000	-0.42200	2.53300
H	1.37000	-0.91100	1.10300
H	-2.10700	-1.67300	-1.27200
H	-3.46500	-0.95400	-0.39600
H	-2.25300	-1.88300	0.49700
H	0.70300	-0.34800	-3.36500
H	0.66500	1.21900	-2.54600
H	-0.84400	0.29900	-2.80400
H	2.40100	1.33100	-0.52400
H	2.24700	1.13300	1.23900
H	2.03900	2.73200	0.50200
H	0.16000	-1.17400	3.24900
H	-1.29400	-0.38700	2.61900
H	0.21200	0.54700	2.84300
Br	4.02600	-1.80900	0.01200

[TPA]Cl

N	0.11000	-0.00400	0.00200
C	-0.92200	1.02500	-0.47500
C	-0.80300	1.47700	-1.92700
C	-1.86200	2.55300	-2.21300
C	0.03300	-1.28800	-0.82800
C	-1.26000	-2.08800	-0.71000
C	-1.27000	-3.21400	-1.75400
C	1.53600	0.52500	-0.16100
C	1.85300	1.84200	0.54000
C	3.32600	2.21000	0.31200
C	-0.21400	-0.28000	1.47100
C	0.68700	-1.28600	2.18100
C	0.20200	-1.48900	3.62400
H	-0.81300	1.88200	0.20200
H	-1.91500	0.58400	-0.29300
H	-0.96000	0.63000	-2.61100
H	0.19600	1.88500	-2.13900
H	-2.87300	2.17000	-2.00800
H	-1.81600	2.86400	-3.26500
H	-1.70300	3.44400	-1.58800
H	0.89500	-1.89500	-0.52500
H	0.20700	-0.97700	-1.86600
H	-2.14400	-1.44500	-0.84600
H	-1.34200	-2.52900	0.29400
H	-2.18500	-3.81500	-1.65700
H	-0.41000	-3.88900	-1.62800
H	-1.23800	-2.81100	-2.77700
H	1.70100	0.61300	-1.24200
H	2.19600	-0.27300	0.20200
H	1.66200	1.76400	1.62000
H	1.21500	2.65100	0.15500
H	3.99800	1.43900	0.71800
H	3.56200	3.16000	0.81000
H	3.54800	2.32400	-0.75900
H	-1.25900	-0.61600	1.48200
H	-0.18000	0.69300	1.97600
H	1.72800	-0.93200	2.19700
H	0.68200	-2.25200	1.65600
H	0.84800	-2.20700	4.14500
H	-0.82700	-1.87900	3.64700
H	0.22000	-0.54500	4.18700
Cl	-4.40800	-0.01700	-0.14800

[DEA]Cl

N	-0.00400	-0.02600	0.18800
C	-1.25400	-0.43000	-0.54600
H	-0.02400	-0.43300	1.13200
C	1.27300	-0.43600	-0.49400
H	1.21500	-1.51900	-0.66200
C	2.48600	-0.05900	0.34200
H	1.27900	0.06800	-1.46800
H	2.47200	-0.56400	1.31900
H	2.53600	1.02700	0.50400
H	3.39800	-0.37000	-0.18600
C	-2.49800	-0.04600	0.23900
H	-1.19500	-1.51300	-0.71100
H	-1.21700	0.07400	-1.52000
H	-2.54900	1.04000	0.39800
H	-2.52700	-0.55000	1.21600
H	-3.38900	-0.35200	-0.32500
H	-0.00300	1.04100	0.30200
Cl	0.00100	3.04800	0.27300

[BHDE]Cl

N	0.38000	-1.14800	0.58700
C	1.40200	-1.72800	1.53100
C	0.79700	-1.36900	-0.86800
C	-0.85800	1.09000	0.19800
C	-2.14300	1.22300	0.75200
C	-3.13400	1.95100	0.08600
C	-2.84800	2.56500	-1.13900
C	-1.56600	2.45400	-1.69000
C	-0.57500	1.72600	-1.02400
H	-1.33300	2.94400	-2.63700
H	0.43100	1.64700	-1.44400
H	-4.12700	2.04600	0.52900
H	-3.61900	3.13700	-1.65700
H	-2.36800	0.76300	1.71700
C	2.22500	-1.00100	-1.26400
H	0.06800	-0.82500	-1.48000
H	0.66000	-2.44400	-1.04500
C	-0.92600	-1.86800	0.79300
C	0.21700	0.34900	0.95000
H	1.20600	0.79500	0.79400
H	0.00000	0.34300	2.02500
H	2.34200	-1.41800	-2.27900
H	2.95800	-1.51600	-0.62400

O	2.49300	0.40000	-1.32000
Cl	4.07200	0.95900	1.22000
H	3.03400	0.63500	-0.50900
H	2.31200	-1.11600	1.50000
H	1.61100	-2.76000	1.22800
H	0.97700	-1.71300	2.54100
H	-0.75400	-2.94000	0.65200
H	-1.65600	-1.50400	0.06400
H	-1.27600	-1.67400	1.81300

Betaine

O	1.57200	0.15200	-2.09200
C	1.41000	1.18700	-1.39000
O	1.92100	2.32800	-1.56100
C	0.48400	1.14900	-0.13900
N	-0.21100	-0.16400	0.21300
C	0.80400	-1.24200	0.50000
C	-1.03700	0.06600	1.45200
C	-1.12200	-0.60000	-0.90600
H	1.07300	1.42900	0.74300
H	-0.31400	1.89100	-0.27000
H	1.39600	-1.39600	-0.40700
H	1.43800	-0.90600	1.32700
H	0.26600	-2.15300	0.78200
H	-1.53900	-0.87200	1.71400
H	-1.77700	0.84500	1.24200
H	-0.37300	0.38000	2.26400
H	-1.85800	0.19200	-1.07800
H	-0.50800	-0.76200	-1.79600
H	-1.62500	-1.52300	-0.59800

Menthol

O	0.43700	2.55800	-0.42700
C	-0.09800	1.32500	0.11700
C	0.68000	0.08300	-0.36600
C	0.04000	-1.18600	0.23400
C	-1.45500	-1.29900	-0.09700
C	-2.23800	-0.06500	0.37800
C	-3.72700	-0.15300	0.02100
C	-1.59500	1.20900	-0.19700
C	2.21200	0.19300	-0.13200
C	2.62100	0.13600	1.34900
C	2.98500	-0.85700	-0.94700
H	0.32700	2.51500	-1.39600
H	0.03300	1.43500	1.20600
H	0.53200	0.03800	-1.46500
H	0.16100	-1.17300	1.33100
H	0.57200	-2.07900	-0.12800
H	-1.87500	-2.20900	0.36200
H	-1.58500	-1.40600	-1.19000
H	-2.15100	-0.01700	1.48000
H	-3.86300	-0.20200	-1.07200
H	-4.27900	0.72400	0.39000
H	-4.18700	-1.05200	0.45800
H	-1.72000	1.20700	-1.29800
H	-2.11100	2.10600	0.18300
H	2.50300	1.18500	-0.51600
H	2.08800	0.88300	1.95500
H	2.42500	-0.85500	1.78600
H	3.69900	0.33400	1.45400
H	2.78100	-1.87900	-0.59300
H	4.07000	-0.69100	-0.86400
H	2.71800	-0.81000	-2.01500

Thymol

C	0.50400	-0.68400	-0.91600
C	1.85300	-0.32500	-0.81000
C	2.26900	0.68400	0.07400
C	3.72500	1.07300	0.16400
C	1.29000	1.32100	0.84900
C	-0.05900	0.95900	0.73300
C	-0.49300	-0.04300	-0.14400
C	-1.94900	-0.47500	-0.25800
C	-2.95000	0.65000	0.04400
C	-2.22300	-1.70400	0.63500
O	0.09800	-1.67900	-1.78000
H	2.59000	-0.84600	-1.43000
H	3.90400	1.74300	1.01600
H	4.05400	1.59700	-0.74800
H	4.37100	0.19000	0.27900
H	1.58000	2.11000	1.54800
H	-0.79600	1.48000	1.34700
H	-2.10800	-0.79100	-1.30200
H	-2.91500	0.95600	1.10100
H	-3.97300	0.30400	-0.16200
H	-2.76000	1.53900	-0.57500
H	-3.25600	-2.06200	0.49700
H	-2.09200	-1.44600	1.69800
H	-1.54100	-2.53300	0.39800
H	0.87800	-2.01800	-2.25800

[TBP]Br

P	0.47200	-0.11600	-0.15100
C	-1.14100	-0.45200	0.66200
C	1.24600	1.39900	0.54600
C	1.65400	-1.48700	0.17200
H	2.56200	-1.20900	-0.39300
C	1.16100	-2.89200	-0.20400
H	1.91000	-1.43200	1.24200
H	0.88600	-2.92700	-1.27100
H	0.25000	-3.13900	0.36500
C	2.23200	-3.95900	0.07300
H	3.14100	-3.71400	-0.50200
C	1.76000	-5.37300	-0.28100
H	2.51600	-3.91700	1.13700
H	1.49600	-5.44800	-1.34700
H	0.87100	-5.65300	0.30500
H	2.54400	-6.11500	-0.07600
C	0.37400	2.66200	0.61200
H	2.15100	1.55600	-0.06900
H	1.59000	1.11400	1.55300
H	0.06800	2.96700	-0.40000
C	1.12300	3.82500	1.28100
H	-0.55200	2.45900	1.17400
H	2.05000	4.02800	0.71900
H	1.43400	3.51700	2.29400
C	0.27700	5.09900	1.36400
H	-0.64100	4.93000	1.94800
H	-0.02100	5.44500	0.36200
H	0.83500	5.91400	1.84700
H	-1.57000	-1.33000	0.15300
C	-1.05700	-0.67700	2.18000
H	-1.79800	0.40000	0.42800
H	-0.39700	-1.53200	2.40000
H	-0.60600	0.20200	2.66900
C	-2.44100	-0.93900	2.79300
H	-3.10000	-0.08300	2.57300
C	-2.38100	-1.17100	4.30600
H	-2.89300	-1.81500	2.29900
H	-1.75400	-2.04200	4.55000
H	-1.95900	-0.29700	4.82600
H	-3.38500	-1.35400	4.71800
C	0.24000	-0.00100	-1.97100
H	1.23900	0.26600	-2.36100
C	-0.84700	0.95600	-2.48300
H	0.02600	-1.03000	-2.30200
H	-0.61100	1.99100	-2.19200

H	-1.81900	0.71000	-2.02600
C	-0.97900	0.88300	-4.01200
H	-0.00400	1.11600	-4.47000
C	-2.04800	1.83500	-4.55700
H	-1.22000	-0.15400	-4.30300
H	-2.12500	1.75900	-5.65200
H	-1.81100	2.88100	-4.31000
H	-3.03800	1.60600	-4.13400
Br	4.08800	0.73700	-2.08500

[MTPP]Cl

P	-0.26500	-0.02500	0.63500
C	-0.60800	1.54500	-0.22800
C	1.52500	-0.15700	0.96500
C	-0.79300	-1.42800	-0.40600
C	-1.92000	2.05400	-0.24000
C	0.42700	2.22100	-0.89600
C	-2.18300	3.24500	-0.92100
C	-1.15400	3.92200	-1.58700
C	0.14700	3.41000	-1.57500
H	-1.36800	4.85300	-2.11500
H	0.95100	3.93700	-2.09200
H	-2.73700	1.53600	0.27300
H	-3.19800	3.64700	-0.92900
H	1.44500	1.83000	-0.88500
C	2.08700	0.59200	2.01500
C	2.33700	-0.97500	0.16300
C	3.71100	-1.04400	0.41500
C	3.46000	0.51500	2.25800
C	4.27100	-0.30200	1.46000
H	1.90500	-1.56000	-0.64900
H	1.46700	1.23400	2.64300
H	3.89600	1.09300	3.07300
H	4.34100	-1.68100	-0.20700
H	5.34300	-0.35900	1.65400
C	-1.07100	-1.23500	-1.76900
C	-0.89900	-2.70800	0.16700
C	-1.45700	-2.32400	-2.55500
C	-1.28800	-3.78800	-0.62800
C	-1.56700	-3.59700	-1.98600
H	-1.87200	-4.44400	-2.60300
H	-1.67500	-2.17400	-3.61300
H	-0.68200	-2.87100	1.22400
H	-1.37400	-4.78000	-0.18300
H	-0.99200	-0.24400	-2.21700

C	-1.18100	-0.06700	2.20700
H	-0.95500	-1.00500	2.72900
H	-2.26200	-0.00400	1.99800
H	-0.87200	0.78300	2.82800
Cl	-4.93600	0.35500	1.57200

[ATPP]Br

P	-0.18400	-0.20300	0.19600
C	-0.65200	1.53700	-0.09000
C	1.62200	-0.32400	0.42400
C	-0.68700	-1.20900	-1.24300
C	-1.99900	1.91400	0.06400
C	0.30600	2.47200	-0.51500
C	-2.37400	3.23400	-0.19800
C	-1.42100	4.17000	-0.61700
C	-0.08400	3.78900	-0.77700
H	-1.72100	5.19900	-0.82000
H	0.66000	4.51600	-1.10600
H	-2.76000	1.19100	0.38000
H	-3.41700	3.53200	-0.07500
H	1.34900	2.18200	-0.64200
C	2.24700	0.42300	1.44100
C	2.38200	-1.17300	-0.39800
C	3.76200	-1.27400	-0.20000
C	3.62600	0.31300	1.62900
C	4.38400	-0.53300	0.81100
H	1.90600	-1.75000	-1.19000
H	1.66900	1.09000	2.08100
H	4.11000	0.89400	2.41600
H	4.35100	-1.93100	-0.84200
H	5.46100	-0.61300	0.96100
C	-0.87500	-2.59500	-1.10200
C	-0.86200	-0.59200	-2.49300
C	-1.24000	-3.35700	-2.21500
C	-1.22500	-1.36500	-3.59900
C	-1.41500	-2.74400	-3.46100
H	-1.70100	-3.34400	-4.32600
H	-1.38800	-4.43200	-2.10500
H	-0.72200	0.48300	-2.60700
H	-1.36200	-0.88500	-4.56900
H	-0.74000	-3.08800	-0.13900
C	-1.07900	-0.84900	1.68500
H	-0.77800	-1.90100	1.78800
H	-2.15500	-0.82300	1.41000

C	-0.82300	-0.08000	2.94600
C	-0.22900	-0.60100	4.02700
H	-1.18300	0.95200	2.96900
H	0.13800	-1.63000	4.04100
H	-0.09800	-0.01100	4.93500
Br	-4.79800	-0.58400	1.12400

HBD's:

1,2,4-triazole

N	0.60300	-1.10100	0.00000
C	0.99600	0.17600	0.00000
C	-0.76100	-0.99800	0.00000
N	-1.23100	0.25000	0.00000
N	-0.08200	0.98400	0.00000
H	-0.11700	2.00200	0.00000
H	-1.42600	-1.85800	0.00000
H	2.01700	0.54500	0.00000

2,6-xylenol

C	-1.27700	0.00800	0.06500
C	-0.02500	0.65300	0.00100
C	-1.29100	-1.39400	0.06600
C	-0.10500	-2.13400	0.00500
C	1.12200	-1.46700	-0.05800
C	1.18700	-0.06600	-0.06100
H	2.05300	-2.03700	-0.10600
C	2.50500	0.66800	-0.12700
H	-2.25400	-1.90900	0.11500
H	-0.13800	-3.22500	0.00600
C	-2.54700	0.81700	0.13000
O	-0.04300	2.03300	0.00200
H	-3.42400	0.15800	0.17300
H	-2.56300	1.47100	1.01600
H	-2.65200	1.47400	-0.74700
H	3.34100	-0.04200	-0.17000
H	2.66500	1.31100	0.75400
H	2.57400	1.31200	-1.02000
H	0.87200	2.36900	-0.04500

Urea

N	-0.69500	-0.95800	-0.06000
C	0.43500	-0.18600	-0.19600
O	1.49500	-0.64000	-0.67200
N	0.32200	1.11800	0.22700
H	-0.71300	-1.81900	-0.59800
H	-1.59900	-0.51200	0.07800
H	-0.44300	1.38600	0.84000
H	1.19700	1.61100	0.38100

Imidazole

C	0.88000	-0.82100	-0.25800
N	-0.33800	-1.30800	-0.47900
C	-1.20800	-0.28000	-0.14700
C	-0.50400	0.82800	0.27500
N	0.82500	0.46400	0.19800
H	1.81800	-1.34700	-0.40800
H	-2.28400	-0.39700	-0.23200
H	-0.81200	1.81100	0.61300
H	1.62200	1.05000	0.43800

Phenol

C	1.10400	0.22400	-0.14800
C	0.63600	-0.75300	0.74300
C	-0.74100	-0.97100	0.87000
C	-1.65300	-0.22300	0.11600
C	-1.17500	0.75000	-0.77100
C	0.19700	0.97900	-0.90800
O	2.44400	0.48600	-0.31800
H	1.34600	-1.33800	1.33300
H	-1.09800	-1.73300	1.56500
H	-2.72500	-0.39700	0.21800
H	-1.87500	1.34100	-1.36500
H	0.57600	1.73600	-1.59700
H	2.96300	-0.10300	0.26300

Lactic acid

C	1.10000	-0.52100	0.55000
C	-0.32600	-0.01600	0.27600
O	-0.32900	1.43000	0.34900
C	-0.81000	-0.46800	-1.10000

O	1.40900	-1.70200	0.58000
O	2.00700	0.45400	0.75000
H	-0.97100	-0.43600	1.06200
H	-0.77400	1.69800	1.17300
H	-0.75400	-1.56200	-1.18000
H	-0.19100	-0.02400	-1.89200
H	-1.85200	-0.15700	-1.24400
H	1.49100	1.30400	0.67600

Ethylene glycol

O	0.79000	1.50500	0.34500
C	-0.42100	0.75700	0.12800
C	-0.14800	-0.55700	-0.58900
O	0.79300	-1.36900	0.14800
H	1.42700	0.87200	0.72800
H	-0.92900	0.55900	1.09100
H	-1.08200	1.38800	-0.48300
H	-1.09500	-1.09700	-0.75700
H	0.32600	-0.36700	-1.56200
H	0.34100	-1.69100	0.95100

Acetic acid

C	-0.49500	0.27900	0.13200
O	-0.96900	1.24400	0.71700
O	-1.27000	-0.62500	-0.52200
H	-2.20700	-0.34800	-0.42100
C	0.96500	-0.06400	0.04300
H	1.56200	0.70700	0.53900
H	1.14600	-1.03800	0.52200
H	1.26800	-0.15500	-1.00900

Glycerol

O	-0.63300	-0.33000	-1.67900
C	-0.12000	0.85100	-1.00700
C	0.05900	0.64200	0.49800
O	-1.21900	0.49200	1.15600
C	0.95400	-0.55900	0.82500
O	0.27300	-1.80100	0.54200
H	-1.59500	-0.35900	-1.52500
H	0.85600	1.06400	-1.46600
H	-0.78700	1.70800	-1.18900

H	0.52700	1.55300	0.90500
H	-1.39100	-0.47300	1.17900
H	1.90000	-0.48500	0.26100
H	1.18900	-0.57600	1.89800
H	-0.01300	-1.72600	-0.39700

Ethanolamine (EA)

N	-1.08500	-0.78000	-0.07400
O	1.64000	-0.79100	0.18000
C	-0.42200	0.48600	0.30500
C	1.01500	0.44500	-0.21500
H	-1.91300	-0.93900	0.50300
H	-1.40900	-0.73600	-1.04300
H	0.88800	-1.43100	0.13100
H	-0.93100	1.39100	-0.07200
H	-0.40800	0.54100	1.40400
H	1.60700	1.27400	0.19900
H	1.01800	0.53900	-1.31800

Diethylene glycol (DEG)

C	1.49100	1.22400	1.43100
C	1.22500	0.67200	0.04400
O	0.41000	2.04400	1.91600
H	2.38100	1.86700	1.39900
H	1.69000	0.39200	2.12900
H	2.11900	0.12900	-0.31800
H	1.00500	1.49400	-0.66200
O	0.10000	-0.21600	0.12700
C	-0.29100	-0.73200	-1.15500
H	0.51600	-1.35700	-1.58100
H	-0.49100	0.10300	-1.85200
C	-1.54000	-1.56900	-0.96400
H	-1.82200	-2.02000	-1.92500
O	-2.67000	-0.78900	-0.53000
H	-1.33300	-2.38400	-0.24700
H	-2.40000	-0.34600	0.29600
H	-0.39100	1.48800	1.89400

Levulinic acid

C	-1.69000	1.54800	-0.91900
H	-1.54500	2.62300	-1.07100
H	-1.96000	1.07700	-1.87900
H	-2.52900	1.36100	-0.23400
C	-0.44000	0.90200	-0.40900
C	-0.55700	-0.50400	0.13600
H	-0.93100	-0.40600	1.17200
H	-1.36100	-1.01900	-0.40900
C	0.71700	-1.37200	0.08700
H	0.43500	-2.42200	0.22200
H	1.18000	-1.28400	-0.91000
C	1.79200	-1.06300	1.12100
O	2.24600	0.20100	1.16600
H	1.73400	0.76500	0.48600
O	2.26200	-1.91100	1.87300
O	0.64700	1.50300	-0.43200

Guaiacol

C	0.99900	-0.83500	-0.53500
C	0.34800	-2.04500	-0.76600
C	-1.01400	-2.17800	-0.45700
C	-1.71900	-1.09900	0.08200
C	-1.07100	0.12400	0.31800
C	0.28500	0.25900	0.01100
H	-2.77900	-1.19700	0.32300
O	1.04900	1.38900	0.18700
C	0.40700	2.55400	0.73900
H	-1.62700	0.96200	0.73800
H	-1.51700	-3.12800	-0.64100
O	2.33300	-0.70400	-0.83700
H	2.60000	0.20900	-0.60100
H	0.02100	2.34700	1.74800
H	-0.41200	2.89600	0.08800
H	1.18400	3.32300	0.79100
H	0.91500	-2.87700	-1.18800

Furfuryl alcohol

C	-1.36900	-0.84700	0.69100
C	-0.11500	-0.20400	0.21500
C	0.45800	1.02100	0.44100
C	1.66100	1.07200	-0.34000
C	1.74200	-0.12400	-0.99600
O	0.67000	-0.92100	-0.67200
O	-2.40000	-0.93400	-0.32500
H	-1.18000	-1.88500	0.99600
H	-1.73000	-0.29000	1.57000
H	0.06700	1.79700	1.09400
H	2.37300	1.89000	-0.40300
H	2.45600	-0.55500	-1.69000
H	-2.63200	-0.02100	-0.57900

2,3-butanediol

C	-0.82900	0.27200	0.01300
C	0.70500	0.40500	0.06400
O	-1.40700	1.58200	-0.18300
H	-1.16700	-0.12800	0.99100
C	-1.32800	-0.62900	-1.10600
C	1.42100	-0.88400	0.44700
O	1.04900	1.48900	0.97200
H	1.05200	0.75900	-0.92000
H	1.06200	-1.25600	1.42000
H	2.50400	-0.71000	0.51800
H	1.25200	-1.67000	-0.30200
H	-2.42600	-0.60200	-1.14700
H	-0.93600	-0.29500	-2.07900
H	-1.02300	-1.67100	-0.94300
H	-0.86400	2.17900	0.37300
H	0.93500	1.15700	1.88300

1,2-propanediol

C	-1.49200	-0.36900	-0.04600
C	-0.18900	0.39300	-0.25100
H	-1.31600	-1.45700	-0.05800
H	-2.21200	-0.12400	-0.83900
H	-1.94600	-0.10900	0.92200
H	-0.37800	1.47700	-0.25800
O	0.39700	0.12800	-1.55500
C	0.84600	0.08300	0.83200

H	0.48200	0.41300	1.81500
O	2.08300	0.77400	0.59000
H	1.01400	-1.01100	0.87400
H	0.44400	-0.84100	-1.66400
H	2.26700	0.64200	-0.36300

Triethylene glycol

C	0.16300	1.35100	1.45500
C	-1.02500	0.43200	1.70100
O	0.93700	0.96600	0.29600
H	0.80900	1.38200	2.34900
H	-0.19500	2.37000	1.25100
H	-1.52400	0.74800	2.63300
H	-0.70100	-0.61300	1.83400
O	-1.97900	0.53000	0.62900
C	-2.11300	-0.60800	-0.24600
H	-3.13700	-1.01000	-0.15500
H	-1.40500	-1.40200	0.04400
C	-1.87400	-0.18700	-1.68500
H	-2.11100	-1.02500	-2.35700
O	-0.50400	0.18900	-1.94400
H	-2.54300	0.65500	-1.93700
C	1.93200	-0.04800	0.58400
C	2.51000	-0.58500	-0.71500
H	1.48400	-0.87600	1.16000
H	2.73600	0.40800	1.18900
H	2.80400	0.26300	-1.36000
O	1.64600	-1.49200	-1.41400
H	3.42300	-1.14900	-0.46900
H	0.83600	-0.98700	-1.68900
H	-0.16900	0.68800	-1.15400

1,4-butanediol

C	-0.37700	1.42400	-0.91300
C	0.71900	0.35500	-0.94100
C	0.98600	-0.39500	0.37900
C	-0.07100	-1.40300	0.82700
O	-1.71700	0.90100	-0.85000
O	-1.33000	-0.79900	1.24300
H	-0.19300	2.11800	-0.06800
H	-0.33000	2.01600	-1.83900
H	1.65400	0.86200	-1.23600
H	0.49100	-0.36800	-1.74200

H	1.16200	0.33000	1.19400
H	1.92700	-0.96100	0.27100
H	0.32000	-2.01200	1.65700
H	-0.33800	-2.07900	0.00300
H	-1.74300	0.31100	-0.05100
H	-1.16200	-0.30100	2.06500

Diethanolamine

N	-0.33300	-0.58800	-0.14500
C	-0.12900	0.21500	2.17100
C	-0.02100	-0.99300	1.24100
O	-1.40400	0.86000	1.99400
C	0.35900	0.46000	-2.25100
C	0.82200	-0.06200	-0.89700
O	-0.63600	1.49300	-2.11000
H	-0.71900	-1.39000	-0.64800
H	-0.05400	-0.10300	3.22100
H	0.69000	0.93200	1.97400
H	-0.76500	-1.74400	1.54300
H	0.98200	-1.45100	1.33300
H	-1.57200	0.75700	1.02900
H	1.20300	0.90000	-2.79800
H	-0.04200	-0.37500	-2.85600
H	1.26500	0.76400	-0.32000
H	1.61000	-0.82600	-1.04800
H	-1.25600	1.15100	-1.43400

Octanoic acid

C	1.76400	-0.63600	-0.32600
H	1.73600	-0.66000	-1.42700
H	2.33000	0.26800	-0.04800
C	2.49800	-1.87500	0.19000
H	2.54600	-1.87400	1.29200
H	1.95500	-2.79600	-0.07800
C	3.91100	-2.02100	-0.32000
O	4.50600	-3.14200	0.17000
H	5.41800	-3.18400	-0.19300
O	4.48800	-1.25500	-1.07900
C	0.33600	-0.54200	0.22500
H	0.37100	-0.52500	1.32900
H	-0.22200	-1.45500	-0.05000
C	-0.43200	0.68800	-0.27500
H	-0.46800	0.67100	-1.37900

H	0.12400	1.60200	0.00100
C	-1.86100	0.77900	0.27600
H	-1.82400	0.79600	1.38000
H	-2.41500	-0.13700	0.00200
C	-2.63800	2.00500	-0.22000
H	-2.08400	2.92000	0.05500
H	-2.67500	1.98800	-1.32300
C	-4.06300	2.08300	0.33900
H	-4.05600	2.13400	1.43900
H	-4.59500	2.97200	-0.03400
H	-4.65100	1.19700	0.05100

1,2-butanediol

C	2.14200	0.10300	0.19100
C	0.85100	-0.59200	-0.25200
H	2.21500	1.11900	-0.22500
H	3.02600	-0.45500	-0.14900
H	2.19600	0.18100	1.28800
H	0.82200	-0.67200	-1.35100
C	-0.42000	0.11800	0.21900
H	0.83100	-1.62200	0.14400
O	-0.54500	1.45000	-0.35000
H	-0.41400	0.20300	1.32100
C	-1.68700	-0.61600	-0.20500
H	-1.69600	-0.71600	-1.30700
O	-2.87300	0.06000	0.24700
H	-1.70400	-1.62300	0.23400
H	-2.73600	0.99900	0.01200
H	-0.01000	2.06300	0.18300

Hexanoic acid

C	2.26300	-1.97100	1.42900
H	2.31500	-2.72200	2.23100
H	2.60300	-2.45100	0.49800
H	2.98000	-1.17200	1.67200
C	0.84400	-1.41200	1.27400
H	0.14300	-2.23800	1.06200
H	0.51600	-0.96800	2.23000
C	0.73000	-0.35900	0.16500
H	1.43100	0.46900	0.37700
H	1.06000	-0.80200	-0.79100
C	-0.68700	0.20500	0.00100
H	-1.01900	0.65600	0.95000

H	-1.38900	-0.61600	-0.21700
C	-0.76600	1.24900	-1.11400
H	-0.07800	2.08900	-0.91600
H	-0.43900	0.82400	-2.07800
C	-2.14000	1.83600	-1.32100
O	-3.14400	1.57300	-0.67400
O	-2.15300	2.73100	-2.34700
H	-3.06700	3.08100	-2.43100

Methyl diethanolamine (MDEA)

C	-1.20000	-0.65800	0.56900
N	0.00000	0.06600	0.10300
C	1.24200	-0.61000	0.52900
H	1.09400	-1.69200	0.39500
H	1.46400	-0.42800	1.60100
C	2.43200	-0.17000	-0.32200
H	2.70200	0.88000	-0.11300
O	2.14400	-0.34000	-1.72300
H	3.30500	-0.79300	-0.08400
H	1.19600	-0.09700	-1.80000
C	-0.02000	1.47600	0.52600
H	-1.01400	-1.73300	0.42800
C	-2.43300	-0.26300	-0.24200
H	-1.39400	-0.48500	1.64800
H	-2.73700	0.77600	-0.02000
H	-3.27300	-0.92000	0.02200
O	-2.18400	-0.41800	-1.65200
H	-1.24700	-0.14200	-1.75700
H	0.84800	2.00700	0.11700
H	-0.00500	1.57300	1.63100
H	-0.92100	1.97300	0.14500

Ethylenecyanohydrin (ECH)

C	0.19300	0.78600	-0.25800
C	-0.86200	-0.33700	-0.14200
C	1.55600	0.30200	-0.08400
H	-0.00100	1.56300	0.49600
H	0.11600	1.26000	-1.25000
O	-0.92000	-0.91700	1.16500
H	-0.68200	-1.10300	-0.91200
H	-1.84400	0.11700	-0.32700
N	2.63400	-0.11400	0.06200
H	-0.19100	-1.55700	1.25000