**Supplementary Materials**

**Structural Investigation, Proton and Electron Affinities, Gas Phase Basicities and Ionization Energies of Captopril**

Samaneh Naderi, Hamed Bahrami\*, Morteza Vahedpour, Mozhgan Sabzehzari

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**S1**

**Conformer 1**

S -3.30250700 0.83406300 -1.22270000

O -0.57809500 -1.38736600 -0.73153200

O 1.97962600 -2.13460800 -0.54446600

O 3.72082800 -0.81407300 -0.13103300

N 0.49813000 0.36132700 0.20462500

C 1.63860100 0.26855800 -0.74361300

C 2.34552400 1.61702500 -0.58456600

C 2.06978100 1.99952700 0.87648300

C 0.62827500 1.53087200 1.10435200

C -0.57965200 -0.44103500 0.07393700

C -1.79718800 -0.19935800 0.96072700

C 2.56101400 -0.93785200 -0.43006700

C -3.08428200 -0.38021000 0.14587600

C -1.76121200 -1.18618800 2.14605200

H 1.23818300 0.11753600 -1.75037900

H 1.89640300 2.34639200 -1.26445300

H 3.40777600 1.53386200 -0.80638400

H 2.75370300 1.45896500 1.53487900

H 2.18410700 3.06699700 1.06995600

H 0.43713400 1.24774800 2.14068700

H -0.09013600 2.30447600 0.81470500

H -1.77956000 0.82205500 1.34506400

H -3.13994900 -1.38570000 -0.26879000

H -3.94778500 -0.23024400 0.79635600

H -0.86432300 -1.04824600 2.75532100

H -2.63176400 -1.03566000 2.78935400

H -1.76996500 -2.21762500 1.78680200

H 1.01994900 -2.02656100 -0.76043400

H -2.46460700 0.23205300 -2.09069300

**Conformer 2**

S -3.17250200 1.06930500 -1.10998700

O -0.46596600 -1.43947000 -0.86473300

O 2.12896000 -2.02915500 -0.67852400

O 3.76849500 -0.63620900 -0.11439200

N 0.47095200 0.29392200 0.23438100

C 1.63119200 0.35401000 -0.69299300

C 2.24202200 1.72914600 -0.41155600

C 1.91455400 1.97366000 1.06823900

C 0.50419200 1.39388200 1.22458400

C -0.55000400 -0.55970200 0.00671400

C -1.81231600 -0.46883600 0.86193700

C 2.62599800 -0.81048100 -0.45351400

C -3.04585800 -0.43403500 -0.05156500

C -1.86979300 -1.68541700 1.80706600

H 1.25664000 0.25940400 -1.71634200

H 1.75651100 2.47872800 -1.04256100

H 3.31140300 1.73458100 -0.61420200

H 2.62133200 1.42744200 1.69722900

H 1.95364500 3.02727000 1.34865100

H 0.31536000 1.01743400 2.23132700

H -0.25917100 2.13917000 0.97839400

H -1.79845900 0.44300000 1.46181000

H -3.00762800 -1.26881300 -0.75186400

H -3.95792400 -0.52624100 0.53903100

H -1.00265200 -1.71285000 2.47211100

H -2.76886800 -1.64268800 2.42700700

H -1.88475200 -2.61428800 1.23344100

H 1.16810800 -1.96598800 -0.90864200

H -3.53200500 1.92282300 -0.12853800

**Conformer 3**

S -4.48917700 0.24442500 -0.24124200

O -0.24882000 -1.53964200 -0.69690300

O 2.18813500 -2.18003000 0.16956200

O 3.88247200 -0.78508900 0.52765500

N 0.71702400 0.42043200 -0.12885500

C 2.01367000 0.06464200 -0.76280900

C 2.74656800 1.40639900 -0.84411000

C 2.22051200 2.17715000 0.37488600

C 0.73807000 1.79150800 0.42916900

C -0.35529600 -0.39946000 -0.21779100

C -1.70102400 0.08649800 0.31435100

C 2.79573300 -0.99747300 0.05413200

C -2.81107200 -0.39716700 -0.63761900

C -1.88818100 -0.43516000 1.75135400

H 1.80977000 -0.36745800 -1.74685400

H 2.47096900 1.91735500 -1.77117100

H 3.82592200 1.26860400 -0.82397400

H 2.73419000 1.83492100 1.27615100

H 2.35727600 3.25640000 0.29404200

H 0.33478600 1.80602200 1.44269200

H 0.13478700 2.46052800 -0.19429500

H -1.71524400 1.17931100 0.33109600

H -2.57899500 -0.14135400 -1.67158400

H -2.89890200 -1.48247700 -0.58961900

H -1.12000700 -0.04454700 2.42347400

H -2.86402100 -0.13169600 2.13350400

H -1.82965600 -1.52622400 1.76790800

H 1.29114300 -2.14388600 -0.24773400

H -4.27254200 1.51713700 -0.63366700

**Conformer 4**

S -4.48917700 0.24442500 -0.24124200

O -0.24882000 -1.53964200 -0.69690300

O 2.18813500 -2.18003000 0.16956200

O 3.88247200 -0.78508900 0.52765500

N 0.71702400 0.42043200 -0.12885500

C 2.01367000 0.06464200 -0.76280900

C 2.74656800 1.40639900 -0.84411000

C 2.22051200 2.17715000 0.37488600

C 0.73807000 1.79150800 0.42916900

C -0.35529600 -0.39946000 -0.21779100

C -1.70102400 0.08649800 0.31435100

C 2.79573300 -0.99747300 0.05413200

C -2.81107200 -0.39716700 -0.63761900

C -1.88818100 -0.43516000 1.75135400

H 1.80977000 -0.36745800 -1.74685400

H 2.47096900 1.91735500 -1.77117100

H 3.82592200 1.26860400 -0.82397400

H 2.73419000 1.83492100 1.27615100

H 2.35727600 3.25640000 0.29404200

H 0.33478600 1.80602200 1.44269200

H 0.13478700 2.46052800 -0.19429500

H -1.71524400 1.17931100 0.33109600

H -2.57899500 -0.14135400 -1.67158400

H -2.89890200 -1.48247700 -0.58961900

H -1.12000700 -0.04454700 2.42347400

H -2.86402100 -0.13169600 2.13350400

H -1.82965600 -1.52622400 1.76790800

H 1.29114300 -2.14388600 -0.24773400

H -4.27254200 1.51713700 -0.63366700

**Conformer 5**

S -3.51853100 0.53616200 -1.24035900

O -0.58862100 -1.34683500 -0.76352800

O 3.23798600 -1.46249400 -1.20657400

O 2.48994700 -1.32778000 0.91129300

N 0.45889300 0.46677300 0.07452700

C 1.63054900 0.22547700 -0.76060000

C 2.40999700 1.55629800 -0.67065700

C 2.06703000 2.07266100 0.73509700

C 0.59945100 1.66132500 0.92808500

C -0.60264700 -0.38549300 -0.00032900

C -1.79200100 -0.12404200 0.92617700

C 2.46415900 -0.93960600 -0.22789500

C -3.10357300 -0.49633700 0.22858200

C -1.61188200 -0.95787800 2.21227700

H 1.33315200 -0.01799500 -1.78037500

H 2.02943200 2.23687600 -1.43675800

H 3.47999100 1.42840100 -0.83861000

H 2.69213000 1.57708000 1.48130500

H 2.20800100 3.14985400 0.83705000

H 0.37600000 1.43168800 1.97139600

H -0.08358500 2.44968100 0.59315600

H -1.83227000 0.93592400 1.18835900

H -3.09014300 -1.54166000 -0.07719700

H -3.93853000 -0.35061400 0.91665100

H -0.68177200 -0.70718300 2.72798100

H -2.44218600 -0.78063800 2.90113900

H -1.58131000 -2.02352000 1.97324400

H 3.76101200 -2.17683700 -0.81205500

H -2.62666300 -0.03462300 -2.07517100

**Conformer 6**

S -3.43745100 0.82490000 -1.12658900

O -0.46703100 -1.32231100 -0.96568600

O 3.30732700 -1.15406900 -1.39100000

O 2.56925500 -1.37229300 0.72318600

N 0.43906400 0.41802200 0.14461800

C 1.63164200 0.37581100 -0.69477200

C 2.34204700 1.70961900 -0.37025800

C 1.94491500 1.97511800 1.09017800

C 0.49510500 1.47525000 1.16979900

C -0.56336800 -0.47728900 -0.08276900

C -1.79442100 -0.43027200 0.82849100

C 2.51773700 -0.81925500 -0.34505700

C -3.06707800 -0.59417600 -0.00903700

C -1.67981800 -1.56276200 1.86916000

H 1.35828800 0.29201600 -1.74641800

H 1.94396600 2.48692100 -1.02767900

H 3.42040400 1.65968400 -0.52586600

H 2.57510300 1.38937500 1.76317700

H 2.03410800 3.02616800 1.36990200

H 0.25514200 1.08169100 2.15921100

H -0.21548900 2.27508100 0.93241800

H -1.84287000 0.52708200 1.35257400

H -2.95750400 -1.45180100 -0.67331600

H -3.93142100 -0.76567000 0.63364500

H -0.77187700 -1.46078100 2.46893400

H -2.53911300 -1.55056300 2.54509200

H -1.64200500 -2.53382200 1.37042700

H 3.86207800 -1.89705500 -1.10874700

H -3.86000500 1.67424200 -0.16666900

**Conformer 7**

S -3.43745100 0.82490000 -1.12658900

O -0.46703100 -1.32231100 -0.96568600

O 3.30732700 -1.15406900 -1.39100000

O 2.56925500 -1.37229300 0.72318600

N 0.43906400 0.41802200 0.14461800

C 1.63164200 0.37581100 -0.69477200

C 2.34204700 1.70961900 -0.37025800

C 1.94491500 1.97511800 1.09017800

C 0.49510500 1.47525000 1.16979900

C -0.56336800 -0.47728900 -0.08276900

C -1.79442100 -0.43027200 0.82849100

C 2.51773700 -0.81925500 -0.34505700

C -3.06707800 -0.59417600 -0.00903700

C -1.67981800 -1.56276200 1.86916000

H 1.35828800 0.29201600 -1.74641800

H 1.94396600 2.48692100 -1.02767900

H 3.42040400 1.65968400 -0.52586600

H 2.57510300 1.38937500 1.76317700

H 2.03410800 3.02616800 1.36990200

H 0.25514200 1.08169100 2.15921100

H -0.21548900 2.27508100 0.93241800

H -1.84287000 0.52708200 1.35257400

H -2.95750400 -1.45180100 -0.67331600

H -3.93142100 -0.76567000 0.63364500

H -0.77187700 -1.46078100 2.46893400

H -2.53911300 -1.55056300 2.54509200

H -1.64200500 -2.53382200 1.37042700

H 3.86207800 -1.89705500 -1.10874700

H -3.86000500 1.67424200 -0.16666900

**Conformer 8**

S -3.95882800 -0.70463400 -0.26654100

O -0.73797800 -1.11629300 -0.53770700

O 1.41793000 -2.31268000 0.49223600

O 3.44734700 -1.42671700 0.69756900

N 0.75400800 0.53529700 -0.18570000

C 1.87952400 -0.26265700 -0.74029700

C 2.96669600 0.78460600 -0.99369500

C 2.71122100 1.83936600 0.09204200

C 1.18206500 1.90696000 0.17202800

C -0.51269200 0.05829600 -0.19996700

C -1.64377400 0.98482000 0.23639500

C 2.33815400 -1.38111400 0.23134800

C -2.91486400 0.76989900 -0.61381300

C -1.88541600 0.84761100 1.75170600

H 1.53805900 -0.74937500 -1.65847900

H 2.83262700 1.21670300 -1.98953400

H 3.96012200 0.34470700 -0.93035500

H 3.12648700 1.49825500 1.04313500

H 3.14868200 2.81124400 -0.14069900

H 0.82390800 2.18174600 1.16488500

H 0.78247300 2.62523400 -0.55233000

H -1.33498300 2.01609300 0.03655100

H -3.58788400 1.61179900 -0.43732900

H -2.66118000 0.77575400 -1.67508400

H -0.99096800 1.10726000 2.32317000

H -2.69297000 1.51496000 2.06303100

H -2.17567700 -0.17160900 2.00672100

H 0.56553300 -2.07980900 0.04844700

H -3.01491200 -1.61709900 -0.56883300

**Conformer 9**

S -4.49010800 0.12951200 -0.22433800

O -0.22902900 -1.42432100 -0.82038500

O 2.13323800 -2.27146100 0.01794100

O 3.82698100 -0.98848200 0.66898700

N 0.76247200 0.43520500 -0.01829600

C 2.07530500 0.07964800 -0.62564700

C 2.89599100 1.38096000 -0.56013500

C 1.87548700 2.48935300 -0.25581200

C 0.82857800 1.77155600 0.59795400

C -0.33154600 -0.33304700 -0.23703800

C -1.69311700 0.13284600 0.27775200

C 2.77240900 -1.10410000 0.09926400

C -2.80118400 -0.51692100 -0.56935700

C -1.81910800 -0.21454200 1.77353600

H 1.88432700 -0.24107700 -1.65456500

H 3.44355100 1.55205100 -1.48737100

H 3.62903400 1.29047700 0.24285700

H 2.32041700 3.34050600 0.26210500

H 1.40912900 2.85784800 -1.17434500

H 1.16080800 1.68540600 1.63864400

H -0.14418500 2.25833600 0.58979100

H -1.77378000 1.21756100 0.16242500

H -2.59684300 -0.40737800 -1.63341200

H -2.85696900 -1.58638000 -0.36636800

H -1.06637000 0.30033100 2.37448300

H -2.80536700 0.07533900 2.13944200

H -1.69537600 -1.29027300 1.92435800

H 1.25501300 -2.14396900 -0.42217900

H -4.32536500 1.33218700 -0.81382700

**Conformer 10**

S -3.75046700 -0.32883000 -0.99927300

O -0.65349700 -1.32240900 -0.22181300

O 1.78557500 -2.28662600 0.28451100

O 3.69301800 -1.14416900 0.23712100

N 0.66088500 0.48701000 0.06262900

C 1.75420000 -0.08819200 -0.76532300

C 2.63644700 1.12261900 -1.07861400

C 2.46870700 2.01707900 0.15704800

C 0.98726500 1.85852700 0.51990800

C -0.51972500 -0.16031700 0.19884200

C -1.69479200 0.56186800 0.84995900

C 2.51931800 -1.21453500 -0.02259000

C -2.71559800 0.98826800 -0.23582700

C -2.30425300 -0.28900700 1.97148500

H 1.31067200 -0.53234300 -1.66091600

H 2.26020900 1.62571100 -1.97397500

H 3.66965800 0.82553500 -1.24816700

H 3.09809300 1.64432000 0.96821100

H 2.73217700 3.05959800 -0.02659200

H 0.80698600 1.96509400 1.59059000

H 0.36959200 2.58955600 -0.01232000

H -1.33689800 1.49772400 1.28612900

H -3.44301000 1.66235100 0.22152400

H -2.21068000 1.54649900 -1.02748600

H -1.57409200 -0.46046000 2.76665800

H -3.16641500 0.22445100 2.40467900

H -2.63432300 -1.25491000 1.59219500

H 0.84287700 -2.13888100 0.02376700

H -2.73373600 -1.15427600 -1.32221100

**Conformer 11**

S -4.23527000 0.65253700 -0.12460300

O 0.02156800 -1.59588300 -0.84851000

O 2.54006300 -2.05494200 -0.20129800

O 3.98114700 -0.54994500 0.57004500

N 0.67404200 0.33018700 0.13056400

C 2.00347000 0.30168900 -0.54320800

C 2.57044600 1.71589900 -0.33627000

C 1.35787200 2.58056500 0.03454700

C 0.47103300 1.61724800 0.82691900

C -0.25390100 -0.62072700 -0.13248700

C -1.66335700 -0.47528800 0.44416300

C 2.94350500 -0.80261100 0.01371900

C -2.55580400 0.12861300 -0.66379300

C -2.16794200 -1.83566500 0.93885900

H 1.83138700 0.07501800 -1.60067600

H 3.09147000 2.06993600 -1.22622200

H 3.29591400 1.68620500 0.47821600

H 1.63003600 3.46330800 0.61533300

H 0.82633300 2.91645900 -0.86094200

H 0.80346200 1.53643300 1.86766300

H -0.57747000 1.90664000 0.82171900

H -1.65069200 0.21674700 1.28744200

H -2.11383400 1.04808100 -1.05492000

H -2.64463800 -0.56680800 -1.49926500

H -1.50501400 -2.24007100 1.70714800

H -3.16156300 -1.73160100 1.37882800

H -2.20881500 -2.55538000 0.11963600

H 1.63201000 -2.05238100 -0.59688000

H -4.77672000 -0.57667000 -0.01397300

**Conformer 12**

S -4.50932200 0.21880300 -0.29787400

O -0.21917400 -1.51288600 -0.78392600

O 3.54782100 -1.70606000 -0.44905900

O 2.42450100 -1.04719400 1.38599600

N 0.68238300 0.48599400 -0.25524400

C 1.99184000 0.06263200 -0.74083000

C 2.79873300 1.38022400 -0.77656600

C 2.18866400 2.20000000 0.37082900

C 0.69559200 1.84316800 0.32209900

C -0.36458800 -0.38938800 -0.31383000

C -1.71201100 0.07471200 0.24594600

C 2.63669400 -0.95046600 0.20491600

C -2.82947300 -0.43259600 -0.68135700

C -1.85083400 -0.44412300 1.68818300

H 1.90741200 -0.40434900 -1.72186300

H 2.62691800 1.87079800 -1.73839700

H 3.87216800 1.21767600 -0.67224400

H 2.61333800 1.88347400 1.32595800

H 2.35876400 3.27243200 0.26283000

H 0.24123900 1.85632800 1.31405900

H 0.14152900 2.53781500 -0.31960700

H -1.75507600 1.16665500 0.25825100

H -2.64635100 -0.10253000 -1.70550400

H -2.85505400 -1.52088700 -0.69693300

H -1.02468100 -0.10206600 2.31624900

H -2.78164300 -0.08887400 2.13501000

H -1.84561400 -1.53709800 1.69976100

H 3.94189700 -2.31022200 0.19842000

H -4.77526500 -0.57781000 0.75628700

**Conformer 13**

S -4.29040700 0.51082300 -0.16791000

O 0.00995900 -1.58088500 -0.85002400

O 2.52427000 -2.06391700 -0.20131200

O 3.97502300 -0.56942000 0.57222500

N 0.67753800 0.33881100 0.12948400

C 2.00634300 0.29657500 -0.54531500

C 2.58663400 1.70569600 -0.34226600

C 1.38129200 2.58320900 0.02099400

C 0.48386800 1.63190900 0.81631100

C -0.25806000 -0.60575400 -0.13185000

C -1.66631200 -0.45802900 0.44897900

C 2.93665000 -0.81471500 0.01391800

C -2.56921600 0.10155800 -0.67386300

C -2.15627100 -1.80784800 0.98669600

H 1.83123100 0.06921900 -1.60212300

H 3.11380300 2.05109200 -1.23198700

H 3.30925000 1.67234900 0.47462600

H 1.66009000 3.46658100 0.59774800

H 0.85492600 2.91876900 -0.87764800

H 0.81065600 1.55613200 1.85924400

H -0.56205000 1.93051300 0.80313100

H -1.65129500 0.25870900 1.27236200

H -2.12866300 0.98891800 -1.13229300

H -2.67892500 -0.64687900 -1.46087000

H -1.51861200 -2.15608600 1.80273600

H -3.17509300 -1.70944000 1.36409500

H -2.13821000 -2.56246300 0.19892700

H 1.61680400 -2.05469900 -0.59771800

H -3.98375900 1.59061800 0.58120700

**Conformer 14**

S -4.52444200 0.10829000 -0.23064500

O -0.21807900 -1.52467700 -0.76275400

O 3.54163500 -1.71093500 -0.44303900

O 2.43238400 -1.02758300 1.39183600

N 0.67833100 0.48329800 -0.26094300

C 1.98796300 0.05805500 -0.74481500

C 2.79249000 1.37667900 -0.79240300

C 2.18193800 2.20513500 0.34854000

C 0.68940300 1.84578000 0.30269000

C -0.36607600 -0.39636100 -0.30608100

C -1.71486000 0.06847000 0.25024700

C 2.63660400 -0.94574000 0.20835000

C -2.83275300 -0.48624600 -0.64922000

C -1.84128900 -0.40359200 1.70997500

H 1.90289300 -0.41715000 -1.72183000

H 2.61939500 1.85900800 -1.75820900

H 3.86628000 1.21692900 -0.68734200

H 2.60686100 1.89646100 1.30608600

H 2.35090700 3.27689100 0.23204100

H 0.23416300 1.86832800 1.29403000

H 0.13548700 2.53377500 -0.34675400

H -1.76553800 1.16100800 0.22530600

H -2.63834000 -0.26056000 -1.69785700

H -2.87991000 -1.57175200 -0.56101200

H -1.05560200 0.02268400 2.33829700

H -2.80948600 -0.10939900 2.11863500

H -1.75493000 -1.49185500 1.76080100

H 3.93849200 -2.30871100 0.20867600

H -4.35595600 1.38109100 -0.64599600

**Conformer 15**

S -3.36952400 1.02769200 -0.97493700

O -0.45346100 -1.24295300 -1.12270700

O 2.46427400 -1.42613700 0.56914700

O 3.40606100 -0.98371000 -1.42353800

N 0.44713100 0.36234800 0.17957100

C 1.62256900 0.45800700 -0.68473300

C 2.29508400 1.77157200 -0.22650900

C 1.91178200 1.87394200 1.25756100

C 0.48101200 1.31855800 1.30116100

C -0.55136300 -0.50557500 -0.14823900

C -1.78409400 -0.57495700 0.76047800

C 2.58286300 -0.72648900 -0.58334000

C -3.05504300 -0.56279400 -0.09718800

C -1.70708100 -1.86590200 1.59960700

H 1.32254800 0.49302200 -1.73221900

H 1.86258600 2.60052200 -0.79259400

H 3.37079600 1.77126000 -0.40384000

H 2.57255100 1.24949200 1.86386500

H 1.96753600 2.89397600 1.64109300

H 0.26394300 0.82457900 2.25032700

H -0.25752100 2.11311000 1.14665600

H -1.81145300 0.28257400 1.43648000

H -2.96554000 -1.30698500 -0.88904800

H -3.92997600 -0.80708500 0.50645000

H -0.80627200 -1.88191500 2.21875000

H -2.57484400 -1.94688100 2.25971500

H -1.68144900 -2.74150500 0.94724800

H 3.11118200 -2.14688500 0.52601600

H -3.77099000 1.72744900 0.10709000

**Conformer 16**

S -2.89229700 1.10034300 -1.02349200

O -1.03891200 -1.88171400 -0.94367100

O 1.20607800 1.83110400 -0.91643600

O 1.29853400 2.45614500 1.24306900

N 0.77991800 -0.81217100 -0.15125800

C 1.49909400 0.10472900 0.73207600

C 2.97558800 -0.32317000 0.54504500

C 3.02881800 -0.82679000 -0.90568300

C 1.66531800 -1.49775500 -1.11290500

C -0.55830500 -1.08145000 -0.14848900

C -1.43380700 -0.39994600 0.91102700

C 1.31284300 1.58882200 0.40604000

C -2.83264700 -0.12622000 0.34909900

C -1.52566500 -1.31845000 2.14820400

H 1.19155700 -0.00632100 1.77174300

H 3.18658900 -1.13747700 1.24324300

H 3.67377800 0.48770400 0.75757500

H 3.14282600 0.01384600 -1.59289900

H 3.85731800 -1.51608700 -1.07571200

H 1.27746400 -1.38515400 -2.12591100

H 1.68789100 -2.56865600 -0.88750000

H -0.99847100 0.55579100 1.21157900

H -3.29294400 -1.05182900 0.00595100

H -3.46217800 0.30201000 1.13140100

H -0.54191400 -1.50480100 2.58762600

H -2.15353800 -0.86130800 2.91731300

H -1.95977300 -2.28352200 1.87581000

H 1.07105300 2.78479700 -1.02850300

H -2.37536700 0.28780700 -1.96721200

**Conformer 17**

S -2.95948000 1.12507800 -1.00533600

O -1.08769300 -1.91379500 -0.88504100

O 1.50197800 2.46120000 1.12631400

O 1.30616900 1.86249400 -1.03597000

N 0.74473600 -0.82524100 -0.15547700

C 1.47926600 0.12776700 0.66893100

C 2.93609200 -0.38949600 0.57424100

C 3.01164500 -0.96999200 -0.84682300

C 1.62080400 -1.57793000 -1.07510200

C -0.59593500 -1.08069300 -0.13229400

C -1.45848900 -0.35381900 0.90899000

C 1.40029800 1.55559000 0.12225500

C -2.86640100 -0.10878600 0.35668500

C -1.52683200 -1.22158200 2.18410000

H 1.12944200 0.13258800 1.70068700

H 3.07119800 -1.17445600 1.32311800

H 3.67175400 0.39213100 0.77023300

H 3.19563600 -0.17226200 -1.56902700

H 3.80672800 -1.70984400 -0.95111100

H 1.26983300 -1.47056700 -2.10203100

H 1.58002400 -2.64174600 -0.82204200

H -1.02107900 0.61528300 1.16035000

H -3.30661700 -1.04479100 0.01518500

H -3.50070900 0.30352300 1.14392400

H -0.53451400 -1.39425700 2.60996000

H -2.13846300 -0.73289600 2.94699800

H -1.96829500 -2.19544000 1.95909300

H 1.48560300 3.34363100 0.72430900

H -2.36834400 0.35900000 -1.94425600

**Conformer 18**

S -4.18495900 0.59450400 0.00723200

O 0.05445900 -1.62011200 -0.86170200

O 2.57431400 -2.02837800 -0.18039100

O 3.97365100 -0.49273300 0.60688300

N 0.65691000 0.32202800 0.11810400

C 1.99598400 0.31665700 -0.53687400

C 2.53267700 1.74194600 -0.32668300

C 1.29703800 2.58544100 0.01489100

C 0.41462200 1.61125100 0.79886400

C -0.24839100 -0.64754600 -0.15461800

C -1.66604700 -0.52710800 0.40920100

C 2.94924500 -0.76750500 0.03673700

C -2.55641300 0.07533100 -0.69803700

C -2.16177800 -1.89781600 0.88928800

H 1.84337900 0.08374500 -1.59604700

H 3.06510300 2.10080600 -1.20793300

H 3.24201700 1.73008900 0.50234800

H 1.54094800 3.47784500 0.59344900

H 0.77559900 2.90384300 -0.89283500

H 0.72895200 1.54619700 1.84629500

H -0.63901200 1.87995700 0.77048100

H -1.65857100 0.15873100 1.25907100

H -2.08227200 0.95400000 -1.13880600

H -2.71655000 -0.66562500 -1.48197000

H -1.52461100 -2.28102300 1.68972600

H -3.18099600 -1.82109100 1.27147200

H -2.14452300 -2.61838900 0.07060800

H 1.67205600 -2.04580600 -0.58798800

H -4.72156800 1.01633600 -1.15524900

**Conformer 19**

S -4.46125100 0.22740500 -0.18359500

O -0.21881100 -1.53730400 -0.76622500

O 3.55634300 -1.70290000 -0.40716000

O 2.42519500 -1.01060100 1.41085100

N 0.67487500 0.47279200 -0.26760100

C 1.98745000 0.04630800 -0.74180000

C 2.78595700 1.36768600 -0.81008300

C 2.16727800 2.21390500 0.31338700

C 0.67672600 1.84642400 0.26920900

C -0.36885000 -0.40654700 -0.31678800

C -1.71828100 0.06380500 0.23370500

C 2.63849900 -0.93934500 0.22830500

C -2.83275500 -0.51919900 -0.64731800

C -1.83213400 -0.37286600 1.70805000

H 1.90641200 -0.44520400 -1.71110000

H 2.61412200 1.83167400 -1.78501800

H 3.86006700 1.21487100 -0.69835200

H 2.59060000 1.92557400 1.27801000

H 2.33096500 3.28414700 0.17743900

H 0.21781600 1.88615500 1.25827500

H 0.12128300 2.51802400 -0.39553500

H -1.77392800 1.15513700 0.17960400

H -2.63727700 -0.29363000 -1.69571400

H -2.87695800 -1.60029600 -0.52639700

H -1.02010500 0.04244900 2.30954800

H -2.78002100 -0.04548000 2.13863600

H -1.77757800 -1.46171300 1.78062200

H 3.95422300 -2.28884200 0.25457700

H -5.19888700 -0.46547800 -1.07360900

**Conformer 20**

S -3.92581900 -0.85937500 -0.19329000

O -0.71826800 -1.12015000 -0.62439400

O 2.84540200 -2.32482400 -0.12631300

O 1.98006100 -1.11928800 1.56549300

N 0.71544600 0.58836000 -0.32274100

C 1.84233200 -0.25534600 -0.71017400

C 2.98905900 0.75799200 -0.92474200

C 2.65436000 1.88704200 0.06195100

C 1.12145300 1.96382700 0.01890300

C -0.54139800 0.05279800 -0.30585300

C -1.68936600 0.96352300 0.13547300

C 2.19275500 -1.25812500 0.38905300

C -2.98481500 0.65821400 -0.64350400

C -1.86315600 0.89962300 1.66434900

H 1.60859600 -0.82025400 -1.61232300

H 2.94967300 1.11985400 -1.95566500

H 3.97359000 0.31719200 -0.76389500

H 2.98330700 1.61795800 1.06815100

H 3.12122900 2.83652100 -0.20505600

H 0.70123100 2.27575200 0.97577300

H 0.78210600 2.66580000 -0.75205000

H -1.42713900 1.99346500 -0.13293600

H -3.69485200 1.46949700 -0.46769200

H -2.77851200 0.63139800 -1.71465000

H -0.95142600 1.20360700 2.18350100

H -2.67389100 1.56252500 1.97860800

H -2.11444100 -0.11270000 1.98124400

H 3.06572200 -2.91407600 0.61110600

H -2.92510800 -1.71823900 -0.47332300

**Conformer 21**

S -3.60246100 0.99161400 -0.29042100

O -0.33681200 -2.44387000 -0.64966100

O 1.24365700 2.75025500 0.68648600

O 0.70865500 1.68737700 -1.22375200

N 1.09599400 -0.83969100 0.02299700

C 1.49394800 0.39193000 0.69404300

C 3.03620000 0.26341100 0.78109200

C 3.39220000 -0.54754600 -0.47325900

C 2.23589100 -1.54482800 -0.59609100

C -0.16052600 -1.37060900 -0.08616800

C -1.34928900 -0.59047800 0.48880800

C 1.09416200 1.64729400 -0.08491200

C -2.23026400 -0.16394200 -0.70419000

C -2.09414900 -1.47243600 1.50048400

H 1.06154500 0.47519800 1.69299500

H 3.28612600 -0.29746200 1.68543100

H 3.53073200 1.23315400 0.84053700

H 3.42201300 0.10447500 -1.35015300

H 4.36078100 -1.04287400 -0.39078900

H 1.99414800 -1.80911000 -1.62579400

H 2.43225600 -2.47612400 -0.05480400

H -1.01597600 0.31763200 0.99539300

H -1.63106000 0.38986900 -1.42858400

H -2.63415400 -1.04088300 -1.20945000

H -1.44213000 -1.75353300 2.33207800

H -2.95142600 -0.93948400 1.91690400

H -2.43948800 -2.39009100 1.01991900

H 0.98936400 3.51828000 0.15220200

H -4.42833900 0.09608900 0.28644600

**Conformer 22**

S -3.57964800 0.03546700 -1.15908500

O -0.51975700 -1.35698900 -0.47086700

O 1.93770500 -2.29957900 -0.22639500

O 3.75323500 -1.09077800 0.19557100

N 0.65412800 0.41902400 0.27303000

C 1.80899400 0.10718500 -0.61679300

C 2.66560500 1.38424200 -0.59916500

C 1.73115100 2.48275300 -0.07510700

C 0.83674100 1.73565500 0.91749500

C -0.47186100 -0.33268500 0.23035000

C -1.69419300 0.09478400 1.04144600

C 2.60446600 -1.14686200 -0.16071800

C -2.65363200 0.93024400 0.15778700

C -2.36381800 -1.12031900 1.69368400

H 1.40894200 -0.10884800 -1.61287900

H 3.07222600 1.60431300 -1.58658500

H 3.50859000 1.23029500 0.07615800

H 2.26995600 3.30732800 0.39436500

H 1.11795800 2.89511500 -0.88197000

H 1.33429900 1.61313100 1.88594900

H -0.11807300 2.23049200 1.07952300

H -1.36684400 0.76613100 1.83992000

H -3.43753200 1.34789800 0.79315900

H -2.12115100 1.76940400 -0.29513100

H -1.67742200 -1.61139400 2.38758400

H -3.24675200 -0.80174000 2.25381300

H -2.67229500 -1.84694900 0.94419800

H 0.99242400 -2.12806500 -0.46444700

H -2.51903500 -0.59895500 -1.69984500

**Conformer 23**

S -3.90565200 0.76306000 -0.20918500

O -0.48509600 -2.33517700 -0.69166500

O 1.49411600 2.75780400 0.52023100

O 1.04458200 1.66511100 -1.39584800

N 1.04793400 -0.82648900 -0.01892200

C 1.51213000 0.38839400 0.63645400

C 3.02086900 0.11152600 0.85790300

C 3.39360400 -0.77214100 -0.34183500

C 2.15410800 -1.65125000 -0.54317500

C -0.24123000 -1.26123000 -0.15575300

C -1.37223100 -0.39077200 0.40552200

C 1.31118700 1.63884700 -0.22363600

C -2.51432300 -0.36890500 -0.62597900

C -1.81294300 -0.95688500 1.76632700

H 1.00960000 0.56079600 1.59020300

H 3.13596200 -0.44129800 1.79381000

H 3.60573100 1.02835300 0.93489600

H 3.56678700 -0.15479700 -1.22704500

H 4.29440000 -1.36110300 -0.16329300

H 1.96745800 -1.90713500 -1.58654300

H 2.21237800 -2.58805900 0.02023100

H -1.02986300 0.63754900 0.54573600

H -2.13850600 -0.10156300 -1.61324900

H -2.96129800 -1.35973700 -0.70820900

H -1.00124300 -0.91545700 2.49832200

H -2.65561600 -0.38503200 2.15892800

H -2.11631900 -2.00104000 1.65788000

H 1.38643100 3.52075700 -0.06807200

H -3.25686000 1.91681500 -0.47088700

**Conformer 24**

S -4.50972300 0.14506200 -0.21911500

O -0.22131700 -1.50031600 -0.83370800

O 2.31065300 -1.07707200 1.31419200

O 3.57534900 -1.71747100 -0.43161900

N 0.69900800 0.47396600 -0.24900800

C 1.99957500 0.07230200 -0.78352300

C 2.80618800 1.39064000 -0.77514500

C 2.21289700 2.16761100 0.40960200

C 0.71905400 1.81573500 0.36238800

C -0.35576700 -0.39018300 -0.33109700

C -1.69881300 0.06623800 0.24709900

C 2.70696700 -1.01786400 0.02156200

C -2.82489400 -0.44799600 -0.66619000

C -1.82567200 -0.45371200 1.69031600

H 1.89160200 -0.33905300 -1.78718900

H 2.62106900 1.91999700 -1.71363600

H 3.88003100 1.21986000 -0.69525900

H 2.64782800 1.81600300 1.34809600

H 2.38403800 3.24309100 0.34099500

H 0.26883800 1.80579700 1.35650300

H 0.16456800 2.52926600 -0.25840400

H -1.74054900 1.15932900 0.25978800

H -2.63270900 -0.18730600 -1.70699600

H -2.88029300 -1.53552200 -0.61624200

H -1.03925100 -0.04928400 2.33240100

H -2.79264100 -0.17041000 2.10940500

H -1.74363000 -1.54349700 1.70501300

H 2.81418600 -1.79349700 1.73015500

H -4.33527600 1.42872300 -0.59672400

**Conformer 25**

S -4.49320100 0.26071700 -0.28608500

O -0.22188900 -1.48852100 -0.85231300

O 2.31246500 -1.09608300 1.30490100

O 3.58308300 -1.70911600 -0.44621200

N 0.70221300 0.47526600 -0.23826800

C 2.00178300 0.07943900 -0.77908300

C 2.80773300 1.39799800 -0.75993100

C 2.21765800 2.16265900 0.43436400

C 0.72387000 1.80997800 0.38943800

C -0.35451700 -0.38473200 -0.33472300

C -1.69685900 0.06921600 0.24667600

C 2.71136600 -1.01814000 0.01378500

C -2.82059200 -0.39238900 -0.69696700

C -1.83991000 -0.50235700 1.66812100

H 1.89183800 -0.32240700 -1.78638100

H 2.61896400 1.93647900 -1.69244300

H 3.88192900 1.22706700 -0.68534800

H 2.65671100 1.80295100 1.36789400

H 2.38719300 3.23894100 0.37538400

H 0.27844300 1.78746800 1.38561400

H 0.16527800 2.52995000 -0.21958900

H -1.73041300 1.16020600 0.30073200

H -2.63524500 -0.02612800 -1.70825200

H -2.85666600 -1.47903500 -0.75362700

H -1.01521200 -0.18393700 2.31071800

H -2.77087900 -0.16179600 2.12582900

H -1.83808700 -1.59510300 1.63915500

H 2.81889500 -1.81552300 1.71205000

H -4.76948100 -0.57773900 0.73241500

**Conformer 26**

S -4.36749900 0.33213500 -0.26760400

O 0.03107100 -1.49422800 -0.84628300

O 3.53842900 -1.45736400 -0.84868500

O 2.57145500 -1.31855000 1.17902400

N 0.65155600 0.48807100 0.01948500

C 2.00292500 0.32128100 -0.52132900

C 2.73997000 1.61327700 -0.09051800

C 1.60748200 2.63052800 0.11135700

C 0.47278600 1.78202200 0.69566800

C -0.26403700 -0.50452000 -0.18566200

C -1.66760600 -0.34401000 0.41054100

C 2.69169400 -0.91334900 0.05256100

C -2.63014600 -0.03571800 -0.75509100

C -2.04581700 -1.61986600 1.17403700

H 1.96485900 0.21581800 -1.60778000

H 3.47720600 1.92339400 -0.83114300

H 3.25913600 1.44287200 0.85647200

H 1.89156100 3.45533200 0.76718800

H 1.29818800 3.05223500 -0.84941100

H 0.57788000 1.67312700 1.78173300

H -0.50910700 2.20563700 0.48414100

H -1.68490400 0.49836500 1.10601700

H -2.26401400 0.79590200 -1.36008300

H -2.69945600 -0.90537100 -1.41085500

H -1.36594600 -1.78415200 2.01339900

H -3.06284700 -1.54037100 1.56143200

H -1.98104300 -2.48667700 0.51389500

H 3.96632800 -2.21498400 -0.42161100

H -4.11991700 1.52148400 0.32005600

**Conformer 27**

S -4.48471100 0.05468100 -0.24074100

O -0.15512700 -1.39174200 -0.85681500

O 2.18063800 -1.34614300 1.27275800

O 3.33989700 -1.93001300 -0.56575400

N 0.75090000 0.54526200 -0.15595600

C 2.07568500 0.11903400 -0.62292100

C 3.00084100 1.30493500 -0.25046800

C 2.04567400 2.50396400 -0.16829900

C 0.77193700 1.89458700 0.42662400

C -0.31061700 -0.29956300 -0.32102200

C -1.67614500 0.13601300 0.21948100

C 2.58435200 -1.17762500 -0.00796600

C -2.77790000 -0.51709000 -0.63080200

C -1.77411900 -0.24824900 1.70761700

H 2.05718800 -0.05485500 -1.70096900

H 3.80140100 1.43083200 -0.97900900

H 3.45904600 1.12704300 0.72622200

H 2.44079200 3.32001300 0.43910900

H 1.83737200 2.89523100 -1.16832600

H 0.83179300 1.84760200 1.52088400

H -0.12320000 2.45585700 0.15873000

H -1.77715900 1.22194200 0.13233300

H -2.59457900 -0.36179900 -1.69342800

H -2.79266800 -1.59467800 -0.46678500

H -1.01242400 0.25763100 2.30519200

H -2.75542800 0.02233900 2.10107600

H -1.63551800 -1.32594700 1.82768400

H 2.56171600 -2.18230800 1.58007300

H -4.36077500 1.29652400 -0.75421800

**Conformer 28**

S -4.26689400 0.55683500 -0.18861300

O 0.08653700 -1.54828600 -0.87778100

O 2.52782600 -1.26564300 1.12765000

O 3.63956800 -1.37597700 -0.82585100

N 0.64435900 0.43894500 0.02257000

C 1.99115000 0.35807000 -0.55435800

C 2.67952400 1.65820500 -0.06981400

C 1.50852000 2.61837800 0.18030000

C 0.41748400 1.70181100 0.74417300

C -0.23778300 -0.57943900 -0.20086400

C -1.64648100 -0.45602500 0.39399000

C 2.79274500 -0.86773300 -0.13832200

C -2.57217400 0.07212500 -0.72266100

C -2.09497300 -1.81258900 0.94745000

H 1.93363400 0.31539700 -1.64444800

H 3.39998400 2.02528500 -0.80038900

H 3.21333200 1.47001900 0.86576300

H 1.76361100 3.43065100 0.86297200

H 1.17129300 3.06099100 -0.76151600

H 0.53928000 1.56014200 1.82499800

H -0.58469900 2.08919400 0.56106700

H -1.64565600 0.27177400 1.20824400

H -2.16774500 0.99096500 -1.15392900

H -2.64465200 -0.65692800 -1.53068800

H -1.41046000 -2.15782100 1.72571700

H -3.09062500 -1.73536600 1.38931500

H -2.10682000 -2.56521100 0.15698100

H 3.09168500 -2.03346200 1.30462100

H -4.76189200 -0.68516400 -0.02040800

**Conformer 29**

S -2.62058200 1.30150700 -0.99851300

O -0.88296100 -1.97380600 -1.10997600

O 1.43225100 1.92882700 -0.74427000

O 0.73013100 2.35201300 1.34912300

N 0.80268700 -0.80941200 -0.17298000

C 1.41299100 0.09354300 0.80511400

C 2.91674900 -0.25458800 0.70722900

C 3.10598400 -0.70102100 -0.75175200

C 1.78535400 -1.39808900 -1.10452900

C -0.51103200 -1.17628300 -0.25845800

C -1.50206500 -0.62398400 0.77638200

C 1.14179500 1.57389500 0.52412900

C -2.79429700 -0.18397800 0.07846500

C -1.79924100 -1.73256100 1.80723000

H 1.03373800 -0.08723100 1.81040000

H 3.11794800 -1.08230500 1.39249300

H 3.55867300 0.57945500 0.99578500

H 3.25806700 0.16708200 -1.39433100

H 3.96392600 -1.36466300 -0.87097100

H 1.47197800 -1.22954800 -2.13555200

H 1.82663600 -2.48032300 -0.94747400

H -1.08439300 0.23680000 1.30155600

H -3.13709100 -0.97562700 -0.58842500

H -3.57710200 0.01003400 0.81272400

H -0.89033100 -2.04526200 2.32897400

H -2.51099200 -1.37714000 2.55685900

H -2.22169400 -2.60984100 1.31233100

H 1.19976800 2.86411600 -0.84818500

H -2.47141600 2.19834800 -0.00097600

**Conformer 30**

S -3.76291200 0.66069000 -0.11464200

O -0.23611000 -2.39030400 -0.76734700

O 1.06020100 2.83626000 0.62692100

O 0.40058800 1.78338000 -1.24997600

N 1.16589700 -0.74161700 -0.12306400

C 1.52654100 0.52306100 0.51207800

C 3.07905800 0.57892400 0.39453800

C 3.48660600 -0.88732700 0.19704000

C 2.34328200 -1.45462100 -0.64491300

C -0.07570200 -1.31627700 -0.20164000

C -1.26622000 -0.60427100 0.45159700

C 0.91621800 1.74518200 -0.16410600

C -2.30846800 -0.33402800 -0.65169900

C -1.81752800 -1.48454700 1.58411100

H 1.23176000 0.54159800 1.56556800

H 3.52609100 1.05266700 1.26818800

H 3.36188300 1.16478700 -0.48463500

H 4.45889400 -0.98741800 -0.28832200

H 3.53302200 -1.40411900 1.16005400

H 2.47859100 -1.23923200 -1.71125300

H 2.19333100 -2.52757600 -0.53764900

H -0.96424200 0.35577300 0.87557100

H -1.84959200 0.16890900 -1.50217700

H -2.71813800 -1.28030100 -1.00679300

H -1.07574900 -1.62045600 2.37625200

H -2.70388100 -1.02229000 2.02247500

H -2.08415000 -2.47011200 1.19696900

H 0.70262500 3.59705300 0.14404200

H -3.14528700 1.85973600 -0.12138500

**Conformer 31**

S 3.78887100 0.84222700 -0.21119500

O 0.76366500 1.06530500 -0.60189000

O -1.33227000 2.32334000 0.48781200

O -3.37453400 1.48601800 0.75767100

N -0.76375800 -0.54375000 -0.19699800

C -1.88006700 0.28367700 -0.72558500

C -3.00153100 -0.73312300 -0.95446400

C -2.74063500 -1.80671200 0.11153800

C -1.21206200 -1.91113600 0.14576600

C 0.51415500 -0.09718900 -0.25087400

C 1.63971600 -1.04631300 0.14997300

C -2.28156700 1.41374500 0.25689100

C 2.92055000 -0.73423000 -0.64751200

C 1.85221000 -1.02124400 1.67561500

H -1.54724000 0.76137600 -1.65179400

H -2.91017800 -1.15789200 -1.95829000

H -3.98083700 -0.26863200 -0.85577500

H -3.11871100 -1.46668500 1.07847200

H -3.20868600 -2.76487000 -0.11886400

H -0.83266200 -2.21526600 1.12174200

H -0.85020900 -2.62407900 -0.60390500

H 1.35073700 -2.06342200 -0.13841200

H 3.63028300 -1.54738800 -0.49678800

H 2.68834600 -0.68830500 -1.71175600

H 0.95082800 -1.32069700 2.21466800

H 2.65402900 -1.71109200 1.95239800

H 2.13577700 -0.02133300 2.00526900

H -0.49831200 2.07237100 0.01943800

H 4.94170900 0.26438000 0.18488300

**Conformer 32**

S -4.35912400 0.35718400 -0.24921300

O 0.01820200 -1.47506300 -0.89354400

O 2.45782400 -1.32557000 1.11607800

O 3.56658800 -1.49244100 -0.83519000

N 0.67133700 0.47913800 0.01209100

C 2.01230400 0.32629800 -0.56510900

C 2.76917800 1.58725300 -0.08125000

C 1.65143200 2.61143000 0.15803400

C 0.50766800 1.75945400 0.71977700

C -0.25890500 -0.49591600 -0.21017800

C -1.65632400 -0.33342600 0.40070800

C 2.74634200 -0.94107900 -0.14873400

C -2.62713600 -0.01126600 -0.75443400

C -2.03495200 -1.61464300 1.15524300

H 1.95250600 0.28650200 -1.65517300

H 3.51267200 1.91151500 -0.80897100

H 3.28651700 1.37349500 0.85807500

H 1.94732500 3.41183800 0.83828600

H 1.34444300 3.06702300 -0.78788200

H 0.61084200 1.62290800 1.80311400

H -0.46951000 2.19959200 0.52030000

H -1.66549500 0.50277300 1.10360500

H -2.26279900 0.82486500 -1.35415800

H -2.70369400 -0.87435400 -1.41788600

H -1.35321400 -1.78744000 1.99169400

H -3.05016800 -1.53602400 1.54746000

H -1.97512000 -2.47604700 0.48755100

H 2.97819400 -2.12352300 1.29304300

H -4.10441600 1.54393200 0.34062600

**Conformer 33**

S -3.93719800 0.71588500 -0.18399300

O -0.45431200 -2.27931900 -0.78037500

O 1.24699000 1.58233900 -1.39262200

O 1.27906300 2.79539100 0.50065500

N 1.05850300 -0.79001300 -0.02191600

C 1.50096300 0.40104500 0.69679200

C 3.00546600 0.11968900 0.94144200

C 3.41422800 -0.72819400 -0.27228400

C 2.18022700 -1.59754600 -0.54063100

C -0.22528900 -1.22717100 -0.19643600

C -1.36816400 -0.38434700 0.38390200

C 1.32034300 1.72454300 -0.05083600

C -2.52104200 -0.37035500 -0.63521000

C -1.78499300 -0.97474300 1.74246700

H 0.97696000 0.52682100 1.64505500

H 3.09904900 -0.45981600 1.86352200

H 3.58430200 1.03602200 1.06185700

H 3.61888900 -0.08566300 -1.13206300

H 4.30680700 -1.32587800 -0.08164600

H 2.02556700 -1.81883700 -1.59720800

H 2.22036000 -2.55290100 -0.00780500

H -1.04185500 0.64814200 0.53611500

H -2.16168200 -0.07850500 -1.62203000

H -2.94536800 -1.36979000 -0.73247300

H -0.96678800 -0.92869600 2.46655600

H -2.63289400 -0.42228300 2.15070100

H -2.07257000 -2.02237400 1.62392900

H 1.16685000 2.47206300 -1.77043200

H -3.29632900 1.89281800 -0.34328400

**Conformer 34**

S -3.09998200 0.56968700 -1.34051100

O -0.40352600 -1.54955800 -0.53057900

O 2.15893200 -2.16124200 -0.42498500

O 3.82340500 -0.77168400 0.06008400

N 0.54953700 0.29073400 0.35448400

C 1.70786000 0.23059000 -0.57936900

C 2.38639000 1.60678300 -0.44352800

C 1.36842800 2.49116100 0.29344400

C 0.63542600 1.49679600 1.19660500

C -0.48290100 -0.57909800 0.23374900

C -1.75375600 -0.35151000 1.05871800

C 2.67719400 -0.94355500 -0.26828700

C -2.67217900 0.73136400 0.44154400

C -2.49078100 -1.67715700 1.27742300

H 1.30848800 0.06086600 -1.58405600

H 2.66825200 2.00796500 -1.41736000

H 3.30001800 1.48858500 0.14070800

H 1.84092400 3.29518500 0.86014500

H 0.65891200 2.94123700 -0.40723300

H 1.22045900 1.27831300 2.09764800

H -0.34880700 1.84017600 1.50479500

H -1.45900800 0.03382500 2.04150400

H -3.59285200 0.78269300 1.02552400

H -2.20677300 1.71722100 0.49255400

H -1.85664000 -2.39212500 1.80495300

H -3.38978400 -1.50970600 1.87659500

H -2.77289800 -2.13668500 0.32993400

H 1.18967900 -2.09057200 -0.62179100

H -3.69158800 -0.63947200 -1.27508700

**Conformer 35**

S -3.92116400 -0.82282900 -0.20363200

O -0.72346600 -1.10277100 -0.68192800

O 1.83799600 -1.13158400 1.50330000

O 2.86514100 -2.35207800 -0.08178500

N 0.73726200 0.57000300 -0.31723000

C 1.85403000 -0.26983600 -0.75027500

C 3.00941900 0.74048100 -0.93090200

C 2.68947500 1.84053400 0.09208100

C 1.15771800 1.93393500 0.05324500

C -0.52862100 0.05612300 -0.32564400

C -1.66395800 0.97080600 0.14159200

C 2.23091000 -1.37835300 0.23251200

C -2.96835300 0.69349800 -0.63258200

C -1.82936800 0.88151000 1.67016600

H 1.60860800 -0.78476900 -1.67912200

H 2.97002900 1.13912900 -1.94813500

H 3.98810800 0.28087100 -0.79130100

H 3.01852500 1.53857800 1.08931300

H 3.16503600 2.79350300 -0.14527300

H 0.74010100 2.23120800 1.01606000

H 0.82614300 2.65601600 -0.70237200

H -1.39253900 2.00281000 -0.10950500

H -3.66860800 1.50851300 -0.43605600

H -2.77064900 0.68440100 -1.70550500

H -0.91224900 1.16864100 2.18963100

H -2.63160900 1.54638800 2.00146200

H -2.09014800 -0.13362500 1.97019000

H 2.12056500 -1.88971600 2.03748200

H -2.93839900 -1.68744800 -0.52598800

**Conformer 36**

S -3.85618300 0.85051400 -0.22493000

O -0.45499800 -2.27942000 -0.78503700

O 1.09826800 1.60091400 -1.34558300

O 1.41964100 2.78973100 0.53628600

N 1.06032100 -0.79263000 -0.02773100

C 1.51341700 0.38738300 0.70273400

C 3.01843400 0.09805100 0.92934800

C 3.41240600 -0.72061200 -0.30879600

C 2.17664200 -1.58718100 -0.57814400

C -0.22331800 -1.23279300 -0.19119000

C -1.36543700 -0.39987300 0.40415300

C 1.33303400 1.72513300 -0.02117200

C -2.47149100 -0.28263700 -0.66029000

C -1.84934200 -1.07367300 1.69926100

H 0.99972900 0.50061100 1.65852300

H 3.12005400 -0.50469100 1.83559200

H 3.59744800 1.01150500 1.06630800

H 3.60304300 -0.05776600 -1.15684900

H 4.30956600 -1.31969000 -0.14632200

H 2.00747900 -1.78819200 -1.63660700

H 2.22631800 -2.55273100 -0.06493800

H -1.02749000 0.61096000 0.64293600

H -2.06017100 0.14230100 -1.57757600

H -2.86832900 -1.26483500 -0.91145300

H -1.04093500 -1.15408400 2.43132700

H -2.65264000 -0.49277700 2.15703000

H -2.21383900 -2.08238600 1.48933300

H 1.01906500 2.49801400 -1.70610300

H -4.51197600 0.02135400 0.61104700

**Conformer 37**

S -3.59792200 0.91849500 -0.15242700

O -0.30990400 -2.45089200 -0.66668100

O 1.16311700 2.75604200 0.67278600

O 0.73071000 1.67518400 -1.25364000

N 1.10010700 -0.83699200 0.03087800

C 1.47474600 0.40511000 0.69651800

C 3.01723300 0.29633500 0.80201000

C 3.39811500 -0.51798700 -0.44285400

C 2.25485300 -1.52934200 -0.57500800

C -0.14975000 -1.37847300 -0.09813300

C -1.35102100 -0.61221500 0.47146400

C 1.07114800 1.64819700 -0.10011700

C -2.22214200 -0.18257500 -0.72302700

C -2.10208800 -1.50812000 1.46966500

H 1.02987500 0.49125000 1.68945900

H 3.26339400 -0.25525400 1.71307600

H 3.49926400 1.27253300 0.86068800

H 3.43176000 0.12921400 -1.32305800

H 4.37110200 -1.00175500 -0.34491800

H 2.02704600 -1.79832100 -1.60667400

H 2.45642300 -2.45716700 -0.02978500

H -1.02308700 0.29259500 0.98860100

H -1.61955200 0.37447000 -1.44002900

H -2.63738300 -1.06473600 -1.20958300

H -1.46155000 -1.77389100 2.31518000

H -2.98549800 -1.00011600 1.86149800

H -2.41685700 -2.43136700 0.98002700

H 0.90772400 3.51595600 0.12756200

H -3.99461100 1.30136100 -1.38220300

**Conformer 38**

S -2.89697000 1.06369300 -1.12295600

O -1.07652800 -2.01982900 -0.78499800

O 1.52861400 2.44298300 1.15593100

O 1.29232900 1.89487100 -1.01554300

N 0.73303100 -0.82404100 -0.17445500

C 1.47309100 0.12148300 0.65326200

C 2.93090100 -0.39524200 0.54792200

C 2.99404000 -0.97890200 -0.87182700

C 1.60743500 -1.60265300 -1.07341900

C -0.59881000 -1.12098800 -0.10567900

C -1.46907300 -0.34816100 0.89677800

C 1.40022100 1.55844100 0.13265700

C -2.86000700 -0.09889800 0.30338000

C -1.58187200 -1.17626800 2.19423500

H 1.13044900 0.11516300 1.68779000

H 3.07278300 -1.17909500 1.29672400

H 3.66744200 0.38726000 0.73701700

H 3.15714300 -0.18117100 -1.59939600

H 3.79600200 -1.70990400 -0.98576000

H 1.24818000 -1.53100000 -2.10050800

H 1.57629300 -2.65797500 -0.78501500

H -1.01707600 0.61822500 1.13554100

H -3.25644900 -1.03420600 -0.09236000

H -3.54166700 0.26505900 1.07342300

H -0.60201000 -1.35231500 2.64711900

H -2.20250300 -0.65728900 2.92939700

H -2.03302600 -2.14904900 1.98497000

H 1.53759800 3.33243900 0.76990600

H -2.64374000 2.18598100 -0.41733600

**Conformer 39**

S -2.52237600 1.31040500 -1.08739100

O -1.25375800 -1.89694700 -0.79939600

O 0.76508400 2.11374900 -0.38184400

O 2.45199000 2.13679800 1.05570500

N 0.60059800 -0.71485900 -0.27980500

C 1.48432800 -0.01744500 0.67106500

C 2.84708700 -0.70581900 0.45368100

C 2.82949200 -1.02770300 -1.04667600

C 1.38082300 -1.45846900 -1.29986100

C -0.71113200 -1.06327000 -0.08513400

C -1.51203900 -0.33887700 1.00161900

C 1.61371900 1.51066600 0.46226300

C -2.80110400 0.21453900 0.37404700

C -1.84168400 -1.30775200 2.15130800

H 1.14197500 -0.14938400 1.69864400

H 2.87973300 -1.62734900 1.04152700

H 3.66988000 -0.06558900 0.76669200

H 3.07348200 -0.13274500 -1.62685700

H 3.54173000 -1.80590400 -1.32389000

H 1.02056400 -1.21865100 -2.30137000

H 1.23320200 -2.53100500 -1.14702500

H -0.94485900 0.50537900 1.39976900

H -3.45532800 -0.59845300 0.06276300

H -3.33416600 0.82767500 1.10219800

H -0.93449300 -1.65661500 2.65245600

H -2.46795400 -0.81508500 2.89969900

H -2.37503500 -2.18112000 1.77041000

H 0.08943400 1.50633200 -0.73420000

H -2.42779300 0.31602200 -1.99351400

**Conformer 40**

S -2.63299100 1.28920600 -1.04009500

O -1.11819000 -1.98810700 -0.85781100

O 0.78579500 2.05180000 -0.55919800

O 2.16645000 2.27323400 1.16919500

N 0.65950500 -0.70936400 -0.30137900

C 1.47216000 0.03191300 0.67964600

C 2.88199700 -0.57432700 0.50813500

C 2.92465700 -0.93515100 -0.98311200

C 1.51099100 -1.45464600 -1.26256500

C -0.64618700 -1.11678100 -0.14384800

C -1.51021900 -0.43579900 0.92504800

C 1.51003800 1.55946700 0.45872900

C -2.82782700 0.01839600 0.28172500

C -1.78319000 -1.42880800 2.07110500

H 1.10877000 -0.11600600 1.69719300

H 2.95856400 -1.47635800 1.12144600

H 3.65718700 0.12176200 0.82541300

H 3.13459800 -0.04449700 -1.58284500

H 3.68717200 -1.67885400 -1.21814500

H 1.17082800 -1.27958300 -2.28390000

H 1.41615100 -2.52632400 -1.06591100

H -1.00591400 0.44414200 1.33167600

H -3.30263500 -0.82913600 -0.21303400

H -3.51177300 0.40252900 1.03928000

H -0.85630400 -1.73904300 2.56163400

H -2.42548600 -0.97211100 2.82831600

H -2.27724300 -2.32388400 1.68744400

H 0.27068900 1.34102300 -0.98015500

H -2.38023800 2.33358900 -0.22390300

**Conformer 41**

S -4.04535500 -0.03319300 -0.27370000

O -1.24512700 -1.64331800 -0.50484300

O 2.56363400 2.38050200 0.13563800

O 1.74300600 1.25972200 -1.63611400

N 0.74970500 -0.78610300 0.07954100

C 1.66573600 0.22965100 0.57978600

C 2.94435300 -0.58440700 0.90246600

C 2.92685500 -1.69397000 -0.15895300

C 1.43876900 -2.03280400 -0.30945300

C -0.60732200 -0.69409100 -0.06149400

C -1.29109000 0.60336000 0.38650100

C 1.96807300 1.31554600 -0.45647800

C -2.49957500 0.93858200 -0.51185900

C -1.64185000 0.53496300 1.88406800

H 1.28600900 0.72312800 1.47539900

H 2.83951500 -1.00691700 1.90512100

H 3.84428400 0.03102600 0.88897500

H 3.32590800 -1.31905200 -1.10476200

H 3.52042400 -2.56131700 0.13366700

H 1.15922500 -2.31444500 -1.32499700

H 1.12678400 -2.84445100 0.35523500

H -0.59292000 1.43454500 0.23893600

H -2.80345600 1.96903100 -0.31437700

H -2.20907700 0.87796100 -1.56117800

H -0.74904000 0.39718300 2.50005700

H -2.13051600 1.46025700 2.20072300

H -2.32702200 -0.28980900 2.08183600

H 2.76584200 3.02552600 -0.55933600

H -3.49401200 -1.22509400 -0.57783400

**Conformer 42**

S -3.80856600 0.60151600 -0.08625700

O -0.21558700 -2.30633400 -0.88747200

O 0.78138600 1.76536300 -1.33228300

O 0.69770600 2.79790500 0.66483200

N 1.17704900 -0.70220800 -0.11874200

C 1.51786700 0.53234300 0.59251800

C 3.07249900 0.58857700 0.52054600

C 3.48523900 -0.86872500 0.27136200

C 2.36993900 -1.39590100 -0.63205500

C -0.06273800 -1.26686300 -0.25847900

C -1.26160200 -0.58835600 0.41697900

C 0.94110200 1.81640000 0.00886500

C -2.32884500 -0.32878300 -0.66343700

C -1.76946600 -1.49669800 1.54901300

H 1.18922200 0.49824600 1.63391500

H 3.49272000 1.02249300 1.42769500

H 3.38084300 1.21138300 -0.32338100

H 4.47271100 -0.94902400 -0.18611400

H 3.50052800 -1.42801800 1.21132000

H 2.54129000 -1.13585600 -1.68304300

H 2.21447600 -2.47207000 -0.57552200

H -0.97512900 0.37304600 0.84953000

H -1.89805400 0.20082700 -1.51375300

H -2.71470300 -1.27869400 -1.03524600

H -1.00881300 -1.62229000 2.32457700

H -2.65930500 -1.06465100 2.00958600

H -2.01820000 -2.48401100 1.15401700

H 0.46977800 2.63796500 -1.61798200

H -3.18165000 1.77442000 0.14323400

**Conformer 43**

S 3.41480700 -1.18661100 -0.80177600

O 0.64715700 0.88122800 -1.35494000

O -2.48383700 1.76701200 0.03255000

O -3.73857400 0.48550300 -1.28605900

N -0.51745200 -0.13068200 0.30748500

C -1.63818300 -0.45428400 -0.60017900

C -2.20230100 -1.76781900 -0.03070600

C -1.94568500 -1.62746200 1.47648400

C -0.56521600 -0.96173200 1.53956800

C 0.62387900 0.44789800 -0.21189500

C 1.82617700 0.61210200 0.72221100

C -2.72474400 0.63784300 -0.66187900

C 3.13214900 0.47945000 -0.06781000

C 1.74152900 1.99272800 1.40709000

H -1.26341200 -0.55838100 -1.61907200

H -1.63634500 -2.61011300 -0.43760700

H -3.25104800 -1.90129000 -0.29172200

H -2.70240700 -0.98149600 1.93145000

H -1.95986900 -2.58058000 2.00692600

H -0.43274700 -0.34976600 2.43406000

H 0.22916900 -1.71364700 1.51442400

H 1.81307300 -0.16357100 1.49019700

H 3.17976500 1.22170000 -0.86346000

H 3.97957900 0.63994700 0.60115300

H 0.83978600 2.08351200 2.01922300

H 2.60248200 2.14554200 2.06275300

H 1.73064600 2.79225100 0.66233200

H -1.61147500 1.68305000 0.44782300

H 2.58445300 -1.02889100 -1.85218200

**Conformer 44**

S -3.21280700 0.51333600 -1.33416000

O -0.37367700 -1.58669300 -0.50184500

O 3.24356700 -1.43855500 -1.14586900

O 2.60640900 -1.20470900 0.99917000

N 0.42663400 0.41791400 0.13507400

C 1.60578200 0.22347800 -0.70434400

C 2.31959000 1.59115400 -0.63403100

C 1.96334900 2.10263900 0.76990700

C 0.51541500 1.62916800 0.96876200

C -0.52342500 -0.56834700 0.15907000

C -1.77046300 -0.34467300 1.02532000

C 2.50315800 -0.88704000 -0.15776300

C -2.72567800 0.71510100 0.43032700

C -2.47568200 -1.67722700 1.29240500

H 1.31624900 -0.04814800 -1.71902000

H 1.90094500 2.24562500 -1.40315200

H 3.39341500 1.51340600 -0.80898200

H 2.61050900 1.63671000 1.51595600

H 2.05842600 3.18565600 0.86472900

H 0.29923400 1.40668600 2.01554300

H -0.19308000 2.39143600 0.62553000

H -1.44409100 0.06555400 1.98931700

H -3.62807900 0.76373900 1.04263200

H -2.27256100 1.70693000 0.45099100

H -1.80956600 -2.37066500 1.80843200

H -3.35953500 -1.51735100 1.91645700

H -2.77712900 -2.15975200 0.36188400

H 3.80825200 -2.11405600 -0.74067400

H -3.76718800 -0.71040800 -1.22816200

**Conformer 45**

S -3.64696200 -0.28033300 -1.09831900

O -0.51579600 -1.28575500 -0.38766000

O 2.21776500 -1.44256900 1.17343600

O 2.88723900 -2.08824800 -0.87597100

N 0.65735200 0.57372000 0.08420900

C 1.81550400 0.05617200 -0.65551100

C 2.88617900 1.16147000 -0.48661500

C 2.06018000 2.43226700 -0.24570000

C 0.88571600 1.93304000 0.60282300

C -0.47270100 -0.18769500 0.16138200

C -1.67756400 0.36644000 0.92511600

C 2.33879400 -1.28704800 -0.16529400

C -2.71844500 0.93458600 -0.06963600

C -2.24734200 -0.69709200 1.87167700

H 1.55656100 -0.09490900 -1.70594800

H 3.53956500 1.22108300 -1.35666600

H 3.50635900 0.94740300 0.38809700

H 2.62781000 3.22007100 0.25235100

H 1.68923000 2.83032600 -1.19461700

H 1.15048500 1.90386100 1.66670400

H -0.00087700 2.55607800 0.48545800

H -1.35577200 1.21878000 1.53048500

H -3.49506800 1.45725200 0.49308400

H -2.24654800 1.66564100 -0.73030600

H -1.50655900 -0.97481000 2.62565300

H -3.13115000 -0.30898600 2.38518500

H -2.53177500 -1.59411500 1.32371400

H 2.58610600 -2.31220100 1.38994800

H -2.57403200 -1.00644500 -1.47739700

**Conformer 46**

S -3.77633500 0.70454700 -0.12831700

O -0.25261600 -2.30790900 -0.85192800

O 0.70255900 1.76184200 -1.30416900

O 0.87184400 2.82696800 0.67059200

N 1.16989200 -0.70737500 -0.13175000

C 1.54335400 0.51930900 0.57695600

C 3.09745600 0.54655900 0.48297500

C 3.47960400 -0.91923900 0.23871800

C 2.34442900 -1.42984500 -0.64925200

C -0.07858900 -1.25693900 -0.24663800

C -1.26210400 -0.54509500 0.42029700

C 0.99001000 1.82312200 0.01502500

C -2.33985500 -0.31826900 -0.65724300

C -1.75960400 -1.40912000 1.59049600

H 1.23173600 0.48628300 1.62401900

H 3.53795400 0.98063800 1.38020500

H 3.40502200 1.15796300 -0.36983600

H 4.46016100 -1.02191800 -0.22908900

H 3.49446000 -1.47310500 1.18198600

H 2.51076500 -1.18129800 -1.70385400

H 2.16732600 -2.50208600 -0.58336100

H -0.96987900 0.43031800 0.81391300

H -1.91548500 0.23605100 -1.49625600

H -2.69451400 -1.27196100 -1.04574300

H -0.97090300 -1.55946500 2.33284100

H -2.59898400 -0.92493900 2.09371000

H -2.07487600 -2.39080900 1.22964600

H 0.41149900 2.64696500 -1.57325900

H -4.42465800 -0.24386500 0.57643200

**Conformer 47**

S 4.13338400 -0.35051100 -0.87603400

O 0.01674200 -1.44100900 1.39738700

O -2.00774300 -2.27359400 -0.08222900

O -3.48138400 -0.98165400 -1.13161900

N -0.67054800 0.40485600 0.30910100

C -2.10398700 0.07818900 0.55999000

C -2.83122000 1.38577800 0.23796000

C -1.95873200 2.01611900 -0.85470500

C -0.53507500 1.70781000 -0.38310900

C 0.30789200 -0.37182800 0.83462100

C 1.79599000 -0.00792600 0.72114600

C -2.60236400 -1.10305200 -0.31699400

C 2.29962700 -0.31241000 -0.70672600

C 2.19850900 1.38066800 1.23872800

H -2.21123400 -0.22234900 1.60590700

H -2.85497800 2.02222100 1.12739900

H -3.85152100 1.19790400 -0.09021100

H -2.15969900 1.53218000 -1.81322800

H -2.12184600 3.08842400 -0.97262500

H 0.17779400 1.64383800 -1.20502000

H -0.19155000 2.47130500 0.31940300

H 2.24957300 -0.75003700 1.38199500

H 1.90389100 -1.26567600 -1.05859900

H 1.98556300 0.45610700 -1.41553800

H 1.72646100 1.59265700 2.20149000

H 3.27958800 1.40832600 1.38292300

H 1.94528900 2.18365500 0.54498300

H -1.28796400 -2.15350200 0.58815300

H 4.32556500 -1.50088200 -0.19797400

**Conformer 48**

S -4.03238100 -0.07644000 -0.29423200

O -1.19649700 -1.61740900 -0.57460300

O 1.83377900 1.13247500 -1.60669900

O 2.36723400 2.50543600 0.09305000

N 0.77261000 -0.75315000 0.08369500

C 1.66235500 0.26287200 0.63751200

C 2.94655800 -0.54222400 0.95892800

C 2.96826800 -1.62956400 -0.12549300

C 1.48803800 -1.97802700 -0.32733300

C -0.58308400 -0.67842000 -0.07746100

C -1.29581900 0.58703500 0.41470300

C 1.98479600 1.43146400 -0.29788000

C -2.50486200 0.93503900 -0.47775200

C -1.65537000 0.45130900 1.90588500

H 1.25681100 0.71591400 1.54213800

H 2.82961300 -0.98899600 1.94965900

H 3.83665900 0.08762300 0.97797800

H 3.39331300 -1.23399000 -1.05089600

H 3.55938600 -2.49825500 0.16809200

H 1.23951100 -2.22967900 -1.35890900

H 1.16656400 -2.81448800 0.30081300

H -0.61313100 1.43795400 0.31030000

H -2.83090200 1.94989700 -0.23941100

H -2.20718500 0.92441000 -1.52708000

H -0.76383200 0.30687400 2.52176800

H -2.16380800 1.35358200 2.25554900

H -2.32505100 -0.39423500 2.06516800

H 2.08492600 1.92119300 -2.11229000

H -3.45445800 -1.24363800 -0.64167800

**Conformer 49**

S 2.38374100 -1.39996900 -1.43288800

O 0.26866800 -0.81179500 1.88753200

O -1.85036100 -2.02589500 0.81945500

O -3.31050300 -1.11393200 -0.58886500

N -0.35467200 0.51079900 0.17883400

C -1.79002900 0.39412400 0.54965700

C -2.44269800 1.54702800 -0.21358600

C -1.60419600 1.64453100 -1.49446300

C -0.17137600 1.35225500 -1.02405100

C 0.59540300 -0.04629000 0.96549000

C 2.08264900 0.31359900 0.83964000

C -2.39516200 -0.98727800 0.18399000

C 2.75936500 0.16014900 -0.53014800

C 2.34914400 1.71184700 1.43411300

H -1.87022200 0.50391400 1.63463500

H -2.36116600 2.46545700 0.37493400

H -3.49369100 1.34600600 -0.41266900

H -1.92930800 0.88033100 -2.20338100

H -1.67903500 2.61606700 -1.98518100

H 0.39866100 0.81539700 -1.78202500

H 0.35822800 2.27449400 -0.76626000

H 2.54686300 -0.41798100 1.50539600

H 2.48088900 0.95398800 -1.22331800

H 3.83904300 0.23414600 -0.38748800

H 1.94203400 1.78432000 2.44491500

H 3.42522400 1.89523600 1.49249400

H 1.90831300 2.50775800 0.82864900

H -1.09316000 -1.71722900 1.37740700

H 2.70914500 -2.24482100 -0.43256600

**Conformer 50**

S -2.43104900 -0.68374900 1.68528400

O -0.26355400 -1.14582800 -1.74256700

O 1.63329200 -2.21588900 -0.27265000

O 3.11890800 -1.11447200 0.96156300

N 0.42039600 0.53917200 -0.41959200

C 1.85105900 0.18471000 -0.64855000

C 2.60497800 1.41675100 -0.14814200

C 1.72642700 1.91834900 1.00495400

C 0.30105700 1.71516500 0.48086200

C -0.55187800 -0.13572800 -1.07251200

C -2.04080100 0.23735600 -1.02605800

C 2.26844000 -1.10618800 0.10856500

C -2.79057300 -0.76786100 -0.12322700

C -2.47105400 1.68804000 -0.78222700

H 1.99265900 -0.00076500 -1.71662700

H 2.65849400 2.16245900 -0.94678700

H 3.61485100 1.16166400 0.16713400

H 1.90014600 1.30671000 1.89297300

H 1.91322000 2.96063800 1.26786300

H -0.42044700 1.51550300 1.27165800

H -0.02518800 2.58796600 -0.08870800

H -2.35361000 -0.02497300 -2.04317000

H -3.86301000 -0.57896000 -0.20017000

H -2.60785900 -1.78658200 -0.46137700

H -1.91296300 2.38738200 -1.40856100

H -3.52640800 1.78595700 -1.05191500

H -2.37112400 1.99253700 0.25935400

H 0.95415300 -1.98887900 -0.95995900

H -1.29400600 -1.40891400 1.65813700

**Conformer 51**

S 4.13534100 -0.46402500 -0.84060800

O -0.00287300 -1.45687100 1.39557200

O -2.03312600 -2.26129100 -0.09250300

O -3.49038300 -0.94938300 -1.13992800

N -0.66792800 0.40059500 0.31325900

C -2.10538000 0.08894200 0.55860900

C -2.81666600 1.40573800 0.23856200

C -1.93505800 2.02784200 -0.85159000

C -0.51559000 1.70132000 -0.37905900

C 0.30097300 -0.38848200 0.83915500

C 1.79271300 -0.03801000 0.73348000

C -2.61448300 -1.08368100 -0.32388200

C 2.30269700 -0.38088200 -0.68297800

C 2.19969700 1.36033500 1.22182200

H -2.21919700 -0.21376700 1.60321300

H -2.83407300 2.04053800 1.12936300

H -3.83869100 1.23096200 -0.09145500

H -2.14066900 1.54818600 -1.81125000

H -2.08524400 3.10226200 -0.96764800

H 0.19691000 1.62744500 -1.20079300

H -0.16227800 2.46088800 0.32297200

H 2.24179100 -0.76726500 1.41036900

H 1.96948100 -1.38262300 -0.96010500

H 1.92482400 0.31033700 -1.43745700

H 1.67747700 1.62344200 2.14517400

H 3.26883100 1.36611000 1.44254200

H 2.01111000 2.14394500 0.48572300

H -1.31324200 -2.15207000 0.57967800

H 4.37064100 0.86349100 -0.82324500

**Conformer 52**

S 4.11925200 -0.34135100 -0.91392200

O -0.12940200 -1.43253600 1.42292300

O -2.22295200 -2.26302800 0.04620900

O -3.50955900 -0.98389700 -1.23717300

N -0.64830200 0.34189100 0.14046500

C -2.10723900 0.14880200 0.38555300

C -2.75498700 1.47094300 -0.06076800

C -1.59636900 2.47461700 -0.14802400

C -0.41880600 1.60334700 -0.58847700

C 0.25574200 -0.45398300 0.76246000

C 1.76713400 -0.19353600 0.67658400

C -2.68439200 -1.08184600 -0.36558700

C 2.29390000 -0.13107000 -0.77179700

C 2.21620900 0.97932600 1.56507700

H -2.23675100 -0.03541900 1.45665000

H -3.53711200 1.78298600 0.63188700

H -3.21969600 1.32123700 -1.03649300

H -1.79335400 3.28795800 -0.84830300

H -1.38132300 2.91382400 0.83070500

H -0.44826000 1.42083700 -1.66841900

H 0.54597100 2.03268300 -0.33665100

H 2.17132400 -1.10442300 1.12324300

H 1.81433500 -0.88962600 -1.39197200

H 2.10825200 0.83638900 -1.23872600

H 1.86274700 0.83820300 2.58883700

H 3.30664500 1.02166500 1.58598500

H 1.85285000 1.94753900 1.21216000

H -1.50051700 -2.12526500 0.70980300

H 4.15312000 -1.64412400 -0.56502200

**Conformer 53**

S 3.17470800 -1.33997300 -0.74570200

O 0.50578100 1.18663500 -1.32437300

O -2.59557300 1.66696800 0.33445000

O -3.84038600 0.43944400 -1.04403000

N -0.48288500 -0.07861600 0.27806700

C -1.62811000 -0.38726900 -0.60592800

C -2.04744400 -1.80550800 -0.18275500

C -1.71380500 -1.82917400 1.31542600

C -0.39237200 -1.05428800 1.39741300

C 0.58429800 0.62874100 -0.24082500

C 1.84721300 0.77814500 0.61633600

C -2.79887700 0.60575700 -0.47075400

C 3.07895900 0.42756900 -0.22851900

C 1.93484400 2.23244000 1.12089700

H -1.30699200 -0.33129200 -1.64672100

H -1.43948100 -2.53676500 -0.72179400

H -3.09583900 -1.99753600 -0.40609900

H -2.49363200 -1.31575500 1.88579800

H -1.61672300 -2.83788800 1.71963300

H -0.26393700 -0.54532200 2.35492800

H 0.45939900 -1.72142800 1.23869900

H 1.81129600 0.11100100 1.47950300

H 3.05483700 0.99228900 -1.16104600

H 3.99534600 0.68634800 0.30284800

H 1.07788000 2.48748600 1.75076900

H 2.83974400 2.37555700 1.71692100

H 1.95635200 2.92790900 0.27946800

H -1.69252200 1.60645100 0.68368300

H 3.55232100 -1.83404000 0.45205700

**Conformer 54**

S 2.57261800 -1.52137700 -1.26136900

O 0.27272500 -0.71002400 1.91623300

O -1.78827400 -2.03958000 0.85600200

O -3.26883800 -1.20833000 -0.58125500

N -0.37797500 0.51336200 0.14651000

C -1.80845800 0.37280400 0.53686900

C -2.50264900 1.49314300 -0.23778200

C -1.67034000 1.61028700 -1.52030500

C -0.22838200 1.37784700 -1.04778000

C 0.58814700 0.02216900 0.96594400

C 2.06834400 0.39236500 0.80728600

C -2.36807100 -1.03247200 0.19877000

C 2.71019300 0.17916000 -0.57199600

C 2.32419400 1.82305600 1.32498700

H -1.87905300 0.49960900 1.62042600

H -2.45542500 2.41971100 0.34155000

H -3.54578400 1.25162400 -0.43347400

H -1.96708000 0.82828600 -2.22249600

H -1.78101100 2.57373100 -2.02000900

H 0.37003900 0.88552100 -1.81385400

H 0.25709000 2.31974900 -0.77639100

H 2.55262500 -0.30380000 1.49436600

H 2.37443000 0.90469700 -1.31128000

H 3.78757100 0.32415300 -0.46388100

H 1.91578000 1.94767400 2.33032200

H 3.39949700 2.01298800 1.37541000

H 1.88294900 2.58577000 0.67876700

H -1.05676000 -1.69195000 1.42427200

H 1.22629700 -1.57594800 -1.33118500

**Conformer 55**

S -3.98670000 -0.10282600 -0.23850700

O -1.14652800 -1.57547100 -0.75678200

O 1.64064100 1.46897000 -1.54211400

O 2.06472000 2.62284200 0.34269000

N 0.83986200 -0.75221000 -0.07992300

C 1.73622800 0.24011400 0.51776400

C 3.13566300 -0.44635200 0.48303900

C 2.81789300 -1.94090700 0.33170100

C 1.56569300 -1.94437100 -0.54548100

C -0.52392700 -0.68606200 -0.18633100

C -1.23662700 0.49769500 0.47728500

C 1.81707600 1.57915400 -0.20705200

C -2.47218300 0.94070400 -0.33245500

C -1.55228400 0.16388800 1.94721300

H 1.45007100 0.47016100 1.54623500

H 3.71468900 -0.20360200 1.37387800

H 3.69776800 -0.09587300 -0.38640400

H 3.64507000 -2.49869000 -0.11048300

H 2.59149800 -2.38492200 1.30535200

H 1.81422000 -1.85002000 -1.60888300

H 0.93417100 -2.82295500 -0.42580900

H -0.56966800 1.36578600 0.47208200

H -2.80060100 1.91360000 0.03989600

H -2.20289300 1.06558400 -1.38214600

H -0.63992300 -0.03666300 2.51495100

H -2.06680700 1.00328900 2.42201800

H -2.20166500 -0.70944900 2.01384200

H 1.75651700 2.35336200 -1.92217900

H -3.41014300 -1.21282800 -0.74123300

**Conformer 56**

S 2.31630600 -1.57559700 -1.31282200

O 0.25708500 -0.68875600 1.88870300

O -1.77105900 -2.07184500 0.93415000

O -3.14235000 -1.40502900 -0.68168900

N -0.37896400 0.52479400 0.10379200

C -1.82333400 0.31232000 0.40901300

C -2.55873300 1.33865300 -0.47004400

C -1.48005500 2.33779200 -0.91056100

C -0.22586800 1.46804200 -1.01713400

C 0.57326600 0.03479500 0.92987600

C 2.06122700 0.37419800 0.75997800

C -2.30728600 -1.14225400 0.14568600

C 2.68537100 0.08696300 -0.61546100

C 2.38920300 1.79752300 1.25502800

H -1.96207000 0.50627400 1.47745900

H -3.37978700 1.80934100 0.07154200

H -2.98631300 0.81889900 -1.32857700

H -1.72169800 2.83157000 -1.85325800

H -1.32678700 3.11189100 -0.15246000

H -0.20375800 0.92020900 -1.96605800

H 0.69198600 2.04168800 -0.92556500

H 2.52534700 -0.31937100 1.46537700

H 2.34770800 0.78068200 -1.38552700

H 3.76760000 0.20733500 -0.53664600

H 1.99856900 1.95063900 2.26347700

H 3.47278700 1.93734500 1.29218500

H 1.97840100 2.57785000 0.61015900

H -1.04926600 -1.66825600 1.47994700

H 2.80696500 -2.29324300 -0.28104000

**Conformer 57**

S -3.21173200 0.58955600 -1.29396700

O -0.38619500 -1.55785800 -0.58945300

O 2.49446600 -1.25907300 0.91022400

O 3.28235300 -1.41302000 -1.19012000

N 0.45004400 0.39665900 0.14860400

C 1.60326300 0.25790500 -0.74089000

C 2.32519000 1.61600000 -0.59774000

C 1.99884900 2.04737000 0.83971500

C 0.55385600 1.56606500 1.03864100

C -0.51541100 -0.57430700 0.12585100

C -1.75313900 -0.37931900 1.01299500

C 2.53429500 -0.90425200 -0.39618300

C -2.70382200 0.71311900 0.47155500

C -2.46807100 -1.71629400 1.22704900

H 1.27739200 0.06957700 -1.76375500

H 1.89489300 2.31832200 -1.31654200

H 3.39372300 1.54242900 -0.80189300

H 2.66048500 1.54241500 1.54723000

H 2.09764000 3.12318500 0.99376100

H 0.35145800 1.29341000 2.07651900

H -0.15731200 2.34610600 0.74451300

H -1.41721000 -0.01325200 1.99142600

H -3.59891400 0.74602600 1.09556100

H -2.23983500 1.69853800 0.52789800

H -1.80692000 -2.43595500 1.71304200

H -3.34948800 -1.57573400 1.85910200

H -2.77446000 -2.15785500 0.27814000

H 3.11481300 -1.99587700 1.01881300

H -3.78391200 -0.62895500 -1.23174300

**Conformer 58**

S 3.76214000 0.97601000 -0.18142400

O 0.75190800 1.07455900 -0.68848900

O -2.81236200 2.34858800 -0.10718300

O -1.93926900 1.13832500 1.57710700

N -0.72097400 -0.59215000 -0.31855100

C -1.83753200 0.26753900 -0.69827900

C -3.00109400 -0.72821200 -0.90535000

C -2.67311900 -1.86644000 0.07325600

C -1.14198400 -1.96396200 0.01491300

C 0.54823400 -0.08268300 -0.34113400

C 1.69038800 -1.00466800 0.09027100

C -2.16488600 1.27600100 0.40293700

C 2.98714600 -0.63940600 -0.65424400

C 1.84569600 -0.99741400 1.62223400

H -1.60148700 0.82925300 -1.60198200

H -2.97711000 -1.08646900 -1.93802500

H -3.97764900 -0.27416300 -0.73301000

H -2.98842600 -1.59708700 1.08381400

H -3.15606400 -2.80805300 -0.19328200

H -0.71710400 -2.29172200 0.96439000

H -0.82021800 -2.66430800 -0.76552600

H 1.44610300 -2.02647300 -0.22517900

H 3.72803700 -1.41820200 -0.47357500

H 2.79500800 -0.60078400 -1.72674700

H 0.93023600 -1.31989100 2.12244200

H 2.65275800 -1.67204400 1.92222100

H 2.09033000 0.00485800 1.97507300

H -3.01418100 2.94334600 0.63107600

H 4.94304200 0.45431400 0.21185300

**Conformer 59**

S -2.23933700 -0.88975000 1.58753500

O -0.09674700 -0.97252400 -1.87886500

O 3.16613100 -1.58800800 -0.43708400

O 1.39852100 -1.52570200 0.94893800

N 0.37732000 0.70880300 -0.47280300

C 1.79016500 0.34130900 -0.57425900

C 2.51640800 1.46373500 0.19929700

C 1.48868600 1.88225900 1.25914200

C 0.14652400 1.77664700 0.52407700

C -0.51336100 -0.05447300 -1.17532300

C -2.03506300 0.15708200 -1.10061400

C 2.04837400 -1.02273500 0.06605100

C -2.64967900 -0.94647800 -0.21138800

C -2.60038100 1.55229200 -0.80808100

H 2.10358700 0.27986100 -1.61602700

H 2.72277500 2.28795300 -0.48884300

H 3.46782200 1.13329000 0.61803300

H 1.50753100 1.18556300 2.10059000

H 1.66414100 2.88682400 1.64800900

H -0.66637400 1.51020300 1.19616800

H -0.09910400 2.71822700 0.02255800

H -2.33957800 -0.10873900 -2.11895400

H -3.73863300 -0.87205800 -0.24767200

H -2.36820600 -1.92669400 -0.59371000

H -2.08625300 2.32548900 -1.38408100

H -3.65336200 1.57458200 -1.10338500

H -2.55357600 1.81490700 0.24857200

H 3.29322900 -2.43463800 0.01756200

H -0.95913100 -1.30833400 1.47291600

**Conformer 60**

S -2.54054200 -0.43626000 1.73099800

O -0.15303100 -1.40204900 -1.57806000

O 1.79138900 -2.21347300 -0.00491700

O 3.21174100 -0.91402600 1.10669800

N 0.43775900 0.45565100 -0.45731900

C 1.88712300 0.14529800 -0.62688600

C 2.57527400 1.45799500 -0.24934800

C 1.65015700 2.03847600 0.82711400

C 0.24866100 1.71949200 0.29811400

C -0.49273500 -0.33131300 -1.03959700

C -1.99600800 -0.00892400 -1.08295900

C 2.36198700 -1.03898900 0.26182300

C -2.74750400 -0.87592800 -0.04877200

C -2.46880400 1.44778400 -1.11688900

H 2.05593200 -0.14297100 -1.66811300

H 2.61461700 2.11668700 -1.12211300

H 3.58759200 1.28310500 0.10933400

H 1.82634100 1.52974400 1.77751200

H 1.78801700 3.10959400 0.98312400

H -0.48420700 1.57927700 1.09088600

H -0.09376000 2.50844700 -0.37577800

H -2.26885000 -0.45270200 -2.04691700

H -3.81431300 -0.87445700 -0.27689900

H -2.39854800 -1.90627000 -0.12083700

H -1.92060200 2.02960100 -1.86145900

H -3.52397900 1.46639500 -1.40521300

H -2.38330800 1.95313700 -0.15534800

H 1.09598500 -2.09335900 -0.70249900

H -3.40624500 0.59740800 1.75420800

**Conformer 61**

S -3.98513500 0.76400100 -0.13813400

O -0.52972300 -2.29366000 -0.69414800

O 1.15097400 1.72338000 -1.41232100

O 1.79529000 2.78426900 0.44001400

N 1.01079600 -0.71538200 -0.19709800

C 1.50489000 0.40547800 0.62666700

C 2.94469400 -0.01873100 0.99388900

C 3.37992500 -0.87432400 -0.20445700

C 2.10831700 -1.64431500 -0.57200600

C -0.28641900 -1.19878200 -0.21283400

C -1.39905300 -0.32046500 0.36939800

C 1.49877800 1.75996200 -0.11063400

C -2.59933600 -0.35527500 -0.59585400

C -1.75951500 -0.83696300 1.77395400

H 0.90269900 0.54652100 1.52386100

H 2.91405000 -0.62532400 1.90286100

H 3.58174600 0.84441600 1.18382100

H 3.69858800 -0.23582300 -1.03386100

H 4.20809000 -1.54330000 0.03277700

H 2.04146000 -1.90677600 -1.62824500

H 2.00484300 -2.57064700 0.00066300

H -1.06109200 0.71626600 0.44794300

H -2.28780300 -0.11890300 -1.61381900

H -3.03063700 -1.35620300 -0.61786000

H -0.91481400 -0.75681100 2.46385300

H -2.58819300 -0.25757900 2.18369700

H -2.05618000 -1.88739600 1.72334400

H 0.94261700 0.80033700 -1.63644400

H -3.35479700 1.92345700 -0.41988100

**Conformer 62**

S -4.54038200 0.20070500 -0.19266800

O -0.30772100 -1.39025600 -1.09044400

O 2.40315200 -1.49850100 1.14824700

O 4.00486400 -1.22381800 -0.37323100

N 0.72316500 0.32830200 -0.02830000

C 2.00387600 0.05702500 -0.71537000

C 2.67420300 1.44049200 -0.79810000

C 2.16497900 2.14660200 0.46637500

C 0.70324300 1.69249200 0.55764700

C -0.39841400 -0.40472100 -0.37461600

C -1.73435700 0.01689500 0.24512000

C 2.90530400 -0.95221900 0.02413400

C -2.87516600 -0.39848400 -0.69889800

C -1.86474100 -0.62427000 1.64026500

H 1.80866800 -0.38106500 -1.69485000

H 2.32287500 1.95994500 -1.69393900

H 3.75860000 1.35852200 -0.85460500

H 2.72439200 1.80552600 1.34240100

H 2.25102800 3.23308700 0.41899500

H 0.32650500 1.67894300 1.58206400

H 0.05899600 2.35026600 -0.03555500

H -1.75889100 1.10439500 0.35920000

H -2.68015300 -0.06508400 -1.71764300

H -2.95945800 -1.48477300 -0.73287400

H -1.08839400 -0.26865400 2.32296000

H -2.83455000 -0.37762500 2.07522000

H -1.78525700 -1.71237700 1.56735100

H 1.50493100 -1.15503200 1.27413100

H -4.34125000 1.50226600 -0.48799400

**Conformer 63**

S -4.51863700 0.31844500 -0.26438100

O -0.30512800 -1.38647700 -1.09270000

O 2.40822700 -1.50631400 1.13938100

O 4.00691000 -1.22286200 -0.38387800

N 0.72550300 0.32676500 -0.02179500

C 2.00528400 0.06088200 -0.71311300

C 2.67485000 1.44529100 -0.78772700

C 2.16648500 2.14341200 0.48151500

C 0.70507900 1.68837200 0.57124300

C -0.39628100 -0.40402900 -0.37236800

C -1.73259600 0.02023900 0.24486600

C 2.90837600 -0.95312500 0.01749000

C -2.87069100 -0.36959700 -0.71304900

C -1.87508300 -0.63582100 1.63105700

H 1.80842400 -0.37052100 -1.69523800

H 2.32244000 1.97016500 -1.67992800

H 3.75923600 1.36412800 -0.84581300

H 2.72694700 1.79732900 1.35494300

H 2.25185700 3.23018200 0.44052300

H 0.32906600 1.66912300 1.59584600

H 0.05967000 2.34847300 -0.01767100

H -1.75467100 1.10540500 0.37256900

H -2.67611500 0.03040000 -1.70908400

H -2.94216100 -1.45106900 -0.81566600

H -1.06340500 -0.34214600 2.30200200

H -2.81191300 -0.33039400 2.10078200

H -1.86711300 -1.72571400 1.54237200

H 1.51067300 -1.16214000 1.26819900

H -4.82586800 -0.56420200 0.70691400

**Conformer 64**

S 2.33673000 -1.85267700 -0.86378700

O 0.28500900 -0.46357900 1.96069100

O -3.09562400 -1.54447100 0.83401500

O -1.39483500 -1.74228700 -0.62168400

N -0.38265000 0.76398300 0.20498600

C -1.76541500 0.39205000 0.50268700

C -2.60395400 1.32479400 -0.40074400

C -1.67206200 1.60049000 -1.58852500

C -0.28814700 1.69342700 -0.93504300

C 0.60029700 0.24304800 1.00997100

C 2.08528300 0.52094000 0.73115200

C -2.01834500 -1.07777700 0.16758100

C 2.60822500 -0.05292600 -0.59949600

C 2.47049700 2.00392900 0.88818800

H -1.98787200 0.52829400 1.56093700

H -2.81672000 2.24768300 0.14529200

H -3.55795300 0.88091300 -0.68730100

H -1.69540200 0.76409400 -2.29115800

H -1.93215100 2.50994500 -2.13292200

H 0.50582100 1.40954100 -1.62299800

H -0.09219500 2.71322400 -0.58452900

H 2.57300700 -0.03868800 1.53158400

H 2.23425800 0.49517000 -1.46432800

H 3.69538300 0.05591500 -0.61207100

H 2.09677000 2.40532000 1.83365400

H 3.55940600 2.10370600 0.89371300

H 2.08905700 2.62873800 0.07781500

H -3.22099100 -2.46956200 0.57285600

H 0.98578200 -1.82450800 -0.87364200

**Conformer 65**

S -4.36402300 0.64348800 -0.15291800

O -0.20932800 -1.44517600 -1.14237800

O 2.62649700 -1.52442400 0.96192200

O 4.12376700 -0.82936400 -0.53135200

N 0.69129000 0.22564500 0.10040200

C 1.95375100 0.18955200 -0.66857700

C 2.44335800 1.64702000 -0.63684800

C 1.94646800 2.14605100 0.72770600

C 0.56425900 1.49390400 0.86663000

C -0.36504100 -0.57122900 -0.30276400

C -1.73008800 -0.35054900 0.35727400

C 3.01171300 -0.76797500 -0.08366500

C -2.71141700 0.09421800 -0.74784800

C -2.16792600 -1.64670900 1.05521100

H 1.75291400 -0.17153200 -1.67809100

H 1.96732300 2.20661700 -1.44686300

H 3.52284300 1.71101500 -0.76528400

H 2.61233100 1.79746500 1.52258700

H 1.89016700 3.23334700 0.79570400

H 0.29530000 1.30219400 1.90692700

H -0.20989800 2.12806800 0.42356300

H -1.67525900 0.44638500 1.10032100

H -2.32094300 0.96922000 -1.27249000

H -2.83423100 -0.69613700 -1.48800300

H -1.45386200 -1.93710900 1.83069000

H -3.13791700 -1.51071700 1.53723900

H -2.23462400 -2.46468700 0.33495800

H 1.69593000 -1.32610500 1.14925800

H -4.88268200 -0.57733000 0.08510500

**Conformer 66**

S 4.08833400 -0.64253700 -0.74791500

O -0.10654400 -1.31392900 1.52469000

O -3.46134100 -1.73001500 0.19913900

O -1.83198100 -1.41712500 -1.32052500

N -0.66252100 0.53917900 0.38698600

C -2.07248500 0.16912400 0.51457900

C -2.82210800 1.40249400 -0.03471700

C -1.84599100 1.97520600 -1.07245600

C -0.47261400 1.75552400 -0.42453700

C 0.26641300 -0.30312900 0.93760700

C 1.77384300 -0.02213600 0.80926400

C -2.39368000 -1.07676100 -0.31127100

C 2.26052400 -0.46930400 -0.58382100

C 2.23027400 1.38821200 1.21123600

H -2.32438800 -0.04637600 1.55253100

H -2.98071700 2.11299800 0.78107100

H -3.79846000 1.14783600 -0.44886400

H -1.91163100 1.40965500 -2.00450100

H -2.03085100 3.02718900 -1.29661900

H 0.31271000 1.62014000 -1.16842400

H -0.20206600 2.60439500 0.21218300

H 2.19783100 -0.72481200 1.52943600

H 1.87961200 -1.46893800 -0.79845600

H 1.90753400 0.18863100 -1.37876200

H 1.74086700 1.70905600 2.13442400

H 3.30610000 1.38264100 1.39879000

H 2.03322800 2.13863600 0.44289600

H -3.63513800 -2.49219300 -0.37384400

H 4.38353500 0.67066100 -0.82585700

**Conformer 67**

S -1.11926142 -4.43840872 -1.22590676

O -1.51809292 0.05022749 -0.20629513

O 2.40822700 -1.50631400 1.13938100

O 4.00691000 -1.22286200 -0.38387800

N 0.72550300 0.32676500 -0.02179500

C 2.00528400 0.06088200 -0.71311300

C 2.67485000 1.44529100 -0.78772700

C 2.16648500 2.14341200 0.48151500

C 0.70507900 1.68837200 0.57124300

C -0.39628100 -0.40402900 -0.37236800

C -0.16884894 -1.75969030 -1.04851592

C 2.90837600 -0.95312500 0.01749000

C -1.35903459 -2.68074863 -0.73237803

C 0.02358057 -1.53945781 -2.56070351

H 1.80842400 -0.37052100 -1.69523800

H 2.32244000 1.97016500 -1.67992800

H 3.75923600 1.36412800 -0.84581300

H 2.72694700 1.79732900 1.35494300

H 2.25185700 3.23018200 0.44052300

H 0.32906600 1.66912300 1.59584600

H 0.05967000 2.34847300 -0.01767100

H 0.73534719 -2.22639321 -0.64976993

H -1.52272475 -2.72554217 0.34518506

H -2.27727985 -2.29905741 -1.17550029

H 0.87795626 -0.88977271 -2.76851309

H 0.20920227 -2.49118353 -3.06204214

H -0.86781903 -1.08145292 -2.99823471

H 1.51067300 -1.16214000 1.26819900

H -1.38030337 -4.29536149 -2.54054176

**Conformer 68**

S -3.76005700 -0.94159600 -0.19297300

O -0.75451100 -1.05186400 -0.75708400

O 1.77547200 -1.16601300 1.50798400

O 2.85204700 -2.36470800 -0.06048000

N 0.74325600 0.57348800 -0.31045800

C 1.85171600 -0.28002100 -0.73606900

C 3.02310600 0.71385300 -0.90506000

C 2.70655200 1.81897100 0.11353100

C 1.17713900 1.93369600 0.05438300

C -0.53440900 0.08775300 -0.36522900

C -1.66526600 1.01246800 0.09221000

C 2.20576600 -1.39633500 0.24665400

C -2.97015000 0.67103300 -0.64921800

C -1.81327300 0.98123900 1.62457500

H 1.60693100 -0.78979200 -1.66817600

H 3.00044500 1.11256100 -1.92279100

H 3.99363800 0.24072500 -0.75432900

H 3.01745400 1.51184700 1.11514000

H 3.19929000 2.76489600 -0.11711200

H 0.75156100 2.24652600 1.00864500

H 0.86608100 2.65465100 -0.71153400

H -1.41332700 2.03738000 -0.20714800

H -3.70177600 1.45568700 -0.45651900

H -2.78398300 0.64151100 -1.72286100

H -0.89382400 1.28943100 2.12650500

H -2.61356200 1.65692500 1.93979800

H -2.06569600 -0.02466000 1.96162100

H 2.04206400 -1.93145600 2.03996100

H -4.91831400 -0.41039000 0.25155500

**Conformer 69**

S -3.92546200 0.57522200 -0.03153000

O -0.34770400 -2.29464200 -0.81696000

O 0.86466300 1.86177300 -1.41518700

O 1.13476700 2.88504200 0.54804100

N 1.12345400 -0.64810900 -0.29580900

C 1.53410400 0.51875500 0.51224700

C 3.08036200 0.39712200 0.59107700

C 3.34098100 -1.10034200 0.38911700

C 2.28708300 -1.50034500 -0.64453900

C -0.14500600 -1.20867400 -0.29809200

C -1.28759500 -0.42897300 0.36158500

C 1.14508700 1.87152900 -0.09429700

C -2.49525700 -0.43402600 -0.59556700

C -1.60752300 -1.08224700 1.71845800

H 1.10228900 0.48381500 1.51421300

H 3.45654900 0.79441100 1.53314100

H 3.54166600 0.97169100 -0.21761100

H 4.35823700 -1.30815400 0.05320700

H 3.17464200 -1.64732500 1.32194400

H 2.62431900 -1.28464200 -1.66416400

H 1.98621300 -2.54563200 -0.60758200

H -1.00066000 0.61069200 0.53399100

H -2.20589200 -0.09268500 -1.59013700

H -2.87993500 -1.44845200 -0.70302100

H -0.75712400 -1.02302000 2.40336500

H -2.45456300 -0.57717000 2.18490000

H -1.85855200 -2.13633800 1.57898300

H 0.87871500 0.93949100 -1.72069300

H -3.34992700 1.78234500 -0.21247500

**Conformer 70**

S -3.97692000 -0.20747300 -0.23032900

O -1.26406000 -1.58115100 -0.56386900

O 2.61820200 2.34612400 0.09612100

O 1.78414200 1.20447800 -1.65559600

N 0.73403000 -0.78160400 0.10067000

C 1.66329600 0.22881500 0.58402900

C 2.92092100 -0.60142700 0.94431000

C 2.89728200 -1.73402200 -0.09257400

C 1.40506600 -2.04584100 -0.26200100

C -0.61520200 -0.65510200 -0.09681000

C -1.28600700 0.66219400 0.31073800

C 2.00105800 1.28163400 -0.47555800

C -2.53511700 0.90983800 -0.55460300

C -1.58202000 0.68830500 1.82128300

H 1.28412500 0.75523400 1.46087700

H 2.79243200 -0.99923500 1.95431500

H 3.83305100 -0.00416000 0.93106700

H 3.32038700 -1.38867500 -1.03924500

H 3.46781900 -2.60640600 0.22946300

H 1.13587800 -2.33467700 -1.27841300

H 1.06723000 -2.84331900 0.40716300

H -0.60500700 1.48895600 0.07754600

H -2.87759300 1.93287400 -0.39923200

H -2.27612500 0.79744500 -1.60685900

H -0.67255600 0.58019600 2.41727600

H -2.05190400 1.63623400 2.09875300

H -2.26482200 -0.11889700 2.08882200

H 2.84227200 2.96816400 -0.61289400

H -4.82460600 0.76509900 0.16580700

**Conformer 71**

S -3.96016600 -0.86346300 -0.21490700

O -0.77771500 -1.03330000 -0.88173900

O 1.85870200 -1.49263600 1.45321400

O 3.44123400 -1.95186200 -0.04334500

N 0.71806200 0.47158400 -0.08886500

C 1.84608900 -0.27709600 -0.68512000

C 2.86605000 0.81677400 -1.04475500

C 2.62949200 1.87778800 0.03896700

C 1.10508800 1.87579600 0.20563900

C -0.57572500 0.04125100 -0.33471000

C -1.71545900 0.93383200 0.16505100

C 2.46400600 -1.32513500 0.26180500

C -3.01953500 0.66846400 -0.61122300

C -1.87996000 0.80513000 1.69231700

H 1.49488500 -0.83347600 -1.55486600

H 2.63053300 1.22083400 -2.03320800

H 3.88201300 0.42555700 -1.06884400

H 3.11474600 1.58082700 0.97341800

H 3.00682200 2.86483000 -0.23217800

H 0.78967600 2.17447600 1.20649000

H 0.63865200 2.55451800 -0.51633400

H -1.44784600 1.97422600 -0.05498100

H -3.72334600 1.47380900 -0.39011000

H -2.82744000 0.68663700 -1.68440600

H -0.97394200 1.10655300 2.22308300

H -2.69628100 1.44537900 2.03609500

H -2.12562100 -0.22054200 1.97040000

H 1.09281600 -0.89845500 1.48890200

H -3.01749200 -1.71930200 -0.65575200

**Conformer 72**

S 4.08628600 -0.51718800 -0.77201200

O -0.08228900 -1.26321200 1.56861700

O -1.72768900 -1.45277100 -1.21819600

O -3.44627500 -1.80363400 0.18862200

N -0.68563600 0.52825500 0.35927400

C -2.09300100 0.15876800 0.54074900

C -2.86278500 1.36190400 -0.04841700

C -1.90702500 1.91459700 -1.11506900

C -0.52527900 1.73404600 -0.47435500

C 0.26428000 -0.26778600 0.94005200

C 1.76530200 0.04118900 0.79239600

C -2.49525200 -1.14603900 -0.14554500

C 2.25432400 -0.39028500 -0.60516400

C 2.20066400 1.45731900 1.19492400

H -2.31745100 0.00401300 1.59604100

H -3.02302100 2.10002000 0.74207300

H -3.84002700 1.07657500 -0.43870700

H -1.97491400 1.32207500 -2.03045400

H -2.10799900 2.95670200 -1.36919100

H 0.25932800 1.60354000 -1.21973900

H -0.26997800 2.60008000 0.14524900

H 2.20194100 -0.65594100 1.51145700

H 1.81805500 -1.35022100 -0.88158000

H 1.97128900 0.33212700 -1.37322000

H 1.76713000 1.73818700 2.15816600

H 3.28721300 1.48767100 1.29361500

H 1.92094800 2.21359600 0.45943200

H -2.06937800 -2.28609000 -1.57673000

H 4.23839900 -1.59045700 0.03108300

**Conformer 73**

S -2.49883700 -0.80121400 1.61139200

O -0.18306500 -0.97702300 -1.82171100

O 1.67218500 -2.24396000 -0.46692600

O 3.04988200 -1.32222900 1.01363300

N 0.43831500 0.51561100 -0.26402600

C 1.87671200 0.18457100 -0.48800700

C 2.65477400 1.34687000 0.15783200

C 1.59659400 2.41074800 0.49400900

C 0.33719600 1.58292400 0.74973300

C -0.50686300 -0.06202400 -1.03949400

C -2.00310900 0.28868600 -1.01789600

C 2.26304900 -1.19710900 0.11040900

C -2.76798500 -0.78679800 -0.21336400

C -2.48478600 1.70950700 -0.69976900

H 2.03179100 0.12422700 -1.56861000

H 3.43163700 1.72098900 -0.50971600

H 3.14279800 0.97952700 1.06132900

H 1.87218300 3.01955800 1.35671400

H 1.42909200 3.08163700 -0.35390200

H 0.35360900 1.13532300 1.74862100

H -0.58094100 2.14503800 0.64634500

H -2.26930100 0.08822300 -2.06130200

H -3.84004500 -0.61779700 -0.33204000

H -2.54492000 -1.77896900 -0.60278400

H -1.86703900 2.47102300 -1.18163900

H -3.50006800 1.82462000 -1.08999000

H -2.52848400 1.91004700 0.37164600

H 1.01642300 -1.92241300 -1.13952600

H -1.33905400 -1.48943300 1.60006900

**Conformer 74**

S -3.23267200 0.53438000 -1.16959700

O -1.13790900 -2.07305300 -0.17397300

O 2.12381600 2.44432600 0.76358000

O 1.23740600 1.72818800 -1.17675400

N 0.74230000 -0.84664500 0.00240300

C 1.62312100 0.13004500 0.63262400

C 3.02719800 -0.51694100 0.49720800

C 2.91890500 -1.31423200 -0.80964700

C 1.48649800 -1.85500400 -0.77949500

C -0.59543200 -1.06160900 0.24318900

C -1.38127300 0.00684900 1.01363800

C 1.61167000 1.49415300 -0.05788900

C -1.98236800 1.07597700 0.06532400

C -2.43479700 -0.65246300 1.90968000

H 1.37729900 0.28941900 1.68360200

H 3.18066000 -1.18766700 1.34663700

H 3.82934300 0.22196400 0.50398300

H 3.05808000 -0.65429800 -1.66958800

H 3.66026600 -2.11213800 -0.87497600

H 1.04210300 -1.96377900 -1.76925200

H 1.41958300 -2.82718300 -0.28064500

H -0.69401200 0.56709600 1.65743300

H -2.41989500 1.87186100 0.67155800

H -1.19988400 1.52378300 -0.54798600

H -1.96179300 -1.27429400 2.67374700

H -3.03563000 0.10882200 2.41603300

H -3.08996400 -1.29789900 1.32430600

H 2.13754500 3.27903700 0.27057800

H -4.20469000 0.19538000 -0.29931100

**Conformer 75**

S 4.06198600 0.02079800 -0.26897600

O 1.23673600 1.63619200 -0.49129800

O -1.73818300 -1.38908800 -1.59841200

O -2.77783200 -2.34310400 0.12715700

N -0.77177000 0.68893700 -0.10259900

C -1.67167100 -0.25895800 0.58119600

C -2.88084300 0.61618100 0.98323400

C -2.92767100 1.68417100 -0.11818000

C -1.45022100 1.97883400 -0.39246900

C 0.61106900 0.66476000 -0.09153400

C 1.30593200 -0.60206900 0.41626700

C -2.11836600 -1.43898200 -0.30626500

C 2.52206500 -0.96780600 -0.46274700

C 1.65451900 -0.45207400 1.90868800

H -1.20602300 -0.70212100 1.46065900

H -2.67563200 1.07801500 1.95276100

H -3.79171300 0.02559200 1.07529700

H -3.41540300 1.28763400 -1.01365000

H -3.47274200 2.57922300 0.18423500

H -1.24639400 2.29548300 -1.41573000

H -1.05088100 2.75064600 0.27212200

H 0.61704800 -1.44711300 0.31153200

H 2.83075300 -1.98528000 -0.21354400

H 2.23635800 -0.96654300 -1.51596600

H 0.75996000 -0.29539800 2.51752500

H 2.15256000 -1.35532000 2.26962000

H 2.32956200 0.38962700 2.06389800

H -1.20268300 -0.58756400 -1.72177100

H 3.51119900 1.20145800 -0.61390000

**Conformer 76**

S -2.34965300 -0.87716500 1.54078600

O -0.09888100 -0.96572700 -1.87007300

O 1.38951400 -1.51718100 0.91367500

O 3.17416800 -1.66558200 -0.44422700

N 0.41266100 0.67547100 -0.43062600

C 1.82942600 0.32902700 -0.58774500

C 2.56249200 1.43605000 0.20242600

C 1.55790000 1.81985100 1.29653600

C 0.20230400 1.72964400 0.58540000

C -0.49321900 -0.04652200 -1.15585400

C -2.00902400 0.22248300 -1.10766400

C 2.20430000 -1.05935800 -0.07168800

C -2.69445100 -0.87916900 -0.27297800

C -2.52560800 1.63072800 -0.79000700

H 2.10822400 0.32100600 -1.64136000

H 2.74476600 2.28177000 -0.46613900

H 3.52697600 1.10117000 0.58526100

H 1.59767600 1.10141000 2.11889400

H 1.73678700 2.81432700 1.70897500

H -0.60271400 1.45801500 1.26565000

H -0.04618100 2.68078300 0.10416700

H -2.29567600 -0.00053700 -2.14149200

H -3.77823000 -0.76579900 -0.34413400

H -2.43371300 -1.85963800 -0.66899200

H -1.97674100 2.39505400 -1.34513600

H -3.57374300 1.69884100 -1.09558100

H -2.48019700 1.87070100 0.27208900

H 1.72971100 -2.38848500 1.16924400

H -1.07425200 -1.31074400 1.45482200

**Conformer 77**

S -3.95864900 -0.25180000 -0.26494900

O -1.21087600 -1.55347400 -0.63172400

O 1.88846200 1.06101500 -1.62461300

O 2.39872200 2.48514700 0.03958600

N 0.75846100 -0.74785400 0.10878300

C 1.65977000 0.26723200 0.64219100

C 2.92499500 -0.55160700 1.00122700

C 2.94122600 -1.66769200 -0.05400000

C 1.45752300 -1.99065700 -0.27512800

C -0.58887100 -0.63816400 -0.10938100

C -1.29185400 0.64658000 0.34564300

C 2.01421100 1.40182300 -0.32320400

C -2.53689400 0.90757700 -0.52168300

C -1.60469300 0.59805700 1.85248800

H 1.25417600 0.75570000 1.52801800

H 2.78676900 -0.96960100 2.00174600

H 3.82662300 0.06190000 1.01565000

H 3.39198700 -1.30646000 -0.98124900

H 3.50810600 -2.54042400 0.27362900

H 1.22119200 -2.25057300 -1.30762500

H 1.11007600 -2.81312400 0.35753500

H -0.62593300 1.49864800 0.16303900

H -2.90145800 1.91557500 -0.32441100

H -2.26639100 0.84764400 -1.57559300

H -0.69933200 0.48130500 2.45259100

H -2.09605600 1.52309400 2.16683000

H -2.27369200 -0.23408200 2.07455100

H 2.15915100 1.82970300 -2.15043900

H -4.82900200 0.68407500 0.16853700

**Conformer 78**

S -2.62712600 1.11565700 -1.16466900

O -1.07676100 -2.09819800 -0.67300200

O 1.50975300 1.66092100 -1.02877700

O 1.49747800 2.47414900 1.06751800

N 0.68558400 -0.83631300 -0.07468200

C 1.43994000 0.07482700 0.78012600

C 2.86779000 -0.52560700 0.75189800

C 2.97907300 -1.12161000 -0.66006300

C 1.56087100 -1.62318100 -0.97002500

C -0.63780900 -1.19227300 0.01995300

C -1.53997900 -0.44789900 1.01932200

C 1.47071200 1.53225200 0.31423800

C -1.95141300 0.96395100 0.54079000

C -2.75859100 -1.31193500 1.36140400

H 1.04600500 0.10172200 1.79531800

H 2.91823300 -1.31235100 1.50923500

H 3.63835500 0.21169700 0.98298900

H 3.27500600 -0.35109700 -1.37408900

H 3.71560500 -1.92504600 -0.71096100

H 1.27266000 -1.47110200 -2.01124100

H 1.43022800 -2.68531700 -0.74658300

H -0.97602100 -0.28487800 1.94621300

H -2.67754600 1.37449100 1.24489900

H -1.10273300 1.64780400 0.53982500

H -2.45120500 -2.26462700 1.79656200

H -3.39537300 -0.79255800 2.08300200

H -3.34223300 -1.54363700 0.46996600

H 1.54813300 2.60879500 -1.23039400

H -3.69149400 0.30366200 -1.00903700

**Conformer 79**

S -4.51863700 0.31844500 -0.26438100

O -0.30512800 -1.38647700 -1.09270000

O 2.40822700 -1.50631400 1.13938100

O 4.00691000 -1.22286200 -0.38387800

N 0.72550300 0.32676500 -0.02179500

C 2.00528400 0.06088200 -0.71311300

C 2.67485000 1.44529100 -0.78772700

C 2.16648500 2.14341200 0.48151500

C 0.70507900 1.68837200 0.57124300

C -0.39628100 -0.40402900 -0.37236800

C -1.73259600 0.02023900 0.24486600

C 2.90837600 -0.95312500 0.01749000

C -2.87069100 -0.36959700 -0.71304900

C -1.87508300 -0.63582100 1.63105700

H 1.80842400 -0.37052100 -1.69523800

H 2.32244000 1.97016500 -1.67992800

H 3.75923600 1.36412800 -0.84581300

H 2.72694700 1.79732900 1.35494300

H 2.25185700 3.23018200 0.44052300

H 0.32906600 1.66912300 1.59584600

H 0.05967000 2.34847300 -0.01767100

H -1.75467100 1.10540500 0.37256900

H -2.67611500 0.03040000 -1.70908400

H -2.94216100 -1.45106900 -0.81566600

H -1.06340500 -0.34214600 2.30200200

H -2.81191300 -0.33039400 2.10078200

H -1.86711300 -1.72571400 1.54237200

H 1.51067300 -1.16214000 1.26819900

H -4.82586800 -0.56420200 0.70691400

**Conformer 80**

S 4.08173600 -0.62159000 -0.73083800

O -0.10687500 -1.27652300 1.57432700

O -1.73250700 -1.43964000 -1.22248400

O -3.46861200 -1.77384300 0.16699600

N -0.68272300 0.52593900 0.36762900

C -2.09515200 0.17120800 0.53755500

C -2.84668500 1.38473800 -0.05327800

C -1.87933700 1.92549800 -1.11563700

C -0.50194000 1.72540100 -0.47074200

C 0.25477500 -0.28336900 0.95163000

C 1.75992100 0.00953900 0.81362300

C -2.50669400 -1.12684400 -0.15635500

C 2.25207300 -0.46786400 -0.56698000

C 2.20151600 1.43447600 1.17917300

H -2.32899300 0.01532700 1.59061200

H -3.00037800 2.12405200 0.73742200

H -3.82597000 1.11268700 -0.44790200

H -1.95230700 1.33500100 -2.03190800

H -2.06522900 2.97049800 -1.36939800

H 0.28196100 1.57822600 -1.21416700

H -0.23341300 2.59003700 0.14524800

H 2.19099200 -0.66955600 1.55191900

H 1.88570900 -1.47874700 -0.75291500

H 1.88934000 0.16370100 -1.37890200

H 1.70679400 1.77431500 2.09261200

H 3.27683800 1.44457600 1.36935400

H 1.99898700 2.16266500 0.39107100

H -2.07960700 -2.26854800 -1.58603900

H 4.35965400 0.69297900 -0.84164400

**Conformer 81**

S -2.33724300 1.85125500 -0.82148900

O -0.24768500 0.19438300 2.08337800

O 1.49250600 1.77438400 -0.32794500

O 3.29188600 1.30649700 0.93517600

N 0.35490600 -0.65873100 0.09461000

C 1.76215600 -0.49481700 0.46682800

C 2.50997900 -1.39525300 -0.53838400

C 1.62606100 -1.33905900 -1.79104600

C 0.19582100 -1.28953300 -1.23053900

C -0.59661800 -0.29444200 1.01501100

C -2.09485400 -0.52631800 0.75438100

C 2.26981400 0.94606100 0.41226200

C -2.67763300 0.06403300 -0.53886800

C -2.46293900 -2.01663400 0.89550700

H 1.91943900 -0.80954700 1.49818600

H 2.54608600 -2.41154200 -0.13726600

H 3.53507800 -1.06521600 -0.70724300

H 1.83301300 -0.42966700 -2.36061800

H 1.77434500 -2.19084700 -2.45669600

H -0.45811600 -0.70573500 -1.87749200

H -0.22293700 -2.29628100 -1.13161700

H -2.55206100 0.01198700 1.58678100

H -2.39335600 -0.50595500 -1.42259800

H -3.76709000 0.01256600 -0.47517300

H -2.08526400 -2.41894600 1.83833100

H -3.54998400 -2.13525500 0.89334300

H -2.06375000 -2.62433300 0.07955900

H 1.90234500 2.65239300 -0.28721600

H -0.99059900 1.78108900 -0.75450700

**Conformer 82**

S -2.62032500 -0.36973800 1.64687900

O 0.09089900 -1.46009800 -1.52102200

O 3.34139100 -1.54929700 -0.08789500

O 1.63244100 -1.25047700 1.34457900

N 0.43243200 0.53335200 -0.55393100

C 1.86993100 0.25082900 -0.56265300

C 2.49821200 1.55546900 -0.02551500

C 1.41558200 2.10584000 0.91321700

C 0.10845100 1.77216100 0.18411400

C -0.39161800 -0.41839700 -1.08093100

C -1.92086900 -0.24800000 -1.17104300

C 2.21633200 -0.93181800 0.34166900

C -2.62148100 -1.06513000 -0.06432300

C -2.50542000 1.15452800 -1.37217000

H 2.20793400 0.00642600 -1.56949300

H 2.66807600 2.23779600 -0.86295500

H 3.45731200 1.38455700 0.46525500

H 1.44655300 1.58478900 1.87263500

H 1.51903200 3.17606900 1.10122900

H -0.71561600 1.60333600 0.87449100

H -0.16299800 2.57181600 -0.51332100

H -2.13173100 -0.81350900 -2.08529300

H -3.65987700 -1.24803400 -0.34477900

H -2.13187100 -2.03476800 0.02938600

H -1.97214200 1.69691700 -2.15688100

H -3.54904500 1.06554700 -1.68927700

H -2.48886800 1.76055000 -0.46681300

H 3.52845700 -2.26868200 0.53392600

H -3.64961500 0.48561200 1.47984500

**Conformer 83**

S -2.41168900 1.71661300 -0.97365200

O -0.15550100 0.36070900 2.03283600

O 3.34925500 1.07671900 1.08755600

O 1.85522600 1.75931300 -0.45081200

N 0.32697000 -0.62333500 0.07169700

C 1.75289100 -0.53046000 0.38115000

C 2.40312500 -1.43236300 -0.68964300

C 1.47568800 -1.26711600 -1.90207100

C 0.07231000 -1.13653100 -1.28598900

C -0.56392900 -0.17246900 1.00567500

C -2.07368900 -0.44644800 0.86984600

C 2.27578300 0.90193100 0.28053800

C -2.80608900 0.01210500 -0.39952800

C -2.37103100 -1.93091400 1.16412900

H 1.94153700 -0.87999500 1.39556600

H 2.39540600 -2.46475800 -0.32977900

H 3.43859500 -1.15838400 -0.89629100

H 1.72438600 -0.35198400 -2.44314700

H 1.54002500 -2.10211500 -2.60185000

H -0.54107700 -0.43864700 -1.85575700

H -0.43625700 -2.10585100 -1.24476700

H -2.48043500 0.13930500 1.69807400

H -2.58914800 -0.62657200 -1.25641200

H -3.88025000 -0.06024000 -0.21742600

H -1.92565400 -2.22962500 2.11560100

H -3.45008000 -2.09516400 1.23169500

H -1.98237300 -2.58962500 0.38284900

H 3.65628100 1.98761500 0.96366200

H -2.49490800 2.31324600 0.23324700

**Conformer 84**

S -2.56185700 -0.58099000 1.68949500

O -0.05697200 -1.22211400 -1.71545000

O 1.87634400 -2.23187400 -0.25471400

O 3.17031700 -1.09649300 1.15107300

N 0.43869900 0.44505700 -0.29560100

C 1.90055500 0.19705900 -0.46496200

C 2.58030400 1.45985600 0.09898300

C 1.44455700 2.47227600 0.32060100

C 0.23981700 1.58131100 0.62232900

C -0.45034200 -0.25880000 -1.02929700

C -1.96355500 0.01658000 -1.08398700

C 2.37951400 -1.10265600 0.24264500

C -2.71223300 -0.92581800 -0.11549300

C -2.49424900 1.45599700 -1.06901000

H 2.08444900 0.06481900 -1.53491200

H 3.35025700 1.83008800 -0.57873800

H 3.06529900 1.20218300 1.04124100

H 1.65671200 3.16961700 1.13280500

H 1.25350900 3.05560300 -0.58529900

H 0.26064300 1.21753800 1.65411100

H -0.71372000 2.06477000 0.45429600

H -2.19413200 -0.38825600 -2.07484400

H -3.77256000 -0.94388500 -0.37192100

H -2.33197900 -1.94104900 -0.23386500

H -1.87434000 2.12172200 -1.67426500

H -3.49769200 1.46244300 -1.50431200

H -2.57802500 1.87769700 -0.06664400

H 1.19847000 -2.01407100 -0.94630600

H -3.45179300 0.43023200 1.74781500

**Conformer 85**

S 2.45648500 -1.54324200 -1.19422000

O 0.06278800 -0.67574500 1.88143000

O -1.58138000 -1.81855600 -0.59328400

O -3.20887100 -1.49973600 0.92833800

N -0.39974000 0.60572000 0.09957700

C -1.83706900 0.38128500 0.31473900

C -2.51610400 1.17906500 -0.82588700

C -1.47408300 2.24072400 -1.20214500

C -0.14653300 1.49345100 -1.04337700

C 0.48151400 0.03706900 0.97524700

C 1.98861400 0.34218200 0.90523100

C -2.27758700 -1.07613000 0.29320100

C 2.70895600 0.11337300 -0.43120800

C 2.29417100 1.74434700 1.47209900

H -2.12648200 0.75862700 1.29791900

H -3.47057600 1.59638500 -0.50583900

H -2.70408500 0.52253300 -1.67964800

H -1.61269200 2.63330600 -2.21108200

H -1.51411600 3.08077000 -0.50241700

H 0.08295400 0.90941600 -1.94290300

H 0.68495900 2.16784900 -0.84591400

H 2.39548300 -0.38336200 1.61427500

H 2.39630100 0.81542200 -1.20402300

H 3.77918100 0.26885800 -0.28011800

H 1.82978400 1.86827800 2.45286200

H 3.37307800 1.87486100 1.59314800

H 1.93579700 2.54785300 0.82328300

H -1.93022200 -2.72109700 -0.54689100

H 2.86349400 -2.26777200 -0.13145400

**Conformer 86**

S 2.42208300 1.73859000 0.89551400

O 0.18003900 0.25346100 -2.06137600

O -1.67622100 1.75422400 0.32710000

O -3.34831600 1.17844300 -1.06226700

N -0.36391300 -0.62437100 -0.06602500

C -1.78380000 -0.53544200 -0.41201000

C -2.46288800 -1.38970300 0.67905500

C -1.56106800 -1.19022200 1.90535900

C -0.14336200 -1.08411100 1.31653300

C 0.55554100 -0.23640000 -1.00119700

C 2.05745800 -0.52650100 -0.81627600

C -2.35489700 0.88214900 -0.44878900

C 2.76855700 -0.01300500 0.44372400

C 2.33778100 -2.02871200 -1.02578100

H -1.95189000 -0.93310000 -1.41247600

H -2.45517600 -2.43496000 0.35866200

H -3.50048600 -1.10008500 0.84779700

H -1.81800000 -0.25960400 2.41588700

H -1.64340300 -2.00279300 2.62909700

H 0.45815100 -0.36578100 1.87410300

H 0.36506400 -2.05410400 1.32689200

H 2.49247900 0.00802300 -1.66457300

H 2.50506600 -0.58545500 1.33347000

H 3.84460600 -0.13136500 0.30172600

H 1.90646600 -2.37058300 -1.96911500

H 3.41526300 -2.21175000 -1.06304100

H 1.92426100 -2.64030000 -0.21956400

H -2.10889600 2.61649500 0.23325100

H 2.63661100 2.26119000 -0.32953200

**Conformer 87**

S -2.00231900 1.90746000 -0.82195200

O -0.42746000 0.05087500 2.13693600

O 1.46027600 1.94039900 -0.08589000

O 3.44604900 1.20869500 0.58361100

N 0.31560700 -0.59263700 0.10547200

C 1.71395500 -0.44187100 0.54396200

C 2.47273600 -1.46314100 -0.31773400

C 1.69526800 -1.43738700 -1.64018200

C 0.22923100 -1.28656600 -1.20007500

C -0.69165800 -0.35296000 1.01151700

C -2.16976100 -0.55141600 0.63015800

C 2.28793400 0.97941800 0.35512700

C -2.64758400 0.19035800 -0.62807300

C -2.59408300 -2.03219000 0.60713000

H 1.78680000 -0.64995800 1.61133100

H 2.40651600 -2.44961100 0.14965000

H 3.52461500 -1.20087900 -0.41932100

H 1.99940800 -0.57389400 -2.23846000

H 1.84523200 -2.33084700 -2.24807300

H -0.34692000 -0.70926400 -1.92413000

H -0.24352300 -2.26511600 -1.08188100

H -2.67446800 -0.08849800 1.48183800

H -2.35258300 -0.31543000 -1.54777200

H -3.73818100 0.22829000 -0.62595600

H -2.28331400 -2.53383300 1.52625700

H -3.68286200 -2.10705600 0.53913500

H -2.17435500 -2.57741200 -0.24103900

H 0.55119900 1.61056500 -0.20102100

H -2.39685900 2.36681400 0.38413100

**Conformer 88**

S 2.58794500 -0.26137900 1.61926600

O 1.13135400 1.91187500 -1.50157800

O -2.12918100 -2.29599700 0.55907000

O -2.36082100 -1.06093100 -1.30730400

N -0.44235300 0.81840400 -0.33606200

C -0.99334300 -0.21567000 0.53493100

C -1.84715100 0.59719100 1.53978800

C -2.38970300 1.74495100 0.67729000

C -1.22432600 2.07433700 -0.26377800

C 0.75729600 0.85921600 -0.99212100

C 1.69892600 -0.35725800 -1.12543200

C -1.88794200 -1.20532900 -0.21052600

C 2.91609700 -0.16895200 -0.19832400

C 1.14072600 -1.78459300 -1.09351400

H -0.21011200 -0.76570500 1.05241500

H -1.18545700 0.97674800 2.32308000

H -2.62006600 -0.00756800 2.01497900

H -3.25880800 1.41049800 0.10564500

H -2.69266400 2.60895800 1.27073800

H -1.54667300 2.37487000 -1.26162800

H -0.58413700 2.87050500 0.12583400

H 2.09817100 -0.19697800 -2.13311500

H 3.64142400 -0.96316500 -0.38622700

H 3.40149700 0.78374400 -0.40368400

H 0.25106700 -1.87929700 -1.71861000

H 1.89477100 -2.46504600 -1.49998000

H 0.90671400 -2.13399000 -0.08706500

H -2.72787000 -2.87455100 0.06264500

H 2.16719800 1.01127900 1.76776000

**Conformer 89**

S -2.37242300 1.27054300 -1.13922000

O -1.20513000 -2.04925600 -0.66382100

O 1.00178600 1.86867400 -0.82797100

O 2.25658000 2.25786300 0.96756800

N 0.58721400 -0.77692800 -0.16721700

C 1.42191600 0.01930900 0.74473600

C 2.78214900 -0.70938200 0.71427400

C 2.86406500 -1.20961200 -0.73480000

C 1.42372300 -1.62865500 -1.05559200

C -0.72881700 -1.15612000 0.01770900

C -1.58144300 -0.42192200 1.06653600

C 1.60050300 1.49125200 0.31472700

C -1.95237200 1.02091000 0.64041400

C -2.83153500 -1.24887100 1.38925500

H 1.01013300 0.04484800 1.75369300

H 2.74840300 -1.55181500 1.41061800

H 3.59909800 -0.05179200 1.00853600

H 3.18963000 -0.40115900 -1.39589700

H 3.56382900 -2.03714700 -0.85836800

H 1.14829200 -1.47882400 -2.10053800

H 1.23131600 -2.67766700 -0.81714100

H -0.99778300 -0.32547800 1.98973400

H -2.78836200 1.36343600 1.25151800

H -1.13040800 1.71744300 0.80646600

H -2.56306500 -2.25422800 1.71699300

H -3.39998900 -0.76369000 2.18681500

H -3.47561300 -1.35851400 0.51547600

H 0.45991800 1.13712100 -1.17418900

H -3.16215100 0.18757800 -1.28544600

**Conformer 90**

S 2.56191100 -0.47121100 1.59376800

O 0.97311100 2.23891700 -1.22567600

O -1.90617600 -2.45864000 0.24127800

O -2.29422600 -1.00002500 -1.42734900

N -0.50594700 0.88005200 -0.22717800

C -0.96220200 -0.29950300 0.50026100

C -1.86019200 0.30311300 1.60873500

C -2.50293100 1.50940700 0.90973800

C -1.38005500 2.05085500 0.01630900

C 0.68578200 1.10314600 -0.85928100

C 1.72042800 -0.00867000 -1.14479500

C -1.78313500 -1.25120300 -0.36776000

C 2.88608500 0.08121300 -0.13972300

C 1.24933600 -1.44104100 -1.42026400

H -0.13037100 -0.84559800 0.93993400

H -1.21421600 0.62671000 2.42901500

H -2.57704300 -0.41715100 2.00459300

H -3.35266400 1.18743900 0.30273000

H -2.86150300 2.26051300 1.61523400

H -1.73919000 2.45627400 -0.93061500

H -0.79527500 2.83306100 0.50741600

H 2.15441300 0.36073900 -2.08024500

H 3.74339800 -0.48155500 -0.51215700

H 3.19359700 1.12266800 -0.04086700

H 0.42211300 -1.45242200 -2.13260000

H 2.07300200 -2.00624100 -1.86709800

H 0.93937500 -1.98148600 -0.52502700

H -2.46713600 -3.01149200 -0.32378200

H 2.66219000 -1.79836600 1.37809200

**Conformer 91**

S -2.56721000 -0.49076200 1.61944000

O 0.05851700 -1.33962200 -1.63545100

O 1.51208100 -1.32531600 1.18732600

O 3.30039900 -1.63602700 -0.13976400

N 0.45524800 0.56445700 -0.52041200

C 1.89193700 0.26857200 -0.58197000

C 2.54270200 1.51246500 0.06347500

C 1.47914800 1.99750400 1.05751300

C 0.15996200 1.74561300 0.31794800

C -0.39433500 -0.32200400 -1.11546300

C -1.91957000 -0.10638000 -1.18491800

C 2.31037000 -1.01106700 0.14139900

C -2.63694800 -1.00284100 -0.15434100

C -2.47401300 1.32069000 -1.25827300

H 2.20959000 0.12499900 -1.61471500

H 2.71493100 2.26346900 -0.71251700

H 3.50475400 1.28338100 0.52302400

H 1.51203600 1.39915400 1.97082300

H 1.60055800 3.04664200 1.33298600

H -0.66150300 1.53545300 1.00044300

H -0.10277100 2.60404700 -0.30916000

H -2.14511700 -0.58281800 -2.14542000

H -3.68810300 -1.11020200 -0.42604800

H -2.19025100 -1.99718600 -0.17377600

H -1.92886400 1.91970700 -1.99186800

H -3.51867900 1.28196000 -1.58183500

H -2.44666200 1.84477500 -0.30315700

H 1.86775600 -2.13778300 1.57815000

H -3.56255000 0.41780200 1.57581000

**Conformer 92**

S 4.00647500 0.31540500 -0.68873500

O 0.45963100 -2.35885700 1.16265300

O -1.68900400 2.65997100 -0.28379200

O -2.19104100 1.27083900 1.41531800

N -0.82281000 -0.86167900 0.09165700

C -1.15928700 0.36906300 -0.60822400

C -2.25563200 -0.09032800 -1.60153500

C -3.01134700 -1.16275300 -0.80201700

C -1.91553800 -1.85723300 0.01992200

C 0.35663100 -1.23680500 0.68153700

C 1.58549400 -0.30426200 0.70477000

C -1.72913000 1.44501600 0.31956700

C 2.28908900 -0.35368100 -0.66670900

C 1.36093800 1.11719500 1.24080800

H -0.30623400 0.79320800 -1.13509600

H -1.76529600 -0.52836100 -2.47490900

H -2.88354700 0.73314900 -1.94387800

H -3.74352900 -0.69414200 -0.14056800

H -3.54487300 -1.86271300 -1.44662400

H -2.24362000 -2.13251200 1.02308700

H -1.53726600 -2.76320200 -0.46094100

H 2.24045900 -0.82006800 1.40942000

H 2.41185900 -1.39361200 -0.97494700

H 1.71813500 0.15348900 -1.44686700

H 0.71318000 1.10693500 2.11973100

H 2.31898900 1.54500700 1.54392600

H 0.92529500 1.79458100 0.50205300

H -2.09764900 3.29861700 0.32044500

H 3.68617500 1.62199700 -0.59880400

**Conformer 93**

S 3.02266700 -0.58497500 -1.20579500

O 1.26986100 -1.03641500 1.98621600

O -2.38082500 1.85054700 -1.19207900

O -2.62413300 1.02907400 0.88985800

N -0.35040700 -0.66374200 0.47976100

C -1.02435800 -0.01651300 -0.63435600

C -1.71475900 -1.20161200 -1.35436900

C -2.11428800 -2.12028700 -0.18972200

C -0.96585000 -1.96559700 0.81924500

C 0.81617400 -0.31689900 1.10364500

C 1.58456800 0.96931800 0.73793300

C -2.08182600 0.99287700 -0.18233500

C 2.23867200 0.98954000 -0.65687600

C 0.80719200 2.27312500 0.99414700

H -0.33118600 0.49177600 -1.30031000

H -0.97408300 -1.68560300 -1.99572700

H -2.55208700 -0.88542700 -1.97803000

H -3.05581600 -1.78505500 0.25090300

H -2.24339000 -3.15665800 -0.50507700

H -1.30631200 -1.96578700 1.85560300

H -0.20878700 -2.74748800 0.71984600

H 2.40175300 0.93387800 1.46246700

H 1.52254800 1.22239900 -1.44753600

H 2.98877700 1.78266300 -0.67453600

H 0.32204700 2.25383100 1.97217700

H 1.49576400 3.12263000 0.97765300

H 0.04277800 2.46460300 0.23804700

H -3.08860100 2.43389100 -0.87777700

H 3.68439600 -0.84322100 -0.05914100

**Conformer 94**

S -3.99610800 0.36291400 0.72304000

O -0.45933900 -2.23066200 -1.29499200

O 2.22178400 1.15885900 -1.34693800

O 1.79873700 2.65957000 0.27321300

N 0.80830400 -0.82320200 -0.09324400

C 1.15395400 0.36968600 0.66967300

C 2.22077500 -0.15776700 1.65998800

C 2.97356300 -1.20914500 0.83021000

C 1.88745300 -1.83542000 -0.05863000

C -0.36110300 -1.14678600 -0.73044000

C -1.58741500 -0.21163300 -0.70100800

C 1.73848800 1.52978700 -0.14251400

C -2.27684600 -0.30213200 0.67661100

C -1.37106800 1.22624700 -1.19277100

H 0.29988400 0.78223000 1.20311200

H 1.70331300 -0.62576400 2.50156400

H 2.85396600 0.63863700 2.05220400

H 3.73881300 -0.72905800 0.21606700

H 3.46974400 -1.95354800 1.45451700

H 2.23602700 -2.05403700 -1.06912200

H 1.48608800 -2.76403800 0.35511900

H -2.24728000 -0.70592300 -1.41761600

H -2.30360400 -1.33626000 1.02179400

H -1.75180500 0.28484300 1.43351000

H -0.82000700 1.23619400 -2.13603600

H -2.34125500 1.69554000 -1.36551600

H -0.83927400 1.85424600 -0.47541400

H 2.58942200 1.95326200 -1.76465500

H -4.55069400 -0.59969000 -0.04243200

**Conformer 95**

S -3.03597100 0.93175400 -1.23628300

O -0.52467300 -1.45314600 -0.90209700

O 2.55810100 -1.66990400 0.56425500

O 3.71830000 -0.76772600 -1.10675000

N 0.49292500 0.13957900 0.33941400

C 1.60168000 0.25856100 -0.63131300

C 2.12188100 1.69121800 -0.41388400

C 1.85817900 1.93196500 1.07909900

C 0.49545700 1.26463700 1.30537400

C -0.58621800 -0.66699900 0.02855800

C -1.83101100 -0.58487900 0.92525000

C 2.72794400 -0.77504600 -0.42841300

C -2.76812600 0.59297700 0.55361500

C -2.57643900 -1.92494600 0.90140900

H 1.22418900 0.09373000 -1.64093600

H 1.53457200 2.38393600 -1.02249600

H 3.16814100 1.78685300 -0.70056100

H 2.62696200 1.44323300 1.68483600

H 1.84290200 2.98868000 1.34991900

H 0.36522500 0.90780500 2.32929700

H -0.31145400 1.96738800 1.07934100

H -1.50457300 -0.39443000 1.95449500

H -3.73451100 0.43206000 1.03421300

H -2.38138700 1.54056600 0.93010900

H -1.92768900 -2.74075200 1.22613000

H -3.43912000 -1.88454700 1.57145400

H -2.91999600 -2.17106800 -0.10408000

H 1.68567700 -1.51912600 0.95898900

H -3.37779100 -0.31816100 -1.60752800

**Conformer 96**

S 3.66746300 -0.28997300 -0.80144000

O 1.31130500 -1.23844200 1.64752100

O -2.64286200 1.90498600 -0.89452600

O -2.61801700 0.91818900 1.12890700

N -0.41824100 -0.71739500 0.31885000

C -1.19516300 0.03986800 -0.65321900

C -1.94835400 -1.06859000 -1.42994800

C -2.23491800 -2.11205800 -0.34010500

C -0.98990900 -2.06248200 0.55664800

C 0.77745300 -0.41197200 0.91324500

C 1.50619300 0.91591500 0.64076800

C -2.20948000 0.98169400 0.00032800

C 2.24577800 0.88275900 -0.71198200

C 0.67576100 2.20288900 0.79347700

H -0.56704800 0.62639100 -1.32141600

H -1.27487900 -1.47354700 -2.18976700

H -2.84071400 -0.69466600 -1.93320400

H -3.12415000 -1.83049200 0.22845000

H -2.40307700 -3.10826800 -0.75156000

H -1.21815700 -2.19441500 1.61493800

H -0.24618500 -2.81617600 0.28480100

H 2.26717200 0.92407300 1.42323500

H 1.56276100 0.67504100 -1.53804300

H 2.68925300 1.86320100 -0.89773000

H 0.03705100 2.15992500 1.67822800

H 1.35388900 3.05194400 0.91315600

H 0.04809200 2.41878000 -0.07354900

H -3.31319400 2.44758000 -0.45159500

H 3.10987800 -1.27405300 -0.06532600

**Conformer 97**

S -4.01749200 0.26872200 0.68445400

O -0.41545500 -2.28680600 -1.25887700

O 2.21387700 1.18623800 -1.34059100

O 1.69697800 2.68954400 0.24936400

N 0.82434700 -0.82564600 -0.09224600

C 1.13525300 0.38105500 0.66391000

C 2.21261800 -0.11059600 1.66160800

C 2.99376800 -1.15042300 0.84373800

C 1.92488400 -1.81399600 -0.03828100

C -0.34011000 -1.18920800 -0.71905000

C -1.58342800 -0.27626400 -0.71428200

C 1.69024600 1.55269300 -0.15168200

C -2.28912400 -0.37101800 0.65395800

C -1.37675900 1.16155800 -1.21202200

H 0.26800600 0.77273700 1.19184200

H 1.70458700 -0.58389300 2.50597000

H 2.82484100 0.70461600 2.04865600

H 3.74645200 -0.65704200 0.22471000

H 3.50853200 -1.87496900 1.47631300

H 2.28131600 -2.04094500 -1.04418900

H 1.54232600 -2.74444200 0.38900100

H -2.23092200 -0.78146400 -1.43336800

H -2.39526200 -1.42002600 0.93667100

H -1.73063100 0.12729400 1.44831400

H -0.75209000 1.17791700 -2.10806000

H -2.34289700 1.59299300 -1.48261700

H -0.92592400 1.82118500 -0.46730800

H 2.56173900 1.98872900 -1.75980400

H -3.71790200 1.58266200 0.64179600

**Conformer 98**

S 2.60964300 -0.31332700 1.58787200

O 0.90999100 2.12508200 -1.39397500

O -2.28833600 -0.97513100 -1.32114200

O -1.93224900 -2.48511300 0.30436200

N -0.51843000 0.82632700 -0.25212500

C -0.94165500 -0.30480700 0.57159900

C -1.81922500 0.36702400 1.65567900

C -2.48846600 1.52131300 0.89701500

C -1.39671800 2.00501700 -0.06570800

C 0.65293800 1.01711600 -0.93164200

C 1.69949700 -0.09684700 -1.15702000

C -1.75198600 -1.38209000 -0.14862200

C 2.88821200 0.09136600 -0.19279600

C 1.24864600 -1.55438500 -1.30199800

H -0.09160500 -0.80244200 1.03287800

H -1.15635700 0.74896700 2.43644800

H -2.51792200 -0.33270900 2.11533300

H -3.35672900 1.15848700 0.34135700

H -2.82811400 2.31771100 1.56099400

H -1.78636800 2.34139500 -1.02774900

H -0.80491500 2.82418300 0.35068700

H 2.10297900 0.20294500 -2.13031700

H 3.74318700 -0.49205100 -0.53800300

H 3.18457900 1.14076500 -0.19024200

H 0.40543500 -1.63801100 -1.99086800

H 2.07032000 -2.14074200 -1.72428600

H 0.96878300 -2.02663100 -0.36010400

H -2.80540400 -1.71856100 -1.66830600

H 2.68416100 -1.65532100 1.47810800

**Conformer 99**

S 2.59952700 -0.48969000 -1.62703200

O 0.86659800 -1.77022200 1.80069100

O -2.26372500 1.44339000 0.75903700

O -1.15050000 2.52645700 -0.86531700

N -0.52578800 -0.76584000 0.35808000

C -0.91221700 0.12556400 -0.73568600

C -2.02435600 -0.66887400 -1.46803200

C -2.66443100 -1.51405300 -0.35922400

C -1.48259800 -1.87997600 0.54205900

C 0.66162600 -0.83018300 1.04010100

C 1.72372300 0.28851000 0.98376400

C -1.42624700 1.49609500 -0.30103700

C 2.21813600 0.80904600 -0.37363800

C 1.32293200 1.46201500 1.90141400

H -0.08435900 0.31117300 -1.41424400

H -1.54293300 -1.30879200 -2.21172200

H -2.72700400 -0.01781700 -1.99102300

H -3.39670000 -0.92317100 0.19417500

H -3.16908100 -2.39854000 -0.75150600

H -1.75068700 -1.97246700 1.59496100

H -1.00495100 -2.81796500 0.24310000

H 2.57452900 -0.20926400 1.45591900

H 1.50315200 1.47383900 -0.86023300

H 3.12127800 1.39792600 -0.20279700

H 1.03699700 1.09399300 2.88883700

H 2.16776800 2.14478500 2.02669300

H 0.49108000 2.03959500 1.49367300

H -2.56189100 2.34885800 0.93637400

H 3.31250000 -1.29210100 -0.80987500

**Conformer 100**

S -3.81908300 -0.97860400 -0.20795600

O -0.79022000 -0.96685600 -0.98704900

O 1.80558700 -1.52922000 1.44566000

O 3.43588300 -1.95742000 -0.00871400

N 0.71746300 0.46753400 -0.07978100

C 1.84515100 -0.28517900 -0.67325800

C 2.87649800 0.80065500 -1.02147300

C 2.64327500 1.85641100 0.06782200

C 1.11813100 1.86557300 0.22856800

C -0.57889400 0.07301800 -0.38595100

C -1.72036200 0.96901400 0.10735300

C 2.44571700 -1.34101900 0.27623300

C -3.02274800 0.63334200 -0.64013500

C -1.87054600 0.90150000 1.63895800

H 1.49407000 -0.83522200 -1.54726200

H 2.65024100 1.21298900 -2.00871200

H 3.88892700 0.40017700 -1.04166100

H 3.12215100 1.54918300 1.00228700

H 3.02940600 2.84245000 -0.19473000

H 0.80359200 2.16037200 1.23067900

H 0.66049800 2.55508700 -0.48893600

H -1.47506900 2.00404700 -0.16282700

H -3.75439400 1.42101800 -0.45979700

H -2.83158600 0.59445800 -1.71180900

H -0.96412800 1.22536800 2.15373600

H -2.68620000 1.55266300 1.96494500

H -2.10634500 -0.11581700 1.95569000

H 1.03931700 -0.93405700 1.46647100

H -4.81472300 -0.45969900 0.53979800

**Conformer 101**

S 3.66263400 -0.37598300 -0.74565700

O 1.24292400 -1.13668900 1.73417700

O -2.57049500 0.86686100 1.07740900

O -2.66151400 1.93204300 -0.90049000

N -0.43295300 -0.67446200 0.31771900

C -1.17681400 0.04097000 -0.71339500

C -1.91178900 -1.10017500 -1.45785900

C -2.23433500 -2.09654700 -0.33434200

C -1.02567700 -2.00022600 0.60883900

C 0.74850600 -0.35033700 0.93118200

C 1.50806600 0.94607500 0.59868000

C -2.19968700 1.06185800 -0.20588600

C 2.26539800 0.82912800 -0.73936800

C 0.69856100 2.25304600 0.67333100

H -0.52370000 0.58644300 -1.39169800

H -1.21730200 -1.53994900 -2.17838500

H -2.78594800 -0.74419700 -2.00393900

H -3.14855200 -1.79999500 0.18493900

H -2.37988400 -3.11104200 -0.70799100

H -1.29787700 -2.07047700 1.66296400

H -0.27697100 -2.77205500 0.41354600

H 2.25870000 0.98140700 1.39034700

H 1.59105200 0.59489900 -1.56512100

H 2.73316500 1.78919500 -0.96699200

H 0.06540300 2.27273800 1.56350200

H 1.38957800 3.09733700 0.74161000

H 0.06867100 2.42798300 -0.20063000

H -3.23767500 1.53877700 1.28757800

H 3.06917300 -1.31455800 0.02089600

**Conformer 102**

S -3.72424800 0.66699100 -0.13914300

O -0.18769700 -2.41627000 -0.72805600

O 0.86155700 2.89560300 0.54621800

O 0.37341600 1.73166300 -1.27997400

N 1.18192100 -0.73634000 -0.09874300

C 1.51354700 0.54738100 0.50754600

C 3.06135200 0.64915700 0.35333100

C 3.51156400 -0.80758200 0.17761300

C 2.36939400 -1.42702600 -0.62769900

C -0.05192000 -1.33306300 -0.17564800

C -1.25652700 -0.63124500 0.46019600

C 0.84607900 1.74614200 -0.18081800

C -2.28075200 -0.35213400 -0.65888100

C -1.82828500 -1.52015100 1.57530100

H 1.23972300 0.55376300 1.57116300

H 3.52403700 1.14935700 1.20579600

H 3.30193900 1.22473500 -0.54461100

H 4.47588000 -0.88543100 -0.32698200

H 3.59556500 -1.30196400 1.14974200

H 2.47640600 -1.23273500 -1.70092200

H 2.25495200 -2.50114800 -0.49177400

H -0.96666400 0.32721000 0.89629000

H -1.80516700 0.14317900 -1.50432600

H -2.69772700 -1.29459800 -1.01565500

H -1.10241400 -1.66197700 2.38122100

H -2.72344400 -1.06095700 1.99894100

H -2.08638700 -2.50304600 1.17610900

H 1.24104100 2.74870700 1.42214400

H -3.09814200 1.86059000 -0.19079800

**Conformer 103**

S 3.96397000 0.17834400 -0.30599800

O 1.26631900 1.59051800 -0.49196600

O -1.75323000 -1.36440500 -1.61025700

O -2.79741300 -2.32896800 0.10698100

N -0.76430100 0.68517400 -0.09611300

C -1.67669700 -0.25558900 0.57885800

C -2.87740000 0.63070000 0.98275600

C -2.90443100 1.71087900 -0.10769700

C -1.42187200 1.98821800 -0.37220100

C 0.61927800 0.63742900 -0.09075500

C 1.29863600 -0.63797300 0.41386300

C -2.13275000 -1.42455500 -0.31841600

C 2.52556900 -0.98152000 -0.45303500

C 1.63327700 -0.50211000 1.91068500

H -1.21990600 -0.71093000 1.45694400

H -2.67205600 1.08000600 1.95812500

H -3.79642500 0.05112100 1.06363100

H -3.39314300 1.33033600 -1.00962300

H -3.43917100 2.60981900 0.20165300

H -1.20882000 2.31499800 -1.39033000

H -1.01496600 2.74603100 0.30405700

H 0.61405400 -1.48405200 0.28924100

H 2.87880900 -1.97235800 -0.16853100

H 2.23381400 -1.01977600 -1.50338600

H 0.73536300 -0.34167600 2.51326200

H 2.11916400 -1.41251300 2.27122300

H 2.31297900 0.33455500 2.07370100

H -1.21292400 -0.56435000 -1.72451200

H 4.88273900 -0.78097300 -0.06910600

**Conformer 104**

S -3.70982500 0.77386600 -0.13216600

O -0.23323500 -2.37379900 -0.77851000

O 0.96108300 2.90093400 0.52241400

O 0.47098200 1.73450000 -1.30197100

N 1.17107600 -0.74486200 -0.09341100

C 1.52495100 0.52893300 0.52161700

C 3.07966600 0.58474800 0.40989000

C 3.49249200 -0.88059300 0.21213600

C 2.34744700 -1.45237500 -0.62372600

C -0.07596100 -1.30699200 -0.19994500

C -1.26857100 -0.59453200 0.44857800

C 0.91615800 1.74526900 -0.19137100

C -2.26782300 -0.23587100 -0.66990700

C -1.86809500 -1.51639800 1.52160300

H 1.22107300 0.54591700 1.57641200

H 3.53396300 1.05106500 1.28571900

H 3.36273100 1.17319600 -0.46697400

H 4.46263700 -0.97505400 -0.27829300

H 3.54648300 -1.39670900 1.17501300

H 2.47449600 -1.23509500 -1.69039200

H 2.20412200 -2.52611000 -0.51531700

H -0.96014400 0.33701600 0.92810700

H -1.77503900 0.38329700 -1.42057400

H -2.62178600 -1.14001600 -1.16432300

H -1.12819700 -1.75980700 2.28933900

H -2.71160300 -1.02945400 2.01496700

H -2.20549000 -2.45253800 1.07198800

H 1.30413300 2.74817800 1.41211700

H -4.41992700 -0.21791800 0.44202200

**Conformer 105**

S 2.39780300 -0.91636400 -1.59460700

O 0.78205100 -1.36529800 2.15779800

O -2.00244500 1.82934200 0.62588200

O -0.93934800 2.40948400 -1.26857300

N -0.60962400 -0.64944700 0.54202800

C -1.01569900 0.07067400 -0.66939200

C -2.32733900 -0.63891800 -1.12132300

C -2.26222100 -2.00942600 -0.43642100

C -1.58657900 -1.69776400 0.89760400

C 0.59192300 -0.61650300 1.20509500

C 1.72076300 0.38229600 0.86569600

C -1.28375500 1.55796800 -0.48602200

C 2.14514300 0.61121900 -0.59208100

C 1.49361900 1.72805600 1.58580800

H -0.26276300 -0.02383700 -1.44930600

H -2.38646200 -0.69008100 -2.20875500

H -3.19528900 -0.08271100 -0.75996900

H -3.24882100 -2.45992700 -0.31393000

H -1.64052300 -2.69766400 -1.01550500

H -2.30068000 -1.31384000 1.63506000

H -1.06133900 -2.53937400 1.34338700

H 2.56800900 -0.09662200 1.36327900

H 1.43223500 1.20989600 -1.15929800

H 3.08168300 1.17211100 -0.58561100

H 1.25382200 1.56008700 2.63749700

H 2.40274100 2.33368400 1.53822000

H 0.68736300 2.31004400 1.13630800

H -2.16548600 2.78469900 0.63940500

H 3.16082700 -1.57234200 -0.69592000

**Conformer 106**

S -2.89787800 0.98379600 -1.18181800

O -1.09565000 -2.05119700 -0.65893300

O 1.64809400 2.54891300 0.99449100

O 1.12637500 1.85662800 -1.05172000

N 0.73129000 -0.83643500 -0.14527800

C 1.49256700 0.13543400 0.62591800

C 2.95339700 -0.36694800 0.47451600

C 2.95963100 -0.99401600 -0.92758100

C 1.58059400 -1.65349500 -1.03377000

C -0.60342800 -1.11861600 -0.04031100

C -1.45218000 -0.27839600 0.92430500

C 1.37834400 1.57184000 0.08107600

C -2.85044200 -0.05023800 0.33803200

C -1.55438000 -1.02055900 2.27351200

H 1.18676900 0.12576900 1.67707200

H 3.14354000 -1.12571300 1.23861900

H 3.68893200 0.43022000 0.59886300

H 3.06447700 -0.21572300 -1.68627900

H 3.77281000 -1.70915900 -1.05965600

H 1.17508400 -1.64713100 -2.04568800

H 1.58528700 -2.69082500 -0.68408900

H -0.98885200 0.69820800 1.09114800

H -3.27382000 -1.00758700 0.03269200

H -3.50581700 0.39062000 1.09086200

H -0.57055700 -1.18512600 2.72303000

H -2.15675300 -0.44816000 2.98376500

H -2.02206200 -1.99780700 2.13268000

H 1.81035600 2.17142800 1.86811800

H -2.51752800 2.14049800 -0.59999300

**Conformer 107**

S 2.22034100 -1.39156700 -1.16809900

O 0.36049500 -0.44215100 2.08041100

O -1.26644600 -1.86173900 -0.59654600

O -3.27034000 -1.62779900 0.33108600

N -0.41998300 0.64453000 0.27030200

C -1.79289100 0.23178900 0.61765000

C -2.66993300 1.30402400 -0.04914400

C -1.87838800 1.64981300 -1.31686300

C -0.41575500 1.61778800 -0.84864200

C 0.59845100 0.27805300 1.11719000

C 2.07772300 0.64334100 0.87306200

C -2.17702200 -1.17700100 0.11660600

C 2.80809300 -0.63558400 0.40984800

C 2.47824600 1.87936500 0.05942400

H -1.90749800 0.20174800 1.70043000

H -2.74021600 2.17370500 0.61027400

H -3.67738100 0.93832000 -0.24192000

H -2.04759200 0.89086700 -2.08596500

H -2.14450200 2.61861200 -1.74242900

H 0.26151400 1.30120600 -1.64165300

H -0.10352900 2.60309900 -0.49525500

H 2.43573100 0.80818800 1.89537300

H 3.88016900 -0.45049700 0.32817300

H 2.65487000 -1.42450100 1.14588500

H 1.97818900 2.78048000 0.41974700

H 3.55371600 2.03999800 0.17822100

H 2.27947500 1.78431400 -1.00865400

H -0.42374500 -1.37890700 -0.65163000

H 2.65440600 -0.42929800 -2.00751900

**Conformer 108**

S 2.58918700 -0.21892200 1.61714100

O 1.01484100 2.02591300 -1.39414700

O -2.19680300 -1.16167000 -1.39371000

O -2.21538800 -2.35106400 0.49184600

N -0.56223400 0.77189600 -0.39112100

C -0.98691700 -0.28593000 0.55105600

C -1.80432700 0.47831300 1.61408100

C -2.44763100 1.61430100 0.80911500

C -1.34050400 2.02545000 -0.16509600

C 0.68910900 0.92885800 -0.96397400

C 1.70311800 -0.22555600 -1.13513300

C -1.85066900 -1.37639000 -0.10720500

C 2.89946400 0.00683000 -0.18880100

C 1.23741600 -1.68548400 -1.17632700

H -0.13100300 -0.77382400 1.01025000

H -1.11490800 0.87947900 2.36172100

H -2.51643100 -0.17394400 2.11870700

H -3.32790400 1.25047000 0.27084100

H -2.76592600 2.45005000 1.43382100

H -1.70968000 2.42105800 -1.11224300

H -0.67388100 2.77844900 0.26212600

H 2.10441000 0.00287000 -2.12928800

H 3.73033100 -0.63968400 -0.47437100

H 3.23471000 1.03989100 -0.28053400

H 0.39125700 -1.82555700 -1.85119900

H 2.05588900 -2.30174000 -1.55960100

H 0.96331300 -2.08896500 -0.20146000

H -1.76205100 -0.33979100 -1.67911700

H 2.61497500 -1.56706600 1.63573000

**Conformer 109**

S 2.89234400 -0.80153700 -1.15198800

O 1.27817600 -0.73993700 2.08355100

O -2.45921400 1.30242300 0.80338800

O -2.68971700 1.50052500 -1.40504700

N -0.41386100 -0.48637400 0.62342500

C -1.01855400 -0.05407100 -0.64794300

C -1.59876100 -1.35714700 -1.23676100

C -2.04062900 -2.12805800 0.01477000

C -0.94025500 -1.81923900 1.03719600

C 0.81621400 -0.11655800 1.13987400

C 1.60450600 1.08999600 0.59235900

C -2.13327900 0.99714300 -0.46733700

C 2.24751800 0.88627300 -0.79501000

C 0.86280500 2.43716300 0.65744000

H -0.28850900 0.38730900 -1.32080100

H -0.79926400 -1.89281200 -1.75479100

H -2.40071800 -1.15831700 -1.94691900

H -3.01153400 -1.76394200 0.36359000

H -2.13631600 -3.20014000 -0.16183000

H -1.29736300 -1.79018300 2.06759100

H -0.12121300 -2.54093200 0.99730000

H 2.42725500 1.13829700 1.30959900

H 1.54685700 1.08277700 -1.60858600

H 3.05957800 1.60690600 -0.90697700

H 0.43850200 2.60595600 1.64996000

H 1.56531900 3.25114900 0.45917700

H 0.05905000 2.52066000 -0.07669300

H -1.85249100 0.81544300 1.38710100

H 3.59902100 -0.95007400 -0.01254100

**Conformer 110**

S 3.98469200 0.41598700 -0.74780400

O 0.53520000 -2.27384600 1.17609400

O -2.08970300 1.32023700 1.46219700

O -2.12227200 2.58207600 -0.37524200

N -0.85308600 -0.77599900 0.23267200

C -1.17917100 0.38387800 -0.61600700

C -2.16882400 -0.19143600 -1.65069500

C -2.93754300 -1.24311900 -0.83884200

C -1.86176300 -1.86130500 0.06214900

C 0.38936100 -1.14877800 0.72210700

C 1.59823600 -0.19222700 0.69694200

C -1.83534300 1.54630800 0.15963300

C 2.26966200 -0.25540400 -0.69367100

C 1.37916200 1.23619700 1.21357200

H -0.29818700 0.79702800 -1.10176400

H -1.60264800 -0.66660800 -2.45664300

H -2.79585600 0.58651500 -2.08477800

H -3.71829600 -0.76413300 -0.24108500

H -3.41887500 -1.99396400 -1.46669700

H -2.24023800 -2.19088000 1.03074900

H -1.37309100 -2.72196200 -0.40114600

H 2.27629300 -0.69134700 1.39320200

H 2.29487300 -1.28287600 -1.05807400

H 1.73214800 0.34440300 -1.43143200

H 0.87080200 1.23461700 2.18047900

H 2.35050100 1.71423900 1.35121100

H 0.80951900 1.86720400 0.52893900

H -1.73443000 0.44315400 1.68507500

H 4.55555300 -0.57160500 -0.02739600

**Conformer 111**

S -2.63741600 0.01396900 1.59713000

O -1.14864700 -1.69319000 -1.61976000

O 2.26746200 1.25678200 -1.24223300

O 2.41467600 2.14453000 0.79736700

N 0.51655000 -0.68880900 -0.48638800

C 1.02282500 0.19595200 0.58696000

C 1.79450800 -0.76488200 1.51585500

C 2.35875500 -1.80838000 0.54373400

C 1.21947100 -2.00529900 -0.45997800

C -0.74620700 -0.68495900 -1.05609000

C -1.67777400 0.54624400 -1.06235100

C 1.96127300 1.30293000 0.07161800

C -2.92687900 0.22638500 -0.21624700

C -1.13908300 1.95757600 -0.79814300

H 0.20921800 0.67754400 1.12368900

H 1.08686200 -1.22782900 2.20911200

H 2.54924300 -0.23848200 2.09921200

H 3.25461300 -1.42228100 0.04862200

H 2.63105100 -2.74386700 1.03438700

H 1.55516700 -2.27838000 -1.46134000

H 0.51332000 -2.77427300 -0.13703800

H -2.03613200 0.53187200 -2.09866700

H -3.63617500 1.05215200 -0.29360000

H -3.41397600 -0.67331800 -0.58703300

H -0.22918700 2.16875500 -1.36203800

H -1.88997200 2.68063300 -1.12888700

H -0.94895800 2.15667100 0.25698700

H 1.76687500 0.52086100 -1.63389600

H -2.29840400 -1.29027900 1.54597700

**Conformer 112**

S 4.00912000 0.31558200 -0.70965500

O 0.49066000 -2.32061600 1.14635500

O -2.07054400 1.33410000 1.46442200

O -2.02753200 2.62255400 -0.35444800

N -0.86801200 -0.77909200 0.22918800

C -1.16183500 0.39470500 -0.61217800

C -2.16474500 -0.14675800 -1.65299900

C -2.95879900 -1.18799100 -0.85232100

C -1.89732200 -1.84188100 0.03998100

C 0.36737500 -1.18525700 0.71351800

C 1.59332000 -0.25009100 0.71017200

C -1.78708300 1.56929700 0.16931300

C 2.28434400 -0.32895400 -0.66927800

C 1.38492700 1.18229000 1.22133700

H -0.26922200 0.78646100 -1.09424800

H -1.60944700 -0.62766800 -2.46307400

H -2.77285600 0.64980200 -2.08029200

H -3.72705000 -0.69682500 -0.24822500

H -3.45877100 -1.91982200 -1.48801100

H -2.28348100 -2.17915800 1.00287600

H -1.42529800 -2.70467800 -0.43650500

H 2.25771700 -0.75542300 1.41406100

H 2.38965100 -1.37486100 -0.96298800

H 1.71522900 0.17627800 -1.45172900

H 0.80622500 1.19500400 2.14751000

H 2.35744300 1.62418500 1.44749100

H 0.89078900 1.83943200 0.50261800

H -1.74849300 0.44221700 1.67950100

H 3.70596100 1.62893500 -0.67472100

**Conformer 113**

S -3.82797500 0.05863800 -0.55023900

O -1.12380700 -1.77723400 -0.44215100

O 2.17107900 2.65302200 0.27587300

O 1.04401200 1.70253800 -1.38507000

N 0.86423300 -0.79824300 -0.03772000

C 1.75799700 0.25528200 0.42891200

C 3.18648200 -0.31727400 0.17381200

C 2.96744300 -1.83266400 0.06392700

C 1.60045100 -1.93609200 -0.61196000

C -0.50586000 -0.82756100 0.02553800

C -1.23611600 0.31758600 0.73210600

C 1.59202100 1.58039400 -0.32922800

C -2.26955800 0.97868500 -0.20881600

C -1.83497700 -0.18890500 2.05461900

H 1.61057600 0.43910800 1.50115800

H 3.88540400 -0.03430400 0.96275800

H 3.57334800 0.07205800 -0.77174400

H 3.75839800 -2.32510400 -0.50394500

H 2.92870800 -2.28786500 1.05774100

H 1.67540300 -1.83081200 -1.70020200

H 1.06309100 -2.85898700 -0.40098900

H -0.52793800 1.11523200 0.97227400

H -2.61058200 1.90880900 0.25123100

H -1.79318000 1.23889200 -1.15447000

H -1.04945500 -0.53342500 2.73385700

H -2.38714700 0.61359400 2.55084500

H -2.52336400 -1.01417300 1.87525300

H 2.54999900 2.40865000 1.12989700

H -3.23286000 -1.06547600 -0.99849300

**Conformer 114**

S -2.88418700 1.37936600 0.32827800

O -0.09470900 -2.65013600 -0.81483200

O 0.14685000 2.62320300 -0.17498500

O 1.89409900 1.76025600 -1.22888800

N 0.95447600 -0.81148400 -0.03684100

C 1.06928600 0.47922300 0.64661200

C 2.44352800 0.36725800 1.34291900

C 3.28925400 -0.46058600 0.35755300

C 2.28135100 -1.38370700 -0.35431100

C -0.16875600 -1.56786500 -0.25105600

C -1.51302100 -1.02466800 0.26672000

C 1.07843200 1.66009600 -0.35255900

C -2.06262900 0.06538100 -0.68502900

C -2.51903200 -2.16248700 0.46210800

H 0.26764300 0.60886700 1.37426200

H 2.30262900 -0.17017700 2.28466200

H 2.88062600 1.34094200 1.56974400

H 3.77132700 0.19753200 -0.36388300

H 4.06405400 -1.03173200 0.87171400

H 2.43695400 -1.41286100 -1.43410600

H 2.30629300 -2.41262900 0.01051400

H -1.32793800 -0.56642200 1.24382400

H -1.27783700 0.53234000 -1.27921500

H -2.79211300 -0.36751600 -1.36925300

H -2.16604800 -2.87383300 1.21118100

H -3.48000000 -1.76081000 0.79346900

H -2.66152800 -2.71024900 -0.47035200

H -0.58451400 2.34037700 0.40372700

H -3.23427600 2.19424300 -0.68894900

**Conformer 115**

S 3.66773700 -0.35886100 -0.77476200

O 1.29431300 -1.14455400 1.68000200

O -2.51685600 1.10963000 1.11681200

O -2.90031100 1.72956100 -0.98965900

N -0.50635600 -0.61033700 0.44353600

C -1.20884400 0.05177400 -0.67134800

C -1.86401500 -1.11931500 -1.43360400

C -2.20749900 -2.10866200 -0.31211100

C -1.01259800 -1.99983500 0.64196800

C 0.75685400 -0.33032800 0.94157300

C 1.50918500 0.96108600 0.57869800

C -2.28660900 1.05491900 -0.20909900

C 2.24333900 0.81158300 -0.77240300

C 0.71416300 2.27756600 0.64101000

H -0.52876200 0.60503500 -1.31463500

H -1.12801100 -1.55297200 -2.11624100

H -2.72138600 -0.78950900 -2.01935100

H -3.13390200 -1.81049600 0.18714500

H -2.34304800 -3.12851400 -0.67413800

H -1.27032700 -2.16961500 1.68815200

H -0.21417700 -2.70183900 0.38929500

H 2.27686900 1.00609800 1.35362000

H 1.55768700 0.54138400 -1.57770800

H 2.68601200 1.77362000 -1.03773700

H 0.12122200 2.34627600 1.55581300

H 1.41861200 3.11313600 0.64764500

H 0.04719600 2.43109400 -0.20891500

H -1.88073800 0.51805500 1.55296600

H 3.09243700 -1.31744900 -0.01980900

**Conformer 116**

S 2.29762200 -0.90262400 -1.68001400

O 0.85580500 -1.42028200 2.08579400

O -1.72605900 1.98463000 0.77363000

O -1.23224200 2.38156900 -1.36334100

N -0.64077100 -0.58541700 0.61949500

C -1.04433800 0.10516700 -0.62154800

C -2.35975500 -0.60603600 -1.04571300

C -2.23340700 -1.99933300 -0.42307800

C -1.55722600 -1.71931200 0.91781400

C 0.62644800 -0.62325800 1.18759400

C 1.75157200 0.37101700 0.82151500

C -1.31464000 1.60023700 -0.45515800

C 2.11106500 0.61657100 -0.65077600

C 1.58355500 1.70865800 1.57384700

H -0.30082200 -0.02115900 -1.40503100

H -2.46622500 -0.60781600 -2.13012500

H -3.22445900 -0.08257300 -0.62685500

H -3.19757700 -2.49783900 -0.30912000

H -1.59030200 -2.63474800 -1.03822000

H -2.28509000 -1.42694400 1.68295900

H -0.97777500 -2.55002400 1.31369600

H 2.61221900 -0.13162100 1.26993600

H 1.38045600 1.23103100 -1.17743200

H 3.05306800 1.16711200 -0.67963300

H 1.39431600 1.52849900 2.63447000

H 2.50448800 2.29210400 1.49450400

H 0.77127200 2.31831000 1.17550800

H -1.62354900 1.23172300 1.37829700

H 3.11376200 -1.56575600 -0.83485300

**Conformer** **117**

S 3.91242000 0.28070600 -0.81331000

O 0.49735000 -2.06781800 1.52126800

O -2.11282600 1.53552600 1.35649300

O -1.90531400 2.64261600 -0.56820800

N -0.92274700 -0.73293200 0.37451500

C -1.24984000 0.33489600 -0.59110000

C -2.37331500 -0.26876700 -1.49293000

C -2.33748100 -1.77439700 -1.19915600

C -1.91392900 -1.83308500 0.26803700

C 0.32899600 -1.02594200 0.90641400

C 1.53562600 -0.08020800 0.72601500

C -1.76674500 1.62738200 0.05723700

C 2.18746000 -0.34639300 -0.64970900

C 1.33211600 1.41009700 1.03237900

H -0.38534100 0.60603300 -1.19293600

H -2.20807600 -0.02001700 -2.54071300

H -3.34216800 0.14998300 -1.21021700

H -3.29927700 -2.25769400 -1.37971600

H -1.58623900 -2.27356300 -1.81819300

H -2.76399300 -1.64446800 0.93351600

H -1.44330300 -2.76365500 0.57459000

H 2.22169300 -0.47639500 1.47795100

H 2.19284900 -1.41420700 -0.87080100

H 1.65082500 0.15738200 -1.45662800

H 0.80819700 1.55377100 1.97987700

H 2.30949600 1.88771400 1.11956200

H 0.78731000 1.94572900 0.25342400

H -1.84924600 0.65610700 1.67528200

H 4.47677800 -0.61156100 0.02682400

**Conformer** **118**

S 2.51413000 -0.00269400 1.62491000

O 1.04504300 1.68073400 -1.78089700

O -2.30209600 -1.35839000 -1.20331000

O -2.17776300 -2.26524600 0.83032000

N -0.61219100 0.70232000 -0.58544100

C -1.06247100 -0.16254500 0.52981900

C -1.94656800 0.75796800 1.42871200

C -1.62050600 2.18102400 0.95864400

C -1.34211800 1.99682300 -0.53187100

C 0.65692600 0.70639600 -1.15395900

C 1.62455600 -0.49974400 -1.08584200

C -1.88284500 -1.37501200 0.08042400

C 2.82685100 -0.13493300 -0.18992700

C 1.11064900 -1.92620900 -0.85908800

H -0.21055600 -0.52280200 1.10052000

H -1.73445900 0.58505100 2.48326600

H -3.00462000 0.53614000 1.26790000

H -2.43457600 2.88238800 1.15103900

H -0.72155100 2.55596900 1.45568000

H -2.27542300 1.91901500 -1.10091500

H -0.72655900 2.77011500 -0.98263900

H 2.03899000 -0.47805400 -2.10029000

H 3.63257400 -0.85405300 -0.34306900

H 3.20087900 0.84853300 -0.47419100

H 0.27118100 -2.16577800 -1.51395100

H 1.91475400 -2.62634200 -1.10407600

H 0.80866200 -2.13255400 0.16747300

H -1.89711300 -0.58744400 -1.63594600

H 2.48875200 -1.32271500 1.89836800

**Conformer** **119**

S 2.56923800 0.10496900 1.58142500

O 1.18560200 1.37545200 -1.87522600

O -2.38593700 -1.36093500 -1.09749800

O -2.41562600 -2.02911000 1.02996900

N -0.56395900 0.62324400 -0.64655200

C -1.09548200 -0.08577200 0.54183200

C -1.90877000 0.99018500 1.33013700

C -1.50023800 2.32753300 0.69816000

C -1.21767400 1.95332100 -0.75571600

C 0.71471000 0.48962600 -1.17697700

C 1.58903000 -0.77149900 -0.97968500

C -2.01304300 -1.26420700 0.19731300

C 2.84882300 -0.38138800 -0.17959100

C 0.99338100 -2.10620100 -0.51586100

H -0.28284100 -0.46166000 1.15785500

H -1.69710700 0.92789500 2.39708800

H -2.98014400 0.81887100 1.20161500

H -2.27605600 3.08953700 0.79290400

H -0.58797100 2.71458300 1.16129400

H -2.14890500 1.86040400 -1.32574400

H -0.55546900 2.63352100 -1.28386300

H 1.95312900 -0.92801500 -2.00219400

H 3.52189600 -1.23897700 -0.13089400

H 3.37446800 0.43266400 -0.67464000

H 0.08786100 -2.37018200 -1.06411200

H 1.72349400 -2.89544100 -0.71662800

H 0.77609500 -2.13794400 0.55201700

H -1.89937500 -0.68292900 -1.59639800

H 2.29409700 1.40261700 1.33913100

**S2**

**Conf. 1 (N)H+**

S -3.54850000 -1.12346900 0.12568700

O -0.73182000 0.34425100 1.63449400

O 3.91733200 0.93339900 0.68533700

O 2.50227000 1.42950300 -0.94414500

N 0.54254600 -0.12677000 -0.28408000

C 1.77599700 -0.25760800 0.58678800

C 2.22993600 -1.72864700 0.43951600

C 1.65829900 -2.16030600 -0.91816200

C 0.29299100 -1.48335900 -0.95959700

C -0.72480000 0.41232200 0.45271600

C -1.76126200 0.99457900 -0.47107100

C 2.76821300 0.78376900 0.03892400

C -3.17680300 0.68033200 0.03929100

C -1.50894900 2.52094900 -0.58489300

H 1.49568600 -0.00583000 1.61092400

H 1.79941800 -2.32133900 1.24924300

H 3.31433200 -1.83420000 0.49091700

H 2.28757100 -1.80898700 -1.73987100

H 1.56363900 -3.24266900 -1.00821100

H -0.10370300 -1.30953300 -1.95776200

H -0.45495100 -2.00907800 -0.36478400

H -1.63662700 0.54526100 -1.46084800

H -3.35191800 1.12922000 1.01610000

H -3.89655300 1.11038000 -0.65763600

H -0.51138100 2.75132000 -0.96816100

H -2.23465700 2.94556000 -1.28050100

H -1.63029700 3.00773000 0.38444700

H 3.98735900 0.38533200 1.47954800

H -3.29775900 -1.27743400 1.44132400

H 0.82401800 0.56776300 -1.00373300

**Conf. 1 (O2)H+**

S -2.78301400 1.24796200 -1.16624300

O -0.53054100 -1.57761100 -0.68232600

O 3.76243200 -0.78739300 -0.28815300

O 1.97398600 -1.99353100 -0.69670000

N 0.40477900 0.24618000 0.31898900

C 1.57102800 0.35587100 -0.62080200

C 2.16998700 1.72530800 -0.26678000

C 1.83879900 1.91156700 1.21943800

C 0.41847500 1.35789400 1.32214600

C -0.60926800 -0.58023700 0.13732300

C -1.92561300 -0.44368600 0.86199700

C 2.46848100 -0.89788000 -0.52114300

C -3.05348200 -0.29165400 -0.17889200

C -2.16174200 -1.66363500 1.77725200

H 1.17935000 0.34039700 -1.64283800

H 1.67147800 2.48960300 -0.86694600

H 3.23394000 1.81196100 -0.50043600

H 2.51884200 1.33705500 1.85475900

H 1.88876100 2.95325800 1.53428600

H 0.17766400 0.97066700 2.31068300

H -0.32159600 2.10671300 1.03150100

H -1.90194600 0.45910400 1.47321700

H -3.07188000 -1.15229600 -0.84535700

H -4.00562800 -0.22709600 0.34699100

H -1.36467400 -1.77141600 2.51674300

H -3.10127300 -1.53128000 2.31601100

H -2.22027100 -2.58440000 1.19533400

H 4.05286200 0.12924300 -0.18817300

H -3.41878600 0.84907200 -2.28467300

H 0.43093000 -1.84424100 -0.86994700

**Conf. 1 (O3)H+**

S -2.95445100 1.18245300 -1.13651500

O -0.57472500 -1.51242900 -0.76231900

O 2.07506700 -1.94323800 -0.86240100

O 3.69565300 -0.64664600 0.02827700

N 0.42354700 0.27334200 0.26975700

C 1.59006200 0.37517900 -0.67224800

C 2.16896200 1.76176300 -0.37697000

C 1.86160100 1.97938000 1.10980500

C 0.46184500 1.38973800 1.27784600

C -0.58988300 -0.54300900 0.11667800

C -1.86152900 -0.45092700 0.91626200

C 2.60457000 -0.75596300 -0.43458500

C -3.06779300 -0.29597000 -0.03605100

C -2.01379800 -1.69005200 1.82500800

H 1.21376000 0.28220700 -1.69433300

H 1.65662500 2.50211600 -0.99494600

H 3.23361100 1.79921800 -0.60152900

H 2.58362100 1.44548200 1.73098100

H 1.88470300 3.03101500 1.39383600

H 0.27365300 0.99279400 2.27404600

H -0.31681900 2.10807800 1.01319500

H -1.81176300 0.44245500 1.53699500

H -3.20873300 -1.18671000 -0.64578700

H -3.96215900 -0.16448900 0.57320800

H -1.17801400 -1.78480400 2.52233400

H -2.92765700 -1.59031500 2.41316000

H -2.08169000 -2.60560700 1.23550300

H 0.32661000 -1.76711900 -1.06031200

H -2.58368800 0.52652500 -2.25422200

H 2.71214900 -2.66582500 -0.72911200

**Conf. 1 (O4)H+**

S -2.87398000 1.15732200 -1.26808000

O -0.56754400 -1.54064900 -0.65722800

O 1.92909600 -2.01049400 -0.69406000

O 3.74324200 -0.84139300 -0.28980400

N 0.41686300 0.27209900 0.31815400

C 1.57681100 0.34673700 -0.63261200

C 2.20711700 1.70779500 -0.30134100

C 1.89039800 1.92156000 1.18427800

C 0.46070100 1.39716300 1.30603100

C -0.61188100 -0.53994200 0.16405900

C -1.90617900 -0.37784600 0.91604100

C 2.44774700 -0.92510800 -0.52452700

C -3.07025000 -0.25359500 -0.09108300

C -2.11753600 -1.56574300 1.87908400

H 1.17804400 0.32610900 -1.65160900

H 1.72104500 2.47458400 -0.90845300

H 3.27098600 1.76773700 -0.54363600

H 2.56414700 1.34338400 1.82306600

H 1.96316900 2.96652400 1.48350800

H 0.22130700 1.02803600 2.30169000

H -0.27037800 2.15233100 1.00848700

H -1.86371000 0.54705600 1.49031100

H -3.20113500 -1.17399400 -0.65715300

H -3.98642400 -0.07210400 0.47086900

H -1.31051200 -1.64077100 2.61179500

H -3.05135300 -1.42156100 2.42526800

H -2.17760100 -2.50801600 1.33257100

H 0.38498500 -1.83012000 -0.85495800

H -2.53083000 0.42399100 -2.34563900

H 4.05397200 0.06914900 -0.19476700

**Conf. 1 (S)H+**

S -3.27059500 -0.80003800 -1.00132800

O -0.91839900 -1.13831200 -0.01779700

O 1.42676600 -2.12249900 1.09337700

O 3.40946800 -1.13961600 0.86794200

N 0.64328600 0.48399400 -0.22993900

C 1.68592600 -0.47991900 -0.69928400

C 2.71423200 0.41691300 -1.39039800

C 2.62081600 1.74341800 -0.62476400

C 1.12466200 1.89087600 -0.32597400

C -0.59212100 0.07293100 0.04472700

C -1.68101600 1.07652100 0.43514500

C 2.27811300 -1.26995100 0.49912800

C -3.05339700 0.38558300 0.43403800

C -1.47898500 1.64460400 1.86047600

H 1.21499600 -1.19201400 -1.38099500

H 2.43615000 0.55126700 -2.43912300

H 3.70912700 -0.02178500 -1.34591000

H 3.18643300 1.67636000 0.30634800

H 3.00090200 2.59241400 -1.19284200

H 0.93821700 2.43364500 0.59866200

H 0.59953700 2.39392900 -1.14417900

H -1.68831800 1.90213200 -0.28386200

H -3.21099900 -0.21119100 1.32993000

H -3.86174400 1.10879200 0.32714800

H -0.58694400 2.26461300 1.92368900

H -2.32880100 2.26931800 2.14502300

H -1.38395600 0.83549000 2.58801000

H 0.54871900 -2.08299300 0.67023500

H -3.16610900 -1.99334900 -0.37990700

H -4.63275600 -0.79642200 -1.03815600

**Conf. 2 (N)H+**

S -3.53550900 -1.11473300 0.15066000

O -0.69876600 0.37903600 1.66873800

O 3.92327300 0.99160300 0.54472800

O 2.45595600 1.37177700 -1.06988600

N 0.53381900 -0.16147800 -0.25558300

C 1.79577700 -0.22598700 0.58254200

C 2.26289800 -1.69870400 0.51274500

C 1.64408600 -2.22470100 -0.79022300

C 0.27039600 -1.56410300 -0.81991200

C -0.71089100 0.42050200 0.48638000

C -1.75277200 1.01263600 -0.42902800

C 2.75799000 0.79033800 -0.05754900

C -3.15861000 0.68546300 0.09918000

C -1.50305200 2.54135200 -0.51438100

H 1.54338900 0.08338300 1.59808600

H 1.87147900 -2.24166800 1.37534300

H 3.34975900 -1.78941600 0.52716800

H 2.23634800 -1.92330800 -1.65805600

H 1.55829700 -3.31144700 -0.80415900

H -0.17228000 -1.46538400 -1.80914900

H -0.44299200 -2.05134500 -0.15438100

H -1.63263100 0.58144200 -1.42757600

H -3.26863800 1.03952700 1.12472800

H -3.90494000 1.19529000 -0.50908600

H -0.50280500 2.77818800 -0.88633400

H -2.22449500 2.97843500 -1.20654500

H -1.63084700 3.00880400 0.46360300

H 4.02326300 0.49204600 1.36723200

H -3.83696500 -1.24898000 -1.15781800

H 0.78683500 0.48040800 -1.03170900

**Conf. 2 (O2)H+**

S -3.08610500 1.29632200 -0.84029900

O -0.30200700 -1.32189300 -1.16031200

O 3.62186800 -0.93953900 -1.00093500

O 2.28130800 -1.48806400 0.67931900

N 0.36536900 0.33900300 0.13916800

C 1.62503600 0.42456200 -0.64093000

C 2.20783000 1.78735000 -0.21186800

C 1.74551800 1.93146500 1.24504200

C 0.33082200 1.34264000 1.24676000

C -0.54174800 -0.55480200 -0.11318700

C -1.80236000 -0.75667400 0.68590900

C 2.52527800 -0.77103100 -0.24757500

C -3.04860300 -0.41350400 -0.16542900

C -1.86425600 -2.20319700 1.22790900

H 1.39535700 0.37866400 -1.70695400

H 1.78234200 2.57380300 -0.83928600

H 3.29246500 1.82536300 -0.31587200

H 2.39165900 1.35841000 1.91257500

H 1.74494500 2.96723800 1.58285100

H 0.08074600 0.85242100 2.18605900

H -0.43038200 2.08660900 1.00373900

H -1.77302000 -0.07094900 1.53172800

H -3.12754600 -1.06938200 -1.03608800

H -3.94066500 -0.58826100 0.43556700

H -0.96813200 -2.45930500 1.79583600

H -2.72748300 -2.29900100 1.88803400

H -1.98848300 -2.94318100 0.43048300

H 3.67579100 -0.31994300 -1.74095700

H -3.50879100 1.90035100 0.28955500

H -0.95315200 -2.03188700 -1.25103900

**Conf. 2 (O3)H+**

S -2.93490100 1.06596600 -1.25702800

O -0.57363900 -1.52015800 -0.73336400

O 2.07379200 -1.95148900 -0.85276100

O 3.69744100 -0.64975200 0.02403500

N 0.42805100 0.27896100 0.26969300

C 1.59086500 0.36863800 -0.67850300

C 2.17491600 1.75589200 -0.39677700

C 1.87539000 1.98534100 1.08981300

C 0.47362700 1.40290900 1.26720900

C -0.58901800 -0.53533200 0.12548200

C -1.86631100 -0.42776700 0.91776400

C 2.60496500 -0.76181700 -0.43540700

C -3.06061700 -0.32257200 -0.05543700

C -2.01134500 -1.63959600 1.86423700

H 1.20805300 0.26889200 -1.69754700

H 1.66192400 2.49274200 -1.01841700

H 3.23859400 1.78872200 -0.62644500

H 2.59710900 1.45162000 1.71146300

H 1.90513800 3.03859000 1.36733200

H 0.28540500 1.01615600 2.26748600

H -0.30061600 2.12500300 0.99993400

H -1.82978100 0.48575200 1.51007800

H -3.14140000 -1.22520800 -0.66109500

H -3.98124100 -0.22672800 0.51947900

H -1.17650600 -1.70637900 2.56591200

H -2.92766900 -1.53051400 2.44673700

H -2.06965900 -2.57274200 1.30187400

H 0.32563400 -1.77453300 -1.03762500

H -3.27899900 2.05125800 -0.40168600

H 2.71049500 -2.67379600 -0.71644700

**Conf. 2 (O4)H+**

S -2.87999600 1.03423000 -1.36989100

O -0.54943100 -1.56060700 -0.62777400

O 1.98839600 -2.00255100 -0.66388000

O 3.73540500 -0.65144500 -0.30284500

N 0.41021700 0.28522800 0.31279300

C 1.57454500 0.36182200 -0.63524700

C 2.22085400 1.71395300 -0.30499500

C 1.88291900 1.93585900 1.17418100

C 0.44841700 1.42309900 1.28712000

C -0.60691600 -0.53853700 0.17041100

C -1.91291100 -0.37778500 0.90530100

C 2.45617700 -0.88706600 -0.51942500

C -3.06152800 -0.30927400 -0.12462300

C -2.11406500 -1.54182200 1.89934900

H 1.17545500 0.33769400 -1.65472900

H 1.75848100 2.48550000 -0.92440300

H 3.28918200 1.71135000 -0.51000500

H 2.54963600 1.35428000 1.81614400

H 1.95954700 2.98116700 1.47185000

H 0.19052200 1.06681200 2.28300100

H -0.27392700 2.17878600 0.96988200

H -1.89326200 0.56416400 1.45274900

H -3.11430700 -1.23359000 -0.69987700

H -4.00758000 -0.19237200 0.40319000

H -1.31121300 -1.58413000 2.63927700

H -3.05387300 -1.39774100 2.43507500

H -2.15603000 -2.49940800 1.37826000

H 0.39511500 -1.84166700 -0.83056800

H -3.24660800 2.05179700 -0.56290600

H 4.22736500 -1.49158300 -0.29466700

**Conf. 2 (S)H+**

S -3.61201300 -0.65145700 -0.98372700

O -0.80734900 -1.27387000 -0.17047700

O 1.71507600 -2.23867500 0.90299000

O 3.45370500 -0.86074900 0.82965700

N 0.61138600 0.44292300 -0.22396300

C 1.69903600 -0.43616200 -0.77559800

C 2.63089100 0.56404500 -1.45994300

C 2.53422600 1.82234600 -0.58570400

C 1.06399300 1.87250000 -0.15394900

C -0.59303700 0.01169700 0.02962300

C -1.68746100 0.90204500 0.58516500

C 2.39211000 -1.19436200 0.39581700

C -3.12639900 0.33642700 0.49583900

C -1.40268100 1.19715500 2.08451000

H 1.24868100 -1.15112800 -1.46496200

H 2.27223100 0.75756400 -2.47411500

H 3.64621300 0.17631200 -1.51863900

H 3.18207900 1.72085700 0.28485400

H 2.81675600 2.72909300 -1.11979000

H 0.92824200 2.26378800 0.85143300

H 0.45019500 2.45001100 -0.84927800

H -1.64601000 1.84303100 0.02770800

H -3.31154700 -0.35110300 1.32368400

H -3.82290700 1.16615700 0.60993000

H -0.46553900 1.72758400 2.24415200

H -2.20675000 1.82077600 2.47934200

H -1.37601900 0.26949500 2.65995100

H 0.88642700 -2.40266600 0.43109300

H -3.28206500 0.25514000 -1.93028800

H -1.76300100 -1.41985200 -0.43961100

**Conf. 3 (N)H+**

S 4.50719000 0.10309900 -0.35718900

O 0.30572700 0.45858400 1.76634600

O -3.70590400 -1.74462100 0.45019000

O -2.04192700 -1.84242400 -1.00962300

N -0.77373400 0.33298100 -0.32559400

C -2.10094800 0.10300500 0.36805300

C -2.98642700 1.30786300 -0.02309800

C -1.96811400 2.42888300 -0.27013800

C -0.82625600 1.71785900 -0.98975800

C 0.47534900 0.20160000 0.62359400

C 1.71594600 -0.24727100 -0.09541300

C -2.60994900 -1.25930100 -0.12127300

C 2.97248200 0.28250400 0.62870000

C 1.68205800 -1.79319600 -0.20082800

H -1.90277000 0.09217300 1.44200100

H -3.69805000 1.55357500 0.76549900

H -3.55046500 1.09051300 -0.93421300

H -2.37350600 3.23898200 -0.87691500

H -1.62168600 2.85495700 0.67448600

H -1.03857900 1.55460200 -2.04674400

H 0.14445600 2.20251500 -0.89379100

H 1.69448800 0.16233400 -1.11222700

H 2.88032700 1.35507500 0.80703200

H 3.09221700 -0.19587900 1.60050700

H 0.78962200 -2.16581800 -0.70950100

H 2.54658200 -2.11469500 -0.78251100

H 1.73313100 -2.24833900 0.79061900

H -4.04270500 -1.19380700 1.17065900

H 4.77358300 -1.17854500 -0.03464200

H -0.71356100 -0.41207600 -1.04039300

**Conf. 3 (O2)H+**

S -4.28127100 0.67513100 -0.09412400

O 0.02530500 -1.56112700 -0.96172600

O 3.90672700 -1.21183100 -0.31645000

O 2.28669900 -1.23426700 1.19923300

N 0.60717500 0.40988200 -0.13541200

C 1.97058200 0.23334100 -0.69328900

C 2.57639900 1.64763900 -0.58029100

C 1.92142200 2.21687700 0.68667000

C 0.48439800 1.68514700 0.63616200

C -0.30646800 -0.51288200 -0.23389700

C -1.68590300 -0.40554200 0.35629300

C 2.71923500 -0.81632500 0.16471200

C -2.64741600 0.15633700 -0.73724200

C -2.15188600 -1.75115300 0.93572100

H 1.90038000 -0.11872700 -1.72416200

H 2.30132300 2.23058000 -1.46251000

H 3.66478400 1.62888400 -0.51896500

H 2.42554700 1.84560800 1.58076800

H 1.94237000 3.30572900 0.71558500

H 0.07388500 1.48434700 1.62428200

H -0.18459500 2.35793800 0.09531200

H -1.64723400 0.32307100 1.16589100

H -2.22815500 1.06231000 -1.17866600

H -2.78202000 -0.56508100 -1.54568300

H -1.42756900 -2.16163700 1.64182600

H -3.08806300 -1.59799900 1.47262000

H -2.35495700 -2.49797500 0.15801000

H 4.11763000 -0.82689400 -1.17766900

H -4.84762600 -0.54783100 -0.05481900

H -0.64761000 -2.25641500 -0.91544600

**Conf. 3 (O3)H+**

S -4.39618400 0.48879400 -0.34468500

O -0.27496400 -1.60869600 -0.62295900

O 2.32136800 -2.09984900 -0.14776200

O 3.87311600 -0.62146700 0.56334300

N 0.67874100 0.39817800 -0.05732800

C 1.98364600 0.17048300 -0.76758600

C 2.61304700 1.56601900 -0.80945200

C 2.10638000 2.23322600 0.47532700

C 0.65597200 1.76263500 0.57844700

C -0.35510600 -0.41144700 -0.10076300

C -1.71794500 -0.04231800 0.41169700

C 2.86255000 -0.84996300 -0.02256900

C -2.76681000 -0.26039500 -0.71698600

C -2.02713500 -0.86241500 1.68126200

H 1.77066800 -0.23113900 -1.76163800

H 2.25400100 2.09551000 -1.69486300

H 3.69893000 1.50687600 -0.85886200

H 2.68500400 1.89124600 1.33559700

H 2.16843300 3.32036700 0.43780600

H 0.29308400 1.68611200 1.60206000

H -0.01663600 2.40054500 0.00164600

H -1.72282200 1.01711200 0.66462000

H -2.44239300 0.23486300 -1.63433800

H -2.88376000 -1.32013500 -0.93944100

H -1.27537700 -0.70585000 2.45848200

H -2.98791800 -0.53936100 2.08322700

H -2.07869500 -1.92933900 1.45590300

H 0.64084900 -1.96112000 -0.67942600

H -4.87537900 -0.51176000 0.42127100

H 2.87600100 -2.75673100 0.30699000

**Conf. 3 (O4)H+**

S -4.42081200 0.40931700 -0.43617600

O -0.26698900 -1.62804700 -0.46740200

O 2.21508400 -2.09178500 0.04983500

O 3.97355800 -0.72179900 0.24998800

N 0.66789200 0.41623500 -0.04980000

C 1.96881400 0.15626900 -0.75745800

C 2.65122700 1.53081800 -0.76915600

C 2.11780100 2.21857800 0.49314300

C 0.64855800 1.80164300 0.52638300

C -0.36947800 -0.39961500 -0.05530000

C -1.74061100 0.02022900 0.39372800

C 2.73147500 -0.99828700 -0.09486000

C -2.77521300 -0.34952000 -0.70681700

C -2.05380000 -0.63871500 1.75330700

H 1.74004200 -0.19744800 -1.76798000

H 2.33725600 2.07338800 -1.66382800

H 3.73523700 1.44317900 -0.79117100

H 2.63956300 1.85590300 1.38243100

H 2.22573600 3.30225500 0.46063000

H 0.22281500 1.77950200 1.52790700

H 0.03678500 2.44245200 -0.11273300

H -1.75888300 1.10347700 0.51125500

H -2.45122900 0.03870700 -1.67436700

H -2.87245400 -1.42986200 -0.80250900

H -1.31412700 -0.37459300 2.51295900

H -3.02450400 -0.28465500 2.10201200

H -2.08433300 -1.72623900 1.66271800

H 0.67569700 -1.97499700 -0.41775100

H -4.89544900 -0.51092000 0.42709200

H 4.39971700 -1.51820700 0.61357400

**Conf. 3 (S)H+**

S -4.48841500 0.11970200 -0.22650600

O -0.33584100 -1.43024400 -0.79714700

O 2.07591000 -2.25596000 0.23704000

O 3.75062200 -0.88857300 0.75540000

N 0.78947800 0.45120400 -0.21019100

C 2.08490200 -0.02936300 -0.77626100

C 2.91491600 1.25142100 -0.88166900

C 2.41184700 2.11102400 0.28702100

C 0.90316000 1.83508700 0.31947300

C -0.31996500 -0.29128200 -0.31029500

C -1.64240700 0.27621900 0.25426000

C 2.73317100 -1.09044000 0.15437400

C -2.72613600 -0.29703400 -0.66724400

C -1.78284500 -0.15999100 1.72431100

H 1.88833300 -0.49356300 -1.74574800

H 2.71531400 1.73966700 -1.83939100

H 3.97956400 1.03708700 -0.81322200

H 2.87678300 1.77931500 1.21714300

H 2.62348500 3.17281600 0.16017700

H 0.48770100 1.90504200 1.32620900

H 0.36177200 2.52499400 -0.33671900

H -1.64416500 1.36742000 0.18433000

H -2.64694700 0.05639100 -1.69683300

H -2.71429600 -1.38815000 -0.68323100

H -0.91386800 0.15730600 2.30219100

H -2.65248600 0.28890800 2.21458800

H -1.84652000 -1.24819500 1.80281800

H 1.25407000 -2.23125300 -0.29262600

H -4.49252300 -0.22628900 1.08543300

H -4.37330700 1.44921200 0.02414300

**Conf. 4 (N)H+**

S 4.53890800 -0.06747400 -0.27132800

O 0.32019700 0.54748300 1.73552000

O -3.66738200 -1.78736000 0.47533500

O -2.02655700 -1.85197400 -1.01240600

N -0.78009300 0.33968400 -0.33705700

C -2.09447500 0.08649000 0.37481600

C -3.00577500 1.27696700 -0.00169500

C -2.01059300 2.41316500 -0.27211900

C -0.87203700 1.71688400 -1.01095200

C 0.48084300 0.25286100 0.60046700

C 1.71822500 -0.21616900 -0.11118900

C -2.58887400 -1.28224700 -0.11206700

C 2.97750500 0.31027100 0.61125600

C 1.67137300 -1.76526200 -0.18193000

H -1.88169800 0.07699400 1.44585000

H -3.70510800 1.51392500 0.80044500

H -3.58444900 1.04829300 -0.90075100

H -2.44050600 3.21435800 -0.87384000

H -1.65241400 2.84778400 0.66413900

H -1.10444800 1.54129700 -2.06180900

H 0.09165800 2.21945100 -0.93896100

H 1.69490600 0.17268400 -1.13638500

H 2.91194800 1.38492300 0.78267500

H 3.06959400 -0.16578800 1.58834100

H 0.80739500 -2.14029300 -0.73551400

H 2.57203300 -2.10395100 -0.69507600

H 1.65893600 -2.19551400 0.82182200

H -4.00072900 -1.24533700 1.20402400

H 4.44535500 0.92048500 -1.18564900

H -0.71156200 -0.41046300 -1.04578500

**Conf. 4 (O2)H+**

S -4.47760100 0.24690000 -0.33719200

O -0.28595300 -1.61651100 -0.46018700

O 3.96289700 -0.91864300 0.37180800

O 2.13864300 -2.11095300 0.10765100

N 0.68562000 0.41599200 -0.08397600

C 1.99068000 0.10660600 -0.76057800

C 2.67738600 1.47978600 -0.81774400

C 2.15188400 2.21587300 0.42120800

C 0.67821900 1.81369100 0.45426900

C -0.37196100 -0.38029400 -0.08493400

C -1.73516500 0.08153700 0.34781400

C 2.71725000 -1.05378700 -0.04148700

C -2.80405900 -0.42705300 -0.65813000

C -1.99735800 -0.42490800 1.78474600

H 1.77350600 -0.27922800 -1.76134800

H 2.36061600 1.99258200 -1.72887500

H 3.76698400 1.42214600 -0.87512400

H 2.65824200 1.87870500 1.32995500

H 2.27419400 3.29624000 0.35336800

H 0.24777200 1.82491600 1.45384800

H 0.07952900 2.44764500 -0.20384600

H -1.75569600 1.17213600 0.34625300

H -2.52107800 -0.19735200 -1.68590600

H -2.90296800 -1.50956600 -0.58074200

H -1.27459400 -0.02326900 2.49888600

H -2.99271200 -0.10001000 2.08963600

H -1.95673000 -1.51521700 1.82400500

H 4.33522400 -0.04729100 0.18071300

H -4.27469600 1.45242300 -0.90846600

H 0.65874500 -1.97705400 -0.37461100

**Conf. 4 (O3)H+**

S -4.46709100 0.29470400 -0.26052200

O -0.30109100 -1.59099800 -0.61359000

O 2.27325700 -2.12634400 -0.07967200

O 3.84824600 -0.66398800 0.61303200

N 0.69071800 0.41108800 -0.10040000

C 2.00329900 0.13078500 -0.77716600

C 2.66691400 1.50919700 -0.84726600

C 2.15125500 2.22611500 0.40678300

C 0.68748300 1.79441900 0.49084800

C -0.36098500 -0.37595500 -0.13291800

C -1.71737500 0.03587600 0.36552400

C 2.84290800 -0.88669400 0.01600100

C -2.80250300 -0.34632800 -0.67922500

C -1.96519100 -0.62592700 1.73986900

H 1.79998000 -0.29581700 -1.76279200

H 2.33805900 2.02039200 -1.75487900

H 3.75180000 1.42305600 -0.87280100

H 2.70252000 1.89439600 1.28877100

H 2.24209200 3.30981600 0.33994500

H 0.29837700 1.76040000 1.50705000

H 0.04548500 2.43006000 -0.12257400

H -1.72812500 1.11904700 0.48772000

H -2.52990100 0.00044000 -1.67666400

H -2.90946100 -1.42994100 -0.72727500

H -1.22668400 -0.31329000 2.48165100

H -2.95142500 -0.32571500 2.09513600

H -1.94025400 -1.71431900 1.65704800

H 0.60691800 -1.96656700 -0.64243800

H -4.26156600 1.55835500 -0.68645600

H 2.80250600 -2.78146600 0.40684700

**Conf. 4 (O4)H+**

S -4.48170500 0.23435400 -0.34099300

O -0.28551200 -1.61761400 -0.45296500

O 2.18119900 -2.10272300 0.11108300

O 3.96013900 -0.75700700 0.29327500

N 0.67600400 0.42404100 -0.08695500

C 1.98383000 0.12436200 -0.76548500

C 2.68777400 1.48764300 -0.80290400

C 2.14423500 2.21770400 0.43101100

C 0.66804600 1.82478400 0.44833300

C -0.37384500 -0.37601100 -0.08067700

C -1.74036000 0.07661100 0.35194800

C 2.71778100 -1.02276100 -0.05905100

C -2.80470400 -0.43286400 -0.65834600

C -2.00442600 -0.43363600 1.78662100

H 1.76613100 -0.25339100 -1.76976600

H 2.39705400 2.01029500 -1.71710500

H 3.77049200 1.38310000 -0.80423600

H 2.64400100 1.87032100 1.33886400

H 2.27084000 3.29822300 0.37187900

H 0.22241500 1.83826000 1.44127500

H 0.07931700 2.45668700 -0.22088700

H -1.76429500 1.16701300 0.35253800

H -2.51947400 -0.19929700 -1.68463500

H -2.90077400 -1.51591200 -0.58433600

H -1.28502800 -0.02977500 2.50289200

H -3.00176400 -0.11357800 2.09010400

H -1.95981600 -1.52391700 1.82424400

H 0.65099700 -1.97739400 -0.37936700

H -4.27931500 1.44439700 -0.90276600

H 4.36787500 -1.54921000 0.68603800

**Conf. 4 (S)H+**

S -4.44329400 0.11459600 -0.04797800

O -0.33870100 -1.43037800 -0.79046200

O 2.06152400 -2.25831700 0.26667100

O 3.74701500 -0.89835700 0.76945200

N 0.79421600 0.45075600 -0.21943800

C 2.08908600 -0.04446900 -0.77366200

C 2.92780900 1.22958100 -0.89125000

C 2.42309600 2.10821500 0.26247200

C 0.91271000 1.84200900 0.28932300

C -0.31931500 -0.28544200 -0.31640200

C -1.64102200 0.29648100 0.23166600

C 2.72788700 -1.09908200 0.17089200

C -2.72494600 -0.32622900 -0.65817200

C -1.78499400 -0.07906900 1.71988400

H 1.89386700 -0.51912400 -1.73842300

H 2.73729900 1.70614200 -1.85671100

H 3.99056900 1.00926900 -0.81328400

H 2.88018000 1.78657900 1.20001800

H 2.64222200 3.16684100 0.12246700

H 0.49072400 1.93050500 1.29159600

H 0.37983600 2.52447500 -0.38150400

H -1.64782700 1.38386400 0.11560100

H -2.66886000 -0.01015700 -1.69832100

H -2.70085800 -1.41517500 -0.60128300

H -0.94360800 0.30679500 2.29611400

H -2.69180400 0.33861400 2.16686800

H -1.80150100 -1.16452300 1.84339800

H 1.24001300 -2.23298300 -0.26356000

H -4.52252300 1.40610200 -0.45889100

H -5.16510700 -0.36160800 -1.09416800

**Conf. 5 (N)H+**

S -3.56257300 -1.11743700 0.09580500

O -0.74503200 0.31350600 1.63653900

O 3.91108100 0.74227500 0.74487200

O 2.54297600 1.46980900 -0.89561600

N 0.54172200 -0.10938100 -0.28557700

C 1.77308000 -0.25639900 0.58940500

C 2.19804300 -1.73411600 0.46119600

C 1.64512100 -2.16095300 -0.90526900

C 0.29171200 -1.46194300 -0.97618400

C -0.73036200 0.40878400 0.45712300

C -1.76581500 1.00563700 -0.45941200

C 2.78363900 0.75544900 0.05072900

C -3.18264400 0.68547400 0.04372000

C -1.51379200 2.53331100 -0.54994500

H 1.50824900 0.01230000 1.61204900

H 1.73512800 -2.31003800 1.26502700

H 3.27753800 -1.84731700 0.55021100

H 2.29527700 -1.82509300 -1.71763800

H 1.53221400 -3.24169100 -0.99473700

H -0.08136400 -1.27686300 -1.98147200

H -0.47664100 -1.97957600 -0.40058500

H -1.63995500 0.57086300 -1.45564500

H -3.35718600 1.11703700 1.02845000

H -3.90056600 1.13058500 -0.64568600

H -0.51511600 2.76965200 -0.92687000

H -2.23759300 2.96886700 -1.24075600

H -1.63739800 3.00551800 0.42631900

H 4.52877100 1.40160000 0.38543900

H -3.29679100 -1.30095200 1.40473600

H 0.80847000 0.59359700 -0.99722500

**Conf. 5 (O2)H+**

S -2.82208600 1.18541400 -1.20705400

O -0.53694800 -1.57625800 -0.65372600

O 3.73808600 -0.63045700 -0.29519400

O 2.00484400 -1.99338000 -0.67663300

N 0.39963100 0.27029800 0.31052500

C 1.57015600 0.36720700 -0.62759400

C 2.20242700 1.72116200 -0.27814900

C 1.85182500 1.92426900 1.20077500

C 0.42065600 1.39910000 1.29714100

C -0.61051400 -0.55929200 0.14892100

C -1.92415300 -0.41467300 0.87684100

C 2.46185900 -0.87505900 -0.51932900

C -3.06367100 -0.31719500 -0.15711700

C -2.13563600 -1.60172200 1.84018500

H 1.17846200 0.35081800 -1.65018000

H 1.73747100 2.49541100 -0.89223100

H 3.27214600 1.73001400 -0.47554300

H 2.51843300 1.34127900 1.84159100

H 1.91726800 2.96696300 1.50992900

H 0.15835500 1.03018800 2.28726200

H -0.30431800 2.15360800 0.98332800

H -1.90673300 0.51099200 1.45290000

H -3.07893600 -1.20328500 -0.78944900

H -4.01111500 -0.24339000 0.37609400

H -1.33274200 -1.66789700 2.57829500

H -3.07396900 -1.46338000 2.37952800

H -2.18351500 -2.54533900 1.29486900

H 4.23717800 -1.46638100 -0.29286000

H -3.46965200 0.73591600 -2.29920300

H 0.41208200 -1.84624600 -0.85075200

**Conf. 5 (O3)H+**

S 2.70501000 0.29904700 -1.45685700

O -0.09100700 0.62172800 1.36298900

O 0.05493600 2.81520300 -0.98783400

O -1.99453700 1.86410600 1.70365100

N -0.66112200 -0.59082600 -0.36828300

C -1.81611500 0.30120100 -0.20656400

C -3.00017200 -0.67226600 -0.27721300

C -2.52142100 -1.65660800 -1.37477400

C -0.98037000 -1.76997900 -1.21171600

C 0.23637700 -0.37602000 0.54970400

C 1.52104000 -1.09500900 0.75507000

C -1.45039200 1.06065500 1.04749500

C 2.70138100 -0.18191300 0.31358200

C 1.68065100 -1.54600500 2.22126000

H -1.83482600 1.03286800 -1.02084700

H -3.93187100 -0.17101300 -0.53343300

H -3.13343700 -1.17860700 0.68186900

H -3.00326000 -2.62965500 -1.28851700

H -2.75850400 -1.25834300 -2.36305400

H -0.67307200 -2.67453600 -0.68719900

H -0.44070500 -1.70498600 -2.15583300

H 1.51130800 -1.96433100 0.09326400

H 2.75515400 0.70723300 0.94181000

H 3.61986000 -0.74927100 0.46717000

H 0.86579200 -2.20347300 2.53214200

H 2.61423000 -2.10203200 2.31973300

H 1.71434100 -0.69184000 2.89888000

H 0.21172700 3.52812700 -0.35628600

H 1.87135900 1.35649500 -1.33386500

H -0.02141700 3.26177600 -1.83966000

**Conf. 5 (O4)H+**

S -2.90258200 0.54849400 -1.48182300

O 0.03036200 -1.35307600 0.17755600

O 1.56381800 -1.92676000 -1.54565000

O 2.28762600 -1.91865600 0.54767200

N 0.44231900 0.79112800 0.04276300

C 1.65433200 0.24042600 -0.58178600

C 2.76079100 1.07539000 0.06211200

C 2.10081400 2.47536700 0.12145600

C 0.59251600 2.22283800 0.39126900

C -0.38916300 -0.14303300 0.42280200

C -1.71620200 0.06823700 1.07830700

C 1.51560000 -1.28452100 -0.37045200

C -2.85377400 -0.36229800 0.11678600

C -1.80035200 -0.69133300 2.41722400

H 1.61165300 0.41236400 -1.66064400

H 3.68348200 1.06685100 -0.51623300

H 2.98933600 0.71102700 1.06827000

H 2.54438900 3.10830600 0.88901700

H 2.22304800 2.98555800 -0.83570600

H 0.32015200 2.36896800 1.43697500

H -0.05908300 2.83216600 -0.23489200

H -1.81834200 1.14165900 1.25543500

H -2.81454000 -1.43396100 -0.07599200

H -3.80142100 -0.15059700 0.61271500

H -1.02585600 -0.36488500 3.11562100

H -2.76778200 -0.49366800 2.88171700

H -1.70378200 -1.76802500 2.26885400

H 1.69034000 -2.87724600 -1.40144800

H -2.19849100 -0.34722700 -2.20350000

H 2.23016500 -1.52359600 1.42669800

**Conf. 5 (S)H+**

S -3.28148300 -0.99633200 -0.87949900

O -0.92122100 -1.15525400 -0.05384300

O 2.95963300 -2.13609100 0.44230500

O 1.88431000 -0.67196200 1.77743800

N 0.59252300 0.48939700 -0.37672900

C 1.66513500 -0.48349600 -0.63887700

C 2.74875800 0.35878100 -1.34352400

C 2.56287200 1.75840300 -0.73979400

C 1.04323800 1.88903500 -0.57455700

C -0.62782900 0.05459900 -0.04889000

C -1.72559700 1.05499800 0.33374100

C 2.15601400 -1.08589800 0.68131600

C -3.07655000 0.32965800 0.42652800

C -1.47471300 1.69457900 1.71988900

H 1.29746300 -1.29833600 -1.26242900

H 2.54946800 0.36849500 -2.41789200

H 3.74759600 -0.04918300 -1.19430800

H 3.04843800 1.82110600 0.23658000

H 2.97121200 2.54900700 -1.36938300

H 0.77717600 2.51875200 0.27202100

H 0.57673000 2.29758900 -1.47703100

H -1.78633700 1.84172000 -0.42549000

H -3.19725700 -0.18218000 1.37901900

H -3.91142300 1.01228400 0.26904100

H -0.59671800 2.33694100 1.71532300

H -2.32810800 2.30902000 2.01653600

H -1.31906500 0.92106600 2.47481400

H 3.27690000 -2.48097000 1.29203300

H -3.11434300 -2.12525300 -0.16081600

H -4.64541500 -1.04201500 -0.86112800

**Conf. 6 (N)H+**

S -3.54566900 -1.11384000 0.11791200

O -0.71162700 0.35234800 1.67228500

O 3.92165900 0.80428100 0.61559100

O 2.49895600 1.41362000 -1.02653200

N 0.53243100 -0.14311400 -0.25738900

C 1.79261900 -0.22347700 0.58612600

C 2.23071600 -1.70216100 0.53787800

C 1.63167400 -2.22334400 -0.77562400

C 0.26835400 -1.54290900 -0.83767900

C -0.71682200 0.41857200 0.49143300

C -1.75877200 1.02330900 -0.41685000

C 2.77463900 0.76257500 -0.04468200

C -3.16560000 0.68619700 0.10258800

C -1.51310600 2.55357300 -0.47733600

H 1.55575600 0.10425400 1.59833500

H 1.80496900 -2.22854600 1.39437000

H 3.31410900 -1.79889200 0.59232800

H 2.24601200 -1.93587600 -1.63324400

H 1.52785900 -3.30860800 -0.78894200

H -0.14998900 -1.43289000 -1.83633900

H -0.46713700 -2.02379200 -0.19189600

H -1.63575300 0.60826000 -1.42196800

H -3.27635100 1.01968600 1.13491100

H -3.91068300 1.20896700 -0.49621200

H -0.51207600 2.79879000 -0.84189700

H -2.23325700 3.00048400 -1.16456600

H -1.64486700 3.00496700 0.50764600

H 4.52135200 1.44498900 0.19697800

H -3.84138700 -1.22203900 -1.19429900

H 0.77102100 0.50747500 -1.02593500

**Conf. 6 (O2)H+**

S -3.08013600 1.30365400 -0.83627500

O -0.31078800 -1.32846400 -1.16252500

O 3.62675800 -0.72979600 -1.04437500

O 2.31681300 -1.54224600 0.60526600

N 0.36378500 0.31820700 0.15353700

C 1.61795800 0.42712500 -0.63515600

C 2.17718900 1.79969200 -0.21472500

C 1.72427200 1.93918400 1.24543000

C 0.32070900 1.32317600 1.26101600

C -0.54757600 -0.56677100 -0.11041800

C -1.81325900 -0.76551000 0.68287500

C 2.54080000 -0.74341600 -0.26449600

C -3.05420800 -0.41024700 -0.17101500

C -1.88762000 -2.21418300 1.21677000

H 1.39790300 0.37155300 -1.70103500

H 1.72758100 2.57408600 -0.84012900

H 3.25721600 1.84961200 -0.34299700

H 2.38654600 1.38158000 1.91107200

H 1.70559900 2.97514700 1.58237700

H 0.08495600 0.83012500 2.20280400

H -0.45516100 2.05320000 1.02232700

H -1.78277700 -0.08473500 1.53268600

H -3.13348400 -1.06055300 -1.04587900

H -3.94972600 -0.58369400 0.42523000

H -0.99624600 -2.47896500 1.78823900

H -2.75481100 -2.30848800 1.87193200

H -2.01169800 -2.94909200 0.41473200

H 4.20943100 -1.46484000 -0.79233100

H -3.50631100 1.90266600 0.29494600

H -0.97518800 -2.02378200 -1.26693900

**Conf. 6 (O3)H+**

S 2.97782200 0.73908600 -0.93638900

O 0.07299500 0.42919700 1.31902000

O 0.05321300 2.62116500 -0.93899300

O -1.66201500 1.74968800 2.06563800

N -0.78874200 -0.42849700 -0.50159000

C -1.83755600 0.50439700 -0.06627100

C -3.09972500 -0.36645900 -0.12180300

C -2.84024800 -1.20101700 -1.40125900

C -1.30486500 -1.43717300 -1.45960300

C 0.21518500 -0.43243600 0.32781500

C 1.41428800 -1.32203700 0.30482300

C -1.27043600 1.03015800 1.23118800

C 2.71534100 -0.49673900 0.39890900

C 1.32503100 -2.34343300 1.46506800

H -1.87612400 1.34953400 -0.76021000

H -4.00805800 0.23029600 -0.18378500

H -3.16600200 -1.00339300 0.76368900

H -3.38672400 -2.14325900 -1.39358900

H -3.15833600 -0.64187300 -2.28283300

H -1.01488200 -2.43215100 -1.12239500

H -0.88801500 -1.25854600 -2.45059000

H 1.40279000 -1.85514000 -0.64935800

H 2.73527600 0.07858400 1.32541700

H 3.56259700 -1.18176700 0.41810800

H 0.41961700 -2.95111400 1.40066100

H 2.18244400 -3.01625400 1.41328500

H 1.33834800 -1.83977200 2.43301800

H 0.03358700 3.58457600 -0.93421600

H 3.12288700 -0.13442100 -1.95458800

H 0.96098200 2.37685400 -1.16777800

**Conf. 6 (O4)H+**

S -2.87956400 0.26844400 -1.55354900

O -0.02263100 -1.30647200 0.25584400

O 1.50786300 -2.07247000 -1.39850700

O 2.20840500 -1.92210500 0.69733200

N 0.47879000 0.80322400 -0.02717500

C 1.66583700 0.15979300 -0.61044400

C 2.80749400 0.99706600 -0.03526100

C 2.20214500 2.42189800 -0.07613700

C 0.68745500 2.24761400 0.21977300

C -0.39360200 -0.06753100 0.40852900

C -1.71135500 0.23602500 1.05210800

C 1.47092500 -1.33736500 -0.28078800

C -2.85374500 -0.33809800 0.18058200

C -1.76156500 -0.32731600 2.48779700

H 1.62234200 0.24774700 -1.69935200

H 3.72444300 0.91100100 -0.61634300

H 3.03060300 0.69916600 0.99360100

H 2.67525200 3.09271200 0.63990000

H 2.33503100 2.85457800 -1.06935100

H 0.43048300 2.47771100 1.25428000

H 0.05810200 2.84027600 -0.44433100

H -1.81441000 1.32378200 1.08247500

H -2.76067700 -1.42252600 0.10780800

H -3.80744500 -0.12019900 0.66061600

H -0.97178300 0.09374600 3.11491400

H -2.71834400 -0.06608100 2.94270400

H -1.66634300 -1.41439500 2.48874000

H 1.58607700 -3.01344000 -1.17813700

H -3.38418500 1.49106700 -1.28621200

H 2.15171700 -1.45697100 1.54138800

**Conf. 6 (S)H+**

S -3.33039100 -1.10321100 -0.74087900

O -0.92376900 -1.15372900 -0.08005700

O 2.94791800 -2.13964300 0.47127700

O 1.87324500 -0.65472000 1.78427300

N 0.59617600 0.48685100 -0.38561400

C 1.66551900 -0.49387200 -0.63454100

C 2.75421000 0.33600000 -1.34431200

C 2.58044500 1.73934000 -0.74596400

C 1.06236700 1.88355700 -0.57088400

C -0.62906200 0.05522400 -0.06517100

C -1.73121400 1.05459900 0.31439700

C 2.14849500 -1.08366400 0.69488300

C -3.06650700 0.30981600 0.46175300

C -1.46839100 1.74093800 1.67612700

H 1.29625700 -1.31462400 -1.24913200

H 2.55406700 0.34229700 -2.41865000

H 3.75001500 -0.07907600 -1.19437400

H 3.07214300 1.80280000 0.22715700

H 2.99093500 2.52453700 -1.38088100

H 0.81166400 2.50622700 0.28501400

H 0.59436500 2.30895200 -1.46478000

H -1.82297500 1.81870600 -0.46593200

H -3.11484900 -0.21092200 1.41775000

H -3.91768600 0.97992400 0.36030400

H -0.62701000 2.42821900 1.62708100

H -2.34219800 2.31997400 1.98416900

H -1.25176000 0.99628900 2.44457400

H 3.25691700 -2.47974500 1.32603600

H -4.54070100 -0.69662300 -1.22976500

H -2.67047500 -0.67041400 -1.83688200