Electronic Supplementary Information

Theoretical Study of Ni^{I}–Ni^{III} Cycle Mediated by Heterogeneous Zinc in C–N Cross-Coupling Reaction

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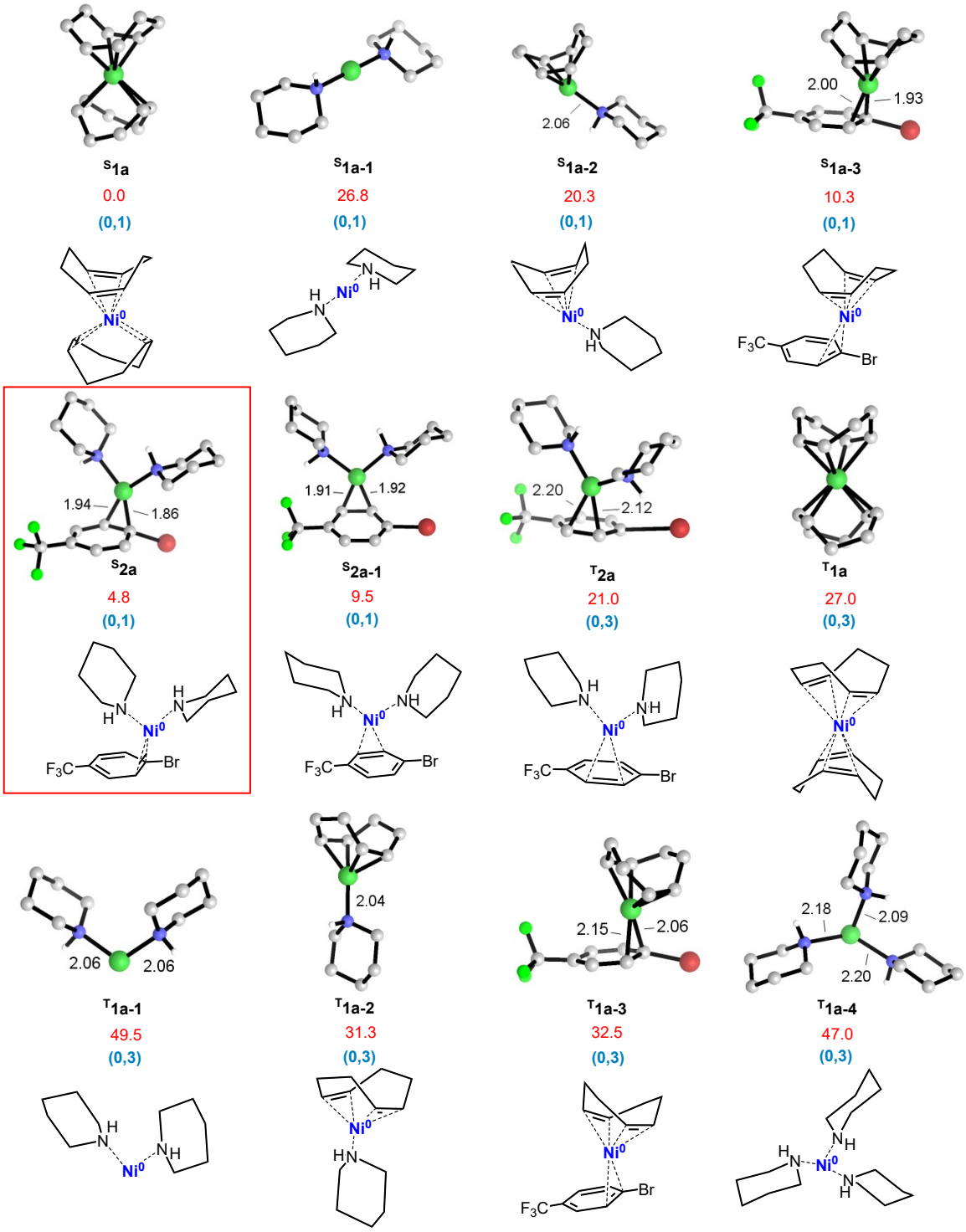

Fig. S1 Relative stability of Ni(0) complexes. The Gibbs free energies are given in kcal/mol. The blue values in parentheses represent the charge and spin multiplicity, respectively.

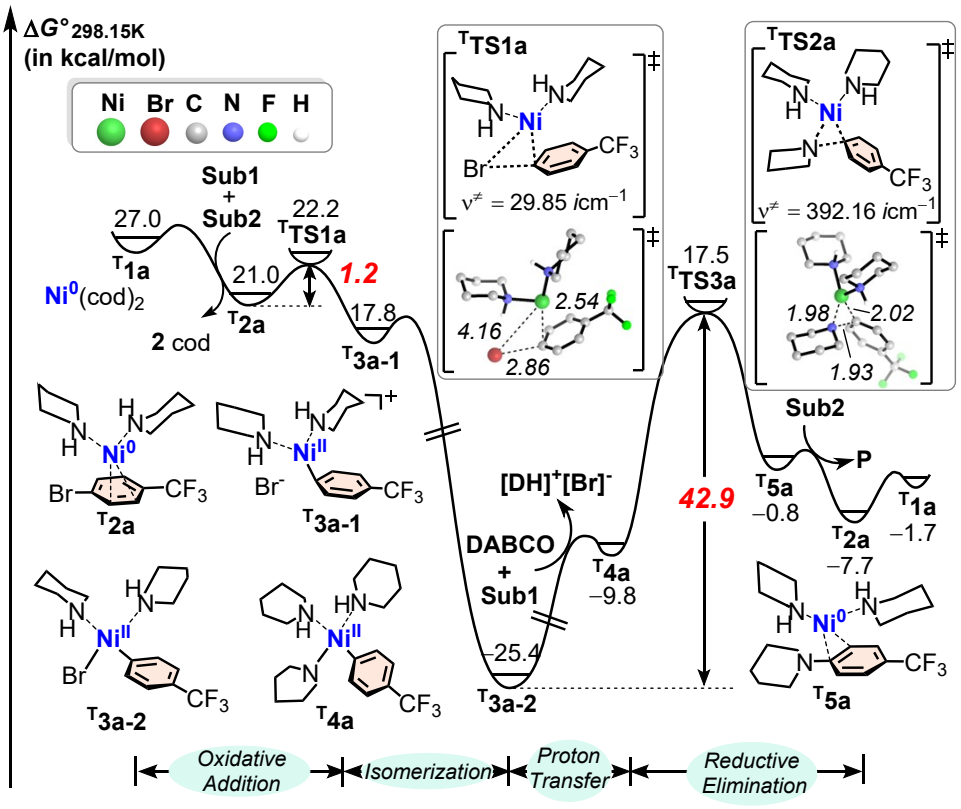

Fig. S2 Triplet Gibbs energy profiles ($\Delta G°_{298.15}$) for Ni^0–Ni^{II}–Ni^0 catalytic cycle in the C–N cross-coupling reaction. The relative Gibbs free energies are given in kcal/mol. The bond distances are given in angstroms.

Table S1 Gibbs activation energies (kcal/mol) of the key transition states of the Ni^0 process calculated at the level of SMD(DMA)/(U)M06/[6-311++G(d,p)/SDD(Ni,Zn)].

$\Delta G°‡_{singlet}$			$\Delta G°‡_{triplet}$	
^{S}TS1a	^{S}TS2a	^{S}TS3a	^{T}TS1a	^{T}TS3a
16.6	22.3	29.8	1.2	42.9

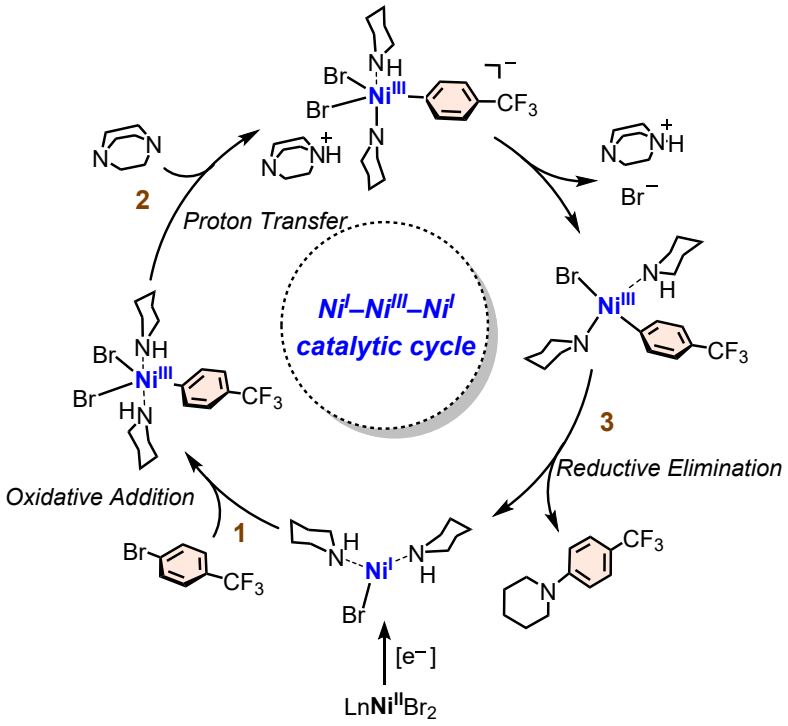

Fig. S3 The proposed Ni^{I}–Ni^{III}–Ni^{I} catalytic cycle process.

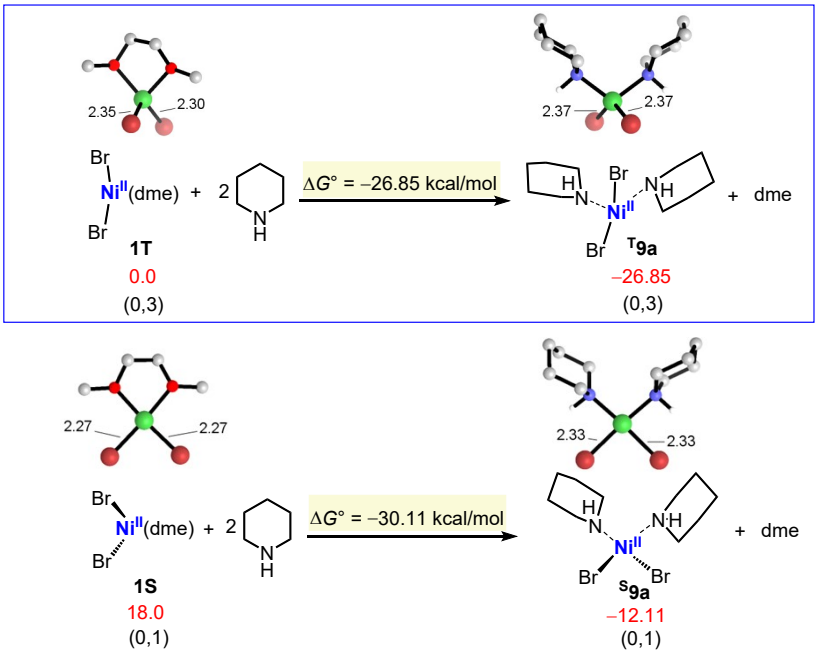

Fig. S4 Relative stability of Ni(II) complexes. The Gibbs free energies are given in kcal/mol.

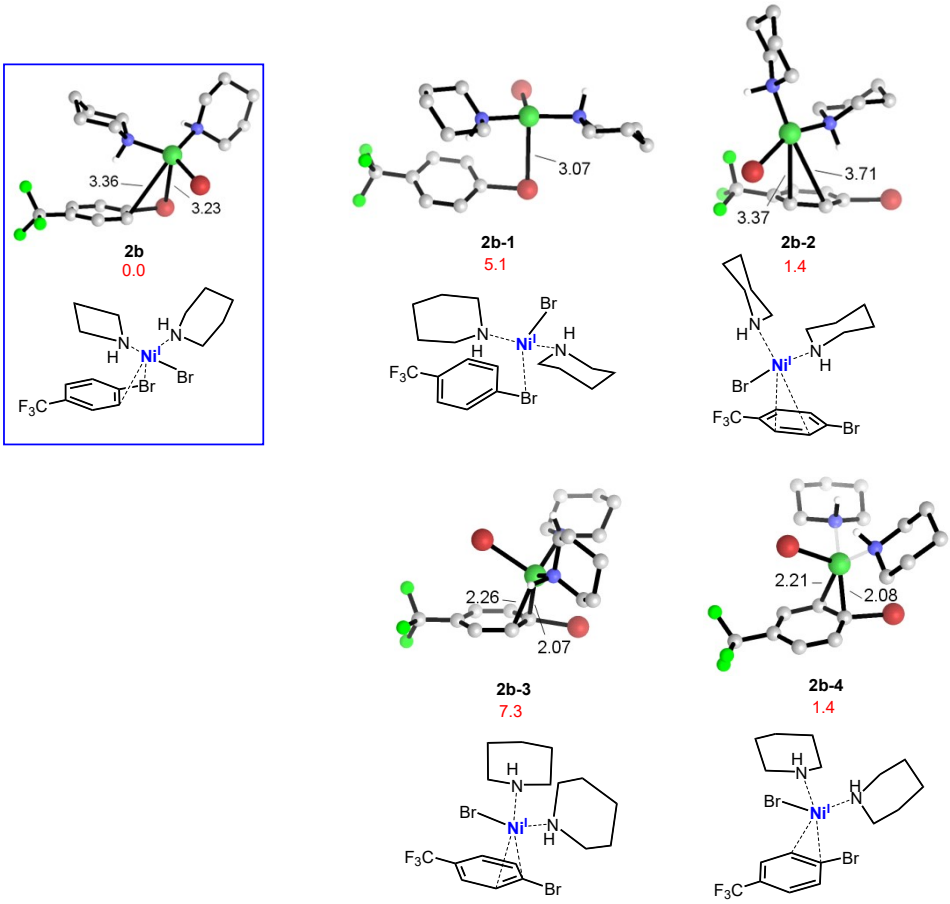

Fig. S5 Relative stability of Ni(I) complexes. The Gibbs free energies are given in kcal/mol. Selected bond lengths are given in angstroms.

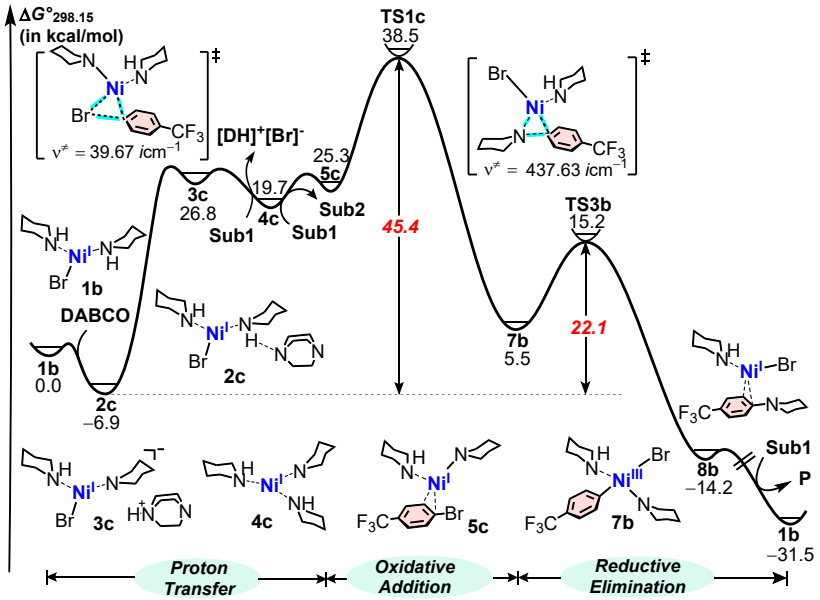

Fig. S6 Gibbs energy profiles ($\Delta G°_{298.15}$) for alternative Ni^{I}–Ni^{III}–Ni^{I} catalytic cycle in the C–N cross-coupling reaction. The relative Gibbs free energies are given in kcal/mol. The bond distances are given in angstroms.

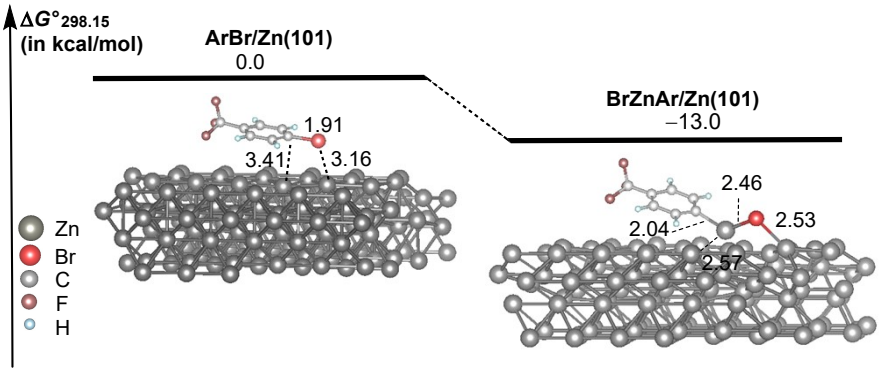

Fig. S7 Thermodynamic evaluation of the formation of organozinc BrZnAr.

Cartesian Coordinates of Optimized Structures

1T

Gibbs free energy before correction = -5621.12693100
Gibbs free energy after correction = -5621.11314089

Ni	0.20662800	-0.13246100	0.27563300
Br	-0.51307400	2.01268400	-0.34126000
C	-0.33190300	-0.92670800	-2.52675900
H	0.73192400	-0.68312800	-2.60035000
H	-0.57030400	-1.76949000	-3.18775700
C	-2.41230300	0.09833100	1.86698500
H	-3.03931200	-0.43846800	2.58983100
H	-3.03985000	0.53662500	1.08059400
O	-1.45201900	-0.80950100	1.32143700
O	-0.57974900	-1.30774300	-1.17266100
C	-1.96310700	-1.56003300	-0.89667800
H	-2.30957000	-2.40513400	-1.50732700
H	-2.55594600	-0.66665100	-1.15064100
C	-2.03416600	-1.88679400	0.56699800
H	-1.44177000	-2.78223700	0.79155600
H	-3.06871600	-2.05610600	0.88856600
H	-0.93408300	-0.05015900	-2.79986900
H	-1.85789300	0.88828900	2.37935800
Br	2.48458700	-0.42055500	0.35682700

1S

Gibbs free energy before correction = -5621.11062500
Gibbs free energy after correction = -5621.09683489

Ni	0.00000000	0.00000000	0.11473900
Br	0.75765900	1.41360500	-1.48805700
C	-0.75417200	-2.57787900	1.55813800
H	-1.35471800	-2.82610400	0.68348700
H	0.24263200	-3.03146900	1.46939900

C	0.75417200	2.57787900	1.55813800
H	1.24940900	2.93003100	2.47140700
H	-0.24263200	3.03146900	1.46939900
O	0.64504800	1.15148100	1.62005500
O	-0.64504800	-1.15148100	1.62005500
C	0.00000000	-0.74500000	2.83212900
H	1.02406400	-1.14933900	2.85578000
H	-0.55921900	-1.13398700	3.69352300
C	0.00000000	0.74500000	2.83212900
H	0.55921900	1.13398700	3.69352300
H	-1.02406400	1.14933900	2.85578000
H	-1.24940900	-2.93003100	2.47140700
H	1.35471800	2.82610400	0.68348700
Br	-0.75765900	-1.41360500	-1.48805700

S1a

Gibbs free energy before correction = -792.64379500

Gibbs free energy after correction = -792.63000471

C	-1.34926300	-1.62997600	-0.20237700
C	-1.50745700	-0.82527300	-1.31232200
C	-1.50755300	0.82530900	1.31241600
C	-2.59153600	0.21032500	-1.51377800
C	-1.34970000	1.62995700	0.20243200
C	-2.16892900	1.61230900	-1.06161800
H	-0.72854200	-2.52088200	-0.33056400
H	-2.85676400	0.24892300	-2.57963400
H	-0.72883100	2.52076800	0.33037800
H	-0.97709900	-1.13576500	-2.21549400
H	-0.97651400	1.13559800	2.21526700
H	-3.50904500	-0.09990700	-0.99596900
H	-1.55818700	2.06901700	-1.85714800
H	-3.05772200	2.26179700	-0.96340100
C	-2.16832700	-1.61244400	1.06179500
H	-1.55743900	-2.06901700	1.85730000
H	-3.05702400	-2.26209300	0.96378400
C	-2.59126400	-0.21053900	1.51398400
H	-3.50888800	0.09943600	0.99623100
H	-2.85643500	-0.24927400	2.57985300
C	1.50774400	-1.31213300	0.82569700
C	1.34991900	-0.20188600	1.62987600
C	1.34909500	0.20168400	-1.62976600
C	2.16880800	1.06234100	1.61173200
C	1.50728600	1.31229200	-0.82589800
C	2.59124400	1.51429600	0.20960700

H	0.97675600	-2.21491600	1.13623000
H	1.55776500	1.85782800	2.06810400
H	0.97636600	2.21495900	-1.13691700
H	0.72915100	-0.32959300	2.52082400
H	0.72856200	0.32959900	-2.52085600
H	3.05768400	0.96473600	2.26116800
H	2.85635400	2.58019200	0.24802900
H	3.50890300	0.99659300	-0.10044000
C	2.59154300	-1.51386900	-0.21004400
H	2.85699200	-2.57969100	-0.24831300
H	3.50907200	-0.99583100	0.09971700
C	2.16841400	-1.06230100	-1.61201400
H	3.05693900	-0.96434000	-2.26187700
H	1.55751200	-1.85805900	-2.06811800
Ni	0.00001000	-0.00002200	0.00012600

S1a-1

Gibbs free energy before correction = -672.50176200

Gibbs free energy after correction = -672.48797185

Ni	0.00001300	0.00036300	-0.45912200
C	-2.49519300	1.21748300	0.20300200
C	-4.01372400	1.25548900	0.12920200
C	-4.61684900	-0.00689900	0.73187200
C	-4.02857800	-1.23997700	0.05790600
C	-2.50967000	-1.22442000	0.13286500
H	-4.38197500	2.15530100	0.64172400
H	-2.16098100	1.20677300	1.25132600
H	-2.04422700	2.09633900	-0.27453900
H	-4.38730300	-0.03887400	1.81044200
H	-5.71199400	0.00224700	0.64150500
H	-4.40785100	-2.16307500	0.51838700
H	-4.33500100	-1.26238800	-1.00141900
H	-2.17530500	-1.27802500	1.17981100
H	-2.06912600	-2.07958600	-0.39471000
H	-4.31956400	1.34217000	-0.92700700
N	-1.92378400	0.01068600	-0.44517200
H	-2.21119500	0.04059300	-1.42981100
C	2.49468700	-1.21740900	0.20252700
C	4.01321300	-1.25600700	0.12898600
C	4.61673700	0.00600400	0.73205900
C	4.02908800	1.23948100	0.05827300
C	2.51016900	1.22453300	0.13299100
H	4.38102400	-2.15607400	0.64137700
H	2.16030500	-1.20686200	1.25079600

H	2.04343300	-2.09593200	-0.27535600
H	4.38699700	0.03782400	1.81059300
H	5.71189500	-0.00356200	0.64190200
H	4.40868500	2.16232000	0.51900500
H	4.33569300	1.26199100	-1.00099800
H	2.17566300	1.27806700	1.17989700
H	2.07005100	2.07999800	-0.39446100
H	4.31923000	-1.34255700	-0.92718200
N	1.92386500	-0.01019200	-0.44539400
H	2.21134300	-0.03998800	-1.43000900

S1a-2

Gibbs free energy before correction = -732.56410600

Gibbs free energy after correction = -732.55031557

C	1.20969800	1.59455300	0.45048900
C	2.10843900	1.31769400	-0.58688200
C	1.29016700	-1.35262400	0.71609000
C	3.42302200	0.58010700	-0.43311300
C	1.97711000	-1.51183300	-0.48136400
C	3.30382700	-0.89321400	-0.84760800
H	0.54913700	2.46393900	0.36577800
H	4.19795200	1.06276100	-1.04778700
H	1.66099600	-2.34560900	-1.11831100
H	2.02506800	1.94715600	-1.48153200
H	0.49820800	-2.07423500	0.93863400
H	3.78373800	0.65947100	0.60194200
H	3.40789800	-0.95975200	-1.94188000
H	4.15173400	-1.47252600	-0.43626400
C	1.30173000	0.98632500	1.83271300
H	0.30291600	1.06446300	2.29319300
H	1.97129300	1.56883700	2.49185300
C	1.75562200	-0.49997400	1.88124600
H	2.85103300	-0.54744100	1.95578000
H	1.37867400	-0.93460100	2.81797600
Ni	0.53753700	0.01916100	-0.57700200
C	-2.19147900	1.19125700	-0.26114500
C	-3.70247800	1.12644700	-0.42473600
C	-4.28865800	-0.00155800	0.41424400
C	-3.59930100	-1.31637200	0.07332400
C	-2.09081100	-1.19178400	0.22360600
H	-4.14289000	2.09567400	-0.15082700
H	-1.93384200	1.44599800	0.77979000
H	-1.75277200	1.96571400	-0.90328100
H	-4.13405600	0.22295200	1.48328300

H	-5.37393100	-0.07878800	0.26085500
H	-3.96536200	-2.13386300	0.71064400
H	-3.83232000	-1.59487700	-0.96841000
H	-1.82778200	-0.99944500	1.27703600
H	-1.58386900	-2.11900900	-0.07408600
H	-3.94067800	0.95662600	-1.48841700
N	-1.51674700	-0.08694800	-0.57064200
H	-1.70627800	-0.29546000	-1.55661900

^{S}1a-3

Gibbs free energy before correction = -3620.89986800

Gibbs free energy after correction = -3620.88607762

C	-2.02901100	1.67072800	-1.35885700
C	-0.71999800	2.07894800	-1.29334300
C	-2.14607200	0.70669000	1.39604400
C	-0.09271900	2.95950400	-0.24748900
C	-0.96244300	1.38094800	1.55182800
C	-0.68697500	2.81289000	1.16541000
H	-2.31699500	1.08917600	-2.24023000
H	0.97850100	2.70356300	-0.20758100
H	-0.18890300	0.88974500	2.14858900
H	-0.07789200	1.83936200	-2.14436700
H	-2.23753000	-0.25429800	1.90968600
H	-0.13323600	4.01843900	-0.55335400
H	0.02915300	3.23807300	1.88120000
H	-1.59930100	3.41327000	1.26310300
C	-3.16099500	2.12989400	-0.47273100
H	-4.08324200	2.16430600	-1.06836400
H	-2.98401600	3.15984300	-0.14050700
C	-3.40047800	1.20534900	0.73209300
H	-4.05493800	1.71193900	1.46126400
H	-3.96318900	0.32234700	0.39233100
Ni	-0.87724300	0.23746400	-0.26694100
C	0.37780400	-0.98330300	-1.22607400
C	-0.11895300	-1.51935500	0.01333000
C	0.73327100	-1.68693500	1.14332400
C	1.98856300	-1.14543000	1.11596100
C	2.45676000	-0.48948200	-0.05820000
C	1.69217200	-0.43901900	-1.19904900
H	-0.08036300	-1.22762200	-2.18537700
H	0.36357000	-2.20076100	2.02970400
H	2.63475500	-1.21489500	1.98958300
H	2.09564400	0.00068400	-2.11014600
Br	-1.72622800	-2.59378900	-0.09763700

C	3.78222900	0.18133200	-0.00217200
F	3.72883600	1.32495900	0.71365600
F	4.25897800	0.51139900	-1.20882700
F	4.71438900	-0.58037000	0.59580000

S2a

Gibbs free energy before correction = -3812.43212200

Gibbs free energy after correction = -3812.41833181

Ni	0.36740900	0.11564700	-0.45861200
C	-1.03101400	-0.84729900	-1.40203800
C	-0.21343800	-1.65121200	-0.49263300
C	-0.81408000	-2.12766300	0.72613700
C	-2.06458700	-1.72162400	1.09240400
C	-2.85066300	-0.90545400	0.21845500
C	-2.35893000	-0.51754100	-1.00169800
H	-0.80315400	-0.82562700	-2.47120600
H	-0.24812700	-2.80064800	1.37068100
H	-2.48364100	-2.04018600	2.04692600
H	-2.99051300	0.04421600	-1.69033900
C	-4.18055200	-0.45941400	0.69145200
F	-4.92602000	0.10452800	-0.26926800
F	-4.08681800	0.45609600	1.68435200
F	-4.90932300	-1.46889900	1.20768000
C	3.25216700	0.01150800	-0.18041900
C	4.54765100	0.20697100	0.59099800
C	4.56685200	-0.66483700	1.84098500
C	3.32705900	-0.40213500	2.68743600
C	2.06451400	-0.58217100	1.85928400
H	5.40273000	-0.01865000	-0.06180100
H	3.16694600	-1.02325200	-0.54554700
H	3.20386600	0.67189400	-1.05689300
H	4.57993100	-1.72618700	1.53995500
H	5.48137000	-0.48927100	2.42435800
H	3.29407400	-1.07073500	3.55915700
H	3.35770400	0.62923900	3.07750600
H	1.97642100	-1.62446400	1.51583800
H	1.16159600	-0.35121300	2.44098900
H	4.63621500	1.26886800	0.87834100
N	2.05436400	0.26496200	0.64985700
H	2.10883900	1.23686900	0.97001800
C	1.20731500	2.93552100	-1.19565400
C	0.83742000	4.39532800	-1.40936400
C	0.17578600	4.97114300	-0.16343600
C	-1.02067300	4.11808700	0.23892400

C	-0.61187100	2.66326900	0.41069100
H	1.73632200	4.96626900	-1.68112000
H	1.96964200	2.85783800	-0.40335400
H	1.63471100	2.49193700	-2.10444700
H	0.90709500	4.98343300	0.66253800
H	-0.12885000	6.01329700	-0.33163100
H	-1.47400600	4.48407300	1.17084100
H	-1.79817500	4.18116400	-0.54091600
H	0.09488300	2.56257400	1.25061700
H	-1.48084500	2.02880700	0.63683500
H	0.14288500	4.46731700	-2.26308900
N	0.05491200	2.10826900	-0.78706500
H	-0.62502600	2.13926700	-1.55147100
Br	1.09789800	-2.89337000	-1.30614900

S2a-1

Gibbs free energy before correction = -3812.42479900

Gibbs free energy after correction = -3812.41100881

Ni	-0.19506700	0.23867700	-0.54604500
C	0.80131700	-1.30628100	-1.10947600
C	1.60082600	-1.85225700	-0.06124200
C	1.10768800	-2.52454900	1.02091300
C	-0.29678100	-2.75787500	1.08946700
C	-1.12358700	-2.32045800	0.09080300
C	-0.64336100	-1.55075100	-1.03881500
H	1.28551700	-1.13249300	-2.07533700
H	1.76579900	-2.89733100	1.80216200
H	-0.69769800	-3.30927400	1.93745400
H	-1.22676400	-1.61754500	-1.96432200
C	-2.57967900	-2.60915100	0.14022200
F	-3.01702700	-3.20670000	-0.98437600
F	-3.32321000	-1.47876600	0.25516800
F	-2.94034700	-3.39505100	1.16149700
C	2.06950700	2.04959900	-1.04347300
C	2.99337800	3.19190400	-0.65104100
C	3.66657900	2.90139400	0.68525400
C	2.61841200	2.59973300	1.74997200
C	1.70565900	1.47080000	1.29594300
H	3.73855400	3.35199100	-1.44306200
H	2.64890700	1.12593100	-1.19803300
H	1.53415900	2.26424600	-1.97881800
H	4.33035900	2.02682800	0.57387700
H	4.30224600	3.74361600	0.99193400
H	3.09113900	2.32882200	2.70462200

H	2.01202000	3.50193900	1.93811500
H	2.28448300	0.54274300	1.17552400
H	0.91378200	1.27021300	2.03116200
H	2.40483400	4.12172400	-0.57350000
N	1.06109500	1.74799000	-0.00554300
H	0.49706600	2.59405300	0.11901000
C	-2.19121900	2.31416600	-1.21846500
C	-3.58343600	2.91433800	-1.08746100
C	-3.86970600	3.31020100	0.35632400
C	-3.64495200	2.12449700	1.28751900
C	-2.24765200	1.55444100	1.09844100
H	-3.67878000	3.77754500	-1.76104500
H	-1.42790400	3.07445700	-0.98725300
H	-2.00105100	1.96204600	-2.24108800
H	-3.19307400	4.13138700	0.64796100
H	-4.89395600	3.69509900	0.45666800
H	-3.79002500	2.41230400	2.33832300
H	-4.38207500	1.33320600	1.06730600
H	-1.49082600	2.30186600	1.38649700
H	-2.08557900	0.66595900	1.72484100
H	-4.32446200	2.16748600	-1.41849900
N	-1.97821200	1.17722200	-0.30243200
H	-2.65729800	0.45521600	-0.55320300
Br	3.48998900	-1.58243800	-0.19360300

^{T}1a

Gibbs free energy before correction = -792.59443000

Gibbs free energy after correction = -792.58063971

C	-1.45225900	-1.10158700	-1.19139400
C	-1.65170400	0.21275000	-1.56566400
C	-1.65529300	-0.21280200	1.56540200
C	-2.72341800	1.13069300	-1.03477400
C	-1.45566800	1.10142400	1.19189600
C	-2.27978600	1.90156600	0.21391200
H	-0.80597600	-1.70438200	-1.83433700
H	-2.99335600	1.85665100	-1.81474200
H	-0.81013400	1.70426200	1.83553100
H	-1.09624000	0.56760200	-2.43657200
H	-1.10003500	-0.56823100	2.43621200
H	-3.64270500	0.56536300	-0.83132300
H	-1.67028100	2.76120600	-0.10605200
H	-3.16351700	2.33390800	0.72173700
C	-2.27821400	-1.90210200	-0.21524200
H	-1.66906200	-2.76139500	0.10634100

H	-3.16050500	-2.33495800	-0.72511800
C	-2.72537200	-1.13110500	1.03210600
H	-3.64413500	-0.56592900	0.82598000
H	-2.99726500	-1.85683200	1.81161100
C	1.45260500	-1.10169700	1.19166800
C	1.65195700	0.21275100	1.56564800
C	1.65469700	-0.21266100	-1.56571100
C	2.72373600	1.13049000	1.03450500
C	1.45508000	1.10147200	-1.19155000
C	2.27992900	1.90147700	-0.21402800
H	0.80649100	-1.70451800	1.83475000
H	2.99410100	1.85629900	1.81446800
H	0.80966700	1.70453200	-1.83511800
H	1.09657100	0.56769700	2.43657400
H	1.09927100	-0.56788300	-2.43648200
H	3.64278900	0.56489500	0.83073800
H	1.67085900	2.76135600	0.10611200
H	3.16362500	2.33337800	-0.72227600
C	2.27817700	-1.90201100	0.21503500
H	1.66897400	-2.76137900	-0.10625000
H	3.16077300	-2.33483300	0.72443100
C	2.72476800	-1.13112300	-1.03262800
H	3.64376900	-0.56611200	-0.82703200
H	2.99618300	-1.85707300	-1.81209500
Ni	0.00016900	0.00075600	0.00027900

P

Gibbs free energy before correction = -819.33436500

Gibbs free energy after correction = -819.32057484

C	-2.93880800	-1.26447300	-0.58804800
C	-3.41730500	-1.20345500	0.85764700
C	-4.21520500	0.07541700	1.09934700
C	-3.44133700	1.30978500	0.64200800
C	-2.95809200	1.12279400	-0.79119900
H	-4.02371800	-2.09021200	1.08969700
H	-3.80375300	-1.26369000	-1.26868100
H	-2.38405800	-2.18239800	-0.79870900
H	-5.15925100	0.01721600	0.53134100
H	-4.49126600	0.16362300	2.15920100
H	-4.06716700	2.21044400	0.71270000
H	-2.56944000	1.47135100	1.29688500
H	-3.82363900	0.98520000	-1.45726300
H	-2.41749200	1.99545000	-1.16960500
H	-2.53707800	-1.23149900	1.52139400

N	-2.13763700	-0.08219100	-0.91264100
C	-0.02704700	-1.22758300	-0.47461500
C	-0.79082600	-0.04224000	-0.59429100
C	-0.10198200	1.17808500	-0.41896700
C	1.26094800	1.21098300	-0.17130300
C	1.99550300	0.03387600	-0.07517700
C	1.33122700	-1.18426100	-0.22645900
H	-0.49430100	-2.20147000	-0.58753100
H	-0.63072100	2.12532600	-0.46703100
H	1.75120300	2.17408600	-0.04381900
H	1.88834600	-2.11812700	-0.14760400
C	3.45305200	0.02751200	0.20654900
F	4.14865900	-0.64481700	-0.73091600
F	3.74462500	-0.58043800	1.37373300
F	3.97616300	1.25874300	0.27102400

^{T}1a-1

Gibbs free energy before correction = -672.46488000

Gibbs free energy after correction = -672.45108985

Ni	-0.00035900	-1.79214000	0.00009200
C	-1.60911200	0.43900600	-1.16526300
C	-2.91599000	1.19741000	-1.33745100
C	-3.42155300	1.71116500	0.00582800
C	-3.53268700	0.56493200	1.00452400
C	-2.20873500	-0.17318700	1.12195200
H	-2.77273600	2.02334700	-2.04842800
H	-0.82012300	1.11760200	-0.80283000
H	-1.26032000	0.00773500	-2.11374100
H	-2.71406900	2.46253300	0.39564400
H	-4.38868200	2.21900300	-0.11252700
H	-3.84064600	0.93082800	1.99415800
H	-4.30873000	-0.14335900	0.66942400
H	-1.43487300	0.49603000	1.53006800
H	-2.28068400	-1.03969800	1.79406400
H	-3.66616400	0.52091800	-1.77999100
N	-1.71614200	-0.65803700	-0.18311800
H	-2.40417700	-1.32845200	-0.54189400
C	1.60926200	0.43947200	1.16523600
C	2.91713400	1.19608500	1.33774200
C	3.42322900	1.70989800	-0.00531400
C	3.53289000	0.56402900	-1.00458700
C	2.20804700	-0.17238700	-1.12235700
H	2.77499600	2.02182500	2.04916700
H	0.82110600	1.11928800	0.80325800

H	1.26003200	0.00802200	2.11346600
H	2.71662000	2.46232100	-0.39467700
H	4.39099100	2.21649000	0.11318700
H	3.84127100	0.93003400	-1.99404600
H	4.30804900	-0.14539200	-0.66984100
H	1.43501500	0.49788900	-1.53030100
H	2.27893400	-1.03875600	-1.79479600
H	3.66646900	0.51839000	1.77986800
N	1.71482700	-0.65718700	0.18246600
H	2.40206600	-1.32865900	0.54089600

^{T}1a-2

Gibbs free energy before correction = -732.53929400

Gibbs free energy after correction = -732.52550357

C	1.25492900	1.58131200	0.03262900
C	1.53924200	0.96465000	-1.20321300
C	1.94384100	-0.89081000	1.24400800
C	2.85948000	0.28349900	-1.51008500
C	1.97895600	-1.57628200	0.00464800
C	2.86469100	-1.21473600	-1.16748000
H	0.46858300	2.34285900	0.03250300
H	3.09507200	0.40556900	-2.57761200
H	1.59984100	-2.60462700	0.00806200
H	0.92727600	1.26353700	-2.05951600
H	1.53311000	-1.44401700	2.09393400
H	3.67276500	0.79697800	-0.97469500
H	2.49982400	-1.77419600	-2.04169500
H	3.90783500	-1.55954500	-1.00951000
C	2.20283500	1.64301100	1.21035300
H	1.62616900	1.99679100	2.07802900
H	2.99674500	2.40228000	1.05221600
C	2.83875700	0.29073300	1.56646900
H	3.80296000	0.17562500	1.04790000
H	3.08470600	0.28315000	2.63863200
Ni	0.38059600	-0.30299800	0.02377900
C	-2.22217100	1.19192600	-0.24253500
C	-3.71792900	1.17188700	-0.51380100
C	-4.41237600	0.12977100	0.35528900
C	-3.76338200	-1.23655700	0.16848800
C	-2.26678700	-1.15531500	0.42031300
H	-4.13608100	2.17313000	-0.34000300
H	-2.02119200	1.49969300	0.79655300
H	-1.70153200	1.89881300	-0.90188500
H	-4.33007000	0.42807100	1.41403700

H	-5.48506400	0.08362600	0.12229900
H	-4.20893300	-1.98307300	0.84047900
H	-3.93329500	-1.59060900	-0.86197100
H	-2.06563200	-0.87802000	1.46880200
H	-1.76816800	-2.11785900	0.23317200
H	-3.88505200	0.93653400	-1.57835800
N	-1.60131000	-0.13453400	-0.41992000
H	-1.72788700	-0.40754100	-1.39823900

^{T}1a-3

Gibbs free energy before correction = -3620.85377400

Gibbs free energy after correction = -3620.83998362

C	-2.65951500	0.64238900	-0.75988900
C	-1.82260900	1.36643100	-1.57226300
C	-1.24772400	1.40527300	1.67150000
C	-1.47865400	2.82887700	-1.46056500
C	-0.61572200	2.35059400	0.87807100
C	-1.31409800	3.34131100	-0.02268700
H	-2.87488200	-0.38732900	-1.05660100
H	-0.53158900	2.98188500	-1.99821900
H	0.44840000	2.52159700	1.07009600
H	-1.46854700	0.87186800	-2.47977600
H	-0.63907100	0.92439800	2.44453700
H	-2.22901200	3.43787000	-1.99432000
H	-0.73272200	4.27258400	-0.04995000
H	-2.28738600	3.61095900	0.40678300
C	-3.45944600	1.19598000	0.39330000
H	-4.39619600	0.62929600	0.47621900
H	-3.75379400	2.23003200	0.17529100
C	-2.72481200	1.11765400	1.74203500
H	-3.21741700	1.78835900	2.46718200
H	-2.83782900	0.10108700	2.14734600
Ni	-0.59719500	0.43693700	-0.03649400
C	0.46202600	-1.00190800	-1.23809000
C	-0.07925300	-1.55275700	-0.01740500
C	0.77346600	-1.61267800	1.13659700
C	2.00844300	-1.02462700	1.11903800
C	2.51344800	-0.40575200	-0.07107200
C	1.72742100	-0.40420100	-1.22368000
H	-0.08486000	-1.10294300	-2.17426000
H	0.40170600	-2.08440900	2.04543000
H	2.61780500	-1.02509700	2.02249100
H	2.10183400	0.04511700	-2.14242700
Br	-1.51292200	-2.83557000	-0.14682900

C	3.77752600	0.34506900	0.00467100
F	3.66395300	1.48568000	0.73422600
F	4.24146200	0.71734600	-1.19702100
F	4.76062000	-0.35352500	0.60987100

^{T}1a-4

Gibbs free energy before correction = -924.04316100

Gibbs free energy after correction = -924.02937085

Ni	-0.19256500	-0.11904100	-0.92995700
C	-2.36999000	-1.05733900	0.89587300
C	-3.77908900	-1.14929000	1.46312800
C	-4.79520800	-1.35380800	0.34680600
C	-4.64720600	-0.26077300	-0.70477300
C	-3.21541000	-0.19469800	-1.21444700
H	-3.82986100	-1.96401400	2.19985000
H	-2.08612100	-2.01626900	0.42672800
H	-1.63466900	-0.85367800	1.68703800
H	-4.62207100	-2.33579200	-0.12529700
H	-5.81776300	-1.37306100	0.74894400
H	-5.33211800	-0.42911100	-1.54853400
H	-4.91776500	0.71346300	-0.26357500
H	-2.94734500	-1.12764500	-1.74308900
H	-3.07363900	0.62140500	-1.93784300
H	-4.00863400	-0.21522200	2.00357400
N	-2.22233200	-0.02065100	-0.14096800
H	-2.38581200	0.88960100	0.29564200
C	1.53564800	-1.78697600	1.05599500
C	2.52391200	-2.89585900	1.39180300
C	3.84684700	-2.67418700	0.66814100
C	3.61185200	-2.52130000	-0.83051400
C	2.59782600	-1.42044200	-1.10411000
H	2.67235200	-2.94686100	2.48005200
H	1.90697100	-0.82553200	1.44924500
H	0.55695900	-1.97047400	1.52120100
H	4.32159400	-1.75634800	1.05523800
H	4.54405900	-3.49898400	0.87152900
H	4.55178900	-2.30198300	-1.35737500
H	3.22880200	-3.47050000	-1.24169500
H	3.00723900	-0.44678800	-0.78509800
H	2.36257700	-1.33204100	-2.17655600
H	2.09297400	-3.86282100	1.08232500
N	1.32619600	-1.61702200	-0.39119000
H	0.90009400	-2.47626900	-0.75059600
C	0.10090700	2.12994600	1.05722000

C	0.88245400	3.27076900	1.69087100
C	1.25427400	4.31173400	0.64146700
C	1.99313000	3.65459800	-0.51877600
C	1.18301600	2.50065700	-1.08952200
H	0.29222500	3.72002300	2.50208400
H	-0.85550500	2.50592900	0.65804400
H	-0.13276900	1.34390900	1.78948400
H	0.33391200	4.78669500	0.26165600
H	1.86224300	5.11173500	1.08621400
H	2.20998800	4.38302600	-1.31281300
H	2.96447800	3.26874800	-0.16589700
H	0.24027700	2.86747700	-1.52935500
H	1.72336800	1.97430500	-1.89058400
H	1.79947000	2.86453500	2.15033200
N	0.81585400	1.50202400	-0.06805600
H	1.68871100	1.11704100	0.30442800

^{S}TS1a

Gibbs free energy before correction = -3812.41644800

Gibbs free energy after correction = -3812.40265781

Ni	0.66429700	-0.32782200	0.30643400
C	-1.21429400	-1.39909700	0.68928400
C	-0.92092900	-0.06455200	1.12466900
C	-1.92855700	0.93451300	1.07673100
C	-3.08654900	0.67145800	0.38672400
C	-3.31197000	-0.59604900	-0.20428600
C	-2.39427900	-1.62103400	-0.03547500
H	-0.62660800	-2.25212000	1.02922300
H	-1.75267800	1.91668500	1.51516500
H	-3.83971900	1.45257200	0.27346700
H	-2.61588200	-2.61867900	-0.41258000
C	-4.58124900	-0.80103900	-0.94077000
F	-4.69549500	-2.03011600	-1.46213700
F	-4.72109800	0.06787300	-1.96487500
F	-5.66823900	-0.60762000	-0.16394700
C	1.48643900	2.54160200	0.43195200
C	1.93584300	3.83747900	-0.22575500
C	0.89957200	4.31793900	-1.23413300
C	0.60254800	3.21911200	-2.24720100
C	0.18670700	1.93680200	-1.54240600
H	2.11967400	4.59770100	0.54665900
H	0.57407900	2.71122300	1.02486500
H	2.25142400	2.14956100	1.11577700
H	-0.02998200	4.57997100	-0.70080900

H	1.24232100	5.23115100	-1.73989000
H	-0.18820000	3.52732900	-2.94591200
H	1.50381100	3.02147000	-2.85183700
H	-0.76382700	2.08623100	-1.00647700
H	0.03131600	1.11628000	-2.25743900
H	2.89711500	3.66525600	-0.73907800
N	1.17535600	1.48205200	-0.54536100
H	2.04058700	1.28198800	-1.05537100
C	3.52987900	-0.96065900	0.17890700
C	4.69675600	-1.85859000	-0.20136300
C	4.74319400	-2.06912400	-1.71011700
C	3.40559600	-2.59974500	-2.21228100
C	2.26834300	-1.68603500	-1.78223200
H	5.63480900	-1.41993700	0.16677400
H	3.67586700	0.04484700	-0.24801800
H	3.44510100	-0.84264900	1.26759300
H	4.95919400	-1.10628500	-2.20344000
H	5.55883300	-2.75320900	-1.98187000
H	3.40462200	-2.69937000	-3.30681000
H	3.22974600	-3.60732300	-1.79946600
H	2.37691400	-0.69801800	-2.25827500
H	1.29116400	-2.08662800	-2.08300500
H	4.57901300	-2.83181700	0.30421500
N	2.23490700	-1.46558800	-0.32206900
H	2.07814100	-2.37654900	0.11890900
Br	0.35177700	-0.07757200	2.87784700

^{T}TS1a

Gibbs free energy before correction = -3812.39571900

Gibbs free energy after correction = -3812.38192881

Ni	-0.03314600	0.06413800	0.23503600
C	-0.18654000	-2.49379000	-1.38640800
C	0.74925300	-2.26701500	-0.38854400
C	0.39966300	-1.89579700	0.90912000
C	-0.97185200	-1.69380900	1.20606400
C	-1.92312200	-1.91047500	0.19372400
C	-1.54055800	-2.33226700	-1.08345300
H	0.11084200	-2.80336300	-2.38827500
H	1.14999800	-1.82097500	1.69792200
H	-1.28979800	-1.44479300	2.21720800
H	-2.30326900	-2.51124000	-1.84212800
C	-3.38129100	-1.72859700	0.46371300
F	-4.05104200	-2.88723100	0.37213100
F	-3.95533700	-0.89482000	-0.42434800

F	-3.62461100	-1.22654100	1.67981600
C	-2.15358700	1.97049000	0.86180500
C	-3.00614500	3.19006100	0.55380000
C	-3.65607900	3.05716400	-0.81797000
C	-2.59216500	2.81641900	-1.88181700
C	-1.74639700	1.60485600	-1.52731800
H	-3.76232200	3.31397200	1.34142000
H	-2.78637300	1.07257800	0.92795400
H	-1.62892100	2.07295900	1.82128800
H	-4.35576900	2.20377000	-0.80592600
H	-4.24866300	3.95100500	-1.05607900
H	-3.04627600	2.66678600	-2.87118300
H	-1.93886300	3.70156100	-1.95964500
H	-2.36785600	0.69623700	-1.52458500
H	-0.93584700	1.44883400	-2.25204500
H	-2.36884000	4.08990400	0.57655000
N	-1.13541000	1.70936400	-0.18174400
H	-0.50123900	2.51323900	-0.19220000
C	2.07238500	1.59894400	1.57448500
C	3.51644400	2.06655600	1.68274400
C	3.92153800	2.86121000	0.44637400
C	3.65418600	2.05219400	-0.81764100
C	2.20273600	1.60039100	-0.86533800
H	3.64637100	2.66188200	2.59746800
H	1.38641200	2.46300200	1.57618200
H	1.79544600	0.95821000	2.42417200
H	3.33755300	3.79699300	0.40969500
H	4.97961400	3.15229600	0.50422800
H	3.89212000	2.63563300	-1.71844500
H	4.28889600	1.15048500	-0.83076400
H	1.53423100	2.47358300	-0.94316800
H	2.01359900	0.95566600	-1.73554800
H	4.16676700	1.18106300	1.78003300
N	1.82625800	0.83747000	0.33919500
H	2.43591800	0.00161400	0.33696400
Br	3.58332900	-1.88875700	-0.43322000

S3a

Gibbs free energy before correction = -3812.48336600

Gibbs free energy after correction = -3812.46957581

Ni	-0.83544600	-0.44921000	0.00799100
C	1.76256700	-0.32282500	1.22005000
C	1.04343400	-0.35739200	0.01942500
C	1.77430900	-0.33520900	-1.17782000

C	3.16138900	-0.26029300	-1.17775800
C	3.85464000	-0.21600000	0.03372300
C	3.15327100	-0.24830200	1.23624000
H	1.23016000	-0.36226000	2.17318400
H	1.25001800	-0.38444600	-2.13488900
H	3.71480200	-0.24120400	-2.11786700
H	3.69118500	-0.22015100	2.18261400
C	5.33851400	-0.12093100	-0.00615300
F	5.90022400	-0.15375700	1.20925800
F	5.75602600	1.01680500	-0.59545500
F	5.89089200	-1.12125200	-0.71866900
C	-0.48527500	2.17681800	-1.21475500
C	-0.91242000	3.63450500	-1.25191900
C	-0.45726200	4.36340600	0.00695600
C	-0.94977900	3.63619400	1.25274400
C	-0.52250000	2.17814400	1.23039800
H	-0.50473200	4.10964500	-2.15456000
H	0.60983800	2.08985300	-1.20081700
H	-0.85164000	1.62184100	-2.08899000
H	0.64461100	4.40140500	0.02324500
H	-0.81050500	5.40342700	0.00104100
H	-0.56894100	4.11253900	2.16639100
H	-2.05116000	3.68543500	1.30226900
H	0.57241700	2.09006500	1.24994800
H	-0.91599700	1.62444000	2.09357000
H	-2.01177500	3.68351800	-1.33445800
N	-0.99543800	1.49833900	0.00067600
H	-2.00921200	1.63954900	-0.01498300
C	-3.53665300	-0.17992500	-1.24224600
C	-5.00999500	-0.55448300	-1.27418400
C	-5.72402900	-0.03685300	-0.03122300
C	-5.02974000	-0.54063600	1.22843200
C	-3.55615300	-0.16604700	1.21574600
H	-5.46965000	-0.15864400	-2.19019100
H	-3.43074100	0.91555500	-1.30780400
H	-2.98767800	-0.61289600	-2.09001600
H	-5.70963800	1.06621300	-0.03713800
H	-6.77993500	-0.33940300	-0.03779100
H	-5.50382600	-0.13508300	2.13276500
H	-5.11678300	-1.63839000	1.28451300
H	-3.45113800	0.93007400	1.27064500
H	-3.02078200	-0.58952500	2.07688400
H	-5.09656700	-1.65277500	-1.31966400
N	-2.87211700	-0.63954300	-0.00527400

H	-2.93562300	-1.66221200	-0.00010400
Br	-0.66775800	-2.75392700	0.01195700

^{T}3a-1

Gibbs free energy before correction = -3812.39761800

Gibbs free energy after correction = -3812.38382781

Ni	0.15595300	0.15666300	-0.00802500
C	-0.48211300	-1.92011400	-1.50650300
C	0.41452400	-1.84075900	-0.43171200
C	-0.03848400	-1.79878700	0.89418400
C	-1.42742800	-1.78701800	1.14416000
C	-2.31222900	-1.83922700	0.07449500
C	-1.84949600	-1.91020700	-1.24942600
H	-0.12549100	-1.97775500	-2.53509700
H	0.66745100	-1.83602700	1.72515100
H	-1.79811300	-1.74004600	2.16679200
H	-2.56479900	-1.93820100	-2.07148200
C	-3.78007900	-1.68926700	0.29917600
F	-4.49860800	-2.51703500	-0.47150300
F	-4.19239800	-0.44033900	-0.00549700
F	-4.13784700	-1.91231300	1.56734500
C	-1.67403900	2.14374600	1.06866700
C	-2.45669000	3.44424000	0.99657300
C	-3.29405800	3.49579900	-0.27546400
C	-2.40788400	3.28673800	-1.49750000
C	-1.62496700	1.99044000	-1.37482800
H	-3.08689800	3.53982000	1.89160000
H	-2.36543600	1.28834200	1.13317500
H	-1.02359000	2.10769500	1.95278400
H	-4.05600200	2.69825900	-0.23967300
H	-3.83483400	4.44927500	-0.34669400
H	-3.00273700	3.26717900	-2.42120700
H	-1.69922300	4.12661500	-1.59011800
H	-2.31358400	1.12997000	-1.35891600
H	-0.93741900	1.84655900	-2.21936800
H	-1.74982500	4.29057800	1.01027500
N	-0.82709200	1.92290500	-0.12709600
H	-0.13124200	2.67368900	-0.16011600
C	2.38695800	1.47976700	1.36808500
C	3.87352600	1.77761400	1.49965300
C	4.39448300	2.47245300	0.24654200
C	4.06497000	1.65162700	-0.99528000
C	2.57273700	1.36376300	-1.06537600
H	4.05347900	2.38840400	2.39551600

H	1.81145200	2.41967800	1.31883600
H	2.01414200	0.91046400	2.23241300
H	3.92187800	3.46592200	0.16047800
H	5.47728000	2.64411100	0.32146300
H	4.39009900	2.16841800	-1.90929500
H	4.59869800	0.68735000	-0.95671600
H	2.00409100	2.30026100	-1.19582800
H	2.33058900	0.70762500	-1.91465100
H	4.41187700	0.82592500	1.64470500
N	2.08590900	0.70343800	0.15649100
H	2.57095100	-0.20916300	0.21528900
Br	3.27314600	-2.37438800	-0.12046200

^{T}3a-2

Gibbs free energy before correction = -3812.46940000

Gibbs free energy after correction = -3812.45560981

Ni	0.88393000	-0.06544700	0.59105300
C	-1.66205700	-1.24182500	-0.47030100
C	-1.03920800	-0.15107900	0.14718500
C	-1.87070400	0.89564000	0.58035300
C	-3.24713000	0.86692800	0.39310200
C	-3.83360800	-0.23064700	-0.24050100
C	-3.04151500	-1.29052400	-0.66988700
H	-1.06866300	-2.09612800	-0.80800700
H	-1.43479900	1.76022600	1.09112300
H	-3.87419300	1.69050100	0.73789200
H	-3.49841400	-2.15136000	-1.15578200
C	-5.31307900	-0.23925300	-0.40846200
F	-5.75876300	-1.30384400	-1.08701500
F	-5.75339600	0.85264700	-1.06066900
F	-5.95284100	-0.23816300	0.77657500
C	2.21503600	2.49202700	0.61095700
C	2.88953600	3.70967800	0.00052200
C	1.94640300	4.43713000	-0.94920500
C	1.40795600	3.47314400	-1.99916900
C	0.75151600	2.27325300	-1.33760200
H	3.23664300	4.37352500	0.80425400
H	1.37120800	2.79342100	1.25373500
H	2.91528000	1.91773500	1.23361500
H	1.10280100	4.85510700	-0.37485500
H	2.45699600	5.28509700	-1.42564300
H	0.68059500	3.96903800	-2.65670700
H	2.23380000	3.12356100	-2.64129300
H	-0.11965800	2.59203600	-0.74617500

H	0.39408400	1.54508900	-2.07702900
H	3.78556500	3.37891000	-0.55048600
N	1.66777700	1.57333500	-0.41384000
H	2.46098100	1.23315600	-0.96613000
C	3.22925400	-1.64977900	-0.10861300
C	3.93284500	-2.80346600	-0.80459900
C	3.78945200	-2.69747900	-2.31746800
C	2.31917300	-2.58811300	-2.70214500
C	1.66027200	-1.42800100	-1.97388900
H	4.98986400	-2.81735000	-0.50497400
H	3.71476200	-0.69263800	-0.36073300
H	3.25520300	-1.75430900	0.98335100
H	4.32395600	-1.79998200	-2.67160500
H	4.25659600	-3.56021900	-2.81150600
H	2.20103100	-2.45173000	-3.78588300
H	1.79484900	-3.52153300	-2.43754000
H	2.12673900	-0.48011900	-2.28378000
H	0.58945800	-1.35915100	-2.20400800
H	3.48925300	-3.75115200	-0.45689000
N	1.80791400	-1.53350800	-0.50834200
H	1.32947300	-2.38856900	-0.20667900
Br	1.15962400	-0.71145700	2.87902400

S4a

Gibbs free energy before correction = -4064.05466700

Gibbs free energy after correction = -4064.04087686

Ni	0.67669600	0.03178100	-0.18211500
Br	1.18141900	0.63712900	2.76580300
C	-0.56174900	2.70536200	0.45844800
C	-0.29687600	4.19588500	0.58485500
C	-0.05978500	4.82860400	-0.77964200
C	1.05460100	4.09181500	-1.50947500
C	0.77521900	2.59810300	-1.57017400
H	-1.14395600	4.67045500	1.09965000
H	-1.47407900	2.52323000	-0.12731000
H	-0.66970200	2.23073400	1.43981700
H	-0.98688800	4.76448600	-1.37344400
H	0.18087500	5.89606400	-0.68115900
H	1.18759600	4.47761400	-2.52965900
H	2.01050500	4.24753000	-0.98102700
H	-0.13582600	2.39379900	-2.15307400
H	1.60253400	2.07172800	-2.06236800
H	0.58903700	4.34759100	1.22591400
N	0.55997700	2.01475400	-0.22609800

H	1.37777800	2.22019600	0.36009600
C	3.10021300	-0.30167200	-1.87974100
C	4.53758700	0.02694300	-2.24885400
C	5.50410300	-0.55263300	-1.22334000
C	5.12524600	-0.09665200	0.18041800
C	3.67170600	-0.41712700	0.48797600
H	4.75309900	-0.35263100	-3.25722900
H	2.94778600	-1.39263600	-1.90495800
H	2.38989400	0.13835700	-2.59318800
H	5.46167300	-1.65389500	-1.26972700
H	6.53790300	-0.26612700	-1.46058800
H	5.76987200	-0.56746400	0.93584200
H	5.27691300	0.99255500	0.26952100
H	3.52963200	-1.51127200	0.48754600
H	3.34466500	-0.04820100	1.46815100
H	4.65050300	1.12382200	-2.28964200
N	2.74855500	0.16543700	-0.51772300
H	2.94622700	1.17109000	-0.50477300
C	-1.88593200	-0.08310800	-1.44330800
C	-1.19919300	-0.10586000	-0.22296200
C	-1.96097100	-0.19307000	0.95291100
C	-3.34780300	-0.25105900	0.91045200
C	-4.00992700	-0.22048100	-0.31956400
C	-3.27815600	-0.13779300	-1.50032300
H	-1.33304600	-0.02148700	-2.38461300
H	-1.44260400	-0.18099400	1.91514600
H	-3.92722300	-0.31331400	1.83318000
H	-3.79085600	-0.11396300	-2.46065600
C	-5.49626600	-0.28733500	-0.32120000
F	-5.95026300	-1.42836200	0.23268500
F	-6.02499200	-0.21708400	-1.54976700
F	-6.04730800	0.70931000	0.39773800
C	0.27250900	-2.66669100	-1.32466600
C	0.73908000	-4.11325000	-1.33017600
C	0.38376100	-4.80438900	-0.01898800
C	0.92057400	-4.00956100	1.16560700
C	0.44848900	-2.56696700	1.10976100
H	0.29297200	-4.63590100	-2.18746000
H	-0.82159100	-2.60895300	-1.24513400
H	0.56569200	-2.14422500	-2.24521000
H	-0.71351900	-4.87663400	0.06404100
H	0.77097400	-5.83251200	-0.00687900
H	0.60612200	-4.45839400	2.11799500
H	2.02452100	-4.02692900	1.15624000

H	-0.64791800	-2.51317900	1.17291300
H	0.85342200	-1.94564200	1.92036700
H	1.83284800	-4.13533400	-1.47791600
N	0.83730100	-1.92555100	-0.17180700
H	1.85062600	-2.05055200	-0.23887700

^{T}4a

Gibbs free energy before correction = -1491.82223100

Gibbs free energy after correction = -1491.80844074

Ni	0.86232700	0.14036400	-0.23947600
C	-1.92857600	-0.70706400	-0.89115100
C	-1.08503700	-0.14503900	0.08810300
C	-1.73270600	0.39099000	1.21474900
C	-3.11675800	0.36390600	1.37570200
C	-3.90960600	-0.20835000	0.38450600
C	-3.31249800	-0.74226500	-0.75856200
H	-1.49472400	-1.13328700	-1.80207500
H	-1.14177900	0.85955800	2.00884700
H	-3.57923300	0.78842500	2.26592100
H	-3.93685800	-1.18362800	-1.53734500
C	-5.39350900	-0.24471900	0.49118700
F	-5.84735500	0.22305000	1.66130700
F	-5.88027200	-1.49282800	0.35465200
F	-5.98761300	0.48340700	-0.47444800
C	2.09261300	-1.66606100	-2.21033600
C	2.82093700	-2.90138400	-2.71710100
C	1.99912100	-4.15792900	-2.45613600
C	1.62255800	-4.24871600	-0.98200200
C	0.91741900	-2.97972000	-0.52965400
H	3.04110600	-2.78646200	-3.78774100
H	1.15920700	-1.51514100	-2.77820300
H	2.70224000	-0.75990400	-2.33554100
H	1.07827300	-4.12147600	-3.06231300
H	2.55064800	-5.05388300	-2.77279400
H	0.97698000	-5.11770200	-0.79183000
H	2.53315200	-4.38819600	-0.37505800
H	-0.03358700	-2.85935200	-1.07184100
H	0.67645000	-3.01175000	0.54133600
H	3.79067100	-2.97978600	-2.19751000
N	1.71613000	-1.76693500	-0.78479300
H	2.58282700	-1.84682600	-0.24464800
C	3.19272000	0.66161600	1.51379400
C	3.83567600	0.93181300	2.86474100
C	3.64679000	-0.25538400	3.80141800

C	2.17092600	-0.62108600	3.90489600
C	1.57583300	-0.85139300	2.52436700
H	4.90123700	1.16207600	2.72659000
H	3.69123600	-0.18468800	1.01389100
H	3.27294200	1.52841700	0.84518400
H	4.20653200	-1.12006100	3.40680200
H	4.06263500	-0.03628000	4.79441400
H	2.02760300	-1.51957400	4.52120200
H	1.61994100	0.19682700	4.39892300
H	2.06482800	-1.71279200	2.04214700
H	0.50130700	-1.07010000	2.57756800
H	3.36861500	1.82968200	3.30424000
N	1.76322800	0.30977200	1.63354800
H	1.28370500	1.10629700	2.06382200
C	0.99152700	3.08535700	-0.11146700
C	1.59845900	4.32136800	-0.77638900
C	0.99285900	4.53093100	-2.15940400
C	1.08686600	3.25281300	-2.98453000
C	0.49613300	2.08474600	-2.19636000
H	1.44827000	5.21040200	-0.14486600
H	-0.09017900	3.29718000	0.07893500
H	1.45626700	2.93611900	0.87757500
H	-0.07139100	4.80217900	-2.04542200
H	1.47578200	5.37218100	-2.67793000
H	0.56695100	3.36858000	-3.94792100
H	2.14366100	3.03170200	-3.20877800
H	-0.59544200	2.28650500	-2.06363100
H	0.56727900	1.15247100	-2.78529800
H	2.68730000	4.16825600	-0.86861000
N	1.15308300	1.89782000	-0.91711500

S5a

Gibbs free energy before correction = -4408.98373900

Gibbs free energy after correction = -4408.96994887

Ni	-0.45644100	0.69385100	0.35329200
Br	0.78745300	0.05905300	-2.33831600
C	-0.08325600	-2.29407100	0.36002100
C	0.74947000	-3.49710200	0.77296900
C	0.85781400	-3.59336200	2.28884900
C	1.39233300	-2.28521400	2.85432900
C	0.54839000	-1.10590700	2.39598500
H	0.28861700	-4.40252500	0.35290200
H	-1.11590100	-2.41933700	0.71344700
H	-0.10362400	-2.16211700	-0.72920700

H	-0.13970200	-3.79206000	2.71652600
H	1.50257300	-4.43401000	2.58154700
H	1.41208300	-2.30333500	3.95309200
H	2.43073100	-2.12998700	2.51659200
H	-0.47528500	-1.18670400	2.79360300
H	0.97523800	-0.16648600	2.77059200
H	1.75734300	-3.41163800	0.33862900
N	0.42940100	-1.01609100	0.92157200
H	1.37785200	-0.92799200	0.53239500
C	1.08125600	2.55674300	2.11309100
C	2.39512800	3.09777000	2.65300700
C	3.08608600	3.96596200	1.60847700
C	3.25052000	3.19700300	0.30303800
C	1.92226700	2.62799900	-0.17122300
H	2.20894700	3.66186900	3.57741400
H	0.39902000	3.39313300	1.89030100
H	0.57519600	1.91601400	2.84787600
H	2.47239900	4.86428100	1.42605700
H	4.05937100	4.31736000	1.97766300
H	3.67055700	3.83971700	-0.48335000
H	3.96634700	2.37045600	0.45187100
H	1.23980200	3.46099400	-0.41221200
H	2.00894100	2.01572800	-1.07795400
H	3.04446100	2.24657900	2.92321200
N	1.26839000	1.78449200	0.86182900
H	1.94845100	1.05064000	1.07934300
C	-2.93768700	-0.35881000	1.32466700
C	-2.11831000	-0.17974900	0.20293200
C	-2.57032400	-0.69270300	-1.02303600
C	-3.78354600	-1.36061200	-1.12159900
C	-4.58008900	-1.53247900	0.01363600
C	-4.15602400	-1.03215300	1.24100500
H	-2.63004500	0.03110100	2.29869000
H	-1.93184300	-0.58505400	-1.90344200
H	-4.11999400	-1.75792900	-2.08067400
H	-4.77286200	-1.16423800	2.12863300
C	-5.86789500	-2.26305100	-0.13264800
F	-6.66407200	-1.69924800	-1.06110900
F	-6.57504700	-2.31546200	1.00354900
F	-5.68554200	-3.53565900	-0.53532700
C	4.88984600	-1.91574200	-2.16382700
C	3.59603500	-2.29835700	-1.41003900
H	4.69344900	-1.12947200	-2.90869500
H	5.32108300	-2.77626700	-2.69555800

H	2.70584800	-1.85338400	-1.87956600
H	3.46152600	-3.38994400	-1.37029600
C	5.38596600	-0.14628200	-0.64741600
H	6.09910800	0.18474300	0.12198700
H	5.36789400	0.62146100	-1.43519000
C	3.97583700	-0.37522700	-0.05575800
H	3.90054700	0.01789600	0.97325200
H	3.19849200	0.10197300	-0.67421700
C	4.75325000	-2.51015600	0.66728000
H	4.85535700	-2.06860700	1.67015100
H	4.46080000	-3.56358500	0.79879700
C	6.06532100	-2.37414500	-0.14198100
H	6.89817600	-2.04699200	0.49689600
H	6.35523800	-3.33131600	-0.59908000
N	3.66802000	-1.80828100	-0.02510800
N	5.89167300	-1.39737400	-1.22314700
C	-2.37686200	2.89486300	0.83362700
C	-2.70996900	4.35216800	0.55733600
C	-3.14338500	4.54566600	-0.89092800
C	-2.09340400	3.98282500	-1.84142100
C	-1.77519200	2.53596700	-1.50554000
H	-3.49246700	4.68464300	1.25326100
H	-3.26306400	2.26004400	0.69900100
H	-2.01843700	2.75075100	1.86178200
H	-4.09759700	4.01771500	-1.05478700
H	-3.32915500	5.60806500	-1.10008700
H	-2.42991200	4.04779000	-2.88550700
H	-1.16753200	4.57978900	-1.76891900
H	-2.66630100	1.90302500	-1.62434500
H	-0.98321200	2.11000400	-2.13641800
H	-1.81738500	4.96820300	0.76383700
N	-1.33289200	2.39918300	-0.09483700
H	-0.55327200	3.05309000	0.00388100

^{S}TS2a

Gibbs free energy before correction = -4408.94695200

Gibbs free energy after correction = -4408.93316187

Ni	-0.20065100	0.65761300	0.41435500
Br	0.76699300	0.30038300	-2.64982000
C	-0.11784500	-2.26788400	0.86905800
C	0.45556000	-3.51487100	1.53917800
C	0.55848900	-3.30418200	3.04112100
C	1.36336400	-2.04379300	3.30698000
C	0.77516700	-0.84725900	2.56036600

H	-0.19621100	-4.36999500	1.30333700
H	-1.15634300	-2.18310800	1.24248600
H	-0.19751300	-2.41662600	-0.21889400
H	-0.45570500	-3.18303600	3.46034400
H	1.00549500	-4.17623700	3.54014600
H	1.39731000	-1.81152700	4.38228000
H	2.40591400	-2.20066200	2.98543600
H	-0.21152500	-0.61844900	3.02392100
H	1.42061700	0.02045000	2.75840000
H	1.45054500	-3.76622900	1.14014600
N	0.63473800	-1.02653200	1.10992100
H	2.02825500	-1.40341500	0.41188300
C	1.51890300	2.55335200	2.07721600
C	2.90292400	2.99669900	2.52361700
C	3.56997100	3.83394800	1.43894200
C	3.57033000	3.08671600	0.11045900
C	2.17382000	2.59781300	-0.24507900
H	2.82741700	3.55816800	3.46539600
H	0.89120700	3.43820600	1.88492800
H	1.01264900	1.96636800	2.85348700
H	3.01030800	4.77737800	1.32327500
H	4.59318800	4.10804300	1.73084900
H	3.94565800	3.72790800	-0.69974800
H	4.25662800	2.22593500	0.17214700
H	1.52634300	3.48060000	-0.38823400
H	2.13227000	2.02967400	-1.18299800
H	3.51025300	2.09835400	2.73394200
N	1.56722400	1.76560000	0.82405300
H	2.20366800	0.98032600	0.98495700
C	-2.80320900	-0.18292900	1.30230900
C	-1.89080900	-0.14324400	0.23758400
C	-2.30047500	-0.71220400	-0.98142300
C	-3.54396800	-1.31336200	-1.11808500
C	-4.42602600	-1.35577000	-0.03368000
C	-4.05613400	-0.78254600	1.17943600
H	-2.53495300	0.24779700	2.27131200
H	-1.60838000	-0.68280100	-1.82769000
H	-3.84114200	-1.75878700	-2.06947300
H	-4.74039800	-0.80606700	2.02658400
C	-5.75002200	-2.00312700	-0.22512200
F	-6.49325800	-1.37503300	-1.15863000
F	-6.48713000	-2.03710400	0.89330300
F	-5.63524900	-3.27565700	-0.65346700
C	3.84938800	-3.09513900	-2.00222000

C	2.56775900	-2.58805200	-1.31608700
H	3.77780700	-2.96266500	-3.08962800
H	4.00664100	-4.16376000	-1.80502400
H	1.94638300	-1.94947300	-1.96007600
H	1.95503200	-3.40756100	-0.92436700
C	4.76503400	-0.93242300	-1.63520900
H	5.68926400	-0.37851800	-1.42533800
H	4.47568600	-0.72606500	-2.67534400
C	3.64439100	-0.50223600	-0.67464800
H	4.03041000	0.03100800	0.20437800
H	2.87323800	0.09149900	-1.17973200
C	3.93144800	-2.46095800	0.70804800
H	4.09569200	-1.85133200	1.60533600
H	3.46014000	-3.40398400	1.00822100
C	5.22580700	-2.69015800	-0.09980400
H	6.03974700	-2.05876100	0.27981000
H	5.54612000	-3.73611700	-0.01456700
N	2.96935200	-1.72841800	-0.16016800
N	5.02290200	-2.36787400	-1.51287900
C	-1.86704100	3.00397000	1.02775600
C	-2.14360900	4.47771900	0.77531100
C	-2.82821200	4.67566100	-0.57181600
C	-2.02038000	4.01223600	-1.68083500
C	-1.74600000	2.55190000	-1.36024800
H	-2.75470700	4.88198800	1.59438800
H	-2.80707700	2.43629300	1.07519600
H	-1.34375600	2.84990400	1.98131100
H	-3.83196600	4.21986100	-0.53526900
H	-2.97367000	5.74481300	-0.77961000
H	-2.54298600	4.08288200	-2.64531500
H	-1.05722900	4.53863300	-1.80387700
H	-2.68661600	1.98606000	-1.29336200
H	-1.11100300	2.06520800	-2.11242600
H	-1.18625500	5.02803100	0.78988000
N	-1.05329200	2.40985900	-0.05723400
H	-0.22047900	2.99564300	-0.13649400

S6a

Gibbs free energy before correction = -1491.83881600

Gibbs free energy after correction = -1491.82502574

Ni	-0.74339900	0.08745700	0.00325400
C	1.87846600	-0.05006900	-1.17780300
C	1.13122500	-0.04654700	0.01480700
C	1.86103000	-0.03050600	1.21473600

C	3.25409000	-0.04253000	1.23664400
C	3.96070700	-0.06033500	0.03709500
C	3.26821900	-0.06126700	-1.17531800
H	1.36398300	-0.05500800	-2.14250500
H	1.33339200	-0.01985400	2.17238600
H	3.78977500	-0.03707000	2.18485600
H	3.82407900	-0.07029300	-2.11437100
C	5.44747400	-0.08442200	0.00148900
F	6.00315000	-0.04864400	1.21964600
F	5.95466000	0.95548500	-0.68864500
F	5.92055500	-1.18827900	-0.60890200
C	-3.39377800	-0.32362900	1.21228900
C	-4.90896400	-0.19974300	1.24095300
C	-5.52199300	-0.81944100	-0.00896900
C	-4.90269800	-0.20587100	-1.25884400
C	-3.38763800	-0.32929200	-1.22218400
H	-5.30013800	-0.67574700	2.15129300
H	-3.08597100	-1.37925100	1.22198800
H	-2.93443200	0.16717400	2.08265800
H	-5.32888700	-1.90569100	-0.00578200
H	-6.61339400	-0.69120800	-0.01203500
H	-5.28935000	-0.68639100	-2.16873900
H	-5.17759000	0.86117400	-1.32056900
H	-3.07924000	-1.38478100	-1.22555200
H	-2.92415300	0.15786300	-2.09242000
H	-5.18394200	0.86764600	1.29607000
N	-2.79957300	0.26277500	-0.00484600
H	-3.05340400	1.25431900	-0.00784400
C	-1.04562800	2.75111200	1.22464600
C	-0.71068600	4.23419500	1.24791600
C	-1.22998200	4.92388800	-0.00794300
C	-0.69522900	4.22879200	-1.25432900
C	-1.02990400	2.74566400	-1.22876200
H	-1.13292200	4.68951400	2.15433100
H	-2.13693400	2.61317000	1.26252600
H	-0.61692500	2.22496000	2.08866400
H	-2.33233200	4.88349500	-0.01457200
H	-0.95253100	5.98671500	-0.00854300
H	-1.10661200	4.68002800	-2.16774400
H	0.39991900	4.34783000	-1.30345800
H	-2.12057800	2.60693900	-1.28009000
H	-0.58972500	2.21587000	-2.08475200
H	0.38383200	4.35302900	1.30984000
N	-0.54136400	2.08678900	0.00260600

H	0.47422900	2.21693500	0.00901400
C	-0.44990800	-2.48138500	1.18341600
C	-0.98755900	-3.91133100	1.25063500
C	-0.58082800	-4.68199700	0.00056600
C	-0.97697300	-3.90912300	-1.25150600
C	-0.44085700	-2.47891900	-1.17719500
H	-0.62031100	-4.41575500	2.15797500
H	0.66616500	-2.54097700	1.22624300
H	-0.76174600	-1.92440400	2.08413500
H	0.51582300	-4.81261200	0.00509600
H	-1.01531900	-5.69281300	-0.00221900
H	-0.60152100	-4.41155100	-2.15660200
H	-2.07711800	-3.87458400	-1.33088600
H	0.67555600	-2.53746900	-1.21190500
H	-0.74663700	-1.92047700	-2.07909800
H	-2.08835600	-3.87619900	1.32033400
N	-0.92739000	-1.79725800	0.00199000

^{S}TS3a

Gibbs free energy before correction = -1491.81577800

Gibbs free energy after correction = -1491.80198774

Ni	0.77406300	0.18147900	0.02019500
C	-1.81505800	-0.14519200	1.19755100
C	-1.02084700	-0.23316200	0.00467500
C	-1.76561600	-0.15111800	-1.21854800
C	-3.14651100	-0.09390200	-1.24435200
C	-3.89032300	-0.07018700	-0.05656400
C	-3.19384100	-0.08646900	1.16269300
H	-1.32083100	-0.11336300	2.17070800
H	-1.23167300	-0.12597500	-2.17086800
H	-3.66145000	-0.03539200	-2.20368400
H	-3.75219000	-0.02134100	2.09899600
C	-5.36321300	-0.05461400	-0.05236900
F	-5.89044200	0.22476700	-1.25683100
F	-5.87575600	0.85044000	0.81228100
F	-5.91280600	-1.23602600	0.32694800
C	3.36598700	-0.40703500	-1.26498500
C	4.88498100	-0.44869900	-1.32791800
C	5.44958500	-1.18978700	-0.12167600
C	4.93394100	-0.56552600	1.16958400
C	3.41378800	-0.52197100	1.16961100
H	5.20265300	-0.92160800	-2.26794900
H	2.95757500	-1.42726300	-1.33562800
H	2.94238500	0.17152300	-2.09815900

H	5.13037400	-2.24558500	-0.16442700
H	6.54815700	-1.18988400	-0.14314500
H	5.28721700	-1.12364700	2.04813400
H	5.32458200	0.46161000	1.26523800
H	3.00702100	-1.54531900	1.15645400
H	3.02184700	-0.02691400	2.06972800
H	5.27302400	0.58381800	-1.34213300
N	2.85930400	0.17235500	-0.00683100
H	3.19203700	1.13971200	0.03250000
C	1.12066000	2.81648000	-1.18463300
C	0.82961100	4.30891700	-1.19623500
C	1.36585500	4.97294900	0.06630200
C	0.81073300	4.28099900	1.30552800
C	1.10071500	2.78880800	1.26462100
H	1.26629500	4.76000600	-2.09804200
H	2.20766800	2.64344200	-1.21578200
H	0.68044300	2.31125000	-2.05549600
H	2.46673900	4.90272000	0.07367900
H	1.11743100	6.04299100	0.07629100
H	1.23473500	4.71111900	2.22348400
H	-0.28049700	4.43182900	1.35564100
H	2.18677900	2.61351600	1.30960800
H	0.64595300	2.26466400	2.11654100
H	-0.26094800	4.45996500	-1.25876800
N	0.59682200	2.15235200	0.02839000
H	-0.41925400	2.28597800	0.02137300
C	0.06902900	-2.42902100	-1.16746700
C	0.93433000	-3.68390100	-1.17100200
C	0.66849000	-4.51680500	0.07328200
C	0.89022100	-3.66103300	1.31065800
C	0.03925200	-2.39728700	1.25196800
H	0.73256200	-4.26099100	-2.08600700
H	-0.99547700	-2.74199100	-1.28527300
H	0.30794000	-1.80999200	-2.04379900
H	-0.37774200	-4.86835200	0.05709100
H	1.30401300	-5.41328900	0.09351900
H	0.64496200	-4.21829500	2.22737400
H	1.95661700	-3.38770800	1.37681700
H	-1.03072000	-2.69519200	1.35765400
H	0.27012300	-1.75793400	2.11596600
H	2.00014300	-3.39881500	-1.19663500
N	0.22504100	-1.63384700	0.03381400

^{T}TS3a

Gibbs free energy before correction = -1491.77904200
Gibbs free energy after correction = -1491.76820862

Ni	-0.97131800	-0.06074400	0.20401100
C	1.88108700	-1.05616400	0.71905100
C	1.03947800	-0.10628000	0.04793600
C	1.68022400	0.62744200	-1.00388900
C	3.02266700	0.48708600	-1.29862700
C	3.82435300	-0.41669100	-0.58432200
C	3.21936000	-1.19706800	0.41948500
H	1.45466900	-1.70434100	1.48929200
H	1.09411600	1.32194900	-1.61177800
H	3.45704700	1.06118200	-2.11788700
H	3.81670700	-1.94617000	0.94513200
C	5.24780400	-0.62816100	-0.89186500
F	5.71227900	0.19635900	-1.84544700
F	5.52065200	-1.88791700	-1.31651400
F	6.05273100	-0.45778900	0.18530800
C	-2.72747800	-1.95466700	1.48093000
C	-3.71531700	-3.10878800	1.53728500
C	-3.15761700	-4.33216500	0.81979400
C	-2.74726800	-3.97137400	-0.60310800
C	-1.78011900	-2.79846200	-0.60219600
H	-3.95331900	-3.33792500	2.58535200
H	-1.80397300	-2.21548600	2.02565600
H	-3.13719200	-1.04593600	1.94429800
H	-2.27488600	-4.70248300	1.36777900
H	-3.89358700	-5.14776800	0.81686600
H	-2.28377100	-4.82874600	-1.11075300
H	-3.64107700	-3.69818200	-1.18893200
H	-0.84613600	-3.07272300	-0.08498300
H	-1.50930800	-2.49392900	-1.62195100
H	-4.65706000	-2.79508400	1.05659900
N	-2.32279100	-1.61543200	0.09837900
H	-3.16212200	-1.31286400	-0.40397800
C	-3.02083100	1.84269600	-0.64546700
C	-3.62437000	2.86953400	-1.59131600
C	-3.86415100	2.26060100	-2.96773800
C	-2.57876400	1.64366600	-3.50661200
C	-2.00771900	0.64343400	-2.51374600
H	-4.55771100	3.26092000	-1.16294400
H	-3.73508300	1.02229800	-0.46683100
H	-2.78084300	2.28462400	0.33192600
H	-4.63633500	1.47667200	-2.88857300
H	-4.25271100	3.01703200	-3.66327000

H	-2.75197900	1.14720200	-4.47157600
H	-1.83338800	2.43693700	-3.68416500
H	-2.70728300	-0.19786900	-2.38455500
H	-1.05260200	0.22584800	-2.86059100
H	-2.93092800	3.72236000	-1.68087900
N	-1.78630400	1.23415500	-1.18045900
H	-1.09679400	1.98407000	-1.28614600
C	0.72407400	2.41875300	1.17177000
C	0.03712100	3.39347800	2.12371700
C	0.15689800	2.91121600	3.56387700
C	-0.32857300	1.47215500	3.68440800
C	0.38989700	0.58666500	2.67243900
H	0.47235600	4.39776600	2.00873400
H	1.82106800	2.43614200	1.37154400
H	0.58968700	2.75042000	0.13243600
H	1.21634000	2.95678300	3.86993000
H	-0.39620700	3.57184600	4.24661700
H	-0.16876600	1.08775500	4.70304400
H	-1.41356100	1.42614800	3.48515700
H	1.47121600	0.54085700	2.93674200
H	0.00670800	-0.44549400	2.73416700
H	-1.02822800	3.46936000	1.84722000
N	0.21000100	1.07704200	1.32179700

S7a

Gibbs free energy before correction = -1491.85227700

Gibbs free energy after correction = -1491.83848674

Ni	-0.52006900	-0.30455600	-0.50983300
C	0.80886800	-2.30222000	1.21417600
C	1.09651400	-3.72875000	1.65549400
C	1.68595200	-4.53422200	0.50367300
C	0.76351700	-4.47271200	-0.70785300
C	0.47624100	-3.02865900	-1.09025000
H	1.77637500	-3.71729900	2.51920100
H	1.74661200	-1.78685800	0.95236000
H	0.33354200	-1.71863400	2.01596500
H	2.66805100	-4.10969400	0.23198700
H	1.86397200	-5.57566000	0.80566000
H	1.20075900	-5.00135800	-1.56670700
H	-0.18851300	-4.97820000	-0.47264600
H	1.40426800	-2.53178700	-1.41528800
H	-0.23452400	-2.96815400	-1.92595800
H	0.15823400	-4.20042500	1.99378800
N	-0.07045100	-2.23577400	0.02873200

H	-0.95473900	-2.67758400	0.29743900
C	-2.94072000	-0.45723700	1.09285300
C	-4.44795900	-0.36617300	1.27576000
C	-5.14984500	-1.48526000	0.51559800
C	-4.73018000	-1.47661200	-0.94966500
C	-3.21488100	-1.53290400	-1.07736400
H	-4.69526600	-0.39800900	2.34634000
H	-2.55775200	-1.38978200	1.53911400
H	-2.42430700	0.37683200	1.58876200
H	-4.87537100	-2.45458700	0.96529900
H	-6.24088600	-1.39319200	0.60710200
H	-5.17902400	-2.31893500	-1.49490000
H	-5.09397500	-0.55354300	-1.43165200
H	-2.84319200	-2.49372000	-0.68600300
H	-2.89728000	-1.46361900	-2.12636600
H	-4.78966200	0.61204200	0.89669300
N	-2.54313300	-0.45511400	-0.32825100
H	-2.86140900	0.43272000	-0.72124700
C	3.65250000	-0.37403200	-0.75422400
C	4.54513100	0.57653900	-1.54477300
C	5.62637700	1.16253300	-0.64010000
C	5.02448700	1.75811000	0.62987100
C	4.12389700	0.73641900	1.31349900
H	4.99500000	0.04953400	-2.39831600
H	4.25639800	-1.21371000	-0.37108300
H	2.86623700	-0.81438100	-1.37509400
H	6.32700500	0.35863500	-0.35652800
H	6.21562600	1.91652300	-1.18037300
H	5.81541900	2.08674200	1.31883200
H	4.42036400	2.64687000	0.38233700
H	4.71309300	-0.15395100	1.58450500
H	3.70006100	1.11977000	2.24501400
H	3.92177600	1.38749900	-1.95681300
N	3.06813000	0.29632300	0.40376400
C	1.03092100	0.80406400	-0.86315600
C	1.87501700	0.99695900	0.30155500
C	1.43525100	1.84549900	1.31781500
C	0.22949300	2.57762200	1.19314500
C	-0.57108200	2.46541500	0.08881900
C	-0.23291100	1.52925200	-0.96727300
H	1.52588300	0.52563100	-1.79681300
H	2.02898000	2.00385200	2.21376300
H	-0.04215900	3.26300100	1.99542300
H	-0.61178100	1.77024200	-1.96943800

C	-1.77646000	3.29515600	-0.07882400
F	-2.90616700	2.55516800	-0.27131900
F	-1.71416900	4.09543100	-1.16861200
F	-2.03838300	4.09606700	0.96421700

^{T}5a

Gibbs free energy before correction = -1491.80760000

Gibbs free energy after correction = -1491.79676662

Ni	1.00307300	-0.04828700	0.32413500
C	-2.16762200	-1.47458400	1.24967500
C	-1.08080300	-1.66436100	0.37401400
C	-1.26035000	-1.27888700	-1.01309200
C	-2.47143300	-0.81244900	-1.46007500
C	-3.58957800	-0.69533400	-0.59555800
C	-3.38823100	-0.99976500	0.80615900
H	-2.06706000	-1.71358500	2.30818100
H	-0.44018700	-1.41085600	-1.72000600
H	-2.58098700	-0.54948300	-2.51350100
H	-4.22099900	-0.91105800	1.50410700
C	-4.82449500	-0.06638400	-1.01503100
F	-4.97868100	-0.00738700	-2.35476800
F	-4.99264000	1.23845100	-0.58982700
F	-5.93989200	-0.68027200	-0.52408600
C	1.44119300	2.15947700	2.11006400
C	1.29162500	3.60826300	2.54574600
C	-0.15911600	4.05967900	2.42674800
C	-0.67439500	3.81803500	1.01315700
C	-0.47952200	2.36596900	0.60942400
H	1.65891700	3.72136900	3.57515400
H	0.87492800	1.49714700	2.78611300
H	2.49052000	1.83458000	2.13380400
H	-0.77613100	3.48793100	3.14021200
H	-0.25914100	5.11904600	2.69980900
H	-1.73772300	4.08164300	0.92793000
H	-0.12696900	4.46258000	0.30511700
H	-1.08642400	1.70270000	1.24973700
H	-0.78834500	2.18772100	-0.42999400
H	1.93008200	4.24108400	1.90667200
N	0.92524800	1.91803500	0.74443100
H	1.49345800	2.47067800	0.09652400
C	3.62298800	0.31556000	-0.97736600
C	4.57953100	0.25160700	-2.15837300
C	4.05544800	1.08391300	-3.32274500
C	2.63484300	0.66288700	-3.68058700

C	1.73392200	0.71879700	-2.45640500
H	5.57668100	0.59223900	-1.84547000
H	3.56258700	1.34683600	-0.59255500
H	3.96401800	-0.32115500	-0.14882200
H	4.05497700	2.14875000	-3.03440700
H	4.71878700	0.99321400	-4.19380100
H	2.22097300	1.30217500	-4.47310600
H	2.64169000	-0.36806700	-4.07254500
H	1.65269400	1.75728100	-2.09653400
H	0.71555000	0.37571800	-2.68557000
H	4.68542100	-0.80037700	-2.47322800
N	2.24893400	-0.09152500	-1.33416100
H	2.29003100	-1.06367100	-1.65463600
C	0.86576500	-3.11325500	0.20375300
C	2.33118800	-3.29404500	0.55167300
C	2.53066400	-3.33429400	2.05965300
C	1.89003700	-2.11300800	2.70245800
C	0.43541800	-1.97686900	2.28902800
H	2.69605400	-4.21698200	0.08004200
H	0.27844700	-3.98549100	0.55264100
H	0.73026000	-3.04108600	-0.88220900
H	2.05553200	-4.24427100	2.46286500
H	3.59802900	-3.39384400	2.31279500
H	1.94075700	-2.17251900	3.79871700
H	2.43579500	-1.20045600	2.40406400
H	-0.14305500	-2.84231000	2.66900900
H	-0.00494200	-1.06676300	2.72186800
H	2.91300300	-2.46275200	0.12011900
N	0.29227200	-1.89633500	0.82249300

1b

Gibbs free energy before correction = -3244.16526600

Gibbs free energy after correction = -3244.15147570

Ni	0.37782200	-0.92822000	-0.01145900
Br	2.36682300	-2.11975000	0.02561900
C	-2.15319000	0.01161700	-1.18857000
C	-3.65974900	-0.09580400	-1.35984400
C	-4.36932100	0.11213200	-0.02743200
C	-3.82681100	-0.85729900	1.01557100
C	-2.31622100	-0.73246800	1.13303900
H	-3.99660700	0.63625200	-2.10711800
H	-1.87986400	1.02820700	-0.86623600
H	-1.62314700	-0.18841700	-2.12890000
H	-4.19887500	1.14661700	0.31607000

H	-5.45527800	-0.00840700	-0.14222800
H	-4.28653700	-0.68126700	1.99817700
H	-4.07915900	-1.89127100	0.72592200
H	-2.04333200	0.26827300	1.49973800
H	-1.90456600	-1.46477700	1.83918300
H	-3.90546300	-1.09465100	-1.75782400
N	-1.63019800	-0.92118100	-0.16591700
H	-1.86544600	-1.86643400	-0.48509700
C	0.23746200	1.92237500	1.12613300
C	0.90190900	3.27900300	1.30416500
C	1.11938900	3.95337500	-0.04529700
C	1.89627200	3.03227600	-0.97854400
C	1.20528200	1.68276800	-1.09838600
H	0.28871800	3.90682200	1.96606300
H	-0.77239900	2.04970800	0.70411200
H	0.12853500	1.39894100	2.08568900
H	0.13944400	4.18330100	-0.49708900
H	1.64261300	4.91153200	0.07936100
H	2.00716500	3.48088800	-1.97578100
H	2.91399300	2.87831700	-0.58211600
H	0.21782300	1.80292700	-1.57119100
H	1.78426700	0.98567200	-1.71942100
H	1.87325300	3.13733600	1.80713600
N	0.98437800	1.03993200	0.21210900
H	1.90763300	0.88274400	0.62740400

2b

Gibbs free energy before correction = -6384.06552600

Gibbs free energy after correction = -6384.05173565

Ni	-1.26271900	-0.02371700	-0.65411000
Br	-1.53287500	-1.70097500	-2.25271900
C	-0.17390100	2.31829100	0.93933600
C	0.99086600	3.23556900	1.27667600
C	1.48045500	3.96744800	0.03285900
C	1.81751300	2.97080900	-1.06965700
C	0.63448600	2.05872800	-1.35117600
H	0.68805800	3.94366600	2.06084200
H	-1.03999100	2.90932300	0.60113500
H	-0.49255100	1.74132600	1.81945600
H	0.68765700	4.64695600	-0.32316700
H	2.35139800	4.59392600	0.26957900
H	2.11338400	3.48687200	-1.99378500
H	2.67836900	2.35280500	-0.76017600
H	-0.21364300	2.63549000	-1.75333000

H	0.88793800	1.28761100	-2.09278300
H	1.81187800	2.62744500	1.69484100
N	0.15233200	1.36348600	-0.13708900
H	0.93991900	0.80317400	0.20206800
C	-3.82283600	-0.50618700	0.68833900
C	-5.11163700	-0.06191900	1.36108100
C	-5.84057900	0.96399100	0.50172600
C	-4.91409000	2.12666500	0.16738700
C	-3.63011900	1.62266000	-0.47298000
H	-5.74675500	-0.93804100	1.55479900
H	-4.03487200	-1.02837700	-0.25751700
H	-3.25810100	-1.20557400	1.31901100
H	-6.16907700	0.48280500	-0.43497700
H	-6.74737200	1.32237800	1.00819700
H	-5.40497600	2.84349400	-0.50596300
H	-4.66153600	2.67608000	1.09008700
H	-3.84687800	1.13578200	-1.43759300
H	-2.93107500	2.44641500	-0.67516800
H	-4.87118200	0.38161500	2.34209500
N	-2.92956300	0.62174900	0.35740600
H	-2.66572000	1.07639800	1.23600000
C	2.10728300	-0.74214900	2.02737600
C	1.25382100	-1.43658400	1.17513900
C	1.59798200	-1.71947700	-0.14165800
C	2.82869000	-1.28140500	-0.62067400
C	3.69194900	-0.58421000	0.21890800
C	3.33572500	-0.31496400	1.54006200
H	1.81574300	-0.52598700	3.05295200
H	0.89313600	-2.22287600	-0.80235200
H	3.10565000	-1.48349800	-1.65272000
H	4.01534000	0.23475500	2.19001100
Br	-0.45945300	-1.95018800	1.80771800
C	5.00700200	-0.06997900	-0.27120100
F	6.02174200	-0.48970500	0.49893500
F	5.04786700	1.27433100	-0.24305000
F	5.27570200	-0.44568900	-1.52398700

TS1b

Gibbs free energy before correction = -6384.04457500

Gibbs free energy after correction = -6384.03078465

Ni	0.74122100	-0.00025500	-0.00424300
Br	0.16381400	-0.00085100	2.36141600
C	1.50990500	2.95192300	-0.97903400
C	2.08459800	4.30342700	-0.58516100
C	3.48435900	4.14650300	-0.00525400

C	3.46513600	3.14697800	1.14307500
C	2.83315700	1.83310200	0.71229100
H	2.09145400	4.96625500	-1.46184500
H	2.12417900	2.49053000	-1.76641500
H	0.49709800	3.05842200	-1.38665000
H	4.16350600	3.78089400	-0.79370700
H	3.87911500	5.11576300	0.32914000
H	4.47881500	2.95717800	1.52309800
H	2.88095700	3.55849300	1.98339800
H	3.43793600	1.35075200	-0.07418700
H	2.76280900	1.13700100	1.55775800
H	1.42214500	4.77014200	0.16300100
N	1.47375000	2.00468400	0.15193400
H	0.88035400	2.40194300	0.88689700
C	2.81506000	-1.86237500	0.69047300
C	3.42938100	-3.18341500	1.12509100
C	3.41492800	-4.19382800	-0.01387600
C	2.00522200	-4.33009200	-0.57478300
C	1.45055100	-2.97173400	-0.97347000
H	4.45146700	-3.00857100	1.48946500
H	3.41740100	-1.39837200	-0.10882500
H	2.76958900	-1.15706900	1.53009300
H	4.09046000	-3.84840200	-0.81443200
H	3.79607800	-5.16706300	0.32479100
H	1.98894200	-5.00081600	-1.44528000
H	1.34366800	-4.77765300	0.18577500
H	2.06333500	-2.52779300	-1.77193400
H	0.43118400	-3.06306500	-1.36802800
H	2.84952600	-3.57631600	1.97723700
N	1.44527600	-2.01546500	0.15033200
H	0.85599500	-2.39766500	0.89651700
C	-1.74760100	1.24176800	-0.65091600
C	-1.09106800	0.01968000	-0.75547900
C	-1.77468300	-1.19029400	-0.64658200
C	-3.11781100	-1.16618100	-0.30464200
C	-3.77506900	0.05233400	-0.12656000
C	-3.09449000	1.25268400	-0.30791500
H	-1.21684700	2.18152700	-0.78244700
H	-1.26398000	-2.14169100	-0.77325900
H	-3.66080400	-2.10227600	-0.17487400
H	-3.60888700	2.20308900	-0.18282300
Br	0.57811800	-0.00211400	-2.35827400
C	-5.21897400	0.02268900	0.24393400
F	-5.74163600	1.24413400	0.39545300

F	-5.42136800	-0.63907900	1.39677200
F	-5.96100600	-0.61148300	-0.68074000

3b

Gibbs free energy before correction = -6384.05184500

Gibbs free energy after correction = -6384.03805465

Ni	-0.73620000	0.00108200	0.06100500
Br	-0.54539100	0.00252900	2.40929400
C	-1.25985500	-3.00500400	-0.91695500
C	-1.87302100	-4.35882200	-0.59882300
C	-3.37109300	-4.22401200	-0.35694800
C	-3.63805200	-3.18520000	0.72414900
C	-2.96030600	-1.86497400	0.39119300
H	-1.66707600	-5.05447800	-1.42436400
H	-1.68882200	-2.59196900	-1.83983600
H	-0.17665700	-3.07816900	-1.07656700
H	-3.86007200	-3.90722600	-1.29342700
H	-3.81093700	-5.19210200	-0.08064600
H	-4.71584900	-3.01743300	0.85785000
H	-3.24833200	-3.54691000	1.69051400
H	-3.38982100	-1.42771800	-0.52488600
H	-3.10010300	-1.13973800	1.20371000
H	-1.38616000	-4.77487600	0.29918400
N	-1.50635500	-2.01845400	0.15413300
H	-1.09275400	-2.38352000	1.01753700
C	-2.93036100	1.89499400	0.39231900
C	-3.59282400	3.22277600	0.72587900
C	-3.31556600	4.25797500	-0.35606900
C	-1.81632200	4.37596300	-0.59944900
C	-1.21833500	3.01532100	-0.91785400
H	-4.67224400	3.06706700	0.86104500
H	-3.36623200	1.46257200	-0.52308100
H	-3.07748000	1.17156800	1.20515300
H	-3.80909000	3.94613200	-1.29182500
H	-3.74427400	5.23105800	-0.07982000
H	-1.60345500	5.06904400	-1.42539500
H	-1.32406000	4.78687700	0.29796500
H	-1.65219000	2.60712300	-1.84058000
H	-0.13442400	3.07643000	-1.07797000
H	-3.19776200	3.58042600	1.69158800
N	-1.47523500	2.03155800	0.15324400
H	-1.05565100	2.39095200	1.01609700
C	1.84732800	-1.23670600	0.07645000
C	1.19009100	-0.01914300	0.06436600

C	1.87274500	1.18796700	0.06745800
C	3.26263500	1.16788800	0.05059400
C	3.94314800	-0.04958700	0.04140000
C	3.24090000	-1.24982600	0.05953800
H	1.30313000	-2.17858300	0.11504200
H	1.34751900	2.14090000	0.09926900
H	3.81953800	2.10492300	0.04954700
H	3.77138200	-2.19966400	0.06553800
Br	-0.66117100	0.00083900	-2.26453300
C	5.43398200	-0.01925100	0.01010600
F	5.98067700	-1.23916300	0.05434100
F	5.94121600	0.67811000	1.04118800
F	5.89540700	0.57830400	-1.10243800

4b

Gibbs free energy before correction = -6384.05348900

Gibbs free energy after correction = -6384.03969865

Ni	0.98263400	0.00014600	0.04735900
Br	1.62426000	0.00021300	2.49358200
C	0.18728400	2.77230900	-0.85063300
C	0.24269400	4.25859900	-0.53311900
C	1.67635500	4.76130900	-0.45092300
C	2.46317200	3.91997600	0.54325000
C	2.37912300	2.44781300	0.17918700
H	-0.32763600	4.80001500	-1.30020300
H	0.61415800	2.55084600	-1.83792700
H	-0.84666000	2.41393300	-0.84060100
H	2.14887300	4.68272900	-1.44392000
H	1.69841300	5.82237600	-0.16824800
H	3.52113400	4.21435000	0.56921200
H	2.06454500	4.06543400	1.56114800
H	2.79825000	2.26146600	-0.81767700
H	2.91422700	1.82074200	0.90098500
H	-0.26767200	4.43581300	0.42808900
N	0.96431800	1.98039800	0.13477900
H	0.55582300	2.14342000	1.06229400
C	2.38053700	-2.44667400	0.17867300
C	2.46562900	-3.91885200	0.54247000
C	1.67889800	-4.76045800	-0.45153600
C	0.24487700	-4.25864300	-0.53296400
C	0.18833700	-2.77233300	-0.85017400
H	3.52378500	-4.21257500	0.56791200
H	2.79915800	-2.25994000	-0.81832400
H	2.91553200	-1.81938700	0.90037000

H	2.15092300	-4.68135100	-1.44472300
H	1.70174900	-5.82157500	-0.16910800
H	-0.32545600	-4.80029900	-1.29987900
H	-0.26490500	-4.43637900	0.42845300
H	0.61451000	-2.55042700	-1.83767500
H	-0.84582700	-2.41461000	-0.83944400
H	2.06752100	-4.06472100	1.56050800
N	0.96544200	-1.98008400	0.13491500
H	0.55749600	-2.14331200	1.06263600
C	-1.59849700	-0.00007200	-1.10484400
C	-0.92949700	-0.00034700	0.11631600
C	-1.61243400	-0.00123000	1.32114200
C	-3.00910200	-0.00160900	1.30724300
C	-3.68863500	-0.00117700	0.09615000
C	-2.98773400	-0.00044500	-1.11098400
H	-1.04438900	0.00045900	-2.04304200
H	-1.07455700	-0.00149000	2.26736000
H	-3.55648400	-0.00219600	2.24751500
H	-3.52827100	-0.00015300	-2.05744100
Br	1.87465800	0.00045200	-2.22561900
C	-5.18078500	-0.00083500	0.03928800
F	-5.65153200	-1.07297500	-0.61924600
F	-5.65096400	1.07383400	-0.61555900
F	-5.74747500	-0.00271700	1.25012600

5b

Gibbs free energy before correction = -6728.98735700

Gibbs free energy after correction = -6728.97356665

Ni	-0.03104000	0.41052200	0.03385300
Br	0.68043300	0.67206700	2.43454100
C	0.34659000	-2.25747700	-1.29085400
C	1.12730800	-3.56317000	-1.31403200
C	0.76164200	-4.45059100	-0.13527000
C	0.93713400	-3.67018500	1.15735000
C	0.15400000	-2.36813700	1.12287900
H	0.93272800	-4.06622900	-2.27156000
H	-0.73068100	-2.46068000	-1.37804500
H	0.63920100	-1.60491800	-2.11794300
H	-0.29034400	-4.76771700	-0.22859400
H	1.37123400	-5.36447400	-0.12952700
H	0.60337200	-4.25323500	2.02712400
H	2.00508800	-3.44560400	1.31753400
H	-0.92119400	-2.57289100	1.01556400
H	0.30287600	-1.79258400	2.03967400

H	2.20683500	-3.33918500	-1.28725500
N	0.55319700	-1.51058700	-0.02404100
H	1.57806700	-1.30674200	0.05378400
C	-1.78491900	2.76435600	-0.75005800
C	-2.28625600	4.14851600	-0.36708000
C	-1.14857400	5.15472200	-0.27972300
C	-0.07138600	4.63469600	0.66057100
C	0.39607600	3.25634700	0.22725000
H	-3.04191800	4.46168400	-1.10048500
H	-1.33731600	2.75713000	-1.75318500
H	-2.60924100	2.04425800	-0.74292800
H	-0.71309400	5.30159200	-1.28195500
H	-1.52117600	6.13271800	0.05378100
H	0.79668100	5.30761200	0.68641400
H	-0.46318500	4.57899700	1.69034500
H	0.82034800	3.28030800	-0.78391900
H	1.15424800	2.85401500	0.90701000
H	-2.79732000	4.08210400	0.60787800
N	-0.73662300	2.28780100	0.18650400
H	-1.14817300	2.26305100	1.12637900
C	-2.42766800	-0.50947200	-1.15577800
C	-1.83195700	-0.20340800	0.06193600
C	-2.53296300	-0.25806100	1.25637100
C	-3.87779900	-0.62796300	1.23192100
C	-4.48827900	-0.93606400	0.02138400
C	-3.76710200	-0.88303000	-1.17161400
H	-1.87017400	-0.43641900	-2.08883800
H	-2.04672000	-0.01734800	2.20088200
H	-4.44173600	-0.67033100	2.16146600
H	-4.25425200	-1.12322800	-2.11656600
Br	0.88456100	0.93121700	-2.19749700
C	-5.92281900	-1.34528800	-0.04352900
F	-6.54020600	-1.26354800	1.13951600
F	-6.05920100	-2.61142600	-0.47266300
F	-6.61706000	-0.58342100	-0.90496800
C	5.54604400	-0.65083400	-1.39282600
C	4.06375900	-1.09056600	-1.34030300
H	5.69235700	0.17629100	-2.10222600
H	6.19738400	-1.47786900	-1.70988900
H	3.43578900	-0.53982100	-2.05540500
H	3.95977600	-2.16416400	-1.55708500
C	5.17809700	0.95921700	0.32274900
H	5.50633700	1.27833000	1.32261100
H	5.39046500	1.78414200	-0.37262200

C	3.67855800	0.58813300	0.31517400
H	3.19229700	0.77133600	1.28260200
H	3.11311600	1.14598100	-0.44521100
C	4.27213400	-1.63186200	0.97988600
H	3.85253500	-1.42101400	1.97522900
H	4.10398700	-2.69823500	0.76640700
C	5.77588500	-1.27259500	0.89863500
H	6.16072900	-0.94015600	1.87321400
H	6.37552100	-2.13844200	0.58352100
N	3.51438600	-0.84248000	0.00091800
N	5.99090500	-0.19558400	-0.07192500

TS2b

Gibbs free energy before correction = -6728.97118500

Gibbs free energy after correction = -6728.95739465

Ni	0.06050400	0.37379400	0.06386600
Br	0.66280400	0.77521200	2.53225800
C	0.40889900	-2.25504400	-1.18012800
C	1.11784900	-3.60605300	-1.21085800
C	0.73808000	-4.44638900	-0.00384500
C	1.01452400	-3.64890600	1.25877900
C	0.33201400	-2.28630800	1.21257500
H	0.85598900	-4.11258500	-2.15123200
H	-0.67836500	-2.44423500	-1.23707500
H	0.68061400	-1.65210100	-2.05274000
H	-0.33663700	-4.69046800	-0.05361200
H	1.28272000	-5.40114500	0.00223400
H	0.65724300	-4.17945500	2.15355500
H	2.10044400	-3.51993800	1.38508300
H	-0.76069100	-2.45268100	1.20178000
H	0.56491300	-1.71060600	2.11255200
H	2.21011300	-3.45915400	-1.22568500
N	0.71254300	-1.47922600	0.03595000
H	2.13696200	-1.15462100	0.01865200
C	-1.74921600	2.74593800	-0.69571700
C	-2.24190200	4.13677300	-0.32596300
C	-1.10545700	5.14858500	-0.31235600
C	0.01318200	4.65613200	0.59464400
C	0.46537400	3.26709700	0.17845300
H	-3.03142100	4.43244900	-1.03076600
H	-1.35318500	2.71583800	-1.72049200
H	-2.56763600	2.02064700	-0.63235700
H	-0.71309400	5.27020700	-1.33583600
H	-1.46706800	6.13458100	0.01024500

H	0.87670900	5.33532900	0.56846000
H	-0.33687900	4.62461400	1.64072500
H	0.85979700	3.27017400	-0.84576800
H	1.24710900	2.88471900	0.84431700
H	-2.70754700	4.09301700	0.67301000
N	-0.65679400	2.29346200	0.19552500
H	-1.02153400	2.27498300	1.15398200
C	-2.34279200	-0.54274900	-1.17494300
C	-1.73199200	-0.26816400	0.04529900
C	-2.44783300	-0.32904400	1.23374400
C	-3.79945100	-0.67125500	1.20463100
C	-4.41531800	-0.94816400	-0.01122100
C	-3.68905600	-0.88868500	-1.20125600
H	-1.78193500	-0.46329600	-2.10578900
H	-1.95964400	-0.10522100	2.18237600
H	-4.36631800	-0.71682800	2.13251600
H	-4.17989600	-1.10271400	-2.15089600
Br	0.84185100	0.90686700	-2.25960200
C	-5.85429800	-1.33508300	-0.08356900
F	-6.47591700	-1.25198600	1.09792400
F	-6.00937000	-2.59746700	-0.52024700
F	-6.53703500	-0.55956800	-0.94311300
C	5.28007900	-0.57053900	-1.49555400
C	3.83590700	-1.10460500	-1.41792000
H	5.33027500	0.33001000	-2.12182700
H	5.94502200	-1.32315300	-1.93833000
H	3.14912900	-0.59722800	-2.10644400
H	3.78809900	-2.18481600	-1.60078300
C	4.99401300	0.89891000	0.35381700
H	5.31197700	1.08862900	1.38755700
H	5.22116600	1.79643200	-0.23597400
C	3.48931700	0.58080800	0.29178900
H	2.96658300	0.75491100	1.23981800
H	2.96693700	1.13672900	-0.49714500
C	4.10046900	-1.68182700	0.92292300
H	3.73995800	-1.42950800	1.92902500
H	3.87574600	-2.73662400	0.72681100
C	5.59923900	-1.36806700	0.72839600
H	6.07458900	-1.14500300	1.69198300
H	6.12125000	-2.22775900	0.28829700
N	3.31905600	-0.86479500	-0.04104500
N	5.77841600	-0.22259600	-0.16368800

6b

Gibbs free energy before correction = -6728.97414700
Gibbs free energy after correction = -6728.96035665

Ni	0.01642700	0.31125400	0.07660000
Br	0.71930600	0.66232300	2.52824300
C	0.29113500	-2.30927200	-1.18538700
C	1.11387600	-3.59765900	-1.20868300
C	0.79511500	-4.47248300	-0.00718300
C	0.93832600	-3.65591900	1.26690200
C	0.12013100	-2.37096700	1.18019400
H	0.91683100	-4.12692300	-2.15265500
H	-0.77904400	-2.58723100	-1.27044300
H	0.53977800	-1.68320400	-2.04908800
H	-0.24438100	-4.83295300	-0.08824600
H	1.43874700	-5.36360800	0.01525400
H	0.60788300	-4.22816300	2.14641500
H	1.99776300	-3.40152100	1.43463000
H	-0.94871400	-2.65127900	1.08870400
H	0.23508900	-1.78792600	2.09849400
H	2.18730100	-3.34559300	-1.20442800
N	0.53510400	-1.54789500	0.03996700
H	2.38666600	-1.07823800	0.00338100
C	-1.69322900	2.76028900	-0.66670300
C	-2.15780500	4.16611800	-0.31865500
C	-0.99570000	5.14888700	-0.30294500
C	0.09818300	4.63895000	0.62461200
C	0.52019700	3.23332400	0.23239600
H	-2.93149300	4.47522800	-1.03551600
H	-1.28982400	2.71218500	-1.68851700
H	-2.52846600	2.05311300	-0.60679200
H	-0.58748400	5.24659600	-1.32298300
H	-1.33537100	6.14846900	0.00168900
H	0.97769000	5.29787500	0.60344900
H	-0.26835600	4.62950500	1.66556000
H	0.93775800	3.21648100	-0.78328100
H	1.27738200	2.83716600	0.91875400
H	-2.63538800	4.14658700	0.67555800
N	-0.61994500	2.28538500	0.23329000
H	-0.99504100	2.26616700	1.18736000
C	-2.41054500	-0.55615200	-1.17945200
C	-1.78861100	-0.29141500	0.03866000
C	-2.51789800	-0.31303200	1.22257000
C	-3.88197800	-0.59915000	1.19223300
C	-4.50378000	-0.86452800	-0.02377300
C	-3.76975800	-0.84527000	-1.21071700

H	-1.84271200	-0.51588900	-2.10905800
H	-2.02627900	-0.10105500	2.17281500
H	-4.45503300	-0.61256600	2.11749000
H	-4.26548800	-1.05055500	-2.16000500
Br	0.87321400	0.85865900	-2.23574200
C	-5.95512600	-1.19760500	-0.09999400
F	-6.57521400	-1.10305100	1.08181000
F	-6.15595800	-2.45007600	-0.54794900
F	-6.61047700	-0.39126200	-0.95329600
C	5.34874200	-0.50401000	-1.52029800
C	3.91691100	-1.06526000	-1.44475600
H	5.37740100	0.40717600	-2.13121200
H	6.01927100	-1.23937800	-1.98133000
H	3.20887300	-0.57487700	-2.12336100
H	3.88258800	-2.14855000	-1.60713800
C	5.07036600	0.94644500	0.34970000
H	5.38301600	1.11389600	1.38826200
H	5.30271600	1.85349500	-0.22181900
C	3.56580800	0.64355700	0.27433000
H	3.02534300	0.80860600	1.21416200
H	3.04595400	1.18330600	-0.52672000
C	4.19076700	-1.63800200	0.91899900
H	3.83559200	-1.36457600	1.91997700
H	3.94463500	-2.68884700	0.73022700
C	5.68408500	-1.32735800	0.69527100
H	6.17606800	-1.12024700	1.65321400
H	6.19119700	-2.18394500	0.23388400
N	3.41310800	-0.81418200	-0.05605000
N	5.84872400	-0.17125000	-0.18549500

7b

Gibbs free energy before correction = -3811.85917000

Gibbs free energy after correction = -3811.84537997

Ni	0.95526800	-0.00423400	-0.00264800
C	1.05721900	-2.59005400	-1.22009400
C	2.30774200	-3.47161600	-1.25506800
C	2.38767500	-4.33739900	-0.00585200
C	2.31352500	-3.47179400	1.24384600
C	1.06227900	-2.59111800	1.21447000
H	2.28729500	-4.08140200	-2.16814800
H	0.15325500	-3.22809400	-1.25957600
H	1.02780800	-1.90464800	-2.07655900
H	1.55228300	-5.05745100	-0.00392700
H	3.31499900	-4.92667100	-0.00806600

H	2.29736300	-4.08172800	2.15692700
H	3.19199900	-2.81099500	1.29585600
H	0.15938500	-3.23046200	1.25666800
H	1.03472400	-1.90622400	2.07143900
H	3.18625600	-2.81118200	-1.31103600
N	1.01284800	-1.81880600	-0.00234000
C	1.30012800	2.58368500	-1.22503800
C	1.03540100	4.07979600	-1.24370800
C	1.58758000	4.74128600	0.01313600
C	1.01749000	4.07083200	1.25713500
C	1.28210300	2.57480100	1.23128500
H	1.48150700	4.51400000	-2.14910200
H	2.37650800	2.36661400	-1.23754600
H	0.84853300	2.07898000	-2.09025000
H	2.68624800	4.64479600	0.02065100
H	1.36267600	5.81654400	0.01537300
H	1.45064900	4.49836800	2.17193100
H	-0.07024400	4.24639600	1.30633500
H	2.35825400	2.35741000	1.25791800
H	0.81753400	2.06439700	2.08621200
H	-0.05151700	4.25574700	-1.30718600
N	0.75404200	1.94511000	-0.00311600
H	-0.25496700	2.12067000	-0.01005200
C	-1.63637100	-0.20453100	1.21575400
C	-0.93221900	-0.14277100	0.00962400
C	-1.65827500	-0.13795300	-1.18865400
C	-3.04763600	-0.18462700	-1.18094900
C	-3.73312800	-0.23870100	0.03371900
C	-3.02898700	-0.24923100	1.23426400
H	-1.09923800	-0.21606600	2.16669200
H	-1.13750900	-0.09230600	-2.14764200
H	-3.60600300	-0.17685100	-2.11786300
H	-3.56402700	-0.29195100	2.18129400
Br	3.35023800	0.05095500	-0.00520100
C	-5.22238100	-0.27312200	0.00211500
F	-5.73659000	0.82211900	-0.58779100
F	-5.76873700	-0.35038000	1.22148700
F	-5.68697400	-1.32083000	-0.70279300

TS3b

Gibbs free energy before correction = -3811.84336600

Gibbs free energy after correction = -3811.82957597

Ni	1.07751600	-0.04455100	0.00224000
C	0.67353800	-2.60409100	-1.21251200

C	1.93734800	-3.46136700	-1.25831000
C	2.04399300	-4.32963600	-0.01309700
C	1.96666200	-3.46103700	1.23403400
C	0.70108900	-2.60530500	1.21812200
H	1.91915900	-4.06917300	-2.17348100
H	-0.22502000	-3.24903400	-1.23160100
H	0.63642800	-1.93523500	-2.08021800
H	1.21832000	-5.06106000	-0.00330000
H	2.97926400	-4.90607000	-0.02408000
H	1.97124000	-4.06849100	2.14962500
H	2.83473800	-2.78460500	1.27240400
H	-0.19618300	-3.25112200	1.25669100
H	0.68272400	-1.93713900	2.08704600
H	2.80534200	-2.78647700	-1.31823400
N	0.68431500	-1.80885300	0.00321000
C	1.27795800	2.56038100	-1.22730800
C	0.96275300	4.04678000	-1.25299100
C	1.50571700	4.73362700	-0.00560900
C	0.97171800	4.05095600	1.24792800
C	1.28674700	2.56445300	1.22512800
H	1.38363700	4.49184700	-2.16533100
H	2.36198900	2.38154600	-1.25386700
H	0.83462200	2.03560400	-2.08528500
H	2.60710000	4.67326400	-0.00946200
H	1.24616700	5.80113400	-0.00645800
H	1.39895600	4.49918600	2.15575500
H	-0.12092500	4.18954100	1.30694500
H	2.37093500	2.38560900	1.24458200
H	0.84946100	2.04254500	2.08796400
H	-0.13027700	4.18523200	-1.30478800
N	0.77549200	1.90531600	0.00185000
H	-0.24333800	2.01859100	0.00537100
C	-1.49867200	-0.44280500	1.23142900
C	-0.79413100	-0.49375300	0.01756500
C	-1.51469400	-0.42720700	-1.18933700
C	-2.89179800	-0.27671500	-1.17637400
C	-3.57844700	-0.21530700	0.03958000
C	-2.87983600	-0.29362700	1.24257200
H	-0.96710200	-0.49945200	2.18145600
H	-0.99505200	-0.47090800	-2.14660000
H	-3.44328000	-0.20391700	-2.11408100
H	-3.41240300	-0.23615000	2.18973500
Br	3.44979700	0.03872400	-0.00536300
C	-5.05864800	-0.05028300	0.00284800

F	-5.41803600	1.10958200	-0.57674500
F	-5.61596100	-0.06765000	1.21880200
F	-5.65114400	-1.01957800	-0.71685900

8b

Gibbs free energy before correction = -3811.90380800

Gibbs free energy after correction = -3811.89001797

Ni	0.77207100	0.34840600	-0.12634100
C	2.78531500	-2.07871300	-0.95813100
C	4.12785100	-1.37420100	-1.00612500
C	4.84332700	-1.49018600	0.32986000
C	3.94516700	-0.92882200	1.41957400
C	2.58777800	-1.61085900	1.43822700
H	4.72175300	-1.81039800	-1.82091200
H	2.92594200	-3.16200600	-0.78370000
H	2.27436800	-1.96207900	-1.91667400
H	5.06852600	-2.55010400	0.53808700
H	5.80354400	-0.95694500	0.30734800
H	4.40005500	-1.04070900	2.41338900
H	3.78477500	0.14588900	1.23891000
H	2.68294400	-2.66971300	1.74527700
H	1.94977100	-1.10279900	2.16979100
H	3.95551100	-0.31149400	-1.23984600
N	1.93861600	-1.53811600	0.12053300
C	-1.38510400	2.13087300	-1.05690900
C	-2.74556900	2.78692000	-0.88519700
C	-2.78554100	3.61217100	0.39610200
C	-2.38990300	2.75558900	1.59346400
C	-1.03907300	2.09827900	1.36018300
H	-2.97037900	3.40869500	-1.76320300
H	-0.59309300	2.88488400	-1.18023900
H	-1.35867700	1.48083500	-1.94304400
H	-2.07795600	4.45351700	0.30502900
H	-3.78196900	4.05072600	0.54482700
H	-2.35645900	3.35411300	2.51472400
H	-3.14739000	1.96867400	1.75114500
H	-0.24081800	2.85146200	1.27732800
H	-0.76939600	1.42363900	2.18561000
H	-3.51784000	1.99989800	-0.84376100
N	-1.00884000	1.31128700	0.11148700
H	-1.71774400	0.57579600	0.20340700
C	-0.24480600	-1.95597600	1.21335000
C	0.54238900	-1.74380600	0.05359700
C	-0.12921400	-1.65224900	-1.19587100

C	-1.51728500	-1.70671400	-1.25801700
C	-2.27140900	-1.86278400	-0.10015900
C	-1.62479000	-1.99814900	1.13185500
H	0.22483000	-2.09449500	2.18213900
H	0.42465900	-1.55677800	-2.12536000
H	-2.00607500	-1.61074400	-2.22539600
H	-2.20698000	-2.14244800	2.04051600
Br	2.33695900	2.09372300	-0.39163700
C	-3.75589100	-1.76596900	-0.14113600
F	-4.17726700	-0.51800200	0.16337800
F	-4.34620200	-2.58223600	0.74310600
F	-4.26001700	-2.05173100	-1.34678100

8b

Gibbs free energy before correction = -3811.90530400

Gibbs free energy after correction = -3811.89151397

Ni	1.05423200	-0.46878800	-0.00650900
C	0.62969500	2.18728200	-1.21305400
C	0.00655800	3.57344300	-1.27049000
C	0.36244000	4.37126300	-0.01993400
C	0.01972900	3.58684100	1.24266400
C	0.64530500	2.20160700	1.19422200
H	0.35872700	4.08707800	-2.17546000
H	1.72314500	2.27487500	-1.15055800
H	0.42272000	1.59257800	-2.10795200
H	1.44455000	4.58448900	-0.02642800
H	-0.15142500	5.34194100	-0.02262400
H	0.37935600	4.11112500	2.13853900
H	-1.07313000	3.49473100	1.34618700
H	1.73755500	2.29160900	1.11617400
H	0.45154000	1.61831300	2.09938600
H	-1.08745800	3.48346800	-1.36227000
N	0.20707800	1.43666000	-0.00231200
C	3.68570400	-0.51641500	-1.21238200
C	5.18574800	-0.26917100	-1.23454100
C	5.84160400	-0.82760300	0.02265500
C	5.17156700	-0.25597700	1.26636400
C	3.67177800	-0.50318100	1.22964100
H	5.61827800	-0.71827400	-2.13967100
H	3.47018400	-1.59591700	-1.23338400
H	3.18891900	-0.06720000	-2.08366900
H	5.73737100	-1.92580400	0.02782600
H	6.91886400	-0.61148800	0.02760800
H	5.59358700	-0.69573500	2.18099200

H	5.35643600	0.83019100	1.31937100
H	3.45615300	-1.58247600	1.26002500
H	3.16564900	-0.04471600	2.09061700
H	5.37110100	0.81641700	-1.29671600
N	3.03660300	0.02139000	0.00208600
H	3.18087700	1.03497700	-0.00291400
C	-1.83569500	0.71000200	-1.18789100
C	-1.15127800	0.97630800	0.01029900
C	-1.80101300	0.68341500	1.21909100
C	-3.07234000	0.12970100	1.23014500
C	-3.73142600	-0.14284100	0.03675300
C	-3.10518000	0.15791600	-1.17097500
H	-1.38011200	0.91838100	-2.15117000
H	-1.31592400	0.86763500	2.17289300
H	-3.54729000	-0.09087900	2.18356300
H	-3.61372600	-0.04165400	-2.11352300
Br	0.59316500	-2.72933500	-0.02169900
C	-5.11402300	-0.69542600	0.01522200
F	-5.23323700	-1.71719800	-0.84920500
F	-6.01724500	0.22374000	-0.37439900
F	-5.51018600	-1.14323300	1.21246200

2c

Gibbs free energy before correction = -3589.10127200

Gibbs free energy after correction = -3589.08748160

Ni	-0.81283600	-0.39311300	0.00917400
Br	-0.43666200	-2.68053400	0.01682800
C	-0.23371300	2.21674800	1.22838100
C	0.57299900	3.50625000	1.26041800
C	0.31289900	4.33386400	0.00716400
C	0.57641500	3.50411400	-1.24392500
C	-0.22802300	2.21328200	-1.21132300
H	0.33285400	4.07638600	2.16900400
H	-1.31305400	2.43936700	1.25954700
H	-0.00614100	1.58115200	2.09609100
H	-0.73990100	4.66397300	0.00553900
H	0.92856500	5.24391100	0.00706300
H	0.33666800	4.07191800	-2.15409900
H	1.64918900	3.24836900	-1.29912800
H	-1.30744300	2.43455900	-1.24855800
H	0.00426000	1.57595600	-2.07658700
H	1.64536100	3.24819900	1.31760700
N	0.03509500	1.42897400	0.01032700
H	1.05071500	1.22657900	0.01435500

C	-3.47697500	-0.27694300	1.21163800
C	-4.95217800	0.09265700	1.23229900
C	-5.65137000	-0.41893900	-0.02172200
C	-4.93604300	0.08519900	-1.26967200
C	-3.46107600	-0.28356300	-1.22764000
H	-5.42151100	-0.31225300	2.14001900
H	-3.35293800	-1.37086600	1.24249100
H	-2.94526300	0.13610500	2.08034500
H	-5.63794400	-1.52209400	-0.01832500
H	-6.70743000	-0.11562800	-0.02937100
H	-5.39334400	-0.32560500	-2.18089700
H	-5.03043500	1.18250500	-1.33148700
H	-3.33611500	-1.37759900	-1.25108100
H	-2.91841700	0.12502000	-2.09170200
H	-5.04674500	1.19038200	1.28604900
N	-2.78729400	0.19424000	-0.00486200
H	-2.83248500	1.21684400	-0.00763100
C	5.25803900	-0.03500200	-0.11917100
C	4.16926600	1.05708400	0.01586200
H	6.01524200	0.05531300	0.67246000
H	5.77805400	0.03760200	-1.08504700
H	4.27398200	1.61773200	0.95593400
H	4.21600900	1.78064200	-0.81059500
C	3.88498100	-1.45619000	1.21267200
H	3.51048400	-2.48486200	1.31956200
H	4.57429500	-1.26500200	2.04755700
C	2.72160600	-0.43772200	1.19366100
H	1.74779000	-0.94851100	1.13120600
H	2.71847700	0.19848900	2.09144400
C	2.70447000	-0.39133100	-1.19752200
H	1.67422000	-0.78048000	-1.23378800
H	2.85216500	0.26704000	-2.06664900
C	3.73443000	-1.54305400	-1.16417500
H	3.23273600	-2.51441300	-1.04292000
H	4.32366800	-1.58466200	-2.09124100
N	2.84130400	0.43225600	0.01330100
N	4.65269900	-1.36817600	-0.03372100

3c

Gibbs free energy before correction = -3589.04906400

Gibbs free energy after correction = -3589.03527360

Ni	-0.73786800	0.15265800	-0.68378900
Br	0.37396000	-1.38470200	-2.19652900
C	-0.67638300	2.57688900	0.96528700

C	-0.40663700	4.06690100	0.74684500
C	-1.67237100	4.75904100	0.25309700
C	-2.24918000	4.02576900	-0.95267400
C	-2.40615800	2.53580700	-0.63994100
H	-0.04196200	4.53792000	1.67391500
H	-1.41061700	2.49970500	1.81045300
H	0.24360300	2.08095400	1.31839400
H	-2.42030900	4.74623100	1.06618300
H	-1.48367600	5.81819100	0.02164600
H	-3.21450500	4.46548900	-1.25089600
H	-1.56459800	4.13309000	-1.81138000
H	-3.19699900	2.44877400	0.15174600
H	-2.80354100	2.01093300	-1.52404500
H	0.39365800	4.17046700	-0.00692000
N	-1.17069000	1.91746800	-0.21965500
H	4.38579200	-1.76288300	-0.51311700
C	-2.74853700	-1.96907700	-0.36057900
C	-3.44784600	-3.12049600	0.34626000
C	-3.87055500	-2.71445100	1.75312000
C	-2.67458500	-2.17569300	2.52929600
C	-2.00028300	-1.04978300	1.75951600
H	-4.31335800	-3.44915300	-0.24690900
H	-3.45057400	-1.12922900	-0.50458400
H	-2.37716300	-2.26148700	-1.35121300
H	-4.64101300	-1.92747700	1.68610700
H	-4.32972400	-3.56110100	2.28243100
H	-2.97746400	-1.81680000	3.52338400
H	-1.94356100	-2.98596600	2.69104300
H	-2.68986000	-0.19445200	1.65588600
H	-1.10814400	-0.68154900	2.28546200
H	-2.75547000	-3.97763200	0.40245100
N	-1.60272700	-1.43703500	0.39694200
H	-0.89331500	-2.17331400	0.45774400
C	3.98398200	0.49793500	1.91660200
C	4.79097200	-0.53123900	1.10017700
H	4.49917000	1.46585800	1.92240600
H	3.87844000	0.16397600	2.95578700
H	5.65770400	-0.09650200	0.59250800
H	5.11701100	-1.39324800	1.69013400
C	2.76037200	1.11918500	-0.03989800
H	1.74636800	1.28816000	-0.43398900
H	3.30377400	2.07180200	-0.06014100
C	3.47746100	0.06002000	-0.89701800
H	2.81025800	-0.38274600	-1.64743600

H	4.39305400	0.42512900	-1.37217600
C	2.66543400	-1.69179900	0.63883200
H	2.06876300	-2.09040100	-0.19230200
H	3.02457200	-2.50769500	1.27424800
C	1.91866300	-0.58801300	1.40797200
H	0.92447400	-0.42779600	0.95567400
H	1.78337900	-0.87082000	2.45925000
N	3.88138700	-1.05314700	0.02816700
N	2.64794900	0.67953500	1.35190100

4c

Gibbs free energy before correction = -923.51300300

Gibbs free energy after correction = -923.49921256

Ni	-0.11905700	-0.65741000	-0.03077400
C	-2.48625300	-2.08904400	0.96886300
C	-3.74040800	-1.27584500	1.29337900
C	-4.62919000	-1.16800500	0.05916600
C	-3.82934900	-0.66702500	-1.13832300
C	-2.57382400	-1.52090200	-1.32785400
H	-4.29264600	-1.73100500	2.13114100
H	-2.82183300	-3.13512100	0.76003200
H	-1.83675900	-2.14523500	1.85675400
H	-5.02864700	-2.17038500	-0.17715700
H	-5.50050200	-0.52428900	0.25215200
H	-4.44765600	-0.67460400	-2.05019800
H	-3.51995600	0.37904000	-0.96418300
H	-2.91564400	-2.54755900	-1.61031500
H	-1.99096300	-1.14301600	-2.18368500
H	-3.43188200	-0.26684500	1.61867000
N	-1.73735300	-1.55917000	-0.14873400
C	2.61254700	-0.85710200	1.21874500
C	4.04192500	-1.37751100	1.24021200
C	4.81516100	-0.87858400	0.02510900
C	4.07582400	-1.23936500	-1.25792900
C	2.64642700	-0.72073000	-1.21704700
H	4.53292600	-1.07106600	2.17463200
H	2.61330300	0.24023800	1.31659700
H	2.02495800	-1.25753100	2.05576500
H	4.91831300	0.21819500	0.08684700
H	5.83356500	-1.29116300	0.01618900
H	4.59144500	-0.83333300	-2.13960900
H	4.05517000	-2.33578300	-1.37642800
H	2.64911900	0.38071600	-1.19048400
H	2.08152100	-1.02321100	-2.10912000

H	4.02104700	-2.48030200	1.23680300
N	1.90271600	-1.19070500	-0.03180900
H	1.86745600	-2.21127600	-0.08985800
C	-0.31814400	1.99257700	1.26169200
C	-0.11131000	3.49759400	1.33893600
C	-0.61178900	4.17423400	0.06812100
C	0.03975500	3.54663500	-1.15850600
C	-0.17083600	2.04007000	-1.16660500
H	-0.62257800	3.89597300	2.22672400
H	-1.39457800	1.75821800	1.21092500
H	0.08460000	1.48282200	2.14805100
H	-1.70574400	4.05011100	-0.00041800
H	-0.41771500	5.25532600	0.10067400
H	-0.36101000	3.98123500	-2.08520500
H	1.12281700	3.75659100	-1.14957900
H	-1.24444700	1.80553500	-1.25734600
H	0.33804700	1.56605100	-2.01748400
H	0.96409600	3.70562300	1.46982700
N	0.30505300	1.38833000	0.06903600
H	1.31164800	1.56237400	0.13374900

5c

Gibbs free energy before correction = -3811.82241200

Gibbs free energy after correction = -3811.80862197

Ni	0.42114200	0.01385300	0.51078500
C	2.10030700	1.92180700	1.90308400
C	3.29366500	2.74109400	1.41070600
C	2.81565200	4.03153800	0.75599800
C	1.77912300	3.73160000	-0.32010300
C	0.65027100	2.88162400	0.26132600
H	3.97629100	2.95346300	2.24704100
H	1.61601800	2.48840200	2.73050000
H	2.44309900	0.96555500	2.32959100
H	2.35562200	4.67514800	1.52598200
H	3.66202400	4.59655100	0.33941700
H	1.37536000	4.66050700	-0.74968400
H	2.25419700	3.17127000	-1.14403400
H	0.11891100	3.49230700	1.02675500
H	-0.08973600	2.63829400	-0.51850500
H	3.85898200	2.14236700	0.67681000
N	1.14548500	1.65670200	0.84852700
C	2.86727300	-1.00944400	-0.72807200
C	3.62266300	-1.76144900	-1.81136600
C	3.25881300	-1.22221000	-3.18989300

C	1.74830900	-1.25198800	-3.39227300
C	1.03811400	-0.52083800	-2.26424300
H	4.70324100	-1.68254600	-1.62782600
H	3.15342600	0.05413400	-0.72856600
H	3.08301100	-1.40609800	0.27384900
H	3.61433400	-0.18175800	-3.27581400
H	3.76625700	-1.79606300	-3.97735800
H	1.46858300	-0.80229600	-4.35511000
H	1.39766900	-2.29754700	-3.41320500
H	1.30873500	0.54761800	-2.26476600
H	-0.05412700	-0.58573000	-2.36376400
H	3.36518700	-2.83220900	-1.75088000
N	1.40359300	-1.05292100	-0.93423000
H	1.12105500	-2.03740700	-0.91203800
C	-1.28823100	-0.21235200	1.55009200
C	-0.92672000	-1.42582000	0.87878700
C	-1.65504400	-1.86759300	-0.26398800
C	-2.61822000	-1.06235100	-0.80512200
C	-2.94505200	0.17672600	-0.18401600
C	-2.32605800	0.57453100	0.97197100
H	-1.00638200	-0.03741000	2.58794700
H	-1.41843600	-2.82897300	-0.71886500
H	-3.14994900	-1.37129500	-1.70428500
H	-2.62999600	1.48998300	1.47656100
Br	0.09652500	-2.72958900	1.86817000
C	-4.00248600	1.00630200	-0.82263700
F	-3.66511800	1.35097100	-2.08016500
F	-4.25355600	2.14137900	-0.16190200
F	-5.16816200	0.34297800	-0.92451900

TS1c

Gibbs free energy before correction = -3811.78419600

Gibbs free energy after correction = -3811.77040597

Ni	-0.83292900	-0.16464000	0.02677400
C	0.22928100	2.20458000	1.23699600
C	1.53724300	2.99395800	1.29790900
C	1.67699500	3.86630300	0.05609600
C	1.52292900	3.02418800	-1.20482800
C	0.21630600	2.23222200	-1.14799400
H	1.57944000	3.60199400	2.21422800
H	-0.61506000	2.93883400	1.32011700
H	0.15264400	1.53816900	2.11328300
H	0.88718000	4.63858200	0.07028700
H	2.63747500	4.40110600	0.05700300

H	1.55305500	3.65485400	-2.10624200
H	2.35818300	2.30803900	-1.27363600
H	-0.62996000	2.96700800	-1.20530800
H	0.13162100	1.58582500	-2.03854600
H	2.37234000	2.27515000	1.33863000
N	0.13806800	1.41803400	0.03561300
C	-3.54685800	0.24199200	1.19505400
C	-4.91418700	0.90877200	1.20270200
C	-5.65927000	0.61862400	-0.09564900
C	-4.81609300	1.03554200	-1.29574600
C	-3.45118200	0.36530600	-1.24891500
H	-5.48901400	0.56583900	2.07399200
H	-3.65275900	-0.85425500	1.17536300
H	-2.96115800	0.49250300	2.09042700
H	-5.86867900	-0.46256600	-0.15875200
H	-6.63193000	1.12794900	-0.10791000
H	-5.31993800	0.78543000	-2.23954700
H	-4.68213000	2.13041000	-1.29011300
H	-3.55553700	-0.72685900	-1.34821200
H	-2.79889000	0.70357600	-2.06582500
H	-4.78554600	1.99816300	1.31853100
N	-2.73944100	0.60990300	0.01852400
H	-2.50744000	1.60498800	0.07614800
C	1.10428500	-1.56504500	-1.22610000
C	0.43679100	-1.65746900	0.00737000
C	1.12895400	-1.57644800	1.22695200
C	2.44201700	-1.14206000	1.20114000
C	3.07182700	-0.87440000	-0.01539300
C	2.41664600	-1.13131100	-1.22222300
H	0.56362100	-1.72435000	-2.15645500
H	0.60730000	-1.74287400	2.16686500
H	2.97729900	-0.97580500	2.13371600
H	2.93389200	-0.95694800	-2.16410900
Br	-1.39558500	-2.57535300	0.02098400
C	4.48358500	-0.39067100	-0.04015200
F	4.69919100	0.45256100	-1.06009800
F	5.36007400	-1.39727800	-0.18607600
F	4.81245500	0.25054600	1.08836000

2b-1

Gibbs free energy before correction = -6384.06335800

Gibbs free energy after correction = -6384.04956765

Ni	1.43330100	0.70085500	-0.30800700
Br	1.22092200	0.12363100	-2.65947500
C	4.02205600	-0.78121600	-0.37127000

C	5.52499800	-0.80113900	-0.15045500
C	5.85618400	-0.45791400	1.29751700
C	5.22763100	0.87535000	1.68659000
C	3.73248400	0.86781800	1.40946500
H	5.92562900	-1.78738700	-0.42396500
H	3.54375600	-1.55852700	0.24604200
H	3.73746400	-0.97427900	-1.41320200
H	5.45967600	-1.25060100	1.95464200
H	6.94343900	-0.43215600	1.45359000
H	5.40543400	1.10309000	2.74693400
H	5.69296300	1.68679100	1.10236800
H	3.22629700	0.13047100	2.05476400
H	3.27690100	1.84669000	1.61559800
H	5.99738600	-0.06591600	-0.82359000
N	3.41439900	0.50741100	0.01145700
H	3.82042700	1.22525600	-0.59586000
C	-0.94686100	2.38200300	-0.76082800
C	-2.30550200	2.90477300	-0.32467800
C	-2.22903600	3.52893400	1.06431800
C	-1.63052400	2.54236800	2.06043600
C	-0.28478100	2.03540900	1.56671900
H	-2.67826100	3.62888700	-1.06285100
H	-0.22615200	3.20847100	-0.86839100
H	-0.98526100	1.86018100	-1.72566500
H	-1.59402600	4.42997000	1.02191200
H	-3.22317100	3.85817300	1.39699100
H	-1.51497500	2.99993800	3.05283100
H	-2.31224100	1.68180200	2.18098000
H	0.43846200	2.86490400	1.50335600
H	0.14304000	1.28318400	2.24790000
H	-3.02450100	2.06636000	-0.31111800
N	-0.37193300	1.43676800	0.21775600
H	-1.02134600	0.64818900	0.27661000
C	-1.44488600	-1.54438000	-0.75692300
C	-1.01050200	-1.74571700	0.54757100
C	-1.86422900	-1.62829200	1.64012100
C	-3.18837100	-1.27898400	1.41436800
C	-3.63591700	-1.05227400	0.11306900
C	-2.77262500	-1.18658400	-0.96951500
H	-0.73704100	-1.57087700	-1.58525000
H	-1.50059500	-1.78783800	2.65287600
H	-3.87163000	-1.16777300	2.25540300
H	-3.12303200	-0.99802000	-1.98185300
Br	0.83230800	-2.07988400	0.85326300

C	-5.04893100	-0.60258400	-0.07023800
F	-5.39488300	-0.48607400	-1.35469800
F	-5.25356300	0.59592800	0.50537100
F	-5.91805600	-1.44749200	0.50360300

2b-2

Gibbs free energy before correction = -6384.05729000

Gibbs free energy after correction = -6384.04349965

Ni	-1.25896400	0.18075600	-0.55794600
Br	-1.64192100	2.14626400	-1.75958900
C	-0.55400700	-2.67901400	-0.35499100
C	0.45925100	-3.76304900	-0.02434100
C	0.78794000	-3.75544900	1.46365700
C	1.26351900	-2.37063800	1.88675900
C	0.24285400	-1.30789300	1.50883200
H	0.07132700	-4.74040500	-0.34298300
H	-1.50568400	-2.87328700	0.16309400
H	-0.76731300	-2.63836600	-1.43110200
H	-0.11591200	-4.02294500	2.03658900
H	1.54857200	-4.51305800	1.69710200
H	1.45618900	-2.32696600	2.96774700
H	2.22130800	-2.14906300	1.38420000
H	-0.69415800	-1.46759100	2.06219600
H	0.59866600	-0.29597100	1.75070800
H	1.38084300	-3.58037000	-0.60481000
N	-0.09389000	-1.33667300	0.06573700
H	0.78245400	-1.16042000	-0.43688000
C	-3.36510500	-0.75093900	1.46074900
C	-4.83055300	-0.86556500	1.85204000
C	-5.59444100	-1.70610300	0.83574000
C	-5.40048000	-1.14509000	-0.56806300
C	-3.92089900	-1.02220800	-0.89816200
H	-4.91098200	-1.29441900	2.86090300
H	-2.88833700	-1.74374200	1.49374700
H	-2.81334600	-0.09867200	2.15145100
H	-5.21769000	-2.74264000	0.86663100
H	-6.66193800	-1.75024700	1.09232300
H	-5.89482100	-1.77734100	-1.31909500
H	-5.86542100	-0.14695600	-0.63426200
H	-3.45440500	-2.01990200	-0.92481600
H	-3.76285800	-0.55868500	-1.88125200
H	-5.26837900	0.14568200	1.89861000
N	-3.18061300	-0.22292000	0.09759000
H	-3.57293400	0.72321500	0.07803600

C	2.38851400	0.51125300	-1.14668500
C	3.30858200	-0.19089300	-0.37680700
C	3.67003500	0.22609100	0.89942200
C	3.05744800	1.35276200	1.43391100
C	2.10630600	2.04397800	0.68753800
C	1.77837300	1.63604500	-0.60302300
H	2.12202500	0.17302700	-2.14736100
H	4.40227100	-0.33185900	1.47884000
H	3.31564700	1.67966100	2.43882500
H	1.00582200	2.15822300	-1.16864300
Br	4.02466500	-1.81233600	-1.05204000
C	1.33630700	3.16307900	1.31024600
F	0.99341800	4.10097900	0.42197900
F	2.02050600	3.76973300	2.28857200
F	0.19315300	2.71410900	1.86228000

2b-3

Gibbs free energy before correction = -6384.05424900

Gibbs free energy after correction = -6384.04045865

Ni	-0.36843600	-0.12113000	0.02605700
Br	0.78781300	-0.48678500	-2.11191900
C	-2.44467000	-1.89726300	-1.24782000
C	-3.17940600	-3.21301800	-1.45021700
C	-3.98374100	-3.57867500	-0.20894800
C	-3.08138900	-3.58718800	1.01868400
C	-2.34661500	-2.26211300	1.15813300
H	-3.82726200	-3.14219000	-2.33565600
H	-3.16997700	-1.07511700	-1.12419500
H	-1.80318100	-1.64826800	-2.10314600
H	-4.78487900	-2.83378300	-0.06452900
H	-4.47713100	-4.55239100	-0.33529300
H	-3.65785800	-3.78693700	1.93324200
H	-2.33873500	-4.39741300	0.92494600
H	-3.06690400	-1.44863400	1.34345200
H	-1.65538100	-2.28508600	2.01177400
H	-2.44081300	-4.00584700	-1.65782200
N	-1.58464700	-1.89904000	-0.04945800
H	-0.85621300	-2.60564900	-0.18814600
C	-0.71459500	2.72406400	-0.95017700
C	-1.47797100	3.74888900	-1.77458300
C	-2.82625000	4.06127100	-1.13515700
C	-3.61422800	2.77808600	-0.89725200
C	-2.78780700	1.78715000	-0.09311900
H	-0.87350600	4.66035200	-1.88611200

H	-0.47753100	3.13873900	0.04342900
H	0.23281300	2.43809700	-1.42574900
H	-2.65855700	4.56420700	-0.16750200
H	-3.40065500	4.75976900	-1.75924200
H	-4.55798900	2.98558700	-0.37335600
H	-3.87865100	2.31920700	-1.86497700
H	-2.57079800	2.19551400	0.90557800
H	-3.32012200	0.83664600	0.05490600
H	-1.63415800	3.34365100	-2.78876800
N	-1.49167300	1.49116900	-0.72933800
H	-1.68223300	1.08454800	-1.65064100
C	1.18641200	-0.89090600	1.47347800
C	0.82693800	0.46723100	1.61329400
C	1.71049700	1.50721100	1.25772700
C	2.90657000	1.18002200	0.66231100
C	3.25057100	-0.16932300	0.45908900
C	2.41943000	-1.18911300	0.87112800
H	0.59719900	-1.68459700	1.92901200
H	1.44015600	2.54523300	1.43927100
H	3.59088100	1.96683700	0.34766400
H	2.70426400	-2.22934500	0.73432600
Br	-0.69499700	0.87180200	2.72588000
C	4.54894800	-0.45411800	-0.21534100
F	4.76512700	-1.76057500	-0.40227200
F	5.59116600	0.02018800	0.49270700
F	4.62292200	0.13535800	-1.41893600

2b-4

Gibbs free energy before correction = -6384.05389200

Gibbs free energy after correction = -6384.04010165

Ni	-0.42259200	0.11322700	-0.03807800
Br	0.75959200	0.04633800	-2.20198700
C	-3.30332300	-0.75281800	-0.59635000
C	-4.30443200	-1.57321500	-1.39621300
C	-4.11845800	-3.06178200	-1.12885800
C	-2.67608900	-3.46921100	-1.40314000
C	-1.71687300	-2.60781900	-0.59739600
H	-5.32607000	-1.25034200	-1.15060500
H	-3.50099500	-0.86022900	0.48269000
H	-3.38294000	0.31584200	-0.84036600
H	-4.35858100	-3.27270000	-0.07262700
H	-4.81440800	-3.65585100	-1.73707600
H	-2.51101200	-4.52916600	-1.16310100
H	-2.45446500	-3.34523300	-2.47660200

H	-1.86624400	-2.78342500	0.48021300
H	-0.66845900	-2.84203500	-0.82867300
H	-4.15259000	-1.36988500	-2.46965700
N	-1.90991700	-1.16670000	-0.83052900
H	-1.68200400	-0.98255600	-1.81273000
C	-0.06613200	3.10572200	-0.46029800
C	-0.60790000	4.48952400	-0.78156900
C	-1.55307700	4.96667000	0.31495200
C	-2.65278900	3.93832800	0.55108700
C	-2.05638100	2.56713500	0.83237400
H	0.22736400	5.19178000	-0.91561200
H	0.54327200	3.14405000	0.45736000
H	0.56962100	2.70869500	-1.26229700
H	-0.98197800	5.10522200	1.24872500
H	-1.98443100	5.94473800	0.06057700
H	-3.30253700	4.23704800	1.38602100
H	-3.29328300	3.86975700	-0.34455900
H	-1.47876600	2.59369200	1.77116900
H	-2.84171200	1.80822800	0.95427900
H	-1.14794300	4.44909100	-1.74274000
N	-1.13653500	2.11803800	-0.22792600
H	-1.67147000	2.03570600	-1.09773800
C	1.14015200	0.46917300	1.48345900
C	0.54206700	-0.81193400	1.55257800
C	1.24425900	-1.97419100	1.17719300
C	2.49709400	-1.84078100	0.61944400
C	3.07513700	-0.56764800	0.47852200
C	2.42334900	0.56587400	0.92343400
H	0.69420400	1.32796000	1.98303600
H	0.79496300	-2.95617400	1.30857400
H	3.03600300	-2.72567900	0.28973500
H	2.89948600	1.54294000	0.84610000
Br	-1.05479800	-0.97241100	2.61930400
C	4.43682000	-0.40851500	-0.11162600
F	5.35559400	-0.09668000	0.82207300
F	4.47897400	0.58033300	-1.01608600
F	4.86814200	-1.51984600	-0.72047600

S8a

Gibbs free energy before correction = -7017.92847700

Gibbs free energy after correction = -7017.91468675

Ni	-2.14570500	0.01843200	0.51201300
C	0.12702500	1.53406900	1.47128900
C	-0.62532800	1.14600200	0.34957300

C	-0.14462600	1.53207700	-0.91469800
C	1.06497000	2.21816400	-1.05807000
C	1.80084400	2.55527900	0.07076300
C	1.32343000	2.22533900	1.34096100
H	-0.21512300	1.26719000	2.47204000
H	-0.70415000	1.28236700	-1.81685100
H	1.43114400	2.47640700	-2.05144700
H	1.89800100	2.49497600	2.22564500
C	3.15299900	3.16090900	-0.09694600
F	3.58366000	3.77944100	1.00942100
F	3.18727800	4.05866600	-1.09295100
F	4.07518600	2.22693100	-0.39922600
C	-3.32429100	2.12252300	-1.21912600
C	-4.52154300	3.04039700	-1.40345800
C	-4.56197100	4.10179400	-0.31035000
C	-4.52726500	3.45301000	1.06817000
C	-3.33552800	2.51961400	1.19650300
H	-4.47169000	3.49952600	-2.39991500
H	-2.38953500	2.69180300	-1.29844400
H	-3.29919500	1.32320800	-1.97141000
H	-3.68859500	4.76564700	-0.41933200
H	-5.45510900	4.73170400	-0.41719400
H	-4.47889200	4.21011200	1.86250800
H	-5.45305900	2.87591900	1.23311700
H	-2.39009900	3.07173300	1.10606200
H	-3.32723200	1.99721200	2.16269900
H	-5.44532200	2.43754900	-1.37526100
N	-3.34707300	1.49126400	0.12281400
H	-4.26276000	1.03830600	0.19016900
C	-4.44960700	-1.40795200	-0.72904900
C	-5.44476700	-2.55600500	-0.68679800
C	-6.38386700	-2.41375100	0.50438400
C	-5.58635100	-2.29932300	1.79749700
C	-4.58313200	-1.16055400	1.71354900
H	-6.00361700	-2.58728900	-1.63208900
H	-4.98600600	-0.46061900	-0.90070600
H	-3.71251800	-1.53048100	-1.53369500
H	-6.99819300	-1.50688100	0.37493100
H	-7.07891300	-3.26279100	0.55307900
H	-6.24710800	-2.13844400	2.66006300
H	-5.04138000	-3.24001000	1.98135500
H	-5.11538600	-0.19898800	1.63022300
H	-3.95068500	-1.10806200	2.61029400
H	-4.88888700	-3.50538100	-0.61119300

N	-3.69107600	-1.29161800	0.53881200
H	-3.19100200	-2.17925400	0.64856000
Br	-0.77667000	-1.67547300	1.46265700
C	3.05624600	-1.25175900	0.95377500
C	2.55292100	-1.12293300	-0.35113300
C	3.48999000	-0.98671700	-1.38497600
C	4.86276500	-0.98738500	-1.14373200
C	5.32390800	-1.11729600	0.16227000
C	4.42059500	-1.24811900	1.21731700
H	2.36413300	-1.35522800	1.79334900
H	3.14973000	-0.87160600	-2.41734400
H	5.56835200	-0.88388700	-1.96624800
H	4.79110600	-1.34704500	2.23844500
Br	-0.95090500	-1.67588600	-2.42933600
C	6.78057900	-1.13211100	0.48164300
F	7.15542900	-2.29398600	1.04715100
F	7.10849100	-0.17116200	1.36348100
F	7.55642400	-0.95533400	-0.59402300
Zn	0.55325700	-0.99854700	-0.67487400

^{T}8a

Gibbs free energy before correction = -7017.92443600

Gibbs free energy after correction = -7017.91064575

Ni	1.34357400	-0.83829200	-0.14139400
C	1.19852300	1.77658400	-1.48381200
C	0.82595900	1.20713500	-0.25322400
C	0.82334600	2.06317600	0.86709100
C	1.20042900	3.39677600	0.77547700
C	1.59837300	3.91104800	-0.45966000
C	1.60237600	3.10610800	-1.59384300
H	1.17501100	1.16183400	-2.38679200
H	0.51273100	1.67461700	1.83993000
H	1.18636500	4.04253500	1.65363500
H	1.90336800	3.51562900	-2.55615700
C	2.02911200	5.34094600	-0.51809300
F	2.25675600	5.76599700	-1.76466700
F	3.15992900	5.54238000	0.17990000
F	1.10759900	6.15720000	0.01714400
C	3.09517800	-0.18251200	2.31180600
C	4.48635200	-0.14281900	2.92281100
C	5.37136600	0.86680200	2.20211600
C	5.39691200	0.57974300	0.70549700
C	3.98324200	0.53788500	0.14945200
H	4.40761400	0.09148900	3.99345900

H	2.58327000	0.78170200	2.44419900
H	2.46783100	-0.95396900	2.77530700
H	4.97170200	1.88150000	2.36728600
H	6.38863200	0.85524300	2.61621300
H	5.97979400	1.33864100	0.16564900
H	5.88538800	-0.39221400	0.51993000
H	3.49684100	1.51689400	0.26364900
H	3.97206000	0.28640000	-0.92150000
H	4.93538300	-1.14822000	2.84835000
N	3.14546300	-0.45283100	0.86033200
H	3.62160200	-1.35285900	0.75510400
C	2.39164700	-3.68420900	0.61269800
C	2.66745700	-5.10768500	0.15562800
C	3.73146100	-5.13381900	-0.93498500
C	3.33468100	-4.21926400	-2.08774500
C	3.04453600	-2.81610900	-1.58062600
H	2.96907500	-5.71661500	1.01898700
H	3.29104700	-3.26559600	1.09402000
H	1.57672200	-3.63809400	1.34525500
H	4.69114000	-4.78933800	-0.51419800
H	3.89324800	-6.15944100	-1.29342600
H	4.12317900	-4.17798100	-2.85177800
H	2.42956100	-4.61221100	-2.58065300
H	3.96145100	-2.37138300	-1.16011300
H	2.69821400	-2.15572000	-2.38865000
H	1.73065900	-5.54208900	-0.23136600
N	2.01879400	-2.80715600	-0.51590100
H	1.15586400	-3.18778100	-0.91785200
Br	-0.34134000	-1.37258500	-2.15167500
C	-3.78602500	-0.69548300	0.81318800
C	-3.18901900	0.28084500	-0.00111300
C	-4.04923100	1.16938500	-0.66216800
C	-5.43427800	1.09848800	-0.52447100
C	-5.98955400	0.11691600	0.29004200
C	-5.16507800	-0.78677300	0.96024000
H	-3.15333600	-1.40582900	1.35095000
H	-3.64059300	1.94680700	-1.31069600
H	-6.07766500	1.80337000	-1.04838800
H	-5.60713400	-1.55582400	1.59470100
Br	-0.23196600	-1.50577700	1.67065800
C	-7.46639100	-0.02646900	0.43837100
F	-7.83565500	-0.12112600	1.72745500
F	-7.92272300	-1.14343000	-0.15837200
F	-8.14664300	0.99895700	-0.08888500

Zn	-1.16715900	0.26077600	-0.26475700

^{S}TS4a

Gibbs free energy before correction = -7017.88806200

Gibbs free energy after correction = -7017.87427175

Ni	1.06667700	-1.04239900	-0.09745800
C	1.19773000	1.74823200	-1.46506800
C	0.58233300	1.63625600	-0.20658000
C	1.09922500	2.45440400	0.81850400
C	2.18228600	3.30006700	0.61908000
C	2.78902600	3.34835100	-0.63828000
C	2.29171200	2.58466000	-1.68860800
H	0.82129000	1.15257000	-2.29910000
H	0.64664100	2.42740400	1.81366700
H	2.57322800	3.90839100	1.43507000
H	2.76394100	2.62635900	-2.66893200
C	4.06454500	4.10637700	-0.78174400
F	4.38939300	4.35003800	-2.05614100
F	5.09303500	3.41698000	-0.24410800
F	4.03462900	5.28700400	-0.14666300
C	2.57951200	-0.34757300	2.36508000
C	3.93997000	-0.34327100	3.04442400
C	4.96155800	0.46750200	2.25964800
C	5.04093700	-0.04947100	0.83082900
C	3.66274300	-0.03024700	0.19318700
H	3.81600700	0.04770000	4.06349200
H	2.15525000	0.66338200	2.32118000
H	1.86472000	-0.98604300	2.89115000
H	4.65943400	1.52899100	2.23940300
H	5.94529100	0.42429700	2.74605200
H	5.71393600	0.56681200	0.21877300
H	5.44126600	-1.07709800	0.81979500
H	3.27958400	0.99496600	0.17508800
H	3.68656400	-0.39920000	-0.83884800
H	4.29402800	-1.38300900	3.14427700
N	2.67864700	-0.83829400	0.96408300
H	3.06124900	-1.78585900	1.03633700
C	1.40272800	-3.85561400	0.16714800
C	1.56134400	-5.23647500	-0.44787700
C	2.95774700	-5.41666400	-1.02735400
C	3.26095700	-4.30671400	-2.02449800
C	3.08790100	-2.93741200	-1.38449000
H	1.34414500	-5.99309200	0.31795000
H	2.07531800	-3.73866200	1.03057800

H	0.37875700	-3.67618500	0.51862600
H	3.69841200	-5.38631900	-0.21102000
H	3.05250500	-6.40002100	-1.50666300
H	4.28404800	-4.38739000	-2.41538300
H	2.57946000	-4.38430800	-2.88746300
H	3.82491100	-2.80906100	-0.57843800
H	3.23191200	-2.13312700	-2.11654300
H	0.80849400	-5.35963200	-1.24395900
N	1.72909800	-2.78871500	-0.81368600
H	1.08326700	-2.91576400	-1.59905600
Br	-0.66349200	-1.20675300	-1.70624500
C	-4.06151100	-0.21849000	0.72567900
C	-3.32093100	0.82501400	0.14428000
C	-4.05522000	1.82933900	-0.50368200
C	-5.44760900	1.80768500	-0.57518600
C	-6.14299600	0.75549300	0.01116200
C	-5.44905000	-0.26360000	0.66570000
H	-3.53064000	-1.02276200	1.24254400
H	-3.53596500	2.66555100	-0.97790200
H	-5.98761600	2.60381100	-1.08526900
H	-6.00121100	-1.08620200	1.12306500
Br	-0.64742800	-1.16054700	1.89727500
C	-7.63045500	0.67863500	-0.03644900
F	-8.17486200	0.68349600	1.19469500
F	-8.05472500	-0.45778400	-0.61897500
F	-8.18698900	1.69237400	-0.71071700
Zn	-1.26994700	0.75924500	0.17097500

^{T}TS4a

Gibbs free energy before correction = -7017.91668000

Gibbs free energy after correction = -7017.90288975

Ni	-0.90468500	1.01521800	-0.16342900
C	-1.39832200	-1.95618000	-1.34516000
C	-0.83135200	-1.70686700	-0.08331600
C	-1.49109100	-2.27533300	1.02317200
C	-2.65638000	-3.02142900	0.88907900
C	-3.19135700	-3.23266500	-0.38270200
C	-2.56141800	-2.70670600	-1.50642500
H	-0.92345300	-1.53517000	-2.23381400
H	-1.08906600	-2.12984300	2.02910700
H	-3.15650600	-3.43412600	1.76544700
H	-2.98208900	-2.86923200	-2.49755700
C	-4.51863400	-3.90244700	-0.50022900
F	-4.76626100	-4.35655400	-1.73408700

F	-5.51811900	-3.04948100	-0.19452800
F	-4.64523100	-4.94134400	0.33797800
C	-2.99100200	0.76868900	2.05445400
C	-4.42329900	1.01861100	2.49657800
C	-5.41263800	0.27108500	1.61107000
C	-5.19699200	0.64069300	0.14870600
C	-3.75547400	0.37671600	-0.24698500
H	-4.53126500	0.72379500	3.54933100
H	-2.71737600	-0.28780900	2.18173600
H	-2.27741600	1.36644400	2.63410600
H	-5.26142000	-0.81550800	1.73130900
H	-6.44537000	0.48501100	1.91784100
H	-5.86053600	0.06236100	-0.50915800
H	-5.43227200	1.70665500	-0.00982200
H	-3.53391400	-0.69358100	-0.15645200
H	-3.54917800	0.67223600	-1.28722600
H	-4.62848200	2.10173500	2.44649500
N	-2.79617300	1.09740900	0.62463000
H	-3.02215900	2.09168600	0.53058600
C	-1.12536900	3.98029800	0.67516800
C	-0.85501200	5.43485000	0.32487700
C	-1.66628800	5.86124700	-0.89223300
C	-1.40218900	4.92139400	-2.06186700
C	-1.65633500	3.47716000	-1.66091200
H	-1.08343700	6.06498100	1.19527400
H	-2.17900600	3.85961400	0.97322200
H	-0.50170500	3.63669800	1.50860000
H	-2.73973000	5.83402500	-0.64049800
H	-1.43180600	6.89802000	-1.16891000
H	-2.03154900	5.17427000	-2.92603200
H	-0.35344200	5.01892500	-2.38878800
H	-2.71927100	3.33292000	-1.40975900
H	-1.40733900	2.78303100	-2.47416900
H	0.22075500	5.55513600	0.11516300
N	-0.86476700	3.08622200	-0.47373200
H	0.12724600	3.18532300	-0.71394700
Br	0.74037000	0.77272900	-1.98461600
C	3.90837700	-0.08328900	0.80293200
C	3.19256700	-1.14098200	0.21626600
C	3.95234800	-2.14824700	-0.39682800
C	5.34585900	-2.11415000	-0.43296600
C	6.01648900	-1.04750600	0.15572500
C	5.29638600	-0.02723200	0.77883300
H	3.35977100	0.72491400	1.29302900

H	3.45363700	-2.99568600	-0.87256500
H	5.90553000	-2.91179400	-0.91879300
H	5.82823700	0.80664400	1.23949200
Br	0.54651900	1.06476900	1.80671500
C	7.50392600	-0.95562500	0.14530900
F	8.01714000	-0.95194400	1.38976300
F	7.93073600	0.18369100	-0.42941100
F	8.08705800	-1.96530900	-0.51208400
Zn	1.14781800	-1.10998800	0.14163700

S9a

Gibbs free energy before correction = -5815.76249700

Gibbs free energy after correction = -5815.74869360

Ni	0.00005700	-0.61075200	-0.00005000
Br	-1.65062600	-2.25499400	-0.13173900
Br	1.65114400	-2.25463100	0.13177400
C	1.40503700	1.79251800	1.11404000
C	2.76121700	2.46248400	1.26970000
C	3.27486300	2.96108900	-0.07492200
C	3.31297300	1.81977100	-1.08305200
C	1.95115600	1.15327300	-1.19691700
H	2.67445800	3.28455400	1.99314300
H	0.66315600	2.52472800	0.76950500
H	1.05093500	1.37039100	2.06325700
H	2.60439100	3.75324500	-0.44826900
H	4.26987000	3.41272800	0.03547500
H	3.62416800	2.17448400	-2.07502900
H	4.05394700	1.06714600	-0.76514000
H	1.21227400	1.85796000	-1.59870300
H	1.98183000	0.28144600	-1.86270300
H	3.47327100	1.73529300	1.69389200
N	1.46776300	0.69064500	0.12769300
H	2.19106900	0.04966000	0.47233400
C	-1.40549200	1.79213300	-1.11408400
C	-2.76176800	2.46192100	-1.26968600
C	-3.27543600	2.96046200	0.07495100
C	-3.31336700	1.81912400	1.08306700
C	-1.95143600	1.15286600	1.19692100
H	-2.67513800	3.28399100	-1.99314200
H	-0.66366300	2.52445400	-0.76966200
H	-1.05141900	1.36999900	-2.06331000
H	-2.60505300	3.75269500	0.44829500
H	-4.27050300	3.41197600	-0.03541300
H	-3.62462900	2.17376300	2.07504900

H	-4.05419700	1.06636400	0.76513800
H	-1.21267500	1.85769600	1.59867800
H	-1.98195300	0.28103800	1.86270800
H	-3.47374900	1.73463100	-1.69383000
N	-1.46798200	0.69032000	-0.12767900
H	-2.19106100	0.04908000	-0.47230300

^{T}9a

Gibbs free energy before correction = -5815.77436800

Gibbs free energy after correction = -5815.76057766

Ni	-0.00010200	-0.82399000	0.00069900
Br	-0.04498600	-1.76977700	2.17450500
Br	0.04371100	-1.77431700	-2.17151900
C	1.55167000	1.38746700	1.17831600
C	2.87124000	2.10949900	1.39250600
C	3.37682800	2.71425800	0.08902100
C	3.46168400	1.64265000	-0.99024600
C	2.13062900	0.92982300	-1.15706300
H	2.73927600	2.88019900	2.16425700
H	0.77317000	2.09616600	0.85642600
H	1.20054500	0.89256700	2.09184400
H	2.68074800	3.50453400	-0.23819500
H	4.35411800	3.19320700	0.23740100
H	3.76222800	2.07280800	-1.95548100
H	4.23161100	0.90189000	-0.71738400
H	1.35579600	1.63003400	-1.50251000
H	2.18511000	0.11609000	-1.88849800
H	3.61179400	1.39103600	1.78173000
N	1.65079400	0.35421100	0.12151500
H	2.35559100	-0.32696300	0.42809200
C	-1.55069000	1.38564100	-1.18053800
C	-2.87014700	2.10732000	-1.39656700
C	-3.37567700	2.71542500	-0.09461000
C	-3.46054300	1.64668300	0.98750800
C	-2.12962900	0.93395400	1.15592100
H	-2.73806200	2.87609500	-2.17021000
H	-0.77207500	2.09492500	-0.86018400
H	-1.19959400	0.88834900	-2.09276600
H	-2.67957700	3.50655100	0.23048800
H	-4.35297000	3.19400300	-0.24418700
H	-3.76075900	2.07952000	1.95164500
H	-4.23072700	0.90539400	0.71682300
H	-1.35451800	1.63487500	1.49930900
H	-2.18410300	0.12222000	1.88958300

H	-3.61076400	1.38798800	-1.78405200
N	-1.65024000	0.35490400	-0.12115500
H	-2.35541200	-0.32659600	-0.42620900