BEILSTEIN JOURNAL OF ORGANIC CHEMISTRY

Supporting Information

for

Intramolecular interactions governing the conformational behavior of 2-aminopropan-1-ol and its methyl ether: hydrogen bonding, gauche effect, and metallic interactions

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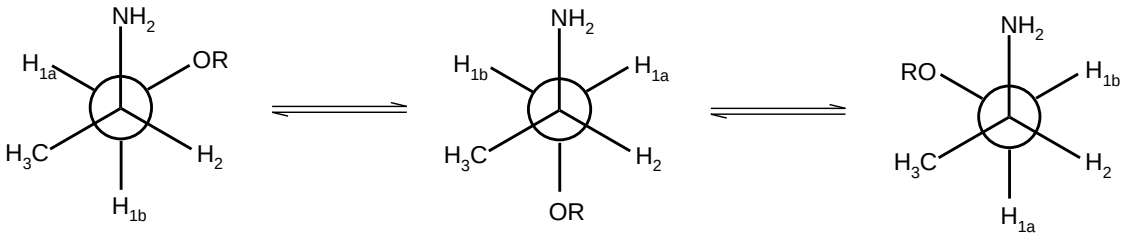
^{1}H NMR spectra of 1, 2, and their complexes with $ZnCl_2$ and $CdCl_2$ and standard coordinates of the conformers of 1, 2, and their complexes with Zn^{2+}

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Content:

Pages S2–S9: ^{1}H NMR spectra of **1**, **2**, and their complexes with $ZnCl_2$ and $CdCl_2$, in 20 mL^{-1} solutions of $CDCl_3$ and CD_3CN at 600.17 MHz.

Pages S10–S46 Standard coordinates of the conformers of **1**, **2**, and their complexes with Zn^{2+} optimized at the B3LYP-GD3BJ/6-311++G(d,p) level.

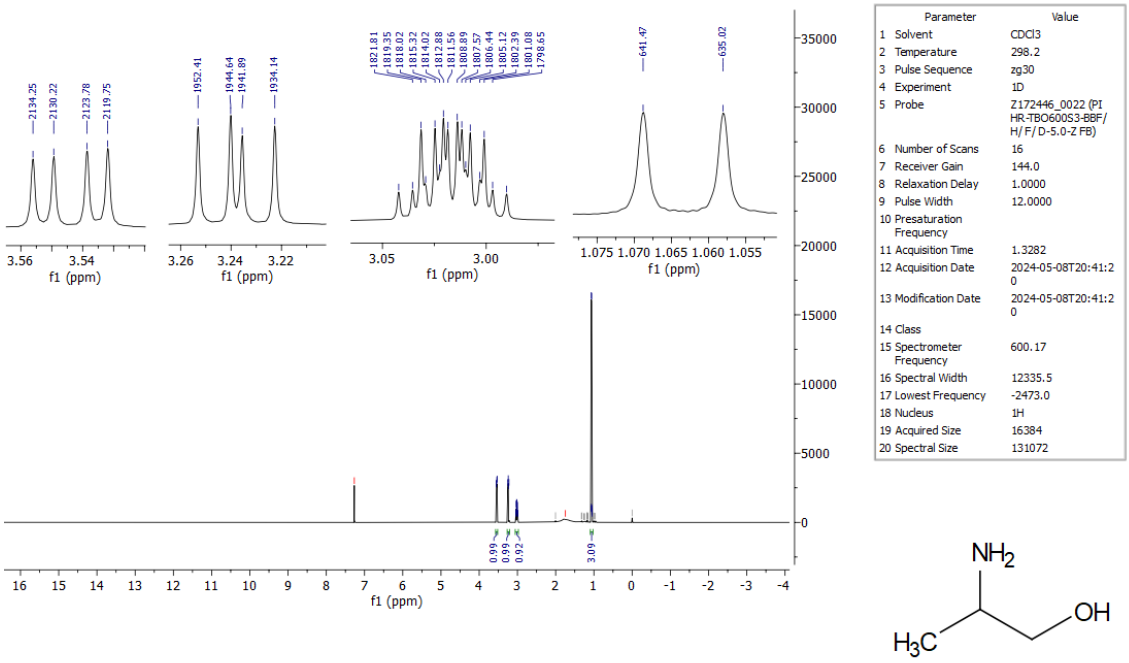


R = H, in $CDCl_3$ [δ_{CH3} = 1.06 ppm (d, 6.45 Hz); δ_{H1a} = 3.24 ppm (dd); δ_{H1b} = 3.54 ppm (dd); δ_{H2} = 3.02 ppm (ddq)]

$^{2}J_{H1a,H1b}$ = 10.52 Hz

$^{3}J_{H1a,H2}$ = 7.77 Hz

$^{3}J_{H1b,H2}$ = 4.03 Hz



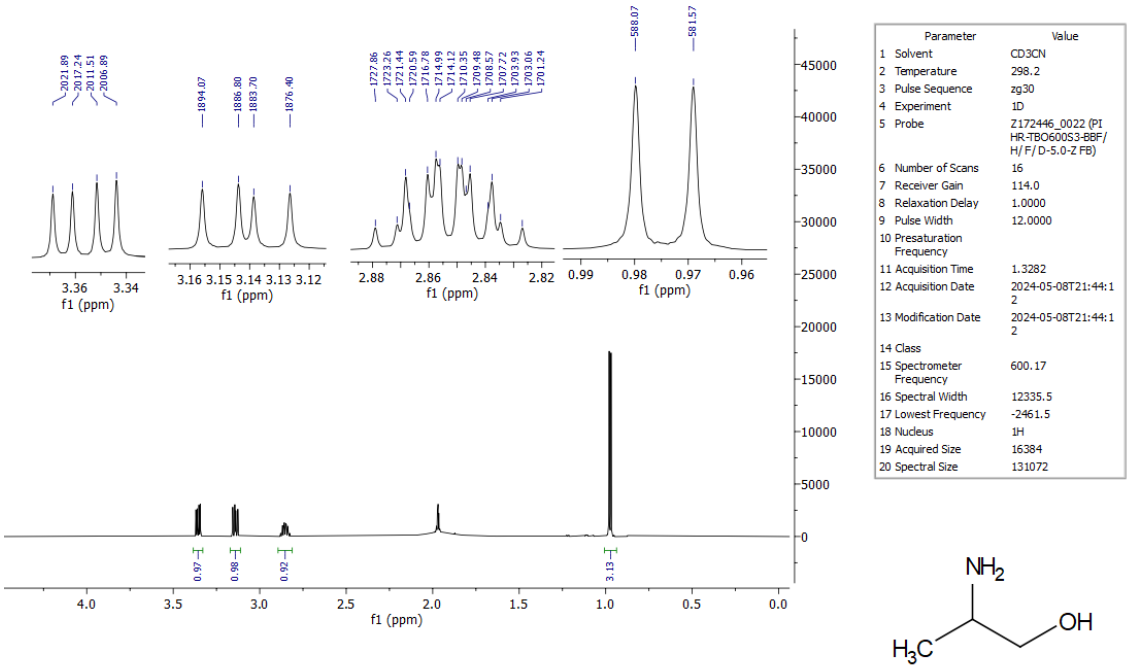
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3 Pulse Sequence	zg30
4 Experiment	1D
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6 Number of Scans	16
7 Receiver Gain	144.0
8 Relaxation Delay	1.0000
9 Pulse Width	12.0000
10 Presaturation Frequency	
11 Acquisition Time	1.3282
12 Acquisition Date	2024-05-08T20:41:20
13 Modification Date	2024-05-08T20:41:20
14 Class	
15 Spectrometer Frequency	600.17
16 Spectral Width	12335.5
17 Lowest Frequency	-2473.0
18 Nucleus	1H
19 Acquired Size	16384
20 Spectral Size	131072

R = H, in CD_3CN [δ_{CH3} = 0.98 ppm (d, 6.50 Hz); δ_{H1a} = 3.14 ppm (dd); δ_{H1b} = 3.36 ppm (dd); δ_{H2} = 2.85 ppm (ddq)]

$^2J_{H1a,H1b}$ = 10.37 Hz

$^3J_{H1a,H2}$ = 7.27 Hz

$^3J_{H1b,H2}$ = 4.65 Hz



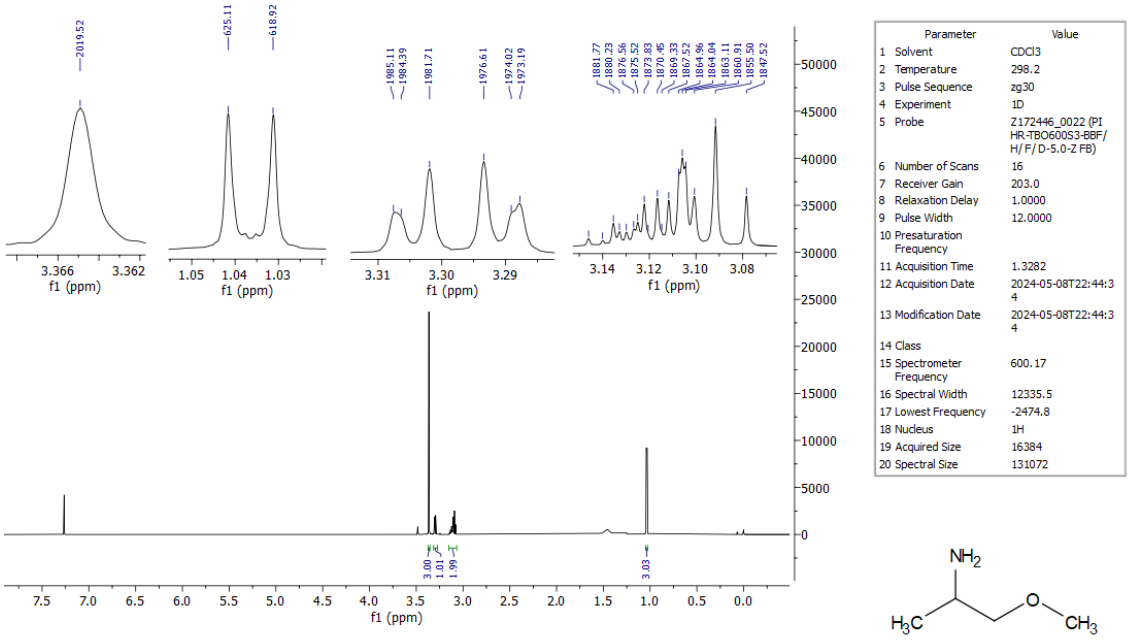
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2	Temperature	298.2
3	Pulse Sequence	zg30
4	Experiment	1D
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6	Number of Scans	16
7	Receiver Gain	114.0
8	Relaxation Delay	1.0000
9	Pulse Width	12.0000
10	Presaturation Frequency	
11	Acquisition Time	1.3282
12	Acquisition Date	2024-05-08T21:44:12
13	Modification Date	2024-05-08T21:44:12
14	Class	
15	Spectrometer Frequency	600.17
16	Spectral Width	12335.5
17	Lowest Frequency	-2461.5
18	Nucleus	1H
19	Acquired Size	16384
20	Spectral Size	131072

R = CH_3, in $CDCl_3$ [δ_{CH3} = 1.04 ppm (d, 6.19 Hz); δ_{OCH3} = 3.36 ppm (s); δ_{H1a} = 3.10 ppm (dd); δ_{H1b} = 3.30 ppm (dd); δ_{H2} = 3.12 ppm (ddq)]

$^2J_{H1a,H1b}$ = 8.50 Hz

$^3J_{H1a,H2}$ = 7.98 Hz

$^3J_{H1b,H2}$ = 3.40 Hz



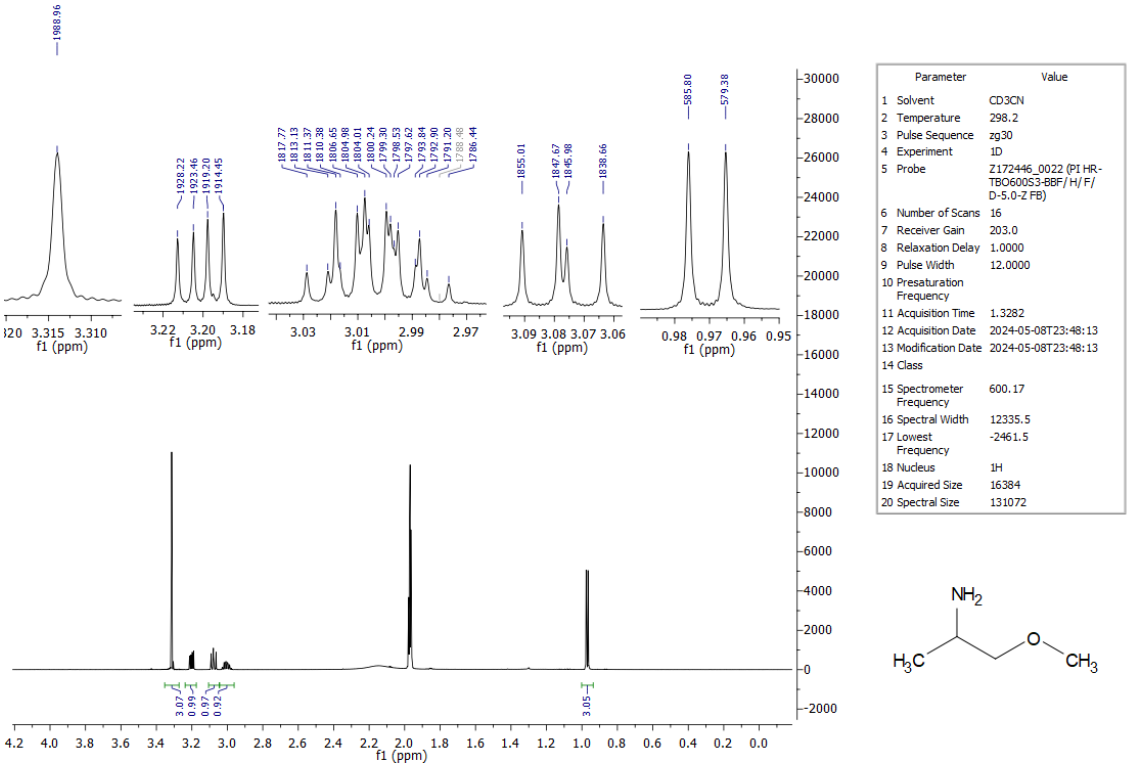
Parameter	Value
1 Solvent	CDCl3
2 Temperature	298.2
3 Pulse Sequence	zg30
4 Experiment	1D
5 Probe	Z172446_0022 (PI HR-TBO600S3-BBF/ H/ F/ D-5.0-Z FB)
6 Number of Scans	16
7 Receiver Gain	203.0
8 Relaxation Delay	1.0000
9 Pulse Width	12.0000
10 Presaturation Frequency	
11 Acquisition Time	1.3282
12 Acquisition Date	2024-05-08T22:44:34
13 Modification Date	2024-05-08T22:44:34
14 Class	
15 Spectrometer Frequency	600.17
16 Spectral Width	12335.5
17 Lowest Frequency	-2474.8
18 Nucleus	1H
19 Acquired Size	16384
20 Spectral Size	131072

R = CH_3, in CD_3CN [δ_{CH3} = 0.97 ppm (d, 6.42 Hz); δ_{OCH3} = 3.31 ppm (s); δ_{H1a} = 3.08 ppm (dd); δ_{H1b} = 3.20 ppm (dd); δ_{H2} = 3.00 ppm (ddq)]

$^{2}J_{H1a,H1b}$ = 9.03 Hz

$^{3}J_{H1a,H2}$ = 7.34 Hz

$^{3}J_{H1b,H2}$ = 4.76 Hz



	Parameter	Value
1	Solvent	CD3CN
2	Temperature	298.2
3	Pulse Sequence	zg30
4	Experiment	1D
5	Probe	Z172446_0022 (PI HR-TBO600S3-BBF/ H/ F/ D-5.0-Z FB)
6	Number of Scans	16
7	Receiver Gain	203.0
8	Relaxation Delay	1.0000
9	Pulse Width	12.0000
10	Presaturation Frequency	
11	Acquisition Time	1.3282
12	Acquisition Date	2024-05-08T23:48:13
13	Modification Date	2024-05-08T23:48:13
14	Class	
15	Spectrometer Frequency	600.17
16	Spectral Width	12335.5
17	Lowest Frequency	-2461.5
18	Nucleus	1H
19	Acquired Size	16384
20	Spectral Size	131072

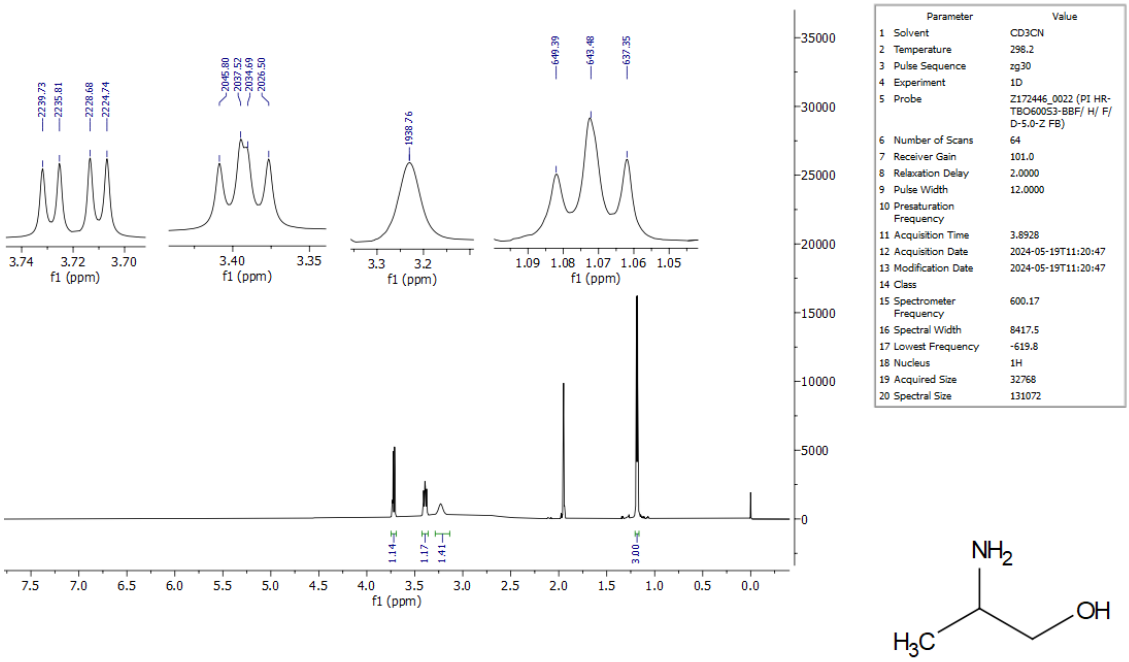
2-Aminopropan-1-ol + $ZnCl_2$ in acetonitrile (saturation)

δ_{CH3} = 1.07 ppm (t, 5.91 Hz); δ_{H1a} = 3.39 ppm (dd); δ_{H1b} = 3.72 ppm (dd); δ_{H2} = 3.22 ppm (s)

$^{2}J_{H1a,H1b}$ = 11.05 Hz

$^{3}J_{H1a,H2}$ = 8.28 Hz

$^{3}J_{H1b,H2}$ = 3.92 Hz



	Parameter	Value
1	Solvent	CD3CN
2	Temperature	298.2
3	Pulse Sequence	zg30
4	Experiment	1D
5	Probe	Z172446_0022 (PI HR-TBO600S3-BBF/ H/ F/ D-5.0-Z FB)
6	Number of Scans	64
7	Receiver Gain	101.0
8	Relaxation Delay	2.0000
9	Pulse Width	12.0000
10	Presaturation Frequency	
11	Acquisition Time	3.8928
12	Acquisition Date	2024-05-19T11:20:47
13	Modification Date	2024-05-19T11:20:47
14	Class	
15	Spectrometer Frequency	600.17
16	Spectral Width	8417.5
17	Lowest Frequency	-619.8
18	Nucleus	1H
19	Acquired Size	32768
20	Spectral Size	131072

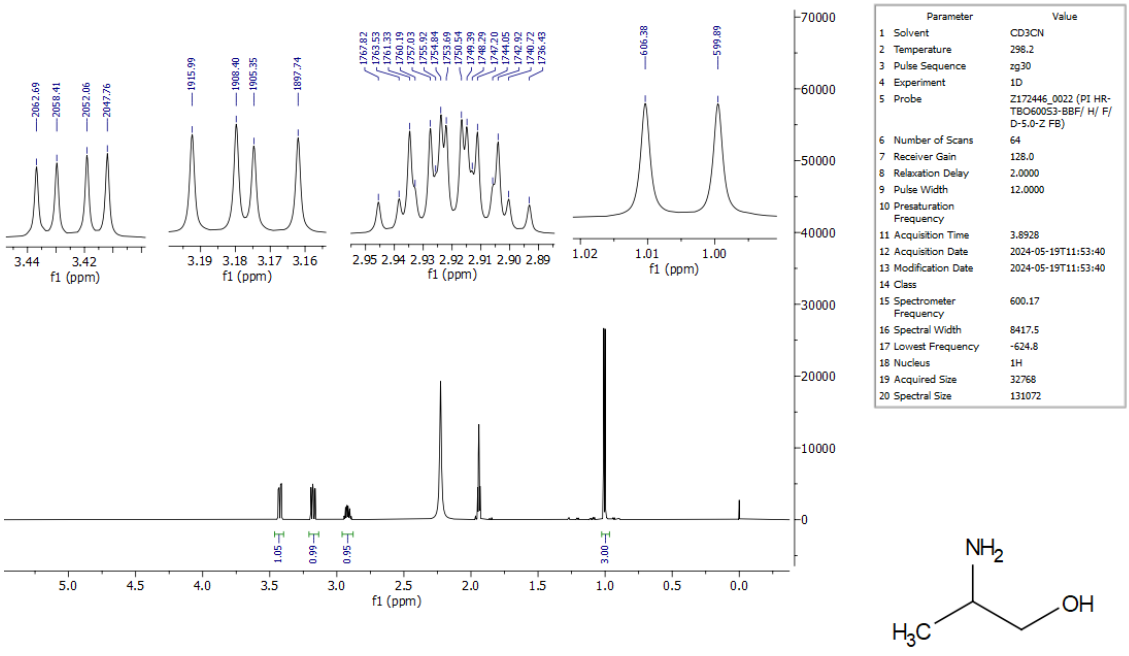
2-Aminopropan-1-ol + $CdCl_2$ in acetonitrile (saturation)

δ_{CH3} = 1.01 ppm (d, 6.49 Hz); δ_{H1a} = 3.18 ppm (dd); δ_{H1b} = 3.42 ppm (dd); δ_{H2} = 2.92 ppm (ddq)

$^{2}J_{H1a,H1b}$ = 10.63 Hz

$^{3}J_{H1a,H2}$ = 7.59 Hz

$^{3}J_{H1b,H2}$ = 4.28 Hz



Parameter	Value
1 Solvent	CD3CN
2 Temperature	298.2
3 Pulse Sequence	zg30
4 Experiment	1D
5 Probe	Z172446_0022 (PI HR-TBO600S3-BBF/ H/ F/ D-5.0-Z FB)
6 Number of Scans	64
7 Receiver Gain	128.0
8 Relaxation Delay	2.0000
9 Pulse Width	12.0000
10 Presaturation Frequency	
11 Acquisition Time	3.8928
12 Acquisition Date	2024-05-19T11:53:40
13 Modification Date	2024-05-19T11:53:40
14 Class	
15 Spectrometer Frequency	600.17
16 Spectral Width	8417.5
17 Lowest Frequency	-624.8
18 Nucleus	1H
19 Acquired Size	32768
20 Spectral Size	131072

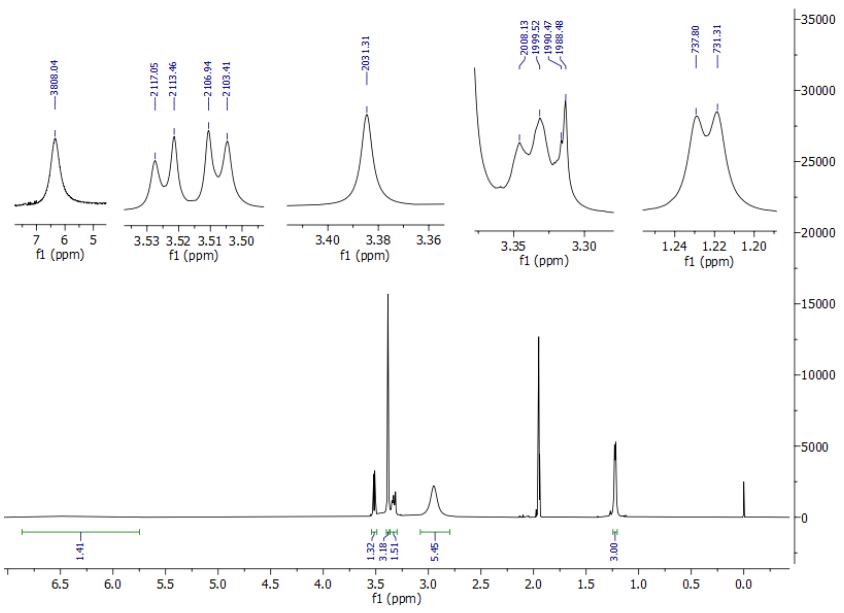
1-Methoxypropan-2-amine + $ZnCl_2$ in acetonitrile (saturation)

δ_{CH3} = 1.22 ppm (d, 6.49 Hz); δ_{OCH3} = 3.38 ppm (s); δ_{H1a} = 3.33 ppm (m); δ_{H1b} = 3.52 ppm (dd); δ_{H2} = 3.33 ppm (m)

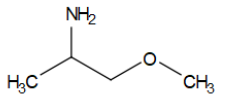
$^{2}J_{H1a,H1b}$ = 10.11 Hz

$^{3}J_{H1a,H2}$ ≈ 8.6 Hz

$^{3}J_{H1b,H2}$ = 3.59 Hz



	Parameter	Value
1	Solvent	CD3CN
2	Temperature	298.2
3	Pulse Sequence	zg30
4	Experiment	1D
5	Probe	Z172446_0022 (PI HR-TBO600S3-BBF/ H/ F/ D-5.0-Z FB)
6	Number of Scans	64
7	Receiver Gain	128.0
8	Relaxation Delay	2.0000
9	Pulse Width	12.0000
10	Presaturation Frequency	
11	Acquisition Time	3.8928
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13	Modification Date	2024-05-19T11:38:07
14	Class	
15	Spectrometer Frequency	600.17
16	Spectral Width	8417.5
17	Lowest Frequency	-619.0
18	Nucleus	1H
19	Acquired Size	32768
20	Spectral Size	131072



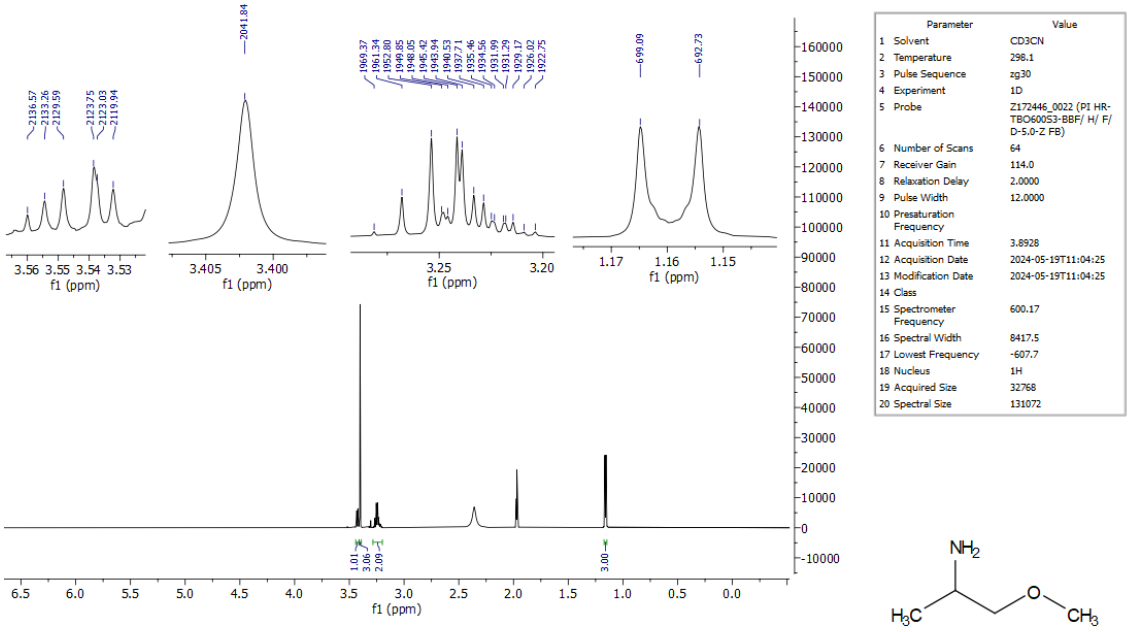
1-Methoxypropan-2-amine + $CdCl_2$ in acetonitrile (saturation)

δ_{CH3} = 1.16 ppm (d, 6.36 Hz); δ_{OCH3} = 3.40 ppm (s); δ_{H1a} = 3.25 ppm (dd); δ_{H1b} = 3.54 ppm (dd); δ_{H2} = 3.22 ppm (m)

$^{2}J_{H1a,H1b}$ = 9.51 Hz

$^{3}J_{H1a,H2}$ = 8.54 Hz

$^{3}J_{H1b,H2}$ = 3.67 Hz



	Parameter	Value
1	Solvent	CD3CN
2	Temperature	298.1
3	Pulse Sequence	zg30
4	Experiment	1D
5	Probe	Z172446_0022 (PI HR-TBO600S3-BBF/ H/ F/ D-5.0-Z FB)
6	Number of Scans	64
7	Receiver Gain	114.0
8	Relaxation Delay	2.0000
9	Pulse Width	12.0000
10	Presaturation Frequency	
11	Acquisition Time	3.8928
12	Acquisition Date	2024-05-19T11:04:25
13	Modification Date	2024-05-19T11:04:25
14	Class	
15	Spectrometer Frequency	600.17
16	Spectral Width	8417.5
17	Lowest Frequency	-607.7
18	Nucleus	1H
19	Acquired Size	32768
20	Spectral Size	131072

Standard coordinates from the geometry-optimized compounds at the B3LYP-GD3BJ/6-311++G(d,p) level

2-Aminopropan-1-ol (1, gas phase)

a1

```
0 1
C 0.80433700 -0.61184300 0.30165600
H 0.87130900 -1.68097600 0.05634900
H 0.73977800 -0.51472500 1.39248000
C -0.45830000 -0.02593400 -0.32406100
H -0.30884500 -0.02792100 -1.41483300
C -0.69113300 1.41188600 0.12759800
H 0.17641200 2.02868000 -0.11003500
H -1.56468000 1.84125400 -0.37261800
H -0.86457900 1.44381500 1.20739600
O 1.93177900 0.09345900 -0.21986900
H 2.72403800 -0.21099800 0.23050800
N -1.59018300 -0.86540700 0.09400600
H -2.47071500 -0.43623500 -0.16910100
H -1.55509400 -1.77737100 -0.35040100
```

G^0 = -249.707023 hartrees, 0 img. freq.

a2

```
0 1
C 0.80021500 -0.64246300 0.28353500
H 0.86856900 -1.69609900 0.00104800
H 0.72409600 -0.59449100 1.37711100
C -0.46091800 -0.02734600 -0.33382500
H -0.32720800 -0.04066400 -1.42666400
C -0.66332400 1.41903100 0.10973600
H 0.17323500 2.04961100 -0.20270400
H -1.56676500 1.84252900 -0.33878400
H -0.76711800 1.47251500 1.19756700
O 2.00582800 -0.04366300 -0.18411900
H 2.08092600 0.83645200 0.19583800
N -1.60611700 -0.83206300 0.11147900
H -2.48088900 -0.42034300 -0.19560600
H -1.56447900 -1.77109900 -0.27188300
```

G^0 = -249.706713 hartrees, 0 img. freq.

a3

```
0 1
C 0.80760200 -0.60622500 0.32857600
H 0.87690500 -1.68013200 0.10486700
H 0.73909300 -0.49731200 1.41229500
C -0.45332800 -0.02606200 -0.32078800
H -0.29431200 -0.03351600 -1.41496000
C -0.69584900 1.41475700 0.11510200
H 0.18049800 2.02977400 -0.09490900
H -1.55290100 1.84581400 -0.41137600
H -0.89946400 1.44980600 1.18904100
O 1.99867000 0.06910800 -0.06711500
H 2.13539300 -0.07553700 -1.00877100
N -1.58979400 -0.86269700 0.08109200
H -2.46753500 -0.45538100 -0.22268500
H -1.52903100 -1.79231400 -0.32156500
```

G^0 = -249.706733 hartrees, 0 img. freq.

a4

```
0 1
C 0.78612300 -0.64373500 0.27005400
H 0.85433100 -1.69460400 -0.04374300
H 0.70229500 -0.61898000 1.36708700
C -0.46945600 -0.01581300 -0.34357500
H -0.33864200 -0.02420000 -1.43120300
C -0.65408700 1.42684800 0.11614200
H 0.23395100 2.01841600 -0.10873800
H -1.52005800 1.87277100 -0.37606300
H -0.82075200 1.46384200 1.19924000
O 1.93069300 0.08803200 -0.17048800
```

H 2.72104600 -0.30271600 0.21237200
N -1.68239300 -0.78387900 -0.04514700
H -1.60021200 -1.74944900 -0.34686600
H -1.87623300 -0.78598500 0.95211400

G^0 = -249.706945 hartrees, 0 img. freq.

a5

0 1
C 0.78451600 -0.66568500 0.26099400
H 0.84981700 -1.70684300 -0.06428900
H 0.69330600 -0.66538400 1.35829100
C -0.46948000 -0.01820100 -0.34982400
H -0.35346500 -0.03946900 -1.43880500
C -0.63584500 1.43307500 0.09455400
H 0.22204200 2.04451900 -0.19767400
H -1.52800300 1.86703800 -0.35940400
H -0.74499600 1.49408500 1.18390400
O 2.00878900 -0.06177200 -0.14942800
H 2.06069800 0.82087100 0.22895400
N -1.69304900 -0.76001300 -0.02682300
H -1.63542400 -1.72447800 -0.33803700
H -1.85808900 -0.77121000 0.97589600

G^0 = -249.706781 hartrees, 0 img. freq.

a6

0 1
C 0.79095000 -0.63297100 0.30229400
H 0.85727200 -1.69510500 0.02658500
H 0.70730900 -0.57789700 1.39176500
C -0.46252500 -0.01663600 -0.34102000
H -0.31991000 -0.03059900 -1.43063500
C -0.66760300 1.42791500 0.10290100
H 0.22835400 2.02133900 -0.08477300
H -1.51353000 1.87356800 -0.42330600
H -0.87486000 1.46788100 1.17848200
O 1.99946000 0.04956500 -0.02732300
H 2.16309700 -0.05527400 -0.97005700
N -1.67661100 -0.79129800 -0.06434300
H -1.56937200 -1.76527300 -0.33001100
H -1.90269000 -0.76592500 0.92588300

G^0 = -249.706781 hartrees, 0 img. freq.

a7

0 1
C 0.78751100 -0.68071600 0.22395600
H 0.85915100 -1.69895900 -0.17204500
H 0.70545400 -0.74147100 1.32017000
C -0.46974100 -0.02385200 -0.33937800
H -0.37295000 -0.02857900 -1.43031000
C -0.61767000 1.42396500 0.13828800
H 0.25622900 2.01821600 -0.13561100
H -1.50688300 1.88473900 -0.30131500
H -0.72264700 1.45618700 1.22889600
O 1.92060400 0.10482100 -0.15142000
H 2.71779400 -0.33496300 0.15587900
N -1.60498200 -0.89592200 -0.00709900
H -1.83377100 -0.82135300 0.98052500
H -2.43292600 -0.61730100 -0.52233100

G^0 = -249.706888 hartrees, 0 img. freq.

a8

0 1
C 0.78500600 -0.70259600 0.21242800
H 0.85194200 -1.71247600 -0.19125700
H 0.69712800 -0.78490700 1.30676600
C -0.47165100 -0.02644600 -0.34776600
H -0.38890600 -0.04258100 -1.43947500
C -0.59739500 1.43077600 0.11461700
H 0.24443600 2.04060900 -0.22823500
H -1.50941100 1.88445200 -0.28215200
H -0.64358900 1.48624200 1.20872900
O 1.99679600 -0.04568400 -0.14823100
H 2.05405700 0.78794000 0.32759000
N -1.61600100 -0.87300000 0.01041000
H -1.80720200 -0.81935600 1.00711400
H -2.45658100 -0.57385700 -0.47176700

G^0 = -249.706225 hartrees, 0 img. freq.

a9

0 1
C 0.79336200 -0.66233600 0.26543900
H 0.85904700 -1.70201400 -0.07212800
H 0.71508500 -0.66855700 1.35711200
C -0.46309900 -0.02183100 -0.33570600
H -0.34616100 -0.02926200 -1.42748100
C -0.63990700 1.42627200 0.13045800
H 0.24399600 2.02520000 -0.10020600
H -1.50836000 1.88623800 -0.34953700
H -0.79417200 1.45891400 1.21467100
O 1.98856800 0.05872500 -0.02775600
H 2.19308500 -0.05698300 -0.96079000
N -1.59586200 -0.90737700 -0.03389100
H -1.81095200 -0.88088400 0.95939600
H -2.43120600 -0.60344100 -0.52290300

G^0 = -249.706640 hartrees, 0 img. freq.

g1

0 1
C -0.82154700 -0.54835100 0.33542100
H -0.79470200 -0.34605800 1.41608800
H -0.82576400 -1.63799400 0.19687400
C 0.43267500 0.03579800 -0.30945200
H 0.24734700 0.05987100 -1.38841000
C 1.64577600 -0.86479900 -0.03022300
H 1.50928200 -1.86954500 -0.44192700
H 2.54827800 -0.43691500 -0.47386100
H 1.81840900 -0.96100200 1.04778400
O -1.97398200 0.03080100 -0.26662200
H -2.73709600 -0.13535900 0.29303000
N 0.60808700 1.42626200 0.12255800
H 0.91805500 1.46476100 1.08978100
H 1.31001800 1.89611200 -0.43877000

G^0 = -249.704006 hartrees, 0 img. freq.

g2 converged to g3

g3

0 1
C -0.75907200 -0.74843900 0.22010200
H -0.65190600 -0.83326400 1.31444200
H -0.79053600 -1.76076700 -0.18959600
C 0.44185700 0.01912100 -0.34012500
H 0.33098600 0.04710900 -1.42920100
C 1.76603900 -0.65731300 0.02009000
H 1.80344800 -1.68314100 -0.35919500
H 2.61225100 -0.10995900 -0.40327400
H 1.89826700 -0.69572700 1.10666600
O -1.97895300 -0.11421900 -0.11690100
H -1.80178100 0.83445900 -0.02600000
N 0.31859500 1.41271900 0.12366800
H 0.62544000 1.50136200 1.08885500
H 0.88234100 2.04443700 -0.43356700

G^0 = -249.711176 hartrees, 0 img. freq.

g4

0 1
C -0.75096200 -0.69561200 0.23595200
H -0.68125400 -0.70343100 1.33069800
H -0.76381700 -1.72925100 -0.13222600
C 0.45698200 0.03547800 -0.32867600
H 0.34004200 0.04611200 -1.42491700
C 1.74831200 -0.70103100 0.01877300
H 1.75124500 -1.71150100 -0.39901700
H 2.61394100 -0.17065500 -0.38745500
H 1.87250700 -0.76325300 1.10315400
O -1.92652900 0.00283000 -0.19045900
H -2.68193600 -0.32010400 0.30785600
N 0.48536500 1.38616000 0.24207200
H 1.23060400 1.93684700 -0.17124900
H -0.39264700 1.85646200 0.04603500

G^0 = -249.708788 hartrees, 0 img. freq.

g5

0 1
C 0.75400800 -0.68113200 -0.27567700
H 0.68025200 -0.65808600 -1.36490500

H 0.76938700 -1.72765600 0.05288900
C -0.45206900 0.03591300 0.32515600
H -0.32017300 0.03228100 1.42377200
C -1.74595400 -0.70662100 -0.00159400
H -1.73595800 -1.71888700 0.41238900
H -2.60888800 -0.18255300 0.41822000
H -1.88464100 -0.76572400 -1.08416400
O 1.98805100 -0.03107000 0.04093700
H 2.16938800 -0.16235400 0.97718200
N -0.50157200 1.39137400 -0.22536400
H -1.19861000 1.95739300 0.24606900
H 0.39993000 1.84557400 -0.11872200

G^0 = -249.708221 hartrees, 0 img. freq.

g6 converged to g3

g7

0 1
C -0.74839300 -0.70283000 0.23875100
H -0.66410600 -0.73488700 1.33496800
H -0.77403500 -1.73384800 -0.13908700
C 0.45763300 0.03668700 -0.34293500
H 0.33727200 0.03522500 -1.43250600
C 1.75564300 -0.68337000 0.01184600
H 1.74771300 -1.71832800 -0.33974600
H 2.60429000 -0.16814500 -0.44073100
H 1.90893000 -0.69752300 1.09690400
O -1.92650300 0.00592400 -0.15530200
H -2.69411300 -0.40648500 0.24983000
N 0.53973200 1.43935900 0.07020000
H -0.35306600 1.89528100 -0.09146300
H 0.73171900 1.50288800 1.06687900

G^0 = -249.708460 hartrees, 0 img. freq.

g8

0 1
C -0.75096100 -0.69159200 0.27557700
H -0.66338200 -0.68809200 1.36585600
H -0.77982500 -1.73720400 -0.05973600
C 0.45081100 0.03422900 -0.34269000
H 0.31981500 0.01556200 -1.43420500
C 1.75352100 -0.68457300 -0.00332700
H 1.73797300 -1.72195000 -0.34706000
H 2.59845800 -0.17572900 -0.47025300
H 1.91940100 -0.69246700 1.07982500
O -1.98817500 -0.03561700 -0.01114400
H -2.19374900 -0.16481300 -0.94267700
N 0.54265700 1.44323800 0.04714000
H -0.37111700 1.88029200 -0.03285100
H 0.81901000 1.51828600 1.02292200

G^0 = -249.708144 hartrees, 0 img. freq.

g9

0 1
C -0.74648900 -0.72838600 0.21390700
H -0.64563000 -0.81544500 1.30646600
H -0.77375900 -1.73857500 -0.20125000
C 0.45963200 0.03618100 -0.35049100
H 0.36295000 0.04005200 -1.44154400
C 1.75947000 -0.66752900 0.03440500
H 1.75899400 -1.70970700 -0.29578200
H 2.61247400 -0.15759400 -0.41539500
H 1.89678700 -0.66075800 1.12142200
O -1.99775700 -0.13828600 -0.12870600
H -2.07917400 0.69398800 0.34757500
N 0.52787500 1.44137300 0.06244200
H -0.25270900 1.98427400 -0.28856100
H 0.57131600 1.53885500 1.07269600

G^0 = -249.707582 hartrees, 0 img. freq.

g10

0 1
C 0.94263600 -0.04610800 0.67410100
H 1.17130300 -0.94645900 1.26100500
H 1.30316400 0.83009300 1.23051400
C -0.57239700 0.07014000 0.46958600
H -1.01651200 0.14246800 1.46973100
C -1.14024400 -1.16750600 -0.22665400
H -0.90259400 -2.07625800 0.33317500

H -2.22422100 -1.08073800 -0.31422500
H -0.71742900 -1.27002300 -1.22871900
O 1.56405100 -0.10990300 -0.61227500
H 2.51764800 -0.14164400 -0.50061000
N -0.97552000 1.27039000 -0.27095400
H -0.68240700 2.11123900 0.21735700
H -0.51269400 1.27866700 -1.17554900

G^0 = -249.707218 hartrees, 0 img. freq.

g11

0 1
C 0.95704000 -0.11880300 0.66248000
H 1.16654200 -1.06100700 1.17488600
H 1.34327000 0.69696800 1.29029600
C -0.56039200 0.05170500 0.48052800
H -0.98899900 0.09090500 1.49026700
C -1.17752700 -1.12828100 -0.26692700
H -0.98911800 -2.06508700 0.26286000
H -2.25578500 -0.99218100 -0.36573900
H -0.74245700 -1.21946300 -1.26585000
O 1.67349300 -0.18019300 -0.56851700
H 1.61210100 0.68069300 -0.99480400
N -0.94498800 1.29841000 -0.19216300
H -0.51306500 2.11565600 0.22630800
H -0.72023900 1.27845900 -1.18142900

G^0 = -249.706703 hartrees, 0 img. freq.

g12

0 1
C 0.95121200 0.02425800 0.67445500
H 1.21378800 -0.82143600 1.32500900
H 1.28906500 0.94090700 1.16385200
C -0.57148700 0.08203300 0.46623300
H -1.02108300 0.17532200 1.46253600
C -1.10491600 -1.19779000 -0.18086700
H -0.81101500 -2.08462100 0.38842700
H -2.19339400 -1.16327000 -0.23863700
H -0.72956200 -1.30575700 -1.20416200
O 1.67750600 -0.03835100 -0.55446300
H 1.56798900 -0.91579400 -0.93311300
N -1.01265100 1.23812200 -0.32114400
H -0.79313200 2.10423600 0.16157400
H -0.50300200 1.25936200 -1.20070100

G^0 = -249.707128 hartrees, 0 img. freq.

g13

0 1
C -0.94275300 0.07008900 0.67677100
H -1.16788200 0.98857700 1.23372100
H -1.29894000 -0.79367400 1.24809600
C 0.56306000 -0.05821700 0.47918200
H 1.00201700 -0.09622000 1.48364800
C 1.14335300 1.15493100 -0.26311800
H 0.95429600 2.08384100 0.28490800
H 2.22556200 1.04801600 -0.37928200
H 0.69604600 1.24620700 -1.25522300
O -1.56109500 0.10605200 -0.61592700
H -2.50770200 -0.02011400 -0.51312000
N 0.83279900 -1.35079700 -0.16159400
H 0.34942500 -1.39013700 -1.05430500
H 1.82438300 -1.46015500 -0.34687400

G^0 = -249.707436 hartrees, 0 img. freq.

g14 converged to g17

g15

0 1
C -0.95247900 0.00296500 0.67632300
H -1.20865200 0.87736600 1.28702100
H -1.28873800 -0.89506900 1.19530500
C 0.56296800 -0.07201800 0.47874500
H 1.00066600 -0.12505700 1.48374000
C 1.11564100 1.18194500 -0.21753000
H 0.87360200 2.09249200 0.34141900
H 2.20398500 1.12466200 -0.30325600
H 0.71557900 1.27804100 -1.23210700
O -1.67163000 0.02189300 -0.56070800
H -1.57224600 0.88974600 -0.96313300
N 0.87305600 -1.33042600 -0.20458800

H 0.32682400 -1.40043900 -1.05830500
H 1.85385000 -1.38125600 -0.45813300

G^0 = -249.706781, 0 img. freq.

g16

0 1
C -0.95459100 -0.20539600 0.61771800
H -1.27922400 0.47156900 1.42043900
H -1.18887900 -1.23359800 0.92924800
C 0.55836100 -0.06591200 0.45749200
H 0.96373500 -0.13153200 1.48278200
C 0.94584500 1.29363100 -0.12089700
H 0.56701500 2.10493300 0.50615900
H 2.03431400 1.39065400 -0.17444700
H 0.53397900 1.40449400 -1.12418500
O -1.61260000 0.11417900 -0.60402400
H -2.55030900 -0.07087800 -0.50687300
N 1.07631900 -1.12954300 -0.41039900
H 2.07665400 -1.02952600 -0.54552600
H 0.91158100 -2.04668000 -0.00849500

G^0 = -249.703560, 0 img. freq.

g17

0 1
C 0.97811500 -0.17156600 0.64897200
H 1.18083300 -1.13815000 1.11624100
H 1.39092400 0.61074400 1.30487600
C -0.53383300 0.04439900 0.50139000
H -0.96360900 0.09379800 1.51365300
C -1.20635500 -1.09432800 -0.26118900
H -1.07725200 -2.03928600 0.27139500
H -2.28024400 -0.91320400 -0.36730100
H -0.77090200 -1.20010600 -1.25658000
O 1.63193300 -0.16205300 -0.60876800
H 1.21506300 0.55674300 -1.10693900
N -0.71363000 1.30609000 -0.24186200
H -1.66022200 1.40023000 -0.59215900
H -0.52221300 2.11200200 0.34494800

G^0 = -249.710175 hartrees, 0 img. freq.

g18 converged to g17

2-Aminopropan-1-ol (1, MeCN - SMD)

a1

```
0 1
C 0.80879500 -0.60271200 0.30023200
H 0.88253200 -1.66922800 0.05148400
H 0.75860100 -0.50673300 1.39220000
C -0.45946200 -0.02486000 -0.31827400
H -0.32400300 -0.03296200 -1.41027300
C -0.71168800 1.41083200 0.12839800
H 0.12535400 2.05507300 -0.14789900
H -1.61658100 1.80820100 -0.34185200
H -0.84189000 1.45485500 1.21483700
O 1.94091900 0.10653500 -0.21906200
H 2.73287600 -0.24314900 0.20466600
N -1.58711400 -0.87665400 0.09941000
H -2.45772300 -0.48252200 -0.24725800
H -1.50259400 -1.79879300 -0.32141100
```

G^0 = -249.719793 hartrees, 0 img. freq.

a2

```
0 1
C 0.79750700 -0.64470500 0.28885600
H 0.85826400 -1.70057200 0.01322500
H 0.73644100 -0.58162200 1.38286700
C -0.46032700 -0.02625500 -0.32651500
H -0.33612800 -0.04873200 -1.41952000
C -0.65828000 1.42169000 0.11007400
H 0.17988700 2.05064800 -0.20317900
H -1.56450100 1.83929600 -0.33888000
H -0.75397300 1.48431200 1.19908800
O 2.00932400 -0.04982800 -0.18603600
H 2.05303400 0.85474300 0.14639400
N -1.61246400 -0.83178900 0.11378100
H -2.47339000 -0.41712900 -0.23320900
H -1.56037800 -1.76417800 -0.28945500
```

G^0 = -249.720203 hartrees, 0 img. freq.

a3

```
0 1
C 0.80896900 -0.60221400 0.33171200
H 0.87892900 -1.67307400 0.10069700
H 0.74913900 -0.49325700 1.41746300
C -0.45196100 -0.02390600 -0.31439700
H -0.29876300 -0.03987300 -1.40598000
C -0.70758400 1.41544400 0.11586700
H 0.14018000 2.05338500 -0.14289500
H -1.59743300 1.81623100 -0.37935400
H -0.86426300 1.46735000 1.19836300
O 2.00517700 0.07194900 -0.07119600
H 2.11809900 -0.06274800 -1.02039900
N -1.58848700 -0.87086000 0.08648300
H -2.45198700 -0.48405800 -0.28549500
H -1.49245600 -1.79947100 -0.31730800
```

G^0 = -249.720069 hartrees, 0 img. freq.

a4

```
0 1
C 0.78343600 -0.63263600 0.26637000
H 0.85779900 -1.68083100 -0.04916700
H 0.70087500 -0.60766600 1.36182600
C -0.47025500 -0.01011600 -0.34988400
H -0.34263400 -0.01596700 -1.43813400
C -0.67842900 1.42602900 0.11892300
H 0.19789800 2.03885000 -0.10052400
H -1.54690200 1.87018300 -0.37443800
H -0.84918800 1.45116300 1.20140600
O 1.93903100 0.09892600 -0.16769400
H 2.71921800 -0.31234100 0.22165700
N -1.67147200 -0.80531100 -0.04548500
H -1.53706000 -1.77073500 -0.33685600
H -1.82046400 -0.82654700 0.96171500
```

G^0 = -249.720258 hartrees, 0 img. freq.

a5

```
0 1
C 0.77397400 -0.66635500 0.26061900
H 0.83262200 -1.70802900 -0.06413500
H 0.68357000 -0.65642700 1.35583200
C -0.46974300 -0.01151100 -0.35681800
H -0.35133100 -0.03362100 -1.44573200
C -0.63548000 1.43569300 0.09670500
H 0.23710000 2.04181700 -0.16231400
H -1.50847200 1.88986700 -0.37855800
H -0.77300100 1.48234200 1.18306100
O 2.00866000 -0.06374100 -0.14759700
H 2.05235200 0.82283900 0.23000300
N -1.69106500 -0.76669200 -0.03019500
H -1.58579500 -1.73995500 -0.30764200
H -1.83137000 -0.76901600 0.97859200
```

G^0 = -249.720548 hartrees, 0 img. freq.

a6

```
0 1
C 0.78382000 -0.63002900 0.30066200
H 0.85147200 -1.68679600 0.01200900
H 0.69278400 -0.58141500 1.38987000
C -0.46175800 -0.00903300 -0.34711000
H -0.31406800 -0.02195200 -1.43430700
C -0.67883000 1.42995600 0.10682400
H 0.20595300 2.03878200 -0.09017500
H -1.53031500 1.87614800 -0.41348000
H -0.87993400 1.46176500 1.18384300
O 2.00195400 0.05201700 -0.02362700
H 2.15028600 -0.04004900 -0.97306600
N -1.66916500 -0.80337800 -0.06408500
H -1.52440800 -1.77234600 -0.33882300
H -1.84264400 -0.81199300 0.93948900
```

G^0 = -249.720503 hartrees, 0 img. freq.

a7

```
0 1
C 0.79738700 -0.66506800 0.22506800
H 0.89006800 -1.68723900 -0.15802400
H 0.71848500 -0.71277600 1.32028400
C -0.46510100 -0.02791300 -0.34611700
H -0.36990200 -0.02269800 -1.43736000
C -0.65378900 1.40953000 0.14354300
H 0.19380000 2.04015200 -0.13646600
H -1.56156000 1.84248200 -0.28717900
H -0.74999700 1.42901300 1.23510300
O 1.93402400 0.11981800 -0.15842400
H 2.72254600 -0.30143700 0.20194100
N -1.59557800 -0.91511600 -0.01685500
H -1.78024300 -0.86823600 0.98377000
H -2.43731700 -0.57128900 -0.47165200
```

G^0 = -249.719706 hartrees, 0 img. freq.

a8

```
0 1
C 0.78820600 -0.69811900 0.21768600
H 0.86814600 -1.71314700 -0.17471200
H 0.70005200 -0.76249900 1.31134500
C -0.46587300 -0.03073500 -0.35375200
H -0.38177600 -0.04250500 -1.44555800
C -0.61116300 1.41855300 0.11783800
H 0.23122500 2.04025500 -0.20298900
H -1.52127000 1.86394200 -0.29364300
H -0.67424500 1.46113100 1.21110800
O 2.00431200 -0.03750100 -0.14604300
H 2.02667600 0.82210700 0.29097700
N -1.61580000 -0.88108600 0.00280600
H -1.78419600 -0.81816100 1.00549600
H -2.45553000 -0.52169800 -0.44395200
```

G^0 = -249.719961 hartrees, 0 img. freq.

a9

```
0 1
C 0.79837500 -0.66232900 0.26200500
H 0.88212300 -1.69659300 -0.09036000
H 0.71275500 -0.68105400 1.35274700
C -0.45646400 -0.02540200 -0.34138000
```

H -0.33809300 -0.02454700 -1.43184000
C -0.65587600 1.41397300 0.13641800
H 0.20325700 2.04078700 -0.11731200
H -1.54630900 1.85086100 -0.32526200
H -0.78731700 1.43786000 1.22411900
O 1.99818700 0.06458400 -0.02215900
H 2.14862000 0.02877300 -0.97496200
N -1.59342900 -0.91301900 -0.03694200
H -1.79486400 -0.87119500 0.96073800
H -2.42787400 -0.56788600 -0.50426500

G^0 = -249.719970 hartrees, 0 img. freq.

g1

0 1
C -0.81606000 -0.56307700 0.30125000
H -0.76696800 -0.43865100 1.39203100
H -0.84894100 -1.63693900 0.08398200
C 0.43623100 0.03127300 -0.32830300
H 0.28644500 0.04808500 -1.41335000
C 1.64710900 -0.85524200 -0.01121100
H 1.52458400 -1.86393500 -0.41817800
H 2.55448300 -0.42270100 -0.44177400
H 1.79261500 -0.93684400 1.07169700
O -1.98581300 0.07872500 -0.22258500
H -2.75526300 -0.31699600 0.20280400
N 0.60961800 1.42847000 0.10740700
H 0.78631300 1.44475100 1.11069800
H 1.44223000 1.81642300 -0.32949100

G^0 = -249.718835 hartrees, 0 img. freq.

g2

0 1
C -0.80926100 -0.59035600 0.31111300
H -0.74566300 -0.49832500 1.39964600
H -0.83400100 -1.65916200 0.06613900
C 0.43084800 0.03304500 -0.32850200
H 0.28016400 0.04089100 -1.41538000
C 1.66055600 -0.82827200 -0.01517800
H 1.54970000 -1.84471700 -0.40615300
H 2.55577900 -0.38790700 -0.46299800
H 1.81943300 -0.89173600 1.06699100
O -2.04530300 0.02731200 -0.06000300
H -2.11844900 -0.01141600 -1.02167400
N 0.57469400 1.43538900 0.09668300
H 0.73267700 1.46538200 1.10264100
H 1.40707400 1.83426500 -0.33056900

G^0 = -249.719577 hartrees, 0 img. freq.

g3

0 1
C -0.75298800 -0.75671300 0.21143900
H -0.64585600 -0.84988100 1.30265000
H -0.79271500 -1.76225200 -0.21296100
C 0.44116300 0.01706000 -0.34665700
H 0.34306300 0.04297800 -1.43692900
C 1.76275100 -0.65248300 0.02731800
H 1.80293700 -1.68192200 -0.34344600
H 2.60655600 -0.10410900 -0.40055500
H 1.88787100 -0.67596800 1.11514200
O -1.98329800 -0.10512000 -0.10841300
H -1.78156800 0.84157700 -0.02383900
N 0.31471000 1.41190500 0.11937000
H 0.60922300 1.47842100 1.09210900
H 0.92834400 2.02159600 -0.41306100

G^0 = -249.723122 hartrees, 0 img. freq.

g4

0 1
C -0.75741200 -0.68957300 0.23055900
H -0.69729300 -0.72008500 1.32552700
H -0.77836700 -1.71721400 -0.15051800
C 0.45725400 0.03506100 -0.32375700
H 0.34876200 0.06299300 -1.41919000
C 1.73819300 -0.71979800 0.01695000
H 1.73124700 -1.72065100 -0.42342100
H 2.61036500 -0.18655900 -0.37220500
H 1.85431900 -0.81574900 1.10104600
O -1.93671700 0.01960800 -0.18264100
H -2.69411700 -0.35545900 0.28079300

N 0.50989700 1.39157900 0.24819400
H 1.26950400 1.91464800 -0.17982400
H -0.34817600 1.88602100 0.01905000

G^0 = -249.721133 hartrees, 0 img. freq.

g5

0 1
C 0.75649400 -0.68685100 -0.26547500
H 0.68191000 -0.70148100 -1.35592600
H 0.77879000 -1.72091800 0.09673900
C -0.45013200 0.03662500 0.32113400
H -0.32196900 0.05458000 1.41622900
C -1.73758600 -0.71613100 0.00012300
H -1.72099600 -1.72055100 0.43236400
H -2.60370800 -0.18755900 0.40875700
H -1.87258500 -0.80416100 -1.08251700
O 1.99545200 -0.02586500 0.03098100
H 2.15350800 -0.10368600 0.98031600
N -0.51202400 1.39719800 -0.23710800
H -1.24735000 1.92631900 0.22436500
H 0.36030000 1.88213000 -0.04311400

G^0 = -249.721314 hartrees, 0 img. freq.

g6

0 1
C -0.75407300 -0.72941700 0.19338100
H -0.66050200 -0.84146800 1.28097900
H -0.79139400 -1.72433900 -0.25559600
C 0.45567300 0.02971400 -0.34451400
H 0.37924000 0.04529000 -1.44201600
C 1.74313500 -0.68809100 0.04670700
H 1.75052600 -1.71117600 -0.33865000
H 2.61462000 -0.16762300 -0.36098900
H 1.84781600 -0.72753000 1.13566100
O -2.00169400 -0.10142000 -0.13171100
H -2.09129200 0.68384200 0.42174000
N 0.45943900 1.39586600 0.21171200
H 1.34093400 1.85192600 -0.00887100
H -0.26088300 1.95814000 -0.23399800

G^0 = -249.721044 hartrees, 0 img. freq.

g7

0 1
C -0.74273500 -0.69189900 0.24512300
H -0.66629500 -0.69572900 1.34053600
H -0.76165500 -1.73061400 -0.10732700
C 0.46014700 0.03663600 -0.34818600
H 0.34039800 0.03158400 -1.43792900
C 1.75298100 -0.68791900 0.01239400
H 1.73015500 -1.72703200 -0.32627300
H 2.60998000 -0.19372100 -0.45169600
H 1.90626200 -0.68696600 1.09725800
O -1.93446400 -0.00582900 -0.16836600
H -2.68494400 -0.39391000 0.29549100
N 0.54555100 1.44603600 0.06974400
H -0.35549600 1.89315800 -0.08079800
H 0.71609800 1.48670800 1.07347600

G^0 = -249.721109 hartrees, 0 img. freq.

g8

0 1
C -0.74342600 -0.68664300 0.28175800
H -0.65250500 -0.67002600 1.37170300
H -0.76458600 -1.73292300 -0.04703800
C 0.45169500 0.03624800 -0.34663200
H 0.31207000 0.01892900 -1.43525700
C 1.75046800 -0.68703000 -0.00501300
H 1.71797300 -1.72989400 -0.33126300
H 2.60032200 -0.20102800 -0.49052100
H 1.92375400 -0.67480400 1.07682700
O -1.99300600 -0.04723500 -0.01483000
H -2.16393000 -0.15318000 -0.95915400
N 0.54703500 1.44996900 0.05337100
H -0.35938800 1.89483300 -0.07181700
H 0.74866500 1.50074400 1.05087800

G^0 = -249.721300 hartrees, 0 img. freq.

g9

0 1
C -0.73393000 -0.72479300 0.22498700
H -0.63763200 -0.77664400 1.31838000
H -0.74644500 -1.74510200 -0.16539500
C 0.46187900 0.03867800 -0.35533600
H 0.36155000 0.03594900 -1.44620700
C 1.76212800 -0.66102200 0.03176600
H 1.75653400 -1.70718000 -0.28633200
H 2.61744300 -0.16394500 -0.43200700
H 1.90319700 -0.63771600 1.11794000
O -1.99882300 -0.15559000 -0.13356500
H -2.07392300 0.70290700 0.30117600
N 0.51958700 1.44919500 0.06254100
H -0.29519200 1.96113400 -0.26423600
H 0.52748100 1.51377900 1.07890800

G^0 = -249.721291 hartrees, 0 img. freq.

g10

0 1
C 0.93806600 -0.02632800 0.67051400
H 1.17116800 -0.90092100 1.29157400
H 1.29230400 0.87144300 1.19216300
C -0.57452500 0.07181400 0.46733800
H -1.00992400 0.14918400 1.46967200
C -1.14045500 -1.17204900 -0.21637700
H -0.86016300 -2.07755700 0.32897000
H -2.23112800 -1.11955600 -0.26087700
H -0.76030300 -1.26092200 -1.23782900
O 1.57707200 -0.13825400 -0.60978500
H 2.52991400 -0.08370300 -0.47664600
N -0.98688100 1.27370300 -0.28008300
H -0.64421500 2.10589400 0.19477900
H -0.53458300 1.26562800 -1.19179300

G^0 = -249.719717 hartrees, 0 img. freq.

g11

0 1
C 0.94822000 -0.11359800 0.66801800
H 1.15133000 -1.04387500 1.20429000
H 1.33135800 0.71880800 1.27256900
C -0.56519900 0.05597100 0.47772900
H -0.98937100 0.10110500 1.48789600
C -1.18740900 -1.12360300 -0.26442400
H -0.96736800 -2.06378500 0.24820100
H -2.27262900 -1.00956500 -0.32552700
H -0.79293600 -1.19321900 -1.28248300
O 1.67693000 -0.20282300 -0.56221300
H 1.58977000 0.64183600 -1.02146300
N -0.93373900 1.31016300 -0.20356100
H -0.46424800 2.10266600 0.22842400
H -0.63885200 1.28484200 -1.17721800

G^0 = -249.720257 hartrees, 0 img. freq.

g12

0 1
C 0.94785300 0.03573900 0.67267700
H 1.20745500 -0.80105300 1.33358700
H 1.27930000 0.96114700 1.14983000
C -0.57243200 0.08273800 0.46750600
H -1.01018700 0.17812900 1.46781300
C -1.10158700 -1.19924400 -0.17448200
H -0.78968000 -2.08001300 0.39377000
H -2.19318100 -1.18373200 -0.21525800
H -0.73507000 -1.30836100 -1.20115400
O 1.68537000 -0.04985200 -0.55435000
H 1.52575000 -0.91832200 -0.94304700
N -1.02021400 1.24498800 -0.31963500
H -0.69916200 2.10240400 0.12476800
H -0.56969000 1.21830600 -1.23226900

G^0 = -249.720298 hartrees, 0 img. freq.

g13

0 1
C -0.94938100 0.06871600 0.67084700
H -1.18078900 0.99411000 1.21143300
H -1.30898700 -0.78132800 1.26130100
C 0.55673600 -0.04854800 0.48198700

H 0.98744000 -0.07203800 1.48918600
C 1.13974000 1.15629400 -0.26636800
H 0.91965700 2.09117700 0.25962700
H 2.22649600 1.06113800 -0.34772600
H 0.72581000 1.22430700 -1.27599700
O -1.58073600 0.07416300 -0.62010100
H -2.53368100 0.01588400 -0.48888000
N 0.86267600 -1.34311200 -0.15412800
H 0.42456800 -1.36968800 -1.07200900
H 1.86407300 -1.41384800 -0.31603500

G^0 = -249.719640 hartrees, 0 img. freq.

g14

0 1
C 0.95408500 -0.19501400 0.65933500
H 1.13622300 -1.19521900 1.05817200
H 1.34657100 0.53896200 1.37231400
C -0.54816100 0.02662800 0.47878700
H -0.97529400 0.03959100 1.48750100
C -1.20747200 -1.09884500 -0.32374000
H -1.06302700 -2.06850300 0.16358000
H -2.28272500 -0.92210300 -0.41857500
H -0.78108800 -1.15550600 -1.32980000
O 1.68664200 -0.12037500 -0.57177600
H 1.69578100 0.80318100 -0.85160000
N -0.77313600 1.36694400 -0.09843100
H -0.59449200 1.34072900 -1.10044700
H -1.75384400 1.61664300 -0.00421200

G^0 = -249.719955 hartrees, 0 img. freq.

g15

0 1
C -0.95847100 0.00520500 0.67671200
H -1.21517900 0.89325700 1.26504300
H -1.29773900 -0.87923600 1.21911600
C 0.55552900 -0.06459100 0.48331500
H 0.98820800 -0.11167000 1.48927100
C 1.10563600 1.18244800 -0.22003900
H 0.85488100 2.09309000 0.33399500
H 2.19473800 1.12338500 -0.29957700
H 0.70593900 1.27510400 -1.23563300
O -1.68499700 -0.00079600 -0.56177700
H -1.53637500 0.84387400 -1.00359600
N 0.89298100 -1.32498000 -0.20169300
H 0.42770200 -1.34267700 -1.10673900
H 1.89077200 -1.35226700 -0.39574100

G^0 = -249.720034, 0 img. freq.

g16

0 1
C -0.95317400 -0.16696300 0.62468800
H -1.26393700 0.55686000 1.38809500
H -1.20376400 -1.17210100 0.98900200
C 0.55721400 -0.06068500 0.44796900
H 0.96625600 -0.13323000 1.46807900
C 0.98524300 1.28232900 -0.13717300
H 0.63268700 2.10699500 0.48879400
H 2.07640800 1.34329000 -0.19264500
H 0.58173900 1.41313400 -1.14359000
O -1.63232400 0.09542300 -0.61004400
H -2.57924100 0.02412100 -0.44521300
N 1.05723600 -1.15393300 -0.40633600
H 2.07122100 -1.10190600 -0.46213200
H 0.84086300 -2.05109900 0.02140600

G^0 = -249.717865, 0 img. freq.

g17

0 1
C 0.97196200 -0.18383200 0.65363300
H 1.16525000 -1.15637200 1.11168100
H 1.38512200 0.59232700 1.31312000
C -0.53352000 0.04381900 0.49399700
H -0.96013200 0.09702400 1.50562500
C -1.21993700 -1.08723100 -0.26590200
H -1.09072900 -2.03609600 0.26128300
H -2.29297100 -0.89359600 -0.35727500
H -0.80526400 -1.19199900 -1.27195100
O 1.64659000 -0.16272300 -0.60656100
H 1.21764700 0.55076600 -1.10539800

```
N -0.70670800 1.31075000 -0.24518200
H -1.67490400 1.42530000 -0.53038000
H -0.48081800 2.10264000 0.35168300

G⁰ = -249.721821 hartrees, 0 img. freq.
```

g18

```
0 1
C -0.96199600 -0.19084400 0.62740500
H -1.27686100 0.51955800 1.40228700
H -1.20955500 -1.19698100 0.97586000
C 0.55359500 -0.07136300 0.44957900
H 0.96412700 -0.15572400 1.46865300
C 0.97108400 1.28611500 -0.11139200
H 0.60414200 2.09882500 0.52200200
H 2.06135900 1.36124600 -0.15814100
H 0.58798800 1.43150800 -1.12638800
O -1.73209700 0.00328700 -0.56306500
H -1.57654200 0.90089500 -0.88034400
N 1.05816200 -1.14221700 -0.42669700
H 2.07148100 -1.08348300 -0.48671200
H 0.84740600 -2.05007000 -0.01937700

G⁰ = -249.718870 hartrees, 0 img. freq.
```

1-Methoxy-2-propylamine (2, gas phase)

a1

```
0 1
C 0.32939900 -0.51952300 0.20150800
H 0.47936900 -1.57765300 -0.06684000
H 0.33496100 -0.45022300 1.29917800
C -1.01516900 -0.03329700 -0.33140700
H -0.94068500 -0.01268700 -1.42937400
C -1.33234400 1.37611600 0.15712700
H -0.53812200 2.06479700 -0.13357900
H -2.27272400 1.73549300 -0.27203900
H -1.42783100 1.38408500 1.24686200
O 1.36103700 0.27254600 -0.35806500
N -2.04465600 -0.96641800 0.14859900
H -2.97241500 -0.61354800 -0.06021000
H -1.95827600 -1.87169900 -0.30241300
C 2.64333800 -0.08396700 0.11389500
H 2.88706400 -1.12652900 -0.13564800
H 3.36317300 0.57545100 -0.37151800
H 2.71844100 0.04109800 1.20317100
```

G^0 = -288.996919 hartrees, 0 img. freq.

a2 converged to a1

a3

```
0 1
C 0.28414400 -0.48616100 0.66963500
H 0.49618300 -1.55788800 0.53191300
H -0.06384100 -0.34199700 1.69467100
C -0.82707800 -0.04944600 -0.29418700
H -0.43988300 -0.11061500 -1.32347500
C -1.25120900 1.39026300 -0.02760600
H -0.39110800 2.05850100 -0.09474500
H -2.00102800 1.72042200 -0.75319500
H -1.68190800 1.47474900 0.97419700
O 1.48110700 0.26434900 0.53952800
N -1.96738700 -0.95136700 -0.08048000
H -2.77948700 -0.63662700 -0.60061600
H -1.75570900 -1.89402900 -0.39199100
C 2.29032200 -0.11302500 -0.55803100
H 1.81906400 0.11281200 -1.52280300
H 3.21731200 0.45579900 -0.48052500
H 2.52618400 -1.18613700 -0.52516300
```

G^0 = -288.995196 hartrees, 0 img. freq.

a4

```
0 1
C 0.32297500 -0.53234400 0.16601200
H 0.48399700 -1.56908000 -0.17065900
H 0.32015100 -0.53724300 1.26941800
C -1.02792900 -0.02630300 -0.34876000
H -0.97475100 -0.00790900 -1.44262400
C -1.32255300 1.38441900 0.15081500
H -0.51694500 2.06524200 -0.12637200
H -2.26298400 1.74594200 -0.26871800
H -1.41119700 1.39155700 1.24362900
O 1.36013900 0.30062100 -0.31836800
N -2.13427900 -0.91704100 0.01736800
H -1.97541100 -1.86526200 -0.30805400
H -2.25335600 -0.95274800 1.02575200
C 2.64189100 -0.10206200 0.11840400
H 2.87988700 -1.11987700 -0.22179100
H 3.36432900 0.59389000 -0.30848500
H 2.71882700 -0.07245100 1.21444300
```

G^0 = -288.996894 hartrees, 0 img. freq.

a5 converged to a4

a6

```
0 1
C 0.25998000 -0.59817400 0.60503800
H 0.44879500 -1.64998100 0.33672600
H -0.10319100 -0.57408000 1.63743400
C -0.82851600 -0.02336000 -0.32074900
H -0.46717900 -0.06074700 -1.35428300
```

C -1.14729900 1.42514000 0.03273100
H -0.24330200 2.03609500 0.01409100
H -1.87750300 1.83706000 -0.66602000
H -1.56768400 1.48701900 1.04301300
O 1.48119000 0.12506800 0.61045300
N -2.05844300 -0.82314200 -0.28296400
H -1.88067400 -1.79240200 -0.52734900
H -2.46593300 -0.81251400 0.64808100
C 2.26039900 -0.04561100 -0.55877800
H 1.79866100 0.41815600 -1.43933000
H 3.22100100 0.43582000 -0.37416000
H 2.42920000 -1.11094100 -0.77052900

G^0 = -288.995286 hartrees, 0 img. freq.

a7

0 1
C 0.32634600 -0.56307000 0.13094000
H 0.48792200 -1.56671100 -0.28332000
H 0.32550700 -0.64931300 1.23129500
C -1.02347500 -0.03357400 -0.34489400
H -0.99436800 -0.01401100 -1.43931000
C -1.29040000 1.38439500 0.16919800
H -0.50274700 2.07026400 -0.14888200
H -2.24968400 1.75476500 -0.20343300
H -1.32602600 1.39177000 1.26460400
O 1.35108100 0.32218700 -0.28412000
N -2.04000700 -1.02412600 0.03722900
H -2.20284200 -0.99675700 1.04027100
H -2.92638400 -0.81680000 -0.41013100
C 2.63815300 -0.11044800 0.10397500
H 2.87928900 -1.09116800 -0.32942300
H 3.35302600 0.62670900 -0.26227600
H 2.72396300 -0.18117000 1.19764600

G^0 = -288.996777 hartrees, 0 img. freq.

a8 converged to a7

a9

0 1
C 0.26013100 -0.67581700 0.54665800
H 0.44354600 -1.69264400 0.17602900
H -0.09687300 -0.74975000 1.57902000
C -0.82806200 -0.01891700 -0.31520400
H -0.49323300 -0.02599300 -1.35834200
C -1.08450100 1.42937600 0.11103200
H -0.16981600 2.02475000 0.05948100
H -1.84002000 1.89401400 -0.52899200
H -1.44550200 1.46368500 1.14478600
O 1.47200500 0.05856200 0.61571000
N -2.00398200 -0.89660100 -0.25715300
H -2.42577200 -0.86439900 0.66728600
H -2.71359900 -0.59519200 -0.91643100
C 2.24930000 -0.00247300 -0.56508500
H 1.77578100 0.52443500 -1.40357900
H 3.20220900 0.47905500 -0.34416200
H 2.43390900 -1.04326600 -0.86511300

G^0 = -288.995156 hartrees, 0 img. freq.

g1

0 1
C -0.34034000 -0.45152100 0.22351200
H -0.37533000 -0.28612600 1.31403200
H -0.44027100 -1.53489200 0.05324800
C 0.99906000 0.03358900 -0.32109800
H 0.89791200 0.08608100 -1.40998500
C 2.10827200 -0.97033700 0.03016500
H 1.92003200 -1.95400700 -0.41117100
H 3.07427200 -0.61431100 -0.33683900
H 2.18997300 -1.09531800 1.11575600
O -1.39856100 0.23343800 -0.41115200
N 1.25620800 1.39901600 0.14817600
H 1.44296400 1.40486000 1.14732100
H 2.06879700 1.79373600 -0.31330900
C -2.66176100 -0.09901600 0.12172500
H -3.40758500 0.46815300 -0.43552100
H -2.87613000 -1.17302000 0.01653300
H -2.73098800 0.16793100 1.18609400

G^0 = -288.993659 hartrees, 0 img. freq.

g2

0 1
C -0.22420700 -0.81158300 0.41252300
H 0.14918900 -1.04426900 1.41506400
H -0.32268800 -1.76003800 -0.13847400
C 0.80038800 0.06967100 -0.31568800
H 0.51448000 0.13478200 -1.37296700
C 2.17752400 -0.60431700 -0.24656900
H 2.15614400 -1.60656400 -0.68717600
H 2.92066800 -0.01818900 -0.79426400
H 2.51357900 -0.69218200 0.79161900
O -1.49489800 -0.22958300 0.61976900
N 0.75887400 1.43053100 0.22475800
H 0.68440700 1.42488200 1.23692600
H 1.59197900 1.95137100 -0.02660800
C -2.16730000 0.13548300 -0.57254200
H -3.17720500 0.42986700 -0.28643500
H -1.67445400 0.98019100 -1.06520200
H -2.22746600 -0.71243600 -1.27028400

G^0 = -288.993390 hartrees, 0 img. freq.

g3

0 1
C -0.21465300 -0.83790800 0.26858100
H -0.29289000 -0.63852200 1.35038400
H 0.06162800 -1.88868100 0.14690000
C 0.89457000 0.03189600 -0.33428600
H 0.80131800 -0.05031500 -1.42215300
C 2.27210700 -0.49804000 0.09164900
H 2.43503900 -1.52382200 -0.25258600
H 3.06785600 0.12708400 -0.32209700
H 2.37222900 -0.48688100 1.18285200
O -1.47863800 -0.70309100 -0.35106900
N 0.67256500 1.44613200 0.00376500
H 0.81928100 1.59786100 0.99883400
H 1.33548800 2.03963500 -0.48505100
C -2.28022600 0.37239300 0.11888200
H -2.42012700 0.30546300 1.20769000
H -1.83811700 1.34082400 -0.12455300
H -3.25134800 0.26910400 -0.36698300

G^0 = -288.993846 hartrees, 0 img. freq.

g4

0 1
C -0.30467200 -0.56549200 0.12728000
H -0.31714600 -0.61552800 1.22605800
H -0.42474700 -1.58311000 -0.27285000
C 1.01598500 0.02862000 -0.33585600
H 0.97852500 0.07496500 -1.43639000
C 2.18484200 -0.86226600 0.07741900
H 2.09977800 -1.85698400 -0.36842800
H 3.13296700 -0.42929100 -0.25312600
H 2.22319600 -0.96161700 1.16533300
O -1.35888800 0.26653800 -0.33327400
N 1.16206600 1.35474500 0.27364400
H 1.99297500 1.82185200 -0.07406400
H 0.36011300 1.92934300 0.03479600
C -2.62875400 -0.14458400 0.12974700
H -3.36353900 0.55162500 -0.27511700
H -2.87034000 -1.16018200 -0.21414000
H -2.67955400 -0.12426000 1.22707300

G^0 = -288.998712 hartrees, 0 img. freq.

g5

0 1
C 0.24975400 -0.58242500 -0.61191600
H -0.09320600 -0.52746700 -1.64772900
H 0.42084400 -1.63590800 -0.34884600
C -0.82427800 0.01486900 0.29700900
H -0.46488800 -0.04451500 1.33801000
C -2.11555800 -0.79427900 0.19817300
H -1.96076200 -1.82599600 0.52676000
H -2.89486800 -0.35685300 0.82823700
H -2.48179800 -0.79956900 -0.83177900
O 1.47787200 0.13582800 -0.57508700
N -1.06341400 1.39516400 -0.13208700
H -1.65055800 1.89154500 0.52929400
H -0.18295100 1.89425100 -0.21080500
C 2.26627700 -0.12121300 0.57242400

H 3.21091200 0.40495100 0.43300600
H 1.79350500 0.24099100 1.49403300
H 2.46751700 -1.19591400 0.68098000

G^0 = -288.996702 hartrees, 0 img. freq.

g6 converged to g4

g7

0 1
C -0.30666400 -0.56306700 0.13074900
H -0.31070300 -0.63205800 1.23144100
H -0.44246000 -1.57852600 -0.27289500
C 1.01879100 0.03016000 -0.34864400
H 0.97591500 0.06760300 -1.44303200
C 2.18841100 -0.85637000 0.06971400
H 2.07560000 -1.87359300 -0.31379600
H 3.12462100 -0.44295300 -0.30839200
H 2.26153800 -0.91475200 1.16151300
O -1.36086100 0.27789700 -0.30599000
N 1.24687900 1.40221100 0.11211500
H 0.42970600 1.96919200 -0.09264900
H 1.37525400 1.41784600 1.12090000
C -2.63368800 -0.15554200 0.12686900
H -3.36676700 0.55363600 -0.25810500
H -2.86814200 -1.15784500 -0.25790100
H -2.69692800 -0.17829300 1.22390800

G^0 = -288.998404 hartrees, 0 img. freq.

g8

0 1
C -0.24882000 -0.58613400 0.60950800
H 0.10105300 -0.54100800 1.64554000
H -0.43272100 -1.64074000 0.35346300
C 0.82286500 0.01049900 -0.31558900
H 0.46685700 -0.06686300 -1.34971000
C 2.12389400 -0.77836300 -0.20199100
H 1.97462700 -1.83085600 -0.45616800
H 2.87806900 -0.36229300 -0.87218300
H 2.51646600 -0.73256600 0.82021100
O -1.47199700 0.13891800 0.58618600
N 1.07625300 1.43177600 -0.06047700
H 0.19177300 1.92524800 0.02215400
H 1.55452900 1.54525700 0.83004500
C -2.27879200 -0.12400900 -0.54803300
H -3.21618200 0.41314400 -0.40229900
H -1.81526200 0.22280000 -1.48002500
H -2.49189000 -1.19785700 -0.64054800

G^0 = -288.996604 hartrees, 0 img. freq.

g9 converged to g7

g10

0 1
C -0.35557700 -0.01637900 0.79054100
H -0.57688300 0.86169000 1.41793500
H -0.62891000 -0.91676800 1.36383200
C 1.13503300 -0.05681100 0.43716500
H 1.67820200 -0.11900700 1.38775300
C 1.57274000 1.21449000 -0.29114600
H 1.34397300 2.10441400 0.30159000
H 2.64645300 1.18418200 -0.48202900
H 1.05174700 1.30461200 -1.24717300
O -1.11070200 0.03721400 -0.40750600
N 1.51962700 -1.22836100 -0.35805700
H 1.31624300 -2.08711200 0.14462500
H 0.96801100 -1.24946800 -1.21125300
C -2.50505800 0.04071700 -0.18535700
H -2.81476300 0.91571600 0.40309700
H -2.98989300 0.07826000 -1.16119800
H -2.82878200 -0.86780700 0.34205600

G^0 = -288.997242 hartrees, 0 img. freq.

g11 converged to g10

g12 converged to g10

g13

0 1
C -0.35628400 0.03331200 0.79629500

H -0.56209900 0.94500900 1.37678100
H -0.63745500 -0.83913800 1.40125000
C 1.12494100 -0.04894300 0.44869700
H 1.66252400 -0.08000800 1.40410400
C 1.59328100 1.18457500 -0.33713400
H 1.43006100 2.10468900 0.23358800
H 2.66178600 1.11248700 -0.55896900
H 1.04817500 1.26578900 -1.27996400
O -1.10630000 0.04636900 -0.40992200
N 1.36680500 -1.32996800 -0.22600400
H 0.79836500 -1.37992700 -1.06643400
H 2.33790000 -1.40926500 -0.50927500
C -2.50119800 0.02455100 -0.19151900
H -2.98411000 0.03402800 -1.16897400
H -2.80637800 -0.88024900 0.35212300
H -2.83045100 0.90445100 0.37914300

G^0 = -288.997440 hartrees, 0 img. freq.

g14 converged to g13

g15 converged to g13

g16

0 1
C -0.37512000 -0.18073500 0.73095700
H -0.62753300 0.50614000 1.55479800
H -0.60617600 -1.20287400 1.07466500
C 1.11797600 -0.06638000 0.43297700
H 1.61368900 -0.13251700 1.41758000
C 1.47318900 1.28260900 -0.18895600
H 1.16543200 2.10392900 0.46352800
H 2.55367100 1.36176300 -0.34172600
H 0.97353400 1.39264400 -1.15163700
O -1.14365700 0.13195100 -0.41102800
N 1.53731400 -1.14499400 -0.46943700
H 2.52775600 -1.07551800 -0.67735000
H 1.37487900 -2.05630500 -0.05352600
C -2.52954100 -0.00558100 -0.18915500
H -2.87862000 0.66148100 0.61294200
H -3.03465800 0.26040500 -1.11795200
H -2.79294000 -1.03927400 0.07802300

G^0 = -288.993499, 0 img. freq.

g17

0 1
C 0.31266800 -0.44297800 0.95570000
H 0.16162900 -1.38273800 1.49462100
H 0.69721500 0.29630400 1.67651400
C -1.04836800 0.02178300 0.41807200
H -1.74365000 -0.06377400 1.27210600
C -1.55098600 -0.88787400 -0.69947400
H -1.63341500 -1.92003800 -0.35030900
H -2.53914700 -0.56841400 -1.04394800
H -0.86143000 -0.86514000 -1.54442400
O 1.29165600 -0.71995000 -0.02734100
N -0.96301800 1.40444600 -0.07950400
H -1.85126100 1.69839300 -0.47306900
H -0.74239200 2.04810600 0.67438000
C 2.00433300 0.41044100 -0.51129400
H 1.35613200 1.08636500 -1.07353800
H 2.46218000 0.96579900 0.32016400
H 2.79613100 0.02538000 -1.15526000

G^0 = -288.993935 hartrees, 0 img. freq.

g18

0 1
C -0.33885600 -0.22149300 1.07348800
H -0.46392600 0.71249500 1.64157900
H -0.34699200 -1.04992100 1.78584500
C 1.02997800 -0.19477400 0.35140100
H 1.75034500 -0.54628600 1.10906300
C 1.48752000 1.20330200 -0.07447000
H 1.55091400 1.87002800 0.79054300
H 2.48143700 1.15387900 -0.52919300
H 0.80914400 1.64090600 -0.80770000
O -1.47026600 -0.45685300 0.25660800
N 0.98774700 -1.07889100 -0.81863000
H 1.91822900 -1.37472400 -1.08999800
H 0.42429200 -1.90358700 -0.64389800
C -1.78309100 0.57739900 -0.66243000

```
H -1.80196900 1.55660300 -0.16401300
H -1.06873700 0.60136500 -1.49033700
H -2.77814400 0.35969200 -1.05228200

G⁰ = -288.990096 hartrees, 0 img. freq.
```

1-Methoxy-2-propylamine (2, MeCN – SMD)

a1

```
0 1
C 0.33275800 -0.50832600 0.20221300
H 0.48757500 -1.56366300 -0.06863100
H 0.34821600 -0.43673200 1.29982400
C -1.01651800 -0.03237700 -0.32552900
H -0.95411100 -0.01929000 -1.42359000
C -1.35522400 1.37291300 0.15853200
H -0.59587000 2.08662600 -0.16699300
H -2.32129300 1.69692700 -0.24080200
H -1.41020200 1.39701900 1.25184900
O 1.36644000 0.28867800 -0.35775200
N -2.03978900 -0.97952100 0.15222200
H -2.96070100 -0.65789900 -0.13398800
H -1.90523400 -1.88801300 -0.28488300
C 2.65079300 -0.08771400 0.11128300
H 2.88113600 -1.13010900 -0.14777800
H 3.37942000 0.56763100 -0.36843400
H 2.72721700 0.02775500 1.20090100

G⁰ = -289.007363 hartrees, 0 img. freq.
```

a2

```
0 1
C 0.33272300 -0.50827600 0.20216800
H 0.48728500 -1.56390400 -0.06790600
H 0.34859400 -0.43568600 1.29976800
C -1.01652900 -0.03240400 -0.32550100
H -0.95402300 -0.01915800 -1.42366100
C -1.35532700 1.37285200 0.15854400
H -0.59565300 2.08653000 -0.16647700
H -2.32120400 1.69703300 -0.24127900
H -1.41090500 1.39676600 1.25191800
O 1.36659000 0.28817600 -0.35872100
N -2.03968000 -0.97956600 0.15231000
H -2.96090400 -0.65697400 -0.13189000
H -1.90649600 -1.88750700 -0.28639700
C 2.65097100 -0.08753000 0.11185200
H 2.72652200 0.03004200 1.20130500
H 2.88107200 -1.13045200 -0.14531200
H 3.37972500 0.56701000 -0.36885500

G⁰ = -289.007329 hartrees, 0 img. freq.
```

a3

```
0 1
C 0.27573400 -0.54466200 0.65168900
H 0.47209800 -1.60750200 0.44661600
H -0.07424800 -0.45508700 1.68377200
C -0.82167600 -0.03610900 -0.29010800
H -0.44800200 -0.08688300 -1.32208700
C -1.20215300 1.40699900 0.01539200
H -0.33740900 2.06537000 -0.09323300
H -1.98266900 1.75542700 -0.66814400
H -1.57816600 1.49537900 1.04012600
O 1.49300900 0.18941700 0.58225900
N -1.99384600 -0.91183600 -0.10258900
H -2.76139500 -0.58114500 -0.68162700
H -1.77971500 -1.85264900 -0.42527500
C 2.25964200 -0.07057000 -0.58665600
H 1.78468600 0.32614100 -1.49121400
H 3.22382900 0.42287800 -0.45274800
```

H 2.42456800 -1.14835900 -0.71803500

G^0 = -289.005894 hartrees, 0 img. freq.

a4

0 1
C 0.32095400 -0.51984500 0.16170500
H 0.48610800 -1.55301400 -0.17831500
H 0.31764000 -0.52385000 1.26335900
C -1.02995900 -0.02126700 -0.35426500
H -0.98119500 -0.00054800 -1.44841300
C -1.34752000 1.37986700 0.15663500
H -0.55672800 2.08136400 -0.11592200
H -2.29188000 1.73779800 -0.26169000
H -1.43642400 1.37486700 1.24914400
O 1.36374900 0.31806000 -0.32041000
N -2.11966200 -0.93948800 0.01724900
H -1.91074500 -1.88103300 -0.30665200
H -2.18909400 -0.99340600 1.03182000
C 2.64414700 -0.10407000 0.12143800
H 2.87146400 -1.12086500 -0.22671200
H 3.37872000 0.58732400 -0.29464900
H 2.71404000 -0.08480500 1.21748800

G^0 = -289.007532 hartrees, 0 img. freq.

a5

0 1
C 0.32098700 -0.51990200 0.16177600
H 0.48621100 -1.55308100 -0.17818000
H 0.31777300 -0.52385200 1.26343800
C -1.02990700 -0.02134800 -0.35427800
H -0.98091500 -0.00050300 -1.44843000
C -1.34746900 1.37978700 0.15662500
H -0.55659500 2.08123600 -0.11577100
H -2.29174800 1.73785100 -0.26177200
H -1.43651100 1.37473800 1.24912800
O 1.36372200 0.31803300 -0.32046500
N -2.11971000 -0.93943800 0.01705400
H -1.91019400 -1.88132900 -0.30547600
H -2.19024100 -0.99217600 1.03161400
C 2.64410900 -0.10402200 0.12146300
H 2.71397300 -0.08464600 1.21751800
H 2.87144200 -1.12085100 -0.22655700
H 3.37867700 0.58732200 -0.29468600

G^0 = -289.007534 hartrees, 0 img. freq.

a6

0 1
C 0.24715700 -0.62751400 0.58602100
H 0.42780600 -1.66788700 0.27758900
H -0.12784000 -0.63569500 1.61441600
C -0.82376900 -0.00898500 -0.32824600
H -0.46176200 -0.03092700 -1.36077600
C -1.12574000 1.43315000 0.06061800
H -0.21858000 2.04086800 0.03687100
H -1.85733100 1.87268300 -0.62242200
H -1.53464900 1.47695200 1.07667500
O 1.48306500 0.08094400 0.63078800
N -2.06328900 -0.80505900 -0.29592600
H -1.86591300 -1.76966400 -0.55283700
H -2.42542400 -0.83104600 0.65587900
C 2.24505700 -0.02008800 -0.56530400
H 1.78352700 0.52290000 -1.39817200
H 3.22260000 0.41978800 -0.36059200
H 2.37984200 -1.06948600 -0.85998800

G^0 = -289.006287 hartrees, 0 img. freq.

a7

0 1
C 0.33063100 -0.55431800 0.12606000
H 0.50295600 -1.56048100 -0.27947100
H 0.33274500 -0.62817500 1.22548800
C -1.02168900 -0.03539700 -0.35182900
H -0.99972800 -0.00703000 -1.44641300
C -1.31379800 1.37045600 0.17686400
H -0.55197300 2.08307400 -0.14919900
H -2.28715700 1.71831400 -0.18185500
H -1.33391800 1.36705700 1.27265700
O 1.36000000 0.32698100 -0.30119300
N -2.03729000 -1.03270200 0.03204900

H -2.15724600 -1.01927300 1.04344500
H -2.93693900 -0.76546300 -0.35877000
C 2.64510800 -0.10522300 0.11543700
H 2.88664300 -1.09492200 -0.29540900
H 3.37044100 0.62083200 -0.25515500
H 2.71369700 -0.15397800 1.21068200

G^0 = -289.006990 hartrees, 0 img. freq.

a8

0 1
C 0.33063100 -0.55429300 0.12597000
H 0.50304100 -1.56036700 -0.27977800
H 0.33284600 -0.62846800 1.22541900
C -1.02171400 -0.03544400 -0.35174700
H -0.99990000 -0.00708700 -1.44638600
C -1.31380300 1.37044700 0.17677800
H -0.55217900 2.08308100 -0.14970800
H -2.28735500 1.71806900 -0.18169200
H -1.33359800 1.36737700 1.27260700
O 1.35997900 0.32720400 -0.30107000
N -2.03710000 -1.03272300 0.03230000
H -2.15842300 -1.01802000 1.04352800
H -2.93646300 -0.76673700 -0.36003300
C 2.64511800 -0.10534500 0.11543200
H 2.71358200 -0.15455000 1.21065100
H 2.88646500 -1.09489300 -0.29586300
H 3.37045500 0.62084300 -0.25487600

G^0 = -289.006982 hartrees, 0 img freq.

a9

0 1
C 0.25464600 -0.71876300 0.51657700
H 0.44103100 -1.71687600 0.09751700
H -0.11471700 -0.83986600 1.54004400
C -0.81883700 -0.01180400 -0.32110600
H -0.48982100 0.01322500 -1.36471500
C -1.05690800 1.42136100 0.15669100
H -0.14342200 2.01904500 0.09356200
H -1.82598500 1.90464200 -0.45327600
H -1.39386100 1.42457600 1.19948600
O 1.48000500 -0.00429800 0.63361800
N -2.02100100 -0.86262600 -0.28016600
H -2.42417900 -0.83338300 0.65475200
H -2.72898000 -0.48394100 -0.90367800
C 2.23034300 0.04344100 -0.57273500
H 1.74991800 0.66778200 -1.33515900
H 3.20204400 0.47582200 -0.32831800
H 2.37947400 -0.96366800 -0.98455900

G^0 = -289.005720 hartrees, 0 img. freq.

g1

0 1
C -0.34057300 -0.44855700 0.20173500
H -0.36162500 -0.33564800 1.29741600
H -0.46504800 -1.51706100 -0.02377100
C 1.00174600 0.02934200 -0.33477300
H 0.92558100 0.07706600 -1.42627100
C 2.09752400 -0.97632800 0.03968800
H 1.90569100 -1.96063500 -0.39904500
H 3.06951500 -0.62727600 -0.31980600
H 2.16048300 -1.09152100 1.12744800
O -1.40680200 0.28697500 -0.38248800
N 1.27999600 1.39649500 0.14115100
H 1.38908700 1.38019700 1.15397300
H 2.17426200 1.70662400 -0.23143700
C -2.67025000 -0.11507300 0.11959900
H -3.42914500 0.48586400 -0.38424200
H -2.86306500 -1.17788600 -0.08299900
H -2.74197000 0.05270500 1.20308500

G^0 = -289.006203 hartrees, 0 img. freq.

g2

0 1
C -0.27165900 -0.57867000 0.61644400
H 0.08125900 -0.53758200 1.65186600
H -0.40702800 -1.63503800 0.34450500
C 0.79470100 0.02948200 -0.29870300
H 0.42601800 0.01712400 -1.32933400
C 2.05902500 -0.83648900 -0.23400000

H 1.85987600 -1.86149800 -0.56320100
H 2.83782500 -0.41942700 -0.87869900
H 2.44910700 -0.87400900 0.78914900
O -1.53522600 0.07565100 0.62063600
N 1.02647800 1.43830000 0.06004800
H 1.34952800 1.49116400 1.02468000
H 1.78027900 1.81251800 -0.51105700
C -2.24044900 -0.03109600 -0.60718500
H -3.24922800 0.34649900 -0.43097700
H -1.77730700 0.56417100 -1.40258300
H -2.30357600 -1.07659200 -0.93910200

G^0 = -289.005407 hartrees, 0 img. freq.

g3

0 1
C -0.21998300 -0.82758400 0.19475700
H -0.31544500 -0.66734000 1.27802200
H 0.02047200 -1.88242200 0.03443600
C 0.92913700 0.01861900 -0.35396600
H 0.92340100 -0.08934400 -1.44407500
C 2.26314700 -0.51261800 0.18617600
H 2.43065200 -1.55335600 -0.10919900
H 3.09281800 0.08717300 -0.19855800
H 2.28536400 -0.45861500 1.28034100
O -1.47394300 -0.60160500 -0.44606200
N 0.70857200 1.44643700 -0.06193100
H 0.71793100 1.58797400 0.94696400
H 1.48808700 1.98818300 -0.42767700
C -2.32561400 0.32233300 0.22041300
H -2.52735800 -0.00057400 1.25068700
H -1.89750400 1.32889700 0.23924100
H -3.26699600 0.34270400 -0.33245500

G^0 = -289.004345 hartrees, 0 img. freq.

g4

0 1
C -0.31068700 -0.55328100 0.12822500
H -0.32873500 -0.61966300 1.22611000
H -0.43971900 -1.56454200 -0.28161000
C 1.01629600 0.02741200 -0.33033400
H 0.98455900 0.08911000 -1.42881200
C 2.17070000 -0.88552200 0.07047100
H 2.07175800 -1.86879900 -0.39743300
H 3.12504300 -0.45558500 -0.24700000
H 2.20157100 -1.01713700 1.15652000
O -1.36561700 0.29116800 -0.32111600
N 1.19518800 1.35606900 0.28051500
H 2.04092200 1.78841200 -0.08245300
H 0.42195300 1.95713300 0.00840400
C -2.63902600 -0.14915100 0.12308700
H -3.38106500 0.54981200 -0.26592200
H -2.86510000 -1.15684900 -0.25095500
H -2.69626200 -0.16046400 1.21977900

G^0 = -289.008442 hartrees, 0 img. freq.

g5

0 1
C 0.24214000 -0.64800800 -0.57386300
H -0.10568100 -0.68007100 -1.61017100
H 0.40228500 -1.67671900 -0.22411700
C -0.81856800 0.02868700 0.29181700
H -0.46985600 0.02245100 1.33478900
C -2.12761900 -0.75179500 0.22637400
H -1.99669800 -1.76671600 0.61239600
H -2.89830900 -0.26033400 0.82738800
H -2.48901900 -0.81462500 -0.80501600
O 1.48584900 0.05138800 -0.60891300
N -1.02425500 1.40165000 -0.19941900
H -1.63806400 1.90597500 0.43507200
H -0.13583700 1.89640000 -0.19931300
C 2.24358700 -0.06096400 0.58966800
H 3.21325300 0.40152600 0.39850700
H 1.76792800 0.45555200 1.43141900
H 2.39574700 -1.11360700 0.86231400

G^0 = -289.007186 hartrees, 0 img. freq.

g6

0 1
C -0.31065400 -0.55321600 0.12827600

H -0.32891300 -0.61912100 1.22623000
H -0.43956700 -1.56470900 -0.28113600
C 1.01632200 0.02747200 -0.33023100
H 0.98459500 0.08902800 -1.42878700
C 2.17072500 -0.88557500 0.07046300
H 2.07158700 -1.86893500 -0.39729700
H 3.12507100 -0.45579700 -0.24732800
H 2.20188000 -1.01700600 1.15656100
O -1.36567900 0.29094900 -0.32151800
N 1.19531800 1.35609000 0.28054400
H 2.04068400 1.78878600 -0.08294300
H 0.42174800 1.95702500 0.00897100
C -2.63913400 -0.14910600 0.12322800
H -2.86534000 -1.15697600 -0.25028100
H -2.69596500 -0.15976400 1.21995100
H -3.38113500 0.54979700 -0.26601800

G^0 = -289.008435 hartrees, 0 img. freq.

g7

0 1
C -0.30263700 -0.55263500 0.13127400
H -0.31161900 -0.59481200 1.23154300
H -0.43265100 -1.57534000 -0.25122900
C 1.02219500 0.03031000 -0.35365200
H 0.98348800 0.06686500 -1.44824000
C 2.18348200 -0.86193800 0.07257600
H 2.05613800 -1.88069600 -0.30263800
H 3.12797300 -0.46923700 -0.31175800
H 2.25378600 -0.90828700 1.16490600
O -1.36545000 0.27417400 -0.32911400
N 1.25301700 1.40697700 0.11667900
H 0.42818200 1.96811500 -0.08157600
H 1.35158200 1.40043900 1.13079400
C -2.63337800 -0.15882400 0.13689700
H -3.38090400 0.52859500 -0.26236800
H -2.86048400 -1.17595200 -0.20997700
H -2.68098100 -0.14340000 1.23412700

G^0 = -289.008562 hartrees, 0 img. freq.

g8

0 1
C -0.23398300 -0.62228600 0.59255100
H 0.12945400 -0.60819400 1.62476700
H -0.40074000 -1.66765800 0.29611700
C 0.81769900 0.02058600 -0.32183500
H 0.46122400 -0.03671200 -1.35552400
C 2.13247900 -0.74544700 -0.21885600
H 1.99326100 -1.80062400 -0.46903800
H 2.87695200 -0.32625800 -0.90031000
H 2.53220500 -0.68825100 0.79980100
O -1.47774500 0.07597100 0.61460100
N 1.04115600 1.44485500 -0.02133600
H 0.14294500 1.92183100 0.01424800
H 1.43620400 1.52897600 0.91431800
C -2.25276000 -0.09371300 -0.56590600
H -3.22099700 0.37496000 -0.38242700
H -1.79137900 0.38369200 -1.43814900
H -2.40587100 -1.15835100 -0.78698400

G^0 = -289.007280 hartrees, 0 img. freq.

g9

0 1
C -0.30255000 -0.55286500 0.13116600
H -0.31182600 -0.59511800 1.23144500
H -0.43251800 -1.57551400 -0.25146400
C 1.02217600 0.03043800 -0.35349800
H 0.98353600 0.06690300 -1.44814100
C 2.18364500 -0.86172800 0.07259100
H 2.05634600 -1.88053000 -0.30252200
H 3.12804900 -0.46895400 -0.31189800
H 2.25418900 -0.90800200 1.16492900
O -1.36533600 0.27406200 -0.32929100
N 1.25262400 1.40691200 0.11680500
H 0.42821100 1.96832100 -0.08241100
H 1.35024400 1.40079100 1.13101400
C -2.63326700 -0.15885100 0.13699800
H -2.86038700 -1.17601900 -0.20976000
H -2.68072800 -0.14327800 1.23420400
H -3.38081800 0.52855800 -0.26225100

G^0 = -289.008560 hartrees, 0 img. freq.

g10

0 1
C -0.35535600 -0.02709200 0.77854800
H -0.57549900 0.83135800 1.43063200
H -0.62872900 -0.94336800 1.32287300
C 1.13501900 -0.05831400 0.43769500
H 1.66263700 -0.12464500 1.39552200
C 1.58315800 1.21374300 -0.27992200
H 1.31526800 2.10194200 0.29898900
H 2.66645800 1.20890700 -0.42409700
H 1.10694000 1.29315000 -1.26107000
O -1.11685000 0.06424800 -0.41898400
N 1.52740400 -1.23608500 -0.35744800
H 1.25716600 -2.08514300 0.13403200
H 0.99819600 -1.23644800 -1.22682900
C -2.51336200 0.03789300 -0.17663000
H -2.82574700 0.88269300 0.45234100
H -3.01520400 0.10902000 -1.14307300
H -2.81527100 -0.89624000 0.31654400

G^0 = -289.007311 hartrees, 0 img. freq.

g11

0 1
C 0.35526800 0.02717800 0.77861600
H 0.57532600 -0.83102700 1.43100500
H 0.62863400 0.94365000 1.32254900
C -1.13505000 0.05835400 0.43758400
H -1.66272700 0.12478700 1.39536400
C -1.58310800 -1.21381900 -0.27988100
H -1.31543300 -2.10190000 0.29930100
H -2.66636400 -1.20886700 -0.42429000
H -1.10668700 -1.29348600 -1.26090200
O 1.11687900 -0.06468100 -0.41888100
N -1.52737900 1.23609000 -0.35767400
H -1.25820100 2.08517900 0.13435600
H -0.99716700 1.23704100 -1.22645200
C 2.51338600 -0.03772400 -0.17662400
H 2.81508100 0.89712100 0.31532400
H 2.82603500 -0.88165900 0.45335000
H 3.01515100 -0.10995700 -1.14301600

G^0 = -289.007316 hartrees, 0 img. freq.

g12

0 1
C -0.27165700 -0.54309500 0.81570700
H -0.71839700 0.05908900 1.61531800
H -0.13797300 -1.56263700 1.19499300
C 1.09690700 0.02757600 0.42351400
H 1.71039200 0.00303600 1.33186400
C 1.00523300 1.47008500 -0.06978900
H 0.52692400 2.11072200 0.67571000
H 2.00303700 1.86563800 -0.27576200
H 0.42178400 1.52684800 -0.99367300
O -1.15700500 -0.61781600 -0.30573100
N 1.78733900 -0.78901200 -0.59159500
H 1.87948200 -1.74533300 -0.25581600
H 1.20021900 -0.84027000 -1.42188700
C -2.24820700 0.29152200 -0.25519100
H -2.90109600 0.08176100 0.60212000
H -1.91310500 1.33333400 -0.19606800
H -2.82026000 0.15690300 -1.17523000

G^0 = -289.004847 hartrees, 0 img. freq.

g13

0 1
C -0.36502900 0.02634400 0.78561400
H -0.58085500 0.94054700 1.35598900
H -0.64693500 -0.83816800 1.40248500
C 1.11929700 -0.04096400 0.45410500
H 1.64406100 -0.05961100 1.41560700
C 1.59043700 1.18791000 -0.33222200
H 1.38946500 2.11093000 0.22157800
H 2.66739200 1.13037700 -0.51555100
H 1.08102700 1.24902300 -1.29759100
O -1.11915700 0.01831400 -0.42222200
N 1.40374400 -1.32041200 -0.22198700
H 0.88658500 -1.35167800 -1.09767800

H 2.38843200 -1.35979200 -0.47278400
C -2.51714500 0.02544100 -0.18621200
H -3.01376900 0.01889900 -1.15782600
H -2.83021700 -0.86043200 0.38293600
H -2.82348700 0.92388900 0.36680300

G^0 = -289.007059 hartrees, 0 img. freq.

g14

0 1
C 0.31518100 -0.50020400 0.95470500
H 0.17569800 -1.48135200 1.41535500
H 0.65729700 0.20040400 1.72788100
C -1.03985500 -0.03038600 0.41021300
H -1.74234900 -0.19681600 1.23499000
C -1.49108200 -0.86801400 -0.79001700
H -1.50575200 -1.93537200 -0.54670900
H -2.49775500 -0.57476400 -1.10128100
H -0.81476800 -0.72397300 -1.63726100
O 1.34867800 -0.69531900 -0.00942300
N -1.05804600 1.42555800 0.15574700
H -0.56546800 1.63795400 -0.70798700
H -2.01914600 1.71966500 -0.00033100
C 1.96454500 0.49067200 -0.49386400
H 1.36497500 0.98443000 -1.26749000
H 2.15268000 1.20275600 0.31912100
H 2.91875200 0.19829000 -0.93735000

G^0 = -289.002955 hartrees, 0 img. freq.

g15

0 1
C -0.29305000 -0.51033800 0.83978300
H -0.72903500 0.14546400 1.60020500
H -0.19541300 -1.51415500 1.26574300
C 1.08815300 0.00162900 0.43825200
H 1.70017200 -0.02242000 1.34754200
C 1.04833400 1.44079700 -0.08730900
H 0.63821600 2.12683600 0.66075900
H 2.05776100 1.77893600 -0.33978200
H 0.43458100 1.50633500 -0.99035900
O -1.16425200 -0.60752200 -0.29294800
N 1.68388300 -0.95198200 -0.51609700
H 1.09464200 -0.99182700 -1.34524100
H 2.58632100 -0.60199300 -0.82816700
C -2.24866800 0.31114900 -0.28064900
H -2.91242100 0.13115600 0.57501600
H -1.90473000 1.35140600 -0.24726200
H -2.81186200 0.15488400 -1.20265300

G° = -289.004787 hartrees, 0 img. freq.

g16

0 1
C -0.37613300 -0.17015000 0.72175800
H -0.63395100 0.54450700 1.51709100
H -0.60368200 -1.17978700 1.09711700
C 1.11517100 -0.05964100 0.42636900
H 1.60405700 -0.13163700 1.41058700
C 1.49064700 1.28502800 -0.19003700
H 1.18479900 2.10813600 0.46199600
H 2.57375600 1.35064100 -0.33138000
H 1.00781900 1.41347400 -1.16117800
O -1.15567000 0.09965900 -0.43468200
N 1.54848500 -1.15178200 -0.46515800
H 2.55608800 -1.10313800 -0.59340200
H 1.35993700 -2.04937800 -0.02531400
C -2.54507600 0.00524600 -0.17361600
H -2.85792600 0.72413400 0.59655600
H -3.06968600 0.23013500 -1.10380300
H -2.82290400 -1.00478100 0.15844900

G^0 = -289.005336, 0 img. freq.

g17

0 1
C 0.30637900 -0.44477700 0.93500900
H 0.14385800 -1.38527600 1.46899700
H 0.70617800 0.28507900 1.65333700
C -1.05020000 0.03807200 0.41215400
H -1.72067500 -0.01471600 1.28588800
C -1.60884100 -0.88011000 -0.67035900
H -1.71363700 -1.90252900 -0.29615300

H -2.59591300 -0.53529700 -0.99330900
H -0.94809000 -0.89598000 -1.54048600
O 1.28717100 -0.73052400 -0.05804600
N -0.96185900 1.41524900 -0.10962500
H -1.89358900 1.74538000 -0.34917800
H -0.61720100 2.03791000 0.61732800
C 2.05992200 0.38670500 -0.48155900
H 1.46780000 1.09350800 -1.06899100
H 2.49070700 0.91482600 0.37984400
H 2.87264500 -0.00479600 -1.09701500

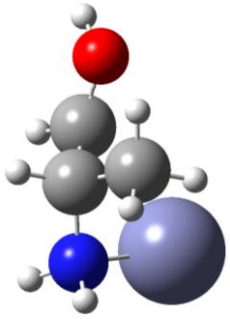
G^0 = -289.004092 hartrees, 0 img. freq.

g18

0 1
C -0.28044900 -0.65657600 0.70295200
H -0.73430600 -0.20063200 1.59017000
H -0.10114000 -1.71421200 0.92894600
C 1.06261200 0.02203700 0.42564000
H 1.59443400 0.00615900 1.39103600
C 0.91889000 1.47599000 -0.01354900
H 0.40368900 2.06561500 0.74935400
H 1.90446000 1.92304200 -0.17599400
H 0.35700900 1.54353000 -0.94847900
O -1.19209600 -0.60799000 -0.39493900
N 1.80324500 -0.72926000 -0.60481000
H 2.72174600 -0.31231300 -0.73395800
H 1.96426600 -1.68193300 -0.28648800
C -2.27898400 0.28867700 -0.21236900
H -2.89752800 -0.00472900 0.64631600
H -1.94296700 1.32152800 -0.06651400
H -2.88803200 0.24191000 -1.11725300

G^0 = -289.002977 hartrees, 0 img. freq.

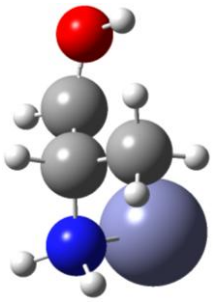
1-Zn^{2+} (gas phase)



a1

2 1
C -1.19700500 -0.71559000 0.52086800
H -1.11349200 -1.16205100 1.51847500
H -0.19408300 -1.22865100 -0.06048400
C -0.91487300 0.80088500 0.44376300
H -1.59536900 1.28075900 1.16195100
C -1.09413000 1.35318000 -0.95580600
H -2.10271400 1.16552500 -1.32446000
H -0.90225600 2.42714100 -0.99453800
H -0.40475100 0.85351600 -1.66711900
O -2.27455700 -1.05875500 -0.18184400
H -2.72577700 -1.85792800 0.13939900
N 0.49284700 1.04299500 0.90053000
H 0.79097700 1.99732200 0.67884900
H 0.62435800 0.92084700 1.91007300
Zn 1.38685600 -0.39527500 -0.20880200

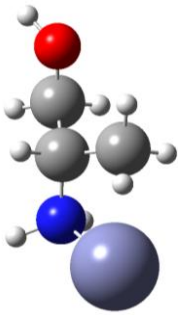
G^0 = -2028.344578 hartrees, 0 img. freq.



a2

2 1
C -1.09839300 -0.80642900 0.46762300
H -0.84926700 -1.27228400 1.42605900
H -0.10393500 -1.17393500 -0.25771500
C -0.98477100 0.74090500 0.46018100
H -1.63260200 1.08145000 1.28075400
C -1.37188800 1.38789400 -0.85618400
H -2.42323000 1.20523000 -1.09111100
H -1.25806900 2.47320000 -0.81023100
H -0.76680400 1.01220500 -1.69486000
O -2.17668800 -1.39679100 -0.02166600
H -2.54781700 -0.99120000 -0.82358900
N 0.42879100 1.09149200 0.82602500
H 0.65203900 2.05342300 0.55435700
H 0.60240600 1.02845900 1.83476600
Zn 1.44898500 -0.32722900 -0.21523300

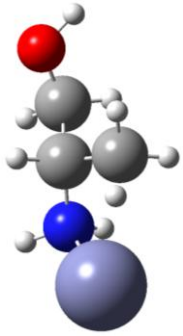
G^0 = -2028.336830 hartrees, 0 img. freq.



a4

2 1
C 2.23504100 -0.56259800 0.30216100
H 2.51187300 -1.56955400 -0.02471200
H 2.12446700 -0.55085400 1.39532700
C 0.86455000 -0.14818900 -0.34511500
H 0.97842400 -0.14863000 -1.42988300
C 0.41123800 1.21735700 0.14679200
H 1.09720300 2.03003100 -0.11642300
H -0.52364500 1.55348200 -0.42608100
H 0.25030700 1.26307800 1.23103800
O 3.11966000 0.42279800 -0.12685100
H 3.98190200 0.06348800 -0.37951100
N -0.22009000 -1.14305900 -0.01205900
H -0.26335600 -1.92814200 -0.67069700
H -0.10406300 -1.55231300 0.92304700
Zn -1.81782400 0.08063400 -0.00086400

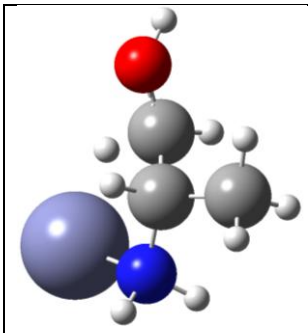
G^0 = -2028.331417 hartrees, 0 img. freq.



a5

2 1
C 2.32280700 -0.55026300 0.29628700
H 2.41905900 -1.60033700 0.00336600
H 2.36594000 -0.45301200 1.38519900
C 0.88221300 -0.06864100 -0.24825900
H 0.95997700 -0.06983200 -1.33669400
C 0.47514900 1.29109700 0.27068400
H 1.11506100 2.10567300 -0.07408500
H -0.53626700 1.56721100 -0.19528300
H 0.37558800 1.34491400 1.35841400
O 3.26553200 0.19204500 -0.38076700
H 3.78191600 0.77105700 0.19816400
N -0.18699800 -1.04041500 0.12424900
H -0.17328100 -1.89311800 -0.44656200
H -0.12252900 -1.34065300 1.10434000
Zn -1.90272500 0.04271600 -0.05775800

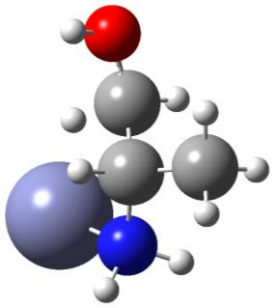
G^0 = -2028.327910 hartrees, 0 img. freq.



a7

2 1
C 0.94192600 -0.87838500 0.34396200
H -0.26954200 -1.25505000 0.18014300
H 1.00661100 -0.87679300 1.43870900
C 1.03470300 0.50698600 -0.33118600
H 1.07528500 0.34010300 -1.41013300
C 2.29290200 1.24139700 0.15533600
H 3.16277900 0.62344300 -0.07957100
H 2.39852000 2.19314900 -0.36787400
H 2.27243400 1.42097300 1.23427500
O 1.70989100 -1.76397500 -0.28349800
H 2.02722200 -2.49383300 0.27581100
N -0.21189800 1.30422400 -0.05349600
H -0.14503800 1.81372500 0.83455000
H -0.35858500 2.01493000 -0.77642300
Zn -1.63275700 -0.13394700 0.01014400

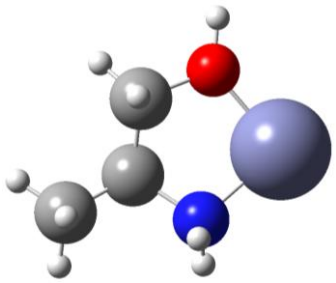
G^0 = -2028.342624 hartrees, 0 img. freq.



a9

2 1
C 0.91502700 -0.87629600 0.30424400
H -0.27019200 -1.26473500 0.02666700
H 0.88288700 -0.84579600 1.39827500
C 1.04126900 0.51722800 -0.35857100
H 1.08114600 0.39975000 -1.44497300
C 2.30122200 1.22401900 0.16493000
H 3.17178900 0.60162300 -0.05611800
H 2.42786700 2.18593200 -0.33457200
H 2.26045800 1.37752400 1.24720100
O 1.74233900 -1.84474500 -0.06627300
H 1.92952000 -1.89236200 -1.01991600
N -0.20270100 1.30730100 -0.05362900
H -0.11888700 1.80229000 0.84129000
H -0.36745300 2.02879300 -0.76179100
Zn -1.63540100 -0.13252900 0.01153000

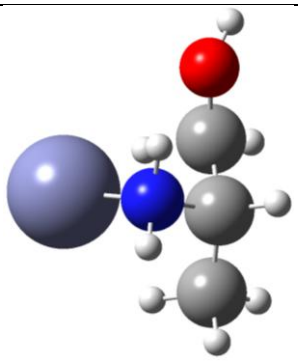
G^0 = -2028.336376 hartrees, 0 img. freq.



g1

2 1
C -0.89017500 1.29367700 0.19476800
H -1.03375700 1.38937800 1.27218200
H -1.39269500 2.10233800 -0.33416500
C -1.35149800 -0.05697500 -0.35944500
H -1.24421300 -0.04877400 -1.44735800
C -2.78464400 -0.37038700 0.04434200
H -3.44837200 0.41099200 -0.33744700
H -3.11544400 -1.31463100 -0.39212300
H -2.90235000 -0.41376100 1.13060500
O 0.57549800 1.42859300 -0.07319800
H 0.90769200 2.34134500 -0.04247100
N -0.39477300 -1.16501600 0.12211800
H -0.62880000 -1.45002900 1.07995000
H -0.51511800 -2.00282800 -0.45442700
Zn 1.38968000 -0.31618500 -0.00073300

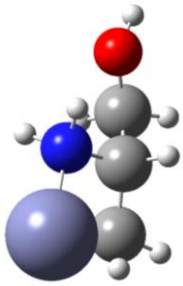
G^0 = -2028.391393 hartrees, 0 img. freq.



g4

2 1
C -1.33682500 -0.42551600 -0.61049100
H -0.27330200 -0.60744500 -1.18946700
H -2.00056100 -0.21026700 -1.45366000
C -1.05248500 0.77670600 0.29586600
H -1.97254800 0.98707400 0.85899100
C -0.55882900 1.99885400 -0.45189000
H -1.28571300 2.33247500 -1.19464500
H -0.35275900 2.83259900 0.22208300
H 0.38240600 1.79090100 -1.00773000
O -1.63075600 -1.52577000 0.12674700
H -2.21830300 -2.15840700 -0.31690300
N 0.00122600 0.31053100 1.25935300
H 0.34284500 1.05869100 1.86997600
H -0.33155400 -0.45902600 1.85277300
Zn 1.28119300 -0.32114700 -0.16239200

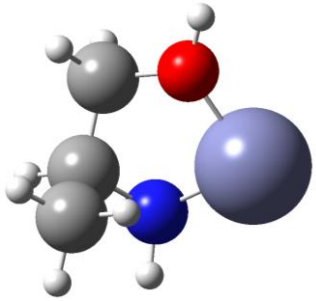
G^0 = -2028.348218 hartrees, 0 img. freq.



g7

```
2 1
C 2.30126400 0.41167200 0.22182400
H 2.26503000 0.57417900 1.30740300
H 2.89172600 1.20915200 -0.23909700
C 0.86588100 0.44471200 -0.35933800
H 0.92634400 0.35377100 -1.44533000
C 0.04254100 1.65392400 0.04543100
H 0.39625200 2.59644300 -0.38578500
H -0.99838400 1.59756200 -0.43431600
H -0.05694100 1.78623200 1.12741900
O 2.75245400 -0.88163500 -0.10475200
H 3.71784500 -0.94393300 -0.10377600
N 0.14883600 -0.80594900 0.12326400
H 0.43657600 -1.63026400 -0.41807200
H 0.38895100 -1.02559400 1.09860100
Zn -1.74290000 -0.22948900 0.00068700
```

G^0 = -2028.335504 hartrees, 0 img. freq.

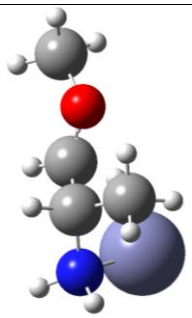


g10

```
2 1
C -1.04316200 -1.25811900 0.53646700
H -1.79105300 -1.89315400 0.06383100
H -0.86972500 -1.56929700 1.56725100
C -1.44212300 0.21974000 0.40335400
H -2.25387500 0.40566900 1.11236500
C -1.85093800 0.62259600 -1.00568100
H -2.71491200 0.03587100 -1.32409500
H -2.13432900 1.67587700 -1.05339400
H -1.05768200 0.44129900 -1.74552200
O 0.23851700 -1.44035400 -0.20613900
H 0.45400300 -2.36348800 -0.41783500
N -0.25398700 1.08882500 0.83860600
H -0.42463000 2.06663800 0.58772600
H -0.11732000 1.07274400 1.85510000
Zn 1.22655500 0.21745300 -0.14904700
```

G^0 = -2028.390269 hartrees, 0 img. freq.

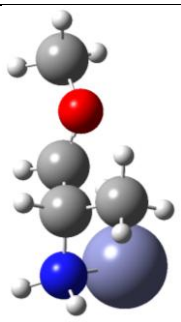
2-Zn^{2+} (gas phase)



a1

```
2 1
C -1.00694900 -0.08647100 0.46714200
H -1.07987400 -0.60972300 1.42999400
H -0.22472600 -0.95457100 -0.18377900
C -0.16151100 1.20770400 0.45398500
H -0.60815900 1.85930100 1.21784100
C -0.13754300 1.88094600 -0.90446700
H -1.14890100 2.11812400 -1.23356000
H 0.44071400 2.80651300 -0.87695500
H 0.30027600 1.21849100 -1.67048900
O -2.11351200 0.00740200 -0.21962700
N 1.23799100 0.88042400 0.88949200
H 1.87254200 1.65089600 0.66435200
H 1.31935800 0.72327800 1.89851000
C -3.23747400 -0.90364100 0.04046500
H -3.25926300 -1.17215500 1.09663700
H -4.12518900 -0.34768400 -0.24958500
H -3.11103600 -1.77679700 -0.60177300
Zn 1.50424300 -0.81096900 -0.21011200
```

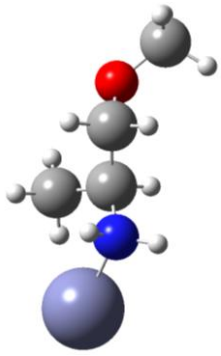
G^0 = -2067.650329 hartrees, 0 img. freq.



a3

```
2 1
C -1.00681400 -0.08639000 0.46732500
H -1.07945100 -0.60985700 1.43007100
H -0.22453100 -0.95469600 -0.18414100
C -0.16154300 1.20788300 0.45403800
H -0.60774100 1.85924400 1.21832400
C -0.13802300 1.88135100 -0.90429500
H -1.14950800 2.11838200 -1.23312600
H 0.44006600 2.80700900 -0.87680900
H 0.29955800 1.21905200 -1.67060300
O -2.11346700 0.00749800 -0.21917000
N 1.23837700 0.88067200 0.88898500
H 1.87274800 1.65089100 0.66247900
H 1.32047900 0.72455500 1.89809500
C -3.23710300 -0.90400800 0.04034600
H -3.25727400 -1.17549700 1.09577400
H -4.12517500 -0.34712700 -0.24682900
H -3.11185300 -1.77538900 -0.60456100
Zn 1.50408900 -0.81114300 -0.21009000
```

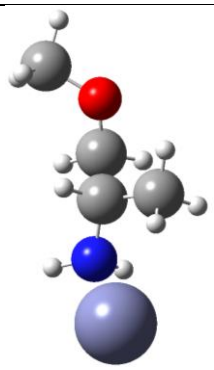
G^0 = -2067.650334 hartrees, 0 img. freq.



a4

2 1
C 1.84049900 -0.41575900 0.62494000
H 2.05336600 -1.47813400 0.46723200
H 1.70909700 -0.20614500 1.69294700
C 0.47833500 -0.01077100 -0.11852400
H 0.66050400 -0.08744600 -1.19113400
C 0.01479100 1.37661200 0.26185200
H 0.72260900 2.15517500 -0.02832600
H -0.91666700 1.62366300 -0.32771500
H -0.19995000 1.48328200 1.32905400
O 2.80073700 0.41348600 0.09197600
N -0.59757500 -0.98508700 0.21521000
H -0.51690300 -1.86887100 -0.29812900
H -0.61220300 -1.22308800 1.21348800
C 3.95158600 -0.18391300 -0.53444200
H 3.63861600 -0.88464200 -1.31871400
H 4.52202400 0.63544100 -0.96184600
H 4.53898800 -0.71984300 0.21888600
Zn -2.38445400 -0.01462300 -0.14803300

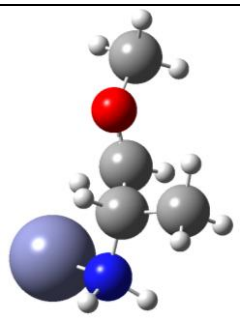
G^0 = -2067.633535 hartrees, 0 img. freq.



a6

2 1
C 1.93318400 -0.37567100 0.75200600
H 2.06265000 -1.45976800 0.68552100
H 1.80361500 -0.03938300 1.78440700
C 0.54343200 0.05144700 -0.03940800
H 0.73097700 -0.14919300 -1.09492100
C 0.18898200 1.49370900 0.21431200
H 0.96862800 2.17442300 -0.12719900
H -0.71972000 1.74101800 -0.38382100
H -0.01935600 1.70352500 1.26681000
O 2.93809900 0.33088200 0.16894500
N -0.54271400 -0.82771400 0.40121500
H -0.45516800 -1.79263800 0.06743100
H -0.63201600 -0.85901200 1.42226500
C 3.82832600 -0.31621600 -0.75755200
H 3.43752200 -0.19926900 -1.77682500
H 4.77020400 0.23000100 -0.69081800
H 3.95757500 -1.36904300 -0.50338400
Zn -2.48580800 -0.06511100 -0.19418900

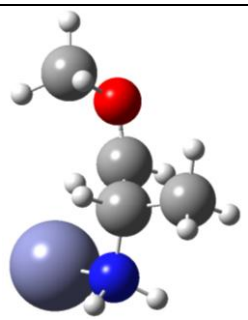
G^0 = -2067.633815 hartrees, 0 img. freq.



a7

2 1
C 0.92417900 -0.14991800 0.22905100
H -0.01984700 -1.10568500 0.05705900
H 1.01056200 -0.20969800 1.32259500
C 0.29107000 1.13774200 -0.34165700
H 0.34538200 1.06975800 -1.43018300
C 1.07275900 2.35589600 0.16842400
H 2.11646800 2.25456900 -0.13684100
H 0.67536000 3.27004400 -0.27577300
H 1.03417700 2.43951600 1.25853900
O 1.96729800 -0.53379800 -0.45307200
N -1.16662700 1.22212000 0.02537500
H -1.29731200 1.65552600 0.94507700
H -1.66994600 1.81662200 -0.63829600
C 2.97928600 -1.41558400 0.14545900
H 2.69150900 -2.44456000 -0.07654700
H 3.90752200 -1.16737000 -0.36273400
H 3.04405700 -1.23063400 1.21765100
Zn -1.70045700 -0.74004600 0.01195800

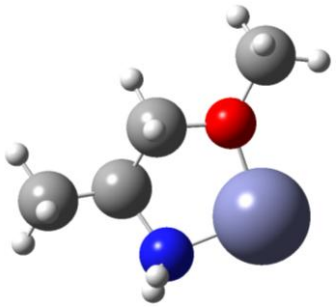
G^0 = -2067.649348 hartrees, 0 img. freq.



a9

2 1
C 0.80153800 -0.26297900 0.67101400
H -0.17124800 -1.08560300 0.39221600
H 0.58508600 -0.01662800 1.71630300
C 0.58318200 0.92759700 -0.30290500
H 0.81066100 0.61671200 -1.32336200
C 1.47812200 2.09556500 0.13716900
H 2.51952300 1.76716600 0.14816600
H 1.38487600 2.92668100 -0.56390900
H 1.22417700 2.44080200 1.14348900
O 1.90033000 -0.97864300 0.61882200
N -0.87050500 1.30380100 -0.28198400
H -1.07487700 1.95981200 0.47910600
H -1.14163800 1.77985800 -1.14630700
C 2.47674200 -1.41076600 -0.64994800
H 2.89209100 -0.55415000 -1.18285100
H 3.26472900 -2.10584100 -0.37659400
H 1.70778900 -1.91606400 -1.24220300
Zn -1.77159300 -0.50689100 -0.00509000

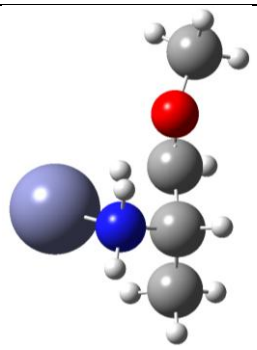
G^0 = -2067.640940 hartrees, 0 img. freq.



g1

2 1
C -0.46446600 1.29838800 0.19055800
H -0.55703200 1.44956700 1.26893000
H -0.59056300 2.24771200 -0.33028800
C -1.47552900 0.28486500 -0.35943100
H -1.37961000 0.24750200 -1.44780800
C -2.89954000 0.63117000 0.04924300
H -3.15534900 1.62540400 -0.32771100
H -3.61238300 -0.07217900 -0.38500700
H -3.01970600 0.64034800 1.13609800
O 0.91325800 0.82767900 -0.08407000
N -1.09971800 -1.13014400 0.11607900
H -1.43864800 -1.29133700 1.07075000
H -1.56174700 -1.83255200 -0.46766100
C 1.98300100 1.86284600 -0.00001700
H 2.91842000 1.36229500 -0.23617500
H 1.75276400 2.62181300 -0.74508200
H 1.99021500 2.26625900 1.01107400
Zn 0.87282700 -1.08129500 0.00102600

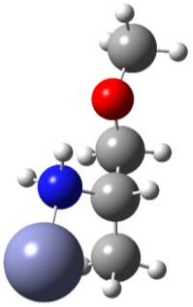
G^0 = -2067.694471 hartrees, 0 img. freq.



g4

2 1
C -0.99229600 0.52954100 -0.44901700
H -0.30618300 -0.37604100 -1.03637600
H -1.41064000 1.02401600 -1.33425900
C 0.07901300 1.33342800 0.30045400
H -0.45082500 2.09381700 0.88857700
C 1.11401800 1.96360300 -0.61324700
H 0.64620000 2.65048400 -1.32033900
H 1.85971500 2.52280200 -0.04484400
H 1.65832700 1.20979100 -1.21488800
O -1.85782800 -0.05217400 0.37416000
N 0.74341700 0.37181100 1.24340200
H 1.54798100 0.78602300 1.72165200
H 0.09584600 0.02909800 1.96127400
C -3.17222900 -0.46430100 -0.13657600
H -3.77635500 -0.64969200 0.74669600
H -3.59392500 0.33850000 -0.74152100
H -3.05010300 -1.38166700 -0.71678400
Zn 1.14225400 -1.02020100 -0.17386600

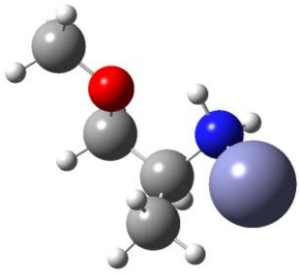
G^0 = -2067.651549 hartrees, 0 img. freq.



g8

2 1
C 1.82607100 0.70816900 0.24151400
H 1.78399200 0.85315100 1.33019300
H 2.35836900 1.55499000 -0.20621800
C 0.39080400 0.61029500 -0.32943600
H 0.45897200 0.48569900 -1.41160200
C -0.50847800 1.77720400 0.02789200
H -0.19818800 2.71742000 -0.43647700
H -1.53400300 1.61592500 -0.42595300
H -0.61214600 1.93939300 1.10453300
O 2.40697000 -0.52597600 -0.09601300
N -0.22376700 -0.66647600 0.19829700
H 0.17113500 -1.48863800 -0.27193300
H -0.02299900 -0.79502700 1.19705000
C 3.84417500 -0.57642100 -0.06052500
H 4.12552200 -1.57675200 -0.37747800
H 4.25578300 0.16813100 -0.75484500
H 4.20710800 -0.36622300 0.95074000
Zn -2.19994600 -0.37834700 -0.01982200

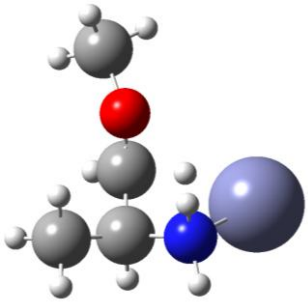
G^0 = -2067.635766 hartrees, 0 img. freq.



g10

2 1
C -1.81506900 0.81298700 0.40913100
H -2.25411900 1.57198400 -0.24765600
H -2.28325500 0.89672400 1.39815200
C -0.28851900 1.02742600 0.55354200
H -0.05972300 1.77891900 1.30900200
C 0.36265000 1.38366300 -0.78427900
H 0.06388500 2.35095400 -1.20371100
H 1.47161100 1.55255100 -0.64477200
H 0.12435000 0.63259100 -1.55524300
O -1.95438800 -0.48522800 -0.12164800
N 0.30452500 -0.29875800 0.99902900
H 0.47133400 -0.35792600 2.00772800
H -0.39004100 -1.02731600 0.73374300
C -3.30799700 -0.87937300 -0.46502900
H -3.70337100 -0.20018900 -1.22551800
H -3.24031100 -1.88949300 -0.85907400
H -3.93947700 -0.85579100 0.42611000
Zn 1.91787200 -0.41827000 -0.14796600

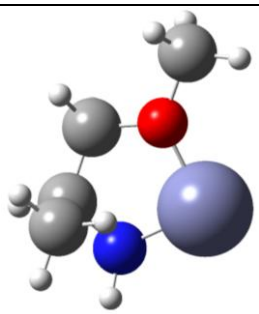
G^0 = -2067.641246 hartrees, 0 img. freq.



g13

2 1
C -0.88992000 -0.16406000 0.67454000
H -1.39392300 -0.29719200 1.63979900
H 0.18694000 -0.87325600 0.95766600
C -0.33884400 1.24597300 0.42037600
H 0.14180400 1.58615800 1.34195900
C -1.44983200 2.22044300 0.00032500
H -2.20546600 2.26661700 0.78718600
H -1.03585200 3.22238200 -0.12375200
H -1.92661600 1.90116800 -0.92737600
O -1.47740900 -0.69554800 -0.38154900
N 0.75126600 1.14675700 -0.62102600
H 0.35336900 1.03642300 -1.56012800
H 1.32633500 1.99331500 -0.64451500
C -2.41751700 -1.81095700 -0.20521300
H -3.00124400 -1.84088600 -1.12080300
H -1.84256600 -2.73240000 -0.08830100
H -3.04885600 -1.62024100 0.66253900
Zn 1.65277200 -0.53511300 0.03783800

G^0 = -2067.649115 hartrees, 0 img. freq.

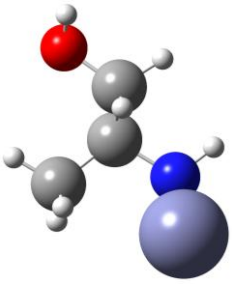


g16

2 1
C 0.18517400 1.35789600 -0.70623000
H 0.38888700 2.36414200 -0.33976900
H 0.41943400 1.29519900 -1.77127400
C -1.27172100 0.98070000 -0.38574300
H -1.91479100 1.54168400 -1.06924400
C -1.66583300 1.23909100 1.06111000
H -1.56119700 2.30143100 1.28953800
H -2.70627100 0.96512500 1.24694100
H -1.03036500 0.69762300 1.77610700
O 1.08863700 0.43278400 0.01000700
N -1.47297400 -0.50900300 -0.69191300
H -2.35899000 -0.83566200 -0.29784600
H -1.51982300 -0.69147800 -1.69946200
C 2.50729500 0.87137700 0.13195700
H 2.50735800 1.80679600 0.68799200
H 3.02606200 0.09305200 0.68551900
H 2.91647300 0.98799500 -0.87010900
Zn 0.16351500 -1.23731800 0.15061300

G^0 = -2067.693348 hartrees, 0 img. freq.

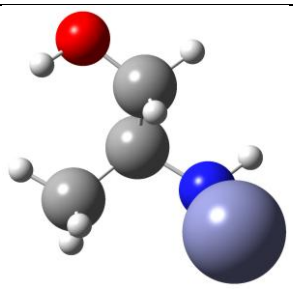
1-Zn^{2+} (implicit MeCN)



a1

2 1
C -1.63214700 -0.80575100 0.08015800
H -1.63580500 -1.52618600 0.90765300
H -1.02078300 -1.21893300 -0.73325000
C -1.02978100 0.50962000 0.55807600
H -1.65914000 0.90866000 1.35905300
C -0.88402200 1.53928000 -0.54994500
H -1.85488800 1.76539100 -0.99163100
H -0.45069700 2.46686700 -0.16775100
H -0.22801500 1.14800000 -1.33918000
O -2.96092700 -0.54287100 -0.36508100
H -3.34401200 -1.37027100 -0.67899200
N 0.31437600 0.21190000 1.13997900
H 0.65734400 1.03406500 1.63740700
H 0.24528000 -0.53418300 1.83285100
Zn 1.73510700 -0.24242100 -0.24717000

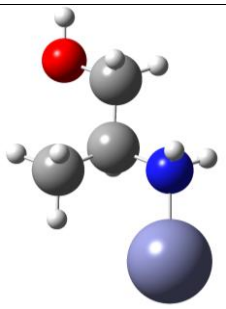
G^0 = -2028.845528 hartrees, 0 img. freq.



a2

2 1
C -1.43121800 -0.82773800 0.26475100
H -1.33667700 -1.38240000 1.20086300
H -0.72824100 -1.26713700 -0.46123800
C -1.04800500 0.63816800 0.49197700
H -1.70118800 1.05930900 1.26165300
C -1.11884700 1.47940200 -0.77258300
H -2.13878100 1.51484900 -1.16100600
H -0.80844100 2.50747300 -0.56917600
H -0.46360100 1.06366800 -1.54684100
O -2.77638500 -0.99270300 -0.16273800
H -2.85203400 -0.68293800 -1.07373300
N 0.35214200 0.65563400 1.01273500
H 0.66453300 1.61818400 1.13863200
H 0.39313900 0.21359000 1.93163300
Zn 1.67686000 -0.30104700 -0.21376300

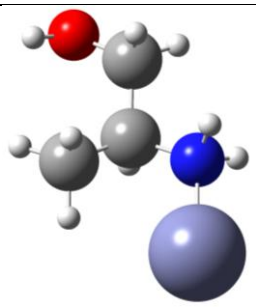
G^0 = -2028.845500 hartrees, 0 img. freq.



a4

2 1
C -2.25770600 0.64041700 0.20780600
H -2.27032900 1.68670300 -0.11967000
H -2.36227200 0.61454800 1.30015600
C -0.93590600 -0.00696300 -0.19615400
H -0.86087900 0.00819300 -1.28536600
C -0.79594400 -1.43042600 0.31707600
H -1.62013600 -2.04770600 -0.04077300
H 0.14170100 -1.87169600 -0.03826700
H -0.79746600 -1.44727500 1.41161400
O -3.30646600 -0.09794300 -0.42222200
H -4.14988000 0.28256200 -0.15063200
N 0.20055700 0.81543000 0.31926300
H 0.16067400 1.76028600 -0.06388100
H 0.12935700 0.90982500 1.33396600
Zn 2.02048000 -0.00126900 -0.10588600

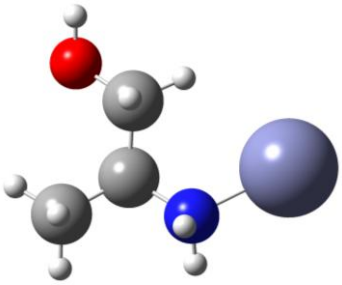
G^0 = -2028.844689 hartrees, 0 img. freq.



a5

2 1
C 2.24463800 -0.65533500 0.23714000
H 2.33198400 -1.68703400 -0.10870400
H 2.17906500 -0.66459400 1.33338700
C 0.97094700 -0.01939800 -0.33629200
H 1.01839300 -0.04653300 -1.42635000
C 0.77268200 1.41210400 0.13861200
H 1.61431800 2.04277100 -0.15479600
H -0.12607700 1.83861800 -0.32071700
H 0.66602200 1.45253800 1.22685700
O 3.42728300 0.01180700 -0.19563000
H 3.48079200 0.86525700 0.25210300
N -0.20313900 -0.86594700 0.05925300
H -0.21307100 -1.72751400 -0.48694300
H -0.09894500 -1.15263800 1.03545600
Zn -2.02594600 0.02073600 -0.01455900

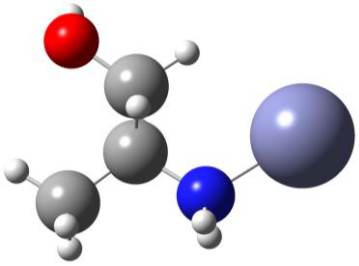
G^0 = -2028.843222 hartrees, 0 img. freq.



a7

2 1
C -1.23204200 0.89539900 0.28731700
H -0.37654000 1.52231400 -0.00552900
H -1.24175500 0.81319800 1.38157700
C -1.07341300 -0.48908000 -0.33171800
H -1.04529500 -0.38191300 -1.41803500
C -2.18214600 -1.45060500 0.07773300
H -3.15472600 -1.05664600 -0.22041700
H -2.04253500 -2.42595200 -0.39531300
H -2.18312300 -1.58713900 1.16437800
O -2.45292700 1.45230300 -0.19417000
H -2.60623000 2.28787100 0.26198400
N 0.25265700 -1.04174900 0.07629100
H 0.20212200 -1.35827500 1.04624400
H 0.46094100 -1.87109900 -0.47901200
Zn 1.89225200 0.19990600 -0.01721800

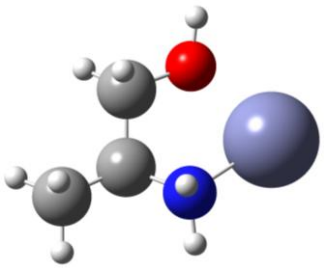
G^0 = -2028.844372 hartrees, 0 img. freq.



a9

2 1
C -1.24280800 0.89225300 0.34157600
H -0.38604300 1.53672900 0.09128200
H -1.27850300 0.77968300 1.42861000
C -1.04162900 -0.47806800 -0.31088900
H -0.93829700 -0.34276000 -1.39082500
C -2.16618300 -1.45904500 -0.01280800
H -3.11641500 -1.06608200 -0.37823500
H -1.97886800 -2.41782400 -0.50346300
H -2.25346800 -1.62834700 1.06522600
O -2.46813800 1.50735000 -0.03617000
H -2.42290200 1.72936700 -0.97490600
N 0.26360400 -1.02367200 0.17112900
H 0.18637500 -1.27057200 1.15946300
H 0.47206700 -1.89200000 -0.32159200
Zn 1.87732200 0.19826200 -0.03971200

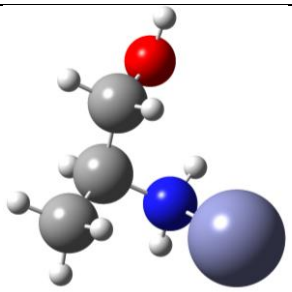
G^0 = -2028.845047 hartrees, 0 img. freq.



g3

2 1
C -1.04899500 1.26165900 0.19488100
H -1.19977700 1.30431100 1.27666300
H -1.67421800 2.00661300 -0.29751900
C -1.36403500 -0.12490000 -0.34312700
H -1.20775500 -0.12602000 -1.42431500
C -2.79130200 -0.53893500 -0.01860500
H -3.50035900 0.16977500 -0.45300700
H -2.99817400 -1.52839400 -0.43267000
H -2.94960900 -0.57282100 1.06308500
O 0.34716100 1.54805000 -0.10609800
H 0.62913500 2.36210600 0.33324300
N -0.36705100 -1.08224700 0.22146100
H -0.55392300 -1.23877200 1.21327300
H -0.44746000 -1.98722700 -0.23912100
Zn 1.49734000 -0.29284000 -0.02466600

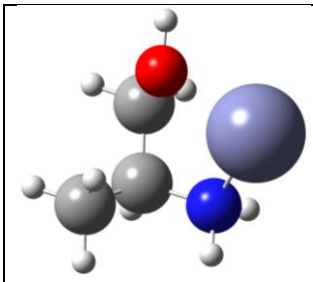
G^0 = -2028.843220 hartrees, 0 img. freq.



g4

2 1
C -1.80437600 -0.21815200 -0.61874200
H -1.08989900 -0.46530800 -1.41517300
H -2.66179400 0.29710200 -1.06272300
C -1.14492900 0.69792500 0.39327600
H -1.86323300 0.91291300 1.19048900
C -0.66218000 1.99272500 -0.23668300
H -1.50579900 2.55769500 -0.63846600
H -0.15334300 2.61617500 0.50232300
H 0.03531500 1.78172400 -1.05515500
O -2.21665700 -1.40318700 0.07212200
H -2.54582300 -2.03937400 -0.57338900
N -0.00053800 -0.03451200 1.01663700
H 0.31521400 0.46311900 1.84894100
H -0.32151800 -0.95284300 1.32615400
Zn 1.63989400 -0.28463700 -0.16811800

G^0 = -2028.849144, 0 img. freq.

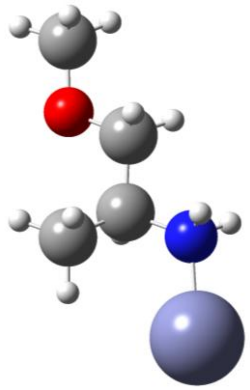


g17

2 1
C 1.17535700 1.11324600 0.64128400
H 2.07043800 1.70864600 0.46128500
H 0.80107500 1.30267200 1.65084900
C 1.46868100 -0.36438600 0.43689000
H 2.18964100 -0.67204400 1.19728700
C 2.02616000 -0.65998500 -0.94857200
H 2.94487100 -0.08759100 -1.09619800
H 2.26372100 -1.72121200 -1.05054600
H 1.31973500 -0.38188200 -1.73411900
O 0.15552700 1.47388500 -0.33063000
H -0.07461900 2.40863500 -0.23906200
N 0.19268300 -1.11731000 0.66310900
H 0.26679200 -2.06539500 0.29677200
H 0.01641900 -1.20645800 1.66360500
Zn -1.41374200 -0.12628400 -0.13080700

G^0 = -2028.842034 hartrees, 0 img. freq.

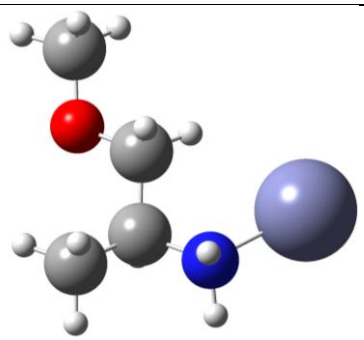
2-Zn^{2+} (implicit MeCN)



a4

2 1
C 1.79896400 -0.49857400 0.19289200
H 1.85092200 -1.54538800 -0.13906800
H 1.87153900 -0.48592800 1.29127700
C 0.46862000 0.11325300 -0.23947000
H 0.40404900 0.08766800 -1.32890500
C 0.27422900 1.53338800 0.26439400
H 1.06528900 2.18129700 -0.11450800
H -0.68949700 1.92943400 -0.07434800
H 0.29767700 1.56110500 1.35840200
O 2.85444000 0.25038900 -0.38078400
N -0.63367100 -0.75345900 0.27482600
H -0.55502300 -1.69366000 -0.11390000
H -0.54545300 -0.85402500 1.28794000
C 4.13086500 -0.25653300 -0.01165700
H 4.25762800 -1.29398100 -0.34743700
H 4.88094300 0.37104500 -0.49407500
H 4.27248000 -0.21714700 1.07616600
Zn -2.51821500 -0.07061700 -0.08386700

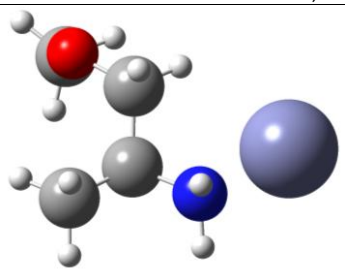
G^0 = -2068.132293 hartrees, 0 img. freq.



a7

2 1
C 1.09769400 -0.27351600 0.16852600
H 0.47602800 -1.11788000 -0.17441800
H 1.09403300 -0.27825100 1.26933500
C 0.50391700 1.03091000 -0.34899700
H 0.48413900 0.99567200 -1.43990000
C 1.27124000 2.25637500 0.13099000
H 2.30978600 2.20291100 -0.19928600
H 0.82684400 3.17349000 -0.26344400
H 1.25972200 2.30440900 1.22513400
O 2.41516700 -0.40154500 -0.32347500
N -0.91882900 1.10890400 0.10201400
H -0.94453800 1.38344900 1.08575500
H -1.39673500 1.85172900 -0.40748800
C 3.04361600 -1.59798600 0.11903900
H 2.52834000 -2.48399600 -0.27412600
H 4.06771900 -1.58279300 -0.25506600
H 3.06033700 -1.65400400 1.21494000
Zn -2.07180000 -0.59464700 -0.01083600

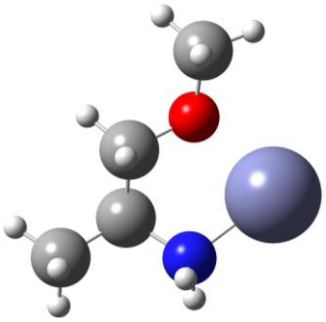
G^0 = -2068.132308 hartrees, 0 img. freq.



a9

2 1
C 1.03253400 -0.29873100 0.70758200
H 0.35858400 -1.16005600 0.56057300
H 0.90792000 0.06228000 1.73273800
C 0.64384600 0.81966300 -0.27028400
H 0.68474200 0.44172600 -1.29327100
C 1.53496200 2.04518700 -0.12918000
H 2.57278300 1.77593600 -0.33623800
H 1.23589800 2.82838000 -0.83022400
H 1.48220700 2.44484900 0.88861400
O 2.37693100 -0.71767700 0.59329300
N -0.78976200 1.16472300 -0.01745100
H -0.87974900 1.62313600 0.89072900
H -1.11157000 1.83678400 -0.71319000
C 2.64625000 -1.46945100 -0.58721400
H 2.61272100 -0.84632900 -1.48759400
H 3.65071500 -1.87984100 -0.47958000
H 1.93020400 -2.29411200 -0.69646000
Zn -2.06923700 -0.46081300 -0.03952400

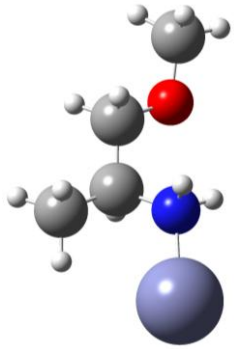
G^0 = -2068.130502 hartrees, 0 img. freq.



g1

2 1
C -0.76409300 1.25823900 0.11404100
H -0.84485100 1.38686100 1.19920800
H -1.14346100 2.15118700 -0.38700800
C -1.52975200 0.03084600 -0.35252300
H -1.43859700 -0.04440400 -1.43804600
C -2.99434400 0.10385100 0.05209900
H -3.46339700 0.98869600 -0.38517800
H -3.53116500 -0.77919000 -0.30146900
H -3.09325300 0.16101300 1.14006400
O 0.62319600 1.08297600 -0.23795700
N -0.85771400 -1.18239500 0.20359300
H -1.07974900 -1.27931200 1.19587200
H -1.20934000 -2.02064900 -0.25646800
C 1.46277400 2.20085400 0.11112700
H 2.47266700 1.95128000 -0.21004700
H 1.11331600 3.09214800 -0.41466800
H 1.44043000 2.36790900 1.19109300
Zn 1.15827700 -0.99751100 -0.01344400

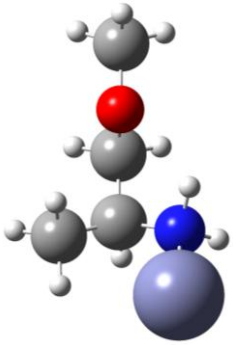
G^0 = -2068.132501, 0 img. freq.



g8

2 1
C 1.90622800 0.64021700 0.08392000
H 1.97702600 0.72889700 1.17837500
H 2.45696500 1.47786900 -0.36321100
C 0.44815700 0.70747400 -0.34219200
H 0.38609500 0.59891400 -1.42685200
C -0.20451800 2.00947700 0.09250600
H 0.31340800 2.86262900 -0.34999100
H -1.24870500 2.03621000 -0.23649300
H -0.18029100 2.11542900 1.18096400
O 2.44845000 -0.60023900 -0.34257900
N -0.29594200 -0.45336700 0.23838600
H 0.09130900 -1.32356900 -0.12658500
H -0.13951300 -0.47930000 1.24846700
C 3.77623400 -0.80159400 0.12597000
H 4.10830200 -1.77135000 -0.24619800
H 4.45092300 -0.02098600 -0.24787400
H 3.81046900 -0.80402000 1.22309700
Zn -2.30328700 -0.42595600 -0.01743300

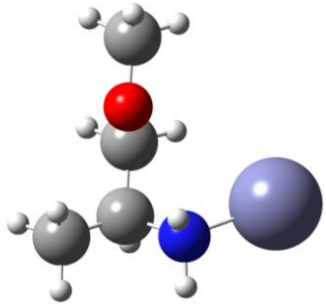
G^0 = -2068.135064 hartrees, 0 img. freq.



g10

2 1
C -1.90933000 0.46844900 0.68932100
H -2.53976600 1.36410600 0.62687600
H -2.11888400 -0.03611700 1.64244200
C -0.44027800 0.87004700 0.60976900
H -0.19879800 1.47418200 1.48523600
C -0.11946600 1.64627300 -0.66121500
H -0.72545100 2.55384000 -0.70638700
H 0.93465800 1.94197400 -0.67087600
H -0.32614400 1.04753500 -1.55058300
O -2.17206600 -0.40999000 -0.39696500
N 0.39866300 -0.37520100 0.69700300
H 0.47096900 -0.67796500 1.66800700
H -0.09864800 -1.12083800 0.20345700
C -3.51255600 -0.88150100 -0.42563500
H -4.22065700 -0.04925300 -0.52370900
H -3.60455200 -1.53431600 -1.29461300
H -3.75304300 -1.45005600 0.48148900
Zn 2.22186600 -0.34087900 -0.14460300

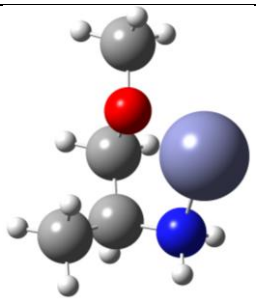
G^0 = -2068.132584 hartrees, 0 img. freq.



g13

2 1
C -1.21544800 -0.15477100 0.77911600
H -2.05087700 -0.03425600 1.48074800
H -0.44731900 -0.77788300 1.26564800
C -0.62998900 1.20852300 0.45318000
H -0.24420100 1.62914000 1.38366500
C -1.63550400 2.16597100 -0.17937500
H -2.48314200 2.31928700 0.49245600
H -1.17070100 3.13572600 -0.37424100
H -2.01095700 1.76349800 -1.12324500
O -1.65018200 -0.77153300 -0.42132800
N 0.54631200 1.03594900 -0.45694800
H 0.21030100 0.78469300 -1.38773600
H 1.02879400 1.92814400 -0.56240300
C -2.19494200 -2.06544100 -0.19883900
H -2.46813800 -2.47491000 -1.17183700
H -1.46051700 -2.72737900 0.27838500
H -3.08898900 -2.01373400 0.43545200
Zn 1.92061000 -0.38458000 0.02426300

G^0 = -2068.134343 hartrees, 0 img. freq.



g16

2 1
C -0.23532000 1.44618900 -0.62831200
H -0.39180600 2.48964000 -0.34737400
H 0.08521800 1.39407900 -1.67390100
C -1.50735900 0.64166400 -0.40358200
H -2.25635700 1.00785900 -1.10930800
C -2.03701800 0.75080900 1.01969000
H -2.25575400 1.79515900 1.25103900
H -2.95805800 0.17385800 1.13053100
H -1.30735300 0.38465000 1.74656000
O 0.80251600 0.88817400 0.20908900
N -1.20352200 -0.78904000 -0.72245200
H -1.96104800 -1.39276500 -0.40792500
H -1.12351100 -0.91785200 -1.73108500
C 2.07153000 1.55743600 0.07592800
H 1.94983400 2.61323300 0.32776900
H 2.75508800 1.08387600 0.77850500
H 2.44893500 1.45710700 -0.94533300
Zn 0.57561200 -1.26825100 0.13275400

G^0 = -2068.131313 hartrees, 0 img. freq.