

Supplementary Material

A DFT study of mono-, bi- and tricyclic examples of semi-conjugated heterocyclic mesomeric betaines

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Table 1. Structures of compound type 6

6a

	angstroms		
	X	Y	Z
C	1.179064000	0.892227000	-0.000095000
C	-1.179060000	-0.892230000	0.000072000
N	-1.207427000	0.523480000	-0.000017000
N	1.207432000	-0.523479000	0.000042000
O	-2.218473000	-1.551641000	0.000158000
O	2.218475000	1.551643000	-0.000119000
C	-0.161863000	1.370253000	-0.000083000
H	-0.358809000	2.432390000	-0.000135000
C	0.161866000	-1.370255000	0.000112000
H	0.358814000	-2.432390000	0.000208000
H	-2.149271000	0.904641000	-0.000018000
H	2.149274000	-0.904643000	0.000070000
Gibbs free energy =	-414.824048	Hartree	

Number of imaginary frequencies: 0

6b

	angstroms		
	X	Y	Z
C	1.164978000	0.883136000	-0.000087000
C	-1.164973000	-0.883148000	0.000085000
N	-1.245000000	0.534995000	-0.000020000
N	1.245005000	-0.534991000	0.000086000
O	-2.189527000	-1.574654000	0.000198000

O	2.189522000	1.574659000	-0.000317000
C	-2.604999000	1.083089000	0.000023000
H	-3.137472000	0.720465000	-0.879583000
H	-3.136661000	0.722616000	0.881024000
H	-2.552134000	2.169495000	-0.001284000
C	2.605002000	-1.083091000	0.000042000
H	3.136464000	-0.723193000	-0.881320000
H	3.137679000	-0.719900000	0.879286000
H	2.552133000	-2.169495000	0.002042000
C	-0.174099000	1.350655000	-0.000002000
H	-0.347410000	2.416854000	-0.000045000
C	0.174099000	-1.350659000	0.000053000
H	0.347421000	-2.416856000	0.000115000

Gibbs free energy = -493.417313 Hartree

Number of imaginary frequencies: 0

6c

	angstroms		
	X	Y	Z
C	1.253854000	0.769623000	-0.094175000
C	-1.192868000	0.647364000	-0.085764000
C	-1.253854000	-0.769623000	-0.094175000
C	1.192868000	-0.647364000	-0.085764000
H	-2.124270000	1.192360000	-0.104511000
H	2.124270000	-1.192360000	-0.104511000
O	-2.285881000	-1.443005000	-0.111064000
C	-0.145728000	2.807418000	-0.002338000

C	0.533275000	3.600047000	-0.926618000
C	-0.935295000	3.384876000	0.991379000
C	0.396289000	4.983106000	-0.862044000
H	1.164862000	3.140015000	-1.673056000
C	-1.062544000	4.770740000	1.048161000
H	-1.431357000	2.756934000	1.721924000
C	-0.399733000	5.571139000	0.120731000
H	0.918753000	5.603105000	-1.581069000
H	-1.672623000	5.220734000	1.822518000
H	-0.496585000	6.649639000	0.167248000
C	0.145728000	-2.807418000	-0.002338000
C	-0.533275000	-3.600047000	-0.926618000
C	0.935295000	-3.384876000	0.991379000
C	-0.396289000	-4.983106000	-0.862044000
H	-1.164862000	-3.140015000	-1.673056000
C	1.062544000	-4.770740000	1.048161000
H	1.431357000	-2.756934000	1.721924000
C	0.399733000	-5.571139000	0.120731000
H	-0.918753000	-5.603105000	-1.581069000
H	1.672623000	-5.220734000	1.822518000
H	0.496585000	-6.649639000	0.167248000
O	2.285881000	1.443005000	-0.111064000
N	0.048570000	-1.367933000	-0.071539000
N	-0.048570000	1.367933000	-0.071539000

Gibbs free energy = -876.876152 Hartree

Number of imaginary frequencies: 0

6d

angstroms

	X	Y	Z
C	1.393954000	-0.487072000	0.000000000
C	-1.055384000	-0.890896000	0.000000000
C	-1.393954000	0.487072000	0.000000000
C	1.055384000	0.890896000	0.000000000
H	-1.834004000	-1.640604000	0.000000000
H	1.834004000	1.640604000	0.000000000
O	-2.525537000	0.961128000	0.000000000
O	2.525537000	-0.961128000	0.000000000
C	0.450890000	-2.768661000	0.000000000
O	-0.451824000	-3.550962000	0.000000000
H	1.520281000	-2.995832000	0.000000000
C	-0.450890000	2.768661000	0.000000000
O	0.451824000	3.550962000	0.000000000
H	-1.520281000	2.995832000	0.000000000
N	-0.220139000	1.333206000	0.000000000
N	0.220139000	-1.333206000	0.000000000

Gibbs free energy = -641.514067 Hartree

Number of imaginary frequencies: 0

6e

angstroms

	X	Y	Z
C	1.145979000	0.879585000	-0.000329000
C	-1.145976000	-0.879588000	0.000288000
N	-1.255533000	0.524286000	-0.000002000
N	1.255535000	-0.524287000	0.000039000
C	-2.601525000	1.109081000	0.000020000
H	-3.142424000	0.759138000	-0.879789000
H	-3.141961000	0.760238000	0.880556000
H	-2.513242000	2.193329000	-0.000666000
C	2.601528000	-1.109084000	0.000062000
H	3.141892000	-0.760506000	-0.880625000
H	3.142499000	-0.758874000	0.879719000
H	2.513245000	-2.193330000	0.001074000
C	-0.182393000	1.329643000	-0.000229000
H	-0.361839000	2.394254000	-0.000403000
C	0.182396000	-1.329645000	0.000251000
H	0.361842000	-2.394256000	0.000455000
S	2.480926000	1.919390000	-0.000885000
S	-2.480924000	-1.919391000	0.000729000

Gibbs free energy = -1139.352549 Hartree

Number of imaginary frequencies: 0

6f

angstroms

	X	Y	Z
C	-1.387069000	0.330421000	-0.000023000
C	1.387069000	-0.330419000	0.000043000
N	0.389490000	-1.306194000	-0.000003000
N	-0.389490000	1.306196000	0.000047000
C	0.823301000	-2.712424000	-0.000002000
H	1.438479000	-2.892922000	-0.881347000
H	1.438056000	-2.893065000	0.881614000
H	-0.057603000	-3.349516000	-0.000257000
C	-0.823301000	2.712426000	0.000053000
H	-1.437930000	2.893116000	-0.881642000
H	-1.438606000	2.892875000	0.881319000
H	0.057603000	3.349518000	0.000466000
N	2.645935000	-0.741413000	0.000089000
N	-2.645936000	0.741414000	-0.000100000
C	3.601011000	0.167727000	0.000111000
N	4.474510000	0.939158000	0.000135000
C	-3.601011000	-0.167726000	-0.000122000
N	-4.474509000	-0.939157000	-0.000147000
C	-0.914860000	-0.996814000	-0.000016000
H	-1.626307000	-1.810547000	-0.000048000
C	0.914859000	0.996816000	0.000053000
H	1.626307000	1.810549000	0.000094000

Gibbs free energy = -638.139786 Hartree

Number of imaginary frequencies: 0

Table 2. Structures of compound type 7

7a

	angstroms		
	X	Y	Z
C	2.068285000	0.907066000	-0.000025000
C	0.855844000	1.583129000	-0.000028000
C	-0.193679000	-0.724316000	0.000008000
C	1.123591000	-1.368006000	0.000050000
H	-1.494259000	2.322439000	-0.000059000
H	2.992163000	1.463384000	-0.000055000
C	-1.535339000	1.241887000	-0.000053000
C	-1.349935000	-1.506332000	0.000007000
H	3.079795000	-0.893629000	0.000015000
C	-2.597658000	-0.914098000	-0.000025000
H	-1.208664000	-2.579317000	0.000032000
H	-3.495374000	-1.519351000	-0.000039000
O	1.290014000	-2.588475000	0.000029000
O	0.622320000	2.795263000	-0.000080000
N	2.160228000	-0.469106000	0.000013000
N	-0.302501000	0.650912000	-0.000023000
C	-2.681492000	0.489539000	-0.000051000
H	-3.638984000	0.994185000	-0.000072000
Gibbs free energy = -607.754562			Hartree
Number of imaginary frequencies: 0			

7b

angstroms

	X	Y	Z
C	3.608598000	0.107815000	0.015445000
C	2.617822000	-0.833717000	-0.023617000
C	1.023210000	0.917524000	0.027075000
C	2.104811000	1.812789000	0.065100000
C	0.290902000	-1.471956000	-0.060710000
C	-0.344874000	1.403758000	0.035243000
C	-1.007182000	-0.942551000	-0.050473000
H	4.646115000	-0.204936000	0.011174000
H	1.871735000	2.871011000	0.100408000
N	1.304489000	-0.433864000	-0.018127000
N	-1.301820000	0.390749000	-0.005875000
H	2.762448000	-1.903768000	-0.059920000
O	-0.661280000	2.593039000	0.073967000
O	0.636985000	-2.655609000	-0.099833000
C	-2.700429000	0.836596000	0.000855000
H	-2.892811000	1.417727000	0.903196000
H	-2.880974000	1.481155000	-0.859890000
H	-3.348952000	-0.035628000	-0.034863000
N	3.372556000	1.444177000	0.060388000
H	-1.838413000	-1.630479000	-0.079543000

Gibbs free energy = -623.799817 Hartree

Number of imaginary frequencies: 0

7c

angstroms

	X	Y	Z
C	2.063994000	0.907923000	0.000028000
C	0.840175000	1.576032000	0.000058000
C	-0.177649000	-0.746295000	0.000039000
C	1.139208000	-1.379276000	-0.000032000
H	-1.562735000	2.264466000	-0.000302000
H	2.981752000	1.474777000	0.000075000
C	-1.558072000	1.182221000	0.000154000
C	-1.345990000	-1.509504000	0.000105000
H	3.091551000	-0.877007000	-0.000212000
C	-2.562451000	-0.863008000	-0.000066000
H	-1.247449000	-2.586770000	0.000224000
H	-3.497529000	-1.410550000	0.000114000
O	1.320386000	-2.596284000	-0.000124000
O	0.600204000	2.783098000	0.000051000
N	2.166673000	-0.462234000	-0.000026000
N	-0.298016000	0.628449000	0.000024000
N	-2.661386000	0.491174000	-0.000111000

Gibbs free energy = -623.803630 Hartree

Number of imaginary frequencies: 0

7d

angstroms

	X	Y	Z
C	3.655274000	0.050795000	0.002630000
C	2.588563000	-0.817874000	0.039995000
C	1.056827000	0.981569000	-0.022460000
C	2.111291000	1.894224000	-0.061530000
C	3.415247000	1.430939000	-0.049036000
C	0.190765000	-1.398576000	0.072045000
C	-0.343376000	1.449376000	-0.034524000
H	4.662140000	-0.345383000	0.013705000
H	1.855555000	2.944470000	-0.100629000
H	4.243601000	2.128639000	-0.078908000
N	1.317835000	-0.348630000	0.027242000
N	-1.260272000	0.442632000	0.008787000
H	2.655078000	-1.897237000	0.080768000
O	-0.610648000	2.652789000	-0.079949000
O	0.571491000	-2.556661000	0.114183000
C	-2.685636000	0.767094000	0.002944000
H	-3.144050000	0.363459000	0.907039000
H	-2.794024000	1.847329000	-0.033994000
H	-3.151145000	0.302309000	-0.867573000
N	-1.029468000	-0.912898000	0.059266000

Gibbs free energy = -623.796199 Hartree

Number of imaginary frequencies: 0

Table 3. Structures of compound type 8

8a

	angstroms		
	X	Y	Z
C	3.661779000	0.051461000	0.000000000
C	2.636601000	-0.840853000	0.000000000
C	1.025284000	0.950317000	0.000000000
C	2.091987000	1.868884000	0.000000000
C	3.396851000	1.447085000	0.000000000
C	0.322435000	-1.435606000	0.000000000
C	-0.322435000	1.435606000	0.000000000
C	-1.025284000	-0.950317000	0.000000000
C	-2.091987000	-1.868884000	0.000000000
H	-1.818549000	-2.915616000	0.000000000
C	-3.396852000	-1.447085000	0.000000000
C	-3.661779000	-0.051461000	0.000000000
C	-2.636602000	0.840853000	0.000000000
H	4.677074000	-0.323733000	0.000000000
H	1.818549000	2.915616000	0.000000000
H	4.210139000	2.161256000	0.000000000
H	-4.210140000	-2.161256000	0.000000000
H	-4.677075000	0.323733000	0.000000000
N	1.314894000	-0.419022000	0.000000000
N	-1.314894000	0.419022000	0.000000000
H	-2.746190000	1.914687000	0.000000000
H	2.746190000	-1.914687000	0.000000000

O -0.646962000 2.627436000 0.000000000
O 0.646962000 -2.627436000 0.000000000
Gibbs free energy = -722.081556 Hartree
Number of imaginary frequencies: 0

8b

angstroms

	X	Y	Z
C	3.619252000	0.093705000	0.000000000
C	2.629124000	-0.838802000	0.000000000
C	1.033081000	0.931425000	0.000000000
C	2.133353000	1.816293000	0.000000000
C	0.305798000	-1.447183000	0.000000000
C	-0.305798000	1.447183000	0.000000000
C	-1.033081000	-0.931425000	0.000000000
C	-2.133353000	-1.816293000	0.000000000
H	-1.907906000	-2.877219000	0.000000000
C	-3.619252000	-0.093705000	0.000000000
C	-2.629124000	0.838802000	0.000000000
H	4.654980000	-0.224013000	0.000000000
H	1.907906000	2.877219000	0.000000000
H	-4.654981000	0.224013000	0.000000000
N	1.305298000	-0.435181000	0.000000000
N	-1.305298000	0.435181000	0.000000000
H	-2.775687000	1.908163000	0.000000000
H	2.775687000	-1.908163000	0.000000000
O	-0.618208000	2.636133000	0.000000000

O	0.618208000	-2.636133000	0.000000000
N	-3.392344000	-1.441783000	0.000000000
N	3.392343000	1.441783000	0.000000000

Gibbs free energy = -754.176895 Hartree

Number of imaginary frequencies: 0

8c

	angstroms		
	X	Y	Z
C	2.655887000	-0.775533000	0.000000000
C	1.009185000	0.967747000	0.000000000
C	2.086422000	1.870414000	0.000000000
C	3.369893000	1.394831000	0.000000000
C	0.343137000	-1.439707000	0.000000000
C	-0.343138000	1.439707000	0.000000000
C	-1.009185000	-0.967747000	0.000000000
C	-2.086423000	-1.870414000	0.000000000
H	-1.853532000	-2.926601000	0.000000000
C	-3.369893000	-1.394831000	0.000000000
C	-2.655887000	0.775533000	0.000000000
H	1.853532000	2.926601000	0.000000000
H	4.226599000	2.056757000	0.000000000
H	-4.226599000	-2.056757000	0.000000000
N	1.313935000	-0.396451000	0.000000000
N	-1.313935000	0.396451000	0.000000000
H	-2.805699000	1.846688000	0.000000000
H	2.805698000	-1.846688000	0.000000000

O	-0.684120000	2.622651000	0.000000000
O	0.684119000	-2.622651000	0.000000000
N	-3.646493000	-0.051718000	0.000000000
N	3.646493000	0.051718000	0.000000000

Gibbs free energy = -754.183300 Hartree

Number of imaginary frequencies: 0

Table 4. Structures of compound type 9-13

9

	angstroms		
	X	Y	Z
C	3.68622600	0.05305200	0.00000000
C	2.69723200	-0.95664800	0.00000000
C	1.02526800	0.96211900	0.00000000
C	2.08453100	1.88417600	0.00000000
C	3.38617700	1.41289200	0.00000000
C	0.31452100	-1.32191400	0.00000000
C	-0.31452200	1.32191400	0.00000000
C	-1.02526800	-0.96211900	0.00000000
C	-2.08453100	-1.88417600	0.00000000
H	-1.85334100	-2.93987900	0.00000000
C	-3.38617700	-1.41289200	0.00000000
C	-3.68622600	-0.05305200	0.00000000
C	-2.69723200	0.95664800	0.00000000
H	0.63831200	-2.35361600	0.00000000
H	4.71096100	-0.29290900	0.00000000

H	1.85334100	2.93987900	0.00000000
H	4.20405600	2.12489800	0.00000000
H	-0.63831200	2.35361600	0.00000000
H	-4.20405600	-2.12489800	0.00000000
H	-4.71096100	0.29290900	0.00000000
O	-2.82264000	2.17317200	0.00000000
O	2.82264000	-2.17317200	0.00000000
N	1.31249400	-0.41805200	0.00000000
N	-1.31249400	0.41805200	0.00000000

Gibbs free energy = -722.074651 Hartree

Number of imaginary frequencies: 0

10

angstroms

	X	Y	Z
C	-3.26771600	-1.67963900	-0.18469400
C	-1.91227600	-2.02893200	-0.09499500
C	-0.95601900	-1.02270500	-0.00469400
C	-1.35412500	0.36157500	0.00959100
C	-2.80349500	0.72911000	-0.17257400
C	-3.70445800	-0.37485500	-0.20393300
C	0.95605900	1.02268100	-0.00463600
C	1.35417800	-0.36160200	0.00967400
C	2.80358100	-0.72910300	-0.17240900
C	3.70450700	0.37488900	-0.20385500
C	3.26774200	1.67966300	-0.18460900
C	1.91229900	2.02892700	-0.09491300

H	-3.99547300	-2.48035500	-0.26479900
H	-1.62736300	-3.06755600	-0.12875600
H	-4.75436600	-0.13239400	-0.30862500
H	4.75441400	0.13245500	-0.30862800
H	3.99547900	2.48039300	-0.26474900
H	1.62736700	3.06754500	-0.12870400
O	-3.14815000	1.91457400	-0.33717000
O	3.14826100	-1.91451200	-0.33735200
N	-0.40277600	1.30722300	0.15936200
N	0.40280400	-1.30725200	0.15940100
C	-0.73439700	2.69938200	0.53679900
H	-0.69645500	3.34629600	-0.34111700
H	-1.73518700	2.73934600	0.94178400
H	0.01348400	3.01460600	1.26355400
C	0.73432000	-2.69939900	0.53698100
H	0.69654600	-3.34636000	-0.34090800
H	1.73501700	-2.73937500	0.94218600
H	-0.01373000	-3.01456300	1.26358900

Gibbs free energy = -800.619750 Hartree

Number of imaginary frequencies: 0

11

angstroms

	X	Y	Z
C	-3.83024300	-0.25151800	-0.02176500
C	-2.92931300	0.78398000	-0.14645100
C	-1.55319900	0.54531700	-0.10561600

C	-1.97472900	-1.75806200	0.20553600
C	-3.32721200	-1.54616000	0.17639300
C	-0.64223000	1.69895000	-0.14138400
C	0.32709700	-0.99765800	-0.01239800
C	1.20303200	0.11833600	0.01385000
C	2.66977200	-0.09328300	-0.08735100
C	3.07892500	-1.46505100	-0.07421300
C	2.18531300	-2.51342600	-0.09212000
C	0.80330400	-2.31209500	-0.07771500
H	-4.89675000	-0.06913300	-0.05647200
H	-3.22922800	1.81569700	-0.26987700
H	-1.55370700	-2.73207200	0.37836600
H	-3.98573800	-2.39336800	0.31685600
H	4.14723500	-1.63957100	-0.11545100
H	2.55792500	-3.53136500	-0.14175200
H	0.14852400	-3.16292500	-0.17403200
N	-1.07586500	-0.73372800	0.03611200
N	0.69006000	1.41367200	0.06147000
O	-1.08876100	2.83807600	-0.26166900
O	3.47090000	0.85823200	-0.20289400
C	1.53690700	2.59987600	0.33578100
H	2.29347000	2.33828700	1.06533200
H	2.03915000	2.92821900	-0.57221200
H	0.86854200	3.37959000	0.69235000

Gibbs free energy = -761.354745 Hartree

Number of imaginary frequencies: 0

12

angstroms

	X	Y	Z
C	3.36861200	-0.78506000	0.00000000
C	2.73661500	0.48595400	-0.00000200
C	0.56550300	-0.77617100	-0.00000100
C	1.26891100	-1.98423700	-0.00000100
C	2.66012000	-1.97030900	0.00000000
C	0.63261500	1.64502800	-0.00000100
C	-0.87225600	-0.70456500	0.00000000
C	-0.74458900	1.81959400	0.00000000
C	-2.85206200	0.64335300	0.00000000
H	-3.19063400	1.67031000	0.00000100
C	-3.66135300	-0.45799000	0.00000000
C	-3.07089700	-1.73441800	0.00000000
C	-1.69947900	-1.84597800	0.00000000
H	1.29392600	2.49575000	-0.00000200
H	4.45024800	-0.77060800	0.00000200
H	0.73824000	-2.92265000	-0.00000100
H	3.19778400	-2.91191900	0.00000100
H	-4.73555000	-0.33043800	0.00000100
H	-3.68697800	-2.62522900	0.00000000
H	-1.24016700	-2.82234600	0.00000000
O	-1.40638700	2.85382700	0.00000000
O	3.26444800	1.58853400	0.00000300
N	-1.48999900	0.52591700	0.00000000
N	1.25907000	0.42318800	-0.00000100

Gibbs free energy = -722.075795 Hartree

Number of imaginary frequencies: 0

13

	angstroms		
	X	Y	Z
C	3.20762800	-0.78721700	-0.00010100
C	2.55514000	0.49978300	-0.00000500
C	1.18551200	0.63083200	0.00001800
C	0.29352500	-0.51118900	-0.00004300
C	0.92382700	-1.78544100	-0.00020800
C	2.28664100	-1.91361400	-0.00025800
C	-1.60924500	0.98749300	-0.00006900
C	-0.71837200	2.05699900	-0.00000300
C	-2.98673000	1.26133300	-0.00017000
H	-3.30132900	2.29584600	-0.00021400
C	-3.89119400	0.21589500	-0.00018200
C	-3.42640700	-1.08442300	-0.00003300
C	-2.04884200	-1.45309600	0.00014200
H	3.20593400	1.36163700	0.00004200
H	0.30391300	-2.66264000	-0.00028400
H	2.72840800	-2.90390500	-0.00039700
H	-1.10886000	3.06442200	-0.00000600
H	-4.95693700	0.41223700	-0.00027600
H	-4.10477100	-1.92706400	0.00002300
O	4.44166600	-0.92579400	-0.00013000
O	-1.65283100	-2.60901000	0.00045400

N	-1.09401400	-0.32022700	-0.00000900
N	0.59810500	1.91279700	0.00007500
C	1.45636300	3.10152300	0.00016900
H	2.08968000	3.09775300	0.88833700
H	2.08970500	3.09787900	-0.88798300
H	0.82827600	3.98936500	0.00022400

Gibbs free energy = -761.343308 Hartree

Number of imaginary frequencies: 0