

Substituted troponimines: When aromatization of conjugate acid leads to very strong neutral organic superbases

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Electronic Supplementary Information

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TI-2

Zero-point correction= 0.225950 (Hartree/Particle)

Thermal correction to Energy= 0.237824

Thermal correction to Enthalpy= 0.238768

Thermal correction to Gibbs Free Energy= 0.188691

Sum of electronic and zero-point Energies= -498.551061

Sum of electronic and thermal Energies= -498.539187

Sum of electronic and thermal Enthalpies= -498.538243

Sum of electronic and thermal Free Energies= -498.588320

C	0.72385300	0.41516600	1.69864100
C	0.77528200	-0.56836900	0.76435000
C	0.08151600	-0.58290700	-0.49673100
C	-0.06944500	1.61386000	1.68525100
C	-0.38898000	0.48463800	-1.17509100
C	-0.59534500	2.25256900	0.59920300
C	-0.16465100	1.88796600	-0.78854300
H	1.25027800	0.22748000	2.63192200
H	1.33842100	-1.46394100	1.01267300
H	-0.85666100	0.33549200	-2.14449300
N	0.31460600	2.68518000	-1.66354600
C	0.60009400	4.06500800	-1.32112300
H	1.43874000	4.40117500	-1.93647500
H	-0.25803400	4.70430500	-1.56505600
H	0.84109800	4.22594100	-0.26354700
H	-0.03781000	-1.55792700	-0.96427100

N	-1.46519300	3.33607800	0.69968400
C	-1.87438400	3.74934200	2.02474100
C	-2.52034600	3.44546400	-0.29840000
H	-1.00183200	4.02734300	2.62255500
H	-2.51349100	4.63008800	1.93737700
H	-2.43138900	2.96550300	2.56341400
H	-2.93125300	4.45798300	-0.27794700
H	-2.12393900	3.25968400	-1.29672900
H	-3.33791300	2.73171700	-0.11308300
H	-0.28377700	2.01748900	2.66922200

TI-3

Zero-point correction= 0.225950 (Hartree/Particle)

Thermal correction to Energy= 0.237903

Thermal correction to Enthalpy= 0.238847

Thermal correction to Gibbs Free Energy= 0.188088

Sum of electronic and zero-point Energies= -498.552715

Sum of electronic and thermal Energies= -498.540761

Sum of electronic and thermal Enthalpies= -498.539817

Sum of electronic and thermal Free Energies= -498.590576

C	-0.12658200	-0.43816400	1.37769100
C	0.23493800	-1.09824900	0.25990900
C	0.31101800	-0.60386000	-1.09584500
C	-0.58920100	0.93926600	1.50899000
C	0.33425700	0.67725600	-1.50761300
C	-0.40773300	1.92825600	0.59242600
C	0.28489100	1.90559200	-0.70138700
H	-0.08491400	-0.98978600	2.31254300

H	0.50882700	-2.14314100	0.38638200
H	0.47043800	0.87686400	-2.56710600
N	0.75481400	2.95355100	-1.28624800
C	0.74899500	4.21227100	-0.57265900
H	1.39799400	4.91868800	-1.09608200
H	-0.25731500	4.65766600	-0.54386800
H	1.09904300	4.12789100	0.46722900
H	0.42412900	-1.36719700	-1.86173100
H	-0.82906900	2.89715200	0.83354400
N	-1.18559100	1.20763100	2.75424100
C	-1.39265900	2.58746600	3.13817200
H	-2.20846700	3.08043200	2.58294700
H	-1.64632800	2.61834100	4.20142500
H	-0.47288500	3.15770800	2.98782600
C	-2.29489700	0.35405100	3.15879600
H	-3.24154700	0.66754400	2.69062000
H	-2.11307500	-0.68376800	2.88011400
H	-2.41638700	0.40088700	4.24500100

TI-4

Zero-point correction=	0.226414 (Hartree/Particle)
Thermal correction to Energy=	0.238206
Thermal correction to Enthalpy=	0.239150
Thermal correction to Gibbs Free Energy=	0.188792
Sum of electronic and zero-point Energies=	-498.551374
Sum of electronic and thermal Energies=	-498.539582
Sum of electronic and thermal Enthalpies=	-498.538638
Sum of electronic and thermal Free Energies=	-498.588997

C	0.54682100	0.02386400	1.69782900
C	1.08637000	-0.72489300	0.69571400
C	1.57148500	-0.28185100	-0.58662200
C	0.42444600	1.47574600	1.65007400
C	1.37741900	0.87773500	-1.24965500
C	0.44795100	2.32216100	0.60475800
C	0.60134500	2.04789400	-0.83625100
H	1.19392500	-1.79038300	0.86614700
H	1.78943000	0.97185400	-2.25049700
N	0.20724400	2.83913900	-1.77055000
C	-0.54539500	4.02670200	-1.42072500
H	-1.01412600	4.42581100	-2.32344600
H	-1.33600100	3.84954800	-0.67725400
H	0.11198800	4.81442400	-1.02333200
H	2.13590400	-1.03888400	-1.12723100
H	0.36151900	3.37677000	0.85466300
H	0.32261100	1.93397100	2.63121400
N	0.19011900	-0.53174800	2.94064500
C	0.57182300	-1.90148800	3.20794700
H	0.37693200	-2.11734600	4.26171000
H	0.01346300	-2.63603200	2.60281500
H	1.64022000	-2.03694300	3.02435700
C	-1.15570900	-0.23687400	3.41653600
H	-1.20831800	-0.40649800	4.49590100
H	-1.41766300	0.80372900	3.22313700
H	-1.91216500	-0.87152000	2.92757600

TI-23

Zero-point correction= 0.299560 (Hartree/Particle)

Thermal correction to Energy= 0.315433

Thermal correction to Enthalpy= 0.316377

Thermal correction to Gibbs Free Energy= 0.258048

Sum of electronic and zero-point Energies= -632.403306

Sum of electronic and thermal Energies= -632.387434

Sum of electronic and thermal Enthalpies= -632.386490

Sum of electronic and thermal Free Energies= -632.444818

C	-0.14816400	-0.06828000	1.44590900
C	-0.05019000	-0.86426400	0.34267700
C	-0.50779500	-0.55740600	-0.98225300
C	-0.82193400	1.19729900	1.59989800
C	-0.64702400	0.69352000	-1.47343400
C	-1.05223900	2.05269000	0.53896100
C	-0.20924100	1.85962600	-0.68573500
H	0.22774700	-0.50117000	2.36861000
H	0.37501800	-1.85372700	0.49040000
H	-1.01360100	0.86116200	-2.48278800
N	0.78865900	2.55457100	-1.05923500
C	1.25774800	3.64169600	-0.22287300
H	2.31709400	3.46819300	-0.00996800
H	1.20320800	4.58079800	-0.78512700
H	0.72198400	3.76928000	0.72735800
N	-1.28908500	1.54985000	2.89458200
C	-1.45798200	0.50978300	3.88703200
H	-0.51655000	0.19099600	4.36694900
H	-2.11870400	0.87984200	4.67820800
H	-1.92735700	-0.36658800	3.43484800

C	-0.74613400	2.78440500	3.43803800
H	-0.86444700	3.59189400	2.71110300
H	-1.30159700	3.05730600	4.34096000
H	0.32000900	2.69416200	3.70184500
H	-0.72299400	-1.39748100	-1.63864200
N	-1.93811400	3.13349400	0.57104100
C	-3.25499300	2.88078800	1.15132400
C	-2.03998300	3.95426000	-0.62577700
H	-3.14594900	2.37633900	2.11038400
H	-3.76458900	3.83595600	1.30285900
H	-3.86908900	2.25477600	0.48622500
H	-2.67976000	4.81109000	-0.40211300
H	-1.06917100	4.33415500	-0.93825900
H	-2.48634200	3.40591000	-1.47186900

TI-24

Zero-point correction= 0.300045 (Hartree/Particle)

Thermal correction to Energy= 0.315926

Thermal correction to Enthalpy= 0.316870

Thermal correction to Gibbs Free Energy= 0.257533

Sum of electronic and zero-point Energies= -632.408728

Sum of electronic and thermal Energies= -632.392847

Sum of electronic and thermal Enthalpies= -632.391903

Sum of electronic and thermal Free Energies= -632.451240

C	0.26732800	0.10650100	1.68105200
C	0.54493600	-0.72855800	0.63632900
C	0.18906600	-0.55044500	-0.74495800
C	-0.55072800	1.30040000	1.58867600

C	-0.12280600	0.59043300	-1.39316000
C	-0.79579800	2.08804100	0.50709200
C	-0.05734000	1.92606200	-0.78643700
H	1.04053000	-1.66670300	0.86028400
H	-0.29805600	0.56465600	-2.46465500
N	0.56370600	2.84796600	-1.41776500
C	0.71830400	4.16752500	-0.83749000
H	1.64127800	4.60352200	-1.22937900
H	-0.10618200	4.82419900	-1.14329700
H	0.75487900	4.17443900	0.25854500
H	0.22878900	-1.45721700	-1.34525400
N	-1.67314500	3.17528300	0.55593700
C	-2.34218100	3.45232900	1.80714100
C	-2.51809700	3.39725200	-0.60957400
H	-1.60820700	3.61532300	2.60137900
H	-2.92421700	4.36977700	1.69738000
H	-3.02452000	2.64427500	2.12042600
H	-2.92479500	4.41130200	-0.57063900
H	-1.93925100	3.29846900	-1.52804500
H	-3.35739200	2.68557700	-0.65212600
H	-1.00699800	1.60330000	2.52178800
N	0.73087500	-0.19292700	2.98948800
C	1.81268900	-1.14844500	3.10338100
C	-0.27686200	-0.41868300	4.01554900
H	2.59736600	-0.90822600	2.38305900
H	2.23521700	-1.07829900	4.11029000
H	1.49959500	-2.19578900	2.94531300
H	0.19713200	-0.37805800	5.00060700

H	-1.05443900	0.34449300	3.99333500
H	-0.76410300	-1.40228200	3.90606000

TI-25

Zero-point correction= 0.300175 (Hartree/Particle)

Thermal correction to Energy= 0.315901

Thermal correction to Enthalpy= 0.316845

Thermal correction to Gibbs Free Energy= 0.257865

Sum of electronic and zero-point Energies= -632.407719

Sum of electronic and thermal Energies= -632.391992

Sum of electronic and thermal Enthalpies= -632.391048

Sum of electronic and thermal Free Energies= -632.450028

C	0.43300500	0.38993500	1.85744500
C	0.57644600	-0.61423400	0.94962500
C	0.03988700	-0.57502900	-0.39874100
C	-0.30118200	1.62246600	1.73099000
C	-0.32262200	0.50149400	-1.12022400
C	-0.67962400	2.30083200	0.61434600
C	-0.17973500	1.91636200	-0.73883200
H	-0.61764200	0.34666700	-2.15464000
N	0.30685300	2.69867500	-1.62696300
C	0.56687400	4.09319600	-1.33016500
H	1.39234000	4.42497500	-1.96608500
H	-0.30489900	4.71155300	-1.57940100
H	0.81765000	4.28883800	-0.28121800
H	0.01604100	-1.52893100	-0.91871200
N	-1.47694300	3.45515800	0.65427900
C	-1.85761400	3.96489700	1.95164100

C	-2.55405700	3.52482600	-0.32303700
H	-0.96686400	4.15978700	2.55531200
H	-2.38490700	4.91192500	1.81472700
H	-2.51747200	3.28132700	2.51311800
H	-2.91922800	4.55382500	-0.38523800
H	-2.19163500	3.23348500	-1.30995000
H	-3.39918500	2.86953500	-0.05739800
H	-0.60320700	2.03446500	2.68866000
H	0.81737100	0.20850900	2.85628300
N	1.29246600	-1.80489400	1.25709800
C	0.49091900	-3.01965300	1.30099400
C	2.21684700	-1.74540200	2.36870700
H	-0.18192400	-3.07947400	0.44441500
H	1.15012500	-3.89263900	1.27283500
H	-0.12294800	-3.07724200	2.21646900
H	2.85790100	-2.63186000	2.33956100
H	2.84862700	-0.85871300	2.27988500
H	1.72267300	-1.72630300	3.35699500

TI-26

Zero-point correction=	0.299697 (Hartree/Particle)
Thermal correction to Energy=	0.315625
Thermal correction to Enthalpy=	0.316570
Thermal correction to Gibbs Free Energy=	0.257449
Sum of electronic and zero-point Energies=	-632.414135
Sum of electronic and thermal Energies=	-632.398207
Sum of electronic and thermal Enthalpies=	-632.397263
Sum of electronic and thermal Free Energies=	-632.456383

C	0.71877200	0.58208100	1.98190400
C	1.15222300	-0.32267400	1.07505600
C	0.75505100	-0.43541300	-0.32172800
C	-0.25414500	1.63083400	1.80754200
C	0.31741300	0.61626500	-1.06024400
C	-0.55516300	2.25264400	0.63436200
C	0.28788500	2.00863200	-0.58398200
H	0.09339500	0.48937000	-2.11337800
N	0.88861100	2.90607400	-1.26552000
C	0.87592100	4.28984700	-0.83033500
H	1.79855400	4.76335800	-1.17614900
H	0.04015000	4.82790700	-1.29558400
H	0.78949800	4.42118500	0.25499600
N	-1.56081400	3.20583900	0.50396400
C	-2.36465800	3.49765900	1.67056100
C	-2.30723200	3.23916900	-0.74505300
H	-1.73009700	3.84555800	2.49046300
H	-3.06563400	4.29787100	1.42470600
H	-2.93978800	2.62511000	2.02111700
H	-2.80308300	4.20861900	-0.84382700
H	-1.63568400	3.11362900	-1.59448500
H	-3.07215500	2.44866600	-0.78958200
H	-0.77974900	1.92383600	2.71032100
H	1.08980600	0.45916600	2.99753700
H	1.85528300	-1.07834400	1.41429700
N	0.97314900	-1.70819100	-0.88564100
C	0.35313400	-2.83197000	-0.19863000
C	0.88453000	-1.83134300	-2.32394700

H	0.44771000	-2.72068500	0.88173300
H	-0.71973400	-2.92333300	-0.43669800
H	0.85001300	-3.76144200	-0.49320000
H	-0.14357400	-1.72172100	-2.71072700
H	1.51744200	-1.08016300	-2.80251300
H	1.24772500	-2.82129100	-2.61407800

TI-27

Zero-point correction= 0.299411 (Hartree/Particle)

Thermal correction to Energy= 0.315541

Thermal correction to Enthalpy= 0.316486

Thermal correction to Gibbs Free Energy= 0.256827

Sum of electronic and zero-point Energies= -632.416559

Sum of electronic and thermal Energies= -632.400428

Sum of electronic and thermal Enthalpies= -632.399484

Sum of electronic and thermal Free Energies= -632.459142

C	-2.29299400	-0.21239300	0.51120200
C	-1.70161000	-0.87877300	-0.51491900
C	-0.52207800	-0.47934600	-1.23646500
C	-1.90248200	1.04792400	1.08053600
C	-0.08428900	0.79923100	-1.39602400
C	-1.21409900	2.04289700	0.45380600
C	-0.97595400	1.93341400	-1.01830400
N	-1.50415600	2.76379900	-1.82643500
C	-1.26628700	2.61158900	-3.25066200
H	-0.35861600	3.15505000	-3.53816500
H	-1.14123300	1.56797900	-3.56272900
H	-2.10766200	3.05399200	-3.78913200

N	-0.65135900	3.12921100	1.12033800
C	-0.84982700	4.48157300	0.61700600
C	-0.58740000	3.07046200	2.56422300
H	-0.97675000	4.46802300	-0.46325200
H	-1.75003800	4.94055600	1.05457400
H	0.01453000	5.10023400	0.88144500
H	0.10122700	3.84422700	2.91620800
H	-1.56323900	3.24306900	3.04813300
H	-0.20912600	2.09588700	2.88198200
H	-2.20684800	1.21289100	2.11005600
H	-3.10991300	-0.71898600	1.01983400
H	-2.08607700	-1.86876700	-0.74771300
H	0.06207200	-1.28873600	-1.66337700
N	1.11504200	1.16049000	-2.02230300
C	1.99093500	0.08338100	-2.42742500
C	1.81828200	2.30523400	-1.46209200
H	1.47966100	-0.57220400	-3.13788600
H	2.86331500	0.50718400	-2.92955700
H	2.33843000	-0.52845300	-1.57823700
H	2.57195600	2.64792000	-2.17613200
H	1.12349500	3.12710900	-1.28117300
H	2.31703200	2.06857600	-0.50955300

TI-34

Zero-point correction= 0.299769 (Hartree/Particle)

Thermal correction to Energy= 0.315650

Thermal correction to Enthalpy= 0.316594

Thermal correction to Gibbs Free Energy= 0.257547

Sum of electronic and zero-point Energies=	-632.412533
Sum of electronic and thermal Energies=	-632.396652
Sum of electronic and thermal Enthalpies=	-632.395708
Sum of electronic and thermal Free Energies=	-632.454756
C	0.30020600 0.23141900 1.65343200
C	1.49813600 -0.09794700 1.10321800
C	2.27461900 0.59888000 0.10298800
C	-0.38203500 1.52580800 1.39709500
C	1.83401900 1.44814200 -0.84254400
C	-0.31054800 2.20525400 0.22707800
C	0.44988800 1.90991100 -1.00054600
N	0.06342300 2.21533200 -2.18652400
C	-1.28527300 2.71183600 -2.36277700
H	-1.59034800 2.55090100 -3.40006200
H	-2.02583400 2.23598700 -1.70292700
H	-1.32847300 3.79559400 -2.17890000
H	1.94479000 -1.03406200 1.42026400
H	3.31890900 0.29941600 0.04517900
H	2.52259700 1.79844900 -1.60619700
N	-0.32259700 -0.59923200 2.60755000
C	0.44544800 -1.69814400 3.14930200
C	-1.69625200 -0.98606800 2.30567500
H	1.40161900 -1.33515500 3.53595300
H	-0.11418900 -2.13713200 3.97960700
H	0.64515200 -2.49933600 2.41671600
H	-2.16882700 -1.37204000 3.21373800
H	-2.26477200 -0.11997800 1.97180800
H	-1.73860500 -1.76825000 1.53123600

H	-0.84661700	3.14711900	0.17143200
N	-1.19572200	1.98996800	2.44889600
C	-0.54951400	2.16797900	3.74354200
C	-2.14269500	3.04545000	2.16373200
H	0.11049400	1.32908800	3.95484300
H	0.02902900	3.10461600	3.78179000
H	-1.31377000	2.20258300	4.52574300
H	-1.67195900	4.03159000	2.01026200
H	-2.72474100	2.79692300	1.27214200
H	-2.82956600	3.13278300	3.01035300

TI-35

Zero-point correction= 0.300177 (Hartree/Particle)

Thermal correction to Energy= 0.316057

Thermal correction to Enthalpy= 0.317002

Thermal correction to Gibbs Free Energy= 0.257492

Sum of electronic and zero-point Energies= -632.416619

Sum of electronic and thermal Energies= -632.400739

Sum of electronic and thermal Enthalpies= -632.399794

Sum of electronic and thermal Free Energies= -632.459305

C	-0.17905000	0.15811100	0.98394800
C	0.48208200	-0.54439000	0.02645800
C	0.80699000	-0.04156200	-1.30508900
C	-0.73079800	1.50310900	0.92093800
C	0.90879000	1.23112000	-1.71657700
C	-0.33992600	2.50333500	0.08397700
C	0.68064900	2.47448600	-0.96299800
N	1.29655700	3.50983200	-1.41978900

C	1.09745500	4.77701600	-0.74931300
H	1.86835500	5.47911200	-1.07682800
H	0.12403400	5.22105000	-1.00817600
H	1.13966800	4.70193500	0.34764800
H	1.01286800	-0.81459600	-2.04046000
H	1.21995200	1.40962600	-2.74245700
H	-0.84604600	3.45690000	0.17615300
N	-1.66799400	1.75225200	1.94256700
C	-2.04216700	3.12122600	2.22271800
C	-2.80138600	0.84328700	2.03873100
H	-1.14699300	3.73848700	2.32898700
H	-2.68736800	3.56743000	1.44700100
H	-2.59105000	3.14567900	3.16840200
H	-3.59621600	1.10522300	1.32177700
H	-2.49406900	-0.18243200	1.83516400
H	-3.22298500	0.88449400	3.04775700
H	-0.32754800	-0.31739200	1.94596400
N	0.84578700	-1.88649700	0.22737500
C	0.32309400	-2.57487100	1.38701800
C	2.23297300	-2.24337200	-0.04208300
H	-0.76008400	-2.44305000	1.44512800
H	0.53280500	-3.64269600	1.28164900
H	0.76996800	-2.23418400	2.33643700
H	2.30747400	-3.32044900	-0.21863600
H	2.60580200	-1.72582100	-0.92552900
H	2.89156000	-1.98353400	0.80196400

Zero-point correction= 0.300828 (Hartree/Particle)

Thermal correction to Energy= 0.316538

Thermal correction to Enthalpy= 0.317482

Thermal correction to Gibbs Free Energy= 0.258107

Sum of electronic and zero-point Energies= -632.410257

Sum of electronic and thermal Energies= -632.394547

Sum of electronic and thermal Enthalpies= -632.393603

Sum of electronic and thermal Free Energies= -632.452978

C	-0.69681000	0.11387400	1.37966200
C	0.01213900	-0.52526700	0.43356300
C	0.59352100	-0.01107600	-0.79999600
C	-1.11086900	1.50749400	1.46686600
C	0.66116900	1.29359300	-1.17242000
C	-0.72521500	2.50283500	0.63510100
C	0.18850700	2.51100400	-0.50999600
N	0.48696800	3.70030300	-0.92361800
C	1.35377200	3.86772800	-2.06881300
H	1.52905100	4.93526400	-2.22409200
H	2.33523100	3.38489800	-1.94328200
H	0.91204700	3.47221500	-2.99713400
H	1.16876000	1.48641200	-2.10838500
H	-1.09843900	3.50335100	0.82223200
N	-1.93941000	1.76286000	2.58968600
C	-2.09056800	3.14066100	3.00929200
C	-3.21803200	1.06329700	2.58391900
H	-1.10988200	3.61203400	3.10294400
H	-2.70637400	3.74684300	2.32293800
H	-2.57550900	3.15271000	3.98962500

H	-3.92849000	1.50658000	1.86638500
H	-3.08865200	0.01261100	2.31900400
H	-3.66305100	1.10862700	3.58220400
H	-1.01758400	-0.49309300	2.22186900
H	0.13157300	-1.59391700	0.58001800
N	1.06671900	-1.03143200	-1.65602800
C	1.29704200	-0.69924800	-3.04595000
C	2.12184500	-1.89143200	-1.13498700
H	0.43264200	-0.17062600	-3.45339600
H	2.19730100	-0.08113500	-3.20704500
H	1.42946200	-1.62974900	-3.60519100
H	3.11135500	-1.41310900	-1.21706300
H	1.95787500	-2.13234800	-0.08495200
H	2.14383100	-2.82841800	-1.69938400

TI-45

Zero-point correction= 0.299532 (Hartree/Particle)

Thermal correction to Energy= 0.315617

Thermal correction to Enthalpy= 0.316562

Thermal correction to Gibbs Free Energy= 0.256137

Sum of electronic and zero-point Energies= -632.402051

Sum of electronic and thermal Energies= -632.385966

Sum of electronic and thermal Enthalpies= -632.385022

Sum of electronic and thermal Free Energies= -632.445447

C	0.56127200	0.20793200	1.61828600
C	1.23684500	-0.44495500	0.61289400
C	1.69649600	0.16327800	-0.62158000
C	0.10591500	1.58727300	1.54912900

C	1.40617400	1.33158600	-1.23019100
C	0.06209100	2.50273200	0.55977900
C	0.50499700	2.41133500	-0.83465300
N	0.22364400	3.27023400	-1.75415200
C	-0.66654800	4.37042800	-1.44707200
H	-0.91418200	4.89219900	-2.37466900
H	-1.60934600	4.05187000	-0.97836700
H	-0.19835800	5.10579400	-0.77532700
H	2.35376300	-0.47967400	-1.20009700
H	1.85438800	1.50828300	-2.20433700
N	0.29510100	-0.37867600	2.87122400
C	1.21862100	-1.29577100	3.49843400
C	-1.08286900	-0.54309100	3.28589400
H	2.24299200	-1.03798000	3.22770100
H	1.10994600	-1.19121400	4.58530600
H	1.05319500	-2.35015600	3.23458100
H	-1.16643400	-0.43720000	4.37382600
H	-1.71605100	0.21487300	2.81990500
H	-1.49055500	-1.53170600	3.01487200
H	-0.33509800	3.47135200	0.84887300
N	1.49061200	-1.83542600	0.77529300
C	0.34293700	-2.69289500	0.53659100
C	2.72516700	-2.38482300	0.26060700
H	-0.54408700	-2.26501700	1.00621200
H	0.13179500	-2.83238700	-0.53765000
H	0.52313400	-3.67840500	0.98101000
H	2.71553500	-2.58134800	-0.82610500
H	3.55650400	-1.71183500	0.48421900

H	2.92085900	-3.33941900	0.76094200
H	-0.25329500	1.93900300	2.51387300

TI-234

Zero-point correction= 0.372708 (Hartree/Particle)

Thermal correction to Energy= 0.392767

Thermal correction to Enthalpy= 0.393711

Thermal correction to Gibbs Free Energy= 0.325827

Sum of electronic and zero-point Energies= -766.256281

Sum of electronic and thermal Energies= -766.236222

Sum of electronic and thermal Enthalpies= -766.235278

Sum of electronic and thermal Free Energies= -766.303162

C	0.20744800	0.26341400	1.45615500
C	1.00951700	-0.34215100	0.54546400
C	1.09642500	-0.09764500	-0.86977200
C	-0.79957400	1.31037800	1.16929500
C	0.77754700	1.03469600	-1.51955700
C	-0.70658500	2.23862500	0.16987700
C	0.34270000	2.28848100	-0.88412000
N	0.71389900	3.45339900	-1.27666200
C	1.69378300	3.55162200	-2.33969800
H	2.13385100	4.55163000	-2.32315800
H	2.50461300	2.81442700	-2.26091100
H	1.22147300	3.42067600	-3.32391700
N	-1.90588800	1.29803100	2.06490100
C	-1.78028500	2.02877100	3.31119900
C	-3.24146200	1.34687400	1.50533100
H	-0.75985000	1.94137300	3.68475200

H	-2.04365000	3.09322200	3.19916700
H	-2.45406200	1.59235600	4.05896400
H	-3.61748400	2.36777600	1.35744000
H	-3.25418100	0.83722700	0.53916700
H	-3.92108500	0.81263800	2.18256900
H	1.61213800	-1.17102900	0.90630800
H	1.49026700	-0.92247700	-1.46003300
N	-1.66147000	3.29526300	0.16425300
C	-1.24328100	4.51367600	0.84701900
C	-2.30176300	3.56592900	-1.10989000
H	-0.68886000	4.25485400	1.75101000
H	-0.60089000	5.14380500	0.21694800
H	-2.13418100	5.08222900	1.14276800
H	-1.65534000	4.10880000	-1.81536000
H	-2.61467600	2.62433400	-1.57046800
H	-3.20086900	4.16524500	-0.92827300
H	0.91155200	1.06619500	-2.59798100
N	0.27317300	-0.15271100	2.82445600
C	-0.68626100	-1.18985900	3.18548900
C	1.59934800	-0.46483900	3.32411100
H	-1.67492800	-0.90963600	2.82464700
H	-0.40582300	-2.16935800	2.75931700
H	-0.72269000	-1.28658700	4.27548600
H	1.98474000	-1.44730400	2.99735600
H	2.30787100	0.30468600	3.01081100
H	1.56252000	-0.48084000	4.41838300

TI-235

Zero-point correction= 0.372030 (Hartree/Particle)

Thermal correction to Energy= 0.392451

Thermal correction to Enthalpy= 0.393396

Thermal correction to Gibbs Free Energy= 0.323903

Sum of electronic and zero-point Energies= -766.258198

Sum of electronic and thermal Energies= -766.237777

Sum of electronic and thermal Enthalpies= -766.236832

Sum of electronic and thermal Free Energies= -766.306325

C	-0.05720600	0.33287600	1.35269100
C	0.75075400	-0.35281900	0.51601700
C	0.86595100	-0.10617400	-0.90888100
C	-0.99218100	1.41894300	1.09023100
C	0.58823600	1.03957000	-1.55164400
C	-0.87407200	2.34807900	0.09018000
C	0.18882400	2.32452500	-0.94323800
N	0.62794000	3.46112700	-1.35109500
C	1.63655700	3.49011700	-2.39111600
H	2.11477700	4.47258800	-2.39093000
H	2.41732000	2.72593300	-2.27151500
H	1.18539200	3.34963900	-3.38419900
N	-2.05427400	1.42727800	2.02978400
C	-1.75133500	1.81739900	3.39189500
C	-3.39405800	1.78238600	1.61381800
H	-0.74549600	1.49766500	3.67313200
H	-1.81084200	2.90887800	3.54037100
H	-2.46270600	1.34772300	4.08072700
H	-3.60082100	2.86036400	1.65166400
H	-3.56283700	1.44511700	0.58982400

H	-4.10071900	1.26124600	2.27224600
H	1.22021000	-0.94460000	-1.50613000
N	-1.74834500	3.46432600	0.09607700
C	-1.31640300	4.58931600	0.91148900
C	-2.30889900	3.87133000	-1.17735800
H	-0.88351300	4.22014300	1.84347000
H	-0.56497200	5.20799200	0.39998900
H	-2.18524300	5.21169500	1.16106200
H	-1.60649500	4.44306200	-1.80058500
H	-2.63037900	2.98622200	-1.73396100
H	-3.19496100	4.48810500	-0.98766500
H	0.72358200	1.06012300	-2.63090000
H	-0.10288000	-0.07595500	2.35881000
N	1.44006400	-1.48843300	1.06425700
C	0.74682400	-2.74544200	0.82795900
C	2.84577200	-1.55923200	0.70232500
H	-0.28684900	-2.66283300	1.17100100
H	0.73593600	-3.04780400	-0.23581500
H	1.23767100	-3.54232300	1.39586000
H	3.02643400	-1.83132000	-0.35318000
H	3.32238600	-0.59475700	0.89263900
H	3.33712800	-2.31235600	1.32646900

TI-236

Zero-point correction= 0.372476 (Hartree/Particle)

Thermal correction to Energy= 0.392969

Thermal correction to Enthalpy= 0.393914

Thermal correction to Gibbs Free Energy= 0.323958

Sum of electronic and zero-point Energies=	-766.265874
Sum of electronic and thermal Energies=	-766.245381
Sum of electronic and thermal Enthalpies=	-766.244436
Sum of electronic and thermal Free Energies=	-766.314392
C	-0.10034900 0.52001300 1.88370100
C	0.77174300 -0.23481400 1.19408600
C	0.98838700 -0.24506400 -0.24863700
C	-1.05153700 1.52286400 1.41265800
C	0.74057800 0.82564300 -1.04107200
C	-0.86069500 2.30821600 0.31384400
C	0.29304900 2.16227200 -0.61649000
N	0.74123200 3.25213700 -1.13146800
C	1.83427300 3.17203100 -2.07724900
H	2.29763700 4.15760000 -2.16956500
H	2.60875600 2.44608900 -1.79070800
H	1.47301500 2.88922200 -3.07718500
N	-2.19253100 1.60312700 2.25605100
C	-2.02658000 2.26504300 3.53467300
C	-3.49847100 1.81838000 1.66816000
H	-1.04159500 2.05215500 3.95760200
H	-2.13083500 3.36078000 3.46029600
H	-2.78319600 1.90395400 4.24046800
H	-3.73521000 2.87604400 1.49070500
H	-3.55867100 1.29809800 0.71037700
H	-4.25020400 1.39188500 2.34430800
N	-1.75901500 3.38145800 0.08127200
C	-1.40955000 4.63697100 0.72948800
C	-2.21803600 3.56452300 -1.28256700

H	-1.04847000	4.44006300	1.74087000
H	-0.62690600	5.18172800	0.18216500
H	-2.30489500	5.26726500	0.80216300
H	-1.47713500	4.05745500	-1.92790400
H	-2.46844400	2.59276000	-1.71756500
H	-3.13113000	4.17082300	-1.26632100
H	0.94341900	0.74146300	-2.10369800
H	-0.17831700	0.30925100	2.94791700
H	1.36437200	-0.95112500	1.75627000
N	1.57562400	-1.42168700	-0.73828900
C	2.07125700	-1.42067200	-2.09696100
C	0.94106700	-2.68272400	-0.38048500
H	2.73074800	-0.56321900	-2.25358500
H	2.65008800	-2.33406200	-2.25836700
H	1.27002100	-1.39070800	-2.85456300
H	1.67212600	-3.49409600	-0.44813000
H	0.55887500	-2.64875500	0.63958200
H	0.09688200	-2.92002300	-1.04756100

TI-237

Zero-point correction= 0.373643 (Hartree/Particle)

Thermal correction to Energy= 0.393524

Thermal correction to Enthalpy= 0.394468

Thermal correction to Gibbs Free Energy= 0.327126

Sum of electronic and zero-point Energies= -766.264207

Sum of electronic and thermal Energies= -766.244326

Sum of electronic and thermal Enthalpies= -766.243382

Sum of electronic and thermal Free Energies= -766.310724

C	0.30701800	0.71439000	1.90088900
C	1.26167400	0.09467300	1.17372300
C	1.35990400	-0.00727000	-0.25921700
C	-0.83836500	1.48139700	1.43420800
C	0.81626000	0.84960700	-1.16268000
C	-0.87616500	2.16752800	0.24905200
C	0.25000400	2.16647100	-0.71669700
N	0.63237800	3.30651400	-1.15894200
C	1.75460300	3.41234000	-2.06875000
H	2.20163700	4.40208800	-1.94236600
H	2.52622000	2.64877200	-1.91124500
H	1.42416200	3.33264200	-3.11214900
N	-1.91632400	1.47727700	2.35194900
C	-1.75239400	2.15296800	3.62189500
C	-3.28199900	1.46046500	1.87757700
H	-0.71125100	2.11967100	3.94913800
H	-2.05474300	3.21327300	3.57704900
H	-2.36596500	1.66485100	4.38819500
H	-3.70713100	2.45899300	1.70408800
H	-3.33840100	0.90681800	0.93917100
H	-3.89564100	0.94193300	2.62566000
H	0.32086400	0.52961400	2.97141600
H	1.97504000	-0.50778300	1.73113700
H	1.89453700	-0.88008700	-0.61816500
N	0.88680400	0.64623800	-2.54147000
C	1.52327400	-0.56546500	-3.00810500
C	-0.25687700	1.05424600	-3.34057900
H	2.55034600	-0.62089400	-2.63647700

H	0.99134200	-1.47918900	-2.69562600
H	1.56277400	-0.54539100	-4.09922700
H	-1.11551600	0.37424100	-3.22121000
H	-0.57454100	2.06002900	-3.06617900
H	0.02850500	1.06712300	-4.39577900
N	-1.93537000	3.08543200	0.02122900
C	-1.77369000	4.38616800	0.65637800
C	-2.43892500	3.19281600	-1.32982200
H	-1.35783100	4.25560500	1.65661500
H	-1.10086800	5.04254700	0.08545700
H	-2.75429100	4.86948800	0.75187000
H	-1.77217900	3.76113600	-1.99924200
H	-2.59335800	2.19374900	-1.74777800
H	-3.40960100	3.70045300	-1.30614300

TI-245

Zero-point correction= 0.373092 (Hartree/Particle)

Thermal correction to Energy= 0.393138

Thermal correction to Enthalpy= 0.394082

Thermal correction to Gibbs Free Energy= 0.325733

Sum of electronic and zero-point Energies= -766.264301

Sum of electronic and thermal Energies= -766.244255

Sum of electronic and thermal Enthalpies= -766.243310

Sum of electronic and thermal Free Energies= -766.311660

C	0.22868700	0.03468400	1.56415100
C	0.39248300	-0.76915200	0.46681900
C	-0.12650500	-0.47386200	-0.85842200
C	-0.51326100	1.29186800	1.55429000

C	-0.34320900	0.72247000	-1.43623600
C	-0.70395500	2.18627100	0.55159700
C	-0.06302200	2.01318700	-0.78895800
N	0.62734100	2.88035200	-1.42388200
C	0.96579600	4.14380100	-0.79705500
H	1.90757800	4.49609100	-1.22632100
H	0.20260000	4.89953900	-1.02143100
H	1.06560600	4.09008900	0.29381800
N	0.62285400	-0.31490000	2.87028000
C	0.71864400	-1.68631300	3.31949400
C	1.56222900	0.57527200	3.52396900
H	-0.08875100	-2.27641600	2.88426000
H	1.66969100	-2.17378600	3.07038100
H	0.59261800	-1.69077100	4.40996400
H	2.60957000	0.33462400	3.27489000
H	1.37478800	1.60901100	3.22613900
H	1.44870000	0.50307300	4.61157500
H	-0.24909000	-1.34341300	-1.50240800
H	-0.96733600	1.49715800	2.51697400
H	-0.62921900	0.76607800	-2.48355500
N	1.17157100	-1.97214700	0.58096700
C	0.47593400	-3.20175500	0.25461500
C	2.45877400	-1.87117000	-0.08589500
H	-0.49373800	-3.22210800	0.75886100
H	0.30129300	-3.35164800	-0.82635800
H	1.06422200	-4.05544600	0.60924500
H	2.38044000	-1.83972200	-1.18750800
H	2.96781700	-0.96243900	0.24344500

H	3.07767500	-2.73352100	0.18712400
N	-1.46516700	3.34683900	0.70912800
C	-2.33306900	3.73834000	-0.39204900
C	-2.04087000	3.60691600	2.00980600
H	-1.82302500	3.60945200	-1.34701100
H	-3.26337400	3.14947500	-0.41475300
H	-2.59413400	4.79490500	-0.28525300
H	-2.80299700	2.86523200	2.30039900
H	-1.25914300	3.61607400	2.77402400
H	-2.51062000	4.59295500	1.99417800

TI-246

Zero-point correction= 0.373942 (Hartree/Particle)

Thermal correction to Energy= 0.393945

Thermal correction to Enthalpy= 0.394890

Thermal correction to Gibbs Free Energy= 0.326845

Sum of electronic and zero-point Energies= -766.278774

Sum of electronic and thermal Energies= -766.258770

Sum of electronic and thermal Enthalpies= -766.257826

Sum of electronic and thermal Free Energies= -766.325871

C	0.59390100	0.15373800	1.48374400
C	0.93114300	-0.49031600	0.33391800
C	0.44189300	-0.22833300	-1.01454800
C	-0.37880200	1.23464200	1.57390300
C	0.08572100	1.00160600	-1.46433500
C	-0.63029500	2.16697800	0.62270100
C	0.18455600	2.21557700	-0.63939300
N	0.83783000	3.22520100	-1.06756800

C	0.91861500	4.43108400	-0.26561600
H	1.89129100	4.89689900	-0.44632000
H	0.15266400	5.14843100	-0.58652300
H	0.79244700	4.27032700	0.81195600
N	1.05629200	-0.29027700	2.73752900
C	1.77837500	-1.54059100	2.80057700
C	1.62013700	0.71815400	3.62246000
H	1.20651100	-2.33094500	2.30760700
H	2.77832000	-1.49139100	2.33635600
H	1.90985400	-1.81624300	3.85066000
H	2.67825900	0.92405100	3.39172700
H	1.07025000	1.65488100	3.53025100
H	1.55535200	0.37740500	4.66085300
H	-0.95210300	1.23595200	2.49432500
H	-0.18858000	1.16157700	-2.50039200
N	-1.60913200	3.14924100	0.75532800
C	-2.34924600	3.53763500	-0.43622400
C	-2.40986700	3.13797900	1.95936000
H	-1.67409600	3.64741300	-1.28496600
H	-3.12179800	2.79988000	-0.70257100
H	-2.83444300	4.50147000	-0.26033100
H	-3.02975700	2.23119200	2.05197700
H	-1.76629700	3.20634900	2.84105800
H	-3.06929800	4.00854500	1.95417900
H	1.64812900	-1.30154900	0.38364700
N	0.52161700	-1.34205700	-1.87378500
C	0.33782400	-1.11642700	-3.29018200
C	-0.13703200	-2.55779900	-1.42054800

H	-0.69764200	-0.84080300	-3.55591800
H	1.00802900	-0.32439900	-3.63255200
H	0.58883800	-2.03527600	-3.82763100
H	0.27969900	-3.42166800	-1.94792700
H	0.01843100	-2.69882100	-0.35080100
H	-1.22428500	-2.53238400	-1.60387100

TI-247

Zero-point correction= 0.373191 (Hartree/Particle)

Thermal correction to Energy= 0.393420

Thermal correction to Enthalpy= 0.394364

Thermal correction to Gibbs Free Energy= 0.325386

Sum of electronic and zero-point Energies= -766.278542

Sum of electronic and thermal Energies= -766.258313

Sum of electronic and thermal Enthalpies= -766.257369

Sum of electronic and thermal Free Energies= -766.326347

C	0.19929500	-0.09627900	1.78850400
C	0.46375500	-0.93121200	0.74396000
C	0.14165000	-0.72899900	-0.64912200
C	-0.50865700	1.16768800	1.66213000
C	0.06229300	0.45973300	-1.29735400
C	-0.48861300	1.99096700	0.58543800
C	0.43466700	1.70015000	-0.55113700
N	1.43802500	2.40415200	-0.89374500
C	1.76401900	3.59053500	-0.12282900
H	2.84173000	3.75842400	-0.18875700
H	1.26390500	4.46333000	-0.55820700
H	1.46925200	3.52612400	0.93151400

N	0.43830900	-0.46783000	3.13538700
C	0.79185500	-1.84368200	3.40078700
C	1.26166900	0.46073300	3.89562400
H	0.05866600	-2.51366100	2.94489900
H	1.79532800	-2.11924500	3.02988800
H	0.78016200	-2.00773100	4.48237000
H	2.33481600	0.35649000	3.66070700
H	0.96933300	1.48950900	3.67883200
H	1.12590800	0.28194600	4.96716200
H	-1.12043600	1.42185100	2.52142800
N	-1.22681000	3.17240200	0.47780300
C	-1.76468300	3.49692100	-0.83549700
C	-2.12567900	3.48554400	1.56634500
H	-1.01379800	3.32634300	-1.60830200
H	-2.64949200	2.89255800	-1.08709200
H	-2.04440800	4.55384500	-0.85738900
H	-2.92481300	2.73587000	1.68927000
H	-1.57127700	3.55355700	2.50663800
H	-2.58755700	4.45695000	1.37652700
H	0.91421500	-1.89330300	0.96492200
H	-0.01058500	-1.63610800	-1.22794700
N	-0.44712900	0.62229000	-2.59359100
C	0.36127200	1.34081400	-3.57048300
C	-1.13603200	-0.50999100	-3.17380300
H	0.89295800	2.16040800	-3.09057300
H	1.11024000	0.68155900	-4.03834100
H	-0.28994300	1.73608700	-4.35704100
H	-0.45524700	-1.32274200	-3.47981800

H	-1.85817000	-0.91187500	-2.45890900
H	-1.67425100	-0.17458700	-4.06553200

TI-345

Zero-point correction= 0.373150 (Hartree/Particle)

Thermal correction to Energy= 0.392994

Thermal correction to Enthalpy= 0.393938

Thermal correction to Gibbs Free Energy= 0.326092

Sum of electronic and zero-point Energies= -766.257340

Sum of electronic and thermal Energies= -766.237496

Sum of electronic and thermal Enthalpies= -766.236552

Sum of electronic and thermal Free Energies= -766.304398

C	0.18172500	0.20628100	1.31755200
C	0.86320900	-0.50168400	0.36913700
C	1.02427600	-0.18230800	-1.03960200
C	-0.67261400	1.38013500	1.02791000
C	0.79408600	0.95159800	-1.72286300
C	-0.59930700	2.21379100	-0.03776200
C	0.27659600	2.21986700	-1.21193300
N	0.54578800	3.26399200	-1.91597600
C	0.05754200	4.55312700	-1.47165600
H	0.55120300	5.33722000	-2.05097400
H	-1.02501800	4.65847100	-1.64048700
H	0.24265400	4.74799500	-0.40528500
N	-1.68745100	1.61449900	2.00908700
C	-1.23982100	2.36544500	3.17634500
C	-2.95014800	2.12940300	1.51341200
H	-0.31606900	1.93535100	3.55863700

H	-1.07597700	3.43027300	2.93410900
H	-2.00304500	2.30417400	3.95867500
H	-2.93442900	3.20861600	1.27846700
H	-3.25174600	1.58449000	0.61647000
H	-3.71089500	1.97929500	2.28640100
H	1.05354100	0.98381200	-2.77739300
H	-1.29996800	3.04322500	-0.02211200
N	0.19877800	-0.18184500	2.68482600
C	-0.82940200	-1.10596900	3.11917100
C	1.48206700	-0.40483900	3.31911900
H	-1.77262400	-0.85600400	2.63209100
H	-0.56718300	-2.15474000	2.90056100
H	-0.97264500	-1.00990600	4.20210500
H	1.86876900	-1.42319000	3.18002100
H	2.21576300	0.30071300	2.92059600
H	1.37632600	-0.21161200	4.39452200
H	1.44390800	-1.00084500	-1.62059700
N	1.44398800	-1.75230900	0.78062300
C	0.68731800	-2.90560200	0.32119200
C	2.86591700	-1.87886400	0.51017400
H	-0.36803000	-2.77546600	0.57032200
H	0.76529100	-3.07967500	-0.76757300
H	1.05533500	-3.80273300	0.83006600
H	3.11269400	-2.00071300	-0.55907400
H	3.38956500	-0.99556000	0.88370700
H	3.25246800	-2.75518000	1.04067000

TI-346

Zero-point correction= 0.373924 (Hartree/Particle)

Thermal correction to Energy= 0.393905

Thermal correction to Enthalpy= 0.394849

Thermal correction to Gibbs Free Energy= 0.326424

Sum of electronic and zero-point Energies= -766.276616

Sum of electronic and thermal Energies= -766.256634

Sum of electronic and thermal Enthalpies= -766.255690

Sum of electronic and thermal Free Energies= -766.324115

C	-0.51157500	-0.01183300	1.51678200
C	0.37459700	-0.57766500	0.66174800
C	1.13899700	0.02282100	-0.42727700
C	-0.85137500	1.43498100	1.52607600
C	0.69792100	1.05771600	-1.18462200
C	-0.89607500	2.18608600	0.40548300
C	-0.54696100	1.80932600	-0.97688400
N	-1.22939500	2.36985800	-1.91063700
C	-0.84796700	2.10976600	-3.28392500
H	-1.67712700	2.38273900	-3.94204900
H	0.01475500	2.72595600	-3.57952400
H	-0.58231700	1.06000900	-3.47596500
N	-1.23599300	1.95068100	2.78420400
C	-0.24101300	1.82099100	3.84069600
C	-1.88295000	3.24419000	2.80415000
H	0.18382600	0.81812500	3.83633100
H	0.57150200	2.55796400	3.73183000
H	-0.72201900	1.97972800	4.81068900
H	-1.20750600	4.07717100	2.54303100
H	-2.72627500	3.25338600	2.10888900

H	-2.26560500	3.42561800	3.81243200
H	1.30244200	1.39603300	-2.01916200
H	0.53079000	-1.64765700	0.73807900
N	2.29875700	-0.69680700	-0.75674500
C	2.96846600	-0.38866800	-2.00039600
C	3.22818400	-0.99622700	0.32135600
H	3.46702700	0.59523500	-1.99531900
H	3.72960000	-1.15118200	-2.18734700
H	2.25113000	-0.41021900	-2.82467700
H	2.68752200	-1.21503600	1.24246700
H	3.83086400	-1.87111800	0.05761900
H	3.91106200	-0.15506500	0.52310400
H	-1.22583600	3.21610300	0.47939700
N	-1.13415800	-0.77744400	2.51902500
C	-2.59084200	-0.72243500	2.56569700
C	-0.62873800	-2.10797200	2.77094900
H	-2.93179500	0.30292300	2.43975900
H	-3.04454800	-1.35497700	1.78657300
H	-2.93383200	-1.07682800	3.54245500
H	-0.85270000	-2.82678500	1.96399100
H	0.45446900	-2.07792000	2.91712400
H	-1.08815300	-2.48569900	3.68851800

TI-347

Zero-point correction= 0.373864 (Hartree/Particle)

Thermal correction to Energy= 0.393577

Thermal correction to Enthalpy= 0.394521

Thermal correction to Gibbs Free Energy= 0.327030

Sum of electronic and zero-point Energies=	-766.264668
Sum of electronic and thermal Energies=	-766.244955
Sum of electronic and thermal Enthalpies=	-766.244011
Sum of electronic and thermal Free Energies=	-766.311501
C	0.21761500 0.38921100 1.74559800
C	1.18509500 -0.02941900 0.88820900
C	1.27714100 0.06546700 -0.54511600
C	-0.98832200 1.12389300 1.33200300
C	0.68260200 0.97059000 -1.36496800
C	-1.07909800 1.85511200 0.19529000
C	-0.02275600 2.14941300 -0.78166600
N	0.15119500 3.37548700 -1.10227000
C	1.19573600 3.75607900 -2.03266500
H	1.52136000 4.76904700 -1.78027200
H	2.06504900 3.08794400 -2.03180900
H	0.80635800 3.78814900 -3.05838300
N	-2.11108800 1.04449400 2.21352400
C	-2.02084700 1.92347300 3.37599300
C	-3.41628500 1.13728300 1.58953600
H	-1.04369900 1.80714600 3.84278000
H	-2.17414300 2.98038600 3.09862800
H	-2.79143900 1.64054600 4.10054200
H	-3.69110500 2.16102700 1.27860300
H	-3.45902700 0.48611300 0.71357600
H	-4.16949400 0.80407400 2.31070300
H	-1.98679300 2.42876400 0.03373300
N	0.31608100 0.05838000 3.13667300
C	-0.41507600 -1.14779800 3.50260400

C	1.64941900	0.07185300	3.70494900
H	-1.42842000	-1.08742200	3.10564400
H	0.07491400	-2.05858200	3.11497000
H	-0.47052900	-1.22392100	4.59374000
H	2.26115800	-0.81006500	3.44160500
H	2.18141200	0.96948900	3.38230600
H	1.56388300	0.08987800	4.79676500
H	1.88953000	-0.71079800	-0.99225200
H	1.96440500	-0.64370300	1.33210200
N	0.76965800	0.92717600	-2.75853300
C	1.52820500	-0.15325200	-3.34803200
C	-0.44021200	1.25262700	-3.50010700
H	2.54936500	-0.15376100	-2.95729500
H	1.08196000	-1.14456100	-3.16166200
H	1.58153000	0.00239600	-4.42789200
H	-1.16783800	0.42569900	-3.48889700
H	-0.92008500	2.13546600	-3.07657800
H	-0.17977300	1.47080200	-4.53944600

TI-2345

Zero-point correction= 0.446249 (Hartree/Particle)

Thermal correction to Energy= 0.470429

Thermal correction to Enthalpy= 0.471373

Thermal correction to Gibbs Free Energy= 0.394175

Sum of electronic and zero-point Energies= -900.110505

Sum of electronic and thermal Energies= -900.086325

Sum of electronic and thermal Enthalpies= -900.085381

Sum of electronic and thermal Free Energies= -900.162579

C	0.16506800	0.01156500	1.52043300
C	0.34163000	-0.77545100	0.42422500
C	-0.21787400	-0.50186800	-0.89932900
C	-0.71872700	1.21071100	1.56933400
C	-0.34858500	0.71727800	-1.43970100
C	-0.79825900	2.13343000	0.57187000
C	0.00381600	1.94120900	-0.68574600
N	0.85375400	2.75320000	-1.17516500
C	1.21093000	3.94367100	-0.42680800
H	2.25960500	4.17568400	-0.63148700
H	0.61035000	4.79106500	-0.77780900
H	1.06487300	3.85610600	0.65716700
N	0.71722200	-0.29464900	2.78713300
C	0.79308700	-1.65053300	3.28360300
C	1.84492300	0.52931200	3.16858600
H	-0.07450200	-2.21609400	2.93739500
H	1.69714900	-2.18865300	2.97052400
H	0.76003700	-1.61775100	4.38131400
H	2.79621500	0.14819800	2.75935800
H	1.70131700	1.54747300	2.79774400
H	1.93330100	0.56990300	4.26134000
N	-1.55845000	3.30270400	0.55696100
C	-2.30997400	3.61044500	-0.64677000
C	-2.11187100	3.89714500	1.75605500
H	-1.73930900	3.35160200	-1.53997500
H	-3.27368900	3.07900200	-0.68431800
H	-2.51187400	4.68541900	-0.68235000
H	-3.02753300	3.41201900	2.11385900

H	-1.37643300	3.87016000	2.55935400
H	-2.32929900	4.94846900	1.53356500
N	-1.61752400	1.30293100	2.68264400
C	-2.53317000	0.18163100	2.76298300
C	-1.09882000	1.67821800	3.98518400
H	-2.96412600	-0.01229100	1.77762800
H	-2.05700900	-0.74576500	3.12657600
H	-3.34844500	0.43219700	3.45196900
H	-0.67131800	0.83142600	4.54173000
H	-0.31611600	2.43239200	3.87204100
H	-1.90876200	2.11839600	4.58198000
H	-0.40918800	-1.36609700	-1.53279500
H	-0.66282300	0.83795600	-2.47312700
N	1.22557000	-1.90659900	0.50658300
C	0.61166800	-3.18728800	0.21159600
C	2.46344200	-1.70441100	-0.22902100
H	-0.32283100	-3.28585800	0.77004200
H	0.39058000	-3.34642800	-0.85956000
H	1.28560800	-3.99114300	0.52722500
H	2.32953800	-1.71018300	-1.32533300
H	2.89977400	-0.74338400	0.05268900
H	3.17286200	-2.49736100	0.03249700

TI-2346

Zero-point correction= 0.448048 (Hartree/Particle)

Thermal correction to Energy= 0.471933

Thermal correction to Enthalpy= 0.472877

Thermal correction to Gibbs Free Energy= 0.396193

Sum of electronic and zero-point Energies= -900.124302
Sum of electronic and thermal Energies= -900.100417
Sum of electronic and thermal Enthalpies= -900.099472
Sum of electronic and thermal Free Energies= -900.176156

C	0.57601900	0.20564700	1.49009300
C	0.89556000	-0.47163500	0.36370500
C	0.41384000	-0.21281200	-0.99492000
C	-0.49084800	1.23663700	1.57506600
C	0.19053100	1.04667700	-1.43531600
C	-0.62073700	2.20000800	0.62443000
C	0.34365600	2.21192300	-0.53867100
N	1.12978200	3.16580600	-0.84554700
C	1.21559300	4.32032200	0.02894100
H	2.22870300	4.72678900	-0.03273800
H	0.52737300	5.09940200	-0.32091600
H	0.97569500	4.11078500	1.07944500
N	1.13026300	-0.14745900	2.74291700
C	1.78082400	-1.43357700	2.86056600
C	1.90799800	0.91561200	3.36465800
H	1.12304700	-2.21780200	2.47698400
H	2.74532600	-1.49201500	2.32667500
H	1.97447900	-1.63234800	3.91895100
H	2.92211700	0.98248700	2.93758900
H	1.41606300	1.87618900	3.20731900
H	1.99315100	0.73848200	4.44196200
N	-1.56688200	3.21742400	0.56830300
C	-2.13643400	3.54948600	-0.72725100
C	-2.43460300	3.53624000	1.68493600

H	-1.36549800	3.56770700	-1.49848900
H	-2.91787200	2.83739700	-1.03421700
H	-2.58309600	4.54637900	-0.67590900
H	-3.26697100	2.83453300	1.81320200
H	-1.86216100	3.55395400	2.61159900
H	-2.83864500	4.54050300	1.51539600
N	-1.51422200	1.02693900	2.55880400
C	-2.16722600	-0.26145800	2.41106800
C	-1.23677500	1.33546400	3.94900200
H	-2.41005800	-0.42805800	1.35860000
H	-1.54759700	-1.10454400	2.76372800
H	-3.10049100	-0.26215200	2.98646900
H	-0.62505800	0.57060600	4.45159700
H	-0.71579000	2.29367300	4.02337100
H	-2.18742100	1.42950000	4.48869900
H	-0.06269800	1.25826700	-2.46798900
H	1.63951600	-1.26018500	0.41887400
N	0.39246100	-1.33982700	-1.83218400
C	0.17259700	-1.11538600	-3.24339200
C	-0.33262800	-2.49594700	-1.32832500
H	-0.84177200	-0.74317200	-3.46890600
H	0.89927900	-0.39276000	-3.62305300
H	0.31449500	-2.05872300	-3.77745700
H	-0.00787100	-3.39581000	-1.85970400
H	-0.13516800	-2.63191700	-0.26428700
H	-1.42266300	-2.39078500	-1.45973900

TI-2347

Zero-point correction= 0.447033 (Hartree/Particle)

Thermal correction to Energy= 0.471267

Thermal correction to Enthalpy= 0.472211

Thermal correction to Gibbs Free Energy= 0.394608

Sum of electronic and zero-point Energies= -900.124371

Sum of electronic and thermal Energies= -900.100137

Sum of electronic and thermal Enthalpies= -900.099193

Sum of electronic and thermal Free Energies= -900.176796

C	0.15452800	-0.16337200	1.71264800
C	0.43064600	-0.99143900	0.66898600
C	0.16834000	-0.80785400	-0.73616700
C	-0.60009300	1.09649000	1.57901600
C	0.14817900	0.40130700	-1.36810600
C	-0.44875900	1.91219200	0.51017900
C	0.54033000	1.59496400	-0.55896900
N	1.58835300	2.24912300	-0.85638400
C	1.91652100	3.40274300	-0.04101100
H	2.99209300	3.58598400	-0.09744900
H	1.39717800	4.28439800	-0.43422600
H	1.62725200	3.28845300	1.01307100
N	0.46613600	-0.51800600	3.06109800
C	0.56424300	-1.92992500	3.36524100
C	1.61137500	0.22027500	3.57565800
H	-0.31497600	-2.45100800	2.97838500
H	1.46751500	-2.41396400	2.95208400
H	0.59395600	-2.05731800	4.45211200
H	2.56150000	-0.12797700	3.13509700
H	1.50473500	1.28287100	3.34707000

H	1.66945200	0.10701700	4.66372400
N	-1.22295400	3.07138100	0.18764200
C	-2.45278900	2.73515500	-0.51513800
C	-1.42149500	4.07381600	1.21859700
H	-2.23459600	2.04767800	-1.33773800
H	-3.19641300	2.26319300	0.14807000
H	-2.89092100	3.64601100	-0.93770500
H	-2.17453900	3.79006900	1.96591400
H	-0.47399300	4.26033500	1.73108800
H	-1.73224900	5.00940700	0.73875800
H	0.88018200	-1.95025000	0.91612800
H	0.05973700	-1.71609400	-1.31951200
N	-0.25005500	0.59710800	-2.67159700
C	0.14735500	1.79046200	-3.40374400
C	-0.60157900	-0.56640900	-3.45460200
H	-0.07985100	2.68586000	-2.82335200
H	1.21743300	1.80654900	-3.64273200
H	-0.42873400	1.83060200	-4.33097700
H	0.26555700	-1.20564500	-3.68136300
H	-1.33798900	-1.16954600	-2.91444300
H	-1.04880000	-0.24556000	-4.39721100
N	-1.61633600	1.40384500	2.54156100
C	-2.56804800	0.32384100	2.74077200
C	-1.18783500	1.98983500	3.80050500
H	-2.88119600	-0.07090200	1.77098800
H	-2.16337800	-0.50292500	3.34598100
H	-3.45324200	0.72240900	3.24904000
H	-0.78022300	1.24634300	4.50188200

H	-0.42632700	2.75134400	3.61555400
H	-2.04490400	2.48233100	4.27578400

TI-2356

Zero-point correction= 0.446044 (Hartree/Particle)

Thermal correction to Energy= 0.469491

Thermal correction to Enthalpy= 0.470435

Thermal correction to Gibbs Free Energy= 0.395191

Sum of electronic and zero-point Energies= -900.115672

Sum of electronic and thermal Energies= -900.092225

Sum of electronic and thermal Enthalpies= -900.091281

Sum of electronic and thermal Free Energies= -900.166524

C	0.30929400	0.33502100	1.71158900
C	0.76197700	-0.50058700	0.74565600
C	0.44215600	-0.34861000	-0.68450800
C	-0.62109200	1.45355800	1.67553500
C	0.11123900	0.83765900	-1.23803900
C	-0.79484600	2.29984900	0.62289200
C	0.09334700	2.15198100	-0.57499700
N	0.75791600	3.08876400	-1.13477800
C	0.81043200	4.40948300	-0.54013900
H	1.74299500	4.88676700	-0.85378400
H	-0.01781400	5.02894800	-0.90573300
H	0.76016900	4.40966900	0.55597400
N	-1.67979900	3.37405300	0.54016300
C	-2.46190400	3.50213300	-0.67476900
C	-2.28089900	3.99995400	1.69814000
H	-1.86967300	3.21669500	-1.54610600

H	-3.37148600	2.88068800	-0.65485500
H	-2.76545800	4.54608800	-0.80411100
H	-3.14445900	3.45722000	2.10310200
H	-1.54438500	4.10274600	2.49444800
H	-2.60506100	5.00417700	1.39951700
N	-1.43115300	1.59707100	2.85574200
C	-2.32935400	0.47662100	3.07511400
C	-0.70423800	1.97200000	4.05370800
H	-2.87420300	0.26461600	2.15220400
H	-1.81569400	-0.44910600	3.39011800
H	-3.05473700	0.74353500	3.85171000
H	-0.07893400	1.16385100	4.47518600
H	-0.05265300	2.82268200	3.83627900
H	-1.41711800	2.27277800	4.82928500
H	-0.02361300	0.88556400	-2.31460500
N	0.51047600	-1.52804700	-1.48927400
C	-0.39817200	-1.57085900	-2.61861300
C	1.86768800	-1.88532300	-1.89449700
H	-1.40201100	-1.27924400	-2.30172600
H	-0.09514000	-0.92254400	-3.45998300
H	-0.43524400	-2.59729700	-2.99752600
H	2.26119000	-1.18368600	-2.64981900
H	2.52022700	-1.88028100	-1.02234500
H	1.86125900	-2.89152200	-2.32596500
H	0.56317600	0.03622000	2.72593900
N	1.56990300	-1.62866000	1.10390500
C	2.48021200	-1.43466900	2.21525200
C	0.81269800	-2.86695100	1.24132900

H	3.00168400	-0.48141800	2.10552400
H	1.99046900	-1.45260700	3.20581400
H	3.22032700	-2.24164500	2.20724200
H	0.18042000	-2.86130100	2.14739200
H	0.18220600	-3.00367100	0.36270400
H	1.50764600	-3.71048400	1.31024400

TI-2357

Zero-point correction= 0.446821 (Hartree/Particle)

Thermal correction to Energy= 0.471199

Thermal correction to Enthalpy= 0.472143

Thermal correction to Gibbs Free Energy= 0.394340

Sum of electronic and zero-point Energies= -900.130243

Sum of electronic and thermal Energies= -900.105866

Sum of electronic and thermal Enthalpies= -900.104922

Sum of electronic and thermal Free Energies= -900.182725

C	-0.03161300	0.09357700	1.94005500
C	0.50660700	-0.79084200	1.04627100
C	0.42802000	-0.67404200	-0.39863500
C	-0.82129800	1.27453900	1.64128300
C	0.35115700	0.49331900	-1.09727900
C	-0.61016100	2.07660200	0.57034800
C	0.51811900	1.77776800	-0.35435000
N	1.53408500	2.50376300	-0.59451000
C	1.66392400	3.74814200	0.13919000
H	2.71349500	4.05172100	0.14483100
H	1.07925900	4.53150000	-0.35697900
H	1.30732000	3.67492400	1.17578700

N	-1.40510400	3.18875400	0.14547100
C	-2.57623000	2.76877200	-0.60860100
C	-1.70975800	4.22319200	1.11900500
H	-2.28035600	2.05004400	-1.37866100
H	-3.34202600	2.29768600	0.03064400
H	-3.02489500	3.63774600	-1.10290700
H	-2.48642800	3.92883800	1.83741400
H	-0.80367300	4.47940500	1.67441300
H	-2.03931500	5.12202100	0.58418800
N	-1.87220600	1.61848000	2.56494300
C	-2.82484200	0.53871800	2.76573800
C	-1.37857100	2.15040700	3.82481300
H	-3.17192200	0.17416300	1.79579900
H	-2.41162500	-0.31881000	3.32477500
H	-3.68824300	0.92341000	3.31872200
H	-0.87309900	1.39755500	4.45615500
H	-0.67239500	2.96072000	3.62896200
H	-2.21777600	2.55689300	4.39919000
H	0.05128800	-0.13657700	2.99686700
N	1.07593300	-2.00575400	1.47975400
C	2.39987500	-2.32556000	0.96652200
C	0.92207500	-2.38069300	2.86676200
H	2.48360100	-2.03398600	-0.08009200
H	3.19552500	-1.80629100	1.52630200
H	2.57444000	-3.40353400	1.04377800
H	1.51785100	-1.75859000	3.55739600
H	-0.12903900	-2.31391600	3.15845900
H	1.24655300	-3.41818700	2.98819500

H	0.41488200	-1.62013400	-0.92718600
N	0.07409900	0.56663700	-2.44173400
C	0.33628700	1.78211900	-3.19853000
C	-0.02901200	-0.66870200	-3.18579900
H	-0.06933000	2.64989800	-2.67639300
H	1.40582300	1.95771900	-3.36323600
H	-0.16829000	1.69961700	-4.16376400
H	0.92757200	-1.21062100	-3.23688000
H	-0.77000500	-1.32851500	-2.72286000
H	-0.35604300	-0.45216300	-4.20389500

TI-2367

Zero-point correction= 0.446154 (Hartree/Particle)

Thermal correction to Energy= 0.470873

Thermal correction to Enthalpy= 0.471817

Thermal correction to Gibbs Free Energy= 0.393345

Sum of electronic and zero-point Energies= -900.126844

Sum of electronic and thermal Energies= -900.102125

Sum of electronic and thermal Enthalpies= -900.101181

Sum of electronic and thermal Free Energies= -900.179653

C	-0.06974100	-0.07903600	2.04275400
C	0.63683300	-0.76187400	1.08368700
C	0.66318300	-0.52938300	-0.32843400
C	-0.94483000	1.04350700	1.88214900
C	0.39097800	0.71806300	-0.85709000
C	-0.80568500	1.93318900	0.83630800
C	0.47160300	1.87139500	0.08378400
N	1.44118300	2.66094700	0.31203600

C	2.68533500	2.47022800	-0.40840300
H	2.91667500	3.38156000	-0.97026800
H	3.48460900	2.33636900	0.32675800
H	2.69321800	1.61401700	-1.09548700
N	-1.76416600	2.81329600	0.37135900
C	-3.17395500	2.52620500	0.50403900
C	-1.43095200	4.20294900	0.13447300
H	-3.33666600	1.45000000	0.43947100
H	-3.60438100	2.87824200	1.45234900
H	-3.70433600	3.01485300	-0.32217700
H	-1.78191100	4.84966400	0.95416300
H	-0.34935500	4.31730200	0.05785700
H	-1.89727900	4.55537000	-0.79380500
N	-1.99542700	1.25349200	2.81860600
C	-2.49869500	0.10849200	3.54423300
C	-1.84983800	2.43406600	3.65099100
H	-2.60570400	-0.74101400	2.86604900
H	-1.85908500	-0.20411700	4.38904700
H	-3.48580800	0.34756200	3.95634000
H	-1.08259400	2.31283900	4.43556300
H	-1.57154300	3.29127500	3.03441300
H	-2.80505800	2.65830700	4.13928900
H	-0.02054200	-0.49278700	3.04690900
N	-0.03239900	0.97764100	-2.14587000
C	0.43065000	2.13791800	-2.87395000
C	-0.76574500	-0.01013900	-2.90538500
H	0.67183700	2.94741300	-2.18311000
H	1.32332500	1.93008200	-3.48478500

H	-0.35987800	2.49231500	-3.54352200
H	-0.12259300	-0.67375400	-3.49969600
H	-1.34979000	-0.63247900	-2.22683000
H	-1.44951400	0.51190600	-3.58435600
H	1.17112500	-1.64304900	1.42917700
N	0.93637200	-1.60547700	-1.21982300
C	2.15889700	-1.46346800	-1.98884700
C	0.71852300	-2.95429400	-0.74537100
H	2.18835400	-0.47956200	-2.46393900
H	3.06971400	-1.57921900	-1.37579000
H	2.18270600	-2.21980700	-2.78097900
H	1.51363700	-3.32908100	-0.07661300
H	-0.23066800	-3.00841700	-0.20762900
H	0.66756900	-3.63401700	-1.60342100

TI-2456

Zero-point correction= 0.445806 (Hartree/Particle)

Thermal correction to Energy= 0.470440

Thermal correction to Enthalpy= 0.471384

Thermal correction to Gibbs Free Energy= 0.392586

Sum of electronic and zero-point Energies= -900.126059

Sum of electronic and thermal Energies= -900.101425

Sum of electronic and thermal Enthalpies= -900.100481

Sum of electronic and thermal Free Energies= -900.179279

C	-0.00543600	0.40844600	2.03094400
C	0.50632000	-0.56237900	1.22162300
C	0.28379300	-0.58695400	-0.25419100
C	-0.91612200	1.47959900	1.62390000

C	0.23519300	0.53949500	-0.99935300
C	-0.79023600	2.22358900	0.50230500
C	0.33151300	1.90277500	-0.44083300
N	1.25388600	2.69246000	-0.82715200
C	1.32244000	4.03745400	-0.28615500
H	2.37663500	4.31083400	-0.18710200
H	0.87139600	4.74316000	-0.99472300
H	0.82274800	4.16643800	0.68119700
N	-1.60393300	3.30824000	0.16973100
C	-1.95734500	3.46677700	-1.23240000
C	-2.67734700	3.62641200	1.08413300
H	-1.07350600	3.34633200	-1.86067200
H	-2.71591300	2.73777600	-1.55904000
H	-2.35323600	4.47332600	-1.39240000
H	-3.43166000	2.82499700	1.15643800
H	-2.27358100	3.80982300	2.08398800
H	-3.17354900	4.53887400	0.74591900
N	0.27668700	-1.86372600	-0.84072900
C	-0.66891700	-2.82265800	-0.29062000
H	-0.35569200	-3.83766000	-0.55476600
H	-0.69084100	-2.74774200	0.79500600
H	-1.68789400	-2.66270100	-0.67982400
H	-1.68285900	1.74264800	2.34570000
H	0.11985700	0.48475600	-2.07616700
N	1.27884900	-1.64048200	1.68581300
C	2.63778000	-1.73553100	1.19633700
C	1.07023300	-2.23762200	2.98357100
H	2.69128800	-1.38783100	0.16366200

H	3.33933200	-1.13797600	1.80238600
H	2.97028600	-2.77964800	1.22070100
H	1.61259400	-1.74149900	3.79899700
H	0.00638600	-2.21510700	3.23197800
H	1.38785400	-3.28782200	2.93035400
N	0.41812100	0.43913300	3.40678500
C	1.39811600	1.48755500	3.63895300
C	-0.64457800	0.45509800	4.39170900
H	2.20400500	1.39821600	2.90672500
H	0.97178600	2.50382900	3.55734700
H	1.82477400	1.37112100	4.64148200
H	-1.17832700	1.42034500	4.46668600
H	-1.37649400	-0.32308600	4.15796500
H	-0.22173200	0.24061400	5.37913700
C	0.36796700	-1.94141100	-2.27988700
H	0.51493300	-2.98715100	-2.56436100
H	-0.53549300	-1.57396500	-2.79821000
H	1.22688700	-1.36454000	-2.63310200

TI-2457

Zero-point correction= 0.446912 (Hartree/Particle)

Thermal correction to Energy= 0.471367

Thermal correction to Enthalpy= 0.472311

Thermal correction to Gibbs Free Energy= 0.393959

Sum of electronic and zero-point Energies= -900.129387

Sum of electronic and thermal Energies= -900.104932

Sum of electronic and thermal Enthalpies= -900.103987

Sum of electronic and thermal Free Energies= -900.182340

C	-0.01092400	0.39009800	1.99550700
C	0.30431100	-0.63064700	1.14117800
C	-0.01661000	-0.63887800	-0.28207900
C	-0.81260500	1.55640100	1.63677000
C	-0.08299900	0.42881900	-1.11301900
C	-0.77163300	2.22052900	0.45867600
C	0.22513000	1.78484300	-0.56298900
N	1.24702800	2.43816300	-0.94649800
C	1.51285900	3.73803000	-0.35653200
H	2.59528300	3.88615000	-0.32492100
H	1.08994200	4.52199500	-0.99486800
H	1.09769600	3.86182900	0.65043300
N	-1.52198200	3.35963900	0.13782200
C	-2.04676700	3.42159800	-1.21830800
C	-2.45530600	3.82137600	1.14061200
H	-1.26689400	3.17046500	-1.93951700
H	-2.88809900	2.72932900	-1.37776600
H	-2.38672000	4.44007400	-1.42496600
H	-3.24759000	3.08569500	1.35987500
H	-1.92632200	4.04350400	2.07188100
H	-2.92541500	4.74303400	0.78999600
H	-1.45358800	1.94125100	2.42499900
N	0.91829200	-1.84110300	1.53782700
C	2.25211100	-2.07474100	1.02149700
C	0.69826000	-2.41627500	2.84575000
H	2.33234200	-1.68670700	0.00376100
H	3.03025200	-1.58769600	1.63474400
H	2.46272600	-3.15050700	1.00082500

H	1.35946000	-2.01822300	3.62668400
H	-0.33424400	-2.24220200	3.15418400
H	0.85336400	-3.50077000	2.77024000
N	0.47779200	0.34606900	3.34921600
C	1.54171000	1.31113200	3.56804400
C	-0.53645600	0.41262000	4.38281900
H	2.30992000	1.18403800	2.80137900
H	1.19243400	2.35978100	3.53162100
H	1.99799000	1.13741400	4.54920100
H	-1.00187300	1.40927700	4.49846100
H	-1.32852000	-0.30993900	4.16884300
H	-0.08699600	0.15217500	5.34735100
H	-0.16876400	-1.63355000	-0.68765200
N	-0.56504000	0.36970000	-2.42065700
C	0.17851100	1.03472300	-3.48208600
C	-1.17051400	-0.87140900	-2.85245500
H	0.67261200	1.92515700	-3.09830300
H	0.95514400	0.37583800	-3.90077500
H	-0.50882600	1.31397300	-4.28735300
H	-0.43484800	-1.67818200	-3.00716900
H	-1.90273000	-1.20627700	-2.11399400
H	-1.68424500	-0.69867500	-3.80237100

TI-3456

Zero-point correction= 0.446656 (Hartree/Particle)

Thermal correction to Energy= 0.470766

Thermal correction to Enthalpy= 0.471711

Thermal correction to Gibbs Free Energy= 0.394925

Sum of electronic and zero-point Energies= -900.114165
Sum of electronic and thermal Energies= -900.090054
Sum of electronic and thermal Enthalpies= -900.089110
Sum of electronic and thermal Free Energies= -900.165896

C	-0.07135700	0.66371400	1.56097100
C	0.18333300	-0.38433900	0.71787200
C	-0.03467900	-0.37679200	-0.74506000
C	-0.53702000	2.01184000	1.13323400
C	0.17766100	0.67629100	-1.55437600
C	-0.19906500	2.62176900	-0.02597100
C	0.52424900	2.04981200	-1.16994200
N	1.26935800	2.71324600	-1.97826100
C	1.58490000	4.08635800	-1.64358200
H	2.50769300	4.37388200	-2.15451500
H	0.79540600	4.76429900	-1.99984500
H	1.71296900	4.26504900	-0.56585700
N	0.81780700	-1.56383000	1.18522100
C	2.02908300	-1.43519600	1.96057700
C	0.08176500	-2.79222200	1.39678300
H	2.56243700	-0.53002000	1.66285200
H	1.86733200	-1.39213600	3.04882800
H	2.67476900	-2.29807300	1.75101900
H	-0.15517500	-2.96293800	2.45968700
H	-0.83992500	-2.76891200	0.81729900
H	0.67191500	-3.65104200	1.04895400
N	0.12090000	0.49966700	2.94245600
C	0.80313000	1.50203200	3.72273200
C	-0.62051000	-0.47315900	3.70508700

H	1.37994700	2.15672500	3.06699800
H	0.11379000	2.12876400	4.30845000
H	1.50479500	1.01705500	4.41577700
H	-1.25995800	0.01841000	4.45614100
H	-1.26173700	-1.05920200	3.04541500
H	0.04081000	-1.16939800	4.24202600
H	0.14629300	0.51309500	-2.62920400
H	-0.57098000	3.62676900	-0.19885000
N	-1.27778100	2.69653800	2.11265300
C	-1.41740500	4.12937900	2.00491600
C	-2.49672700	2.05289600	2.57616000
H	-0.44013200	4.58964700	1.83798600
H	-2.09836800	4.44753800	1.19643500
H	-1.82207800	4.51176800	2.94702000
H	-3.36771400	2.36463000	1.97763200
H	-2.41256000	0.97077900	2.49506600
H	-2.68819300	2.31006700	3.62392400
N	-0.34871100	-1.66021900	-1.32190700
C	-1.40586900	-1.62853400	-2.31696500
C	0.82489800	-2.37302300	-1.80828200
H	-2.26090200	-1.06869900	-1.93152700
H	-1.10425600	-1.17975300	-3.27959000
H	-1.72726400	-2.65565700	-2.52082300
H	1.24843100	-1.91061200	-2.71723200
H	1.59042700	-2.37905700	-1.03138800
H	0.55286400	-3.40794500	-2.04225100

TI-23456

Zero-point correction=	0.519818 (Hartree/Particle)
Thermal correction to Energy=	0.548217
Thermal correction to Enthalpy=	0.549162
Thermal correction to Gibbs Free Energy=	0.462245
Sum of electronic and zero-point Energies=	-1033.968154
Sum of electronic and thermal Energies=	-1033.939755
Sum of electronic and thermal Enthalpies=	-1033.938811
Sum of electronic and thermal Free Energies=	-1034.025728
C	0.04237200 0.62533700 1.67516100
C	0.36176300 -0.31704300 0.74186600
C	0.06200400 -0.17822400 -0.70073200
C	-0.66016700 1.91018800 1.40864800
C	0.19180500 0.98842400 -1.36114900
C	-0.42852200 2.68418300 0.32675600
C	0.55139500 2.26972600 -0.72100000
N	1.48031600 3.06452900 -1.08779900
C	2.33911100 2.65894700 -2.18557400
H	3.33111200 3.09288200 -2.03514700
H	2.44210700 1.57158300 -2.29816300
H	1.95002300 3.06491200 -3.12812700
N	1.06026200 -1.51918100 1.06047700
C	2.28179600 -1.41970000 1.83245300
C	0.27031500 -2.69476100 1.36988800
H	2.80274200 -0.49420700 1.57718900
H	2.11750000 -1.42704400 2.91904300
H	2.93171500 -2.26428000 1.56798300
H	0.00644500 -2.76219300 2.43859400
H	-0.64127700 -2.68819900 0.77061600

H	0.83870900	-3.59758400	1.11192700
N	0.36898500	0.34893100	3.03277500
C	1.03047900	1.41670700	3.75487900
C	-0.61640100	-0.34294500	3.83967700
H	1.75702200	1.90832300	3.10324200
H	0.33081800	2.17470300	4.14047500
H	1.57351400	0.98794400	4.60539700
H	-1.33150200	0.35053300	4.31111600
H	-1.17811300	-1.04534900	3.22176300
H	-0.11327900	-0.91252700	4.63198200
H	0.02078800	1.01246600	-2.43637800
N	-1.59261100	2.24097300	2.42835200
C	-1.71038000	3.61251100	2.88394500
C	-2.87389000	1.57815900	2.27898000
H	-0.72005600	4.07293100	2.91096300
H	-2.35663500	4.23339800	2.25072700
H	-2.11120800	3.60390600	3.90564500
H	-3.50813700	2.05739600	1.51341200
H	-2.72256500	0.53354400	1.99411200
H	-3.41465600	1.59638200	3.23228700
N	-0.31627700	-1.37818000	-1.38853900
C	-1.33772700	-1.19645800	-2.40392300
C	0.81367200	-2.13910900	-1.91093600
H	-2.15507600	-0.59080200	-2.00626200
H	-0.96777900	-0.71884700	-3.32910600
H	-1.73479600	-2.17814400	-2.68172700
H	1.27492900	-1.63957600	-2.78193400
H	1.56353600	-2.25360300	-1.12896600

H	0.46949500	-3.12994500	-2.22499500
N	-1.23884000	3.83164000	0.06481500
C	-0.52374500	5.09551400	-0.04600300
C	-2.15563700	3.62371400	-1.04456200
H	0.18702500	5.18543900	0.77788800
H	0.03817700	5.19967400	-0.98499100
H	-1.25064400	5.91279100	0.02700700
H	-1.65073300	3.58747000	-2.02712500
H	-2.69590100	2.68457800	-0.90106000
H	-2.88230000	4.44280500	-1.07023800

TI-23457

Zero-point correction= 0.520750 (Hartree/Particle)

Thermal correction to Energy= 0.549092

Thermal correction to Enthalpy= 0.550036

Thermal correction to Gibbs Free Energy= 0.464189

Sum of electronic and zero-point Energies= -1033.977363

Sum of electronic and thermal Energies= -1033.949021

Sum of electronic and thermal Enthalpies= -1033.948077

Sum of electronic and thermal Free Energies= -1034.033924

C	-0.23738800	0.28430900	2.00979900
C	0.34559700	-0.56631600	1.10901300
C	0.17792400	-0.44547300	-0.35286000
C	-1.09413100	1.41769300	1.71492300
C	0.11317700	0.75084000	-0.98262300
C	-0.94753300	2.25179100	0.64659300
C	0.25012000	2.01632900	-0.21109200
N	1.19046300	2.86926300	-0.23291900

C	2.34482000	2.58751100	-1.06311700
H	3.23107800	3.03469400	-0.60597200
H	2.52554000	1.51495700	-1.21932000
H	2.20499800	3.05415600	-2.04539500
N	1.16714500	-1.67318400	1.48248000
C	2.57574900	-1.34238800	1.56137400
C	0.74105000	-2.58706100	2.52293700
H	2.86207600	-0.73210600	0.69959500
H	2.82863200	-0.78420600	2.47941100
H	3.17471100	-2.26106700	1.54234800
H	0.97472800	-2.24111200	3.53824900
H	-0.33904300	-2.73808100	2.45421700
H	1.22624000	-3.55849600	2.35818400
N	0.00980100	0.04091800	3.41084900
C	0.71875200	1.14196500	4.04310700
C	-1.16477500	-0.35387100	4.16688800
H	1.59666900	1.39952300	3.44562600
H	0.10633300	2.05352200	4.15644800
H	1.05542400	0.82753800	5.03711000
H	-1.89583300	0.46070300	4.32127000
H	-1.67357500	-1.17566300	3.65691800
H	-0.85410600	-0.70688600	5.15627200
N	0.05316500	-1.62790000	-1.14776400
C	1.29986700	-2.26436600	-1.54284800
C	-0.91677000	-2.58999900	-0.65714300
H	2.03082500	-1.50248600	-1.82236500
H	1.72977400	-2.88155000	-0.74009400
H	1.12103000	-2.89965000	-2.41909500

H	-0.54557600	-3.18862600	0.18859800
H	-1.82632700	-2.06880900	-0.34781000
H	-1.17908400	-3.27626400	-1.47046900
N	-1.82632300	3.24159200	0.28989600
C	-2.94658200	3.50962700	1.16214100
C	-1.44414400	4.26801800	-0.66698000
H	-3.49227500	2.58182800	1.36402600
H	-2.63764900	3.94139900	2.12607500
H	-3.62799200	4.20808000	0.67345500
H	-0.75086600	5.00627100	-0.24629100
H	-0.96723700	3.80793300	-1.53435700
H	-2.34919500	4.77707100	-1.00624500
H	-1.83411800	1.65683400	2.47209100
N	-0.25792000	0.99120400	-2.34783700
C	0.60249300	0.44763700	-3.38403900
C	-1.66590200	0.71361200	-2.59835500
H	1.65025100	0.62701800	-3.13122800
H	0.45962400	-0.63118400	-3.54101400
H	0.39308000	0.96595600	-4.32715600
H	-1.89168400	-0.36411000	-2.57716200
H	-2.27659000	1.21962700	-1.84547300
H	-1.93962300	1.11072400	-3.58219500

TI-23567

Zero-point correction= 0.520945 (Hartree/Particle)

Thermal correction to Energy= 0.549196

Thermal correction to Enthalpy= 0.550140

Thermal correction to Gibbs Free Energy= 0.464329

Sum of electronic and zero-point Energies=	-1033.982193
Sum of electronic and thermal Energies=	-1033.953943
Sum of electronic and thermal Enthalpies=	-1033.952999
Sum of electronic and thermal Free Energies=	-1034.038810
C	0.08431900 0.15011800 2.01429900
C	0.66469400 -0.63976700 1.07656300
C	0.38325600 -0.57018900 -0.37490600
C	-0.83916600 1.25769500 1.82193600
C	0.23965000 0.62720000 -1.00849400
C	-0.73321800 2.09590300 0.75753500
C	0.40663800 1.87716800 -0.19243600
N	1.34934200 2.72297800 -0.30026400
C	2.40729800 2.48008700 -1.26422300
H	3.34052300 2.88092700 -0.85974800
H	2.54883300 1.42178700 -1.51594000
H	2.18739500 3.02248600 -2.19036800
N	1.50249900 -1.72491700 1.44729600
C	2.89050600 -1.55694700 1.04247900
C	1.39206600 -2.23316800 2.79658500
H	2.93553500 -1.11413400 0.04627600
H	3.44265400 -0.89479900 1.73061500
H	3.39501300 -2.52890900 1.01454800
H	1.82219900 -1.56131100 3.56083200
H	0.34088200 -2.40660000 3.04038900
H	1.92523200 -3.18706200 2.85899500
N	0.04991300 -1.79108600 -1.04990900
C	1.10600900 -2.72788300 -1.38456200
C	-1.09439500 -2.45531700 -0.45234800

H	1.97141000	-2.19046200	-1.78109200
H	1.44042900	-3.33124600	-0.52703900
H	0.74649700	-3.40752900	-2.16754100
H	-0.85984900	-2.94293000	0.50972900
H	-1.89142600	-1.72592300	-0.28624700
H	-1.46631100	-3.22292400	-1.14120800
N	-1.64331200	3.09428400	0.37507200
C	-3.05108300	2.93278500	0.66668900
C	-1.18613600	4.47327300	0.36781900
H	-3.33130100	1.88559600	0.54281700
H	-3.33215100	3.23869600	1.68461000
H	-3.62048200	3.53854100	-0.04853800
H	-1.32589400	4.96278600	1.34666300
H	-0.12571400	4.50601200	0.11503400
H	-1.75187200	5.04624400	-0.37610400
N	-0.00909200	0.85868400	-2.35650300
C	0.13670800	-0.17149200	-3.36314300
C	-0.95837300	1.89548000	-2.72136100
H	1.05336200	-0.73617800	-3.19294900
H	-0.69979700	-0.87931700	-3.39723400
H	0.22042500	0.32799500	-4.33531800
H	-1.97424200	1.48797200	-2.84170800
H	-1.00789300	2.66955800	-1.95442600
H	-0.65897300	2.35227600	-3.67098000
H	0.31993800	-0.05165300	3.05568900
N	-1.80241200	1.50323100	2.84151800
C	-2.31397800	0.34300700	3.54089100
C	-1.48229700	2.60284700	3.73440300

H	-2.52639000	-0.45454800	2.82549300
H	-1.62550900	-0.05747400	4.30656700
H	-3.24841900	0.61006900	4.04683300
H	-0.68413600	2.35046200	4.45530500
H	-1.15618900	3.46836200	3.15538100
H	-2.37532700	2.88627900	4.30331500

TI-234567

Zero-point correction= 0.593558 (Hartree/Particle)

Thermal correction to Energy= 0.626097

Thermal correction to Enthalpy= 0.627041

Thermal correction to Gibbs Free Energy= 0.532806

Sum of electronic and zero-point Energies= -1167.838613

Sum of electronic and thermal Energies= -1167.806075

Sum of electronic and thermal Enthalpies= -1167.805130

Sum of electronic and thermal Free Energies= -1167.899366

C	-0.00610600	0.08689400	1.55867800
C	0.59868900	-0.54217400	0.50247700
C	0.41806400	-0.17105500	-0.91850700
C	-0.89079500	1.25887800	1.43919000
C	0.45776600	1.13454800	-1.29590800
C	-0.58933400	2.25807600	0.55983500
C	0.70322900	2.10819600	-0.19074700
N	1.84749600	2.60467600	0.04828400
C	2.02013400	3.43483300	1.22408000
H	2.45179200	4.39621300	0.92721400
H	1.10140400	3.61527700	1.79877800
H	2.74749800	2.94628800	1.88083900

N	-2.04541900	1.35543400	2.25966600
C	-2.78950300	0.13695300	2.49900400
H	-2.35967700	-0.48005000	3.30259600
H	-3.82251000	0.38830200	2.76937000
H	-2.81622900	-0.45955600	1.58315700
C	-1.92631900	2.18644200	3.44033600
H	-1.38275100	3.10187800	3.19257900
H	-2.92540200	2.47039900	3.79431400
H	-1.40144300	1.67858400	4.26737600
N	-1.42565700	3.27287400	0.11171600
C	-0.91811900	4.62627700	0.02679800
C	-2.86506500	3.15359700	0.20502400
H	0.12580200	4.62081100	-0.29320200
H	-1.49427500	5.18604200	-0.71718300
H	-0.98344500	5.16608800	0.98496200
H	-3.30708800	3.79636300	-0.56542800
H	-3.15880600	2.12154100	0.01313100
H	-3.27352300	3.44380800	1.18235300
N	0.17339700	-0.30019000	2.91619000
C	0.19997000	-1.69656600	3.29456800
C	1.15383800	0.50187900	3.62150500
H	-0.53909600	-2.24527800	2.70562500
H	1.17770200	-2.17618500	3.15812600
H	-0.08743500	-1.77739900	4.35119200
H	2.18944800	0.23099600	3.35297600
H	1.00273300	1.55916900	3.38838900
H	1.03182800	0.36945100	4.70294000
N	1.59859600	-1.53569700	0.78823000

C	1.30173500	-2.92675900	0.49552800
C	2.90625300	-1.15164600	0.28260100
H	0.27273100	-3.15859800	0.77876900
H	1.43085900	-3.17876100	-0.56832100
H	1.96553400	-3.56953800	1.08763000
H	3.00652100	-1.29362500	-0.80765700
H	3.09180300	-0.09810900	0.50464500
H	3.67507600	-1.75784700	0.77605500
N	0.31617600	-1.25453500	-1.81434600
C	-0.87854600	-2.06834200	-1.74195400
C	0.90621700	-1.17082300	-3.13067500
H	-1.27653100	-2.04488800	-0.72490700
H	-1.67332900	-1.72418400	-2.42625700
H	-0.64871800	-3.11054900	-1.99718500
H	0.26667400	-0.67661900	-3.87795100
H	1.84389500	-0.61525800	-3.07441100
H	1.12150800	-2.18782800	-3.48123400
N	0.13558300	1.59982300	-2.58384300
C	-1.26311800	1.47792700	-2.96403300
C	0.72052600	2.86674500	-2.97696900
H	-1.63503500	0.48966100	-2.69190300
H	-1.89480700	2.23581900	-2.47192600
H	-1.35985800	1.59551800	-4.04902000
H	0.19648600	3.73702700	-2.54592100
H	1.76392400	2.90565800	-2.66052500
H	0.67917600	2.95791100	-4.06752200

Cartesian Coordination of (Me)₂N-TI Conjugated Acid and Their Thermochemical Values (ωB97X-D/6-31g(d,p))

TI-2

Zero-point correction= 0.241015 (Hartree/Particle)

Thermal correction to Energy= 0.252887

Thermal correction to Enthalpy= 0.253831

Thermal correction to Gibbs Free Energy= 0.203653

Sum of electronic and zero-point Energies= -498.962841

Sum of electronic and thermal Energies= -498.950969

Sum of electronic and thermal Enthalpies= -498.950025

Sum of electronic and thermal Free Energies= -499.000203

C	-0.19048800	0.24152700	1.59066900
C	0.41801000	-0.42892100	0.56073900
C	0.76326000	0.10363500	-0.69534500
C	-0.66703800	1.56914400	1.62746300
C	0.68170300	1.39519400	-1.15510600
C	-0.57657200	2.60338400	0.71971600
C	0.19747300	2.56850800	-0.51803700
C	1.21342000	3.99432000	-2.28399600
H	1.29824000	5.07065300	-2.42282000
H	2.21970100	3.57544200	-2.18634300
H	0.72820000	3.57099100	-3.16789900
H	1.09198000	1.55191000	-2.14657000
H	-0.39432300	-0.33611800	2.48759200
H	0.64764900	-1.47735500	0.71997700
N	0.42584200	3.75201300	-1.08727700
H	0.12981300	4.54511200	-0.52953300

H	1.19917400	-0.60238500	-1.39694300
H	-1.22210400	1.80595000	2.52876300
N	-1.15395500	3.85053600	0.99579800
C	-1.39059000	4.20964500	2.39043700
H	-1.57221900	5.28523200	2.43634000
H	-2.26511200	3.70400500	2.82392800
H	-0.50606800	3.98758900	2.99008100
C	-2.29506800	4.21770000	0.13720500
H	-3.20611100	3.69648700	0.45692700
H	-2.46242200	5.29426700	0.20911100
H	-2.10196000	3.96503500	-0.90611700

TI-3

Zero-point correction= 0.241118 (Hartree/Particle)

Thermal correction to Energy= 0.253580

Thermal correction to Enthalpy= 0.254524

Thermal correction to Gibbs Free Energy= 0.201098

Sum of electronic and zero-point Energies= -498.971363

Sum of electronic and thermal Energies= -498.958901

Sum of electronic and thermal Enthalpies= -498.957956

Sum of electronic and thermal Free Energies= -499.011383

C	-0.65539000	0.18191000	1.30931300
C	0.25706900	-0.38345900	0.48282300
C	0.99442500	0.19091800	-0.59711500
C	-1.15605500	1.54039000	1.33740100
C	1.00738100	1.47126600	-1.03633000
C	-0.68618600	2.57435600	0.50915600
C	0.26514000	2.59529500	-0.52414900

C	1.41412300	4.06669800	-2.19907600
H	1.36156100	5.13255700	-2.41606100
H	2.44593900	3.82810400	-1.92522700
H	1.14107700	3.52267900	-3.10817600
H	1.66213400	1.67910900	-1.87417500
H	-1.13491100	3.54382700	0.68324500
N	-2.12570100	1.81783600	2.24037900
C	-2.66069800	3.16986500	2.37103400
C	-2.68273800	0.78944400	3.12263300
H	-1.87706400	3.88205000	2.64963800
H	-3.13830500	3.49989000	1.44248600
H	-3.41285600	3.18077100	3.15568400
H	-3.49860900	1.22675000	3.69285600
H	-3.09344300	-0.04769000	2.55209700
H	-1.93797000	0.42014800	3.83417300
H	-1.06275400	-0.48851200	2.05354800
H	0.45911100	-1.43519800	0.66248800
N	0.49207400	3.78737500	-1.10927600
H	-0.02928000	4.57471300	-0.75682200
H	1.64193600	-0.49914500	-1.12973300

TI-4

Zero-point correction= 0.241366 (Hartree/Particle)

Thermal correction to Energy= 0.253648

Thermal correction to Enthalpy= 0.254592

Thermal correction to Gibbs Free Energy= 0.202721

Sum of electronic and zero-point Energies= -498.973389

Sum of electronic and thermal Energies= -498.961107

Sum of electronic and thermal Enthalpies= -498.960163
Sum of electronic and thermal Free Energies= -499.012034

C	-0.13106200	0.05480700	1.39949200
C	0.99987300	-0.27954400	0.62861000
C	1.62065100	0.45281300	-0.37295600
C	-0.81694900	1.32058000	1.26178500
C	1.36709800	1.69137000	-0.95074700
C	-0.61761200	2.36463500	0.42179600
C	0.34425800	2.58891800	-0.62779000
C	1.07386200	4.18481200	-2.38227600
H	0.71002700	5.14491700	-2.74479200
H	2.10786700	4.31048800	-2.04556900
H	1.04850800	3.47114800	-3.21162600
H	2.04791100	1.98491800	-1.74067900
H	1.45384900	-1.24264100	0.81645200
N	0.21709500	3.74936300	-1.29449700
H	-0.52993300	4.36886400	-1.02320400
H	2.47980300	-0.05449800	-0.80460200
H	-1.62996700	1.48369400	1.95737300
H	-1.31144300	3.18977000	0.57031800
N	-0.59749800	-0.81402600	2.32082200
C	-1.83476900	-0.57325400	3.06465200
H	-2.10464000	-1.48401800	3.59443300
H	-1.71552600	0.22554800	3.80397400
H	-2.66090500	-0.33124200	2.39144000
C	0.11974800	-2.05749700	2.59541800
H	1.16676500	-1.85777400	2.83968500
H	-0.33460800	-2.54596300	3.45423100

H	0.07200500	-2.74351600	1.74305500
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TI-23

Zero-point correction=	0.314332 (Hartree/Particle)
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Thermal correction to Energy=	0.330675
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Thermal correction to Enthalpy=	0.331619
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Thermal correction to Gibbs Free Energy=	0.271783
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Sum of electronic and zero-point Energies=	-632.817093
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Sum of electronic and thermal Energies=	-632.800751
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Sum of electronic and thermal Enthalpies=	-632.799807
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Sum of electronic and thermal Free Energies=	-632.859643
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C	-0.88836100	-0.35083200	1.29206000
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C	-0.71170300	-1.06947700	0.10015300
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C	-0.28560900	-0.56690300	-1.10924200
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C	-1.02637300	1.01656300	1.49117700
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C	0.04877400	0.76245600	-1.40118500
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C	-1.25566500	1.91695000	0.37315100
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C	-0.25548500	1.91557200	-0.68802300
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H	-0.95396600	-0.96130300	2.18568300
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H	-0.81327100	-2.14680100	0.17850300
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H	0.59042100	0.91743700	-2.32871100
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C	1.32098400	3.27750700	-2.02370500
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H	0.95121300	3.06040300	-3.03057700
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H	1.66470300	4.31114900	-2.00950200
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H	2.17236100	2.62083200	-1.80835600
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N	-1.10510200	1.58620600	2.75877400
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C	-1.13300200	0.70568800	3.91578900
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H	-0.18883700	0.16141200	4.06121800
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H	-1.31850300	1.30991000	4.80492300
H	-1.95108500	-0.01308200	3.82840000
C	-0.33054400	2.80655000	2.97246300
H	-0.51929600	3.53581400	2.18018900
H	-0.63846100	3.26459700	3.91414600
H	0.74886800	2.60712600	3.01536400
H	-0.08727600	-1.28657600	-1.89703300
N	-2.24960600	2.80651200	0.37641700
C	-3.27071600	2.79259800	1.43090700
C	-2.53255400	3.64053900	-0.79904600
H	-2.89897200	3.24160100	2.35270600
H	-4.13509600	3.35103500	1.07927600
H	-3.56715300	1.76326500	1.64374100
H	-2.02337100	4.60567300	-0.74433500
H	-2.22355300	3.12672100	-1.70858300
H	-3.60607600	3.81366600	-0.84340200
N	0.26453000	3.13121200	-1.03988400
H	0.18488000	3.86837800	-0.35953500

TI-24

Zero-point correction=	0.315352 (Hartree/Particle)
Thermal correction to Energy=	0.331487
Thermal correction to Enthalpy=	0.332431
Thermal correction to Gibbs Free Energy=	0.272251
Sum of electronic and zero-point Energies=	-632.843716
Sum of electronic and thermal Energies=	-632.827582
Sum of electronic and thermal Enthalpies=	-632.826638
Sum of electronic and thermal Free Energies=	-632.886818

C	0.27391400	-0.04998800	1.59467500
C	0.81820900	-0.76846700	0.50865900
C	0.90267400	-0.35893200	-0.80713800
C	-0.56328300	1.10883800	1.42396200
C	0.58501700	0.84399600	-1.43607200
C	-0.76192400	1.97088600	0.38249100
C	-0.06082000	1.96048300	-0.90809400
H	1.25207300	-1.73721100	0.71446400
H	0.91980800	0.92618600	-2.46355400
C	0.52155900	3.33920100	-2.88135200
H	0.36453800	4.38023600	-3.15937500
H	1.59904700	3.15245100	-2.81769900
H	0.09627600	2.70580600	-3.66616300
H	1.37767600	-1.08257200	-1.46464100
N	-1.64837500	3.05163900	0.53116600
C	-1.95396300	3.52262400	1.87466600
C	-2.85139500	2.99389800	-0.31480200
H	-1.03174700	3.63923400	2.44763600
H	-2.43083300	4.50127800	1.79027300
H	-2.64433600	2.86355900	2.42279900
H	-3.29864500	3.98858200	-0.37209600
H	-2.60248000	2.66846800	-1.32514000
H	-3.59079400	2.29777300	0.10265300
H	-1.18837700	1.31971300	2.28053900
N	0.42912100	-0.51828600	2.85181300
C	1.06905900	-1.80869900	3.09618500
C	-0.02727000	0.23586300	4.01591300
H	2.11935600	-1.79498500	2.78792900

H	1.02750200	-2.02655700	4.16116100
H	0.54827900	-2.61382400	2.56960500
H	0.48965300	-0.13513100	4.89914700
H	0.21637000	1.29548400	3.91195400
H	-1.10559300	0.12483300	4.17946700
N	-0.12761500	3.10381100	-1.60798100
H	-0.55060800	3.88099700	-1.11916500

TI-25

Zero-point correction= 0.314952 (Hartree/Particle)

Thermal correction to Energy= 0.331169

Thermal correction to Enthalpy= 0.332113

Thermal correction to Gibbs Free Energy= 0.271427

Sum of electronic and zero-point Energies= -632.839496

Sum of electronic and thermal Energies= -632.823278

Sum of electronic and thermal Enthalpies= -632.822334

Sum of electronic and thermal Free Energies= -632.883020

C	0.04113900	0.28959200	1.96852200
C	0.47690500	-0.71624700	1.08884700
C	0.31746100	-0.59747600	-0.33484100
C	-0.51628800	1.53305100	1.69146300
C	-0.09206500	0.44312800	-1.11031300
C	-0.77429500	2.24193400	0.52428200
C	-0.51594300	1.77278800	-0.79378700
H	-0.07131300	0.22694300	-2.17343100
C	-0.47659300	2.41240600	-3.20534100
H	-0.67733200	3.34152800	-3.73669500
H	0.56417200	2.12812900	-3.39353800

H	-1.14108200	1.64282800	-3.60951500
H	0.57775500	-1.47835300	-0.90788600
N	-1.31691300	3.55408200	0.58304000
C	-0.88849500	4.39952100	1.69128700
C	-2.77306300	3.58765300	0.39271800
H	0.19185900	4.31833900	1.82491100
H	-1.12697800	5.43756400	1.44773500
H	-1.38781800	4.16067800	2.64283700
H	-3.09016300	4.62197100	0.24053400
H	-3.05463500	3.00775600	-0.48955800
H	-3.30668800	3.18043400	1.26338600
H	-0.79423100	2.07469300	2.59148700
H	0.12227400	0.07990000	3.02640800
N	1.03419600	-1.85118000	1.57811200
C	1.49390500	-2.92302400	0.69854000
C	1.18180400	-2.03668300	3.01761400
H	2.23030100	-2.55974500	-0.02455100
H	1.97800400	-3.68746000	1.30205000
H	0.66230700	-3.39631000	0.16565400
H	1.66979100	-2.99028100	3.20491000
H	1.80149200	-1.24775900	3.45638400
H	0.20904200	-2.05112400	3.52043200
N	-0.72698200	2.63850600	-1.79523700
H	-0.92152800	3.57919000	-1.46721700

TI-26

Zero-point correction= 0.315408 (Hartree/Particle)

Thermal correction to Energy= 0.331523

Thermal correction to Enthalpy= 0.332467
 Thermal correction to Gibbs Free Energy= 0.272414
 Sum of electronic and zero-point Energies= -632.844872
 Sum of electronic and thermal Energies= -632.828757
 Sum of electronic and thermal Enthalpies= -632.827813
 Sum of electronic and thermal Free Energies= -632.887866

C	-0.00687700	0.25315200	1.97221700
C	0.50331300	-0.67373500	1.12288600
C	0.55043400	-0.61891900	-0.31602400
C	-0.68074000	1.48083200	1.71245000
C	0.42153500	0.58186800	-1.04752700
C	-0.77475600	2.19200000	0.55337000
C	-0.05398300	1.84099500	-0.68226900
H	0.79145200	0.53774700	-2.06140000
C	0.80131900	2.82101200	-2.79762000
H	0.81624800	3.82390400	-3.22162100
H	1.83542200	2.48480100	-2.66233700
H	0.30096400	2.15735400	-3.51121200
N	-1.45612000	3.41806000	0.49109900
C	-1.69506300	4.12903500	1.74072600
C	-2.64722700	3.42177500	-0.37364700
H	-0.77224200	4.18507300	2.32104300
H	-2.01015400	5.14620900	1.49921000
H	-2.48426800	3.66952400	2.35364200
H	-2.92275700	4.45504400	-0.59564600
H	-2.44639800	2.90788300	-1.31444900
H	-3.49474000	2.92869500	0.12031500
H	-1.18308500	1.90078300	2.57637100

H	0.04072700	-0.01209600	3.02477900
H	0.91491000	-1.55815300	1.59039900
N	0.84287100	-1.75540800	-0.98207300
C	1.11603800	-3.00915200	-0.27831500
C	0.93246200	-1.76688500	-2.43832200
H	0.29340100	-3.27250100	0.39104700
H	1.21717600	-3.80576500	-1.01182800
H	2.04876600	-2.95668100	0.29210500
H	0.04540500	-1.30693600	-2.88269400
H	1.82710900	-1.24219600	-2.79281300
H	0.98634800	-2.79672800	-2.78430300
N	0.09167200	2.86608700	-1.53827100
H	-0.22063700	3.75815700	-1.17587000

TI-27

Zero-point correction= 0.314809 (Hartree/Particle)

Thermal correction to Energy= 0.330732

Thermal correction to Enthalpy= 0.331677

Thermal correction to Gibbs Free Energy= 0.272712

Sum of electronic and zero-point Energies= -632.825125

Sum of electronic and thermal Energies= -632.809202

Sum of electronic and thermal Enthalpies= -632.808258

Sum of electronic and thermal Free Energies= -632.867222

C	-1.56814400	-0.43753900	1.12086000
C	-1.04178200	-1.09939300	0.03331800
C	-0.26462500	-0.56780600	-1.00050900
C	-1.51932900	0.93534500	1.38417000
C	0.01310600	0.75327900	-1.34254200

C	-1.15608300	1.99443100	0.56698200
C	-0.72800500	1.88513100	-0.80733900
C	-0.99755600	3.00966000	-3.02908700
H	-0.01016500	3.15468700	-3.47021100
H	-1.43227300	2.09406500	-3.43571900
H	-1.63161400	3.85260900	-3.30288400
N	-1.38069000	3.32323400	0.97904600
C	-0.16751700	4.13511100	1.15134700
C	-2.35633000	3.57099200	2.03429200
H	0.51927900	3.99122900	0.31553900
H	-0.44419900	5.19099500	1.18586700
H	0.35653200	3.87846800	2.08103700
H	-2.58770300	4.63825100	2.03763500
H	-3.27831400	3.02326800	1.83113800
H	-1.98739900	3.30671600	3.03580800
H	-1.89734300	1.22088100	2.35978000
H	-2.03233000	-1.04954800	1.88757100
H	-1.14894400	-2.17969000	0.02484000
H	0.21647700	-1.31642500	-1.61873000
N	0.92540700	1.04424800	-2.33912300
C	1.42851300	-0.02279200	-3.19135800
C	1.91889700	2.08619800	-2.07190600
H	0.60037800	-0.60368800	-3.60276400
H	1.96217600	0.43202900	-4.02714200
H	2.12273300	-0.69604400	-2.66940900
H	2.36342000	2.40603800	-3.01619900
H	1.46216100	2.95816200	-1.60350700
H	2.71618800	1.71251900	-1.41733300

N	-0.94817200	2.96310500	-1.57282700
H	-1.45815800	3.68275300	-1.06979200

TI-34

Zero-point correction= 0.315095 (Hartree/Particle)

Thermal correction to Energy= 0.331342

Thermal correction to Enthalpy= 0.332287

Thermal correction to Gibbs Free Energy= 0.272270

Sum of electronic and zero-point Energies= -632.836679

Sum of electronic and thermal Energies= -632.820432

Sum of electronic and thermal Enthalpies= -632.819488

Sum of electronic and thermal Free Energies= -632.879504

C	0.33079300	0.23723900	1.68235000
C	1.57782300	-0.02044100	1.15808000
C	2.21846300	0.57625400	0.04416800
C	-0.39696200	1.49025700	1.37045300
C	1.69297000	1.34041600	-0.95233800
C	-0.50435400	2.00050700	0.07667700
C	0.36018100	1.85155900	-1.02841600
C	-1.30399600	2.96281500	-2.50379100
H	-1.37490300	3.13139700	-3.57747000
H	-2.11525700	2.29153400	-2.20710000
H	-1.43047900	3.92669700	-1.99676100
H	2.12649200	-0.85025600	1.58587200
H	3.24928200	0.26588200	-0.10200900
H	2.33976800	1.56444000	-1.79618600
N	-0.24489100	-0.59439000	2.61399200
C	0.53052900	-1.69932500	3.15240400

C	-1.68064100	-0.86837900	2.55653700
H	1.47467400	-1.33755200	3.56689600
H	-0.03794100	-2.15496000	3.96400800
H	0.73883200	-2.47354800	2.40080900
H	-2.04855800	-1.09381800	3.56027000
H	-2.23229500	-0.01164200	2.17477700
H	-1.88304400	-1.72982100	1.90823700
H	-1.28184100	2.73684800	-0.07257900
N	-1.07373100	2.08187400	2.38220900
C	-0.69006900	1.91868200	3.78699100
C	-2.03087200	3.14823300	2.11802500
H	0.33037100	1.55154100	3.87333700
H	-0.73691900	2.90096200	4.26065800
H	-1.36116900	1.23797300	4.31810600
H	-1.53671700	4.06115400	1.76445700
H	-2.77241900	2.83048900	1.37998000
H	-2.56104600	3.37404600	3.04215300
N	-0.01573000	2.36727400	-2.21337400
H	0.66574100	2.35850300	-2.95585600

TI-35

Zero-point correction= 0.315572 (Hartree/Particle)

Thermal correction to Energy= 0.332131

Thermal correction to Enthalpy= 0.333075

Thermal correction to Gibbs Free Energy= 0.271153

Sum of electronic and zero-point Energies= -632.849209

Sum of electronic and thermal Energies= -632.832650

Sum of electronic and thermal Enthalpies= -632.831706

Sum of electronic and thermal Free Energies= -632.893628

C	-0.28539700	0.15687600	0.93230700
C	0.64461900	-0.50578700	0.14282900
C	1.31646700	0.08096000	-1.00339800
C	-0.75072400	1.50128300	0.90262500
C	1.37804500	1.36369800	-1.40123100
C	-0.19120700	2.57362800	0.15607400
C	0.78195600	2.55164300	-0.82620300
C	0.74344800	5.02834700	-1.01000500
H	1.28966100	5.76667500	-1.59528400
H	-0.32689600	5.15504000	-1.20987800
H	0.93233700	5.22098400	0.05182700
H	1.84104000	-0.61606000	-1.64527200
H	1.95795300	1.54221700	-2.30395100
H	-0.60241900	3.54936700	0.35909100
N	-1.78672700	1.80265600	1.72993700
C	-2.20729300	3.18123500	1.96068200
C	-2.53230000	0.76095600	2.42897300
H	-1.36773500	3.80269900	2.28617500
H	-2.65934000	3.62306400	1.06601000
H	-2.95010600	3.19393800	2.75533200
H	-3.46651300	1.18307200	2.79463800
H	-2.78321700	-0.05827100	1.75036300
H	-1.98051800	0.36296500	3.28882300
H	-0.69281300	-0.43257100	1.73631100
N	0.92686100	-1.81254500	0.39440100
C	0.12259400	-2.58285400	1.33041600
C	2.08899600	-2.48665500	-0.18033200

H	-0.94320400	-2.42820000	1.13844300
H	0.33277900	-3.64195100	1.18822200
H	0.33988600	-2.32410400	2.37434500
H	1.88352500	-2.89104000	-1.17794900
H	2.95017300	-1.81757700	-0.22834500
H	2.36638700	-3.31503900	0.47109600
N	1.19983200	3.70886100	-1.38885600
H	1.88709200	3.65177400	-2.12190900

TI-36

Zero-point correction= 0.315345 (Hartree/Particle)

Thermal correction to Energy= 0.331918

Thermal correction to Enthalpy= 0.332862

Thermal correction to Gibbs Free Energy= 0.271497

Sum of electronic and zero-point Energies= -632.848918

Sum of electronic and thermal Energies= -632.832345

Sum of electronic and thermal Enthalpies= -632.831401

Sum of electronic and thermal Free Energies= -632.892766

C	-0.46218500	0.30895900	1.43431300
C	0.33250500	-0.31455300	0.54561000
C	0.77720400	0.10975300	-0.77213200
C	-1.12692700	1.60059500	1.35755800
C	0.82961300	1.44432700	-1.15615200
C	-0.67785200	2.62022200	0.53290700
C	0.27381200	2.58047700	-0.52162800
C	1.49415800	4.03337000	-2.14991900
H	1.60718500	5.11032600	-2.26759900
H	2.48315900	3.60626300	-1.95648900

H	1.10535100	3.62801300	-3.09105900
H	1.34347300	1.65439800	-2.08144200
H	-1.11326300	3.59923000	0.69025300
N	-2.14604000	1.81278900	2.22849400
C	-2.73226400	3.13781400	2.36379600
C	-2.70367800	0.74018600	3.04718600
H	-1.97938600	3.87488100	2.66336800
H	-3.19990700	3.46421100	1.42786100
H	-3.49790900	3.11286400	3.13634700
H	-3.71313000	1.01896400	3.34685500
H	-2.78275200	-0.18837500	2.47830600
H	-2.11602600	0.56055000	3.95499400
H	-0.60350700	-0.22419200	2.36728700
H	0.72627700	-1.26801700	0.87857700
N	1.26548600	-0.85512900	-1.58791900
C	1.93145900	-0.50085800	-2.83321900
C	1.12277200	-2.27616300	-1.28055900
H	1.23656100	-0.03104600	-3.53878000
H	2.76927400	0.17985100	-2.64964900
H	2.33083500	-1.40243600	-3.29330800
H	1.19659400	-2.84179900	-2.20841600
H	1.90288400	-2.63228000	-0.59809700
H	0.14180100	-2.48544400	-0.85002900
N	0.58973300	3.78761900	-1.04519400
H	0.15417800	4.59509000	-0.63075200

TI-45

Zero-point correction= 0.314667 (Hartree/Particle)

Thermal correction to Energy=	0.330937
Thermal correction to Enthalpy=	0.331881
Thermal correction to Gibbs Free Energy=	0.272060
Sum of electronic and zero-point Energies=	-632.829372
Sum of electronic and thermal Energies=	-632.813102
Sum of electronic and thermal Enthalpies=	-632.812158
Sum of electronic and thermal Free Energies=	-632.871979

C	0.29834100	0.04567600	1.47736200
C	1.15349000	-0.53986700	0.48515100
C	1.71810400	0.19492900	-0.58112300
C	-0.46310500	1.22130000	1.24423100
C	1.50094800	1.45486700	-1.08951800
C	-0.41097900	2.21247800	0.29592200
C	0.51588800	2.40807700	-0.75630600
C	-0.49544500	4.61796700	-1.31275500
H	-0.29192500	5.38192100	-2.06171100
H	-1.52412800	4.27036700	-1.45446500
H	-0.40232200	5.07793100	-0.32341100
H	2.45430100	-0.35802300	-1.15307600
H	2.13489000	1.71696300	-1.93354200
N	0.14530600	-0.58929100	2.68040000
C	1.28973800	-1.22602900	3.33371600
C	-1.00097300	-0.34772300	3.54500800
H	2.22711900	-0.85493400	2.92127600
H	1.25881000	-0.96554900	4.39420100
H	1.26944600	-2.31598000	3.23879700
H	-0.91384200	0.58765000	4.11319000
H	-1.92908800	-0.33804800	2.96924600

H	-1.06937600	-1.17164900	4.25676000
H	-1.14869900	2.99550300	0.43095200
N	1.49055800	-1.87687900	0.61933000
C	0.40443900	-2.84617000	0.76210200
C	2.65942900	-2.41653900	-0.05490700
H	-0.36626600	-2.47068000	1.43477000
H	-0.05373400	-3.06906800	-0.20998400
H	0.80511200	-3.77191000	1.18051300
H	2.50277700	-2.58268000	-1.13072000
H	3.52221800	-1.76238400	0.08870400
H	2.89695700	-3.38032900	0.39928100
H	-1.21029400	1.41870900	2.00429200
N	0.45906700	3.54031100	-1.49024700
H	1.13905100	3.64711000	-2.22556100

TI-234

Zero-point correction= 0.388130 (Hartree/Particle)

Thermal correction to Energy= 0.408472

Thermal correction to Enthalpy= 0.409416

Thermal correction to Gibbs Free Energy= 0.340410

Sum of electronic and zero-point Energies= -766.680778

Sum of electronic and thermal Energies= -766.660436

Sum of electronic and thermal Enthalpies= -766.659492

Sum of electronic and thermal Free Energies= -766.728498

C	0.38950600	0.38659400	1.57719700
C	1.70572700	0.23213400	1.14688700
C	2.30106100	0.77297900	0.01312100
C	-0.48346500	1.52828400	1.21818000

C	1.77015000	1.54854300	-0.99306500
C	-0.43376900	2.30852400	0.06269800
C	0.52674000	2.20524600	-1.03668200
C	1.10245000	3.12602100	-3.27552000
H	0.57230200	3.74826200	-3.99550400
H	2.05179800	3.61477800	-3.02721400
H	1.30821400	2.16177900	-3.74723900
N	-1.42799600	1.83740000	2.18710600
C	-1.02767600	1.99767200	3.57369400
C	-2.85298900	1.89711900	1.93342600
H	0.05205700	2.13473000	3.64591300
H	-1.50385500	2.89874800	3.97495700
H	-1.31575500	1.14865600	4.20724700
H	-3.25575800	2.91494800	1.98646800
H	-3.08335600	1.47565700	0.95462000
H	-3.37850900	1.29668200	2.68547500
H	2.30383700	-0.51334900	1.65496100
H	3.32727400	0.45600700	-0.15222000
N	-1.30087200	3.41775200	-0.07747300
C	-1.21379300	4.50223500	0.88444900
C	-2.51230200	3.34927000	-0.88414000
H	-0.21518500	4.52397100	1.32440700
H	-1.37475400	5.45353800	0.36570100
H	-1.94878000	4.43453400	1.69637300
H	-2.59508100	4.23156100	-1.53294400
H	-2.49156900	2.45875400	-1.51693100
H	-3.42540700	3.31336300	-0.27806900
H	2.43592500	1.74437800	-1.82443800

N	-0.11278400	-0.50312200	2.48081600
C	-1.49849100	-0.96108600	2.39509400
C	0.76093100	-1.39394500	3.22770600
H	-1.98027100	-0.59126300	1.49194900
H	-1.49385800	-2.05352200	2.33887600
H	-2.08468700	-0.66430700	3.26988400
H	1.13755100	-2.22499000	2.61649200
H	1.60413100	-0.84316000	3.64903200
H	0.18977500	-1.81087100	4.05851200
N	0.25258300	2.96064800	-2.11327500
H	-0.48365500	3.63519000	-1.96760500

TI-235

Zero-point correction= 0.388283 (Hartree/Particle)

Thermal correction to Energy= 0.408657

Thermal correction to Enthalpy= 0.409601

Thermal correction to Gibbs Free Energy= 0.340910

Sum of electronic and zero-point Energies= -766.699396

Sum of electronic and thermal Energies= -766.679023

Sum of electronic and thermal Enthalpies= -766.678079

Sum of electronic and thermal Free Energies= -766.746770

C	-0.21444600	0.25530700	1.12210500
C	0.81230600	-0.34831900	0.39646200
C	1.00858200	-0.07064900	-1.00976300
C	-1.01104300	1.38494400	0.82607900
C	0.71244300	1.05940100	-1.68350900
C	-0.66931700	2.44819500	-0.08660400
C	0.20245200	2.31152000	-1.17787100

C	1.52074100	3.49397800	-2.93199100
H	1.73263100	4.54418700	-3.12953400
H	2.45799800	2.99952600	-2.65415700
H	1.14591000	3.05075200	-3.86006500
N	-2.12780100	1.56824300	1.59699500
C	-2.31692500	0.89461700	2.87051400
C	-3.36565900	2.05495300	0.99794700
H	-1.40378200	0.93539700	3.46819200
H	-3.09512900	1.42527600	3.42225300
H	-2.63322000	-0.15141800	2.75634000
H	-3.68459200	3.00820500	1.43109800
H	-3.25380000	2.16258800	-0.07910500
H	-4.15388200	1.31617000	1.17623600
H	1.44397700	-0.86700300	-1.60169200
N	-1.11873900	3.76476200	0.15486200
C	-1.03852500	4.30848400	1.49785100
C	-2.07482800	4.41672300	-0.73291100
H	-0.16247600	3.90207500	2.00731000
H	-0.91860700	5.39411200	1.42864900
H	-1.92402300	4.10344000	2.11523400
H	-1.78512500	5.46061500	-0.90203300
H	-2.09943100	3.90796100	-1.69853800
H	-3.09254100	4.42507300	-0.32329500
H	0.97497600	1.05824200	-2.73665700
H	-0.52380300	-0.28747100	2.00193100
N	1.54701400	-1.34263500	0.95399300
C	1.32504500	-1.72401600	2.33998800
C	2.50747000	-2.11627000	0.17403000

H	1.34805200	-0.84219000	2.98804400
H	0.36430200	-2.23699900	2.47366100
H	2.11640400	-2.39988000	2.65811400
H	2.01463600	-2.80474800	-0.52211900
H	3.17881200	-1.45913900	-0.38408300
H	3.11755300	-2.70768000	0.85424500
N	0.53551900	3.42440800	-1.87027100
H	0.26663300	4.28239700	-1.41053900

TI-236

Zero-point correction= 0.388020 (Hartree/Particle)

Thermal correction to Energy= 0.408696

Thermal correction to Enthalpy= 0.409640

Thermal correction to Gibbs Free Energy= 0.339462

Sum of electronic and zero-point Energies= -766.702210

Sum of electronic and thermal Energies= -766.681534

Sum of electronic and thermal Enthalpies= -766.680590

Sum of electronic and thermal Free Energies= -766.750769

C	-0.22187700	0.61308300	1.80467000
C	0.57724400	-0.26406300	1.16582600
C	0.88739100	-0.33468400	-0.24687600
C	-1.02238100	1.70711000	1.29485300
C	0.83502400	0.78656300	-1.07071600
C	-0.66993600	2.46969200	0.18034100
C	0.31200800	2.07325300	-0.81743500
C	1.66659100	2.96500300	-2.70520000
H	1.83494800	3.96313600	-3.10755100
H	2.61709100	2.57742200	-2.32215400

H	1.32691300	2.32411400	-3.52610000
N	-2.12873100	2.05437100	2.03767500
C	-2.24658200	1.74863300	3.45388700
C	-3.40315900	2.27442500	1.36533000
H	-1.31254800	1.95981300	3.97810000
H	-3.00818200	2.40578400	3.87889400
H	-2.54846100	0.70976200	3.64628200
H	-3.78179100	3.29102000	1.51568800
H	-3.30316900	2.08248200	0.29782500
H	-4.14389800	1.57182200	1.76334600
N	-1.15518100	3.78564800	0.01161500
C	-1.17797000	4.68154600	1.15547800
C	-2.12197700	4.08790800	-1.04066000
H	-0.31122400	4.48621700	1.78976600
H	-1.10940900	5.71003800	0.78835200
H	-2.08259100	4.59988500	1.77115900
H	-1.92346500	5.08183100	-1.45644300
H	-2.03724100	3.35619700	-1.84663100
H	-3.15717400	4.08284800	-0.67832200
H	1.32026000	0.69197900	-2.03057800
H	-0.34620600	0.41506300	2.86354400
H	1.02283900	-1.02608300	1.79337700
N	1.34800000	-1.51412600	-0.72737300
C	1.78814900	-1.62133300	-2.11106000
C	1.43055400	-2.70490600	0.11446200
H	2.67432200	-1.00396900	-2.29869900
H	2.04735700	-2.65590500	-2.32517300
H	0.99233900	-1.31974100	-2.80012500

H	2.25441300	-2.64563300	0.83438000
H	0.49316400	-2.87077200	0.65080400
H	1.60314400	-3.57154000	-0.52087400
N	0.67339600	3.05782700	-1.65831200
H	0.30993400	3.96498500	-1.39601100

TI-237

Zero-point correction= 0.390409 (Hartree/Particle)

Thermal correction to Energy= 0.410101

Thermal correction to Enthalpy= 0.411046

Thermal correction to Gibbs Free Energy= 0.344729

Sum of electronic and zero-point Energies= -766.689444

Sum of electronic and thermal Energies= -766.669751

Sum of electronic and thermal Enthalpies= -766.668807

Sum of electronic and thermal Free Energies= -766.735124

C	0.27869200	0.99406700	1.94664100
C	1.31502600	0.40430700	1.27331100
C	1.47719000	0.19347400	-0.11094500
C	-0.84151300	1.66594000	1.37525900
C	0.80185300	0.81862000	-1.14244300
C	-0.73228800	2.40528500	0.14048400
C	0.15609700	2.11988200	-0.90723700
C	1.53930200	3.17616900	-2.69517400
H	1.70288500	4.22856300	-2.92701000
H	2.43437200	2.78448000	-2.20296500
H	1.39261100	2.63654500	-3.63303600
N	-1.97321500	1.78296700	2.10682300
C	-2.01338400	1.45992000	3.52779300

C	-3.27634900	1.89880100	1.46258200
H	-1.19653300	1.95079600	4.06043600
H	-2.94850600	1.84044100	3.93908600
H	-1.96680600	0.37904400	3.70479000
H	-3.72456200	2.88575200	1.61005100
H	-3.18872200	1.69336100	0.39669700
H	-3.94364500	1.14899500	1.89611200
H	0.26529700	0.83376400	3.01740700
H	2.03180600	-0.12003800	1.89877800
H	2.17421600	-0.59363000	-0.37054000
N	0.88649200	0.38495000	-2.43639100
C	1.73607700	-0.75264900	-2.75087900
C	-0.24352100	0.56424300	-3.34614900
H	2.76363500	-0.56416800	-2.43013700
H	1.37810400	-1.68023500	-2.28468300
H	1.74415000	-0.89181000	-3.83188800
H	-0.96856400	-0.25099300	-3.23329100
H	-0.74504900	1.51349500	-3.16387600
H	0.12104400	0.56575500	-4.37538000
N	-1.38560900	3.65391200	0.03083300
C	-1.38495200	4.56153700	1.16431900
C	-2.43747600	3.86558000	-0.95738400
H	-0.42772000	4.49597100	1.68615700
H	-1.50123300	5.58352600	0.79224300
H	-2.18814200	4.37511300	1.89063300
H	-2.33721200	4.85843900	-1.40960300
H	-2.35826300	3.12051200	-1.75155800
H	-3.44356500	3.79913700	-0.52520500

N	0.37155500	3.09442900	-1.82752300
H	-0.02487100	3.97465600	-1.52259500

TI-245

Zero-point correction= 0.388605 (Hartree/Particle)

Thermal correction to Energy= 0.408747

Thermal correction to Enthalpy= 0.409692

Thermal correction to Gibbs Free Energy= 0.341437

Sum of electronic and zero-point Energies= -766.698395

Sum of electronic and thermal Energies= -766.678253

Sum of electronic and thermal Enthalpies= -766.677309

Sum of electronic and thermal Free Energies= -766.745564

C	0.28284300	-0.02100700	1.43924300
C	0.55507300	-0.81717800	0.28026900
C	0.13994400	-0.46151300	-1.00836200
C	-0.18919000	1.31767000	1.40385700
C	-0.40406800	0.68639500	-1.56352800
C	-0.58697900	2.19845800	0.42371100
C	-0.66579500	1.93763300	-0.99398400
C	-1.08810300	2.95592100	-3.21839800
H	-1.36847800	3.94983100	-3.56470300
H	-0.12576300	2.68955200	-3.67119800
H	-1.85023200	2.25061800	-3.56309400
N	0.48180400	-0.56108000	2.68183600
C	0.10245300	-1.94010400	2.99328000
C	0.73652900	0.26780300	3.85012300
H	-0.56734700	-2.34138700	2.23606600
H	0.97160200	-2.59840700	3.08294900

H	-0.42935500	-1.92979600	3.94874600
H	1.28180500	-0.33376500	4.58033100
H	1.36620100	1.12100500	3.58999700
H	-0.18499800	0.62718500	4.32848100
H	0.35646000	-1.21288300	-1.75979400
H	-0.33909900	1.72806700	2.39416900
H	-0.54481200	0.62645300	-2.63683100
N	1.24322400	-2.01935600	0.46159100
C	1.10633100	-3.08005400	-0.51934900
C	2.59315400	-1.91938500	1.01267200
H	0.05446900	-3.22701700	-0.77543600
H	1.68144600	-2.90536300	-1.44210800
H	1.47455300	-4.00678900	-0.07327600
H	3.31820900	-1.61115000	0.24666900
H	2.62294300	-1.19789200	1.82971700
H	2.89472500	-2.89410500	1.40428000
N	-0.99831000	3.49869300	0.79778300
C	-2.45585000	3.69076900	0.80919200
C	-0.36389300	4.09928400	1.96335500
H	-2.90703100	3.27322900	-0.09214500
H	-2.91230700	3.20780100	1.68472900
H	-2.67593900	4.76017300	0.84529900
H	-0.75674200	3.71934100	2.91972000
H	0.71464600	3.93480400	1.92698300
H	-0.54947900	5.17548900	1.93781900
N	-1.01824100	2.97988300	-1.77256700
H	-0.99251700	3.87333100	-1.29787800

TI-246

Zero-point correction= 0.389506 (Hartree/Particle)

Thermal correction to Energy= 0.409863

Thermal correction to Enthalpy= 0.410807

Thermal correction to Gibbs Free Energy= 0.341548

Sum of electronic and zero-point Energies= -766.720136

Sum of electronic and thermal Energies= -766.699779

Sum of electronic and thermal Enthalpies= -766.698834

Sum of electronic and thermal Free Energies= -766.768094

C	0.53319700	0.11080500	1.44190300
C	0.70067600	-0.65860300	0.29473900
C	0.39723400	-0.32034000	-1.04688900
C	-0.27866900	1.31056500	1.50442700
C	0.23292300	1.01438200	-1.52945800
C	-0.60194100	2.20578200	0.54055700
C	-0.09454300	2.16314000	-0.84398800
C	0.44725300	3.59181800	-2.79237400
H	0.47973100	4.66488400	-2.97634700
H	1.45745700	3.18666000	-2.92286200
H	-0.21354600	3.13575700	-3.53909100
N	1.01371400	-0.34287200	2.62955700
C	1.60906100	-1.66664500	2.73386400
C	0.95591400	0.46343600	3.84358300
H	0.91471800	-2.43750600	2.38230100
H	2.54006700	-1.73566200	2.15974900
H	1.83457900	-1.87464100	3.77805600
H	1.72361300	0.11511300	4.53373400
H	1.16532000	1.51244900	3.62496000

H	-0.01545300	0.38722800	4.34740000
H	-0.71965900	1.49415400	2.47464700
H	0.44675500	1.15672000	-2.57892500
N	-1.37403600	3.34272600	0.83015100
C	-2.65179900	3.42835000	0.10902600
C	-1.51075900	3.74162100	2.22228200
H	-2.51841400	3.18014200	-0.94403800
H	-3.39611200	2.74472100	0.53914800
H	-3.03363100	4.44935800	0.17664400
H	-2.16574000	3.07464400	2.80373500
H	-0.52826700	3.78394100	2.69727100
H	-1.94873800	4.74138900	2.25052400
H	1.14867100	-1.62756700	0.43721100
N	0.41709600	-1.31309600	-1.97050300
C	0.18415300	-1.04064600	-3.38430600
C	0.70847100	-2.68983900	-1.58977800
H	-0.70822800	-0.42414300	-3.51799600
H	1.04042400	-0.54157500	-3.85300200
H	0.01988200	-1.98335400	-3.90249800
H	1.74908700	-2.81197400	-1.26782500
H	0.04378100	-3.02017700	-0.78626300
H	0.54657800	-3.33808300	-2.44842000
N	-0.03888900	3.36726600	-1.45169100
H	-0.27767400	4.15579900	-0.86805800

TI-247

Zero-point correction= 0.389888 (Hartree/Particle)

Thermal correction to Energy= 0.409716

Thermal correction to Enthalpy= 0.410660
 Thermal correction to Gibbs Free Energy= 0.343272
 Sum of electronic and zero-point Energies= -766.699111
 Sum of electronic and thermal Energies= -766.679283
 Sum of electronic and thermal Enthalpies= -766.678338
 Sum of electronic and thermal Free Energies= -766.745727

C	-1.98952600	-0.74057000	-0.03676400
C	-1.16054600	-1.86923400	-0.20450400
C	0.21502200	-1.91255500	-0.30635000
C	-1.48629300	0.58893800	-0.17362200
C	1.23016900	-0.96957400	-0.07308700
C	-0.21878900	1.10081400	-0.05140700
C	0.99307900	0.37366800	0.31555400
C	3.00581300	0.61146100	1.78631300
H	3.27662300	1.41785000	2.46848800
H	2.66594900	-0.24714600	2.36970800
H	3.89087500	0.31558000	1.22126700
N	-3.32509100	-0.90374700	0.12881600
C	-3.92433200	-2.23269700	0.08389900
C	-4.20976900	0.23922500	0.31557700
H	-3.77844500	-2.70680900	-0.89244300
H	-3.50785200	-2.87969800	0.86239700
H	-4.99498900	-2.14527000	0.25579300
H	-5.17079700	-0.11327800	0.68553900
H	-3.80165800	0.92968400	1.05869900
H	-4.38490100	0.78238700	-0.62120000
H	-2.23763100	1.32993300	-0.40570400
N	-0.02526100	2.49142700	-0.13032200

C	0.85199800	2.94473400	-1.21943400
C	-1.16441600	3.37813100	0.05495700
H	1.72509000	2.29791900	-1.30697300
H	0.31952000	2.94707900	-2.17937200
H	1.19725000	3.95876500	-1.00651100
H	-1.84476800	3.40073900	-0.80972700
H	-1.72286100	3.09005800	0.94800500
H	-0.78445000	4.39113700	0.20229500
H	-1.64858200	-2.82714700	-0.32554000
H	0.58916900	-2.90027800	-0.55431900
N	2.57388700	-1.36533300	-0.15888600
C	3.37145700	-0.67195600	-1.16623600
C	2.91311000	-2.77060600	-0.02631300
H	3.23610800	0.40917000	-1.08637100
H	4.42915500	-0.88848400	-0.99711000
H	3.11038000	-0.98455400	-2.18724100
H	2.38283000	-3.20877900	0.82221100
H	2.69846700	-3.36323000	-0.92946800
H	3.98483900	-2.85069300	0.17097300
N	1.94456600	1.11550000	0.92345800
H	1.63211500	2.06145700	1.10365100

TI-345

Zero-point correction= 0.388352 (Hartree/Particle)

Thermal correction to Energy= 0.408601

Thermal correction to Enthalpy= 0.409545

Thermal correction to Gibbs Free Energy= 0.341575

Sum of electronic and zero-point Energies= -766.690111

Sum of electronic and thermal Energies= -766.669862
Sum of electronic and thermal Enthalpies= -766.668918
Sum of electronic and thermal Free Energies= -766.736889

C	0.24087800	0.23073600	1.30988700
C	1.32796400	-0.20047400	0.55164800
C	1.98095300	0.57776100	-0.46727400
C	-0.40324000	1.54460900	1.17198900
C	1.49930400	1.57312200	-1.24726900
C	-0.58426800	2.23635600	-0.03834400
C	0.21270100	2.20948900	-1.18283400
C	-1.37240100	3.68784200	-2.38923100
H	-1.44820100	4.06572100	-3.40789900
H	-2.23868000	3.04821000	-2.19303800
H	-1.39793400	4.54330500	-1.70336300
N	-0.98814000	2.04553300	2.29028500
C	-0.38846300	1.84262400	3.61023700
C	-1.97105300	3.11623700	2.22771100
H	0.62916900	1.46604200	3.52050200
H	-0.34042500	2.81418200	4.10821100
H	-0.97532000	1.16162500	4.23268600
H	-1.51606200	4.08519100	1.98512800
H	-2.74792200	2.88598800	1.49509700
H	-2.45290000	3.19590000	3.20230800
H	2.14547100	1.90175000	-2.05759700
H	-1.33476000	3.01419800	-0.03227000
N	-0.30687400	-0.59622400	2.27795400
C	-1.74250500	-0.79106000	2.35306300
C	0.48852600	-1.29351500	3.27201700

H	-2.21556200	-0.49929900	1.41340100
H	-1.95012700	-1.85428300	2.51510700
H	-2.21562400	-0.22860800	3.16984700
H	0.57218300	-2.36774400	3.06987100
H	1.49389600	-0.87655100	3.31816800
H	0.01658900	-1.16558200	4.25333800
H	2.95699000	0.21213200	-0.76618000
N	1.82243200	-1.49504700	0.77167700
C	0.93024300	-2.58870200	0.39264900
C	3.21731500	-1.78658400	0.49271500
H	-0.09208100	-2.37331000	0.70224600
H	0.94036500	-2.75789100	-0.69387900
H	1.25627100	-3.50660400	0.88860700
H	3.43368300	-1.93249000	-0.57738700
H	3.86213700	-0.99799000	0.88685600
H	3.47911700	-2.71292500	1.00979000
N	-0.14128800	2.93740500	-2.26175500
H	0.51501700	2.98959200	-3.02397100

TI-346

Zero-point correction= 0.389120 (Hartree/Particle)

Thermal correction to Energy= 0.409821

Thermal correction to Enthalpy= 0.410765

Thermal correction to Gibbs Free Energy= 0.340651

Sum of electronic and zero-point Energies= -766.713540

Sum of electronic and thermal Energies= -766.692838

Sum of electronic and thermal Enthalpies= -766.691894

Sum of electronic and thermal Free Energies= -766.762009

C	-0.42120300	0.02646200	1.55945500
C	0.56766300	-0.49460400	0.77507500
C	1.21652600	0.04763800	-0.39625100
C	-0.85998500	1.44300700	1.47907100
C	0.57753600	0.91892600	-1.29078600
C	-1.01910100	2.08653700	0.27839400
C	-0.52976600	1.73299100	-1.02436900
C	-0.67702400	2.34924500	-3.43180800
H	-1.35510400	2.96027700	-4.02630300
H	0.33935500	2.73599900	-3.56975700
H	-0.72194500	1.32187500	-3.80721700
N	-1.22769400	2.04265900	2.65112000
C	-0.56283300	1.74042200	3.91778800
C	-1.95941900	3.29547400	2.63786200
H	0.26719500	1.05331300	3.77239800
H	-0.16480600	2.66995700	4.33594200
H	-1.26068200	1.30125600	4.63783000
H	-1.33199600	4.14502300	2.33441500
H	-2.82125600	3.23104800	1.96787400
H	-2.33458700	3.48697700	3.64389000
H	0.99080200	0.99681500	-2.28488500
H	0.83221300	-1.52420900	0.97145600
N	2.41575500	-0.48387900	-0.72654200
C	3.02713300	-0.20259500	-2.01874400
C	3.11722900	-1.40236800	0.16233900
H	3.18787700	0.87200300	-2.15009900
H	3.99247000	-0.70177200	-2.07362100
H	2.40755300	-0.57446600	-2.84231000

H	2.99110300	-1.09758400	1.20265100
H	2.76914700	-2.43594100	0.04571400
H	4.18196000	-1.37151500	-0.06668000
H	-1.48932700	3.06265500	0.30826000
N	-1.00299300	-0.73220400	2.55484200
C	-2.44699700	-0.67006900	2.77491600
C	-0.42923200	-2.01862400	2.89953300
H	-2.84475000	0.30385100	2.49996800
H	-2.96068300	-1.43975900	2.18506300
H	-2.66047700	-0.84230500	3.83305400
H	-0.59353600	-2.78349700	2.12597700
H	0.64440100	-1.91837500	3.08020100
H	-0.89589200	-2.36776500	3.82215700
N	-1.08931100	2.41845400	-2.04592900
H	-1.85597100	3.03177400	-1.82380600

TI-347

Zero-point correction= 0.389388 (Hartree/Particle)

Thermal correction to Energy= 0.409413

Thermal correction to Enthalpy= 0.410358

Thermal correction to Gibbs Free Energy= 0.342219

Sum of electronic and zero-point Energies= -766.704373

Sum of electronic and thermal Energies= -766.684348

Sum of electronic and thermal Enthalpies= -766.683403

Sum of electronic and thermal Free Energies= -766.751542

C	-0.11487600	0.05301400	1.66967000
C	0.81682200	-0.43851100	0.79537500
C	1.21636600	0.04257200	-0.48340000

C	-0.74700200	1.37265600	1.47298800
C	0.54788600	0.83960800	-1.36263900
C	-1.20155600	1.78941700	0.21585500
C	-0.73842900	1.46062000	-1.06886400
C	-2.72932900	2.49892400	-2.11326900
H	-3.10657500	2.56452700	-3.13280500
H	-3.43506900	1.91171100	-1.51655900
H	-2.67592800	3.51399200	-1.70237900
N	-1.01703900	2.12209200	2.56253500
C	-0.29698400	1.96920900	3.83040800
C	-1.86881400	3.30046300	2.45984500
H	0.66274300	1.48236200	3.67390400
H	-0.11349000	2.96825600	4.22933400
H	-0.87274100	1.39319600	4.55955400
H	-1.41058400	4.07501100	1.83380200
H	-2.84883200	3.04119900	2.04898400
H	-2.02695000	3.70630600	3.45746600
H	-1.96074100	2.55961600	0.21942300
N	-0.46023200	-0.62278100	2.83362300
C	-1.88451600	-0.77313400	3.12917400
C	0.32312900	-1.78228600	3.21935200
H	-2.42743800	0.14802000	2.91780000
H	-2.33293600	-1.58590800	2.54210700
H	-2.00795000	-1.00110800	4.19034300
H	0.18496500	-2.63858100	2.54204300
H	1.38514800	-1.52810500	3.26058800
H	0.01340300	-2.08923300	4.21979600
H	2.13198500	-0.40486100	-0.85703400

H	1.32611700	-1.34739000	1.09342000
N	0.99806300	1.05172100	-2.69114600
C	1.56196100	2.39031000	-2.90737400
C	1.83128900	0.01228400	-3.28095300
H	0.88330800	3.15551600	-2.52394700
H	2.53579200	2.50628900	-2.41087100
H	1.69401000	2.55534000	-3.97917300
H	2.85577200	-0.00523000	-2.87836900
H	1.37011100	-0.96506200	-3.12635700
H	1.90250100	0.19475600	-4.35555500
N	-1.42823500	1.87019700	-2.14042600
H	-0.99024000	1.63684600	-3.02476200

TI-2345

Zero-point correction= 0.461050 (Hartree/Particle)

Thermal correction to Energy= 0.485824

Thermal correction to Enthalpy= 0.486768

Thermal correction to Gibbs Free Energy= 0.409563

Sum of electronic and zero-point Energies= -900.541690

Sum of electronic and thermal Energies= -900.516916

Sum of electronic and thermal Enthalpies= -900.515972

Sum of electronic and thermal Free Energies= -900.593177

C	0.54754800	0.19594000	1.63148900
C	0.54856400	-0.90936600	0.64561800
C	0.93629300	-0.46650300	-0.58306500
C	-0.66000100	1.01888300	1.53319600
C	1.18556100	0.92101300	-0.87259200
C	-0.53838900	2.03370700	0.61192900

C	0.60113000	2.05310500	-0.32076900
C	1.82448100	3.56817000	-1.86284300
H	1.92496300	4.64599800	-1.98968400
H	2.82851800	3.15413200	-1.71400700
H	1.41459900	3.14480900	-2.79041200
N	1.60658800	0.54440400	2.30302300
C	2.89044800	-0.13493600	2.13458500
C	1.66515000	1.78249300	3.08284000
H	2.73920700	-1.11653600	1.69146800
H	3.51076400	0.46340200	1.46040700
H	3.37944000	-0.22206900	3.10524700
H	2.18258400	2.54733800	2.49762900
H	0.65819700	2.12780800	3.30680300
H	2.21667400	1.59054900	4.00404500
N	-1.47464900	3.05742700	0.45810500
C	-2.14036000	3.21727700	-0.83152800
C	-2.27768900	3.46994800	1.59509400
H	-1.48439600	2.89017800	-1.63914100
H	-3.07328800	2.63875800	-0.88572600
H	-2.38858700	4.27089300	-0.98943600
H	-3.16004000	2.83827700	1.76042700
H	-1.67159700	3.45083700	2.50260800
H	-2.61417500	4.49620500	1.42242300
N	-1.84467700	0.59726400	2.12245600
C	-2.91129500	0.12862000	1.24549200
C	-1.78281900	-0.09867500	3.39514200
H	-2.91722200	0.71228500	0.32538600
H	-2.78012400	-0.93226400	0.98799400

H	-3.87764900	0.25344000	1.74274600
H	-0.98239700	0.31424000	4.01429500
H	-2.72410400	0.04649400	3.93288700
H	-1.62423600	-1.18066700	3.27886300
H	1.03691500	-1.17585400	-1.39979900
H	1.87922200	1.09504600	-1.68928800
N	-0.06553600	-2.09838200	0.99305900
C	0.42492200	-2.78496200	2.18089300
C	-0.46889800	-2.98143900	-0.08770300
H	0.61811100	-2.06579200	2.98160200
H	-0.33392000	-3.48540200	2.53731100
H	1.34988000	-3.34730800	1.98513600
H	-1.00643400	-2.40627600	-0.84501500
H	0.38378700	-3.48602400	-0.56478300
H	-1.13938600	-3.74624800	0.31075200
N	0.98061700	3.30944200	-0.72215700
H	0.39137700	4.05498600	-0.38717600

TI-2346

Zero-point correction= 0.463588 (Hartree/Particle)

Thermal correction to Energy= 0.487465

Thermal correction to Enthalpy= 0.488409

Thermal correction to Gibbs Free Energy= 0.412258

Sum of electronic and zero-point Energies= -900.559429

Sum of electronic and thermal Energies= -900.535552

Sum of electronic and thermal Enthalpies= -900.534608

Sum of electronic and thermal Free Energies= -900.610759

C	0.50940800	0.10374100	1.51686200
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C	0.69653100	-0.67597300	0.40664400
C	0.40261000	-0.32940800	-0.95700300
C	-0.45624800	1.23526100	1.54150500
C	0.41110000	1.01023900	-1.42745600
C	-0.51151300	2.21911800	0.60724800
C	0.19107400	2.17021000	-0.69973500
C	0.97325200	3.60286400	-2.55796500
H	1.13170500	4.67236400	-2.68950100
H	1.93543800	3.09301500	-2.67065100
H	0.29464100	3.25402900	-3.34635700
N	1.03458900	-0.25656900	2.73380600
C	1.63757000	-1.56571400	2.90694000
C	1.67455200	0.78055400	3.54183600
H	0.95513300	-2.34395200	2.55787700
H	2.59929300	-1.66294200	2.38242200
H	1.81374100	-1.72531200	3.97214300
H	2.75972700	0.76712900	3.37847300
H	1.30445600	1.76528700	3.25966300
H	1.47541900	0.61697800	4.60375600
N	-1.27825000	3.39231900	0.75285300
C	-2.49696100	3.44589300	-0.05407600
C	-1.45068600	3.97964900	2.07399700
H	-2.30008100	3.08865700	-1.06765500
H	-3.29330200	2.83090300	0.38707800
H	-2.84812700	4.47923900	-0.11543100
H	-2.26217800	3.51855100	2.64548300
H	-0.52045800	3.88282400	2.63769200
H	-1.66348800	5.04511500	1.94395900

N	-1.54635400	1.15162900	2.46361400
C	-2.48124100	0.10476900	2.05806600
C	-1.34671100	1.17332900	3.90287700
H	-2.68405800	0.18590300	0.98769100
H	-2.10776300	-0.91120600	2.26793400
H	-3.42281900	0.24155100	2.59735900
H	-0.91445300	0.24444500	4.30217400
H	-0.71207400	2.01366100	4.18885100
H	-2.32111800	1.32452900	4.37636600
H	0.64941600	1.15296200	-2.47219600
H	1.25242600	-1.59518200	0.53313000
N	0.32981900	-1.33083700	-1.85529600
C	0.24641900	-1.05881100	-3.28569300
C	0.40163600	-2.72678200	-1.43684900
H	-0.56958700	-0.36303000	-3.49763900
H	1.18287300	-0.64097100	-3.67209000
H	0.04865300	-1.98959600	-3.81336600
H	1.43410400	-3.03977700	-1.24144200
H	-0.19632900	-2.88429300	-0.53741400
H	-0.00235600	-3.35617000	-2.22817000
N	0.42133500	3.37317600	-1.24379900
H	0.07650500	4.14969100	-0.69256300

TI-2347

Zero-point correction= 0.463667 (Hartree/Particle)

Thermal correction to Energy= 0.487383

Thermal correction to Enthalpy= 0.488328

Thermal correction to Gibbs Free Energy= 0.413750

Sum of electronic and zero-point Energies=	-900.547228
Sum of electronic and thermal Energies=	-900.523512
Sum of electronic and thermal Enthalpies=	-900.522567
Sum of electronic and thermal Free Energies=	-900.597145
C	0.30232500 -0.19867400 1.79750900
C	0.78876000 -0.97122400 0.78303500
C	0.47056100 -0.89512900 -0.60652400
C	-0.74276200 0.81194500 1.52631700
C	0.13317400 0.21507500 -1.32532000
C	-0.47872400 1.81991100 0.53593100
C	0.13193200 1.54710700 -0.70737800
C	1.44209000 2.56876400 -2.58889800
H	1.95502200 3.52974200 -2.63877000
H	2.18771100 1.77482200 -2.50741300
H	0.88004100 2.41973800 -3.51225600
N	0.67207500 -0.37608000 3.13361800
C	1.52288000 -1.50896500 3.44925300
C	1.00715700 0.82841000 3.88420800
H	1.06300400 -2.43550600 3.09656200
H	2.53072800 -1.42403200 3.01450400
H	1.62438600 -1.57739700 4.53352300
H	1.94549000 1.28770800 3.53937100
H	0.20975600 1.57003400 3.80786000
H	1.11656600 0.57166500 4.93976200
N	-0.70044200 3.18867900 0.82311200
C	-1.68603500 3.96884400 0.08476700
C	-0.27483000 3.72546500 2.09989500
H	-1.87948800 3.50142300 -0.88278200

H	-2.64347400	4.07281700	0.61102200
H	-1.30086600	4.97777700	-0.09837400
H	-0.95683600	3.50080000	2.93566000
H	0.71542400	3.33747200	2.35047900
H	-0.20163000	4.81353600	2.02060200
H	1.44518900	-1.78951700	1.05458500
H	0.59434900	-1.82357900	-1.15218700
N	-0.09035500	0.18857900	-2.70425100
C	-1.32001000	0.82352100	-3.16978100
C	0.22629000	-1.03295600	-3.41941300
H	-1.43886400	1.81027600	-2.71766800
H	-1.26407400	0.95873100	-4.25246600
H	-2.21024600	0.22071000	-2.93870100
H	1.25871300	-1.32890000	-3.21805800
H	-0.44206700	-1.87014600	-3.16343100
H	0.13203600	-0.84300400	-4.49021800
N	-1.83613900	0.85460000	2.29683200
C	-2.95195000	1.72432700	1.93138800
C	-2.10274700	-0.13689500	3.34682700
H	-3.00524000	1.81656300	0.84475600
H	-3.87715600	1.27488000	2.28764400
H	-2.85824800	2.71708000	2.37534100
H	-1.79832500	-1.13012800	3.01630200
H	-1.57630500	0.09964300	4.27240300
H	-3.17338100	-0.14061300	3.54206800
N	0.57442200	2.60058500	-1.41999700
H	0.56392800	3.45716600	-0.88192300

TI-2356

Zero-point correction= 0.463114 (Hartree/Particle)

Thermal correction to Energy= 0.487408

Thermal correction to Enthalpy= 0.488352

Thermal correction to Gibbs Free Energy= 0.411050

Sum of electronic and zero-point Energies= -900.557949

Sum of electronic and thermal Energies= -900.533654

Sum of electronic and thermal Enthalpies= -900.532710

Sum of electronic and thermal Free Energies= -900.610012

C	-0.01086100	0.02934100	1.65982600
C	0.52454300	-0.76466700	0.68270800
C	0.72250300	-0.32160900	-0.70340900
C	-0.64728400	1.31632800	1.69456400
C	-0.04236000	0.66624300	-1.29160300
C	-1.11099600	2.05341100	0.60176500
C	-0.90444300	1.66680700	-0.77331900
C	-1.35217200	2.40260600	-3.11818000
H	-2.00970300	3.15267200	-3.55689900
H	-0.33088800	2.59356800	-3.47282300
H	-1.67448300	1.42042800	-3.47482800
N	-1.71366600	3.32619000	0.75607000
C	-3.16087200	3.48874700	0.68026300
C	-0.99440000	4.35915000	1.48110400
H	-3.60539000	2.63088200	0.17073700
H	-3.63429300	3.58544500	1.66517200
H	-3.41108600	4.39409400	0.11302400
H	-1.18285200	4.35795200	2.56243200
H	0.07846700	4.23736600	1.32088700

H	-1.28976900	5.33664000	1.08574100
N	-0.91841600	1.77332800	2.97587800
C	-2.29103100	2.01772200	3.40093000
C	-0.01061100	1.46443500	4.06599000
H	-2.99231000	1.71845300	2.62310200
H	-2.50536700	1.40868500	4.28663600
H	-2.46812900	3.06636600	3.66256900
H	-0.24372800	0.51388900	4.57077800
H	1.01912400	1.43409300	3.70642400
H	-0.08197500	2.26011700	4.81259900
H	0.17676600	0.82642600	-2.33684600
N	1.65182600	-0.98087600	-1.45842600
C	1.64345700	-0.88798700	-2.90810100
C	2.92869900	-1.43219100	-0.90081900
H	0.63027900	-1.01562500	-3.29691700
H	2.05427500	0.06312800	-3.27494000
H	2.25785200	-1.69777200	-3.30495400
H	3.73399600	-1.02186900	-1.51726000
H	3.06491300	-1.07407600	0.11602300
H	3.00516400	-2.52372900	-0.90503400
H	-0.08299200	-0.45851500	2.62227000
N	0.94902600	-2.05000600	0.99463900
C	1.15317300	-2.41682900	2.38317700
C	0.45688500	-3.16455800	0.18598100
H	1.73536400	-1.64887600	2.89793400
H	0.21211100	-2.58196000	2.93039800
H	1.72053400	-3.34964400	2.41038700
H	-0.50918900	-3.52513600	0.56415700

H	0.33612900	-2.86920100	-0.85453900
H	1.17524000	-3.98728200	0.22951500
N	-1.46507100	2.49236000	-1.67970200
H	-1.78762200	3.36142200	-1.27415100

TI-2357

Zero-point correction= 0.462498 (Hartree/Particle)

Thermal correction to Energy= 0.487131

Thermal correction to Enthalpy= 0.488075

Thermal correction to Gibbs Free Energy= 0.410152

Sum of electronic and zero-point Energies= -900.567941

Sum of electronic and thermal Energies= -900.543308

Sum of electronic and thermal Enthalpies= -900.542363

Sum of electronic and thermal Free Energies= -900.620286

C	-0.16583700	-0.03418200	1.91946800
C	0.86405300	-0.56973400	1.11340400
C	0.79918900	-0.56494500	-0.32253100
C	-1.10364000	0.93892500	1.57105500
C	0.18909700	0.35841400	-1.13402500
C	-0.85906400	1.93710100	0.52830500
C	-0.14117900	1.70344500	-0.62572800
C	1.38543300	2.74427100	-2.29131000
H	1.72411100	3.77055300	-2.43449600
H	2.21513500	2.15888800	-1.87866600
H	1.12616900	2.33243900	-3.26858800
N	-1.17458400	3.29197000	0.78747000
C	-2.18135500	3.98715400	-0.00424100
C	-0.94844500	3.83810800	2.11201300

H	-2.30351600	3.49563900	-0.97147300
H	-3.16075400	4.02598500	0.49033000
H	-1.86595900	5.02069200	-0.18657000
H	-1.79455000	3.69919900	2.80051500
H	-0.06396300	3.37650600	2.55605200
H	-0.76249800	4.91283300	2.02228300
N	-2.18766500	1.13033200	2.37113900
C	-3.43834400	1.64905300	1.83340200
C	-2.30070000	0.49318800	3.67117800
H	-3.37246100	1.75279400	0.75188400
H	-4.23998300	0.93727100	2.05340300
H	-3.70169700	2.61458700	2.27734400
H	-2.50033700	-0.58358400	3.59227600
H	-1.38949400	0.64852500	4.25426800
H	-3.12539500	0.95805300	4.21277200
H	-0.31666200	-0.53012600	2.86649000
N	1.82218100	-1.32726600	1.69518500
C	2.80915200	-2.04346200	0.89788900
C	1.83653000	-1.53087900	3.13656300
H	3.21349000	-1.39321400	0.11889200
H	3.63079700	-2.35055300	1.54307200
H	2.38725700	-2.94214600	0.43153300
H	1.72730700	-0.57482200	3.65526000
H	1.03589400	-2.20654200	3.46175900
H	2.78934100	-1.97054200	3.42615600
H	1.18534900	-1.45611900	-0.79686400
N	0.04478900	0.14967000	-2.47895900
C	-1.07077000	0.75004600	-3.20662400

C	0.56854800	-1.06624900	-3.07329700
H	-1.32256600	1.72422400	-2.79177400
H	-0.78564000	0.89110600	-4.25165100
H	-1.95479300	0.10153300	-3.17093700
H	1.63492200	-1.17083200	-2.85369300
H	0.04178000	-1.96499200	-2.72368900
H	0.45452100	-1.00176100	-4.15558300
N	0.23554400	2.77555900	-1.39650600
H	0.12261800	3.63358800	-0.87048800

TI-2367

Zero-point correction= 0.461319 (Hartree/Particle)

Thermal correction to Energy= 0.485862

Thermal correction to Enthalpy= 0.486806

Thermal correction to Gibbs Free Energy= 0.409640

Sum of electronic and zero-point Energies= -900.530881

Sum of electronic and thermal Energies= -900.506339

Sum of electronic and thermal Enthalpies= -900.505394

Sum of electronic and thermal Free Energies= -900.582560

C	0.02854600	0.03065400	2.01080000
C	0.68422100	-0.65866200	0.96669800
C	0.76226400	-0.39539300	-0.41582600
C	-0.75955900	1.19734700	1.98124500
C	0.43640600	0.89997900	-0.90849700
C	-0.72243500	2.03044400	0.80626500
C	0.53021700	1.90633800	0.12077400
C	2.97283400	1.73198600	0.42119900
H	3.72438900	2.46190300	0.72092800

H	3.12838000	0.79106300	0.96094800
H	3.05332700	1.53248300	-0.64866100
N	-1.79620600	2.61209400	0.21854600
C	-3.14465700	2.10066600	0.40675900
C	-1.69710000	3.88811500	-0.46980600
H	-3.11246900	1.03129800	0.61139100
H	-3.66635100	2.60105000	1.23080700
H	-3.70695500	2.26745000	-0.51608200
H	-2.26997300	4.65929300	0.06021800
H	-0.65504100	4.20624900	-0.52092800
H	-2.09116300	3.80945500	-1.48790900
N	-1.74128300	1.44226300	2.92806300
C	-2.13889700	0.39596800	3.85027200
C	-1.85924500	2.79203700	3.45967200
H	-2.25259400	-0.54970100	3.31578700
H	-1.42130400	0.25196000	4.67169900
H	-3.10330600	0.65960200	4.29143000
H	-1.13436500	2.98127800	4.26491500
H	-1.70025500	3.52843700	2.66980600
H	-2.86443200	2.94059800	3.86260100
H	0.06094500	-0.48633300	2.96480600
N	-0.19158700	1.19302100	-2.07954100
C	0.21164300	2.34248100	-2.87424500
C	-1.00779100	0.20927700	-2.77148700
H	0.81686400	3.02151900	-2.27102700
H	0.80490000	2.03141200	-3.74433000
H	-0.66620200	2.88411500	-3.23892700
H	-0.42957800	-0.38258200	-3.49087600

H	-1.46074200	-0.46956600	-2.05005000
H	-1.80045800	0.73705500	-3.30959700
H	1.11911500	-1.60335400	1.27936900
N	1.00562700	-1.41074400	-1.34197600
C	2.05802100	-1.17943400	-2.32055200
C	0.87351400	-2.79568800	-0.93272100
H	1.99718300	-0.16164200	-2.71174100
H	3.06213900	-1.33225900	-1.89592200
H	1.93375700	-1.86899100	-3.15964700
H	1.73226900	-3.16192300	-0.34890600
H	-0.03347000	-2.92265100	-0.33758000
H	0.78782700	-3.42151600	-1.82491800
N	1.65588900	2.26343700	0.71464500
H	1.53867200	2.73103200	1.60720200

TI-2456

Zero-point correction= 0.463748 (Hartree/Particle)

Thermal correction to Energy= 0.487656

Thermal correction to Enthalpy= 0.488600

Thermal correction to Gibbs Free Energy= 0.412950

Sum of electronic and zero-point Energies= -900.557730

Sum of electronic and thermal Energies= -900.533823

Sum of electronic and thermal Enthalpies= -900.532878

Sum of electronic and thermal Free Energies= -900.608528

C	0.09710900	0.57481200	2.04026900
C	0.53902300	-0.49255200	1.23838600
C	0.55380500	-0.45473300	-0.20752800
C	-0.83600400	1.58447400	1.57836300

C	0.65357600	0.74961000	-0.96200900
C	-0.85824500	2.23740500	0.39359100
C	0.10545300	1.98636900	-0.68834700
C	1.23035300	3.02904900	-2.62743300
H	1.30051100	4.03810600	-3.03159600
H	2.23353800	2.70321800	-2.32968000
H	0.86923500	2.36569000	-3.42322300
N	-1.72679100	3.32014900	0.14726900
C	-2.70124800	3.08101500	-0.92538700
C	-2.33987000	3.96783600	1.29619700
H	-2.21371100	2.64128300	-1.79663500
H	-3.50246500	2.40552400	-0.59483800
H	-3.14644400	4.03248600	-1.22451000
H	-3.11789000	3.35406200	1.77676800
H	-1.57565400	4.22038000	2.03450800
H	-2.81030100	4.89363100	0.95855700
N	0.66321100	-1.62579300	-0.88526600
C	0.01639400	-2.85328200	-0.41716100
H	0.73267100	-3.57507500	-0.01633800
H	-0.73677400	-2.63232500	0.33548700
H	-0.48957900	-3.30483400	-1.27436000
H	-1.54703000	1.92732300	2.31835800
H	1.12108800	0.66491500	-1.93282300
N	0.98803800	-1.66655500	1.85647200
C	2.33254400	-2.16428300	1.65874400
C	0.16786600	-2.32995000	2.84578200
H	2.74735900	-1.76941300	0.72898900
H	3.01603200	-1.89553200	2.47666600

H	2.32410700	-3.25827600	1.58498300
H	0.40531900	-2.06634100	3.88556500
H	-0.88480700	-2.08953600	2.67455300
H	0.28838600	-3.41453800	2.74214000
N	0.43559600	0.61258200	3.36594000
C	1.80109400	0.28163900	3.76820400
C	-0.31459100	1.40591000	4.32718700
H	2.46447400	0.28951900	2.90271700
H	2.14951300	1.05130100	4.46186300
H	1.87477300	-0.68866400	4.26696000
H	-0.15021700	2.48500800	4.20532500
H	-1.38435500	1.19537200	4.26127700
H	0.00485300	1.11998200	5.32986600
C	1.09119600	-1.66563800	-2.27705100
H	1.28255800	-2.70472600	-2.54429600
H	0.33055200	-1.26393600	-2.95803300
H	2.02620100	-1.11804300	-2.41596300
N	0.33133700	3.03990900	-1.49906400
H	-0.15151200	3.88965300	-1.24305300

TI-2457

Zero-point correction= 0.462426 (Hartree/Particle)

Thermal correction to Energy= 0.486883

Thermal correction to Enthalpy= 0.487827

Thermal correction to Gibbs Free Energy= 0.409793

Sum of electronic and zero-point Energies= -900.558517

Sum of electronic and thermal Energies= -900.534059

Sum of electronic and thermal Enthalpies= -900.533115

Sum of electronic and thermal Free Energies= -900.611150

C	0.38714800	0.77628100	2.02691700
C	0.60544000	-0.37956700	1.16891000
C	0.54206400	-0.30748600	-0.20375800
C	-0.58906400	1.73481300	1.69714800
C	0.31548800	0.77926500	-1.07996400
C	-1.07775200	2.16714300	0.45922200
C	-0.33860300	1.97361200	-0.77686900
C	-0.35976500	4.37513600	-1.39395800
H	0.05141900	4.92299600	-2.24197100
H	-1.36664400	4.75187900	-1.20441200
H	0.25697200	4.58342000	-0.51157800
N	-2.17711200	2.98342800	0.42023800
C	-3.11626700	2.89296400	-0.70012700
C	-2.78857700	3.45119800	1.65306100
H	-2.59704900	2.66212300	-1.62784500
H	-3.86802800	2.11945600	-0.50335000
H	-3.62472800	3.85180100	-0.82135800
H	-3.23590600	2.63498500	2.23673600
H	-2.05877500	3.98003300	2.27235400
H	-3.57669300	4.15939700	1.39764400
H	-1.01854700	2.24505200	2.54618500
N	0.90569500	-1.58603300	1.80977600
C	1.47864000	-2.66440000	1.02716500
C	-0.05601000	-2.05367200	2.80519100
H	2.32847400	-2.29914900	0.44506300
H	1.84488300	-3.43059200	1.71371800
H	0.75737700	-3.14259300	0.34531700

H	0.41129300	-2.83003600	3.41573400
H	-0.35522000	-1.23970300	3.46728400
H	-0.95706500	-2.47347200	2.33609000
N	0.97462800	0.82089300	3.24822900
C	2.23612000	0.13314600	3.53293000
C	0.53633200	1.78520500	4.24652300
H	2.77882500	-0.06982700	2.61210600
H	2.84491000	0.79628500	4.15049000
H	2.08192300	-0.80975900	4.06439200
H	0.72735500	2.81774300	3.92918400
H	-0.53067000	1.66941500	4.46131700
H	1.07657300	1.60010900	5.17353000
H	0.77010800	-1.23149100	-0.72181600
N	0.74535700	0.65224700	-2.42730200
C	1.95027700	-0.12893600	-2.66910200
C	-0.32196900	0.33929200	-3.38144200
H	2.71027100	0.12204300	-1.92691600
H	1.77968100	-1.21704400	-2.65089800
H	2.33928600	0.12587100	-3.65817700
H	-0.68976000	-0.69045900	-3.26156100
H	-1.15960900	1.02822700	-3.25371900
H	0.06195700	0.45457600	-4.39797300
N	-0.36422400	2.95792000	-1.74216300
H	0.28739900	2.71200400	-2.47976400

TI-3456

Zero-point correction= 0.462547 (Hartree/Particle)

Thermal correction to Energy= 0.486514

Thermal correction to Enthalpy= 0.487458
 Thermal correction to Gibbs Free Energy= 0.412144
 Sum of electronic and zero-point Energies= -900.543370
 Sum of electronic and thermal Energies= -900.519403
 Sum of electronic and thermal Enthalpies= -900.518459
 Sum of electronic and thermal Free Energies= -900.593773

C	-0.12570900	0.67940400	1.59040700
C	0.14559300	-0.39081800	0.74366800
C	0.02264800	-0.36960100	-0.71789900
C	-0.44896100	2.06271600	1.19245100
C	0.16673600	0.72736200	-1.51377100
C	0.02089800	2.69466700	0.03734600
C	0.37238000	2.10234800	-1.17775500
C	1.08504400	4.30429300	-2.08099100
H	1.56623500	4.63474700	-3.00059200
H	0.16128900	4.88050800	-1.95111700
H	1.75876300	4.51614900	-1.24496800
N	0.61687400	-1.58462600	1.29155900
C	1.80488700	-1.56471200	2.12062400
C	-0.14427900	-2.82170700	1.29306100
H	2.35138500	-0.63269200	1.96835600
H	1.59658400	-1.67645100	3.19253400
H	2.45930100	-2.39379000	1.82356400
H	-0.38431600	-3.12193100	2.32178300
H	-1.07096000	-2.69442700	0.73707200
H	0.42182000	-3.63821800	0.82842700
N	-0.08763800	0.47160000	2.96682400
C	0.73268600	1.30244900	3.82348100

C	-0.85230500	-0.57043400	3.61779500
H	1.39734200	1.92503200	3.22230600
H	0.13823900	1.95961500	4.47422400
H	1.35800000	0.67077700	4.46560700
H	-1.40266900	-0.14628600	4.46743100
H	-1.57999400	-0.99431600	2.92384000
H	-0.22691300	-1.38421800	4.00448800
H	0.22021100	0.51759600	-2.57908300
H	-0.06801900	3.77076200	0.00587300
N	-1.13977900	2.81047400	2.09380300
C	-1.17471600	4.26178000	2.00966400
C	-2.21596500	2.22984700	2.89757300
H	-0.16746700	4.66781700	1.89254200
H	-1.80908000	4.61894100	1.18746400
H	-1.57737400	4.64820900	2.94651400
H	-3.09521600	2.87100400	2.79152200
H	-2.48575800	1.24031200	2.53408200
H	-1.95664200	2.17151500	3.95814400
N	-0.11933100	-1.62978100	-1.35144500
C	-0.95143500	-1.66090800	-2.54531600
C	1.13815900	-2.34926100	-1.56199900
H	-1.87138400	-1.09748600	-2.37893600
H	-0.45257000	-1.27281600	-3.44916400
H	-1.21622200	-2.70233100	-2.74574000
H	1.70322900	-1.91932200	-2.40467600
H	1.75696300	-2.30181700	-0.66701200
H	0.92202200	-3.39656500	-1.78729100
N	0.82009300	2.88450300	-2.18223300

H	0.95861800	2.45237000	-3.08126400
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TI-23456

Zero-point correction=	0.537230 (Hartree/Particle)
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Thermal correction to Energy=	0.565216
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Thermal correction to Enthalpy=	0.566160
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Thermal correction to Gibbs Free Energy=	0.482656
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Sum of electronic and zero-point Energies=	-1034.391585
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Sum of electronic and thermal Energies=	-1034.363599
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Sum of electronic and thermal Enthalpies=	-1034.362655
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Sum of electronic and thermal Free Energies=	-1034.446159
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C	-0.16402900	0.69230700	1.62080000
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C	0.16726600	-0.36866100	0.80213500
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C	-0.05891200	-0.34972500	-0.64173800
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C	-0.86510200	1.92196600	1.17010400
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C	0.00006600	0.77452700	-1.41292600
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C	-0.30746700	2.73466600	0.14100200
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C	0.22200300	2.13894400	-1.02643200
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C	1.43532900	2.53182000	-3.16340200
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H	2.00830000	3.36844700	-3.56165700
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H	2.11179700	1.68341600	-3.01822200
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H	0.67943500	2.25757300	-3.90654500
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N	0.78177200	-1.49234100	1.37571000
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C	2.14999400	-1.39189400	1.83123900
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C	0.14598000	-2.79050400	1.42867100
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H	2.39091600	-0.35292300	2.06897000
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H	2.28880000	-1.98811300	2.74102000
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H	2.87771200	-1.75286500	1.08723100
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H	0.12013100	-3.15837200	2.46509600
H	-0.87525500	-2.71638600	1.05557200
H	0.66775200	-3.54266500	0.82224400
N	0.09991000	0.66817000	2.98461300
C	0.57218500	1.86291700	3.65414100
C	-0.17269900	-0.47897400	3.83342500
H	1.17719900	2.46363300	2.97254900
H	-0.23488500	2.49873500	4.05105300
H	1.21150700	1.56947100	4.49075000
H	-0.62774600	-0.12691200	4.76664700
H	-0.87782200	-1.15705400	3.35252100
H	0.73183300	-1.04119200	4.08891900
H	-0.00770800	0.60410500	-2.48432200
N	-1.94641800	2.30139400	1.87789900
C	-2.75459700	3.43366100	1.43505500
C	-2.57117100	1.39906500	2.84828500
H	-2.31576900	4.38788400	1.72576900
H	-2.87176700	3.40767100	0.34766800
H	-3.73901700	3.36262400	1.89246600
H	-3.62969900	1.64416200	2.91228300
H	-2.48102200	0.36154400	2.51962300
H	-2.13432300	1.49882100	3.84350200
N	-0.20850900	-1.60803500	-1.28060200
C	-1.10934200	-1.63883400	-2.42296300
C	1.05399100	-2.27610600	-1.59080900
H	-2.03365600	-1.10785600	-2.18811000
H	-0.67687600	-1.21163400	-3.34370900
H	-1.35469000	-2.68284600	-2.63503500

H	1.55094500	-1.80768400	-2.45667000
H	1.73238800	-2.22988400	-0.74063800
H	0.86121000	-3.32570800	-1.82700500
N	-0.23400700	4.14387300	0.22320300
C	0.31630800	4.73842700	1.42576600
C	-1.01608000	5.00974600	-0.65035600
H	1.28009500	4.27821700	1.66215800
H	0.48830500	5.80274200	1.24773000
H	-0.33046600	4.64832700	2.31231400
H	-0.40763700	5.85868700	-0.98212800
H	-1.33152300	4.45353700	-1.53528000
H	-1.91405900	5.42004200	-0.17069700
N	0.83156700	2.94753800	-1.91382100
H	1.01151700	3.88049400	-1.57175800

TI-23457

Zero-point correction= 0.534229 (Hartree/Particle)

Thermal correction to Energy= 0.563570

Thermal correction to Enthalpy= 0.564514

Thermal correction to Gibbs Free Energy= 0.476935

Sum of electronic and zero-point Energies= -1034.403905

Sum of electronic and thermal Energies= -1034.374564

Sum of electronic and thermal Enthalpies= -1034.373620

Sum of electronic and thermal Free Energies= -1034.461199

C	-0.47362500	-0.02901100	2.09155800
C	0.67831900	-0.37178200	1.23637000
C	0.23426200	-0.65372300	-0.10551400
C	-0.83290200	1.29014000	1.92040900

C	0.22502700	0.47585600	-0.92875200
C	-0.26330400	2.14132100	0.91975600
C	0.32680300	1.78915200	-0.32174600
C	1.92967900	2.60596600	-2.02222900
H	2.41541500	3.56250800	-2.21967900
H	2.68392300	1.90815300	-1.62834400
H	1.57535700	2.20059300	-2.97280100
N	1.91902600	-0.14133600	1.60439700
C	3.01967600	-0.19523200	0.65082700
C	2.23034800	0.47527700	2.88835300
H	2.74744700	-0.84369000	-0.18100900
H	3.21962700	0.80872900	0.26226800
H	3.90914600	-0.57414700	1.15602900
H	2.29348300	1.56175100	2.76057300
H	1.44731700	0.25245800	3.61179000
H	3.18829500	0.09525100	3.24535800
N	-1.18277400	-0.99170300	2.72037200
C	-2.53920600	-0.73320200	3.16476900
C	-0.59958700	-2.26672000	3.09567000
H	-2.56690200	-0.20251300	4.12411600
H	-3.06734300	-0.13717200	2.41577400
H	-3.06095800	-1.68494000	3.28345000
H	-1.14504400	-3.09182300	2.62655600
H	0.43996100	-2.31856700	2.76880500
H	-0.62561800	-2.40257700	4.18265000
N	-0.55577400	-1.78903200	-0.25958000
C	0.06606800	-3.09650700	-0.33879700
C	-1.88627400	-1.67137200	-0.82436900

H	0.31631400	-3.38498800	-1.37048600
H	0.98777300	-3.10564500	0.24928500
H	-0.60697600	-3.85740400	0.06981600
H	-2.53496800	-2.43389400	-0.37980300
H	-2.29400400	-0.68794200	-0.58080100
H	-1.92054200	-1.80258500	-1.91488300
N	-0.34594100	3.53989400	1.15627800
C	-0.29703100	3.99160200	2.53856400
C	-1.38738200	4.23095200	0.39129500
H	-1.25333600	3.87850000	3.07212700
H	0.47129100	3.44080200	3.08500300
H	-0.03607300	5.05355100	2.55183200
H	-1.24101400	5.31064700	0.47944900
H	-1.32389100	3.96260900	-0.66445800
H	-2.39383100	3.98645400	0.76254100
H	-1.62157300	1.71068600	2.53644100
N	0.02850200	0.36780600	-2.28846000
C	0.50096600	-0.79827100	-3.00636100
C	-0.95110700	1.19483000	-2.97237800
H	1.35278000	-1.23264600	-2.47845500
H	-0.26175500	-1.57726900	-3.13286600
H	0.83295000	-0.49324400	-4.00406500
H	-1.95842300	0.76073300	-2.91812500
H	-0.96472000	2.19547000	-2.53694400
H	-0.67502900	1.28627400	-4.02637400
N	0.83316500	2.83284500	-1.09667400
H	0.94322000	3.66120700	-0.52388000

TI-23567

Zero-point correction= 0.536568 (Hartree/Particle)

Thermal correction to Energy= 0.564989

Thermal correction to Enthalpy= 0.565933

Thermal correction to Gibbs Free Energy= 0.480111

Sum of electronic and zero-point Energies= -1034.405583

Sum of electronic and thermal Energies= -1034.377163

Sum of electronic and thermal Enthalpies= -1034.376218

Sum of electronic and thermal Free Energies= -1034.462041

C	0.03068700	0.01304900	2.05779200
C	0.83126700	-0.60539000	1.12521100
C	0.43426600	-0.61706300	-0.31047000
C	-0.90555700	1.06526000	1.77138700
C	0.10835200	0.50697900	-1.00368200
C	-0.57318000	2.10784100	0.80947700
C	0.12635700	1.84560100	-0.36144200
C	1.58947600	2.75712000	-2.16842500
H	2.22725900	3.64191300	-2.17690600
H	2.22619000	1.87289200	-2.07821500
H	1.05388500	2.69996600	-3.11914600
N	1.83664900	-1.45401700	1.49443700
C	3.06830800	-1.48184700	0.70994800
C	2.02548600	-1.79500600	2.89232400
H	2.89892200	-1.03827900	-0.26996800
H	3.84652900	-0.89915700	1.21850600
H	3.42477000	-2.50696700	0.58143700
H	2.37060000	-0.93805200	3.48817500
H	1.09456200	-2.17677200	3.31904900

H	2.77463400	-2.58510100	2.95978600
N	0.04147700	-1.88260000	-0.84830000
C	1.01418400	-2.93244600	-1.08407200
C	-1.17546400	-2.38602700	-0.22530400
H	1.87658700	-2.53790700	-1.62546500
H	1.36714500	-3.42107100	-0.16255600
H	0.55167800	-3.69789600	-1.71433300
H	-1.01291800	-2.78219700	0.79162700
H	-1.91887300	-1.58696400	-0.17193600
H	-1.58349800	-3.19255300	-0.84181300
N	-0.67205500	3.46975000	1.18977000
C	-1.58664200	4.37349800	0.50866600
C	-0.24979200	3.85822300	2.52098300
H	-1.77261200	4.01341000	-0.50610600
H	-2.55532300	4.48937500	1.01374100
H	-1.13647500	5.36963600	0.43405900
H	-1.01071500	3.69880100	3.30085600
H	0.64547300	3.29633500	2.79940400
H	0.00229900	4.92286000	2.52116000
N	-0.23285000	0.53737600	-2.34399200
C	0.22931600	-0.46468700	-3.28216100
C	-1.42632100	1.25310300	-2.76292700
H	1.24084900	-0.77754100	-3.01581900
H	-0.40863200	-1.35369500	-3.31985000
H	0.26475300	-0.00453400	-4.27556900
H	-2.28529900	0.57451100	-2.85588600
H	-1.68359800	2.03118900	-2.04351200
H	-1.25820500	1.72734700	-3.73549200

H	0.15487000	-0.24168100	3.10241300
N	-1.95342900	1.22496500	2.59145000
C	-2.12778000	0.36771800	3.75929600
C	-3.06267800	2.11167500	2.25878700
H	-2.11623500	-0.68781600	3.47129100
H	-1.33937200	0.54427900	4.49731600
H	-3.08236300	0.59785400	4.22892500
H	-3.00544800	3.06516400	2.79013800
H	-3.07894900	2.29191800	1.18458300
H	-3.99421800	1.61489500	2.53511400
N	0.68272100	2.86981400	-1.03943900
H	0.67834200	3.73677000	-0.51916400

TI-234567

Zero-point correction= 0.608374 (Hartree/Particle)

Thermal correction to Energy= 0.641337

Thermal correction to Enthalpy= 0.642281

Thermal correction to Gibbs Free Energy= 0.547874

Sum of electronic and zero-point Energies= -1168.240298

Sum of electronic and thermal Energies= -1168.207335

Sum of electronic and thermal Enthalpies= -1168.206391

Sum of electronic and thermal Free Energies= -1168.300798

C	0.12563200	0.11941400	1.55801000
C	0.67937700	-0.50048300	0.43652600
C	0.42568100	-0.15527400	-0.98201700
C	-0.75657400	1.31241400	1.50982300
C	0.43840700	1.16164100	-1.36337000
C	-0.47079900	2.30201100	0.60443100

C	0.72901600	2.02431300	-0.20280000
C	2.34674700	2.99722500	1.37116500
H	3.16091900	3.69690100	1.18262400
H	1.49365700	3.52022900	1.80279000
H	2.67907700	2.22398500	2.06996700
N	-1.87174100	1.37215500	2.33355800
C	-2.54949400	0.15835900	2.74023200
H	-2.17536500	-0.24469300	3.69219900
H	-3.61826900	0.36611400	2.85459600
H	-2.43445100	-0.60927300	1.97260000
C	-2.09647600	2.51952100	3.19309500
H	-1.54219700	3.38235900	2.82080500
H	-3.16047800	2.77839300	3.21582300
H	-1.77776900	2.32302300	4.22745400
N	-1.30035000	3.27891700	0.07418000
C	-0.84696400	4.65920900	0.09907800
C	-2.74139600	3.09563700	0.05698900
H	0.22868700	4.71051600	-0.09372400
H	-1.35334800	5.22589600	-0.68733400
H	-1.04988000	5.15313100	1.06127400
H	-3.14795300	3.64769500	-0.79647400
H	-2.97501800	2.03870900	-0.06741100
H	-3.23624900	3.46108300	0.96527900
N	0.33907600	-0.35928500	2.83306000
C	0.43964300	-1.76427400	3.16750300
C	0.56647200	0.54622200	3.93998000
H	-0.11060600	-2.36098300	2.43898300
H	1.47211000	-2.12511900	3.20390900

H	-0.02736900	-1.91795600	4.14747900
H	1.52898900	0.32411300	4.41846900
H	0.59381100	1.57934300	3.59095100
H	-0.21540400	0.46121900	4.70672700
N	1.70828700	-1.47156400	0.68854400
C	1.53296800	-2.85004500	0.25848200
C	3.02369000	-0.95925300	0.35579300
H	0.52123100	-3.18978000	0.48732200
H	1.70888200	-3.00016900	-0.81613300
H	2.22938400	-3.48392200	0.81779700
H	3.17108900	-0.78804800	-0.72628100
H	3.20159300	-0.01907000	0.88960000
H	3.78344400	-1.67224600	0.68851600
N	0.24419200	-1.20445300	-1.87448000
C	-0.86896100	-2.11659300	-1.68063900
C	0.71404900	-1.09566900	-3.24062000
H	-1.20378000	-2.07585700	-0.64254200
H	-1.72235200	-1.86004800	-2.32639500
H	-0.56937200	-3.14498300	-1.90949800
H	-0.00893500	-0.62194400	-3.91895400
H	1.63840900	-0.51615200	-3.26616100
H	0.92490300	-2.10200300	-3.61612900
N	-0.06503500	1.69602400	-2.54094400
C	-1.45436100	1.44550200	-2.89130300
C	0.44776300	2.96926500	-3.00489700
H	-1.77584700	0.49495800	-2.46568800
H	-2.11689200	2.23854200	-2.51596600
H	-1.56170300	1.39251900	-3.97951000

H	-0.04434500	3.82978700	-2.52540900
H	1.52397600	3.03207600	-2.82616900
H	0.28892800	3.05279000	-4.08383700
N	1.94038500	2.38173100	0.11588100
H	2.67540100	2.02763800	-0.48911300

Cartesian Coordination of (Me)₂N-TI Free Bases and Their Thermochemical Values (M06-2X/6-31g(d,p))

TI-2

Zero-point correction= 0.225468 (Hartree/Particle)

Thermal correction to Energy= 0.237453

Thermal correction to Enthalpy= 0.238397

Thermal correction to Gibbs Free Energy= 0.187990

Sum of electronic and zero-point Energies= -498.482489

Sum of electronic and thermal Energies= -498.470504

Sum of electronic and thermal Enthalpies= -498.469560

Sum of electronic and thermal Free Energies= -498.519967

C	0.71558000	0.41067600	1.70881900
C	0.77252900	-0.57199400	0.77504900
C	0.08604500	-0.58719100	-0.49231400
C	-0.07847500	1.61120400	1.68961600
C	-0.37465100	0.48020000	-1.17662900
C	-0.58519700	2.25505800	0.59850200
C	-0.15635800	1.88595000	-0.78924200
H	1.23813700	0.22351700	2.64429300
H	1.33776500	-1.46526800	1.02575500
H	-0.83099500	0.33255900	-2.15186000
N	0.29903000	2.68962200	-1.66938200
C	0.57285800	4.07167700	-1.31729700
H	1.37069500	4.43569900	-1.96860000
H	-0.31085500	4.69665300	-1.49966600
H	0.86531700	4.21059100	-0.27035200

H	-0.03076800	-1.56284700	-0.95910300
N	-1.44226300	3.35108800	0.68959500
C	-1.86492200	3.75178500	2.01542700
C	-2.50321600	3.44848300	-0.30646800
H	-0.99633000	4.01624900	2.62393000
H	-2.49943000	4.63544600	1.92785500
H	-2.42942300	2.96164500	2.53613700
H	-2.92258800	4.45710600	-0.27904800
H	-2.10628700	3.26801400	-1.30570600
H	-3.31144300	2.72580500	-0.11620100
H	-0.30531000	2.01459900	2.67089000

TI-3

Zero-point correction= 0.225610 (Hartree/Particle)

Thermal correction to Energy= 0.237564

Thermal correction to Enthalpy= 0.238508

Thermal correction to Gibbs Free Energy= 0.187697

Sum of electronic and zero-point Energies= -498.483371

Sum of electronic and thermal Energies= -498.471416

Sum of electronic and thermal Enthalpies= -498.470472

Sum of electronic and thermal Free Energies= -498.521283

C	-0.14520700	-0.44941100	1.37398200
C	0.21133200	-1.10798200	0.25451000
C	0.29664900	-0.60690500	-1.10060200
C	-0.58405500	0.93715700	1.51186600
C	0.33585100	0.67508200	-1.50700900
C	-0.38634700	1.93061100	0.60431200
C	0.29246000	1.90418600	-0.69851600

H	-0.11441800	-1.00330100	2.30810100
H	0.47417000	-2.15628400	0.37612700
H	0.47709800	0.87972900	-2.56516500
N	0.75288000	2.95227700	-1.28766800
C	0.74646300	4.20946300	-0.56906100
H	1.39218400	4.91923800	-1.09017900
H	-0.26233100	4.64789600	-0.53752800
H	1.09625300	4.11755900	0.46932400
H	0.40511800	-1.36791100	-1.86923900
H	-0.78510900	2.90563400	0.85843700
N	-1.16972600	1.20597100	2.76292000
C	-1.37615000	2.58878900	3.13800400
H	-2.18231100	3.07790400	2.56633600
H	-1.64504900	2.62285600	4.19683100
H	-0.45229000	3.15403300	2.99386300
C	-2.29556000	0.36666200	3.15710300
H	-3.23469900	0.70735600	2.69368600
H	-2.13123200	-0.66901900	2.86126000
H	-2.41328200	0.40275600	4.24362300

TI-4

Zero-point correction= 0.225661 (Hartree/Particle)

Thermal correction to Energy= 0.237658

Thermal correction to Enthalpy= 0.238603

Thermal correction to Gibbs Free Energy= 0.187550

Sum of electronic and zero-point Energies= -498.482746

Sum of electronic and thermal Energies= -498.470749

Sum of electronic and thermal Enthalpies= -498.469805

Sum of electronic and thermal Free Energies= -498.520857

C	0.55578300	0.02454800	1.69984500
C	1.07993300	-0.73149400	0.69605400
C	1.54571800	-0.29582400	-0.59795500
C	0.43695500	1.47836000	1.64671800
C	1.34553800	0.85987300	-1.26591800
C	0.44841700	2.32017100	0.59768200
C	0.58521200	2.03956800	-0.84565500
H	1.18735900	-1.79586000	0.87280700
H	1.73903200	0.94644700	-2.27495800
N	0.19342300	2.83628800	-1.77389900
C	-0.54601100	4.02835000	-1.40636500
H	-1.02822500	4.43278400	-2.29856800
H	-1.32041100	3.84866300	-0.64838100
H	0.12444400	4.80835500	-1.01732800
H	2.09728300	-1.05881500	-1.14319300
H	0.37142700	3.37684400	0.84301600
H	0.35062400	1.93734600	2.62945700
N	0.21442000	-0.52028500	2.95260500
C	0.57241300	-1.90041700	3.20179100
H	0.37617100	-2.12457400	4.25301200
H	-0.00289300	-2.61313500	2.58717600
H	1.63681700	-2.05008000	3.00819200
C	-1.13040300	-0.21766100	3.43142900
H	-1.17835900	-0.38761400	4.51036200
H	-1.38506800	0.82382300	3.23450600
H	-1.88796200	-0.85077600	2.94302800

TI-23

Zero-point correction= 0.298986 (Hartree/Particle)

Thermal correction to Energy= 0.314984

Thermal correction to Enthalpy= 0.315928

Thermal correction to Gibbs Free Energy= 0.257278

Sum of electronic and zero-point Energies= -632.309212

Sum of electronic and thermal Energies= -632.293214

Sum of electronic and thermal Enthalpies= -632.292270

Sum of electronic and thermal Free Energies= -632.350920

C	-0.16672000	-0.07735200	1.44516400
C	-0.05759000	-0.86910800	0.34085500
C	-0.51170000	-0.56076100	-0.98773900
C	-0.84329100	1.18972600	1.59951100
C	-0.64366100	0.69098300	-1.47574600
C	-1.05254800	2.05443100	0.54390800
C	-0.20707100	1.85454600	-0.67940000
H	0.20419600	-0.51046500	2.36971000
H	0.37102900	-1.85692300	0.48863900
H	-1.00128600	0.86534900	-2.48747700
N	0.78600700	2.55541500	-1.05016900
C	1.23815900	3.64830800	-0.20783200
H	2.28464700	3.46119700	0.05083600
H	1.22113300	4.57745800	-0.78767300
H	0.66218200	3.79484300	0.71539600
N	-1.31881500	1.53541500	2.89491300
C	-1.44291300	0.48854300	3.88912400
H	-0.48250600	0.19128700	4.34351200
H	-2.09043300	0.84699100	4.69551400

H	-1.90365400	-0.39588600	3.44421000
C	-0.77305400	2.76946900	3.44149300
H	-0.90193900	3.58267800	2.72310800
H	-1.31937400	3.02827400	4.35369100
H	0.29617000	2.67779100	3.69083900
H	-0.72651300	-1.40018200	-1.64506200
N	-1.91138600	3.15846500	0.57542300
C	-3.23562400	2.93393900	1.15671500
C	-2.01572300	3.94543500	-0.64647100
H	-3.14215900	2.44534600	2.12490200
H	-3.73044800	3.90007200	1.28200700
H	-3.85148700	2.30401300	0.49743900
H	-2.65312600	4.80829900	-0.44273200
H	-1.04404900	4.30913000	-0.97532500
H	-2.46801700	3.36820500	-1.47014700

TI-24

Zero-point correction= 0.299404 (Hartree/Particle)

Thermal correction to Energy= 0.315346

Thermal correction to Enthalpy= 0.316290

Thermal correction to Gibbs Free Energy= 0.256926

Sum of electronic and zero-point Energies= -632.315534

Sum of electronic and thermal Energies= -632.299592

Sum of electronic and thermal Enthalpies= -632.298648

Sum of electronic and thermal Free Energies= -632.358012

C	0.28147400	0.11803000	1.69807500
C	0.56664300	-0.72467700	0.66339800
C	0.20871800	-0.56142300	-0.72094700

C	-0.52707300	1.31848900	1.59788400
C	-0.11047100	0.57072200	-1.38006300
C	-0.77135900	2.09918500	0.51048100
C	-0.05482400	1.91776300	-0.79368900
H	1.06749600	-1.65697100	0.89985800
H	-0.28682300	0.53367400	-2.45110200
N	0.52899800	2.83890700	-1.45868000
C	0.67118100	4.17232800	-0.90213400
H	1.55331200	4.63355100	-1.35246500
H	-0.19471700	4.79511200	-1.16095900
H	0.77173100	4.18649900	0.18889700
H	0.25216800	-1.47347500	-1.31278200
N	-1.63174000	3.20091500	0.55873700
C	-2.29749300	3.47422500	1.81392400
C	-2.49501300	3.40939700	-0.59840300
H	-1.55970200	3.64410900	2.60255400
H	-2.89118700	4.38350900	1.70294500
H	-2.96546900	2.65532300	2.12907500
H	-2.89962600	4.42404800	-0.56010200
H	-1.92656000	3.30025100	-1.52226500
H	-3.33430900	2.69719200	-0.61811700
H	-0.96022800	1.64030800	2.53640000
N	0.72236000	-0.17641800	3.01894800
C	1.80077200	-1.13629600	3.14249200
C	-0.32587400	-0.46068500	3.99164300
H	2.60121300	-0.88537600	2.44383400
H	2.19451600	-1.08486100	4.16157700
H	1.48458700	-2.17786400	2.95756800

H	0.10073600	-0.42856400	4.99812100
H	-1.12716900	0.27613300	3.94285000
H	-0.76969500	-1.45757100	3.83278000

TI-25

Zero-point correction= 0.299537 (Hartree/Particle)

Thermal correction to Energy= 0.315283

Thermal correction to Enthalpy= 0.316227

Thermal correction to Gibbs Free Energy= 0.257459

Sum of electronic and zero-point Energies= -632.315077

Sum of electronic and thermal Energies= -632.299331

Sum of electronic and thermal Enthalpies= -632.298387

Sum of electronic and thermal Free Energies= -632.357155

C	0.46273100	0.39644000	1.85559900
C	0.60032900	-0.61239400	0.95233900
C	0.07269300	-0.57410800	-0.40111000
C	-0.26896500	1.63094000	1.72307000
C	-0.28839700	0.49933700	-1.12778300
C	-0.64823200	2.30774800	0.60566100
C	-0.16759500	1.91948200	-0.75385300
H	-0.56928800	0.34136300	-2.16594600
N	0.27211100	2.70932400	-1.65849700
C	0.50981800	4.11038900	-1.36340600
H	1.27133900	4.47604000	-2.05638400
H	-0.39872200	4.70422600	-1.52642900
H	0.83722900	4.29192800	-0.33381400
H	0.06373500	-1.52859100	-0.92083700
N	-1.44081700	3.46639800	0.64790400

C	-1.83558700	3.94919000	1.95287400
C	-2.52915300	3.52448200	-0.32105100
H	-0.95021500	4.14356700	2.56392000
H	-2.37716300	4.88910300	1.82676900
H	-2.48642500	3.24179400	2.49433500
H	-2.91022600	4.54821000	-0.36616100
H	-2.16850200	3.24737000	-1.31269900
H	-3.35875600	2.85230500	-0.05037400
H	-0.56831700	2.04937600	2.67876900
H	0.84546800	0.21705700	2.85534400
N	1.30120700	-1.81067200	1.26537600
C	0.47194500	-3.00971800	1.29694800
C	2.17950800	-1.76395000	2.41553200
H	-0.17424300	-3.06188500	0.42027300
H	1.11499200	-3.89413500	1.29879600
H	-0.16822900	-3.03981900	2.19450300
H	2.80259400	-2.66259400	2.41383800
H	2.82804300	-0.88767500	2.35078200
H	1.63942400	-1.73217000	3.37849000

TI-26

Zero-point correction=	0.299343 (Hartree/Particle)
Thermal correction to Energy=	0.315306
Thermal correction to Enthalpy=	0.316250
Thermal correction to Gibbs Free Energy=	0.257025
Sum of electronic and zero-point Energies=	-632.320714
Sum of electronic and thermal Energies=	-632.304751
Sum of electronic and thermal Enthalpies=	-632.303807

Sum of electronic and thermal Free Energies= -632.363032

C	0.70950000	0.58490500	1.99145800
C	1.15218500	-0.31893500	1.08934500
C	0.76942800	-0.43331700	-0.31333800
C	-0.26608200	1.63247700	1.80609200
C	0.34168900	0.61594800	-1.06003300
C	-0.54759700	2.25731400	0.63074200
C	0.29942500	2.01051300	-0.58500200
H	0.13462900	0.48920600	-2.11665900
N	0.87816100	2.91333200	-1.27611500
C	0.84844700	4.29732700	-0.83590500
H	1.76028500	4.78419200	-1.18982200
H	-0.00061000	4.82363900	-1.29084900
H	0.76940700	4.41746600	0.25040400
N	-1.54480700	3.21958500	0.48795400
C	-2.36756700	3.49303900	1.64705000
C	-2.29011700	3.22983200	-0.76458600
H	-1.74359800	3.82744300	2.48000100
H	-3.06530400	4.29542800	1.40036700
H	-2.94310800	2.61192200	1.97406300
H	-2.81536000	4.18383400	-0.85744300
H	-1.61157400	3.12669600	-1.61180200
H	-3.02972000	2.41560000	-0.80858500
H	-0.80720300	1.92383200	2.70003200
H	1.07154400	0.46411400	3.01046600
H	1.85280800	-1.07517200	1.43300900
N	0.99897900	-1.70856000	-0.86982700
C	0.36948500	-2.82626500	-0.17785700

C	0.88011600	-1.83382500	-2.30663700
H	0.47282400	-2.71572100	0.90155000
H	-0.70493800	-2.90130200	-0.41210300
H	0.85459000	-3.75893200	-0.47963800
H	-0.15633400	-1.71322600	-2.66564200
H	1.50864100	-1.08747900	-2.79755200
H	1.22652700	-2.82816400	-2.59987800

TI-27

Zero-point correction= 0.300339 (Hartree/Particle)

Thermal correction to Energy= 0.316115

Thermal correction to Enthalpy= 0.317060

Thermal correction to Gibbs Free Energy= 0.258591

Sum of electronic and zero-point Energies= -632.319690

Sum of electronic and thermal Energies= -632.303913

Sum of electronic and thermal Enthalpies= -632.302969

Sum of electronic and thermal Free Energies= -632.361438

C	-2.23116300	-0.24956300	0.59012800
C	-1.50771600	-1.02145900	-0.26110800
C	-0.33236600	-0.67315800	-1.00342300
C	-1.94651800	1.10600800	0.96203500
C	0.08278000	0.57321900	-1.39690200
C	-1.21868800	2.01403200	0.25271300
C	-0.80290600	1.75440100	-1.16165800
N	-1.12164400	2.47926100	-2.16211000
C	-2.05168200	3.57931900	-1.97860700
H	-2.54317000	3.77115600	-2.93478000
H	-2.80700400	3.38086700	-1.20951000

H	-1.51801900	4.49238300	-1.68599300
N	-0.95835600	3.31247700	0.72137100
C	0.33165200	3.88665700	0.37294100
C	-1.38367600	3.61296700	2.07213300
H	0.47161700	3.87355000	-0.70877600
H	0.35509800	4.92776000	0.70256300
H	1.17485800	3.35130700	0.83985200
H	-1.13509500	4.65168200	2.29638900
H	-2.46765200	3.49897500	2.15864700
H	-0.90641300	2.96433900	2.82494100
H	-2.35896100	1.41737700	1.91591600
H	-3.04478200	-0.72890100	1.12746700
H	-1.80154300	-2.06569300	-0.33872600
H	0.24910200	-1.52344900	-1.33927400
N	1.22696100	0.75432900	-2.15192100
C	2.09008400	-0.39138200	-2.34866500
C	1.85344700	2.05950200	-2.26367500
H	1.56694400	-1.17645600	-2.90413000
H	2.95787800	-0.08743600	-2.93372100
H	2.43801100	-0.82100300	-1.39707100
H	2.65305600	1.99644900	-3.00318500
H	1.12812900	2.79375200	-2.61307400
H	2.29167700	2.40097600	-1.31297700

TI-34

Zero-point correction=	0.299585 (Hartree/Particle)
Thermal correction to Energy=	0.315537
Thermal correction to Enthalpy=	0.316481

Thermal correction to Gibbs Free Energy= 0.256958
Sum of electronic and zero-point Energies= -632.318916
Sum of electronic and thermal Energies= -632.302963
Sum of electronic and thermal Enthalpies= -632.302019
Sum of electronic and thermal Free Energies= -632.361542

C	0.29908100	0.23264400	1.66769800
C	1.50149500	-0.09003800	1.12541300
C	2.27614600	0.61155100	0.12348700
C	-0.39683000	1.51850900	1.39920500
C	1.83079500	1.44965700	-0.82931600
C	-0.33623100	2.18881600	0.22387200
C	0.44179700	1.90129500	-0.99686800
N	0.06765200	2.21581400	-2.18288300
C	-1.28378300	2.70638400	-2.36457500
H	-1.58403200	2.54505800	-3.40238500
H	-2.02104200	2.22673100	-1.70571000
H	-1.32829200	3.78952600	-2.17972100
H	1.95287000	-1.02096600	1.45116200
H	3.32385500	0.32308700	0.07336600
H	2.51677500	1.80448100	-1.59345000
N	-0.32766900	-0.59487200	2.62334300
C	0.44039800	-1.70286800	3.14893600
C	-1.69332000	-0.99600900	2.29428400
H	1.39704800	-1.34498800	3.53812100
H	-0.12214600	-2.15357900	3.97043200
H	0.63796500	-2.48896300	2.40032400
H	-2.18006500	-1.37739300	3.19642100
H	-2.25910400	-0.13758400	1.93683000

H	-1.70674900	-1.78646000	1.52753900
H	-0.89121800	3.11944700	0.15950000
N	-1.21084200	1.97877000	2.45457700
C	-0.53677700	2.18418900	3.73371000
C	-2.14412600	3.04661000	2.16524400
H	0.13004800	1.35092600	3.94566700
H	0.03928100	3.12265600	3.73661800
H	-1.28693900	2.23552100	4.52811600
H	-1.65525200	4.01999700	1.99199300
H	-2.73755100	2.79379900	1.28248400
H	-2.81725200	3.15593600	3.01966200

TI-35

Zero-point correction= 0.299623 (Hartree/Particle)

Thermal correction to Energy= 0.315615

Thermal correction to Enthalpy= 0.316560

Thermal correction to Gibbs Free Energy= 0.256780

Sum of electronic and zero-point Energies= -632.322885

Sum of electronic and thermal Energies= -632.306892

Sum of electronic and thermal Enthalpies= -632.305948

Sum of electronic and thermal Free Energies= -632.365728

C	-0.18336900	0.15309300	0.98300700
C	0.48092600	-0.54672000	0.02661500
C	0.81267400	-0.04236500	-1.30480600
C	-0.73018800	1.50207700	0.92156800
C	0.91888300	1.23044600	-1.71392400
C	-0.33435300	2.50444200	0.08968600
C	0.68954500	2.47411600	-0.95713900

N	1.30135600	3.51061400	-1.41196400
C	1.09351500	4.77488700	-0.73605100
H	1.87963700	5.47176200	-1.03474800
H	0.13184600	5.22458900	-1.02504700
H	1.09820500	4.68780100	0.35976100
H	1.01935500	-0.81854500	-2.03704100
H	1.23550900	1.41304600	-2.73781400
H	-0.83778200	3.45937400	0.18284900
N	-1.66679800	1.75072900	1.94503600
C	-2.05950900	3.12044600	2.19702600
C	-2.79939100	0.83816700	2.03986200
H	-1.17126800	3.74724300	2.30550000
H	-2.69431500	3.54398900	1.40081300
H	-2.62484300	3.15175400	3.13206800
H	-3.58980200	1.09588200	1.31707600
H	-2.48625800	-0.18695500	1.84348400
H	-3.22387200	0.88733200	3.04675000
H	-0.34033600	-0.32565300	1.94229200
N	0.84079600	-1.89135100	0.22250800
C	0.33547600	-2.56460700	1.39934500
C	2.23101400	-2.24363100	-0.04614600
H	-0.74808700	-2.43916100	1.46310600
H	0.55734000	-3.63098700	1.31035500
H	0.78823000	-2.19843600	2.33590900
H	2.30536200	-3.32066900	-0.21964400
H	2.59882200	-1.72391300	-0.93010200
H	2.88486100	-1.97992900	0.79963700

TI-36

Zero-point correction= 0.299672 (Hartree/Particle)

Thermal correction to Energy= 0.315608

Thermal correction to Enthalpy= 0.316552

Thermal correction to Gibbs Free Energy= 0.257003

Sum of electronic and zero-point Energies= -632.320820

Sum of electronic and thermal Energies= -632.304885

Sum of electronic and thermal Enthalpies= -632.303940

Sum of electronic and thermal Free Energies= -632.363490

C	-0.58394900	0.19737300	1.44209300
C	0.21360200	-0.43721000	0.56782100
C	0.78314000	0.06818500	-0.68079600
C	-1.08786800	1.56976000	1.41272000
C	1.00012000	1.37984200	-0.94680900
C	-0.49826500	2.58537400	0.74063400
C	0.70620500	2.55244600	-0.10392000
N	1.33882700	3.66871500	-0.20218200
C	2.50030300	3.73263700	-1.06533900
H	3.07829900	4.62482700	-0.81514200
H	3.15904100	2.85667700	-0.97995700
H	2.20747100	3.82145200	-2.12243900
H	1.45146100	1.62931600	-1.90073800
H	-0.88296800	3.59208800	0.85875800
N	-2.17493100	1.77488200	2.29239900
C	-2.55413500	3.14571200	2.56527900
C	-3.34095300	0.93760600	2.03627100
H	-1.68469000	3.71041100	2.90841000
H	-2.98271500	3.65837600	1.68769400

H	-3.30557100	3.14500000	3.35896600
H	-3.91575900	1.28788000	1.16359600
H	-3.03952900	-0.09404300	1.84882200
H	-3.99620100	0.95130100	2.91146900
H	-0.89015900	-0.36158000	2.32344400
H	0.49568000	-1.45959500	0.80647400
N	1.21679700	-0.95007800	-1.54839700
C	0.23520100	-1.97005400	-1.89702800
C	2.02629700	-0.56756500	-2.68545300
H	-0.36102500	-2.24443000	-1.02696800
H	-0.45186800	-1.62168600	-2.68426600
H	0.75196300	-2.86329600	-2.25876500
H	1.46239300	-0.00449900	-3.44769000
H	2.86874100	0.04319300	-2.35210700
H	2.41697100	-1.47467100	-3.15328000

TI-45

Zero-point correction= 0.298847 (Hartree/Particle)

Thermal correction to Energy= 0.315076

Thermal correction to Enthalpy= 0.316020

Thermal correction to Gibbs Free Energy= 0.255615

Sum of electronic and zero-point Energies= -632.308640

Sum of electronic and thermal Energies= -632.292410

Sum of electronic and thermal Enthalpies= -632.291466

Sum of electronic and thermal Free Energies= -632.351872

C	0.53766900	0.19128700	1.59922400
C	1.26988700	-0.44352400	0.62009800
C	1.76192700	0.18572900	-0.59218600

C	0.06397000	1.56414000	1.52149100
C	1.47169500	1.35396900	-1.20316600
C	0.03910800	2.48949700	0.53937700
C	0.53796900	2.41808000	-0.83793400
N	0.28481600	3.28405700	-1.75688600
C	-0.63612700	4.36404700	-1.46381000
H	-0.87112700	4.88950200	-2.39160400
H	-1.58029500	4.01879400	-1.01940100
H	-0.19724700	5.09895400	-0.77320500
H	2.45410600	-0.43573500	-1.15242400
H	1.95418000	1.54594600	-2.15812000
N	0.23448600	-0.41630400	2.83041400
C	1.14773700	-1.31561400	3.49679200
C	-1.14353200	-0.52487900	3.26323400
H	2.17540800	-1.05638000	3.24272400
H	1.00917100	-1.19491600	4.57834000
H	0.99131800	-2.37537800	3.24549000
H	-1.22288500	-0.32627500	4.33871800
H	-1.76666700	0.19576300	2.73064700
H	-1.56063400	-1.52890000	3.07954300
H	-0.37955200	3.45034000	0.82435700
N	1.55128800	-1.82680600	0.79358300
C	0.39031600	-2.69274300	0.65484500
C	2.73558100	-2.38484700	0.17656400
H	-0.44386100	-2.28778200	1.23042200
H	0.07029400	-2.80156400	-0.39457400
H	0.63166400	-3.68598000	1.04852500
H	2.63387300	-2.56747100	-0.90682300

H	3.59101100	-1.72558800	0.34139900
H	2.95253700	-3.34610200	0.65311500
H	-0.33292100	1.90287400	2.47648300

TI-234

Zero-point correction= 0.372128 (Hartree/Particle)

Thermal correction to Energy= 0.392253

Thermal correction to Enthalpy= 0.393197

Thermal correction to Gibbs Free Energy= 0.325084

Sum of electronic and zero-point Energies= -766.137795

Sum of electronic and thermal Energies= -766.117670

Sum of electronic and thermal Enthalpies= -766.116725

Sum of electronic and thermal Free Energies= -766.184839

C	0.21883400	0.25941100	1.46794300
C	1.05467000	-0.32499500	0.57379300
C	1.16139700	-0.07761600	-0.84142600
C	-0.79469700	1.29738100	1.16554400
C	0.82553900	1.04243100	-1.50430100
C	-0.70292800	2.22930600	0.16943800
C	0.33756700	2.29051900	-0.89366100
N	0.65675100	3.45864900	-1.32020700
C	1.63294500	3.55955000	-2.38919300
H	2.01888000	4.58046200	-2.41914800
H	2.47750900	2.86827200	-2.27219100
H	1.17009400	3.35676700	-3.36538300
N	-1.90416300	1.28491600	2.05855700
C	-1.78122400	2.04254400	3.29148300
C	-3.23867800	1.35266000	1.49379100

H	-0.75607600	1.98476300	3.65727500
H	-2.06893200	3.09797100	3.15394800
H	-2.44231300	1.60761900	4.05148700
H	-3.60521700	2.37978800	1.36969800
H	-3.24845800	0.86463700	0.51617600
H	-3.92243400	0.80824800	2.15865700
H	1.66960700	-1.13966400	0.94614600
H	1.58919100	-0.89314900	-1.42131700
N	-1.65459100	3.29077500	0.18848300
C	-1.19865400	4.50928300	0.85231700
C	-2.31942800	3.57434200	-1.07241000
H	-0.60590800	4.24512800	1.73048100
H	-0.58381100	5.13452700	0.19203400
H	-2.07446100	5.08013200	1.18617600
H	-1.68144900	4.11538700	-1.78537800
H	-2.64996300	2.63712400	-1.53009500
H	-3.20798600	4.18097200	-0.86471700
H	0.98137100	1.06994700	-2.57996800
N	0.26043500	-0.15675600	2.83726200
C	-0.71188100	-1.19437500	3.17535100
C	1.57567100	-0.50986500	3.34279400
H	-1.69431300	-0.91049600	2.80242400
H	-0.42101000	-2.16812100	2.74436400
H	-0.75889600	-1.29887900	4.26400400
H	1.92936100	-1.50066300	3.00873200
H	2.30681500	0.24151300	3.03791100
H	1.52856200	-0.53425100	4.43597100

TI-235

Zero-point correction= 0.371675 (Hartree/Particle)

Thermal correction to Energy= 0.392115

Thermal correction to Enthalpy= 0.393059

Thermal correction to Gibbs Free Energy= 0.323591

Sum of electronic and zero-point Energies= -766.139124

Sum of electronic and thermal Energies= -766.118684

Sum of electronic and thermal Enthalpies= -766.117740

Sum of electronic and thermal Free Energies= -766.187209

C	-0.07071000	0.32947100	1.35861800
C	0.74440200	-0.35499800	0.52775300
C	0.86865200	-0.11679900	-0.89977000
C	-1.00463000	1.41745000	1.08916500
C	0.59135900	1.02373600	-1.55186300
C	-0.89017300	2.33520200	0.07750600
C	0.17529400	2.31055300	-0.95345400
N	0.60266900	3.44674400	-1.37152800
C	1.61943800	3.46679700	-2.40660100
H	2.09662100	4.44904500	-2.41214800
H	2.39558100	2.70233300	-2.27136700
H	1.17347200	3.31616500	-3.39997500
N	-2.06120400	1.44337900	2.03286000
C	-1.74592000	1.78959700	3.40547300
C	-3.39530400	1.84489400	1.63846100
H	-0.73967000	1.45799900	3.66811200
H	-1.80147900	2.87612000	3.58504300
H	-2.45633300	1.30252800	4.08269000
H	-3.57622800	2.92516200	1.72388600

H	-3.57595800	1.55492200	0.60240000
H	-4.10719900	1.31509500	2.28409800
H	1.23113000	-0.95941400	-1.48738000
N	-1.76126300	3.45384800	0.08077900
C	-1.32857600	4.56435300	0.91738800
C	-2.28850100	3.89201300	-1.19833000
H	-0.94189000	4.17803200	1.86318700
H	-0.54393100	5.16325700	0.43309300
H	-2.19041000	5.20746100	1.13531000
H	-1.57356100	4.48886500	-1.78046500
H	-2.58087500	3.01917400	-1.78912800
H	-3.18698200	4.49222100	-1.01366700
H	0.73525200	1.04128600	-2.63036300
H	-0.11999300	-0.07779000	2.36574800
N	1.43829700	-1.48717500	1.08199600
C	0.76395300	-2.74765000	0.80250600
C	2.84546500	-1.54178200	0.71513200
H	-0.27363600	-2.68871000	1.13742900
H	0.77059400	-3.01673000	-0.26922700
H	1.26382600	-3.55095600	1.35225300
H	3.01959500	-1.79935000	-0.34417100
H	3.31369500	-0.57580900	0.91665800
H	3.34140100	-2.30082200	1.32766400

TI-236

Zero-point correction= 0.372758 (Hartree/Particle)

Thermal correction to Energy= 0.392870

Thermal correction to Enthalpy= 0.393814

Thermal correction to Gibbs Free Energy= 0.325446
Sum of electronic and zero-point Energies= -766.146311
Sum of electronic and thermal Energies= -766.126199
Sum of electronic and thermal Enthalpies= -766.125255
Sum of electronic and thermal Free Energies= -766.193623

C	-0.12065100	0.50829600	1.87953900
C	0.75762200	-0.24572400	1.19666700
C	0.99699700	-0.25026900	-0.24396000
C	-1.06705400	1.51629900	1.40407900
C	0.75713300	0.81913200	-1.04008800
C	-0.87575100	2.29312500	0.29914500
C	0.28363300	2.15176500	-0.62532300
N	0.71636100	3.24324400	-1.14802900
C	1.81907200	3.16550300	-2.08595500
H	2.26309800	4.15723300	-2.19449300
H	2.60183000	2.45952600	-1.77605200
H	1.46993600	2.85353900	-3.08116400
N	-2.20475200	1.60978900	2.24990800
C	-2.01987100	2.23380900	3.54669600
C	-3.50735700	1.88395200	1.67653200
H	-1.03422900	1.99613700	3.95330800
H	-2.11172400	3.33175200	3.50180300
H	-2.77739200	1.86195700	4.24523700
H	-3.71790600	2.95444500	1.54802900
H	-3.58307300	1.40812600	0.69720300
H	-4.26417200	1.44846700	2.34075800
N	-1.77115500	3.36808800	0.06382200
C	-1.42613300	4.61440400	0.73450000

C	-2.19627700	3.57964500	-1.30855500
H	-1.09883200	4.40080000	1.75437500
H	-0.62286700	5.15295800	0.21197200
H	-2.31728600	5.25247100	0.78452200
H	-1.44832600	4.10787700	-1.91506900
H	-2.40910000	2.61385300	-1.77581900
H	-3.12396000	4.16327400	-1.29833900
H	0.98558300	0.73968300	-2.09791200
H	-0.21110400	0.29119500	2.94175900
H	1.34250200	-0.96722400	1.76064400
N	1.60321600	-1.42375800	-0.72264400
C	2.08508100	-1.41822500	-2.08715200
C	0.95543900	-2.68354800	-0.37743700
H	2.73622100	-0.55503500	-2.24634500
H	2.66595900	-2.32857500	-2.25488700
H	1.27265200	-1.38852800	-2.83238200
H	1.67361500	-3.50104700	-0.48492200
H	0.60260000	-2.66612700	0.65329200
H	0.09180100	-2.88992300	-1.02897800

TI-237

Zero-point correction= 0.373213 (Hartree/Particle)

Thermal correction to Energy= 0.393054

Thermal correction to Enthalpy= 0.393999

Thermal correction to Gibbs Free Energy= 0.327253

Sum of electronic and zero-point Energies= -766.146091

Sum of electronic and thermal Energies= -766.126249

Sum of electronic and thermal Enthalpies= -766.125305

Sum of electronic and thermal Free Energies= -766.192051

C	0.28822500	0.71516500	1.89493000
C	1.24380300	0.09005300	1.17239500
C	1.35613600	-0.01317400	-0.26031800
C	-0.85390900	1.48664700	1.42455100
C	0.82170200	0.84459900	-1.16851800
C	-0.89666000	2.15188800	0.22622900
C	0.23459200	2.15546400	-0.73259400
N	0.60051300	3.29518900	-1.18790400
C	1.73275200	3.39656200	-2.09021400
H	2.16306500	4.39483100	-1.98127200
H	2.50837700	2.64500200	-1.90289000
H	1.41465100	3.28579800	-3.13502100
N	-1.92307200	1.51747400	2.34745400
C	-1.72476300	2.11066000	3.65414800
C	-3.29819800	1.54809600	1.90235900
H	-0.66832300	2.10582600	3.92612900
H	-2.07423500	3.15592000	3.69214700
H	-2.28057200	1.54835800	4.41396300
H	-3.69957300	2.56390900	1.77418100
H	-3.38782600	1.02870800	0.94787600
H	-3.90585000	1.02448900	2.65159400
H	0.29674400	0.52915400	2.96519600
H	1.95105100	-0.51388400	1.73582300
H	1.89963700	-0.88192700	-0.61551700
N	0.91711300	0.65069500	-2.54718500
C	1.54356200	-0.57315800	-2.99908200
C	-0.21762600	1.06242800	-3.36030900

H	2.56567500	-0.63492900	-2.61584600
H	0.99670800	-1.47458800	-2.67826000
H	1.58915200	-0.56190800	-4.08959200
H	-1.08030500	0.38692500	-3.24495600
H	-0.52973000	2.07198900	-3.09031700
H	0.08265600	1.06543600	-4.41106800
N	-1.95877400	3.06360400	-0.01214400
C	-1.82983500	4.33607300	0.68659100
C	-2.40018500	3.22753400	-1.38062200
H	-1.54062600	4.15114300	1.72349200
H	-1.07765200	4.98770900	0.21924400
H	-2.80098600	4.84596400	0.68580600
H	-1.70471900	3.81934900	-1.99652400
H	-2.53460300	2.24369800	-1.84049300
H	-3.37217100	3.73271000	-1.37461200

TI-245

Zero-point correction= 0.372486 (Hartree/Particle)

Thermal correction to Energy= 0.392620

Thermal correction to Enthalpy= 0.393564

Thermal correction to Gibbs Free Energy= 0.324983

Sum of electronic and zero-point Energies= -766.145631

Sum of electronic and thermal Energies= -766.125496

Sum of electronic and thermal Enthalpies= -766.124552

Sum of electronic and thermal Free Energies= -766.193133

C	0.23144500	0.04364000	1.58121300
C	0.39211500	-0.76967000	0.49102500
C	-0.11330300	-0.48178700	-0.84250500

C	-0.49518100	1.31171300	1.55652600
C	-0.31808700	0.70924800	-1.43550500
C	-0.67299300	2.19686300	0.54334400
C	-0.04124400	2.00849300	-0.80063100
N	0.62140800	2.88061900	-1.45552800
C	0.95184800	4.15269200	-0.83775900
H	1.88278200	4.51391800	-1.28107600
H	0.17428700	4.89631500	-1.05472900
H	1.06308300	4.10033500	0.25117100
N	0.60622100	-0.30485000	2.89392700
C	0.71354100	-1.67857900	3.33852500
C	1.54837600	0.58208300	3.55161900
H	-0.07302400	-2.27736900	2.87799400
H	1.67880600	-2.14698900	3.10828400
H	0.56408000	-1.68661400	4.42553400
H	2.59287100	0.34340300	3.29173400
H	1.35500900	1.61769000	3.26449100
H	1.43990800	0.49477300	4.63796800
H	-0.23363000	-1.35889000	-1.47793500
H	-0.94883000	1.53354200	2.51620000
H	-0.59301300	0.74377800	-2.48628900
N	1.15755600	-1.98182400	0.62020800
C	0.44231400	-3.20131700	0.28796400
C	2.43492800	-1.90275400	-0.07259100
H	-0.53025900	-3.20578900	0.78710200
H	0.27361400	-3.34253300	-0.79404700
H	1.01795100	-4.06310400	0.64319700
H	2.33072300	-1.86671600	-1.17116900

H	2.96738500	-1.00496900	0.24958300
H	3.03877800	-2.77932300	0.18604800
N	-1.42394000	3.36872200	0.68504100
C	-2.30444200	3.72811800	-0.42025700
C	-2.01436700	3.62755200	1.98064800
H	-1.78613800	3.61649900	-1.37307900
H	-3.21196100	3.10530500	-0.44141500
H	-2.60257800	4.77404200	-0.31024100
H	-2.77465600	2.88014300	2.26080000
H	-1.23805700	3.63699500	2.75027400
H	-2.48690000	4.61178100	1.95763300

TI-246

Zero-point correction= 0.373970 (Hartree/Particle)

Thermal correction to Energy= 0.393748

Thermal correction to Enthalpy= 0.394692

Thermal correction to Gibbs Free Energy= 0.327075

Sum of electronic and zero-point Energies= -766.154268

Sum of electronic and thermal Energies= -766.134490

Sum of electronic and thermal Enthalpies= -766.133546

Sum of electronic and thermal Free Energies= -766.201163

C	0.36335800	0.09814000	1.57870200
C	0.60703500	-0.64553800	0.46539900
C	0.21232700	-0.36004500	-0.90527300
C	-0.42482700	1.32331300	1.62416200
C	-0.02503200	0.87887600	-1.40725900
C	-0.60951700	2.22865600	0.63406100
C	0.13141600	2.13506600	-0.66577600

N	0.78764800	3.08551600	-1.21249400
C	0.98563700	4.33540200	-0.50120400
H	1.92812700	4.77223700	-0.84080100
H	0.18830700	5.04969100	-0.74470900
H	1.00911100	4.22767900	0.58945800
N	0.69592000	-0.37859700	2.86756000
C	1.19745200	-1.73049900	2.97974500
C	1.45406900	0.54810700	3.69963200
H	0.49929300	-2.42831900	2.51183400
H	2.19152900	-1.86383400	2.51929200
H	1.27946400	-1.98322600	4.03989700
H	2.51839400	0.57900100	3.41567700
H	1.05057700	1.55680400	3.60789500
H	1.38389200	0.23745500	4.74599700
H	-0.95374000	1.45008000	2.56241300
H	-0.18422000	1.00610100	-2.47227800
N	-1.45545800	3.33241900	0.76064300
C	-2.26494100	3.68213100	-0.40063500
C	-2.16576200	3.47966500	2.01267200
H	-1.65601800	3.67421700	-1.30489100
H	-3.10583100	2.98523200	-0.53895200
H	-2.66575200	4.68946300	-0.26213500
H	-2.87696100	2.65837600	2.19891600
H	-1.45528100	3.51706500	2.84284300
H	-2.71869600	4.42088700	1.99275200
H	1.07370700	-1.61006100	0.61095000
N	0.12304200	-1.51249900	-1.73757600
C	-0.55857600	-1.33388200	-3.00315500

C	1.37601900	-2.23274100	-1.93618600
H	-1.52370300	-0.85066900	-2.83879400
H	0.01742800	-0.73228100	-3.72805900
H	-0.72896800	-2.31870200	-3.44674900
H	2.06522800	-1.67644000	-2.59283400
H	1.88492900	-2.41646900	-0.99061200
H	1.16268300	-3.20084900	-2.39801300

TI-247

Zero-point correction= 0.373291 (Hartree/Particle)

Thermal correction to Energy= 0.393416

Thermal correction to Enthalpy= 0.394360

Thermal correction to Gibbs Free Energy= 0.325915

Sum of electronic and zero-point Energies= -766.159184

Sum of electronic and thermal Energies= -766.139059

Sum of electronic and thermal Enthalpies= -766.138114

Sum of electronic and thermal Free Energies= -766.206560

C	0.18250700	-0.09736800	1.79198900
C	0.44160900	-0.93306400	0.74688700
C	0.11559600	-0.73033500	-0.64695600
C	-0.52055800	1.17192100	1.66684900
C	0.04931000	0.45878900	-1.29646400
C	-0.48895700	1.99501600	0.59119100
C	0.43086600	1.69724100	-0.54853800
N	1.43046500	2.40292900	-0.89364000
C	1.75251900	3.58834800	-0.11483000
H	2.83108100	3.75127200	-0.16817800
H	1.25986200	4.46199100	-0.55711600

H	1.44173100	3.52156800	0.93399900
N	0.42052400	-0.47057300	3.13971000
C	0.81786900	-1.83924500	3.38542800
C	1.24327600	0.46694600	3.89336700
H	0.09561700	-2.52310700	2.93368800
H	1.82098900	-2.07748600	2.99045200
H	0.83071500	-2.01100700	4.46508100
H	2.30966700	0.39393600	3.62159200
H	0.91584100	1.49049700	3.70489200
H	1.14355900	0.26087900	4.96319200
H	-1.13095200	1.43051700	2.52652500
N	-1.20879800	3.18935200	0.48043600
C	-1.77053600	3.48447800	-0.83225500
C	-2.10664300	3.50178900	1.57169700
H	-1.02204600	3.32296700	-1.61047800
H	-2.64219100	2.85389400	-1.06388300
H	-2.07719700	4.53319600	-0.85821800
H	-2.90656400	2.75290300	1.69015300
H	-1.54689600	3.55944500	2.50913800
H	-2.56264700	4.47617500	1.38478900
H	0.88439400	-1.89814300	0.96961600
H	-0.04927700	-1.63581600	-1.22471800
N	-0.45849800	0.62639400	-2.59337000
C	0.35854100	1.34793100	-3.56401700
C	-1.10833100	-0.52485300	-3.18421200
H	0.85677500	2.18993000	-3.08897400
H	1.13332500	0.69684200	-3.99917900
H	-0.28549600	1.70803200	-4.37212200

H	-0.39839000	-1.32019400	-3.46777200
H	-1.83467200	-0.94020600	-2.48211000
H	-1.63225400	-0.20424400	-4.08897400

TI-345

Zero-point correction= 0.372405 (Hartree/Particle)

Thermal correction to Energy= 0.392521

Thermal correction to Enthalpy= 0.393465

Thermal correction to Gibbs Free Energy= 0.323379

Sum of electronic and zero-point Energies= -766.138372

Sum of electronic and thermal Energies= -766.118256

Sum of electronic and thermal Enthalpies= -766.117312

Sum of electronic and thermal Free Energies= -766.187399

C	0.19346500	0.20365500	1.34462100
C	0.91658600	-0.48573300	0.41394600
C	1.16890200	-0.13428600	-0.97395500
C	-0.62755200	1.40505200	1.05380800
C	0.90298100	0.97661300	-1.68203400
C	-0.57388300	2.21945500	-0.03097200
C	0.24740400	2.20767800	-1.24426200
N	0.38392700	3.21546500	-2.03521000
C	-0.23684300	4.47620400	-1.68288900
H	0.10554900	5.24454500	-2.37874200
H	-1.33320700	4.42721000	-1.76025500
H	0.00490300	4.80566900	-0.66250100
N	-1.60055800	1.68492600	2.06271900
C	-1.06912500	2.38313300	3.23091400
C	-2.83339400	2.30928200	1.61947900

H	-0.15102700	1.90421200	3.56490000
H	-0.86920100	3.44358000	3.00018500
H	-1.80415100	2.33702900	4.04066700
H	-2.73456200	3.38823100	1.40842000
H	-3.20434400	1.81123800	0.72141900
H	-3.57565100	2.20087500	2.41619800
H	1.23278700	1.02138900	-2.71652300
H	-1.25446300	3.06333400	0.00586400
N	0.12223700	-0.23750200	2.69405900
C	-0.95801400	-1.15358700	3.00790300
C	1.35626000	-0.55553700	3.38660000
H	-1.86805500	-0.83181700	2.49984700
H	-0.71478800	-2.18899700	2.71534500
H	-1.14476500	-1.13758100	4.08803600
H	1.68423400	-1.59283700	3.24090400
H	2.15017000	0.11224100	3.04125200
H	1.20535700	-0.37835100	4.45946700
H	1.68587900	-0.92004500	-1.52152300
N	1.45200200	-1.76119300	0.82106800
C	0.75731900	-2.87760100	0.19521100
C	2.89531900	-1.87566300	0.67284900
H	-0.31935700	-2.76679500	0.34202000
H	0.95278000	-2.96564700	-0.88812900
H	1.08086200	-3.80853700	0.67217200
H	3.23406200	-1.92513100	-0.37592800
H	3.38230700	-1.02222500	1.15092600
H	3.23008300	-2.78922200	1.17480500

TI-346

Zero-point correction= 0.373460 (Hartree/Particle)

Thermal correction to Energy= 0.393437

Thermal correction to Enthalpy= 0.394381

Thermal correction to Gibbs Free Energy= 0.326333

Sum of electronic and zero-point Energies= -766.158231

Sum of electronic and thermal Energies= -766.138255

Sum of electronic and thermal Enthalpies= -766.137311

Sum of electronic and thermal Free Energies= -766.205358

C	-0.51112600	-0.01813300	1.52632900
C	0.37895500	-0.58435200	0.67686000
C	1.13429000	0.01578100	-0.42160800
C	-0.86543400	1.42637000	1.52609000
C	0.68224400	1.04012700	-1.18651100
C	-0.92484900	2.17023100	0.40170000
C	-0.56664900	1.78967400	-0.97943400
N	-1.24118800	2.35051500	-1.91672100
C	-0.84738700	2.08714100	-3.28709700
H	-1.68137600	2.33003700	-3.94941500
H	-0.00239800	2.72693500	-3.58098200
H	-0.54896900	1.04469400	-3.46430200
N	-1.24816700	1.94113900	2.78651700
C	-0.23055500	1.82450300	3.82622300
C	-1.87018600	3.24809900	2.79549000
H	0.18788200	0.81884000	3.82791300
H	0.58065900	2.55640800	3.68456200
H	-0.69380600	2.00455200	4.80055300
H	-1.18085200	4.05887000	2.50440000

H	-2.72528600	3.26017500	2.11502800
H	-2.22678600	3.45339000	3.80817700
H	1.28108800	1.37294600	-2.02736800
H	0.54908800	-1.65187100	0.76356000
N	2.29853800	-0.69957100	-0.75031100
C	2.97522100	-0.35710100	-1.98222600
C	3.23139400	-0.97217500	0.33463600
H	3.44482300	0.64031200	-1.95419600
H	3.75760500	-1.09738500	-2.16699300
H	2.26702400	-0.38522000	-2.81400200
H	2.69038400	-1.23330100	1.24421300
H	3.87523400	-1.81194100	0.05836600
H	3.86981900	-0.10204100	0.55528100
H	-1.27318900	3.19485100	0.46801700
N	-1.13307600	-0.77600200	2.53678700
C	-2.59310300	-0.73381500	2.55586900
C	-0.63369200	-2.11219700	2.77638700
H	-2.94096800	0.28371700	2.39198200
H	-3.02145800	-1.39391500	1.78570700
H	-2.94789900	-1.06615200	3.53564100
H	-0.85837500	-2.81597400	1.95708300
H	0.44939900	-2.08617300	2.92422100
H	-1.09971500	-2.49611800	3.68749700

TI-347

Zero-point correction= 0.373788 (Hartree/Particle)

Thermal correction to Energy= 0.393407

Thermal correction to Enthalpy= 0.394351

Thermal correction to Gibbs Free Energy= 0.327323
Sum of electronic and zero-point Energies= -766.146250
Sum of electronic and thermal Energies= -766.126631
Sum of electronic and thermal Enthalpies= -766.125686
Sum of electronic and thermal Free Energies= -766.192715

C	0.21757800	0.38577100	1.75662800
C	1.19979600	-0.01106400	0.90453600
C	1.30560100	0.09460800	-0.52824400
C	-0.98791200	1.12264300	1.34179500
C	0.70005100	0.98523500	-1.35637400
C	-1.08901600	1.84694200	0.20105600
C	-0.05140200	2.14651800	-0.79616300
N	0.06174700	3.36588100	-1.16481700
C	1.09346000	3.75541900	-2.10891300
H	1.33887600	4.80429800	-1.92569600
H	2.00554100	3.15224700	-2.03975900
H	0.72806700	3.67907000	-3.14126800
N	-2.09933300	1.06705100	2.24191000
C	-1.97227900	1.97823200	3.37896500
C	-3.41033700	1.19571600	1.63309600
H	-0.99500100	1.85137800	3.84132600
H	-2.09984900	3.02753500	3.06358400
H	-2.74697900	1.73972900	4.11472600
H	-3.65587100	2.22686600	1.32564100
H	-3.48023500	0.54570900	0.75844700
H	-4.16185900	0.88567300	2.36578100
H	-1.99695300	2.42472200	0.05269700
N	0.30003800	0.03684300	3.14396400

C	-0.46525500	-1.15920900	3.48512400
C	1.63612600	-0.02632700	3.70556000
H	-1.47535900	-1.06947000	3.08743400
H	0.01012400	-2.06979300	3.08071100
H	-0.52028300	-1.25196300	4.57465300
H	2.19798600	-0.93214700	3.41778800
H	2.21006000	0.85070900	3.39925300
H	1.55307000	-0.03068800	4.79708900
H	1.94381200	-0.66287100	-0.97136500
H	1.98123900	-0.62057900	1.35120500
N	0.81060100	0.94217800	-2.74965200
C	1.59606500	-0.13348000	-3.31455900
C	-0.40810100	1.21076500	-3.50358600
H	2.61453500	-0.10128200	-2.91914600
H	1.16970600	-1.12848300	-3.10434400
H	1.64574700	0.00164400	-4.39691100
H	-1.10148300	0.35553300	-3.48173000
H	-0.92010300	2.08256500	-3.09453700
H	-0.14457200	1.42005800	-4.54367300

TI-2345

Zero-point correction= 0.445692 (Hartree/Particle)

Thermal correction to Energy= 0.469871

Thermal correction to Enthalpy= 0.470816

Thermal correction to Gibbs Free Energy= 0.393700

Sum of electronic and zero-point Energies= -899.966508

Sum of electronic and thermal Energies= -899.942328

Sum of electronic and thermal Enthalpies= -899.941384

Sum of electronic and thermal Free Energies= -900.018500

C	0.15742000	0.01051900	1.52511700
C	0.34459000	-0.77192000	0.42613400
C	-0.19025500	-0.48983300	-0.90638400
C	-0.71279200	1.22030200	1.57055200
C	-0.30786200	0.73236100	-1.44337500
C	-0.78511300	2.14104900	0.56936200
C	0.03701000	1.95195400	-0.67697900
N	0.88008800	2.77535700	-1.15533600
C	1.20651800	3.96870500	-0.39357300
H	2.24514400	4.23585200	-0.60220500
H	0.57523200	4.80014800	-0.72949000
H	1.06662500	3.85835500	0.68870000
N	0.67486700	-0.31712000	2.80340900
C	0.75868300	-1.68717300	3.26632700
C	1.80511500	0.49291200	3.21595700
H	-0.08793100	-2.25610600	2.87537900
H	1.68174600	-2.19906300	2.96636100
H	0.69141500	-1.68092300	4.36280100
H	2.75721600	0.10683400	2.81496200
H	1.67552200	1.51777800	2.85811700
H	1.87473200	0.51233700	4.31046000
N	-1.54881400	3.30903900	0.53159700
C	-2.25465700	3.60435100	-0.70679400
C	-2.20551600	3.86191100	1.70195400
H	-1.62008300	3.41092400	-1.57304300
H	-3.17807100	3.01362000	-0.80863400
H	-2.52340200	4.66420800	-0.71663600

H	-3.12623200	3.33670000	1.98285100
H	-1.52874200	3.84511400	2.55466200
H	-2.44614000	4.90646700	1.47513500
N	-1.59712700	1.33127100	2.69480400
C	-2.46050300	0.17552700	2.85621900
C	-1.05517000	1.77070300	3.96991000
H	-2.89747300	-0.09386600	1.89151900
H	-1.93045500	-0.70170200	3.26443400
H	-3.27379100	0.43144900	3.54526700
H	-0.60971300	0.95043100	4.55235100
H	-0.28492500	2.52906000	3.80686200
H	-1.85981500	2.22491400	4.56366300
H	-0.37370500	-1.35230100	-1.54572500
H	-0.60558300	0.86103800	-2.48113600
N	1.21682600	-1.91381900	0.51722300
C	0.58492900	-3.18252500	0.19731800
C	2.44913200	-1.72532100	-0.23618400
H	-0.35576800	-3.27467300	0.74626500
H	0.37264300	-3.31745000	-0.87784500
H	1.24593100	-3.99976800	0.50517700
H	2.29441600	-1.72227600	-1.32905100
H	2.90341500	-0.77262600	0.04582500
H	3.14623100	-2.53361700	0.00961300

TI-2346

Zero-point correction= 0.447356 (Hartree/Particle)

Thermal correction to Energy= 0.471205

Thermal correction to Enthalpy= 0.472150

Thermal correction to Gibbs Free Energy= 0.395957
Sum of electronic and zero-point Energies= -899.980608
Sum of electronic and thermal Energies= -899.956758
Sum of electronic and thermal Enthalpies= -899.955814
Sum of electronic and thermal Free Energies= -900.032007

C	0.56057800	0.19396400	1.48860400
C	0.89046600	-0.48219800	0.36425100
C	0.43105700	-0.21792200	-1.00235200
C	-0.49694200	1.23504300	1.56900200
C	0.20630900	1.04052400	-1.44558400
C	-0.62475100	2.19538200	0.61504300
C	0.33909400	2.21002600	-0.54896000
N	1.09520200	3.18295800	-0.86742500
C	1.15440900	4.34181900	0.00706100
H	2.15520900	4.77471300	-0.06210400
H	0.44094900	5.09983500	-0.33941300
H	0.92427000	4.12096100	1.05671800
N	1.08660700	-0.17478400	2.75242400
C	1.74006200	-1.46259400	2.85416100
C	1.88298500	0.87574000	3.37824300
H	1.08446300	-2.24156500	2.45594900
H	2.70405700	-1.50614700	2.31921000
H	1.93257100	-1.67335900	3.90991100
H	2.90225600	0.91166200	2.96104200
H	1.41547600	1.84658200	3.20855600
H	1.95050900	0.69973900	4.45689200
N	-1.56414300	3.22072100	0.55919700
C	-2.14063600	3.54736000	-0.73647200

C	-2.44238200	3.53071800	1.67256500
H	-1.37338500	3.55821700	-1.51188100
H	-2.92768300	2.83680200	-1.03196000
H	-2.58250700	4.54616200	-0.68329400
H	-3.27857400	2.83032100	1.78380000
H	-1.87589500	3.53374900	2.60287000
H	-2.83922500	4.53789900	1.50585900
N	-1.50726000	1.04744600	2.57204300
C	-2.12495600	-0.26640800	2.49370300
C	-1.20629400	1.40534900	3.94826900
H	-2.39006900	-0.48290300	1.45561700
H	-1.46663700	-1.06976700	2.86628600
H	-3.04067000	-0.26682700	3.09561000
H	-0.60342100	0.64670400	4.47010100
H	-0.66765500	2.35616800	3.97877100
H	-2.14939300	1.53435000	4.49430100
H	-0.02475100	1.25077300	-2.48400700
H	1.62001500	-1.28379700	0.42992600
N	0.43564100	-1.34414500	-1.84389100
C	0.20401500	-1.10654200	-3.25198900
C	-0.29937000	-2.50128800	-1.35137200
H	-0.81239000	-0.73132000	-3.46072100
H	0.92681900	-0.37913500	-3.62859800
H	0.34104700	-2.04532600	-3.79423400
H	0.01052600	-3.39176400	-1.90541500
H	-0.08981900	-2.65820500	-0.29259300
H	-1.38860400	-2.37922600	-1.46978500

TI-2347

Zero-point correction= 0.446976 (Hartree/Particle)

Thermal correction to Energy= 0.470961

Thermal correction to Enthalpy= 0.471906

Thermal correction to Gibbs Free Energy= 0.395060

Sum of electronic and zero-point Energies= -899.981323

Sum of electronic and thermal Energies= -899.957338

Sum of electronic and thermal Enthalpies= -899.956393

Sum of electronic and thermal Free Energies= -900.033239

C	0.16007100	-0.14134400	1.71879800
C	0.36490500	-0.98768800	0.67778700
C	0.01032400	-0.78734900	-0.71142100
C	-0.63754000	1.10659400	1.65184100
C	0.01629300	0.41970900	-1.32551900
C	-0.57735500	1.93999400	0.57641600
C	0.41246600	1.61484200	-0.50598500
N	1.47287300	2.26553300	-0.76061300
C	1.80749100	3.40770100	0.07472700
H	2.89444300	3.45293700	0.17438400
H	1.48111200	4.32552300	-0.42672300
H	1.34744800	3.38090800	1.06956700
N	0.57511200	-0.47316600	3.04381600
C	0.83004300	-1.87117000	3.32232000
C	1.68299100	0.36053800	3.49620300
H	-0.02314800	-2.47212000	2.99796800
H	1.74005900	-2.25858500	2.83142100
H	0.95737800	-1.99566400	4.40193400
H	2.63514600	0.06449500	3.02461200

H	1.48883300	1.40378900	3.23978400
H	1.78904300	0.28099600	4.58349200
N	-1.26452700	3.13545500	0.34645400
C	-1.76152700	3.35610000	-1.00495500
C	-2.12575900	3.73651300	1.35033500
H	-1.03904700	3.02148200	-1.75046900
H	-2.70574200	2.82129900	-1.19070100
H	-1.93672300	4.42635600	-1.14687200
H	-3.07147300	3.19958400	1.49555900
H	-1.61366800	3.78872000	2.30951600
H	-2.34450700	4.75693700	1.01773500
H	0.85685300	-1.93302700	0.89024100
H	-0.18756300	-1.67909900	-1.29873000
N	-0.43052100	0.65115600	-2.63068600
C	0.43398100	1.41091700	-3.52817600
C	-1.06700100	-0.46400800	-3.29994600
H	0.91901600	2.22420300	-2.99234000
H	1.22239900	0.77453800	-3.95940800
H	-0.17137500	1.81660400	-4.34441600
H	-0.35591900	-1.26401000	-3.56571900
H	-1.84228700	-0.88626700	-2.65658600
H	-1.52884600	-0.10119500	-4.22197900
N	-1.59887000	1.32795600	2.69243400
C	-2.48989500	0.19862600	2.89958800
C	-1.13012600	1.87413300	3.95479800
H	-2.86461900	-0.15129900	1.93487900
H	-1.99977600	-0.64156500	3.41773900
H	-3.34337600	0.52638000	3.50428800

H	-0.67436300	1.11606800	4.60941800
H	-0.39317100	2.66078300	3.76891500
H	-1.97923300	2.32538200	4.48447700

TI-2356

Zero-point correction= 0.446396 (Hartree/Particle)

Thermal correction to Energy= 0.470449

Thermal correction to Enthalpy= 0.471393

Thermal correction to Gibbs Free Energy= 0.394080

Sum of electronic and zero-point Energies= -899.970980

Sum of electronic and thermal Energies= -899.946928

Sum of electronic and thermal Enthalpies= -899.945984

Sum of electronic and thermal Free Energies= -900.023297

C	0.31110600	0.33253900	1.70966800
C	0.75268200	-0.51173500	0.74481300
C	0.44789600	-0.35342400	-0.68959000
C	-0.61003000	1.45973400	1.67556600
C	0.10828400	0.83045300	-1.24513900
C	-0.79520400	2.30300500	0.62202600
C	0.06858700	2.15214100	-0.59404500
N	0.68383300	3.09981100	-1.18906800
C	0.72033100	4.42918400	-0.60806300
H	1.62540200	4.92817000	-0.96342700
H	-0.14076900	5.02037700	-0.94417900
H	0.71232300	4.43271500	0.48855900
N	-1.67700900	3.38123800	0.54992100
C	-2.48618400	3.49742800	-0.65042900
C	-2.26979000	4.00181000	1.71713100

H	-1.90180000	3.23146600	-1.53329600
H	-3.37955100	2.85466400	-0.61502700
H	-2.81623100	4.53516200	-0.76082900
H	-3.12683500	3.45315600	2.12795000
H	-1.52416700	4.10363300	2.50560000
H	-2.60007100	5.00408200	1.42006400
N	-1.40246800	1.61683700	2.86881100
C	-2.26475700	0.47485000	3.13202800
C	-0.64185300	2.00345200	4.04477400
H	-2.83648000	0.23837600	2.23182500
H	-1.71354200	-0.43106400	3.43915500
H	-2.96534900	0.73518700	3.93277500
H	0.00533000	1.20185400	4.44300300
H	-0.00965800	2.86286600	3.80624200
H	-1.33586800	2.29212200	4.84160600
H	-0.00723900	0.87527300	-2.32452100
N	0.55090300	-1.52765600	-1.49969200
C	-0.30770000	-1.55483000	-2.66979700
C	1.92736500	-1.85718100	-1.87171500
H	-1.32535500	-1.27228400	-2.39235000
H	0.03297700	-0.88967100	-3.48186800
H	-0.31875900	-2.57495600	-3.06553900
H	2.32296700	-1.13720700	-2.60746500
H	2.55789100	-1.85401800	-0.98438300
H	1.94514200	-2.85637400	-2.31846400
H	0.55942100	0.03049800	2.72503100
N	1.53159500	-1.66003600	1.10497000
C	2.39353000	-1.50556900	2.26182900

C	0.73435500	-2.87945300	1.21210500
H	2.94269500	-0.56428800	2.19301000
H	1.85296100	-1.52765400	3.22473100
H	3.10925900	-2.33360200	2.27349300
H	0.08231800	-2.85447700	2.10301100
H	0.12278900	-2.99378400	0.31778300
H	1.40468500	-3.74094800	1.29694500

TI-2357

Zero-point correction= 0.446554 (Hartree/Particle)

Thermal correction to Energy= 0.470887

Thermal correction to Enthalpy= 0.471831

Thermal correction to Gibbs Free Energy= 0.394256

Sum of electronic and zero-point Energies= -899.979044

Sum of electronic and thermal Energies= -899.954712

Sum of electronic and thermal Enthalpies= -899.953768

Sum of electronic and thermal Free Energies= -900.031343

C	0.21942000	0.18720300	1.90221600
C	0.70069800	-0.71378600	0.99096800
C	0.53667900	-0.64177000	-0.44219000
C	-0.58196500	1.36538300	1.64815700
C	0.31040400	0.48682800	-1.18357400
C	-0.52454000	2.13126700	0.53067500
C	0.45982700	1.82772600	-0.54201300
N	1.35468900	2.60928700	-0.99756600
C	1.50254100	3.90694100	-0.36465800
H	2.50354700	4.29165100	-0.57029500
H	0.76552600	4.60667500	-0.77534400

H	1.34897000	3.86559300	0.72225900
N	-1.39150500	3.22563100	0.19881500
C	-2.67437600	2.76015000	-0.31012600
C	-1.55613300	4.29137600	1.17639100
H	-2.51065200	2.01133300	-1.09109900
H	-3.29855500	2.31189800	0.48094100
H	-3.21964100	3.60334500	-0.74842700
H	-2.20744200	4.01263600	2.01525800
H	-0.57893900	4.57982300	1.57250400
H	-1.98204700	5.16397000	0.66707600
N	-1.51591000	1.74386700	2.68175300
C	-2.42107300	0.66615700	3.05560700
C	-0.86088300	2.31819200	3.84769500
H	-2.87261700	0.24379200	2.15476700
H	-1.93065900	-0.15065900	3.61099500
H	-3.21692900	1.07768900	3.68504400
H	-0.25708500	1.58804600	4.41452900
H	-0.20698100	3.13563700	3.53450200
H	-1.62149000	2.72118700	4.52447400
H	0.32624300	-0.06071000	2.95313300
N	1.39923700	-1.87435000	1.43616400
C	1.89292900	-1.85793400	2.79723200
C	0.74890700	-3.14636700	1.14852500
H	2.42795600	-0.92539300	2.98663400
H	1.09645300	-1.96759300	3.55486300
H	2.58811300	-2.69288900	2.92328500
H	-0.11766000	-3.31954000	1.80933300
H	0.40032700	-3.19073700	0.11750600

H	1.46551200	-3.95878600	1.29955000
H	0.70960900	-1.56604600	-0.97790300
N	-0.00866900	0.45197300	-2.51564200
C	0.03707700	1.64115300	-3.35535300
C	-0.07340100	-0.83372500	-3.17397800
H	-0.44893500	2.47863100	-2.85216500
H	1.06029800	1.94543100	-3.59972800
H	-0.51136100	1.42504100	-4.27427300
H	0.91529900	-1.30486400	-3.27444000
H	-0.71684100	-1.51119500	-2.60256000
H	-0.49943500	-0.70743600	-4.16977700

TI-2367

Zero-point correction= 0.445523 (Hartree/Particle)

Thermal correction to Energy= 0.470235

Thermal correction to Enthalpy= 0.471179

Thermal correction to Gibbs Free Energy= 0.392974

Sum of electronic and zero-point Energies= -899.981931

Sum of electronic and thermal Energies= -899.957219

Sum of electronic and thermal Enthalpies= -899.956274

Sum of electronic and thermal Free Energies= -900.034479

C	-0.11262600	-0.12348000	2.03082800
C	0.58650700	-0.80611800	1.06555100
C	0.62523000	-0.55313800	-0.34407700
C	-0.96717800	1.01777400	1.88199000
C	0.38027300	0.70559100	-0.85765800
C	-0.80761700	1.92148400	0.85170800
C	0.46980700	1.84912100	0.09603600

N	1.44463300	2.63172000	0.32033600
C	2.67971200	2.43609800	-0.41895000
H	2.89792600	3.34098900	-0.99597300
H	3.49096900	2.31493000	0.30438200
H	2.67420400	1.57093200	-1.09436200
N	-1.74986900	2.82774400	0.40441300
C	-3.16576500	2.57326100	0.55115800
C	-1.39105000	4.21402300	0.17600900
H	-3.35096600	1.50069000	0.48999800
H	-3.57545400	2.93540500	1.50527800
H	-3.69060500	3.07804800	-0.26825400
H	-1.74545800	4.86095900	0.99391000
H	-0.30676400	4.30951500	0.11543900
H	-1.84164800	4.57475300	-0.75654700
N	-2.02170200	1.23726000	2.81518700
C	-2.48228400	0.10554300	3.59125700
C	-1.87037100	2.43626500	3.62361900
H	-2.58692700	-0.76838500	2.94467600
H	-1.81383000	-0.16116600	4.42857400
H	-3.46266800	0.34232600	4.01879200
H	-1.08302400	2.33349300	4.38938100
H	-1.61671300	3.28451800	2.98402100
H	-2.81716400	2.65506100	4.12974900
H	-0.07539200	-0.55014800	3.03007100
N	-0.01357000	0.98481000	-2.15153500
C	0.46702700	2.15471900	-2.85502700
C	-0.74001200	0.01133700	-2.93860600
H	0.69164200	2.95532800	-2.14765600

H	1.37236400	1.95437400	-3.44972400
H	-0.31082900	2.51369200	-3.53633400
H	-0.08887100	-0.65065800	-3.52651600
H	-1.33871600	-0.61312400	-2.27508100
H	-1.40318100	0.55028300	-3.62410900
H	1.10452800	-1.70086100	1.40066700
N	0.88753000	-1.61872800	-1.25506400
C	2.09712100	-1.44391600	-2.04170900
C	0.73529100	-2.97376500	-0.76772900
H	2.08871200	-0.46106200	-2.52172900
H	3.01489100	-1.52764400	-1.43474200
H	2.13264100	-2.20560900	-2.82798700
H	1.56666000	-3.31100300	-0.12451500
H	-0.19361100	-3.05830300	-0.19975200
H	0.68438500	-3.65545100	-1.62317300

TI-2456

Zero-point correction= 0.445557 (Hartree/Particle)

Thermal correction to Energy= 0.469920

Thermal correction to Enthalpy= 0.470864

Thermal correction to Gibbs Free Energy= 0.393322

Sum of electronic and zero-point Energies= -899.976811

Sum of electronic and thermal Energies= -899.952448

Sum of electronic and thermal Enthalpies= -899.951504

Sum of electronic and thermal Free Energies= -900.029046

C	0.05851300	0.44877400	1.92381600
C	0.37148200	-0.54344000	1.04398500
C	-0.02587000	-0.53555200	-0.38044200

C	-0.75629500	1.62441400	1.64323600
C	-0.11511400	0.58326300	-1.12868700
C	-0.76192500	2.34288800	0.49244500
C	0.15267500	1.94377400	-0.62845300
N	1.02093100	2.68406000	-1.19410000
C	1.24815700	4.02773600	-0.68724400
H	2.28912000	4.29473700	-0.88286200
H	0.61845300	4.74425200	-1.22976600
H	1.03539400	4.14069800	0.38200700
N	-1.52409600	3.49118700	0.28632100
C	-2.09113300	3.68155700	-1.04309700
C	-2.41789300	3.88159000	1.35605100
H	-1.33903900	3.48329400	-1.80768100
H	-2.95300600	3.02070500	-1.22245500
H	-2.41938100	4.71905800	-1.14394400
H	-3.19086000	3.12255500	1.55808100
H	-1.84997500	4.05048200	2.27514700
H	-2.90876200	4.81709300	1.08111200
N	-0.24119200	-1.77531500	-1.04893500
C	-0.93390800	-2.81086500	-0.30402900
H	-0.25643500	-3.43283200	0.29811500
H	-1.67446200	-2.35550100	0.35897300
H	-1.46568000	-3.45914900	-1.01031200
H	-1.34648100	1.97889500	2.48371000
H	-0.37281000	0.47555600	-2.17984300
N	1.17946700	-1.67413600	1.38600700
C	2.60105400	-1.38756100	1.29473800
C	0.84226200	-2.45631900	2.56188700

H	2.81162800	-0.87065000	0.35382000
H	2.95437400	-0.75947500	2.13011700
H	3.16348900	-2.32820100	1.30540300
H	1.21116300	-2.01994900	3.49902300
H	-0.24430000	-2.56205900	2.62731000
H	1.26976200	-3.46042400	2.44602000
N	0.55061500	0.33888700	3.27677700
C	1.36211000	1.48693500	3.65790600
C	-0.49306300	0.08301200	4.25841900
H	2.13254800	1.65372900	2.90111400
H	0.77853300	2.41750500	3.76704400
H	1.85139600	1.27454400	4.61395900
H	-1.16845400	0.94204100	4.41940500
H	-1.09355700	-0.77383100	3.94483600
H	-0.02737700	-0.15488600	5.22059900
C	0.89878500	-2.30639600	-1.77722300
H	1.62657900	-2.79228700	-1.10548900
H	0.55067900	-3.04981100	-2.50308700
H	1.39886600	-1.50195200	-2.31994600

TI-2457

Zero-point correction= 0.446236 (Hartree/Particle)

Thermal correction to Energy= 0.470676

Thermal correction to Enthalpy= 0.471621

Thermal correction to Gibbs Free Energy= 0.393563

Sum of electronic and zero-point Energies= -899.984936

Sum of electronic and thermal Energies= -899.960496

Sum of electronic and thermal Enthalpies= -899.959552

Sum of electronic and thermal Free Energies= -900.037610

C	-0.00879100	0.38783500	1.99286200
C	0.30063700	-0.63257400	1.13571400
C	-0.02555500	-0.63860500	-0.28836800
C	-0.80238400	1.56282800	1.64034100
C	-0.08921300	0.42969900	-1.11921800
C	-0.75878200	2.22738900	0.46244400
C	0.22565000	1.78606500	-0.57058700
N	1.23595300	2.44658400	-0.96863600
C	1.49705000	3.74621200	-0.36787800
H	2.57261400	3.93137900	-0.40522600
H	0.99995600	4.52888100	-0.95187300
H	1.14491400	3.82381700	0.66719500
N	-1.49105800	3.38032700	0.14358900
C	-2.05455200	3.41310800	-1.20053600
C	-2.41097500	3.84810200	1.15782400
H	-1.29086000	3.15179400	-1.93676700
H	-2.89504000	2.71202300	-1.31952500
H	-2.40663000	4.42577400	-1.41344200
H	-3.20539600	3.11638600	1.38084800
H	-1.86672000	4.05936300	2.08246900
H	-2.87478200	4.77460500	0.81252500
H	-1.43400700	1.95435600	2.43378100
N	0.90232800	-1.85085100	1.53060000
C	2.22732400	-2.10191300	0.99468500
C	0.71582700	-2.39954400	2.85689200
H	2.28450700	-1.75093000	-0.03762300
H	3.01482000	-1.59279700	1.57601700

H	2.43488100	-3.17751000	1.01143800
H	1.41236000	-2.00125500	3.60567200
H	-0.30116500	-2.19556700	3.19652700
H	0.84774500	-3.48726600	2.79153700
N	0.47604500	0.33547900	3.34915500
C	1.51066800	1.33132100	3.58315200
C	-0.55226400	0.39346000	4.37293100
H	2.29017600	1.22800400	2.82442300
H	1.12661700	2.36696800	3.54510300
H	1.95673700	1.16647300	4.57002400
H	-1.01051900	1.39187800	4.49033400
H	-1.34567900	-0.32185500	4.14058800
H	-0.11348300	0.12115100	5.33911800
H	-0.18601800	-1.63295500	-0.69244300
N	-0.57392700	0.37155800	-2.42742700
C	0.17880900	1.03566100	-3.48589500
C	-1.13455100	-0.89180300	-2.85999500
H	0.60273600	1.96984800	-3.12468400
H	1.00784800	0.40591400	-3.84402000
H	-0.49262400	1.23634300	-4.32609300
H	-0.36962000	-1.67367000	-2.99656000
H	-1.86421600	-1.24354200	-2.12736800
H	-1.63873400	-0.73901000	-3.81770400

TI-3456

Zero-point correction= 0.446209 (Hartree/Particle)

Thermal correction to Energy= 0.470327

Thermal correction to Enthalpy= 0.471271

Thermal correction to Gibbs Free Energy= 0.395261
Sum of electronic and zero-point Energies= -899.970869
Sum of electronic and thermal Energies= -899.946751
Sum of electronic and thermal Enthalpies= -899.945807
Sum of electronic and thermal Free Energies= -900.021817

C	-0.07752700	0.67748100	1.56871800
C	0.15648800	-0.37709000	0.72433700
C	-0.04062300	-0.37711600	-0.74136200
C	-0.50220000	2.04149300	1.15099400
C	0.14062700	0.67449300	-1.56260400
C	-0.20257200	2.63726900	-0.02747600
C	0.45570000	2.06306700	-1.20889000
N	1.12006600	2.74246800	-2.07295200
C	1.40728400	4.13005700	-1.76983100
H	2.26937600	4.45147000	-2.35875900
H	0.56183000	4.77241200	-2.05671800
H	1.61856600	4.31591500	-0.70742000
N	0.74172200	-1.56562000	1.22343800
C	1.96230700	-1.47285100	1.98850800
C	0.00067500	-2.80054700	1.37182900
H	2.50932000	-0.57318200	1.69777200
H	1.80914800	-1.44151800	3.07864000
H	2.58986100	-2.34554400	1.76294600
H	-0.13677400	-3.06517300	2.43218600
H	-0.97404100	-2.70424300	0.89633500
H	0.52806400	-3.63386200	0.88548800
N	0.06705300	0.48615500	2.95011200
C	0.76102300	1.43770400	3.78370500

C	-0.65081100	-0.55098100	3.64898800
H	1.33182300	2.12885600	3.16127600
H	0.07560400	2.02895700	4.40918500
H	1.46472500	0.90946700	4.44280100
H	-1.24627400	-0.11616500	4.46714100
H	-1.33066500	-1.06032500	2.96239500
H	0.01648600	-1.30562300	4.09143100
H	0.11881000	0.49564400	-2.63544500
H	-0.55738000	3.65148800	-0.17948500
N	-1.17385200	2.76035400	2.15894500
C	-1.29693000	4.19305500	2.01630900
C	-2.39477500	2.15884700	2.67819400
H	-0.32046600	4.63005000	1.79204800
H	-2.00720600	4.49522000	1.22793200
H	-1.65483100	4.60412000	2.96465700
H	-3.27152700	2.46114200	2.08423200
H	-2.32821900	1.07292900	2.64973900
H	-2.55485900	2.47481400	3.71503700
N	-0.30320000	-1.67686100	-1.30948200
C	-1.27948900	-1.67880700	-2.38660000
C	0.91583800	-2.36800100	-1.71709700
H	-2.16134100	-1.10852800	-2.08808300
H	-0.89835300	-1.26135100	-3.33383800
H	-1.57916700	-2.71371200	-2.58215400
H	1.37960200	-1.89335000	-2.59906100
H	1.63367600	-2.35657300	-0.89541300
H	0.67600300	-3.40663900	-1.96790700

TI-23456

Zero-point correction= 0.518839 (Hartree/Particle)

Thermal correction to Energy= 0.547352

Thermal correction to Enthalpy= 0.548297

Thermal correction to Gibbs Free Energy= 0.461074

Sum of electronic and zero-point Energies= -1033.798619

Sum of electronic and thermal Energies= -1033.770106

Sum of electronic and thermal Enthalpies= -1033.769162

Sum of electronic and thermal Free Energies= -1033.856384

C	0.05199400	0.62052900	1.67640700
C	0.36716400	-0.33827500	0.75533400
C	0.06459500	-0.22591200	-0.68966900
C	-0.63972000	1.91050100	1.40930700
C	0.13401700	0.93327100	-1.37516800
C	-0.45760900	2.67156700	0.30780700
C	0.45144000	2.25444300	-0.79957100
N	1.27221500	3.09909600	-1.29406100
C	2.04888700	2.69189300	-2.45351900
H	2.96677800	3.28240400	-2.48906500
H	2.31017900	1.62640300	-2.45310500
H	1.48941500	2.90363900	-3.37438600
N	1.05103700	-1.53971500	1.10196500
C	2.23486000	-1.45395500	1.93462800
C	0.25192500	-2.72208700	1.37190600
H	2.75324400	-0.51230900	1.74110400
H	2.01710100	-1.50742000	3.01026600
H	2.90389100	-2.28281500	1.66805700
H	-0.03113300	-2.80182600	2.43457500

H	-0.64584000	-2.70584600	0.75366200
H	0.82967900	-3.61894300	1.11370800
N	0.35286700	0.33150900	3.03723300
C	0.98790100	1.38997100	3.79725600
C	-0.66023200	-0.36591600	3.80743300
H	1.70335900	1.92093000	3.16358500
H	0.26867200	2.11477400	4.20790000
H	1.54074800	0.94281400	4.63232000
H	-1.38047900	0.33055200	4.26624100
H	-1.20798700	-1.05552400	3.16214900
H	-0.18097100	-0.94848300	4.60549000
H	-0.03817700	0.91309700	-2.45090400
N	-1.54619600	2.25553300	2.45774100
C	-1.59265600	3.62358300	2.94481500
C	-2.86892100	1.69385400	2.24525800
H	-0.57762400	4.02691900	2.98531800
H	-2.20742600	4.28795200	2.32564100
H	-1.99338400	3.61085000	3.96641800
H	-3.42508100	2.22940000	1.45751100
H	-2.78203700	0.64204900	1.95662300
H	-3.44373700	1.74830500	3.17671700
N	-0.24917900	-1.45328200	-1.36349300
C	-1.22232000	-1.32404300	-2.43476300
C	0.93259500	-2.17267000	-1.83717500
H	-2.07716900	-0.73682500	-2.09304900
H	-0.81516400	-0.85465400	-3.34732900
H	-1.56906200	-2.32462700	-2.71044900
H	1.40136200	-1.65169700	-2.69076800

H	1.65709700	-2.25747200	-1.02834800
H	0.63475600	-3.17389900	-2.16421100
N	-1.24593100	3.85036500	0.10186300
C	-0.49414500	5.10423700	0.15751000
C	-2.03672900	3.77522200	-1.11948000
H	0.16473200	5.09599700	1.02817500
H	0.12315400	5.26961700	-0.73455600
H	-1.20694700	5.92976600	0.26726900
H	-1.42072200	3.81439800	-2.03439400
H	-2.61583800	2.84771000	-1.12451300
H	-2.73216900	4.62028300	-1.14161600

TI-23457

Zero-point correction= 0.519832 (Hartree/Particle)

Thermal correction to Energy= 0.548211

Thermal correction to Enthalpy= 0.549155

Thermal correction to Gibbs Free Energy= 0.462878

Sum of electronic and zero-point Energies= -1033.807498

Sum of electronic and thermal Energies= -1033.779119

Sum of electronic and thermal Enthalpies= -1033.778174

Sum of electronic and thermal Free Energies= -1033.864452

C	-0.23129400	0.27384400	2.00790800
C	0.34540200	-0.57578700	1.10476000
C	0.19760000	-0.44620900	-0.36053900
C	-1.07935500	1.41735400	1.72426900
C	0.13247400	0.74714700	-0.99798300
C	-0.94894600	2.25691400	0.65787800
C	0.21680200	2.03303800	-0.24858800

N	1.10287900	2.93493800	-0.37090800
C	2.20124800	2.66806400	-1.28337400
H	3.06380000	3.27088200	-0.99285200
H	2.49221800	1.60884100	-1.30732000
H	1.90331100	2.95361200	-2.29921300
N	1.14571500	-1.69966000	1.48066400
C	2.55372500	-1.37499100	1.61211300
C	0.68771700	-2.60631800	2.51745700
H	2.87272000	-0.76329800	0.76255500
H	2.76840500	-0.82113400	2.54188300
H	3.14673300	-2.29731800	1.61354800
H	0.93707100	-2.27306800	3.53300900
H	-0.39740900	-2.71795300	2.44846900
H	1.14068300	-3.59177800	2.34418700
N	0.00985900	0.01410600	3.40921200
C	0.69015500	1.12424600	4.06211800
C	-1.17790700	-0.38109000	4.14955600
H	1.56573500	1.40988900	3.47455200
H	0.05161500	2.01614100	4.18190800
H	1.02308200	0.80195700	5.05444200
H	-1.89638800	0.44272800	4.30693600
H	-1.69184700	-1.18854800	3.62299900
H	-0.87766200	-0.74885800	5.13663300
N	0.09993500	-1.63388300	-1.15774900
C	1.35952700	-2.29302500	-1.47803500
C	-0.89116200	-2.58581900	-0.68429200
H	2.12038100	-1.54185800	-1.70391500
H	1.72354200	-2.92220800	-0.65327900

H	1.22206100	-2.91760300	-2.36951500
H	-0.55050300	-3.16494800	0.18746800
H	-1.81132500	-2.05672900	-0.42283500
H	-1.11804900	-3.28839100	-1.49414200
N	-1.82789800	3.26588400	0.34965200
C	-2.90212700	3.52990400	1.28131000
C	-1.46439800	4.32897700	-0.57707100
H	-3.46162900	2.60878400	1.47312600
H	-2.53626100	3.91453500	2.24519700
H	-3.58275200	4.26399300	0.84845500
H	-0.73779100	5.03179900	-0.15365100
H	-1.03224600	3.90372700	-1.48435500
H	-2.37526200	4.86667600	-0.84812200
H	-1.80261200	1.66017100	2.49655300
N	-0.14423400	0.96878800	-2.38877200
C	0.66802400	0.27128900	-3.37329800
C	-1.56891400	0.84106800	-2.67185800
H	1.72288200	0.33881100	-3.09373200
H	0.39927500	-0.78725600	-3.48623700
H	0.54397600	0.77425900	-4.33934800
H	-1.91189800	-0.20387100	-2.59990100
H	-2.14038700	1.44912000	-1.96353800
H	-1.76939900	1.20940700	-3.68371800

TI-23567

Zero-point correction= 0.519559 (Hartree/Particle)

Thermal correction to Energy= 0.548190

Thermal correction to Enthalpy= 0.549134

Thermal correction to Gibbs Free Energy= 0.463220
Sum of electronic and zero-point Energies= -1033.819341
Sum of electronic and thermal Energies= -1033.790710
Sum of electronic and thermal Enthalpies= -1033.789766
Sum of electronic and thermal Free Energies= -1033.875679

C	-0.03087900	0.10704100	2.04993500
C	0.60769500	-0.70752400	1.15078200
C	0.43375000	-0.63022800	-0.30444500
C	-0.92474000	1.21775800	1.80514300
C	0.26100100	0.58227500	-0.91812300
C	-0.76639700	2.03788500	0.72167500
C	0.46495000	1.80968800	-0.09083100
N	1.48712000	2.55783900	-0.00884800
C	2.66345800	2.21139100	-0.78661500
H	3.49468900	2.05248800	-0.09261600
H	2.54934300	1.31616900	-1.41299300
H	2.93577600	3.06274600	-1.41919500
N	1.39798500	-1.79763900	1.58533800
C	2.76051600	-1.80855200	1.07600200
C	1.32921400	-2.17394800	2.97730900
H	2.76788800	-1.50938000	0.02712500
H	3.41575500	-1.11850500	1.63407800
H	3.17547400	-2.81906700	1.15397400
H	1.79621500	-1.43704600	3.65432300
H	0.28497300	-2.30239900	3.27591400
H	1.84790100	-3.12785900	3.10961000
N	0.36560500	-1.82146500	-1.05480200
C	1.24126700	-1.99372900	-2.19453200

C	-0.10826700	-3.05401000	-0.46694900
H	1.41672200	-1.02997600	-2.67567000
H	2.20750400	-2.45070000	-1.92153200
H	0.76045300	-2.65387500	-2.92674900
H	0.69947300	-3.68100700	-0.06124200
H	-0.80019200	-2.83198300	0.34768000
H	-0.64299100	-3.62877100	-1.23448700
N	-1.67463000	2.97624500	0.23403300
C	-3.09326500	2.82256800	0.47084700
C	-1.22937300	4.34326200	0.03250000
H	-3.35081100	1.76286300	0.45640600
H	-3.42869600	3.23828200	1.43278100
H	-3.63075900	3.33580600	-0.33531400
H	-1.42561600	4.97643700	0.91309600
H	-0.15610200	4.35394200	-0.16272300
H	-1.75737900	4.78358900	-0.82152100
N	-0.17452000	0.73338800	-2.24733400
C	-1.43837100	0.07246600	-2.56339500
C	-0.11645100	2.07593600	-2.80804700
H	-1.40266100	-0.96425100	-2.22793300
H	-2.28616700	0.58159300	-2.07875900
H	-1.58985300	0.09234300	-3.64656100
H	-0.86009100	2.75342900	-2.36017400
H	0.87639000	2.50738300	-2.67159000
H	-0.31031500	2.00803300	-3.88206500
H	0.13043000	-0.10681300	3.10210600
N	-1.94190300	1.50485500	2.76143100
C	-2.37111200	0.41995500	3.61973200

C	-1.74133900	2.74282900	3.49775300
H	-2.49391000	-0.49137600	3.03065300
H	-1.67094500	0.20516000	4.44640800
H	-3.33666400	0.67902800	4.06726300
H	-0.92454100	2.66747400	4.23606000
H	-1.50171100	3.55076900	2.80334400
H	-2.66300600	3.00420700	4.02933400

TI-234567

Zero-point correction= 0.593948 (Hartree/Particle)

Thermal correction to Energy= 0.625796

Thermal correction to Enthalpy= 0.626740

Thermal correction to Gibbs Free Energy= 0.534393

Sum of electronic and zero-point Energies= -1167.628706

Sum of electronic and thermal Energies= -1167.596858

Sum of electronic and thermal Enthalpies= -1167.595914

Sum of electronic and thermal Free Energies= -1167.688260

C	0.00633400	0.12223000	1.60019700
C	0.53172900	-0.53190500	0.53484300
C	0.30297100	-0.18711800	-0.90516600
C	-0.87315300	1.31309600	1.47958500
C	0.44788600	1.08777000	-1.34031100
C	-0.60589200	2.29856200	0.59849100
C	0.57152700	2.19762500	-0.34116600
N	1.51314800	3.04644300	-0.45686000
C	1.53737200	4.17315400	0.45766300
H	0.86241100	4.95679500	0.09384400
H	1.22346600	3.90295800	1.47530300

H	2.54954500	4.58066000	0.49934900
N	-2.02444500	1.41262400	2.32419100
C	-2.83040200	0.20202000	2.33163300
H	-2.35556800	-0.62589700	2.88220700
H	-3.79335300	0.42145300	2.80458600
H	-3.02090500	-0.11640300	1.30259700
C	-1.79158400	1.90564000	3.67695500
H	-1.08316800	2.73687700	3.64753700
H	-2.73743300	2.27873700	4.08764000
H	-1.39510700	1.12830100	4.34609000
N	-1.46680300	3.41724000	0.32427800
C	-1.70116100	4.35812800	1.41232700
C	-2.74179700	3.00656000	-0.26023200
H	-0.76684000	4.58576000	1.92927500
H	-2.08903200	5.29154900	0.98873300
H	-2.42898000	3.98067300	2.14494300
H	-3.22418200	3.88113400	-0.71054300
H	-2.56668700	2.26761200	-1.04344200
H	-3.41613400	2.57091200	0.49197100
N	0.24365400	-0.22982300	2.95649900
C	0.30883600	-1.62174400	3.35643300
C	1.26595500	0.58626700	3.58918500
H	-0.44489300	-2.18949000	2.80479100
H	1.28867800	-2.08534900	3.18675800
H	0.06486500	-1.68301600	4.42462300
H	2.28087800	0.28085800	3.28725900
H	1.12474800	1.63534900	3.31304400
H	1.18338400	0.50170900	4.67879900

N	1.54221500	-1.52750400	0.77981200
C	1.21625800	-2.92753100	0.54474900
C	2.80720500	-1.17757700	0.14779000
H	0.21489900	-3.14975400	0.92027800
H	1.25998700	-3.20374600	-0.51901400
H	1.92896900	-3.55061800	1.09881600
H	2.79071700	-1.32167300	-0.94607600
H	3.04734000	-0.13234400	0.35908000
H	3.59683700	-1.81192800	0.56483900
N	0.16148400	-1.33044700	-1.71392300
C	-1.07857300	-2.05741300	-1.50456100
C	0.60682000	-1.36629400	-3.09365200
H	-1.36330300	-2.01064900	-0.45030500
H	-1.90601100	-1.64013700	-2.10164800
H	-0.94676400	-3.10952800	-1.78325500
H	-0.09508800	-0.89910700	-3.79620300
H	1.56692900	-0.85787200	-3.18747900
H	0.74033300	-2.41996000	-3.37053500
N	0.43777400	1.42386600	-2.72973800
C	-0.64230100	2.32868500	-3.09295900
C	1.72609100	1.89892000	-3.23461900
H	-1.60411200	1.83599900	-2.92487200
H	-0.62589800	3.27739800	-2.52855700
H	-0.56323800	2.55919200	-4.15993400
H	1.94959700	2.93287300	-2.94355900
H	2.52345400	1.26325800	-2.84079800
H	1.72063900	1.82073100	-4.32839400

Cartesian Coordination of (Me)₂N-TI Conjugated Acid and Their Thermochemical Values (M06-2X/6-31g(d,p))

TI-2

Zero-point correction= 0.240648 (Hartree/Particle)

Thermal correction to Energy= 0.252576

Thermal correction to Enthalpy= 0.253520

Thermal correction to Gibbs Free Energy= 0.203240

Sum of electronic and zero-point Energies= -498.883784

Sum of electronic and thermal Energies= -498.871856

Sum of electronic and thermal Enthalpies= -498.870911

Sum of electronic and thermal Free Energies= -498.921191

C	-0.15231500	0.25229800	1.60421000
C	0.43448100	-0.42355500	0.56401200
C	0.74837600	0.10643400	-0.70198800
C	-0.63619800	1.57774800	1.64449000
C	0.65779100	1.39839700	-1.16180400
C	-0.57286000	2.61059800	0.73030500
C	0.18979100	2.57498900	-0.51645900
C	1.21322200	3.97610100	-2.29161600
H	1.31633400	5.04987000	-2.43520200
H	2.20977300	3.53629800	-2.19084100
H	0.71658200	3.55482900	-3.16988700
H	1.04564500	1.55448100	-2.16259000
H	-0.33533900	-0.32095200	2.50876900
H	0.67157400	-1.47046300	0.72301500
N	0.42306900	3.75453000	-1.08948400
H	0.14162700	4.55886100	-0.53932200

H	1.16862100	-0.59989200	-1.41303400
H	-1.17661600	1.81508400	2.55462900
N	-1.15278600	3.85104800	1.01053600
C	-1.44206800	4.18151800	2.40300000
H	-1.64529000	5.25251900	2.45755500
H	-2.32150100	3.64951300	2.79195100
H	-0.57454400	3.96163200	3.02727700
C	-2.26438100	4.24835600	0.12354700
H	-3.19423500	3.75595400	0.43335700
H	-2.40006900	5.32997600	0.18632600
H	-2.05824900	3.97732800	-0.91199100

TI-3

Zero-point correction= 0.240800 (Hartree/Particle)

Thermal correction to Energy= 0.253112

Thermal correction to Enthalpy= 0.254057

Thermal correction to Gibbs Free Energy= 0.201825

Sum of electronic and zero-point Energies= -498.892372

Sum of electronic and thermal Energies= -498.880059

Sum of electronic and thermal Enthalpies= -498.879115

Sum of electronic and thermal Free Energies= -498.931346

C	-0.66300900	0.18121000	1.30477100
C	0.26598000	-0.37771500	0.49279800
C	1.02883700	0.20592900	-0.56769800
C	-1.15914300	1.54369600	1.33715200
C	1.03712100	1.48495100	-1.01002300
C	-0.69910600	2.57753300	0.50256700
C	0.26032700	2.60027700	-0.52350400

C	1.39191600	4.05218800	-2.22245900
H	1.31672300	5.10937200	-2.47070900
H	2.42515700	3.84192600	-1.93268700
H	1.13528200	3.47267100	-3.11357500
H	1.70980500	1.70183900	-1.83143900
H	-1.16921500	3.54085800	0.65440000
N	-2.11796000	1.81957900	2.24838600
C	-2.60783000	3.18390500	2.42780400
C	-2.72888300	0.77512700	3.07631500
H	-1.78046100	3.86828200	2.63739400
H	-3.15116400	3.53133600	1.54233500
H	-3.28517900	3.20625700	3.27754600
H	-3.56862300	1.21054800	3.61215100
H	-3.11428300	-0.04072500	2.46021000
H	-2.02261300	0.37838000	3.81167100
H	-1.08107000	-0.49144600	2.04140200
H	0.46914800	-1.42938400	0.67281800
N	0.46817900	3.78350800	-1.12940100
H	-0.07037400	4.56927100	-0.79587500
H	1.70044500	-0.47742700	-1.07953500

TI-4

Zero-point correction= 0.240524 (Hartree/Particle)

Thermal correction to Energy= 0.252849

Thermal correction to Enthalpy= 0.253793

Thermal correction to Gibbs Free Energy= 0.201886

Sum of electronic and zero-point Energies= -498.895243

Sum of electronic and thermal Energies= -498.882918

Sum of electronic and thermal Enthalpies= -498.881974

Sum of electronic and thermal Free Energies= -498.933881

C	-0.13257000	0.05282200	1.40132800
C	1.01105700	-0.27216300	0.64290500
C	1.63012300	0.46476200	-0.35738400
C	-0.83226100	1.31230700	1.25110700
C	1.36949800	1.69764300	-0.94602800
C	-0.63467800	2.35528800	0.40928400
C	0.33649000	2.58745300	-0.63280400
C	1.07926300	4.17827200	-2.37862300
H	0.72959500	5.14458900	-2.73665300
H	2.10993000	4.28694400	-2.02714700
H	1.05389000	3.46748000	-3.21030000
H	2.05137900	1.99347300	-1.73411300
H	1.48006400	-1.22512300	0.84406000
N	0.20711800	3.74448000	-1.30064600
H	-0.54900100	4.35950800	-1.03974100
H	2.49972500	-0.03468300	-0.77816600
H	-1.65864200	1.46550700	1.93347600
H	-1.33948600	3.17391300	0.54425600
N	-0.60065200	-0.81599700	2.31767600
C	-1.81526800	-0.55334300	3.09281100
H	-2.05509400	-1.44192100	3.67113500
H	-1.67452400	0.27906300	3.78925200
H	-2.66374100	-0.34325300	2.43665000
C	0.10338800	-2.07417500	2.56420600
H	1.13891200	-1.88666200	2.86272600
H	-0.39439700	-2.60377100	3.37226100

H	0.09429000	-2.70974300	1.67327300
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TI-23

Zero-point correction=	0.313301 (Hartree/Particle)
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Thermal correction to Energy=	0.329671
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Thermal correction to Enthalpy=	0.330615
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Thermal correction to Gibbs Free Energy=	0.270920
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Sum of electronic and zero-point Energies=	-632.714503
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Sum of electronic and thermal Energies=	-632.698133
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Sum of electronic and thermal Enthalpies=	-632.697189
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Sum of electronic and thermal Free Energies=	-632.756884
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C	-0.88899300	-0.35161800	1.29162100
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C	-0.70829900	-1.07135900	0.09798800
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C	-0.28224300	-0.56875900	-1.11072500
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C	-1.03756800	1.01376100	1.49057200
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C	0.05105600	0.76368600	-1.40207700
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C	-1.26263100	1.91681900	0.37103600
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C	-0.26412400	1.91583600	-0.69439800
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H	-0.94904600	-0.96176900	2.18604400
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H	-0.80570200	-2.14917800	0.17675000
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H	0.60149400	0.92109600	-2.32430500
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C	1.31898000	3.26799700	-2.01867400
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H	0.96772300	3.02711600	-3.02612800
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H	1.65672600	4.30318900	-2.01904500
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H	2.16518600	2.61587900	-1.77165800
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N	-1.12993100	1.58344700	2.75826800
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C	-1.11835800	0.69293600	3.90983100
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H	-0.16423300	0.15856300	4.02310200
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H	-1.28771000	1.29140300	4.80565700
H	-1.92993300	-0.03408900	3.83269100
C	-0.36015700	2.80929200	2.97028700
H	-0.56912500	3.54242700	2.18622700
H	-0.65836400	3.25244300	3.92209200
H	0.72079700	2.61545200	2.99296800
H	-0.08071700	-1.28780300	-1.89843700
N	-2.24432800	2.81404400	0.37955000
C	-3.26412000	2.81144600	1.43983600
C	-2.52614400	3.64815300	-0.80047700
H	-2.89422200	3.28805500	2.34925700
H	-4.13437200	3.35026400	1.07313100
H	-3.54162400	1.78252400	1.67664400
H	-1.98056100	4.59381600	-0.76887100
H	-2.24957400	3.11035600	-1.70698800
H	-3.59395700	3.85468300	-0.81756800
N	0.23900800	3.13847400	-1.05454400
H	0.18216600	3.86381200	-0.35573600

TI-24

Zero-point correction=	0.314848 (Hartree/Particle)
Thermal correction to Energy=	0.330916
Thermal correction to Enthalpy=	0.331860
Thermal correction to Gibbs Free Energy=	0.272201
Sum of electronic and zero-point Energies=	-632.740507
Sum of electronic and thermal Energies=	-632.724440
Sum of electronic and thermal Enthalpies=	-632.723496
Sum of electronic and thermal Free Energies=	-632.783154

C	0.27383500	-0.04644200	1.59976100
C	0.79918600	-0.77579800	0.50934700
C	0.87458600	-0.36641800	-0.80697300
C	-0.55956800	1.11799400	1.43485000
C	0.56468500	0.84083100	-1.43519200
C	-0.76541500	1.97719000	0.39094900
C	-0.06835200	1.96349100	-0.90420900
H	1.21899900	-1.75098600	0.71359600
H	0.89264200	0.91944500	-2.46508600
C	0.53643700	3.32199800	-2.87739100
H	0.40699600	4.36516500	-3.15990100
H	1.60737300	3.10491800	-2.80475700
H	0.09838000	2.69393200	-3.65922900
H	1.33447400	-1.09556100	-1.46958300
N	-1.64589200	3.06040600	0.54041500
C	-1.99578100	3.49201100	1.88698300
C	-2.83198300	3.02848500	-0.33490600
H	-1.09255700	3.59410200	2.49219800
H	-2.47628400	4.46950100	1.81371100
H	-2.69832600	2.80928800	2.38818200
H	-3.25564200	4.03299800	-0.39805400
H	-2.56663700	2.69523200	-1.33784000
H	-3.59154700	2.34840700	0.07131700
H	-1.17573800	1.33277200	2.29688800
N	0.44025800	-0.51128900	2.85379300
C	1.09649400	-1.79623300	3.09005500
C	-0.01525400	0.24116000	4.02045200
H	2.13233900	-1.77630600	2.73804400

H	1.09660000	-1.99926900	4.15829700
H	0.56100300	-2.60720000	2.58830100
H	0.49034300	-0.14557500	4.90299200
H	0.24325000	1.29788900	3.92016800
H	-1.09659200	0.14461700	4.17210300
N	-0.12491800	3.10618100	-1.60475000
H	-0.53532100	3.89424600	-1.12064400

TI-25

Zero-point correction= 0.314950 (Hartree/Particle)

Thermal correction to Energy= 0.331079

Thermal correction to Enthalpy= 0.332023

Thermal correction to Gibbs Free Energy= 0.271820

Sum of electronic and zero-point Energies= -632.735663

Sum of electronic and thermal Energies= -632.719534

Sum of electronic and thermal Enthalpies= -632.718589

Sum of electronic and thermal Free Energies= -632.778792

C	0.09232200	0.31029500	1.97077800
C	0.49461100	-0.70980100	1.08935900
C	0.32494300	-0.59022900	-0.33394200
C	-0.46389200	1.55486000	1.69548500
C	-0.09132300	0.45180900	-1.10604900
C	-0.75387500	2.25822100	0.52971900
C	-0.51529400	1.78299300	-0.79074400
H	-0.08063700	0.23395000	-2.16914900
C	-0.49381800	2.38773300	-3.20759500
H	-0.69286400	3.30833800	-3.75333800
H	0.54506000	2.09397300	-3.39012000

H	-1.16213400	1.61290300	-3.59388600
H	0.58073500	-1.47058800	-0.91011600
N	-1.29890200	3.56600600	0.59332000
C	-0.93214700	4.38448400	1.74388100
C	-2.74957100	3.59894700	0.34901200
H	0.14313900	4.31780900	1.91949800
H	-1.18246300	5.42323800	1.51776700
H	-1.46884100	4.10479600	2.66273700
H	-3.06131300	4.63517700	0.19948100
H	-2.99842300	3.02693400	-0.54752100
H	-3.30801800	3.18051000	1.19803100
H	-0.71695200	2.10523000	2.59787200
H	0.19704400	0.10815800	3.02814300
N	1.03118400	-1.85309600	1.57572000
C	1.47031600	-2.93170600	0.69283000
C	1.18514400	-2.03598800	3.01557900
H	2.21522800	-2.57740500	-0.02563100
H	1.93284300	-3.70813000	1.29734600
H	0.62931600	-3.37934100	0.15325700
H	1.63270500	-3.00911400	3.20174600
H	1.83997100	-1.26859600	3.44118300
H	0.21583500	-2.00169600	3.52340700
N	-0.73984500	2.63806000	-1.79849000
H	-0.92008300	3.58823500	-1.49032600

TI-26

Zero-point correction= 0.314997 (Hartree/Particle)

Thermal correction to Energy= 0.331066

Thermal correction to Enthalpy= 0.332011
 Thermal correction to Gibbs Free Energy= 0.272224
 Sum of electronic and zero-point Energies= -632.741507
 Sum of electronic and thermal Energies= -632.725438
 Sum of electronic and thermal Enthalpies= -632.724494
 Sum of electronic and thermal Free Energies= -632.784280

C	0.00433700	0.25954700	1.97183600
C	0.50137200	-0.67389800	1.12136700
C	0.54532200	-0.61705600	-0.31898200
C	-0.66041400	1.49492200	1.71736100
C	0.40866200	0.58248800	-1.05354100
C	-0.76556100	2.20389200	0.55699000
C	-0.05716000	1.84548600	-0.68623000
H	0.76521800	0.53479100	-2.07164400
C	0.79988800	2.79991500	-2.80799000
H	0.83999600	3.80119800	-3.23300500
H	1.82355100	2.43605600	-2.66682200
H	0.28323300	2.14466700	-3.51742900
N	-1.44340800	3.43004700	0.49875600
C	-1.71734900	4.11202900	1.75824000
C	-2.62649600	3.44003300	-0.38055000
H	-0.80674900	4.16914400	2.35695000
H	-2.04664800	5.12694600	1.52802500
H	-2.50962900	3.62204200	2.34235400
H	-2.89678500	4.47505600	-0.59962900
H	-2.41695900	2.92596300	-1.31881200
H	-3.47664700	2.94724300	0.10822900
H	-1.15061300	1.92109200	2.58542600

H	0.05288600	-0.00732700	3.02418200
H	0.90504000	-1.56326400	1.58621500
N	0.84351000	-1.75098800	-0.98255600
C	1.11396900	-3.00451200	-0.27501300
C	0.93073800	-1.76367700	-2.43994500
H	0.27991200	-3.26991900	0.37899900
H	1.23578900	-3.79694700	-1.00929100
H	2.03378900	-2.94175900	0.31425700
H	0.03482800	-1.31657000	-2.87946600
H	1.81478900	-1.22066500	-2.79282800
H	1.00232700	-2.79358900	-2.78102300
N	0.08969400	2.86539600	-1.54748500
H	-0.20591000	3.76705600	-1.19352800

TI-27

Zero-point correction= 0.314399 (Hartree/Particle)

Thermal correction to Energy= 0.330296

Thermal correction to Enthalpy= 0.331240

Thermal correction to Gibbs Free Energy= 0.272483

Sum of electronic and zero-point Energies= -632.721807

Sum of electronic and thermal Energies= -632.705910

Sum of electronic and thermal Enthalpies= -632.704966

Sum of electronic and thermal Free Energies= -632.763723

C	-1.57860100	-0.43881900	1.11711000
C	-1.04457900	-1.10050900	0.03315600
C	-0.26398900	-0.56495900	-0.99828700
C	-1.53325300	0.93610400	1.37930900
C	0.00592100	0.75677900	-1.34461400

C	-1.16951700	1.99761500	0.56466300
C	-0.73689900	1.89015100	-0.81101700
C	-0.97623500	3.00398200	-3.04024100
H	0.01833700	3.15945200	-3.46164900
H	-1.38927500	2.07792900	-3.44476400
H	-1.61696000	3.83741100	-3.32556900
N	-1.39816200	3.32409700	0.97832600
C	-0.18774300	4.14944900	1.12092400
C	-2.33324900	3.55649400	2.07430400
H	0.47766400	4.01478500	0.26653400
H	-0.47881100	5.20063800	1.16812500
H	0.36065100	3.89216900	2.03590500
H	-2.56843500	4.62225500	2.09543000
H	-3.25762500	3.00295000	1.90107200
H	-1.91996100	3.28209100	3.05531800
H	-1.91341900	1.22243100	2.35411300
H	-2.04585000	-1.05021600	1.88268300
H	-1.14617900	-2.18141300	0.02484300
H	0.22435400	-1.31104800	-1.61444000
N	0.91165500	1.05024200	-2.34753600
C	1.43591800	-0.02805600	-3.17427700
C	1.90311100	2.09728800	-2.08271200
H	0.61646700	-0.62047000	-3.58640700
H	1.98166500	0.41944100	-4.00590800
H	2.12353500	-0.68743400	-2.62643900
H	2.34588600	2.41022200	-3.03026200
H	1.44161800	2.96907800	-1.61823800
H	2.70041200	1.72608700	-1.42676500

N	-0.95199300	2.96372100	-1.57992700
H	-1.46787100	3.69054400	-1.09191400

TI-34

Zero-point correction= 0.314164 (Hartree/Particle)

Thermal correction to Energy= 0.330454

Thermal correction to Enthalpy= 0.331398

Thermal correction to Gibbs Free Energy= 0.271400

Sum of electronic and zero-point Energies= -632.734029

Sum of electronic and thermal Energies= -632.717739

Sum of electronic and thermal Enthalpies= -632.716795

Sum of electronic and thermal Free Energies= -632.776793

C	0.33322300	0.24180200	1.68940600
C	1.57170100	-0.02960500	1.15503400
C	2.21482400	0.56414100	0.03734400
C	-0.39835400	1.49277100	1.37118700
C	1.69193600	1.33243800	-0.95610400
C	-0.50875600	1.99917700	0.07380700
C	0.35833300	1.84942200	-1.02884900
C	-1.29966400	2.97160800	-2.49704900
H	-1.37177900	3.14357200	-3.56962800
H	-2.11012700	2.30156100	-2.19650800
H	-1.41766200	3.93302500	-1.98387300
H	2.11457600	-0.86440600	1.58052500
H	3.24333500	0.24642900	-0.11130900
H	2.33500300	1.55791100	-1.80250800
N	-0.23867900	-0.57599300	2.63810800
C	0.53798500	-1.68991300	3.15917300

C	-1.67327400	-0.86387800	2.56664700
H	1.49221000	-1.33429500	3.55458700
H	-0.02181700	-2.14294700	3.97799600
H	0.72651300	-2.46047600	2.39856700
H	-2.02987300	-1.14477400	3.56011100
H	-2.23488200	0.00595900	2.22990200
H	-1.86624900	-1.69544200	1.87739400
H	-1.28912700	2.73150800	-0.07969900
N	-1.07617100	2.08339500	2.37888000
C	-0.70807600	1.90763300	3.78859700
C	-2.02788800	3.15469800	2.10582500
H	0.32628600	1.58088400	3.87727300
H	-0.80592700	2.87914000	4.27518000
H	-1.35737300	1.18633800	4.29337000
H	-1.52424400	4.05690900	1.73887200
H	-2.76992800	2.83165900	1.37044000
H	-2.55290300	3.39381200	3.02903700
N	-0.01219300	2.36903000	-2.21177500
H	0.67110600	2.35935300	-2.95439500

TI-35

Zero-point correction= 0.314651 (Hartree/Particle)

Thermal correction to Energy= 0.331266

Thermal correction to Enthalpy= 0.332210

Thermal correction to Gibbs Free Energy= 0.270436

Sum of electronic and zero-point Energies= -632.746081

Sum of electronic and thermal Energies= -632.729466

Sum of electronic and thermal Enthalpies= -632.728522

Sum of electronic and thermal Free Energies= -632.790296

C	-0.31543400	0.14520300	0.92755300
C	0.61988000	-0.50988000	0.13572900
C	1.21682000	0.06120300	-1.06321400
C	-0.77692600	1.49233200	0.89482100
C	1.28314900	1.34461500	-1.45594700
C	-0.16818900	2.57442300	0.19556400
C	0.78039900	2.54201900	-0.80918100
C	0.86686100	5.01662700	-0.88439500
H	1.42497200	5.75558300	-1.45651900
H	-0.20358200	5.18787000	-1.04624700
H	1.09302000	5.15478700	0.17842000
H	1.66793100	-0.64973400	-1.74481400
H	1.79643700	1.52315600	-2.39848300
H	-0.50085000	3.56191500	0.47230600
N	-1.83907200	1.79314300	1.68365400
C	-2.32935400	3.16333500	1.80774400
C	-2.53302200	0.76218000	2.45000600
H	-1.58501300	3.81483600	2.27769000
H	-2.59906500	3.57270300	0.82965200
H	-3.21865300	3.16284100	2.43300100
H	-3.44524000	1.18614300	2.86293000
H	-2.80994500	-0.07781700	1.80718400
H	-1.92089600	0.39317400	3.28097300
H	-0.74144300	-0.45109400	1.71519000
N	0.95872500	-1.79420000	0.41571200
C	0.27540900	-2.51887800	1.47771500
C	2.03036100	-2.48985800	-0.29555500

H	-0.80716500	-2.51879100	1.31100600
H	0.61699300	-3.55151100	1.47988500
H	0.48416600	-2.08022600	2.46048900
H	1.70441400	-2.85899600	-1.27442800
H	2.90018000	-1.84223500	-0.42255000
H	2.34256800	-3.34362600	0.30304100
N	1.25469500	3.69526200	-1.33054700
H	1.93411100	3.63278000	-2.07207700

TI-36

Zero-point correction= 0.314316 (Hartree/Particle)

Thermal correction to Energy= 0.331103

Thermal correction to Enthalpy= 0.332047

Thermal correction to Gibbs Free Energy= 0.269334

Sum of electronic and zero-point Energies= -632.745992

Sum of electronic and thermal Energies= -632.729205

Sum of electronic and thermal Enthalpies= -632.728260

Sum of electronic and thermal Free Energies= -632.790973

C	-0.50736400	0.28933200	1.40988900
C	0.29135600	-0.33378500	0.52359500
C	0.77086700	0.10292600	-0.77979700
C	-1.14597800	1.59668100	1.35037900
C	0.83482500	1.44093800	-1.15419300
C	-0.69101800	2.61546100	0.52751300
C	0.26418500	2.57329700	-0.52454200
C	1.49092300	4.02262100	-2.14837200
H	1.59313800	5.09918800	-2.27546000
H	2.48077000	3.60500500	-1.93991100

H	1.11249000	3.60138500	-3.08625800
H	1.37373000	1.65920200	-2.06261700
H	-1.11511700	3.59851300	0.68984100
N	-2.15128800	1.81920100	2.23269700
C	-2.72875200	3.14993500	2.35691300
C	-2.69490500	0.75537800	3.07394000
H	-1.97037300	3.88100000	2.65788200
H	-3.17937700	3.47246200	1.41168500
H	-3.50347300	3.13153700	3.12008900
H	-3.66229900	1.07799900	3.45422600
H	-2.85550100	-0.15671500	2.49500900
H	-2.04803700	0.53278700	3.93007800
H	-0.68072500	-0.26163100	2.32714500
H	0.65592800	-1.30227400	0.84617200
N	1.27312000	-0.85568600	-1.59154800
C	1.93775800	-0.48665900	-2.83447700
C	1.16224100	-2.27864400	-1.27522500
H	1.24652600	0.02615300	-3.51258100
H	2.79536000	0.16593100	-2.63922600
H	2.30081300	-1.38729500	-3.32434000
H	1.30886000	-2.84762100	-2.19153900
H	1.91569400	-2.59906800	-0.54696700
H	0.16662000	-2.51523100	-0.89524800
N	0.57931900	3.78009000	-1.04743100
H	0.13916900	4.58804300	-0.63595000

TI-45

Zero-point correction= 0.314092 (Hartree/Particle)

Thermal correction to Energy=	0.330415
Thermal correction to Enthalpy=	0.331359
Thermal correction to Gibbs Free Energy=	0.271345
Sum of electronic and zero-point Energies=	-632.726366
Sum of electronic and thermal Energies=	-632.710043
Sum of electronic and thermal Enthalpies=	-632.709099
Sum of electronic and thermal Free Energies=	-632.769113

C	0.30265200	0.04859400	1.48043100
C	1.16386800	-0.53693900	0.49295800
C	1.71940100	0.19399800	-0.58156400
C	-0.45489600	1.22962300	1.24691100
C	1.49763100	1.45116800	-1.09778300
C	-0.40331500	2.22076900	0.29847000
C	0.51769900	2.40937900	-0.76276200
C	-0.49834700	4.61389800	-1.31256100
H	-0.30424100	5.37741700	-2.06370600
H	-1.52586600	4.25932100	-1.44235600
H	-0.39561500	5.07075800	-0.32318100
H	2.45368000	-0.36105200	-1.15461300
H	2.12312200	1.70844900	-1.94975700
N	0.14065200	-0.58572400	2.67953900
C	1.27187100	-1.24477600	3.33656200
C	-1.00994100	-0.33822300	3.53902700
H	2.21595400	-0.87789200	2.93627100
H	1.22755200	-0.99488000	4.39898500
H	1.23875600	-2.33345000	3.22680000
H	-0.91317400	0.59047100	4.11602900
H	-1.93022200	-0.30819100	2.95234400

H	-1.09221100	-1.17002000	4.23999400
H	-1.13575500	3.00852100	0.43665400
N	1.50965300	-1.87097800	0.63977500
C	0.42333600	-2.84393100	0.78117200
C	2.66430400	-2.41060000	-0.06064000
H	-0.35047400	-2.46889300	1.45057800
H	-0.02881000	-3.06728100	-0.19374600
H	0.82952000	-3.76775100	1.19832100
H	2.48110000	-2.57331500	-1.13272700
H	3.52721800	-1.75306200	0.06383000
H	2.90885300	-3.37507600	0.38822300
H	-1.19811800	1.42888600	2.01105100
N	0.45786700	3.53774900	-1.49882700
H	1.13211000	3.64105900	-2.24182100

TI-234

Zero-point correction= 0.387592 (Hartree/Particle)

Thermal correction to Energy= 0.407833

Thermal correction to Enthalpy= 0.408778

Thermal correction to Gibbs Free Energy= 0.340098

Sum of electronic and zero-point Energies= -766.553276

Sum of electronic and thermal Energies= -766.533035

Sum of electronic and thermal Enthalpies= -766.532090

Sum of electronic and thermal Free Energies= -766.600770

C	0.40219300	0.39488800	1.58681300
C	1.70902200	0.22381500	1.13224200
C	2.28275600	0.74463200	-0.02323700
C	-0.47692300	1.52629700	1.21782000

C	1.74428300	1.52244500	-1.02602100
C	-0.42858800	2.31543800	0.06634800
C	0.51365700	2.20651300	-1.04786600
C	1.09103900	3.11045400	-3.28810500
H	0.57531700	3.74636500	-4.00583000
H	2.05537600	3.56950600	-3.04228300
H	1.26535600	2.13761000	-3.75394500
N	-1.44223300	1.82257400	2.16907300
C	-1.07968700	1.99028500	3.56607600
C	-2.85903900	1.87375900	1.86672800
H	-0.00192500	2.13137300	3.66092100
H	-1.57224100	2.89052700	3.95035500
H	-1.37876100	1.14126300	4.19389900
H	-3.27196600	2.88762900	1.91857100
H	-3.04640100	1.46561200	0.87184700
H	-3.40397200	1.25718700	2.59243300
H	2.30990400	-0.52162400	1.63713500
H	3.29973000	0.40902800	-0.20982700
N	-1.28581600	3.43198000	-0.04611100
C	-1.22087100	4.47433300	0.96496400
C	-2.47792000	3.40699200	-0.88585500
H	-0.23448600	4.46631800	1.43293900
H	-1.35923100	5.44573200	0.47816000
H	-1.98004100	4.37932700	1.75058700
H	-2.53368200	4.31362000	-1.50320300
H	-2.45067000	2.53736900	-1.54720300
H	-3.40323200	3.35961300	-0.29961300
H	2.39709900	1.70212500	-1.87098600

N	-0.08992000	-0.47399200	2.51592400
C	-1.47482500	-0.94432100	2.43403600
C	0.79548000	-1.36655800	3.24905300
H	-1.95093600	-0.59786900	1.51795800
H	-1.45771600	-2.03770000	2.40610900
H	-2.06829500	-0.63075800	3.29791800
H	1.14945600	-2.20395800	2.63290700
H	1.65290800	-0.81563100	3.63990300
H	0.23952200	-1.77066800	4.09640400
N	0.24352100	2.97226700	-2.11776600
H	-0.47984700	3.66254600	-1.98034700

TI-235

Zero-point correction= 0.388049 (Hartree/Particle)

Thermal correction to Energy= 0.408405

Thermal correction to Enthalpy= 0.409350

Thermal correction to Gibbs Free Energy= 0.340833

Sum of electronic and zero-point Energies= -766.571167

Sum of electronic and thermal Energies= -766.550811

Sum of electronic and thermal Enthalpies= -766.549867

Sum of electronic and thermal Free Energies= -766.618384

C	-0.21461000	0.25072300	1.13450900
C	0.81652000	-0.34718200	0.40686300
C	1.01419200	-0.07060300	-1.00120900
C	-1.00950100	1.38049300	0.83381600
C	0.70896600	1.05471100	-1.68020000
C	-0.66751900	2.44514000	-0.08119800
C	0.19186900	2.30799800	-1.17985100

C	1.49774300	3.46568100	-2.95389400
H	1.71421700	4.51161000	-3.16618800
H	2.43060200	2.96982300	-2.66489500
H	1.12148000	3.00926900	-3.87451300
N	-2.12612500	1.57304500	1.59874300
C	-2.34175700	0.87169100	2.85408100
C	-3.34700700	2.10197400	0.99606500
H	-1.43808000	0.89640200	3.46664800
H	-3.12981800	1.39276600	3.40016100
H	-2.65551300	-0.17089600	2.70728700
H	-3.63466300	3.06620700	1.42736400
H	-3.22573400	2.20371200	-0.08124300
H	-4.15723100	1.38846100	1.17693400
H	1.45478700	-0.86806900	-1.58848900
N	-1.12134400	3.75607900	0.16913100
C	-1.04620700	4.29499700	1.51524300
C	-2.05600300	4.42524900	-0.72906600
H	-0.18736900	3.86386300	2.03392900
H	-0.89942600	5.37765800	1.44893900
H	-1.94472400	4.11093900	2.11969800
H	-1.74059500	5.46129900	-0.90241100
H	-2.08528800	3.90793200	-1.69040400
H	-3.07485800	4.45747800	-0.32293700
H	0.97093400	1.05177000	-2.73383300
H	-0.52376000	-0.29721100	2.01138500
N	1.55244000	-1.33868700	0.96151100
C	1.32742700	-1.72516800	2.34648300
C	2.52710800	-2.09817400	0.18349900

H	1.33031100	-0.84038500	2.99017100
H	0.37250200	-2.25073000	2.47076600
H	2.12881400	-2.38775400	2.66643000
H	2.04546700	-2.79093500	-0.51590100
H	3.18691200	-1.42689900	-0.37096600
H	3.14089900	-2.67955000	0.86855900
N	0.51042700	3.41539200	-1.89024700
H	0.24927800	4.28301300	-1.44337600

TI-236

Zero-point correction= 0.387846 (Hartree/Particle)

Thermal correction to Energy= 0.408336

Thermal correction to Enthalpy= 0.409281

Thermal correction to Gibbs Free Energy= 0.339794

Sum of electronic and zero-point Energies= -766.573411

Sum of electronic and thermal Energies= -766.552921

Sum of electronic and thermal Enthalpies= -766.551976

Sum of electronic and thermal Free Energies= -766.621463

C	-0.21105200	0.61710400	1.81473500
C	0.59647900	-0.25240300	1.17455300
C	0.88911400	-0.33148900	-0.24344400
C	-1.02740400	1.69829400	1.29833300
C	0.80816000	0.77832900	-1.08112300
C	-0.67951500	2.46546700	0.18245700
C	0.28570600	2.06740500	-0.82735300
C	1.61607500	2.92861800	-2.74269900
H	1.78868000	3.92022600	-3.15794900
H	2.56474600	2.53539200	-2.36196600

H	1.26084800	2.27970100	-3.55002300
N	-2.13542500	2.03981900	2.03220900
C	-2.29171400	1.67449800	3.43219900
C	-3.38438100	2.34051100	1.33947000
H	-1.37591200	1.87623900	3.99087600
H	-3.07564100	2.30343300	3.85790800
H	-2.58146300	0.62395500	3.56886700
H	-3.68897600	3.38519300	1.46070600
H	-3.28487800	2.11467800	0.27741800
H	-4.17396600	1.70278200	1.74975100
N	-1.16316200	3.78298500	0.04048500
C	-1.16358800	4.66336500	1.19757400
C	-2.10327800	4.12676600	-1.02365900
H	-0.28025500	4.45960900	1.80654300
H	-1.10781200	5.69638800	0.84169700
H	-2.05102300	4.56928500	1.83610900
H	-1.87633400	5.12648900	-1.41077000
H	-2.01183100	3.41038000	-1.84291700
H	-3.14601200	4.13258800	-0.68414500
H	1.27501000	0.67659400	-2.04927600
H	-0.32088300	0.42923300	2.87760200
H	1.06430400	-1.00173700	1.80169800
N	1.36173900	-1.50833700	-0.71508000
C	1.77472900	-1.62344600	-2.10685200
C	1.49485500	-2.68249600	0.14435300
H	2.64406400	-0.99001300	-2.31820800
H	2.04567300	-2.65611900	-2.31404600
H	0.95698200	-1.33815900	-2.77663700

H	2.33313900	-2.58718300	0.84332500
H	0.57483300	-2.85938600	0.70613500
H	1.67508900	-3.55264700	-0.48358300
N	0.63293400	3.04341400	-1.68545800
H	0.29327300	3.96138100	-1.43045300

TI-237

Zero-point correction= 0.388209 (Hartree/Particle)

Thermal correction to Energy= 0.408254

Thermal correction to Enthalpy= 0.409198

Thermal correction to Gibbs Free Energy= 0.342042

Sum of electronic and zero-point Energies= -766.563232

Sum of electronic and thermal Energies= -766.543187

Sum of electronic and thermal Enthalpies= -766.542243

Sum of electronic and thermal Free Energies= -766.609399

C	0.28312200	0.99675500	1.95640600
C	1.31495900	0.40478300	1.27734400
C	1.47198100	0.19303000	-0.10875300
C	-0.83740100	1.66878300	1.38264300
C	0.79965700	0.82005100	-1.14168000
C	-0.73190400	2.40716200	0.14579400
C	0.14205700	2.11794500	-0.91217000
C	1.49235200	3.15156200	-2.73816100
H	1.65206300	4.20111400	-2.98366500
H	2.39186900	2.76235400	-2.25209300
H	1.32925000	2.59925900	-3.66592700
N	-1.96698500	1.79313500	2.11063800
C	-2.01243800	1.45289300	3.52894400

C	-3.26557900	1.94184600	1.45996700
H	-1.20149300	1.94578100	4.06844200
H	-2.95500100	1.81805700	3.93609400
H	-1.95282600	0.37028600	3.68986400
H	-3.67983700	2.94627400	1.58688600
H	-3.17947100	1.71338900	0.39789100
H	-3.95479000	1.22265900	1.90961100
H	0.27249100	0.84207900	3.02812600
H	2.03383600	-0.12090300	1.89976100
H	2.16324600	-0.59834600	-0.37110500
N	0.90249300	0.39274900	-2.43666700
C	1.77087200	-0.73407600	-2.74178000
C	-0.23056500	0.53792500	-3.35052800
H	2.78842000	-0.53243800	-2.39839900
H	1.41482300	-1.66697100	-2.28451600
H	1.79655200	-0.86501700	-3.82348300
H	-0.92133500	-0.30775600	-3.24694100
H	-0.76914200	1.46462200	-3.15921800
H	0.14037900	0.56027100	-4.37738200
N	-1.39039300	3.65240400	0.05052100
C	-1.39520300	4.54822000	1.19489700
C	-2.43073400	3.87822600	-0.94736700
H	-0.44102300	4.47112600	1.72133900
H	-1.50470900	5.57375300	0.83078800
H	-2.20357200	4.35596100	1.91363100
H	-2.33324300	4.88453100	-1.36940600
H	-2.32705600	3.15478600	-1.75917900
H	-3.44224300	3.78862400	-0.53234700

N	0.33531600	3.08162600	-1.85026400
H	-0.05009300	3.97039200	-1.55401100

TI-245

Zero-point correction= 0.388627 (Hartree/Particle)

Thermal correction to Energy= 0.408528

Thermal correction to Enthalpy= 0.409472

Thermal correction to Gibbs Free Energy= 0.342001

Sum of electronic and zero-point Energies= -766.570139

Sum of electronic and thermal Energies= -766.550239

Sum of electronic and thermal Enthalpies= -766.549294

Sum of electronic and thermal Free Energies= -766.616765

C	0.28924100	-0.01850700	1.44572100
C	0.53885800	-0.82467000	0.28654700
C	0.11936900	-0.46518300	-0.99868400
C	-0.18096400	1.32310900	1.40905300
C	-0.41713400	0.68887500	-1.55513900
C	-0.58605400	2.20478300	0.43072000
C	-0.66856500	1.94375000	-0.98963100
C	-1.06775600	2.93904600	-3.22243000
H	-1.32144800	3.93315800	-3.58652800
H	-0.10618000	2.64055800	-3.65582500
H	-1.84115600	2.24353600	-3.56105000
N	0.50147800	-0.55118200	2.68618700
C	0.14621000	-1.93631300	3.00909000
C	0.75468100	0.28679500	3.85025000
H	-0.54841600	-2.33819000	2.27504200
H	1.02506600	-2.58603300	3.06133500

H	-0.34578100	-1.92686800	3.98533400
H	1.31443400	-0.30565200	4.57685700
H	1.36611900	1.14882700	3.57723900
H	-0.16992400	0.63279100	4.33214900
H	0.32278100	-1.22014900	-1.75079300
H	-0.32770900	1.73266300	2.40032700
H	-0.56125400	0.62794400	-2.62794200
N	1.21501300	-2.03475600	0.47017300
C	1.08715900	-3.07732600	-0.53332500
C	2.57572200	-1.93474300	1.00138600
H	0.03780800	-3.21398000	-0.80423000
H	1.67295000	-2.87995600	-1.44440800
H	1.45084500	-4.01162900	-0.10026500
H	3.28226500	-1.60521700	0.22704000
H	2.61450100	-1.23022100	1.83318800
H	2.88770400	-2.91769000	1.36254000
N	-0.99319700	3.50305800	0.80609100
C	-2.45005700	3.71382500	0.76975100
C	-0.40447600	4.07703200	2.00905800
H	-2.87563700	3.30672600	-0.14800300
H	-2.93537000	3.22927200	1.62821500
H	-2.65574900	4.78581900	0.80860200
H	-0.84083500	3.67811400	2.93798900
H	0.67355200	3.90539800	2.01365900
H	-0.58647000	5.15376500	1.99562600
N	-1.01257500	2.98425800	-1.77437600
H	-0.97516000	3.88631900	-1.31632700

TI-246

Zero-point correction= 0.389120 (Hartree/Particle)

Thermal correction to Energy= 0.409416

Thermal correction to Enthalpy= 0.410360

Thermal correction to Gibbs Free Energy= 0.341437

Sum of electronic and zero-point Energies= -766.591529

Sum of electronic and thermal Energies= -766.571233

Sum of electronic and thermal Enthalpies= -766.570289

Sum of electronic and thermal Free Energies= -766.639212

C	0.54009600	0.11217300	1.44325600
C	0.70313900	-0.66205300	0.29734300
C	0.39415500	-0.32002900	-1.04290700
C	-0.26989400	1.31507500	1.50920100
C	0.23147900	1.01650300	-1.52716700
C	-0.60127400	2.20887800	0.54508000
C	-0.09721800	2.16572100	-0.84275800
C	0.45380800	3.57439200	-2.79587600
H	0.47864100	4.64389000	-2.99774700
H	1.46694100	3.17144600	-2.90744700
H	-0.19751400	3.09827500	-3.53791000
N	1.02075700	-0.33943200	2.62985800
C	1.62989200	-1.65821000	2.72644100
C	0.95484300	0.46519500	3.84581000
H	0.93473800	-2.43371900	2.38696800
H	2.54661600	-1.71632100	2.12920200
H	1.87931700	-1.85926900	3.76608900
H	1.70984700	0.10392800	4.54257100
H	1.17661100	1.51165800	3.62700300

H	-0.02438800	0.39847700	4.33528700
H	-0.70175900	1.49986400	2.48352800
H	0.45012700	1.15640300	-2.57597900
N	-1.36896200	3.34617200	0.83656700
C	-2.63521100	3.45425300	0.09417800
C	-1.54106800	3.71128700	2.23460800
H	-2.49349600	3.18029200	-0.95099700
H	-3.39999100	2.79837700	0.53057300
H	-2.98829600	4.48661000	0.14123000
H	-2.20735300	3.02383200	2.77762100
H	-0.56979900	3.74186200	2.73329800
H	-1.98406700	4.70821700	2.27378900
H	1.14779400	-1.63276100	0.43740300
N	0.41031300	-1.30972000	-1.96693400
C	0.17352200	-1.03386200	-3.38027500
C	0.69843500	-2.68826300	-1.58731600
H	-0.71439500	-0.40920100	-3.50414800
H	1.03048800	-0.53656900	-3.84914400
H	0.00230300	-1.97585200	-3.89686500
H	1.74304200	-2.81313800	-1.27991000
H	0.04530900	-3.00578300	-0.76964200
H	0.51603100	-3.33490200	-2.44264900
N	-0.04495100	3.36743100	-1.45523800
H	-0.26435000	4.16499900	-0.87483600

TI-247

Zero-point correction= 0.389156 (Hartree/Particle)

Thermal correction to Energy= 0.409048

Thermal correction to Enthalpy= 0.409992
 Thermal correction to Gibbs Free Energy= 0.342602
 Sum of electronic and zero-point Energies= -766.571610
 Sum of electronic and thermal Energies= -766.551718
 Sum of electronic and thermal Enthalpies= -766.550774
 Sum of electronic and thermal Free Energies= -766.618164

C	0.13622100	-0.15542700	1.75538800
C	0.24537000	-1.04262100	0.66234900
C	0.14017600	-0.75354900	-0.68298000
C	-0.34560300	1.18102800	1.59672500
C	0.10912400	0.44629700	-1.41671200
C	-0.39187700	2.01331200	0.50477500
C	0.12550800	1.73981500	-0.83543200
C	1.43825900	2.84326400	-2.65922700
H	1.87881400	3.83991300	-2.68792000
H	2.22866100	2.10530500	-2.50764500
H	0.95410400	2.64102000	-3.61591100
N	0.36201600	-0.60512500	3.01134100
C	0.67426400	-2.01038700	3.25205800
C	0.26899400	0.28524000	4.16243500
H	-0.15572800	-2.65929500	2.95403000
H	1.57527900	-2.30811600	2.70738700
H	0.85289900	-2.15372600	4.31526200
H	0.73718500	-0.19778800	5.01769900
H	0.80232200	1.21974800	3.96808000
H	-0.77151400	0.51351500	4.42291500
H	-0.74263800	1.62034600	2.50073500
N	-0.83300500	3.33765700	0.66698100

C	-2.00663600	3.71667100	-0.13686800
C	-0.90410000	3.89793900	2.00912500
H	-1.93038100	3.31405900	-1.14675800
H	-2.93077400	3.34346200	0.32280000
H	-2.05926400	4.80559300	-0.19984200
H	-1.74620200	3.50226000	2.59644400
H	0.03039200	3.71076200	2.54214600
H	-1.03911500	4.97736700	1.91735100
H	0.37611000	-2.09233300	0.88912300
H	0.15126000	-1.64079000	-1.30764100
N	0.12268600	0.39870400	-2.81996600
C	-1.03982200	0.99343200	-3.47709400
C	0.58835500	-0.80737800	-3.48319400
H	-1.23564800	1.99175200	-3.07806900
H	-0.83039300	1.09072600	-4.54523900
H	-1.94125000	0.37743200	-3.35114400
H	1.52218800	-1.14819600	-3.03063100
H	-0.14340800	-1.62979200	-3.46201500
H	0.78665200	-0.56669800	-4.53010200
N	0.48949100	2.82820600	-1.54814600
H	0.42813900	3.68265500	-1.00707100

TI-345

Zero-point correction= 0.386810 (Hartree/Particle)

Thermal correction to Energy= 0.407304

Thermal correction to Enthalpy= 0.408248

Thermal correction to Gibbs Free Energy= 0.339375

Sum of electronic and zero-point Energies= -766.563575

Sum of electronic and thermal Energies= -766.543080
 Sum of electronic and thermal Enthalpies= -766.542136
 Sum of electronic and thermal Free Energies= -766.611010

C	0.24266700	0.23287000	1.30932600
C	1.33298500	-0.20120100	0.55824400
C	1.97379700	0.56032100	-0.48119100
C	-0.40728500	1.54543000	1.16499300
C	1.48935300	1.55314900	-1.26519600
C	-0.58180100	2.24526000	-0.04053500
C	0.21157500	2.20676900	-1.19062900
C	-1.36625800	3.70017100	-2.38182300
H	-1.45537200	4.06236400	-3.40456500
H	-2.22976400	3.06623100	-2.15914500
H	-1.37295800	4.56385100	-1.70653300
N	-1.00077600	2.03408300	2.28363700
C	-0.39712300	1.82788300	3.60392300
C	-1.98025000	3.10908300	2.22105400
H	0.63379000	1.48872900	3.50640100
H	-0.38829600	2.79261900	4.11682000
H	-0.95958700	1.11321100	4.21135500
H	-1.51957000	4.07656600	1.98245600
H	-2.75083600	2.88223000	1.48072100
H	-2.46475900	3.18469100	3.19451300
H	2.12453300	1.86650700	-2.09042200
H	-1.31702000	3.03792000	-0.02831000
N	-0.30300300	-0.58342700	2.28465500
C	-1.74124100	-0.76883400	2.36448500
C	0.49418300	-1.29717300	3.26723100

H	-2.21201100	-0.46764900	1.42623600
H	-1.95426100	-1.83155300	2.52384800
H	-2.20531200	-0.20346300	3.18430300
H	0.58776700	-2.36591500	3.03929200
H	1.49546400	-0.87106800	3.32579600
H	0.01129000	-1.19357300	4.24617600
H	2.94248800	0.18415400	-0.79215800
N	1.83067400	-1.49285900	0.80254600
C	0.93575000	-2.58663400	0.42064500
C	3.22048700	-1.78439500	0.49273800
H	-0.08312500	-2.37763900	0.74823300
H	0.93351200	-2.74004100	-0.66816000
H	1.27717700	-3.50754900	0.90043700
H	3.40869300	-1.93981300	-0.58102100
H	3.86810300	-0.98573000	0.86079100
H	3.49580600	-2.70376600	1.01467600
N	-0.13789000	2.94108300	-2.26425200
H	0.51577900	2.98777500	-3.03088800

TI-346

Zero-point correction= 0.387954 (Hartree/Particle)

Thermal correction to Energy= 0.408645

Thermal correction to Enthalpy= 0.409589

Thermal correction to Gibbs Free Energy= 0.339572

Sum of electronic and zero-point Energies= -766.585974

Sum of electronic and thermal Energies= -766.565283

Sum of electronic and thermal Enthalpies= -766.564339

Sum of electronic and thermal Free Energies= -766.634356

C	-0.40877300	0.03971600	1.57216000
C	0.57702600	-0.48562200	0.78756900
C	1.21710200	0.04937900	-0.39454900
C	-0.86290000	1.45185300	1.48282200
C	0.58006400	0.92451000	-1.28663400
C	-1.03166100	2.08894900	0.27841800
C	-0.52928200	1.73876400	-1.02026800
C	-0.65239600	2.35117100	-3.42652800
H	-1.32755200	2.95517500	-4.03042700
H	0.36439500	2.73979900	-3.55315600
H	-0.68812700	1.31979800	-3.79075500
N	-1.23120900	2.05036900	2.65208300
C	-0.58754800	1.72346200	3.92618800
C	-1.96182500	3.30548400	2.62958200
H	0.32617900	1.15414500	3.76468900
H	-0.32160900	2.66033900	4.42206200
H	-1.25126300	1.15050200	4.58158500
H	-1.33508900	4.14554600	2.30088700
H	-2.83003700	3.22903500	1.96904100
H	-2.32265400	3.51312600	3.63698400
H	0.99257600	1.00235000	-2.28073900
H	0.85043500	-1.51072700	0.99624000
N	2.40611200	-0.49522000	-0.73504500
C	3.01331100	-0.20265000	-2.02747200
C	3.09745100	-1.43340100	0.14291000
H	3.16432900	0.87449300	-2.14736500
H	3.98053700	-0.69706300	-2.08570200
H	2.38965600	-0.56896200	-2.85045000

H	3.01742900	-1.10850600	1.18191700
H	2.69946300	-2.45130300	0.05225200
H	4.15236400	-1.45142900	-0.12624300
H	-1.51965800	3.05653000	0.30092800
N	-0.98331700	-0.70784700	2.58232100
C	-2.43564200	-0.67241900	2.76574900
C	-0.40591000	-1.99434100	2.92430900
H	-2.83929900	0.30307700	2.50324600
H	-2.92089200	-1.43553000	2.14381300
H	-2.67017200	-0.87724300	3.81338700
H	-0.57451500	-2.75726400	2.14992800
H	0.66888500	-1.88989600	3.09521200
H	-0.86775100	-2.34122400	3.85013600
N	-1.07906500	2.42679100	-2.04416500
H	-1.84981600	3.03939500	-1.82877800

TI-347

Zero-point correction= 0.388372 (Hartree/Particle)

Thermal correction to Energy= 0.408537

Thermal correction to Enthalpy= 0.409481

Thermal correction to Gibbs Free Energy= 0.340528

Sum of electronic and zero-point Energies= -766.574579

Sum of electronic and thermal Energies= -766.554414

Sum of electronic and thermal Enthalpies= -766.553470

Sum of electronic and thermal Free Energies= -766.622423

C	0.03452800	0.22927300	1.71336000
C	1.09252000	-0.05286800	0.88039800
C	1.39387100	0.38994100	-0.43175000

C	-0.87798800	1.36214400	1.46945100
C	0.64771100	1.07071500	-1.35041600
C	-1.22347200	1.83139100	0.20279300
C	-0.64398600	1.66794300	-1.07254800
C	-2.51293400	2.93562100	-2.09980800
H	-2.79628800	3.17341700	-3.12389800
H	-3.28798300	2.29950900	-1.66344900
H	-2.45573900	3.87132200	-1.52982100
N	-1.47071000	1.92707300	2.55478700
C	-0.79645900	2.02061500	3.85511000
C	-2.63420100	2.79248100	2.41744200
H	0.27285100	1.85092200	3.75121100
H	-0.94958400	3.03464100	4.23134900
H	-1.20422800	1.30725700	4.57725200
H	-2.36836400	3.79040100	2.04493800
H	-3.36951800	2.34080400	1.74739100
H	-3.09427300	2.90078600	3.39980000
H	-2.00269800	2.58021100	0.20425000
N	-0.16006900	-0.48545200	2.88323700
C	-1.50425100	-0.99265700	3.17094900
C	0.88260300	-1.39136000	3.33500500
H	-2.26702100	-0.27781300	2.86590200
H	-1.68083400	-1.94194200	2.64862200
H	-1.59719500	-1.16474200	4.24587400
H	0.97385800	-2.28486000	2.69997000
H	1.84433300	-0.87455800	3.36847000
H	0.63417000	-1.71651800	4.34656900
H	2.33287800	-0.00221200	-0.81452900

H	1.77387100	-0.82030600	1.22703600
N	1.09343300	1.22941100	-2.69550700
C	2.52162100	1.47787200	-2.86916100
C	0.62972700	0.13376000	-3.55889500
H	2.84849500	2.25369700	-2.17474700
H	3.13787400	0.57836100	-2.72025700
H	2.68885800	1.82855100	-3.89012500
H	1.13207500	-0.81360800	-3.31372800
H	-0.44829700	-0.00430000	-3.44409300
H	0.84223700	0.38534200	-4.60063000
N	-1.24419500	2.23920600	-2.12608900
H	-0.64234000	2.32437100	-2.94020700

TI-2345

Zero-point correction= 0.459277 (Hartree/Particle)

Thermal correction to Energy= 0.484327

Thermal correction to Enthalpy= 0.485272

Thermal correction to Gibbs Free Energy= 0.407153

Sum of electronic and zero-point Energies= -900.387591

Sum of electronic and thermal Energies= -900.362540

Sum of electronic and thermal Enthalpies= -900.361596

Sum of electronic and thermal Free Energies= -900.439715

C	0.52668600	0.18841900	1.66635900
C	0.52154900	-0.92026400	0.68222500
C	0.91659900	-0.47810400	-0.54577300
C	-0.67561400	1.01679700	1.56666200
C	1.17875200	0.90863000	-0.83873000
C	-0.53600000	2.03536300	0.64887400

C	0.60482700	2.04683500	-0.28511900
C	1.83753300	3.53418200	-1.83952300
H	1.94683500	4.60885100	-1.98101700
H	2.83586200	3.11085400	-1.68140400
H	1.42355200	3.09874700	-2.75933200
N	1.60632000	0.56440900	2.28532200
C	2.89213700	-0.09902100	2.05980400
C	1.68629000	1.82588300	3.03019000
H	2.73233800	-1.13547200	1.76895900
H	3.40419500	0.42385400	1.24431600
H	3.48520700	-0.04097000	2.97194500
H	2.13785700	2.58698800	2.38667200
H	0.68784100	2.14620200	3.32045600
H	2.31186700	1.66808300	3.90928700
N	-1.47017600	3.05775300	0.48934300
C	-2.09764300	3.25926600	-0.81527600
C	-2.29861400	3.45852700	1.61386600
H	-1.43507400	2.91360300	-1.60973100
H	-3.05073700	2.71868000	-0.89560300
H	-2.30261700	4.32373600	-0.96310500
H	-3.19220300	2.83351900	1.74137600
H	-1.71513100	3.41111100	2.53498900
H	-2.61743200	4.49165800	1.44901900
N	-1.87419400	0.60559800	2.13640000
C	-2.93793900	0.19914000	1.22221400
C	-1.81839200	-0.19135700	3.35168300
H	-2.96384700	0.87208900	0.36439200
H	-2.78500100	-0.82911900	0.86290800

H	-3.90002700	0.25454700	1.73920500
H	-1.01779600	0.17371600	4.00130300
H	-2.76200900	-0.08634000	3.89381700
H	-1.65781500	-1.25967400	3.14531900
H	1.01352600	-1.19015000	-1.36121100
H	1.86331700	1.07778200	-1.66395400
N	-0.09147800	-2.11038700	1.03276900
C	0.42053900	-2.78913300	2.21892400
C	-0.44514900	-3.01059400	-0.05354000
H	0.61608300	-2.06170900	3.01259000
H	-0.32815000	-3.49523300	2.58539500
H	1.34783200	-3.34287900	2.01004700
H	-0.98664400	-2.45482500	-0.82226700
H	0.43539100	-3.48526900	-0.51037400
H	-1.09471600	-3.79571100	0.33901900
N	0.98881100	3.29877300	-0.69573600
H	0.41632200	4.05728000	-0.35812900

TI-2346

Zero-point correction= 0.462244 (Hartree/Particle)

Thermal correction to Energy= 0.486194

Thermal correction to Enthalpy= 0.487138

Thermal correction to Gibbs Free Energy= 0.410906

Sum of electronic and zero-point Energies= -900.406058

Sum of electronic and thermal Energies= -900.382108

Sum of electronic and thermal Enthalpies= -900.381163

Sum of electronic and thermal Free Energies= -900.457395

C	0.46464800	0.09261200	1.50005500
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C	0.67898600	-0.67127700	0.38597900
C	0.41297000	-0.31583500	-0.98425700
C	-0.47201700	1.24750000	1.53213900
C	0.40760900	1.02421800	-1.44782300
C	-0.52508600	2.23037900	0.59586000
C	0.17169300	2.18186300	-0.71679400
C	0.94263600	3.59983600	-2.58615400
H	1.09182800	4.66867300	-2.72961700
H	1.90866800	3.09408000	-2.68102700
H	0.27262100	3.23232400	-3.37289800
N	0.92945700	-0.30960900	2.73500100
C	1.48831700	-1.64162500	2.88973700
C	1.64180400	0.69106500	3.53413500
H	0.79162100	-2.38672500	2.49904400
H	2.46105800	-1.75319900	2.38816600
H	1.63069700	-1.83063200	3.95525700
H	2.72068600	0.62638700	3.34146600
H	1.30936100	1.69403200	3.26858700
H	1.46096400	0.52469900	4.59872800
N	-1.28633900	3.40838900	0.74084000
C	-2.51432500	3.44159100	-0.05660700
C	-1.46160000	4.00097900	2.06071500
H	-2.31568600	3.09210100	-1.07287900
H	-3.29090600	2.80720100	0.39204500
H	-2.88396600	4.46877300	-0.10718300
H	-2.27431400	3.54203100	2.63166100
H	-0.53001400	3.90642200	2.62297800
H	-1.67488700	5.06532400	1.92312300

N	-1.54065800	1.19211800	2.48717400
C	-2.39737800	0.03680500	2.21906300
C	-1.30117400	1.33246700	3.91840100
H	-2.64208300	-0.00324900	1.15504500
H	-1.92916900	-0.91662000	2.51501600
H	-3.32583100	0.15347500	2.78475300
H	-0.85442300	0.43601700	4.37107500
H	-0.66395000	2.19424400	4.12279900
H	-2.26657100	1.51254400	4.40102200
H	0.64102400	1.17350100	-2.49239000
H	1.22793400	-1.59392400	0.51711100
N	0.38120000	-1.31294600	-1.88735600
C	0.32584600	-1.03110000	-3.31827000
C	0.46365400	-2.71146600	-1.47468400
H	-0.50509900	-0.35683400	-3.54102200
H	1.25924600	-0.57991000	-3.67245400
H	0.17042900	-1.96364600	-3.85616500
H	1.49302200	-3.00373900	-1.23668800
H	-0.16942900	-2.88478000	-0.60261600
H	0.10689300	-3.33874800	-2.28945500
N	0.38109700	3.38203100	-1.27203100
H	0.04620900	4.16524200	-0.72266000

TI-2347

Zero-point correction= 0.461953 (Hartree/Particle)

Thermal correction to Energy= 0.485531

Thermal correction to Enthalpy= 0.486475

Thermal correction to Gibbs Free Energy= 0.411177

Sum of electronic and zero-point Energies=	-900.381396
Sum of electronic and thermal Energies=	-900.357818
Sum of electronic and thermal Enthalpies=	-900.356874
Sum of electronic and thermal Free Energies=	-900.432172
C	0.16452500 -0.20707000 1.73881700
C	0.41554300 -1.04945100 0.67741700
C	0.27726300 -0.79894600 -0.70068200
C	-0.52485500 1.07608900 1.59058000
C	0.21561000 0.38856900 -1.40177500
C	-0.38513500 1.95276200 0.53474900
C	0.25182000 1.68394000 -0.76101400
C	1.53483200 2.83842000 -2.59131700
H	2.03963800 3.80344100 -2.54876500
H	2.27466800 2.03876800 -2.57855500
H	0.96261500 2.77206300 -3.51879400
N	0.37363100 -0.62691500 3.04728500
C	0.53254300 -2.04871600 3.31337300
C	1.33096100 0.17609700 3.81657300
H	-0.27926000 -2.61038300 2.84702600
H	1.49815700 -2.44438300 2.96476900
H	0.47717200 -2.19864600 4.39358000
H	2.34946300 -0.21163500 3.67712700
H	1.31480800 1.21275000 3.48058200
H	1.08200200 0.14384700 4.88012600
N	-0.84337800 3.29230300 0.60549300
C	-2.12472700 3.52458600 -0.06618400
C	-0.73773400 4.03109500 1.85947500
H	-2.12702000 3.05499900 -1.05356900

H	-2.95464200	3.11494800	0.52496100
H	-2.27480000	4.59950900	-0.19313900
H	-1.58600500	3.85664500	2.52753500
H	0.18726000	3.75202900	2.36912400
H	-0.68824700	5.09678200	1.61644000
H	0.72775900	-2.05884800	0.91998000
H	0.32604300	-1.69131500	-1.31589200
N	0.19412500	0.40756400	-2.80684000
C	-0.98951800	1.03746300	-3.39429200
C	0.57355000	-0.80682900	-3.51115900
H	-1.16794700	2.01681600	-2.94422200
H	-0.81886000	1.18220300	-4.46375400
H	-1.88915200	0.41985400	-3.26184000
H	1.52805000	-1.17736300	-3.13106400
H	-0.17956600	-1.60625800	-3.43455200
H	0.69723200	-0.56327300	-4.56828000
N	-1.56928600	1.40280800	2.51909200
C	-2.67038200	0.44749900	2.36062700
C	-1.31455700	1.65292300	3.93478700
H	-2.91640400	0.33561200	1.30197300
H	-2.43104900	-0.54169200	2.78186600
H	-3.54688100	0.84374200	2.88069700
H	-1.13424300	0.73344200	4.50611200
H	-0.47063100	2.33106700	4.06685800
H	-2.20116000	2.14525400	4.34646000
N	0.67704100	2.75890900	-1.41356800
H	0.50294300	3.61257200	-0.88490500

TI-2356

Zero-point correction= 0.461860 (Hartree/Particle)

Thermal correction to Energy= 0.486258

Thermal correction to Enthalpy= 0.487202

Thermal correction to Gibbs Free Energy= 0.409398

Sum of electronic and zero-point Energies= -900.405659

Sum of electronic and thermal Energies= -900.381261

Sum of electronic and thermal Enthalpies= -900.380317

Sum of electronic and thermal Free Energies= -900.458121

C	0.02464300	0.04074400	1.66565700
C	0.55873400	-0.75125800	0.68501000
C	0.72634000	-0.31863000	-0.70948600
C	-0.62948700	1.31970700	1.69926000
C	-0.04944600	0.66643600	-1.29223900
C	-1.09095000	2.06442400	0.60898600
C	-0.89943900	1.67588700	-0.76727100
C	-1.38215100	2.37344900	-3.11424000
H	-2.05660800	3.10483700	-3.55757500
H	-0.36948100	2.56327500	-3.49228200
H	-1.69957000	1.37719500	-3.43287600
N	-1.68074900	3.33794700	0.78000400
C	-3.12177000	3.53168700	0.65565100
C	-0.96680900	4.34835600	1.54301400
H	-3.56765700	2.67901700	0.13795100
H	-3.61972700	3.64363300	1.62660100
H	-3.33432900	4.43939400	0.07660600
H	-1.17169400	4.32073300	2.62065600
H	0.10762600	4.22406900	1.39453000

H	-1.25419900	5.33522900	1.16576300
N	-0.93405100	1.76698700	2.97520400
C	-2.32320400	2.02792600	3.34072100
C	-0.08674600	1.41492300	4.10147000
H	-2.98826300	1.74072300	2.52680300
H	-2.58021200	1.41582700	4.21253500
H	-2.49842100	3.07727400	3.60032000
H	-0.36372500	0.45608900	4.56628600
H	0.95847400	1.37582000	3.79100100
H	-0.18617000	2.19348600	4.86246900
H	0.16014100	0.82182300	-2.34008900
N	1.64116400	-0.98293900	-1.47456300
C	1.60737800	-0.89557900	-2.92552600
C	2.92225800	-1.44595100	-0.93119000
H	0.58403600	-1.01474500	-3.28939200
H	2.01561800	0.05331100	-3.30005200
H	2.20900300	-1.71123200	-3.32926200
H	3.71369000	-1.10136500	-1.60235800
H	3.10243500	-1.02589500	0.05517700
H	2.96261300	-2.53781500	-0.86697100
H	-0.03448500	-0.44580000	2.62997500
N	1.00549100	-2.03081500	0.99596800
C	1.21778900	-2.38700100	2.38714100
C	0.48529700	-3.15216900	0.21051400
H	1.78848700	-1.60464700	2.89290200
H	0.27884200	-2.55875600	2.93587600
H	1.79729900	-3.31194600	2.41627500
H	-0.48933100	-3.47895600	0.59715400

H	0.37299700	-2.87556500	-0.83644400
H	1.18420400	-3.98956000	0.27878200
N	-1.46623000	2.49779400	-1.67424300
H	-1.78128700	3.37850500	-1.28927800

TI-2357

Zero-point correction= 0.461997 (Hartree/Particle)

Thermal correction to Energy= 0.486455

Thermal correction to Enthalpy= 0.487400

Thermal correction to Gibbs Free Energy= 0.410490

Sum of electronic and zero-point Energies= -900.414827

Sum of electronic and thermal Energies= -900.390368

Sum of electronic and thermal Enthalpies= -900.389424

Sum of electronic and thermal Free Energies= -900.466333

C	-0.15630800	-0.03326600	1.93597900
C	0.86213300	-0.57952300	1.12305600
C	0.80252900	-0.56300800	-0.31488600
C	-1.09038600	0.94458100	1.58714300
C	0.20350300	0.36690000	-1.12748200
C	-0.86004300	1.93718300	0.53640600
C	-0.14772200	1.70928400	-0.62356600
C	1.32724600	2.75279800	-2.33656400
H	1.70478600	3.77093000	-2.43008600
H	2.13806600	2.11064300	-1.97627000
H	1.02491800	2.40630900	-3.32722700
N	-1.20469200	3.28300100	0.79374600
C	-2.19963600	3.96836400	-0.02164200
C	-0.98918200	3.84138400	2.11610700

H	-2.29902600	3.46657700	-0.98672300
H	-3.18787000	4.00387000	0.45545100
H	-1.88459500	5.00204500	-0.20495500
H	-1.83994400	3.70775000	2.79975400
H	-0.10812000	3.38074100	2.56859300
H	-0.80228600	4.91514300	2.01677200
N	-2.16354800	1.15265800	2.39564500
C	-3.41044400	1.68950400	1.86304600
C	-2.26881900	0.52426300	3.70149100
H	-3.36809000	1.73379200	0.77546300
H	-4.22684500	1.01722100	2.14278000
H	-3.63015000	2.68560400	2.26122200
H	-2.47845400	-0.55103200	3.62980600
H	-1.34692700	0.67384800	4.26925600
H	-3.08222800	1.00237400	4.24819600
H	-0.30524200	-0.52180300	2.88706400
N	1.80375900	-1.36193600	1.69629700
C	2.78521700	-2.07914900	0.89168300
C	1.80879100	-1.58376200	3.13580900
H	3.19901000	-1.41978700	0.12570900
H	3.59761900	-2.40663600	1.53801900
H	2.35217000	-2.96324400	0.40803100
H	1.73540400	-0.62905300	3.66331100
H	0.97888600	-2.22828900	3.44994100
H	2.74307100	-2.06548100	3.41732500
H	1.18765300	-1.45390500	-0.79051900
N	0.09177300	0.17118400	-2.47892700
C	-1.04054000	0.73235700	-3.21471800

C	0.64920000	-1.03127100	-3.07126900
H	-1.33591500	1.69278800	-2.79544100
H	-0.74708200	0.88672200	-4.25568700
H	-1.89717800	0.04754700	-3.19169400
H	1.70702200	-1.12447300	-2.80973600
H	0.11963500	-1.93965200	-2.75157500
H	0.57271900	-0.95014700	-4.15581200
N	0.20089700	2.78048900	-1.40817600
H	0.08662400	3.64726500	-0.89647500

TI-2367

Zero-point correction= 0.459862 (Hartree/Particle)

Thermal correction to Energy= 0.484583

Thermal correction to Enthalpy= 0.485527

Thermal correction to Gibbs Free Energy= 0.408109

Sum of electronic and zero-point Energies= -900.376738

Sum of electronic and thermal Energies= -900.352017

Sum of electronic and thermal Enthalpies= -900.351073

Sum of electronic and thermal Free Energies= -900.428491

C	0.01399400	0.02279500	2.00951600
C	0.66626200	-0.66674200	0.95972500
C	0.75125400	-0.39116100	-0.41945100
C	-0.76112500	1.19719200	1.98693500
C	0.43325800	0.91128900	-0.90464200
C	-0.72339300	2.03370300	0.80879700
C	0.53349200	1.91276400	0.12903100
C	2.96653200	1.67780800	0.45446600
H	3.73040500	2.38595600	0.77386200

H	3.09320700	0.72379300	0.97998400
H	3.04722800	1.49504700	-0.61888900
N	-1.80207400	2.60884500	0.23177300
C	-3.15121700	2.10322900	0.44425700
C	-1.70931200	3.85192700	-0.51727900
H	-3.11665100	1.03950300	0.67655600
H	-3.66259200	2.62690700	1.26056800
H	-3.71918400	2.25212600	-0.47822200
H	-2.29548500	4.63862900	-0.02611600
H	-0.66864400	4.17484100	-0.57232400
H	-2.09667800	3.72024500	-1.53259200
N	-1.74651700	1.44958900	2.92802900
C	-2.11765000	0.41611300	3.87710500
C	-1.86556300	2.80765700	3.44287700
H	-2.23662000	-0.53729200	3.35795200
H	-1.37880500	0.29055700	4.68225000
H	-3.07220400	0.68629300	4.33450500
H	-1.12903000	3.01151000	4.23334500
H	-1.72458400	3.53169900	2.63763000
H	-2.86570700	2.95010100	3.85956400
H	0.03015300	-0.50609100	2.95750400
N	-0.19475000	1.21242600	-2.07375800
C	0.23210500	2.34989100	-2.87689500
C	-1.00186200	0.22702600	-2.77708200
H	0.83127000	3.03137500	-2.26936200
H	0.83801700	2.02101400	-3.73199200
H	-0.63639700	2.88998000	-3.26529300
H	-0.41726500	-0.34319600	-3.51001800

H	-1.43649700	-0.46998600	-2.06173200
H	-1.80327400	0.75446500	-3.30268300
H	1.08254600	-1.62254700	1.26414900
N	0.98284900	-1.39750300	-1.36062100
C	2.02539300	-1.14476700	-2.34743100
C	0.90845100	-2.78461000	-0.93922600
H	1.94646700	-0.12355300	-2.72794300
H	3.03383600	-1.28791300	-1.93004200
H	1.90083800	-1.83128700	-3.18876900
H	1.78809200	-3.10797200	-0.36148400
H	0.01388200	-2.93942900	-0.33215400
H	0.83971300	-3.41756700	-1.82710000
N	1.65718800	2.23485800	0.74436700
H	1.53818200	2.69338300	1.64344500

TI-2456

Zero-point correction= 0.461984 (Hartree/Particle)

Thermal correction to Energy= 0.486125

Thermal correction to Enthalpy= 0.487070

Thermal correction to Gibbs Free Energy= 0.410872

Sum of electronic and zero-point Energies= -900.406419

Sum of electronic and thermal Energies= -900.382277

Sum of electronic and thermal Enthalpies= -900.381333

Sum of electronic and thermal Free Energies= -900.457531

C	0.08930500	0.57476200	2.03974800
C	0.53772500	-0.48850700	1.23608200
C	0.54989700	-0.45465400	-0.20978800
C	-0.83871800	1.59277800	1.58460700

C	0.63674700	0.74850800	-0.97034900
C	-0.86496800	2.24391800	0.39664600
C	0.09170500	1.98703000	-0.69237000
C	1.24269800	3.01435300	-2.61764200
H	1.34027700	4.02369800	-3.01377600
H	2.22988000	2.66430500	-2.29585400
H	0.88420900	2.36126000	-3.42240400
N	-1.72427000	3.33383900	0.15696800
C	-2.68123800	3.12048400	-0.93953500
C	-2.36951300	3.94365300	1.30984300
H	-2.18204300	2.67859300	-1.80255500
H	-3.49929700	2.45748600	-0.62677800
H	-3.10303000	4.08330500	-1.23595400
H	-3.14515600	3.30176200	1.75538800
H	-1.62235400	4.18515800	2.06924000
H	-2.84663300	4.87001100	0.98439400
N	0.67015300	-1.62702500	-0.88083900
C	0.05502800	-2.86547500	-0.39203000
H	0.78710600	-3.54997800	0.04537900
H	-0.71955600	-2.64532600	0.34029600
H	-0.41575700	-3.35350700	-1.24845900
H	-1.53998600	1.94495000	2.32976000
H	1.09761000	0.66539000	-1.94446400
N	0.98917700	-1.65888600	1.85976500
C	2.33292000	-2.15578400	1.64604300
C	0.15924000	-2.31485200	2.84873600
H	2.67054700	-1.90472400	0.63628000
H	3.06536900	-1.75653800	2.36151400

H	2.33779100	-3.24678800	1.74184300
H	0.36298500	-2.01807300	3.88630700
H	-0.89286700	-2.09656700	2.64301600
H	0.30451800	-3.39839100	2.77308100
N	0.42584600	0.59579500	3.36605600
C	1.79388200	0.24870800	3.75518600
C	-0.30420300	1.41314700	4.32481200
H	2.45589000	0.30781800	2.88934100
H	2.13219200	0.98205100	4.49108800
H	1.87269400	-0.74832300	4.19670000
H	-0.12729600	2.48793500	4.18298500
H	-1.37662500	1.21420700	4.26959800
H	0.02430500	1.13560300	5.32638100
C	1.07051700	-1.66104600	-2.28269800
H	1.25660700	-2.69843600	-2.55820300
H	0.29395200	-1.25328800	-2.94137100
H	1.99992500	-1.10778600	-2.43517100
N	0.31856600	3.03691400	-1.50740400
H	-0.13547800	3.90071500	-1.24304800

TI-2457

Zero-point correction= 0.462110 (Hartree/Particle)

Thermal correction to Energy= 0.486363

Thermal correction to Enthalpy= 0.487307

Thermal correction to Gibbs Free Energy= 0.410328

Sum of electronic and zero-point Energies= -900.403673

Sum of electronic and thermal Energies= -900.379420

Sum of electronic and thermal Enthalpies= -900.378476

Sum of electronic and thermal Free Energies= -900.455455

C	0.29320500	0.69597600	2.03791200
C	0.57344000	-0.42442400	1.15651700
C	0.55975800	-0.31663300	-0.22904700
C	-0.56094000	1.73171900	1.67050400
C	0.30727700	0.75308400	-1.10246000
C	-1.03862100	2.19989600	0.42453500
C	-0.32907900	1.97709500	-0.80532100
C	-0.30712600	4.37072500	-1.44071700
H	0.16648800	4.89827800	-2.26839300
H	-1.31016100	4.77926200	-1.30413800
H	0.26876500	4.55718000	-0.52713000
N	-2.08124300	3.09274600	0.40786300
C	-3.05661600	3.02797500	-0.68563800
C	-2.64707300	3.58317600	1.65560100
H	-2.56817900	2.80211800	-1.63199200
H	-3.81151200	2.26076900	-0.47538100
H	-3.55539300	3.99518800	-0.77311700
H	-3.10965400	2.78227800	2.24892800
H	-1.88343500	4.08248300	2.25803700
H	-3.41340100	4.31960400	1.41486400
H	-0.90152700	2.33138700	2.50113300
N	0.90159000	-1.63097200	1.73051400
C	1.56314100	-2.66680100	0.95627900
C	0.20171700	-2.11074300	2.92318300
H	2.37245500	-2.23724400	0.36062700
H	2.00083000	-3.38586200	1.65092700
H	0.87548800	-3.20819000	0.29064000

H	0.84189800	-2.08469500	3.81134900
H	-0.69041100	-1.51667600	3.11637400
H	-0.10935700	-3.14388800	2.74537100
N	0.75011200	0.61744700	3.34158700
C	2.16138900	0.29224300	3.56807900
C	0.22189000	1.52402100	4.34528700
H	2.51640900	-0.42836500	2.83465000
H	2.77882700	1.19775300	3.50908000
H	2.27106300	-0.13976900	4.56543500
H	0.52472800	2.56880500	4.17884300
H	-0.86954800	1.46676700	4.37665700
H	0.60230100	1.21081900	5.31839500
H	0.82202300	-1.22798100	-0.75159000
N	0.68664600	0.60164800	-2.45696800
C	1.80476300	-0.28342000	-2.75431500
C	-0.42652900	0.40163500	-3.39411700
H	2.61065400	-0.11721000	-2.03730100
H	1.52900700	-1.34938300	-2.74707500
H	2.17363700	-0.04488500	-3.75464700
H	-0.85183400	-0.60699100	-3.29561500
H	-1.21347600	1.13646500	-3.21705000
H	-0.05832300	0.52768200	-4.41484100
N	-0.33746900	2.94931100	-1.78353600
H	0.30926500	2.69433800	-2.52235100

TI-3456

Zero-point correction= 0.461078 (Hartree/Particle)

Thermal correction to Energy= 0.485387

Thermal correction to Enthalpy= 0.486331
 Thermal correction to Gibbs Free Energy= 0.409765
 Sum of electronic and zero-point Energies= -900.392061
 Sum of electronic and thermal Energies= -900.367752
 Sum of electronic and thermal Enthalpies= -900.366808
 Sum of electronic and thermal Free Energies= -900.443374

C	-0.12014200	0.68770700	1.58908200
C	0.13469600	-0.38995600	0.74243300
C	0.02500600	-0.37600000	-0.72018400
C	-0.41724500	2.07762000	1.20012200
C	0.13971900	0.72043200	-1.52479000
C	0.00060500	2.70087200	0.02147000
C	0.31639400	2.10290800	-1.20311400
C	0.94972800	4.31504300	-2.13331500
H	1.39529700	4.65251500	-3.06769900
H	0.02099600	4.87450000	-1.97124100
H	1.64507600	4.53266000	-1.31705400
N	0.56845000	-1.58583000	1.30954100
C	1.74265900	-1.58690800	2.16055100
C	-0.18700600	-2.82663900	1.25832700
H	2.30917900	-0.66533200	2.01405700
H	1.51138400	-1.69122100	3.22813100
H	2.38303900	-2.43131600	1.87557100
H	-0.38186500	-3.18305700	2.27850800
H	-1.13777100	-2.66916200	0.75219000
H	0.36144100	-3.61217900	0.72333000
N	-0.10282300	0.46055500	2.96234100
C	0.72099700	1.26058500	3.84611400

C	-0.90351600	-0.57781400	3.57767300
H	1.40467900	1.87961200	3.26241600
H	0.13125200	1.91840100	4.49989100
H	1.32342500	0.60372500	4.48514700
H	-1.46778900	-0.15389100	4.41897800
H	-1.61870900	-0.97681500	2.85533300
H	-0.30379900	-1.40964300	3.96713700
H	0.19561000	0.50382700	-2.58889200
H	-0.10379400	3.77530800	-0.01694000
N	-1.05013100	2.83979900	2.13526200
C	-1.05206600	4.29212100	2.05191800
C	-2.14735100	2.28761700	2.93620000
H	-0.04055000	4.66596900	1.88060100
H	-1.71821000	4.66640600	1.26257600
H	-1.39645900	4.68455100	3.00934000
H	-2.99713100	2.97004700	2.84735000
H	-2.45851000	1.31687400	2.55382000
H	-1.88290300	2.19758800	3.99345700
N	-0.07455000	-1.64444300	-1.34425400
C	-0.83845600	-1.69592200	-2.58384300
C	1.20751100	-2.33971400	-1.50139800
H	-1.76549600	-1.12970200	-2.47831300
H	-0.28431000	-1.32054100	-3.45971200
H	-1.08836300	-2.74107200	-2.78235300
H	1.80053700	-1.88318800	-2.30970300
H	1.78295400	-2.29712900	-0.57776100
H	1.01625200	-3.38469600	-1.75748800
N	0.70536100	2.88981100	-2.22701200

H	0.81799700	2.45740500	-3.13102200
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TI-23456

Zero-point correction=	0.535466 (Hartree/Particle)
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Thermal correction to Energy=	0.563594
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Thermal correction to Enthalpy=	0.564538
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Thermal correction to Gibbs Free Energy=	0.480400
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Sum of electronic and zero-point Energies=	-1034.219082
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Sum of electronic and thermal Energies=	-1034.190954
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Sum of electronic and thermal Enthalpies=	-1034.190010
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Sum of electronic and thermal Free Energies=	-1034.274149
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C	-0.42540500	0.60839800	1.53708400
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C	0.18279900	-0.34942300	0.76350200
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C	0.80522500	-0.11242800	-0.56144300
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C	-0.43768700	2.06528400	1.25227800
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C	0.21979800	0.71927500	-1.51575300
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C	-0.63383700	2.60118400	-0.00333000
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C	-0.57538400	1.84629900	-1.26719200
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C	-1.28158300	1.87331000	-3.63522500
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H	-2.02304100	2.43731600	-4.19892600
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H	-0.32010300	1.94784200	-4.15657100
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H	-1.58476900	0.82248600	-3.60218000
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N	0.19039600	-1.68997800	1.15711400
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C	0.75435400	-2.14597700	2.40837400
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C	-0.24873500	-2.72067900	0.23927400
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H	1.27129500	-1.32395300	2.90636500
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H	-0.00683900	-2.54407500	3.09191800
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H	1.48299900	-2.94799100	2.22607300
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H	-0.88180500	-3.44011500	0.77126800
H	-0.84672500	-2.27798500	-0.56062300
H	0.58541400	-3.27762400	-0.21535600
N	-1.15319100	0.23606700	2.68987500
C	-0.57008200	0.30930900	4.02175800
C	-2.20242800	-0.75589600	2.53452800
H	0.28379500	0.98907800	4.01402800
H	-1.31030800	0.68874700	4.73471100
H	-0.23785900	-0.67134500	4.38491500
H	-2.98899600	-0.54369300	3.26739400
H	-2.63714200	-0.67664700	1.53566100
H	-1.86763400	-1.79070600	2.68682000
H	0.48681000	0.56587200	-2.55215900
N	-0.32157600	2.91620200	2.36351000
C	0.67044000	3.97426900	2.32405000
C	-1.35242100	3.10538500	3.37571800
H	1.43307700	3.74676600	1.57658100
H	0.24543600	4.96447800	2.10854900
H	1.15965500	4.03558000	3.30369400
H	-1.78063100	4.11369200	3.31178100
H	-2.14753200	2.37397800	3.24101700
H	-0.93063400	2.99062000	4.38028100
N	1.85007600	-0.88872100	-0.90766300
C	2.30275100	-0.95654600	-2.29049000
C	2.75315100	-1.46820800	0.08569800
H	1.47870300	-1.24460000	-2.94877300
H	2.71439500	0.00202400	-2.62803600
H	3.07600700	-1.71969600	-2.36538900

H	3.77531000	-1.32773100	-0.27219000
H	2.65483100	-0.95088200	1.03862800
H	2.57508500	-2.53811600	0.22827000
N	-1.02624300	3.94092800	-0.21639000
C	-0.07120600	4.86357900	-0.82230800
C	-2.04409200	4.56052600	0.61435700
H	0.55262100	4.33106400	-1.54466700
H	-0.61460800	5.65170900	-1.35351600
H	0.58553600	5.34307500	-0.08605000
H	-2.63118800	5.24734300	-0.00538200
H	-2.71192500	3.79220700	1.00783700
H	-1.63665800	5.13884600	1.45117800
N	-1.20312400	2.42087500	-2.29836700
H	-1.67061000	3.29138000	-2.07280400

TI-23457

Zero-point correction= 0.534037 (Hartree/Particle)

Thermal correction to Energy= 0.562250

Thermal correction to Enthalpy= 0.563194

Thermal correction to Gibbs Free Energy= 0.476393

Sum of electronic and zero-point Energies= -1034.208871

Sum of electronic and thermal Energies= -1034.180659

Sum of electronic and thermal Enthalpies= -1034.179714

Sum of electronic and thermal Free Energies= -1034.266516

C	-0.16303700	0.27136600	2.05525000
C	0.38342000	-0.62525500	1.15052400
C	0.38555300	-0.46529700	-0.29716000
C	-0.83418400	1.48793300	1.75659500

C	0.25098300	0.71001400	-1.04212000
C	-0.81259600	2.30799400	0.66024600
C	-0.00702800	2.04631700	-0.51684700
C	1.34059700	3.25637300	-2.26889400
H	1.70635900	4.28305000	-2.23994500
H	2.17493500	2.57203000	-2.11176200
H	0.89889800	3.05811000	-3.24730300
N	0.89963800	-1.86652700	1.59363600
C	2.29869000	-1.82369700	1.99916600
C	0.09356500	-2.70833200	2.46926700
H	2.87545600	-1.19913600	1.31250400
H	2.41385300	-1.42562500	3.01910400
H	2.71489800	-2.83613200	1.97209900
H	0.25299200	-2.49916300	3.53289500
H	-0.96593200	-2.57412000	2.23751500
H	0.35153600	-3.75451600	2.26738900
N	-0.06120200	-0.05323300	3.44915700
C	0.82544500	0.86533500	4.15900300
C	-1.33868500	-0.20528500	4.13649100
H	1.78093600	0.93841900	3.63466900
H	0.40295300	1.88030600	4.26256400
H	1.00948300	0.47023700	5.16156900
H	-1.86615800	0.74904000	4.30588400
H	-1.99324200	-0.86807200	3.56673100
H	-1.15764900	-0.65812800	5.11491000
N	0.47588700	-1.64033700	-1.09943500
C	1.70968800	-2.41867400	-1.10274600
C	-0.70690400	-2.48777500	-1.00859500

H	2.57248900	-1.76437700	-0.95617900
H	1.72316500	-3.18783200	-0.32164100
H	1.81630200	-2.90218700	-2.08066300
H	-0.73183000	-3.08633100	-0.08598100
H	-1.61070700	-1.87580500	-1.06524500
H	-0.70560300	-3.17212600	-1.86282600
N	-1.39935100	3.59354500	0.68753800
C	-1.72927400	4.16027300	1.98987800
C	-2.50341000	3.76968600	-0.26945100
H	-2.59125500	3.67032300	2.46612200
H	-0.86513700	4.09592500	2.65440000
H	-1.97795300	5.21342900	1.84669600
H	-2.75070100	4.83123200	-0.33203700
H	-2.20823500	3.42822200	-1.26355300
H	-3.39723900	3.21456400	0.04325400
H	-1.36968600	1.89412500	2.60991700
N	0.34944500	0.72685000	-2.43730100
C	1.30932700	-0.06605900	-3.18327700
C	-0.87238700	1.01701200	-3.17223500
H	2.20394200	-0.23134900	-2.58171500
H	0.91567900	-1.03703800	-3.50000100
H	1.59729400	0.51080700	-4.07104900
H	-1.52028800	0.13261300	-3.24877600
H	-1.43502600	1.82026300	-2.68850100
H	-0.61420000	1.34403700	-4.18411000
N	0.35490900	3.12821600	-1.20055700
H	0.04981200	3.98785000	-0.75041900

TI-23567

Zero-point correction= 0.535648 (Hartree/Particle)

Thermal correction to Energy= 0.563831

Thermal correction to Enthalpy= 0.564776

Thermal correction to Gibbs Free Energy= 0.480223

Sum of electronic and zero-point Energies= -1034.227384

Sum of electronic and thermal Energies= -1034.199201

Sum of electronic and thermal Enthalpies= -1034.198256

Sum of electronic and thermal Free Energies= -1034.282809

C	0.00120300	0.03239400	2.05552200
C	0.75777700	-0.63612800	1.11808400
C	0.42047000	-0.63603100	-0.32281800
C	-0.90809400	1.11424500	1.80651500
C	0.00859500	0.47914600	-0.99921100
C	-0.60302800	2.12775900	0.81102100
C	0.04081500	1.82819300	-0.38037700
C	1.52795600	2.60797800	-2.20006600
H	2.15664000	3.49512200	-2.27406400
H	2.16488900	1.74457500	-1.98199200
H	1.03927900	2.44475800	-3.16405100
N	1.67778100	-1.58874600	1.50714100
C	3.00234300	-1.51944500	0.88601800
C	1.73829700	-2.00459300	2.89705000
H	2.92944000	-1.06535500	-0.10110600
H	3.67362400	-0.90402000	1.49999200
H	3.43095300	-2.51985200	0.79065000
H	2.13042900	-1.21763400	3.55865600
H	0.74542500	-2.30401000	3.24118600

H	2.39910600	-2.87042800	2.96705900
N	0.16917000	-1.90988500	-0.92563100
C	1.26631300	-2.77967600	-1.32083600
C	-0.86583500	-2.65667100	-0.21947500
H	2.05969400	-2.20501600	-1.80396500
H	1.69761400	-3.33827600	-0.47656600
H	0.88697700	-3.50614600	-2.04688900
H	-0.51168200	-3.07101400	0.73919300
H	-1.72490400	-2.00791100	-0.03274400
H	-1.19102000	-3.48862600	-0.85084000
N	-0.69415900	3.49582500	1.15549200
C	-1.60641200	4.38225700	0.44743800
C	-0.24084200	3.92262600	2.46625900
H	-1.76608200	4.00557300	-0.56677600
H	-2.58506800	4.49102500	0.93411100
H	-1.16327600	5.38111100	0.37231700
H	-0.98202700	3.79160300	3.26846500
H	0.65676200	3.36133800	2.73858000
H	0.01803200	4.98436000	2.42262700
N	-0.41048000	0.49175700	-2.30709300
C	0.07676800	-0.42520100	-3.32150300
C	-1.47493800	1.39052200	-2.72564700
H	1.10422300	-0.71360500	-3.09364500
H	-0.53016200	-1.33156700	-3.40306800
H	0.07508300	0.10088500	-4.28248400
H	-2.16337100	0.84395600	-3.37652700
H	-2.04021100	1.73722000	-1.85801400
H	-1.09984500	2.26564200	-3.27381500

H	0.12785700	-0.24487300	3.09355300
N	-1.89678900	1.34045200	2.68428300
C	-2.03250900	0.52783100	3.88954100
C	-3.01087400	2.22810900	2.35962400
H	-2.12640300	-0.53286400	3.63523400
H	-1.16895300	0.66192900	4.54753000
H	-2.92144300	0.84760300	4.42990200
H	-2.91014200	3.21224600	2.82526100
H	-3.08207000	2.34259600	1.27774200
H	-3.93005400	1.76299100	2.71981200
N	0.56358900	2.82600100	-1.13004200
H	0.60297800	3.71176700	-0.64145800

TI-234567

Zero-point correction= 0.606691 (Hartree/Particle)

Thermal correction to Energy= 0.639678

Thermal correction to Enthalpy= 0.640622

Thermal correction to Gibbs Free Energy= 0.546177

Sum of electronic and zero-point Energies= -1168.034184

Sum of electronic and thermal Energies= -1168.001197

Sum of electronic and thermal Enthalpies= -1168.000253

Sum of electronic and thermal Free Energies= -1168.094698

C	0.15427500	0.14476800	1.54755500
C	0.70180300	-0.50015000	0.43295500
C	0.48643000	-0.13941500	-0.98208500
C	-0.72638300	1.34216700	1.49447400
C	0.45250000	1.18439500	-1.36339100
C	-0.46227000	2.33410600	0.58138000

C	0.74122000	2.05909500	-0.22015800
C	2.35594700	2.93707000	1.41107800
H	3.22711500	3.57371800	1.25919500
H	1.52396500	3.51932100	1.80841600
H	2.60095300	2.13438200	2.11423700
N	-1.83020200	1.40549100	2.33416400
C	-2.51131300	0.19501300	2.74823600
H	-2.15342700	-0.18820500	3.71468300
H	-3.58299100	0.40110100	2.83848000
H	-2.37365700	-0.58295300	1.99435300
C	-2.05768300	2.56392700	3.17918900
H	-1.49961200	3.41984400	2.79300700
H	-3.12176700	2.82257800	3.19537800
H	-1.74159500	2.37938600	4.21673800
N	-1.30595400	3.30127900	0.05595500
C	-0.85019400	4.68323200	0.06883600
C	-2.74920900	3.12533300	0.09623600
H	0.21878600	4.72788500	-0.16360200
H	-1.38550700	5.24999700	-0.69797900
H	-1.01851400	5.17375000	1.03930000
H	-3.18025400	3.65392300	-0.76043900
H	-2.98987300	2.06487600	0.01780800
H	-3.20699900	3.52455200	1.01015600
N	0.35284300	-0.32874600	2.82728600
C	0.43334600	-1.73344700	3.17597900
C	0.52840800	0.57987600	3.94237100
H	-0.10672300	-2.32791000	2.43791500
H	1.46210600	-2.10179500	3.23464000

H	-0.05399200	-1.87278800	4.14835500
H	1.46695800	0.35252100	4.46377500
H	0.57361900	1.61264400	3.59232900
H	-0.28815100	0.49551800	4.67282700
N	1.69079000	-1.51042500	0.70073600
C	1.44191800	-2.89467400	0.31653900
C	3.01243700	-1.08268000	0.27480400
H	0.41166500	-3.17406100	0.54453600
H	1.62178900	-3.08335700	-0.75166600
H	2.10344200	-3.54415400	0.90010500
H	3.10392400	-0.98028700	-0.82133900
H	3.25952900	-0.12509600	0.74711500
H	3.75190300	-1.81532600	0.61077600
N	0.34703500	-1.17893700	-1.89677700
C	-0.75024400	-2.12382200	-1.75279100
C	0.82425300	-1.01943800	-3.25760200
H	-1.13983000	-2.08340000	-0.73386500
H	-1.57210200	-1.89538400	-2.44763400
H	-0.40942500	-3.14389100	-1.96006000
H	0.08385800	-0.56057500	-3.92786500
H	1.72101600	-0.39716700	-3.25937500
H	1.08016600	-2.00792400	-3.65185700
N	-0.10241900	1.69469300	-2.52649600
C	-1.47095100	1.33308900	-2.86826800
C	0.27445000	3.02701400	-2.96158500
H	-1.69582900	0.33878000	-2.48201600
H	-2.19013900	2.04997700	-2.44515400
H	-1.59024600	1.32396800	-3.95623100

H	-0.35279100	3.80777000	-2.50520600
H	1.32149600	3.22069900	-2.71626700
H	0.16740900	3.09786200	-4.04794500
N	1.95751400	2.35729700	0.13330500
H	2.69151900	1.97455000	-0.45985100

Cartesian Coordination of MeO-TI Free Bases and Their Thermochemical Values (ω B97X-D/6-31g(d,p))

TI-2

Zero-point correction= 0.184975 (Hartree/Particle)

Thermal correction to Energy= 0.195416

Thermal correction to Enthalpy= 0.196360

Thermal correction to Gibbs Free Energy= 0.148755

Sum of electronic and zero-point Energies= -479.146282

Sum of electronic and thermal Energies= -479.135841

Sum of electronic and thermal Enthalpies= -479.134897

Sum of electronic and thermal Free Energies= -479.182502

C	-0.77531200	-0.00085200	1.10726700
C	0.03056500	-0.49951600	0.13823500
C	0.96739600	0.25282900	-0.64689300
C	-0.89881000	1.34879800	1.57791200
C	1.02331500	1.58958300	-0.83774100
C	-0.49552700	2.50561700	0.98193600
C	0.09687500	2.63476000	-0.37883600
H	-1.37552400	-0.72136700	1.65815400
H	0.02285400	-1.57438100	-0.01770900
H	1.83391500	1.95784900	-1.46156200
N	-0.15788300	3.71667800	-1.01399400
C	0.41851100	3.90186400	-2.32986900
H	-0.09260200	4.73038900	-2.82564300
H	1.48287200	4.16930000	-2.26194500
H	0.34158400	3.01264300	-2.97155300
H	1.72567000	-0.33635500	-1.15912100

H	-1.41847900	1.44165700	2.52509400
O	-0.64651100	3.71368000	1.54790800
C	-1.16748900	3.80685200	2.85504900
H	-1.12672800	4.86425600	3.11467100
H	-2.20831800	3.46404000	2.89818800
H	-0.56619600	3.22969100	3.56815900

TI-3

Zero-point correction= 0.184674 (Hartree/Particle)

Thermal correction to Energy= 0.195222

Thermal correction to Enthalpy= 0.196166

Thermal correction to Gibbs Free Energy= 0.148240

Sum of electronic and zero-point Energies= -479.143339

Sum of electronic and thermal Energies= -479.132791

Sum of electronic and thermal Enthalpies= -479.131847

Sum of electronic and thermal Free Energies= -479.179773

C	-0.70962300	-0.00068000	1.26405600
C	0.10265000	-0.50209700	0.31086100
C	0.91231600	0.23160200	-0.63310800
C	-0.98533000	1.39078200	1.55561400
C	0.89599400	1.54390700	-0.94598300
C	-0.66316800	2.48999600	0.84262500
C	0.02711000	2.62321600	-0.44286900
H	-1.23259500	-0.70085700	1.91044500
H	0.19155600	-1.58376500	0.25792800
H	1.61909400	1.85855500	-1.69278100
N	-0.11010700	3.76592200	-1.02064900
C	0.54901200	4.01353200	-2.28642000

H	0.17785800	4.95592100	-2.69588700
H	1.63798100	4.11707300	-2.16812600
H	0.36992900	3.22887300	-3.03551000
H	-1.02137900	3.43555700	1.23861400
O	-1.74594400	1.59063500	2.68830000
C	-1.03004100	1.42448800	3.89831200
H	-0.22988200	2.17051500	3.98461300
H	-1.74704400	1.56380100	4.70830200
H	-0.58639900	0.42283300	3.98027900
H	1.63161800	-0.37729000	-1.17687000

TI-4

Zero-point correction= 0.184504 (Hartree/Particle)

Thermal correction to Energy= 0.195129

Thermal correction to Enthalpy= 0.196074

Thermal correction to Gibbs Free Energy= 0.147752

Sum of electronic and zero-point Energies= -479.145617

Sum of electronic and thermal Energies= -479.134992

Sum of electronic and thermal Enthalpies= -479.134047

Sum of electronic and thermal Free Energies= -479.182369

C	-0.55418300	-0.27309300	1.12398900
C	0.20339200	-0.68585800	0.08060600
C	0.55239500	0.06434900	-1.09544400
C	-1.18977300	1.01838700	1.28794300
C	0.43385700	1.38351600	-1.36464100
C	-1.00270600	2.15664300	0.59357300
C	-0.09017500	2.46343000	-0.51700300
H	0.54276000	-1.71591800	0.12671800

H	0.78244600	1.70068100	-2.34305600
N	0.10793200	3.71946000	-0.72082900
C	0.97960100	4.13352400	-1.80114700
H	1.16992800	5.20510500	-1.70737400
H	1.94899700	3.61501200	-1.80277200
H	0.51520000	3.96913600	-2.78475900
H	1.00737200	-0.53474800	-1.88154900
H	-1.92624500	1.05233500	2.08667300
H	-1.57865500	3.02726600	0.89562100
O	-0.83786700	-1.21033800	2.08293300
C	-0.42256000	-0.88608000	3.39914100
H	-0.72580300	-1.72061700	4.03190200
H	0.66669800	-0.76809500	3.44692800
H	-0.89270400	0.03139000	3.77268400

TI-23

Zero-point correction= 0.218152 (Hartree/Particle)

Thermal correction to Energy= 0.231001

Thermal correction to Enthalpy= 0.231945

Thermal correction to Gibbs Free Energy= 0.178998

Sum of electronic and zero-point Energies= -593.591860

Sum of electronic and thermal Energies= -593.579011

Sum of electronic and thermal Enthalpies= -593.578067

Sum of electronic and thermal Free Energies= -593.631014

C	0.57048700	0.07539900	1.79938700
C	1.02631000	-0.71726600	0.80577000
C	0.70460400	-0.61707500	-0.59754200
C	-0.36959900	1.17013300	1.70670000

C	0.22086900	0.45643000	-1.25196900
C	-0.65585600	1.93569600	0.62197000
C	-0.00347600	1.81020400	-0.71444100
H	0.84878400	-0.16189300	2.82293800
H	1.66586900	-1.54825200	1.09101700
H	0.07665400	0.38755000	-2.32649100
N	0.27995300	2.77795600	-1.50029300
C	0.15408800	4.15607200	-1.07624400
H	0.80958600	4.76691400	-1.70261900
H	-0.87233100	4.51200000	-1.21575400
H	0.42768300	4.32579900	-0.02572300
H	0.91646100	-1.50246400	-1.19210000
O	-1.63444300	2.88176600	0.63511500
C	-1.69680000	3.82594000	1.69736500
H	-2.08825800	4.74620100	1.25805600
H	-2.35954000	3.48812400	2.49688400
H	-0.70554100	4.01349900	2.11937100
O	-1.02789300	1.43157200	2.89244300
C	-2.24498200	0.70946400	3.00864000
H	-2.96168200	1.02252600	2.23955400
H	-2.07419100	-0.37036600	2.91909400
H	-2.64990200	0.93106000	3.99741500

TI-24

Zero-point correction=	0.218288 (Hartree/Particle)
Thermal correction to Energy=	0.230954
Thermal correction to Enthalpy=	0.231898
Thermal correction to Gibbs Free Energy=	0.179708

Sum of electronic and zero-point Energies=	-593.606082
Sum of electronic and thermal Energies=	-593.593416
Sum of electronic and thermal Enthalpies=	-593.592471
Sum of electronic and thermal Free Energies=	-593.644661
C	-0.29415000 0.06567000 1.60740100
C	0.03018400 -0.79385500 0.60518400
C	0.02700600 -0.49320600 -0.80214400
C	-0.77668300 1.42096100 1.47113400
C	0.06590300 0.70267400 -1.42576400
C	-0.63144200 2.26204300 0.42174700
C	0.20310800 2.02142900 -0.79631000
H	0.27161800 -1.81871600 0.86028000
H	0.11676500 0.72353200 -2.51026900
N	0.93774500 2.88746900 -1.38077400
C	1.16160600 4.20314400 -0.81833800
H	2.14540200 4.54857500 -1.14828100
H	0.41688400 4.91018700 -1.19954000
H	1.12457000 4.24305700 0.27770800
H	0.04035000 -1.36812500 -1.44867700
H	-1.31995000 1.76081800 2.34560200
O	-1.24394100 3.46501100 0.34845900
C	-2.13950300 3.83969600 1.37305800
H	-2.57037600 4.79059300 1.06097100
H	-2.93556700 3.09539400 1.49382700
H	-1.62147300 3.97252000 2.33030500
O	-0.31514400 -0.28916500 2.92190900
C	0.03952000 -1.60687800 3.27261800
H	1.06847900 -1.83940200 2.97231600

H	-0.04041800	-1.66190600	4.35837100
H	-0.64149900	-2.34039900	2.82317400

TI-25

Zero-point correction= 0.218384 (Hartree/Particle)

Thermal correction to Energy= 0.231175

Thermal correction to Enthalpy= 0.232119

Thermal correction to Gibbs Free Energy= 0.179419

Sum of electronic and zero-point Energies= -593.603786

Sum of electronic and thermal Energies= -593.590994

Sum of electronic and thermal Enthalpies= -593.590050

Sum of electronic and thermal Free Energies= -593.642750

C	-0.21743300	-0.06070800	1.37148300
C	0.17455700	-0.83675200	0.32911200
C	0.18321900	-0.45255900	-1.06678600
C	-0.73276200	1.28428900	1.31366100
C	0.18389600	0.78559300	-1.59059600
C	-0.60444000	2.21116000	0.33464200
C	0.24269300	2.07502500	-0.88369700
H	-0.23510400	-0.50381500	2.36045900
H	0.24707800	0.88204500	-2.67073100
N	0.94322900	2.99316800	-1.43057400
C	1.11865600	4.28827700	-0.80646500
H	2.07684900	4.69667900	-1.13947900
H	0.33175900	4.97701400	-1.13184600
H	1.10533100	4.26551800	0.29026900
H	0.24602800	-1.29418400	-1.75096500
H	-1.30022600	1.57012300	2.19376200

O	-1.24173600	3.41215800	0.34364500
C	-2.14258300	3.69333700	1.38848500
H	-2.58912500	4.65901000	1.15170800
H	-2.92955200	2.93140000	1.45241300
H	-1.63048700	3.76188600	2.35665500
O	0.56724100	-2.13568100	0.45714900
C	0.59664300	-2.70644300	1.74317300
H	-0.40254900	-2.73310900	2.19690000
H	0.96059800	-3.72570600	1.61366900
H	1.27676500	-2.16066700	2.40941500

TI-26

Zero-point correction= 0.217568 (Hartree/Particle)

Thermal correction to Energy= 0.230648

Thermal correction to Enthalpy= 0.231592

Thermal correction to Gibbs Free Energy= 0.176806

Sum of electronic and zero-point Energies= -593.600390

Sum of electronic and thermal Energies= -593.587311

Sum of electronic and thermal Enthalpies= -593.586367

Sum of electronic and thermal Free Energies= -593.641152

C	0.70489700	0.38859700	1.56431100
C	1.23069600	-0.34851300	0.55838200
C	1.01040100	-0.15513700	-0.85798400
C	-0.20639500	1.49734500	1.48328200
C	0.62049000	0.99129600	-1.46347300
C	-0.40275700	2.30540000	0.41138000
C	0.43086100	2.29923000	-0.83249500
H	0.94212600	0.06511400	2.57495800

H	1.85482400	-1.19056300	0.83901400
H	0.56267100	0.97879000	-2.54734600
N	0.86854400	3.33445200	-1.43826200
C	0.70083200	4.66241400	-0.88501700
H	1.54233700	5.27618000	-1.21833300
H	-0.21627800	5.11931800	-1.27249400
H	0.65164400	4.69924600	0.21099900
H	-0.78112000	1.68766800	2.38376600
O	-1.36676400	3.24852200	0.34431700
C	-2.29499400	3.34770500	1.40341300
H	-3.02530500	4.09446500	1.09364700
H	-2.79761300	2.38924700	1.57893100
H	-1.81037300	3.67734800	2.33023900
O	1.29441100	-1.19024400	-1.70678900
C	1.18175500	-2.51376300	-1.22628900
H	0.28210100	-2.65033300	-0.61525000
H	1.11597900	-3.15119500	-2.10947300
H	2.06024800	-2.81961600	-0.64470300

TI-27

Zero-point correction=	0.217989 (Hartree/Particle)
Thermal correction to Energy=	0.230879
Thermal correction to Enthalpy=	0.231823
Thermal correction to Gibbs Free Energy=	0.179062
Sum of electronic and zero-point Energies=	-593.602479
Sum of electronic and thermal Energies=	-593.589589
Sum of electronic and thermal Enthalpies=	-593.588645
Sum of electronic and thermal Free Energies=	-593.641407

C	0.25385400	0.27017700	1.72865000
C	0.82180300	-0.51792300	0.78436800
C	0.77123600	-0.36852400	-0.64685400
C	-0.56142100	1.43685700	1.51093200
C	0.54694400	0.77805100	-1.33756900
C	-0.56301400	2.21633800	0.40346700
C	0.43108400	2.11702600	-0.70300100
H	0.34754800	-0.04882100	2.76321600
H	1.32868300	-1.41358500	1.13460400
N	1.11528400	3.07366600	-1.18682000
C	1.04411500	4.39318600	-0.59333900
H	2.00778400	4.88657100	-0.74365500
H	0.28015100	4.98633500	-1.10609800
H	0.80543100	4.39256700	0.47825300
H	0.97899700	-1.27105800	-1.21213500
H	-1.23876900	1.69226400	2.31988200
O	-1.43251800	3.23232700	0.17060700
C	-2.45824800	3.45961800	1.11098800
H	-3.08092400	4.25142100	0.69496700
H	-3.06304900	2.55764700	1.26495600
H	-2.05089400	3.78806000	2.07541900
O	0.47545600	0.86733100	-2.68095800
C	0.56485800	-0.32097200	-3.43420900
H	-0.20662900	-1.04215100	-3.13646800
H	0.41266000	-0.03193100	-4.47383800
H	1.55195800	-0.78754600	-3.32863800

TI-34

Zero-point correction= 0.218259 (Hartree/Particle)

Thermal correction to Energy= 0.231146

Thermal correction to Enthalpy= 0.232091

Thermal correction to Gibbs Free Energy= 0.179018

Sum of electronic and zero-point Energies= -593.600833

Sum of electronic and thermal Energies= -593.587946

Sum of electronic and thermal Enthalpies= -593.587002

Sum of electronic and thermal Free Energies= -593.640075

C	-0.27300300	0.06243300	1.62920100
C	0.48210300	-0.71192900	0.81189200
C	1.29990700	-0.30478800	-0.30493300
C	-0.36056700	1.52914700	1.58133900
C	1.33967000	0.86028500	-0.97983000
C	-0.01136300	2.34885600	0.56994900
C	0.54488600	2.07082000	-0.76225000
H	0.49440500	-1.77817400	1.00670300
H	1.99595800	0.93269200	-1.84217700
N	0.48831600	2.89353600	-1.75050300
C	-0.26860600	4.12004500	-1.60832300
H	-0.39103000	4.57581100	-2.59374500
H	-1.26769800	3.97271500	-1.17405000
H	0.26063600	4.84946900	-0.97695700
H	1.94841800	-1.09242800	-0.68111200
H	-0.18745700	3.39666500	0.79470600
O	-0.92801900	2.12850900	2.67261300
C	-0.15150000	2.08267900	3.86040000
H	-0.71848700	2.62723000	4.61604700
H	0.00797100	1.05482500	4.20012900

H	0.81659100	2.57528600	3.70720000
O	-1.02723000	-0.43085900	2.64221000
C	-1.08701900	-1.82700800	2.82691900
H	-0.10595400	-2.24334200	3.08737000
H	-1.77908400	-1.98900300	3.65282400
H	-1.46573500	-2.33121400	1.92980200

TI-35

Zero-point correction= 0.217496 (Hartree/Particle)

Thermal correction to Energy= 0.230801

Thermal correction to Enthalpy= 0.231745

Thermal correction to Gibbs Free Energy= 0.176596

Sum of electronic and zero-point Energies= -593.601995

Sum of electronic and thermal Energies= -593.588690

Sum of electronic and thermal Enthalpies= -593.587746

Sum of electronic and thermal Free Energies= -593.642895

C	-0.63127500	0.20134200	1.66432500
C	0.05133000	-0.69911800	0.91311000
C	0.96607200	-0.40925200	-0.17275800
C	-0.60949000	1.63639600	1.56562200
C	1.14415000	0.74987800	-0.83485400
C	-0.13704600	2.43265500	0.57564700
C	0.49299800	2.05870300	-0.68688600
H	-1.26934800	-0.21950000	2.43403500
H	1.86281300	0.74901800	-1.65005400
N	0.64671200	2.84298700	-1.69935000
C	0.05408000	4.16260100	-1.65076300
H	0.12908600	4.62164700	-2.63936700

H	-1.00559600	4.15113600	-1.35689300
H	0.58234400	4.82052700	-0.94431200
H	1.57564100	-1.24143000	-0.50837600
H	-0.26817600	3.49378600	0.75829800
O	-1.24208000	2.30134400	2.58820600
C	-0.75878300	2.04730300	3.89536800
H	0.30553800	2.29902600	3.97613800
H	-1.33491300	2.69008400	4.56165500
H	-0.89924800	1.00412600	4.20097900
O	-0.13572500	-1.99428100	1.28589100
C	0.18504800	-3.04514800	0.39515200
H	1.26605500	-3.21435800	0.32921200
H	-0.28055100	-3.93752500	0.81409800
H	-0.21757900	-2.86618400	-0.60779100

TI-36

Zero-point correction= 0.217377 (Hartree/Particle)

Thermal correction to Energy= 0.230614

Thermal correction to Enthalpy= 0.231558

Thermal correction to Gibbs Free Energy= 0.176959

Sum of electronic and zero-point Energies= -593.598975

Sum of electronic and thermal Energies= -593.585738

Sum of electronic and thermal Enthalpies= -593.584794

Sum of electronic and thermal Free Energies= -593.639393

C	-0.72589900	0.02234400	1.24115900
C	0.09179500	-0.48940800	0.29995500
C	0.95250200	0.23991500	-0.61143300
C	-0.98515100	1.40948800	1.56348900

C	0.91806400	1.56088100	-0.91184000
C	-0.66338800	2.50689100	0.85192700
C	0.02501200	2.62109400	-0.43744400
H	-1.29189600	-0.68028200	1.84766000
H	0.11716500	-1.57055200	0.22047700
H	1.66455700	1.86160200	-1.64015100
N	-0.12407400	3.75791400	-1.02677900
C	0.53164900	3.98410900	-2.29693500
H	0.14943700	4.91141200	-2.73043600
H	1.61946900	4.10344800	-2.17936200
H	0.36728300	3.17597900	-3.02468300
H	-1.01756500	3.45635400	1.24205100
O	-1.73967900	1.59409600	2.70295300
C	-1.01440500	1.41052700	3.90447700
H	-0.21148500	2.15311700	3.99459300
H	-1.72409700	1.53999100	4.72257000
H	-0.57257100	0.40644100	3.96869700
O	1.88977600	-0.46555600	-1.31053500
C	2.32097400	-1.72797100	-0.84486300
H	1.59674200	-2.51972100	-1.07148300
H	3.24612400	-1.94201100	-1.38098200
H	2.52483000	-1.72019300	0.23202100

TI-45

Zero-point correction=	0.217291 (Hartree/Particle)
Thermal correction to Energy=	0.230642
Thermal correction to Enthalpy=	0.231586
Thermal correction to Gibbs Free Energy=	0.176707

Sum of electronic and zero-point Energies=	-593.596526
Sum of electronic and thermal Energies=	-593.583175
Sum of electronic and thermal Enthalpies=	-593.582230
Sum of electronic and thermal Free Energies=	-593.637110
C	0.18099100 0.12806300 1.72563900
C	0.74239000 -0.70757800 0.80540200
C	1.34270600 -0.31699700 -0.45056600
C	0.13665100 1.57280000 1.62971400
C	1.33750700 0.84865000 -1.12545000
C	0.34128400 2.41391600 0.59754100
C	0.69300900 2.12235700 -0.79949900
H	1.85867400 0.87845600 -2.07790600
N	0.56946300 2.95333000 -1.77520600
C	-0.03898200 4.24582100 -1.53433100
H	-0.19593700 4.74494500 -2.49329700
H	-1.01072300 4.17967200 -1.02433600
H	0.60757500 4.89849600 -0.92875100
H	1.90018700 -1.12887800 -0.91185100
H	0.21878900 3.46816900 0.82760700
H	-0.15295300 2.02263100 2.57617000
O	-0.32599700 -0.27687900 2.92301500
C	-1.07118700 -1.47850900 3.01676500
H	-0.42474700 -2.35536200 3.07416200
H	-1.65931300 -1.38975000 3.93187800
H	-1.75272300 -1.58271800 2.16352600
O	0.87546600 -2.03836200 1.12809900
C	0.19916700 -2.94491000 0.27323700
H	0.50199000 -2.83088400 -0.77379800

H	0.46139100	-3.94741400	0.61339900
H	-0.88806300	-2.80947300	0.33823600

TI-234

Zero-point correction= 0.251051 (Hartree/Particle)

Thermal correction to Energy= 0.266465

Thermal correction to Enthalpy= 0.267409

Thermal correction to Gibbs Free Energy= 0.208980

Sum of electronic and zero-point Energies= -708.047950

Sum of electronic and thermal Energies= -708.032537

Sum of electronic and thermal Enthalpies= -708.031593

Sum of electronic and thermal Free Energies= -708.090022

C	0.34497200	0.07391800	1.69151600
C	0.71047200	-0.73743400	0.66831600
C	0.39501200	-0.56801800	-0.72991500
C	-0.54039100	1.24105000	1.60048700
C	0.07104200	0.56513300	-1.37867500
C	-0.69922400	2.04658500	0.52224600
C	0.01809600	1.90851200	-0.78313900
H	1.28642800	-1.62502400	0.90343600
H	-0.06386600	0.53864900	-2.45569000
N	0.47345700	2.87760300	-1.47950300
C	0.49632200	4.22531400	-0.95145000
H	1.29118400	4.77791600	-1.45955200
H	-0.45234100	4.73253900	-1.15748500
H	0.67715900	4.27929200	0.13135900
H	0.49968700	-1.46747600	-1.33208500
O	-1.60470100	3.05938000	0.48195600

C	-1.74038600	3.95649700	1.57654000
H	-2.08073900	4.89988600	1.14385400
H	-2.46682700	3.59572200	2.30628800
H	-0.78198800	4.10992900	2.08138000
O	-1.24222200	1.53839200	2.74062300
C	-2.25126600	0.59302600	3.05895900
H	-2.74642900	0.96342400	3.95769200
H	-2.98147800	0.51138000	2.24512100
H	-1.82048600	-0.39242600	3.26643100
O	0.66843400	-0.16218300	2.98975900
C	1.45787500	-1.28852600	3.29364300
H	1.60803100	-1.26587500	4.37289500
H	0.95229800	-2.22227500	3.01654900
H	2.43096900	-1.24390600	2.78970100

TI-235

Zero-point correction= 0.250692 (Hartree/Particle)

Thermal correction to Energy= 0.266270

Thermal correction to Enthalpy= 0.267214

Thermal correction to Gibbs Free Energy= 0.207909

Sum of electronic and zero-point Energies= -708.047343

Sum of electronic and thermal Energies= -708.031765

Sum of electronic and thermal Enthalpies= -708.030821

Sum of electronic and thermal Free Energies= -708.090125

C	-0.06431900	-0.10849500	1.78538300
C	0.28177200	-0.97371200	0.80121600
C	0.04483800	-0.77752100	-0.61406700
C	-0.75189400	1.15185100	1.66502400

C	-0.14031100	0.39504200	-1.24741400
C	-0.78803400	1.99451800	0.59958800
C	-0.07736500	1.75648500	-0.68442800
H	0.11935600	-0.43203500	2.80555400
H	-0.27607500	0.37580800	-2.32519700
N	0.47084400	2.64271900	-1.42561100
C	0.61469500	4.00686800	-0.96278100
H	1.43534600	4.47215600	-1.51522500
H	-0.29720500	4.57909000	-1.16436100
H	0.83082600	4.09100400	0.11123800
H	0.03213000	-1.67390300	-1.22687300
O	-1.55327800	3.12415000	0.57849200
C	-1.47274200	4.05057300	1.65298700
H	-1.65934400	5.03545900	1.21814600
H	-2.21683800	3.83655900	2.42272500
H	-0.48022300	4.03854400	2.11380200
O	-1.40701200	1.54103900	2.81550200
C	-2.67428700	0.92012000	2.96314700
H	-2.58156600	-0.17277300	2.98448700
H	-3.08504200	1.26727000	3.91260500
H	-3.34722000	1.20710200	2.14599900
O	0.81642700	-2.15516200	1.22453700
C	1.60091200	-2.91393300	0.32531900
H	2.26975600	-2.28008600	-0.26728200
H	2.19756500	-3.58816800	0.94115000
H	0.98128300	-3.51560900	-0.35069100

TI-236

Zero-point correction= 0.250323 (Hartree/Particle)

Thermal correction to Energy= 0.266111

Thermal correction to Enthalpy= 0.267055

Thermal correction to Gibbs Free Energy= 0.206389

Sum of electronic and zero-point Energies= -708.052719

Sum of electronic and thermal Energies= -708.036931

Sum of electronic and thermal Enthalpies= -708.035987

Sum of electronic and thermal Free Energies= -708.096653

C	0.40847500	0.10544500	2.07470500
C	1.07707400	-0.68259100	1.21275300
C	1.08087300	-0.59200800	-0.23540600
C	-0.50070100	1.19432900	1.78454200
C	0.76243900	0.49458800	-0.97473800
C	-0.53519300	1.95502000	0.66349300
C	0.42789200	1.83592800	-0.47481700
H	0.47185900	-0.12937300	3.13410800
H	1.64852300	-1.51629400	1.60867500
H	0.89644500	0.46850100	-2.04961100
N	0.89315300	2.82039300	-1.14590400
C	0.65034200	4.19014500	-0.74664900
H	1.44259200	4.81328100	-1.17057900
H	-0.30680600	4.54827800	-1.14103100
H	0.64205600	4.34321300	0.34161600
O	-1.49114900	2.89358300	0.43414500
C	-1.85498100	3.81169000	1.45703000
H	-2.18314300	4.71651400	0.94103500
H	-2.66463600	3.42596200	2.07961500
H	-1.00108100	4.04670500	2.09924100

O	-1.41294700	1.43973100	2.79175600
C	-2.58156600	0.64245600	2.67586200
H	-2.33982400	-0.42713200	2.71352500
H	-3.22140500	0.89819100	3.52215900
H	-3.10918800	0.85549700	1.73813100
O	1.51431200	-1.76714200	-0.76759500
C	1.64308100	-1.86210800	-2.16822300
H	2.36516600	-1.13184700	-2.55410200
H	2.00440700	-2.87054800	-2.36942600
H	0.67946400	-1.71312200	-2.67049500

TI-237

Zero-point correction= 0.251254 (Hartree/Particle)

Thermal correction to Energy= 0.266668

Thermal correction to Enthalpy= 0.267612

Thermal correction to Gibbs Free Energy= 0.209037

Sum of electronic and zero-point Energies= -708.049228

Sum of electronic and thermal Energies= -708.033814

Sum of electronic and thermal Enthalpies= -708.032870

Sum of electronic and thermal Free Energies= -708.091445

C	0.47526400	0.22388000	1.81119800
C	1.09825100	-0.51212600	0.86372700
C	0.98535300	-0.39906600	-0.56796400
C	-0.49500500	1.27644400	1.60358100
C	0.62777800	0.71608500	-1.25234100
C	-0.58326200	2.07384600	0.51025900
C	0.39938700	2.04048200	-0.61003800
H	0.63392300	-0.03166900	2.85572700

H	1.73185700	-1.32320800	1.21425900
N	0.97755100	3.05064600	-1.12418000
C	0.79979900	4.35734900	-0.52668000
H	1.67226700	4.96901500	-0.76943400
H	-0.08477300	4.84409300	-0.95024500
H	0.67954300	4.33069500	0.56558100
H	1.26719500	-1.28325500	-1.12935200
O	-1.55801800	2.99748400	0.28432700
C	-2.04620700	3.80340300	1.34657000
H	-2.44284200	4.70432600	0.87373100
H	-2.83734100	3.30187200	1.90769200
H	-1.24426800	4.07502600	2.03981100
O	-1.37886200	1.46477500	2.64645500
C	-2.38292900	0.46574600	2.71327400
H	-1.94612700	-0.53423700	2.82509400
H	-2.99399600	0.69347500	3.58831100
H	-3.01046700	0.47944000	1.81319300
O	0.51459900	0.79380700	-2.59064800
C	0.70746600	-0.38145900	-3.34641700
H	0.01202900	-1.17176700	-3.03756600
H	0.51340900	-0.10889500	-4.38335500
H	1.73608100	-0.75081300	-3.25473000

TI-245

Zero-point correction= 0.250551 (Hartree/Particle)

Thermal correction to Energy= 0.266174

Thermal correction to Enthalpy= 0.267118

Thermal correction to Gibbs Free Energy= 0.207555

Sum of electronic and zero-point Energies= -708.049189
Sum of electronic and thermal Energies= -708.033566
Sum of electronic and thermal Enthalpies= -708.032622
Sum of electronic and thermal Free Energies= -708.092185

C	0.12759300	0.09557500	1.53473300
C	0.63497400	-0.66945300	0.52518900
C	0.63294500	-0.31941300	-0.87455400
C	-0.52258000	1.37869200	1.38458300
C	0.48464000	0.87645900	-1.47848600
C	-0.49108400	2.27359500	0.37038000
C	0.35124100	2.19798500	-0.85741200
H	0.59336700	0.91829500	-2.55815600
N	0.89350300	3.18004600	-1.47030900
C	0.88272600	4.52654000	-0.93799100
H	1.76469700	5.04606700	-1.32270900
H	-0.00246500	5.06718300	-1.29018600
H	0.89041700	4.58338500	0.15737000
H	0.86067600	-1.15132200	-1.53630400
H	-1.12037400	1.61721900	2.25660800
O	-1.26603500	3.38419000	0.34763400
C	-2.17165800	3.61420000	1.40367500
H	-2.70470400	4.52904900	1.14581500
H	-2.88653300	2.78831500	1.50259700
H	-1.65028500	3.75595900	2.35790400
O	0.12349600	-0.26581300	2.84913900
C	-0.08636700	-1.61288800	3.23492600
H	0.82600000	-2.20582300	3.15744400
H	-0.41545500	-1.57162700	4.27518900

H	-0.87489800	-2.07761500	2.63074500
O	1.25965700	-1.85758500	0.85161100
C	0.66821500	-3.03541600	0.33926900
H	0.79707200	-3.13163300	-0.74566700
H	1.17575800	-3.87286700	0.82129600
H	-0.40432600	-3.07968500	0.56960000

TI-246

Zero-point correction= 0.251954 (Hartree/Particle)

Thermal correction to Energy= 0.267090

Thermal correction to Enthalpy= 0.268034

Thermal correction to Gibbs Free Energy= 0.210191

Sum of electronic and zero-point Energies= -708.066103

Sum of electronic and thermal Energies= -708.050967

Sum of electronic and thermal Enthalpies= -708.050023

Sum of electronic and thermal Free Energies= -708.107866

C	-0.20732200	0.10417100	1.75659000
C	0.43390700	-0.72532400	0.89858400
C	0.69235500	-0.48743500	-0.50458000
C	-0.82546100	1.37711200	1.45474400
C	0.72754700	0.69758000	-1.16074400
C	-0.54250500	2.19770500	0.42071200
C	0.57693300	2.02446100	-0.55990000
H	0.75974000	-1.70100200	1.23540800
H	1.03152300	0.72982300	-2.19952900
N	1.32671400	2.96387600	-0.99431600
C	1.25368600	4.30982900	-0.46486900
H	2.24235900	4.76622100	-0.56781300

H	0.54965200	4.91177400	-1.04968300
H	0.94815500	4.37238100	0.58752300
H	-1.59562200	1.65513800	2.16469300
O	-1.25617100	3.30985000	0.13879900
C	-2.38662500	3.61126700	0.92804800
H	-2.83121500	4.50251900	0.48626700
H	-3.11258400	2.78973500	0.91048700
H	-2.10601500	3.82172300	1.96705200
O	-0.44708000	-0.21538300	3.05698100
C	-0.00680100	-1.46449700	3.53953500
H	1.08128100	-1.56856500	3.45083300
H	-0.28811600	-1.49683700	4.59212700
H	-0.49013200	-2.29365300	3.00807000
O	0.97645700	-1.67523300	-1.10962000
C	1.34279100	-1.67114000	-2.47013300
H	1.53082500	-2.71257700	-2.73227300
H	0.53850700	-1.27704600	-3.10309200
H	2.25301000	-1.08279500	-2.63989300

TI-247

Zero-point correction= 0.251572 (Hartree/Particle)

Thermal correction to Energy= 0.266857

Thermal correction to Enthalpy= 0.267801

Thermal correction to Gibbs Free Energy= 0.209453

Sum of electronic and zero-point Energies= -708.059910

Sum of electronic and thermal Energies= -708.044625

Sum of electronic and thermal Enthalpies= -708.043681

Sum of electronic and thermal Free Energies= -708.102029

C	-0.24638600	0.12676500	1.61293300
C	0.31694700	-0.67365200	0.67328200
C	0.46492200	-0.39882200	-0.73636800
C	-0.86047500	1.41495000	1.38518900
C	0.51672200	0.80620200	-1.35167600
C	-0.59299700	2.26419800	0.37037800
C	0.50590600	2.10102500	-0.62662700
H	0.65664700	-1.65728600	0.97668800
N	1.35994700	2.98684000	-0.94865000
C	1.39441000	4.25868600	-0.25626800
H	2.41914900	4.63750000	-0.28833700
H	0.75391200	4.97896200	-0.77528300
H	1.06468000	4.21037100	0.78985400
H	0.60102000	-1.28315400	-1.35019300
H	-1.60122100	1.68496200	2.12940800
O	-1.27753300	3.40972100	0.13444100
C	-2.37102900	3.72009300	0.97007600
H	-2.80526500	4.63574900	0.56947600
H	-3.12110100	2.92025800	0.95580900
H	-2.04855900	3.89212900	2.00427100
O	-0.40139300	-0.23205600	2.92305500
C	0.03498300	-1.50791600	3.32245100
H	1.11397000	-1.63401400	3.16599500
H	-0.18373900	-1.58528200	4.38782700
H	-0.49694900	-2.30432200	2.78529400
O	0.65334000	0.99210100	-2.68499000
C	0.71373200	-0.14598800	-3.51105400
H	-0.18673900	-0.76585400	-3.40910600

H	0.78501200	0.22708200	-4.53276100
H	1.59696900	-0.75779400	-3.28724000

TI-345

Zero-point correction= 0.250362 (Hartree/Particle)

Thermal correction to Energy= 0.266169

Thermal correction to Enthalpy= 0.267113

Thermal correction to Gibbs Free Energy= 0.206842

Sum of electronic and zero-point Energies= -708.050172

Sum of electronic and thermal Energies= -708.034365

Sum of electronic and thermal Enthalpies= -708.033421

Sum of electronic and thermal Free Energies= -708.093693

C	0.21094100	-0.06634400	1.65510300
C	0.94903400	-0.74816200	0.73001600
C	1.63151800	-0.17666700	-0.41257800
C	-0.05300800	1.36643900	1.66359600
C	1.42494100	0.99899600	-1.03494900
C	0.04112600	2.26114700	0.65296500
C	0.45561800	2.05851800	-0.73485400
H	2.01829800	1.20923000	-1.92056100
N	0.15855500	2.83421900	-1.71830700
C	-0.77530800	3.91622900	-1.48639900
H	-1.11073500	4.30889800	-2.44938500
H	-1.66135900	3.61493400	-0.90916200
H	-0.29851900	4.74722900	-0.94526700
H	2.39498800	-0.81070300	-0.85099400
H	-0.23179100	3.27425500	0.93188400
O	-0.55412500	1.85945300	2.84096800

C	0.33879900	1.80444200	3.94839000
H	-0.18597300	2.26974800	4.78356800
H	0.59437500	0.77277800	4.20311500
H	1.25029800	2.37418700	3.73167700
O	-0.27337000	-0.78136600	2.71848100
C	-1.67659300	-0.99669400	2.67406800
H	-1.92745700	-1.58154300	3.56021700
H	-2.22214400	-0.04724800	2.69829100
H	-1.95312300	-1.56109100	1.77583500
O	1.07583700	-2.07833000	0.97680400
C	1.54159300	-2.94289000	-0.03862000
H	2.62387000	-2.85456000	-0.19131400
H	1.32356500	-3.95150800	0.31366500
H	1.02681000	-2.77358900	-0.99118800

TI-346

Zero-point correction= 0.251505 (Hartree/Particle)

Thermal correction to Energy= 0.266872

Thermal correction to Enthalpy= 0.267816

Thermal correction to Gibbs Free Energy= 0.208421

Sum of electronic and zero-point Energies= -708.062584

Sum of electronic and thermal Energies= -708.047218

Sum of electronic and thermal Enthalpies= -708.046273

Sum of electronic and thermal Free Energies= -708.105668

C	-0.43974500	-0.04063900	1.79515200
C	0.39603000	-0.62961400	0.90806400
C	1.02244300	-0.07314300	-0.27006600
C	-0.91435000	1.35082700	1.77019700

C	0.89851000	1.15303300	-0.83794100
C	-0.67601600	2.28873200	0.83686200
C	0.08723700	2.28702800	-0.41421600
H	0.66513900	-1.66680900	1.05908200
H	1.47346300	1.32955000	-1.73569700
N	-0.00739800	3.39693600	-1.07128000
C	0.70248800	3.53760300	-2.32257100
H	0.48222800	4.51969200	-2.74772500
H	1.79499300	3.46990100	-2.19907300
H	0.41073700	2.78022900	-3.06682700
H	-1.15518900	3.24587200	1.01890100
O	-1.74678000	1.70425100	2.80139000
C	-1.08010100	2.01812400	4.01287700
H	-1.85146900	2.32552100	4.72009400
H	-0.54803900	1.14938100	4.41554900
H	-0.37288700	2.84386300	3.86414600
O	-0.95728200	-0.70059600	2.85318200
C	-0.63708000	-2.06188600	3.04051400
H	0.43895900	-2.20426500	3.19654500
H	-1.17757100	-2.37242500	3.93403700
H	-0.96260300	-2.66860900	2.18749500
O	1.82576500	-1.03473500	-0.80256700
C	2.54035300	-0.76560200	-1.98788300
H	3.08102300	-1.68226000	-2.22306100
H	1.86505400	-0.51808100	-2.81573700
H	3.25646400	0.05341400	-1.84964600

TI-347

Zero-point correction=	0.250925 (Hartree/Particle)
Thermal correction to Energy=	0.266465
Thermal correction to Enthalpy=	0.267409
Thermal correction to Gibbs Free Energy=	0.208164
Sum of electronic and zero-point Energies=	-708.056148
Sum of electronic and thermal Energies=	-708.040608
Sum of electronic and thermal Enthalpies=	-708.039664
Sum of electronic and thermal Free Energies=	-708.098908

C	0.13783900	0.38658300	1.96845900
C	0.75976000	-0.27850800	0.96499200
C	0.80873500	0.03165000	-0.44252600
C	-0.67861000	1.58545500	1.78602000
C	0.63154800	1.22657000	-1.05878200
C	-0.58138600	2.46690000	0.77102600
C	0.36044900	2.50773000	-0.35676900
H	1.27642000	-1.19618200	1.22445900
C	0.56486000	4.83728500	-0.21326900
H	1.29439500	5.57812300	-0.54873300
H	-0.43015000	5.20917900	-0.49595800
H	0.59920600	4.78185400	0.88364100
H	1.09946700	-0.80976100	-1.06178500
H	-1.28831300	3.29093200	0.82257200
O	-1.58456600	1.87983000	2.76586500
C	-2.60697700	0.91427700	2.96305700
H	-3.28475500	1.33648800	3.70586300
H	-3.15637800	0.73840700	2.03028400
H	-2.20228400	-0.03022600	3.33758500
O	0.15451900	-0.01012100	3.27245400

C	0.87440400	-1.17098300	3.61027000
H	1.93900700	-1.06885400	3.36481600
H	0.76277400	-1.29129500	4.68779400
H	0.47309900	-2.05900300	3.10462100
O	0.72851200	1.40908700	-2.39043900
C	0.98509100	0.29468200	-3.21192500
H	0.21160200	-0.47610500	-3.09919000
H	0.97692900	0.66976500	-4.23514700
H	1.96606800	-0.14754900	-2.99736200
N	0.84397400	3.57551600	-0.86785900

TI-2345

Zero-point correction= 0.283654 (Hartree/Particle)

Thermal correction to Energy= 0.301973

Thermal correction to Enthalpy= 0.302917

Thermal correction to Gibbs Free Energy= 0.237946

Sum of electronic and zero-point Energies= -822.497701

Sum of electronic and thermal Energies= -822.479381

Sum of electronic and thermal Enthalpies= -822.478437

Sum of electronic and thermal Free Energies= -822.543408

C	0.29106100	-0.26809000	1.23915800
C	0.67254600	-0.90375300	0.10070500
C	0.43898100	-0.43929800	-1.25111300
C	-0.52746000	0.94330400	1.32478800
C	0.22634600	0.82040100	-1.66898500
C	-0.58109500	1.96411600	0.43420700
C	0.20606100	2.03144900	-0.83157400
H	0.14799900	1.00944100	-2.73549200

N	0.74799400	3.08142100	-1.31683300
C	0.80177400	4.30509100	-0.54485700
H	1.64404100	4.90154100	-0.90498500
H	-0.11351000	4.88817900	-0.69180000
H	0.92807400	4.14467400	0.53521300
H	0.53867000	-1.21956700	-2.00061700
O	-1.43571100	3.01653100	0.55546500
C	-1.56442300	3.69207700	1.79871600
H	-1.84484600	4.71905100	1.55399100
H	-2.32860600	3.23452900	2.42871900
H	-0.61544300	3.69637500	2.34471000
O	-1.27693500	1.05144600	2.47194100
C	-2.30134800	0.07291700	2.59140000
H	-2.84633800	0.31201000	3.50576100
H	-2.98481700	0.12010800	1.73598600
H	-1.87720700	-0.93231500	2.67527000
O	0.55951500	-0.88117000	2.43713500
C	1.40678200	-0.13131300	3.29684600
H	0.94293700	0.82010700	3.57602000
H	1.55110300	-0.73802300	4.19164200
H	2.37570100	0.05120400	2.81915900
O	1.36625400	-2.08380100	0.15176000
C	0.66658700	-3.19796300	0.68836600
H	-0.28864600	-3.34532300	0.16882800
H	1.30323500	-4.06736500	0.51715800
H	0.48395200	-3.07646100	1.75862300

TI-2346

Zero-point correction= 0.283815 (Hartree/Particle)

Thermal correction to Energy= 0.301951

Thermal correction to Enthalpy= 0.302896

Thermal correction to Gibbs Free Energy= 0.238280

Sum of electronic and zero-point Energies= -822.508949

Sum of electronic and thermal Energies= -822.490813

Sum of electronic and thermal Enthalpies= -822.489869

Sum of electronic and thermal Free Energies= -822.554485

C	0.48662700	0.19363800	1.86606700
C	1.06784500	-0.57840700	0.92072300
C	0.92268100	-0.46998400	-0.51848600
C	-0.49808600	1.26001000	1.64017300
C	0.60418500	0.63892900	-1.22110600
C	-0.56378100	2.03967900	0.53730000
C	0.37557900	1.96226300	-0.62895200
H	1.70815000	-1.39776400	1.22266000
H	0.63853600	0.63386100	-2.30347400
N	0.86866600	2.97596200	-1.22986500
C	0.68387000	4.31238800	-0.70476700
H	1.52439900	4.92831500	-1.03639200
H	-0.23440300	4.75628000	-1.10451900
H	0.63162500	4.36368700	0.39197400
O	-1.53582900	2.96134800	0.32024800
C	-1.99681300	3.79861000	1.37214400
H	-2.35604300	4.70849500	0.88653200
H	-2.80703300	3.33142800	1.93427600
H	-1.18681000	4.04732300	2.06393800
O	-1.39552500	1.46560700	2.65717900

C	-2.32115100	0.40425200	2.82801800
H	-3.02412500	0.72849800	3.59681400
H	-2.86317100	0.20471200	1.89600700
H	-1.82036000	-0.51098800	3.16264500
O	0.67213500	0.00631200	3.19730400
C	1.51701400	-1.04097700	3.61748300
H	1.52368200	-1.00082400	4.70652500
H	1.13877700	-2.01718000	3.28918500
H	2.53834600	-0.90674100	3.24132500
O	1.25071500	-1.66022300	-1.09384000
C	1.28392100	-1.73358300	-2.50094700
H	1.57719000	-2.75544100	-2.74235600
H	0.29971800	-1.52568500	-2.93803300
H	2.01669500	-1.03308200	-2.92041100

TI-2347

Zero-point correction= 0.285076 (Hartree/Particle)

Thermal correction to Energy= 0.302841

Thermal correction to Enthalpy= 0.303785

Thermal correction to Gibbs Free Energy= 0.240248

Sum of electronic and zero-point Energies= -822.502554

Sum of electronic and thermal Energies= -822.484789

Sum of electronic and thermal Enthalpies= -822.483845

Sum of electronic and thermal Free Energies= -822.547382

C	0.44053900	0.19904400	1.74100100
C	0.99117700	-0.54059600	0.74968200
C	0.81100200	-0.39018400	-0.67776200
C	-0.53316000	1.27947700	1.56008500

C	0.52659400	0.75626400	-1.33430500
C	-0.57602600	2.10685500	0.49005500
C	0.39360700	2.06666100	-0.64450400
H	1.63512100	-1.36560200	1.03376500
N	1.01466000	3.06659100	-1.12621900
C	0.91004400	4.35504300	-0.47412700
H	1.81519000	4.92681900	-0.69319800
H	0.05478400	4.90612900	-0.87880000
H	0.78808500	4.29256500	0.61634900
H	1.00125900	-1.28760100	-1.25665900
O	-1.52319800	3.06187800	0.28495300
C	-1.98066800	3.86590600	1.36330100
H	-2.33442400	4.79360900	0.90842700
H	-2.79364900	3.38501100	1.90975400
H	-1.16986800	4.08647000	2.06452300
O	-1.43273000	1.46634400	2.57742000
C	-2.32376100	0.38001500	2.77188800
H	-3.03366700	0.69836100	3.53674300
H	-2.86372700	0.14675700	1.84649500
H	-1.79363300	-0.51195500	3.12182300
O	0.65083900	-0.03000600	3.07029200
C	1.47621600	-1.10860700	3.43602800
H	1.50530400	-1.11143600	4.52582600
H	1.07132000	-2.06546000	3.08050800
H	2.49508300	-0.98671800	3.04669000
O	0.38376000	0.87819300	-2.67125300
C	0.50240400	-0.28616400	-3.45496900
H	-0.23617000	-1.04294200	-3.16049200

H	0.31869700	0.02053500	-4.48445800
H	1.50758500	-0.71954200	-3.37889600

TI-2356

Zero-point correction= 0.283514 (Hartree/Particle)

Thermal correction to Energy= 0.301699

Thermal correction to Enthalpy= 0.302643

Thermal correction to Gibbs Free Energy= 0.237231

Sum of electronic and zero-point Energies= -822.502361

Sum of electronic and thermal Energies= -822.484176

Sum of electronic and thermal Enthalpies= -822.483232

Sum of electronic and thermal Free Energies= -822.548644

C	0.36313500	0.01023300	1.67844300
C	0.97316200	-0.70353800	0.71203200
C	0.88440000	-0.45407100	-0.73043300
C	-0.53915900	1.13289200	1.55775700
C	0.54022100	0.71667400	-1.30974900
C	-0.61628500	2.02508700	0.54261900
C	0.26278400	2.00902800	-0.66303100
H	0.50638400	-0.34210700	2.69614900
H	0.59323300	0.80220400	-2.38856000
N	0.69445100	3.04348700	-1.27962500
C	0.50592800	4.37474900	-0.74412900
H	1.26322100	5.02900100	-1.18470600
H	-0.47891500	4.77111300	-1.01346700
H	0.60279400	4.43199500	0.34893100
O	-1.56713900	2.99991000	0.49675100
C	-1.76947900	3.83604500	1.62914600

H	-2.11927400	4.79313000	1.23602100
H	-2.51399000	3.42131600	2.31203200
H	-0.83535800	3.98617200	2.17875100
O	-1.38835400	1.27003100	2.63763400
C	-2.62678200	0.60341900	2.44237400
H	-2.47370400	-0.46671900	2.25510700
H	-3.19923000	0.73118100	3.36253000
H	-3.17780500	1.04003200	1.60059100
O	1.75769100	-1.76084500	1.08948400
C	1.07583400	-3.00193500	1.17870300
H	0.66628600	-3.29989900	0.20834500
H	1.81314300	-3.73697400	1.50403500
H	0.26593900	-2.94946600	1.91812400
O	1.24261300	-1.56083100	-1.43029200
C	1.30364500	-1.47794200	-2.83592300
H	1.63537100	-2.45760700	-3.17979000
H	0.32197500	-1.25276900	-3.27041500
H	2.02301000	-0.71606300	-3.15897200

TI-2357

Zero-point correction=	0.282872 (Hartree/Particle)
Thermal correction to Energy=	0.301427
Thermal correction to Enthalpy=	0.302372
Thermal correction to Gibbs Free Energy=	0.236200
Sum of electronic and zero-point Energies=	-822.506612
Sum of electronic and thermal Energies=	-822.488057
Sum of electronic and thermal Enthalpies=	-822.487113
Sum of electronic and thermal Free Energies=	-822.553284

C	-0.12309600	-0.07646000	1.68344100
C	0.36884000	-0.86547800	0.70286600
C	0.33637000	-0.62413500	-0.72295700
C	-0.83006000	1.17450600	1.52029600
C	0.28649800	0.59111300	-1.31658000
C	-0.66379700	2.06158600	0.50920100
C	0.34608700	1.88132300	-0.57084300
H	-0.05214800	-0.45055000	2.70029000
N	1.17280200	2.75621400	-0.98309200
C	1.26856900	4.02401700	-0.29008200
H	2.25813300	4.44842200	-0.47559300
H	0.51975300	4.72167300	-0.67930200
H	1.11792200	3.94020000	0.79534700
H	0.37172600	-1.52060100	-1.33241600
O	-1.39165700	3.20156000	0.33440800
C	-1.68766800	4.03175100	1.44766400
H	-1.83097700	5.03475300	1.03946900
H	-2.59287200	3.70828200	1.96515400
H	-0.86124600	4.04164600	2.16542400
O	-1.70938500	1.48417200	2.53565100
C	-2.88488800	0.69062300	2.52015800
H	-2.65214300	-0.37613500	2.62229200
H	-3.49002700	1.01131500	3.36967900
H	-3.44602600	0.84390300	1.59024200
O	0.86628300	-2.09001100	1.08275400
C	2.22915300	-2.30460200	0.76093400
H	2.87516300	-1.61739200	1.32123600
H	2.45827500	-3.33248400	1.04522300

H	2.42479600	-2.17444000	-0.31021600
O	0.21936100	0.79421200	-2.64316200
C	0.16211600	-0.33311800	-3.49064700
H	-0.70324300	-0.96493200	-3.25572100
H	0.06501100	0.05840200	-4.50268800
H	1.07804600	-0.93183400	-3.41704800

TI-2367

Zero-point correction= 0.283550 (Hartree/Particle)

Thermal correction to Energy= 0.301964

Thermal correction to Enthalpy= 0.302908

Thermal correction to Gibbs Free Energy= 0.237229

Sum of electronic and zero-point Energies= -822.499962

Sum of electronic and thermal Energies= -822.481548

Sum of electronic and thermal Enthalpies= -822.480604

Sum of electronic and thermal Free Energies= -822.546283

C	0.28395600	0.04038300	1.95646300
C	0.94144800	-0.77116900	1.09533800
C	0.99803500	-0.70157900	-0.34014000
C	-0.53675600	1.17924400	1.63368200
C	0.77112700	0.40901000	-1.09952000
C	-0.44571200	1.93541400	0.50964700
C	0.62072100	1.76215900	-0.51389300
H	0.28781900	-0.21691100	3.01212700
H	1.43237600	-1.64990700	1.50416000
N	1.33096200	2.70238600	-1.00768800
C	1.22075300	4.04358700	-0.47382100
H	2.14213200	4.58328300	-0.70512700

H	0.38529800	4.57495900	-0.94226900
H	1.06427000	4.06799900	0.61385700
O	-1.29930000	2.94394700	0.17578200
C	-1.75891400	3.85324300	1.16689600
H	-2.00961400	4.77156100	0.63162400
H	-2.64121300	3.47487400	1.68682600
H	-0.97925000	4.06063000	1.90590900
O	-1.48331300	1.50185700	2.58405700
C	-2.63935100	0.68219900	2.51177100
H	-2.38909200	-0.37680900	2.64871200
H	-3.30366800	1.00408500	3.31542300
H	-3.14538500	0.80496600	1.54611400
O	1.31190500	-1.89516900	-0.94302500
C	2.58424300	-1.93358700	-1.57373900
H	3.38342700	-1.72603500	-0.85080500
H	2.70473000	-2.94679400	-1.96036100
H	2.64423100	-1.21744000	-2.39781200
O	0.84410300	0.25721300	-2.44106100
C	0.27732000	1.25149700	-3.28163300
H	0.22243300	0.79535500	-4.27045700
H	-0.73163700	1.51918500	-2.94805900
H	0.89715100	2.15004600	-3.30283400

TI-2456

Zero-point correction= 0.284406 (Hartree/Particle)

Thermal correction to Energy= 0.302318

Thermal correction to Enthalpy= 0.303262

Thermal correction to Gibbs Free Energy= 0.239213

Sum of electronic and zero-point Energies=	-822.508523
Sum of electronic and thermal Energies=	-822.490612
Sum of electronic and thermal Enthalpies=	-822.489667
Sum of electronic and thermal Free Energies=	-822.553716
C	-0.17425100 -0.16092900 1.29023400
C	0.45030300 -0.84304000 0.29704200
C	0.60252100 -0.38399600 -1.08347600
C	-0.82807200 1.12429100 1.22330200
C	0.58328600 0.89792700 -1.51796900
C	-0.60235700 2.11711600 0.33499800
C	0.47960200 2.10941600 -0.69661300
H	0.78024100 1.10620900 -2.56239700
N	1.22450400 3.10116100 -1.00051900
C	1.17958800 4.33888100 -0.24874500
H	2.15999600 4.81676300 -0.32639300
H	0.44056400 5.02240000 -0.68022600
H	0.93379100 4.21324200 0.81363200
H	-1.56989000 1.25546000 2.00326100
O	-1.33054100 3.25460600 0.27115800
C	-2.41812200 3.41019600 1.15668700
H	-2.88642700 4.35859200 0.89492600
H	-3.14431200 2.59665200 1.04117400
H	-2.08174000 3.44716700 2.19990400
O	-0.32182000 -0.78173000 2.51102700
C	0.84352800 -0.72164400 3.32159900
H	1.12595500 0.31982500 3.52106800
H	0.59319900 -1.21350900 4.26289300
H	1.67783600 -1.24395300 2.84329400

O	0.99069900	-2.07072300	0.57625500
C	0.05505600	-3.14062400	0.55666800
H	0.61744200	-4.04595500	0.79142100
H	-0.72441700	-2.98876300	1.31052700
H	-0.39596100	-3.24272900	-0.43590300
O	0.81412400	-1.44349700	-1.90481400
C	1.06271000	-1.19865000	-3.26977800
H	1.22089900	-2.17605200	-3.72554400
H	0.20996900	-0.70614300	-3.75319600
H	1.95965600	-0.58292100	-3.40809300

TI-2457

Zero-point correction= 0.283732 (Hartree/Particle)

Thermal correction to Energy= 0.301922

Thermal correction to Enthalpy= 0.302866

Thermal correction to Gibbs Free Energy= 0.237761

Sum of electronic and zero-point Energies= -822.504148

Sum of electronic and thermal Energies= -822.485957

Sum of electronic and thermal Enthalpies= -822.485013

Sum of electronic and thermal Free Energies= -822.550119

C	0.02775200	0.20257000	1.56237700
C	0.76381900	-0.49552000	0.65298000
C	0.88290800	-0.20810000	-0.76071400
C	-0.73253800	1.40068200	1.28693100
C	0.78374600	0.99154000	-1.37803800
C	-0.54051200	2.29935800	0.29746000
C	0.59661800	2.27982300	-0.66370500
N	1.34765800	3.25737700	-0.97400800

C	1.21191600	4.53128500	-0.29881600
H	0.56279600	5.18678100	-0.88848400
H	0.79501000	4.46662000	0.71392400
H	2.19934900	4.99744400	-0.25014400
H	1.14667100	-1.06266400	-1.37342700
H	-1.53056600	1.56362600	2.00265500
O	-1.35730400	3.35455900	0.04905700
C	-2.49742100	3.52241500	0.86175100
H	-3.02443100	4.38958700	0.46447600
H	-3.15116600	2.64249800	0.81770400
H	-2.22191100	3.71144400	1.90659000
O	-0.10518600	-0.16784700	2.87372700
C	-0.34304200	-1.52803900	3.18719400
H	0.58829300	-2.09085000	3.27822400
H	-0.87010700	-1.53173800	4.14421800
H	-0.97682200	-2.00337700	2.42776000
O	1.47963400	-1.57865300	1.12187500
C	1.23188500	-2.82370200	0.50422800
H	1.72620700	-2.91315600	-0.47165000
H	1.64496700	-3.58662900	1.16698200
H	0.15620900	-3.00194700	0.37567200
O	0.89717700	1.18271100	-2.70989500
C	1.10999600	0.05926800	-3.53187200
H	0.30353900	-0.67780800	-3.42311900
H	1.12412100	0.43399100	-4.55516000
H	2.07003500	-0.42370200	-3.31053600

TI-3456

Zero-point correction= 0.283581 (Hartree/Particle)

Thermal correction to Energy= 0.301887

Thermal correction to Enthalpy= 0.302831

Thermal correction to Gibbs Free Energy= 0.237220

Sum of electronic and zero-point Energies= -822.506271

Sum of electronic and thermal Energies= -822.487966

Sum of electronic and thermal Enthalpies= -822.487021

Sum of electronic and thermal Free Energies= -822.552632

C	0.01297800	-0.17647900	1.45232200
C	0.23947900	-0.92591900	0.34332400
C	0.26062300	-0.47650600	-1.05458200
C	-0.37089200	1.23234200	1.51456200
C	0.19478300	0.78720300	-1.53166800
C	-0.35147800	2.16790300	0.54556900
C	0.07587200	2.07533300	-0.85181000
H	0.28144400	0.93303600	-2.60140200
N	0.29431900	3.10324000	-1.60127900
C	0.17766600	4.43170400	-1.03870700
H	0.52989300	5.15764900	-1.77549700
H	-0.86537800	4.69018400	-0.80048000
H	0.76794500	4.57217300	-0.12096600
H	-0.70693800	3.13926500	0.87387700
O	-0.84454000	1.62200900	2.74405900
C	0.16457500	2.04567900	3.65042600
H	-0.34579000	2.32146500	4.57404000
H	0.87703300	1.23982800	3.85186500
H	0.69592500	2.91924400	3.25238200
O	0.13667900	-0.79431500	2.66727900

C	-1.05290400	-1.43229000	3.12106200
H	-0.81331500	-1.87820300	4.08733400
H	-1.85643700	-0.69930200	3.24534700
H	-1.35614500	-2.21674800	2.42090100
O	0.42496600	-2.26290400	0.53649000
C	1.78644800	-2.66697800	0.56805500
H	2.31168500	-2.17821500	1.39601300
H	1.78283100	-3.74612400	0.72529400
H	2.28556000	-2.44145200	-0.38038500
O	0.39900500	-1.55485300	-1.86867800
C	0.45499600	-1.35409500	-3.26276400
H	1.31891900	-0.74169700	-3.54878600
H	0.55402900	-2.34702000	-3.70104500
H	-0.45981700	-0.87987800	-3.63725200

TI-23456

Zero-point correction= 0.317344 (Hartree/Particle)

Thermal correction to Energy= 0.338046

Thermal correction to Enthalpy= 0.338990

Thermal correction to Gibbs Free Energy= 0.268892

Sum of electronic and zero-point Energies= -936.953720

Sum of electronic and thermal Energies= -936.933018

Sum of electronic and thermal Enthalpies= -936.932074

Sum of electronic and thermal Free Energies= -937.002173

C	0.38793600	-0.19121000	1.35420900
C	0.86666700	-0.82025700	0.25461100
C	0.59969500	-0.42901900	-1.13517900
C	-0.50304200	0.97283600	1.39817100

C	0.37326100	0.82998400	-1.56427700
C	-0.52759400	1.97871900	0.49575300
C	0.35869800	2.02826400	-0.70978200
H	0.28114100	1.03513700	-2.62396700
N	0.96656000	3.06953100	-1.12767000
C	0.97392700	4.28191200	-0.33544700
H	1.89152800	4.83146400	-0.56214200
H	0.12558100	4.91852400	-0.60891200
H	0.93134100	4.11177100	0.74947100
O	-1.39670200	3.02149000	0.52017800
C	-1.73280100	3.64865800	1.74962600
H	-2.02234700	4.66950800	1.49136800
H	-2.55889800	3.14110900	2.25049700
H	-0.87349800	3.67339800	2.42719400
O	-1.32431000	1.03841700	2.49886900
C	-2.27993300	-0.01108600	2.57099000
H	-2.89564900	0.19631300	3.44749500
H	-2.91170500	-0.02394400	1.67513200
H	-1.78981600	-0.98206400	2.69367700
O	0.65865200	-0.76602600	2.56837700
C	1.41728500	0.05352400	3.44623800
H	0.88661700	0.98287200	3.67847100
H	1.55470000	-0.52138400	4.36275600
H	2.39534100	0.28145500	3.00845000
O	1.69247100	-1.89845300	0.39871900
C	1.03285900	-3.11793000	0.70620300
H	1.80935200	-3.88306000	0.75131500
H	0.52716800	-3.05344900	1.67507000

H	0.31399300	-3.37925600	-0.07784000
O	0.68594500	-1.50706700	-1.95365900
C	0.56876100	-1.29497200	-3.34181300
H	0.69261300	-2.27209500	-3.80841400
H	-0.41529600	-0.88684700	-3.60401500
H	1.34740700	-0.61423000	-3.70694600

TI-23457

Zero-point correction= 0.316292 (Hartree/Particle)

Thermal correction to Energy= 0.336636

Thermal correction to Enthalpy= 0.337580

Thermal correction to Gibbs Free Energy= 0.268198

Sum of electronic and zero-point Energies= -936.955673

Sum of electronic and thermal Energies= -936.935328

Sum of electronic and thermal Enthalpies= -936.934384

Sum of electronic and thermal Free Energies= -937.003767

C	0.34965700	-0.20631500	1.33887800
C	0.91600000	-0.79625400	0.25448900
C	0.83117800	-0.35416100	-1.11938200
C	-0.52778100	0.96220300	1.31956300
C	0.66352300	0.91755700	-1.54968800
C	-0.45929600	1.98980400	0.44056000
C	0.56688600	2.08881400	-0.63529500
N	1.27619000	3.10967000	-0.90467600
C	1.22045000	4.26790900	-0.03880200
H	2.16896100	4.80440800	-0.11974600
H	0.42203700	4.94057300	-0.36894600
H	1.04224000	4.02492400	1.01828300

H	1.01985400	-1.14320200	-1.83815600
O	-1.33485100	3.03353200	0.39231100
C	-1.75298500	3.66386600	1.59394700
H	-2.02197600	4.68573700	1.31723700
H	-2.61212700	3.15849600	2.03836600
H	-0.94325200	3.68735400	2.33063700
O	-1.45347000	1.02697600	2.33221400
C	-2.39815900	-0.03491500	2.32944700
H	-3.10938800	0.18766600	3.12627900
H	-2.92805500	-0.08022000	1.37101800
H	-1.91280400	-0.99450300	2.53064800
O	0.49996400	-0.81220300	2.56559300
C	1.23569400	-0.03596700	3.49822900
H	0.73070300	0.91363700	3.70759100
H	1.29125900	-0.62291400	4.41631800
H	2.24807000	0.15818600	3.12606200
O	1.66602500	-1.93679600	0.39930600
C	0.95217700	-3.09512800	0.80522000
H	0.15174200	-3.32933500	0.09136100
H	1.67603000	-3.91169400	0.80866000
H	0.52756000	-2.97367400	1.80494100
O	0.61507600	1.29209800	-2.84051800
C	0.73715800	0.29234600	-3.82866800
H	-0.05146500	-0.46423900	-3.73117400
H	0.63684200	0.80190700	-4.78643100
H	1.71594800	-0.19905600	-3.77658400

TI-23567

Zero-point correction=	0.316158 (Hartree/Particle)
Thermal correction to Energy=	0.337282
Thermal correction to Enthalpy=	0.338226
Thermal correction to Gibbs Free Energy=	0.266756
Sum of electronic and zero-point Energies=	-936.953448
Sum of electronic and thermal Energies=	-936.932324
Sum of electronic and thermal Enthalpies=	-936.931380
Sum of electronic and thermal Free Energies=	-937.002850

C	0.27744000	0.05710100	1.56587100
C	0.86680800	-0.68832100	0.60243500
C	0.79945700	-0.48687300	-0.83355000
C	-0.57443200	1.20873000	1.39105700
C	0.59799800	0.70882200	-1.45071900
C	-0.51647200	2.07935000	0.35348100
C	0.52356400	1.99189400	-0.70755000
H	0.40960600	-0.27629800	2.59161200
N	1.26802400	2.95188600	-1.09821000
C	1.22220700	4.21677500	-0.39431300
H	2.17286500	4.73222700	-0.54883900
H	0.42213900	4.84714800	-0.79693200
H	1.05150300	4.10560300	0.68543300
O	-1.36575900	3.12380300	0.13698900
C	-1.81101800	3.91886900	1.22678500
H	-2.09031900	4.88188000	0.79420100
H	-2.67184200	3.47280500	1.72814100
H	-1.01388100	4.06404700	1.96279800
O	-1.47727100	1.43419700	2.40702900
C	-2.51741100	0.47144100	2.46411000

H	-2.12094900	-0.53971300	2.61531800
H	-3.14822500	0.74323200	3.31181200
H	-3.11332300	0.48327400	1.54318800
O	1.60292200	-1.78258100	0.99246700
C	0.84925500	-2.97856900	1.12057300
H	0.39822100	-3.25985500	0.16397300
H	1.54918100	-3.75227400	1.43994100
H	0.06354300	-2.86643500	1.87930400
O	0.97623800	-1.61578700	-1.59197800
C	2.28395400	-1.75159800	-2.13322600
H	2.29384700	-2.69528000	-2.68133700
H	2.51071400	-0.93010700	-2.82045300
H	3.03011300	-1.78699300	-1.33234400
O	0.58344000	0.69828400	-2.80025900
C	0.08758500	1.82961100	-3.50185500
H	-0.06667200	1.48709700	-4.52549600
H	-0.86598800	2.16929200	-3.08295500
H	0.80290700	2.65371100	-3.47571300

TI-234567

Zero-point correction= 0.348814 (Hartree/Particle)

Thermal correction to Energy= 0.372930

Thermal correction to Enthalpy= 0.373874

Thermal correction to Gibbs Free Energy= 0.295395

Sum of electronic and zero-point Energies= -1051.406886

Sum of electronic and thermal Energies= -1051.382770

Sum of electronic and thermal Enthalpies= -1051.381826

Sum of electronic and thermal Free Energies= -1051.460304

C	0.38354200	-0.17525700	1.37317400
C	0.76156400	-0.83219400	0.24380500
C	0.54021700	-0.41259700	-1.12968600
C	-0.30999900	1.10400500	1.44130400
C	0.52541600	0.87474300	-1.56191300
C	-0.20835800	2.07371700	0.49901900
C	0.76254700	2.00467400	-0.63127700
N	1.65651400	2.86771300	-0.90783300
C	1.86576500	3.98937600	-0.01449900
H	2.93928100	4.18896400	0.03679800
H	1.38477200	4.87722700	-0.43786400
H	1.47032800	3.84287700	0.99775100
O	-0.91959800	3.23405200	0.47311700
C	-2.27985500	3.20954500	0.87789700
H	-2.73932200	4.09522900	0.43578700
H	-2.77847300	2.31126100	0.49418800
H	-2.37779700	3.23934000	1.96441100
O	-1.03550900	1.36369600	2.57646400
C	-2.06972300	0.43227000	2.87067500
H	-2.54688500	0.78843900	3.78476000
H	-2.81063200	0.40604600	2.06184100
H	-1.66399400	-0.56880500	3.03459700
O	0.60815900	-0.79693300	2.57875600
C	1.60582900	-0.16524100	3.36690500
H	1.33537500	0.87298500	3.59000600
H	1.67029200	-0.72917600	4.29866300
H	2.57443000	-0.19292200	2.85524300
O	1.42256900	-2.02791200	0.35796100

C	0.58294700	-3.13999000	0.63615800
H	1.23177100	-4.01750600	0.65367000
H	0.09719100	-3.02612700	1.61060900
H	-0.16867300	-3.25825800	-0.15151000
O	0.38738900	-1.43811700	-2.02673600
C	1.55131500	-1.72479100	-2.79124200
H	1.28830600	-2.55216300	-3.45264200
H	1.84852700	-0.85991200	-3.39338800
H	2.37430100	-2.02673200	-2.13506400
O	0.33683800	1.08720600	-2.88471700
C	0.06040500	2.40333600	-3.33797800
H	-0.25160000	2.29039000	-4.37660100
H	-0.75205100	2.85979500	-2.76110300
H	0.94471700	3.04105800	-3.27232500

Cartesian Coordination of MeO-TI Conjugated Acid and Their Thermochemical Values (ω B97X-D/6-31g(d,p))

TI-2

Zero-point correction= 0.200531 (Hartree/Particle)

Thermal correction to Energy= 0.210880

Thermal correction to Enthalpy= 0.211825

Thermal correction to Gibbs Free Energy= 0.164850

Sum of electronic and zero-point Energies= -479.560485

Sum of electronic and thermal Energies= -479.550136

Sum of electronic and thermal Enthalpies= -479.549191

Sum of electronic and thermal Free Energies= -479.596166

C	-0.08148000	0.21266400	1.62291200
C	0.76303500	-0.35329100	0.70031700
C	1.19385800	0.22445800	-0.50518700
C	-0.71293600	1.47109500	1.60032100
C	0.90422700	1.45210200	-1.05536400
C	-0.66639600	2.48215100	0.66698100
C	0.08575700	2.50524300	-0.58156100
H	-0.30461800	-0.38533100	2.50158400
H	1.13833700	-1.34738000	0.91899100
H	1.38012100	1.64452900	-2.00998800
C	0.60597200	3.89250000	-2.57484500
H	0.30982900	4.88921900	-2.89697700
H	1.69526800	3.87033800	-2.47790500
H	0.29117000	3.17453300	-3.33762700
N	-0.03792500	3.61960300	-1.30042100
H	-0.64049400	4.32973200	-0.90936900

H	1.86131300	-0.39062900	-1.10242400
H	-1.33542200	1.66848500	2.46523500
O	-1.34593400	3.62258600	0.81863500
C	-2.17712300	3.85418800	1.95897500
H	-1.58233900	3.85034200	2.87637400
H	-2.60719700	4.84098300	1.80439200
H	-2.97481400	3.10839600	2.01020500

TI-3

Zero-point correction= 0.199820 (Hartree/Particle)

Thermal correction to Energy= 0.210440

Thermal correction to Enthalpy= 0.211384

Thermal correction to Gibbs Free Energy= 0.163686

Sum of electronic and zero-point Energies= -479.556794

Sum of electronic and thermal Energies= -479.546174

Sum of electronic and thermal Enthalpies= -479.545229

Sum of electronic and thermal Free Energies= -479.592927

C	-0.09471400	0.33328500	1.69815600
C	0.63960700	-0.27712300	0.72927900
C	1.06978400	0.23126200	-0.52983500
C	-0.62897700	1.66145100	1.68662300
C	0.86048300	1.44971100	-1.09566000
C	-0.51259700	2.61325900	0.68485900
C	0.13575300	2.57311000	-0.56679000
H	-0.29861800	-0.25913500	2.58185000
H	0.94487200	-1.29763400	0.93985800
H	1.29994200	1.59281700	-2.07604300
C	0.65662300	3.88099500	-2.63344400

H	0.41743400	4.89177800	-2.95968400
H	1.74545400	3.78292900	-2.59917100
H	0.24652300	3.18002700	-3.36615600
H	-1.01597800	3.54439200	0.93260400
O	-1.33248700	2.10994300	2.72109000
C	-1.57731600	1.31686500	3.88542300
H	-2.17148800	1.95341800	4.53697100
H	-2.14853400	0.41839600	3.63625300
H	-0.64048300	1.05655100	4.38537000
N	0.06545700	3.68145400	-1.31822500
H	-0.44567200	4.46161200	-0.93366200
H	1.65480600	-0.46349500	-1.12534600

TI-4

Zero-point correction= 0.199485 (Hartree/Particle)

Thermal correction to Energy= 0.210176

Thermal correction to Enthalpy= 0.211120

Thermal correction to Gibbs Free Energy= 0.163131

Sum of electronic and zero-point Energies= -479.556447

Sum of electronic and thermal Energies= -479.545756

Sum of electronic and thermal Enthalpies= -479.544812

Sum of electronic and thermal Free Energies= -479.592801

C	-0.25010900	-0.07012300	1.27604800
C	0.77989800	-0.45049600	0.42593700
C	1.34327800	0.27148300	-0.62631400
C	-0.94603900	1.17859800	1.23163900
C	1.07176200	1.52583700	-1.14013900
C	-0.79277100	2.23765300	0.39130100

C	0.10237900	2.45586900	-0.71092400
H	1.18665700	-1.43731500	0.62118500
H	1.68895200	1.82481900	-1.97915900
C	0.76369500	4.06325400	-2.48868600
H	0.41245100	5.04774600	-2.79297500
H	1.82529400	4.13907500	-2.23430100
H	0.63919200	3.37723500	-3.33190300
N	-0.02245900	3.63150900	-1.34466300
H	-0.72199200	4.27395100	-1.00613400
H	2.14672100	-0.25191000	-1.13773000
H	-1.71986000	1.31205300	1.97904200
H	-1.47000800	3.06608400	0.58854900
O	-0.55907400	-0.98994600	2.18002100
C	-1.58867300	-0.79683600	3.15217300
H	-2.56036500	-0.65327300	2.67132200
H	-1.60494100	-1.71765800	3.73065800
H	-1.35147700	0.04282600	3.81156000

TI-23

Zero-point correction= 0.233058 (Hartree/Particle)

Thermal correction to Energy= 0.246185

Thermal correction to Enthalpy= 0.247129

Thermal correction to Gibbs Free Energy= 0.193624

Sum of electronic and zero-point Energies= -594.013313

Sum of electronic and thermal Energies= -594.000185

Sum of electronic and thermal Enthalpies= -593.999241

Sum of electronic and thermal Free Energies= -594.052747

C	1.46165500	1.57821200	0.07899200
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C	0.56395600	2.59358400	0.23595400
C	-0.84866000	2.52500500	0.25829800
C	1.23320200	0.18335900	-0.08954600
C	-1.65835800	1.43765600	0.11468400
C	0.00563200	-0.48973800	-0.09406500
C	-1.31679000	0.06311800	-0.07303900
H	2.50311900	1.87648400	0.08441800
H	0.98832900	3.58520800	0.35741800
H	-2.72231700	1.63975100	0.16258400
C	-3.72648500	-0.54378800	-0.26735600
H	-4.24877900	-1.48315400	-0.44059400
H	-4.08046900	-0.12660600	0.68011800
H	-3.97460700	0.14233900	-1.08271500
H	-1.35803100	3.47313300	0.40170500
O	0.01180000	-1.83331100	-0.26098600
C	0.51737600	-2.64156200	0.82004000
H	0.30710400	-3.67075100	0.53529400
H	1.59077600	-2.50074700	0.93946200
H	-0.00632800	-2.39646300	1.74856200
O	2.26265200	-0.64664300	-0.25625500
C	3.61011200	-0.18200900	-0.34590400
H	3.72958000	0.51948200	-1.17604400
H	3.93612700	0.27154500	0.59442100
H	4.19981800	-1.07505300	-0.54094200
N	-2.30255800	-0.82623500	-0.22428300
H	-1.99187100	-1.77491000	-0.38412300

TI-24

Zero-point correction= 0.233255 (Hartree/Particle)

Thermal correction to Energy= 0.246224

Thermal correction to Enthalpy= 0.247168

Thermal correction to Gibbs Free Energy= 0.193993

Sum of electronic and zero-point Energies= -594.029618

Sum of electronic and thermal Energies= -594.016649

Sum of electronic and thermal Enthalpies= -594.015704

Sum of electronic and thermal Free Energies= -594.068879

C	1.78929000	-0.07338100	0.00001500
C	1.65618300	-1.45541200	-0.00061500
C	0.45965500	-2.16724700	-0.00090500
C	0.74418900	0.89360100	-0.00004700
C	-0.86342000	-1.76032100	-0.00050400
C	-0.61571000	0.76469100	-0.00012700
C	-1.40839300	-0.46664300	0.00001300
H	2.56082400	-2.04972800	-0.00087700
H	-1.58687000	-2.56645000	-0.00066300
C	-3.72413900	-1.34916200	0.00079800
H	-4.71038000	-0.88850200	0.00119400
H	-3.63448800	-1.97502500	-0.89224000
H	-3.63379400	-1.97514400	0.89368100
H	0.58587000	-3.24666300	-0.00146400
H	1.13777200	1.90313900	0.00009100
O	-1.42287800	1.83157500	-0.00013300
C	-0.90027100	3.16066100	-0.00057800
H	-1.77157500	3.81177500	-0.00079700
H	-0.30559100	3.34085200	0.89914400
H	-0.30559400	3.34022300	-0.90042700

O	2.97309400	0.53173400	0.00056000
C	4.18474100	-0.22412000	0.00070500
H	4.25656800	-0.84193100	-0.89890600
H	4.98146000	0.51604200	0.00144900
H	4.25577800	-0.84291100	0.89970500
N	-2.73046900	-0.29063200	0.00048900
H	-3.05117400	0.66628000	0.00075100

TI-25

Zero-point correction= 0.233378 (Hartree/Particle)

Thermal correction to Energy= 0.246340

Thermal correction to Enthalpy= 0.247284

Thermal correction to Gibbs Free Energy= 0.194100

Sum of electronic and zero-point Energies= -594.024165

Sum of electronic and thermal Energies= -594.011204

Sum of electronic and thermal Enthalpies= -594.010259

Sum of electronic and thermal Free Energies= -594.063444

C	1.55084100	0.95814100	-0.00008800
C	2.00382800	-0.34879200	0.00018100
C	1.17494000	-1.50238100	0.00047200
C	0.22961400	1.42799300	-0.00025100
C	-0.18433900	-1.62401300	0.00054700
C	-0.98753400	0.77901600	-0.00012500
C	-1.21454000	-0.64322500	0.00012900
H	2.30091300	1.73985700	-0.00021300
H	-0.53905500	-2.64836600	0.00107800
C	-2.97458500	-2.40244100	-0.00053700
H	-4.06289100	-2.37569400	-0.00312300

H	-2.64225500	-2.94036700	-0.89327900
H	-2.64622500	-2.93982500	0.89402400
H	1.73751900	-2.43168000	0.00077100
H	0.16316800	2.51027200	-0.00060600
O	-2.15694300	1.44446600	-0.00034400
C	-2.20120400	2.86912800	0.00048200
H	-3.25894100	3.12360100	0.00095800
H	-1.72813600	3.27376000	0.90006000
H	-1.72872800	3.27476800	-0.89895600
O	3.29750500	-0.67783900	0.00028100
C	4.29976000	0.33356800	-0.00051300
H	5.24827400	-0.19883900	-0.00067200
H	4.22915100	0.95393100	-0.89970500
H	4.22986800	0.95466900	0.89822700
N	-2.49094100	-1.03221200	-0.00001200
H	-3.17124400	-0.28557800	0.00024500

TI-26

Zero-point correction= 0.232842 (Hartree/Particle)

Thermal correction to Energy= 0.246004

Thermal correction to Enthalpy= 0.246948

Thermal correction to Gibbs Free Energy= 0.192982

Sum of electronic and zero-point Energies= -594.028860

Sum of electronic and thermal Energies= -594.015698

Sum of electronic and thermal Enthalpies= -594.014754

Sum of electronic and thermal Free Energies= -594.068720

C	0.50671300	-2.17516700	-0.00018700
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C	1.66275000	-1.44725800	-0.00000300
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C	1.77117500	-0.03367500	0.00002300
C	-0.84682900	-1.77007600	-0.00031900
C	0.73483000	0.90147800	0.00009300
C	-1.38455400	-0.51026700	-0.00019100
C	-0.65543100	0.76011800	-0.00011900
H	0.64192300	-3.25295700	-0.00022700
H	2.58398700	-2.01558400	0.00014500
H	1.10722600	1.91909700	0.00025100
C	-0.95441800	3.22167900	-0.00000200
H	-1.82011000	3.88193300	-0.00004100
H	-0.35822000	3.43402000	0.89295200
H	-0.35799900	3.43418900	-0.89276900
H	-1.55610700	-2.58868600	-0.00050600
O	-2.70182400	-0.29153000	-0.00018700
C	-3.63441000	-1.37400500	0.00052000
H	-4.61616500	-0.90629000	0.00121400
H	-3.51598400	-1.98344000	-0.89947000
H	-3.51466400	-1.98335500	0.90039100
O	2.96075600	0.55958500	0.00018400
C	4.17900700	-0.18692000	0.00008900
H	4.26039100	-0.80262800	-0.89981900
H	4.96724500	0.56236800	0.00000600
H	4.26054100	-0.80258200	0.90001500
N	-1.42888200	1.85088300	-0.00018100
H	-2.42434300	1.68785400	-0.00027500

TI-27

Zero-point correction= 0.233060 (Hartree/Particle)

Thermal correction to Energy=	0.246029
Thermal correction to Enthalpy=	0.246973
Thermal correction to Gibbs Free Energy=	0.193458
Sum of electronic and zero-point Energies=	-594.014697
Sum of electronic and thermal Energies=	-594.001728
Sum of electronic and thermal Enthalpies=	-594.000784
Sum of electronic and thermal Free Energies=	-594.054298

C	-0.49319400	-0.10128100	1.67595700
C	0.32725900	-0.71856400	0.76362000
C	0.77969900	-0.21663200	-0.46100500
C	-1.04166400	1.18330500	1.59730900
C	0.60621800	1.01702500	-1.06499700
C	-0.86544500	2.18243200	0.66138900
C	-0.03230200	2.19264700	-0.52595400
H	-0.76218300	-0.67048900	2.55969500
H	0.64551600	-1.72942400	0.99687800
C	0.86261700	3.86139000	-2.24759100
H	0.76398400	4.94657500	-2.25147600
H	1.91096600	3.60431400	-2.10297400
H	0.52036400	3.46804700	-3.20392100
H	1.36326900	-0.92288600	-1.03940300
H	-1.68982700	1.44360000	2.42586700
O	-1.47626400	3.37379300	0.79943800
C	-2.37894000	3.63704400	1.87224800
H	-2.74305500	4.64723300	1.69842500
H	-3.21865500	2.93683700	1.85339500
H	-1.86212300	3.59461200	2.83515200
O	1.07248100	1.25059400	-2.29872100

C	1.70396500	0.22974200	-3.06523900
H	1.03264300	-0.62208400	-3.20978300
H	1.91935900	0.69024300	-4.02723600
H	2.63926500	-0.09346500	-2.59843300
N	0.03951800	3.37352200	-1.14109400
H	-0.52594900	4.07791300	-0.68655500

TI-34

Zero-point correction= 0.233077 (Hartree/Particle)

Thermal correction to Energy= 0.246168

Thermal correction to Enthalpy= 0.247112

Thermal correction to Gibbs Free Energy= 0.193672

Sum of electronic and zero-point Energies= -594.015305

Sum of electronic and thermal Energies= -594.002214

Sum of electronic and thermal Enthalpies= -594.001270

Sum of electronic and thermal Free Energies= -594.054711

C	-0.14358400	0.10636700	1.66015200
C	0.48791500	-0.67410700	0.72395800
C	1.02354100	-0.31333600	-0.53431600
C	-0.29401500	1.55674500	1.59299200
C	0.98272000	0.86213100	-1.22247300
C	-0.09121400	2.36286700	0.49398900
C	0.39877900	2.09512300	-0.80867200
H	0.57695000	-1.72784700	0.95847200
H	1.43424800	0.85851600	-2.21081600
C	-0.16064100	4.42053700	-1.51332600
H	-0.09986900	4.95427000	-2.46031200
H	-1.21073000	4.37208600	-1.21200300

H	0.40866600	4.98107200	-0.76531800
H	1.51224000	-1.13228600	-1.05436600
H	-0.34792400	3.39415500	0.70692000
O	-0.77650800	2.22448800	2.63523000
C	-0.45471700	1.93211500	4.00821400
H	-0.46149100	2.90165600	4.50370200
H	-1.20936000	1.27863100	4.44081500
H	0.53436900	1.47963900	4.09435500
O	-0.69616900	-0.39473000	2.76254200
C	-0.69775400	-1.80047300	3.00302200
H	0.32245800	-2.17903700	3.11720000
H	-1.24152200	-1.93151000	3.93589400
H	-1.21420500	-2.32911100	2.19638700
N	0.38638000	3.08776700	-1.70880800
H	0.79169100	2.89211900	-2.61136700

TI-35

Zero-point correction= 0.232729 (Hartree/Particle)

Thermal correction to Energy= 0.245896

Thermal correction to Enthalpy= 0.246840

Thermal correction to Gibbs Free Energy= 0.193366

Sum of electronic and zero-point Energies= -594.023381

Sum of electronic and thermal Energies= -594.010214

Sum of electronic and thermal Enthalpies= -594.009270

Sum of electronic and thermal Free Energies= -594.062745

C	-0.24353200	0.30508700	1.81718100
C	0.07889500	-0.65042800	0.87489600
C	0.39493800	-0.42732300	-0.50784000

C	-0.33391800	1.70231600	1.66395600
C	0.47973800	0.73797900	-1.19081800
C	-0.09275100	2.48629600	0.52693900
C	0.28048700	2.10027400	-0.75809400
H	-0.45060000	-0.11093000	2.79500000
H	0.74093800	0.63261600	-2.24143200
C	0.32862700	4.46619300	-1.50989000
H	0.54964300	4.96696400	-2.45100400
H	-0.69374300	4.72274300	-1.21424900
H	1.02752500	4.83139000	-0.75056100
H	0.59903800	-1.31555600	-1.09374400
H	-0.22922000	3.54456100	0.71368500
O	-0.68313000	2.46277900	2.69797200
C	-0.98510400	1.91106500	3.97981400
H	-1.25172100	2.76549600	4.59793100
H	-1.83326100	1.22337600	3.92145800
H	-0.11110000	1.41057800	4.40565100
O	0.07152600	-1.88642800	1.36664100
C	0.37064000	-3.03400400	0.57015000
H	1.38386600	-2.97908200	0.16250600
H	0.30345400	-3.87526900	1.25633100
H	-0.36457000	-3.15887300	-0.22984500
N	0.47205200	3.03585600	-1.70735800
H	0.74003800	2.72400900	-2.62693000

TI-36

Zero-point correction= 0.232437 (Hartree/Particle)

Thermal correction to Energy= 0.245751

Thermal correction to Enthalpy= 0.246695
 Thermal correction to Gibbs Free Energy= 0.192405
 Sum of electronic and zero-point Energies= -594.021032
 Sum of electronic and thermal Energies= -594.007719
 Sum of electronic and thermal Enthalpies= -594.006775
 Sum of electronic and thermal Free Energies= -594.061064

C	-0.09527100	0.35291300	1.68342900
C	0.63823800	-0.27520400	0.73063300
C	1.08275300	0.21370500	-0.54296500
C	-0.63759400	1.68163300	1.68591100
C	0.85307900	1.45873000	-1.08869300
C	-0.52075400	2.62418800	0.69139100
C	0.13878800	2.56331500	-0.56464600
H	-0.29829000	-0.24037500	2.56701500
H	0.92676000	-1.29126000	0.97197100
H	1.29982300	1.58058400	-2.06810100
C	0.65945100	3.86811900	-2.62704800
H	0.42421400	4.87719500	-2.96166400
H	1.74815900	3.76481700	-2.58925600
H	0.25187300	3.16137000	-3.35632300
H	-1.02044600	3.56022300	0.92631500
O	-1.34324500	2.11595400	2.73241200
C	-1.57482100	1.30991500	3.88676300
H	-2.17054600	1.93402500	4.54924700
H	-2.14171900	0.40873600	3.63503900
H	-0.63497200	1.05044300	4.38271400
O	1.80571000	-0.57072100	-1.34201400
C	2.15997600	-1.90794400	-0.98995900

H	1.27050300	-2.53012400	-0.85598400
H	2.73288500	-2.27847900	-1.83710700
H	2.78670600	-1.92804100	-0.09367200
N	0.06586500	3.67667900	-1.31480600
H	-0.44461200	4.45619000	-0.93058200

TI-45

Zero-point correction= 0.232486 (Hartree/Particle)

Thermal correction to Energy= 0.245782

Thermal correction to Enthalpy= 0.246726

Thermal correction to Gibbs Free Energy= 0.192509

Sum of electronic and zero-point Energies= -594.010683

Sum of electronic and thermal Energies= -593.997387

Sum of electronic and thermal Enthalpies= -593.996443

Sum of electronic and thermal Free Energies= -594.050660

C	-0.48341100	0.11687100	1.81127700
C	0.32113000	-0.54979900	0.86820700
C	0.80349600	0.01808200	-0.32871400
C	-0.78382900	1.50235000	1.79231000
C	0.73451100	1.28178200	-0.86907000
C	-0.51651100	2.50635100	0.90534900
C	0.15319900	2.46113400	-0.34683300
H	1.22222500	1.38054300	-1.83196800
C	0.87241400	3.77167600	-2.33916200
H	0.74764900	4.80699900	-2.65210900
H	1.94442000	3.55813500	-2.28045900
H	0.41357100	3.12878600	-3.09668900
H	1.35495100	-0.67550800	-0.95359400

H	-0.90055900	3.48172700	1.19431600
H	-1.35023000	1.79327200	2.67247700
O	-0.98506400	-0.47204700	2.89268400
C	-1.41333500	-1.84407200	2.94342600
H	-0.58010400	-2.50061000	3.18584600
H	-2.15754700	-1.86564000	3.73760600
H	-1.87017900	-2.14255200	1.99835100
O	0.61347400	-1.81454400	1.19919300
C	1.41702500	-2.64211000	0.36424700
H	2.41583000	-2.21540500	0.23047200
H	1.49884900	-3.58870100	0.89437500
H	0.93834700	-2.81137000	-0.60542800
N	0.22972800	3.60625200	-1.04706000
H	-0.18771900	4.42713800	-0.63715200

TI-234

Zero-point correction= 0.264953 (Hartree/Particle)

Thermal correction to Energy= 0.280953

Thermal correction to Enthalpy= 0.281897

Thermal correction to Gibbs Free Energy= 0.221257

Sum of electronic and zero-point Energies= -708.473795

Sum of electronic and thermal Energies= -708.457795

Sum of electronic and thermal Enthalpies= -708.456851

Sum of electronic and thermal Free Energies= -708.517491

C	1.54240900	-0.67169100	-0.11212500
C	1.16378400	-2.00145500	-0.13235900
C	-0.13002800	-2.52637700	-0.06985900
C	0.67192900	0.48503400	-0.06216500

C	-1.35942400	-1.91673200	0.02896200
C	-0.70691700	0.54441900	-0.05002900
C	-1.67052900	-0.54242700	0.05454800
H	1.95594300	-2.73678400	-0.18881000
H	-2.20709400	-2.58967300	0.07260100
C	-4.09206600	-1.02642800	0.29220900
H	-4.98300000	-0.40623700	0.37469300
H	-4.20049600	-1.67046100	-0.58580000
H	-4.01883100	-1.64727700	1.19022800
H	-0.17044800	-3.61189400	-0.09372800
O	-1.32263900	1.74278900	-0.03814000
C	-0.98145500	2.76894000	-0.99370800
H	-1.91990900	3.27555300	-1.21663300
H	-0.26615600	3.46753400	-0.56433900
H	-0.56732500	2.32578000	-1.90049400
O	1.31406200	1.67328100	-0.08486400
C	1.67650000	2.19152400	1.20352100
H	2.35772800	1.50749700	1.71595300
H	2.18297300	3.13581100	1.01164400
H	0.78135100	2.36398000	1.80930400
O	2.81419800	-0.29473500	-0.13195400
C	3.86279700	-1.25955800	-0.19925300
H	4.78314900	-0.67989500	-0.20303900
H	3.84538000	-1.91876100	0.67373500
H	3.79349400	-1.84307400	-1.12176800
N	-2.94131900	-0.15179400	0.16288600
H	-3.08450600	0.84829300	0.16745800

TI-235

Zero-point correction= 0.265899 (Hartree/Particle)

Thermal correction to Energy= 0.281691

Thermal correction to Enthalpy= 0.282635

Thermal correction to Gibbs Free Energy= 0.222929

Sum of electronic and zero-point Energies= -708.476299

Sum of electronic and thermal Energies= -708.460507

Sum of electronic and thermal Enthalpies= -708.459563

Sum of electronic and thermal Free Energies= -708.519269

C	-1.31952900	0.97258500	-0.06015300
C	-2.02230400	-0.21340400	0.04133900
C	-1.46846100	-1.52456000	0.06310600
C	0.06189800	1.21176600	-0.14595300
C	-0.16383200	-1.90292500	-0.01186100
C	1.12044900	0.27927900	-0.11168300
C	1.03918900	-1.13374500	-0.10618100
H	-1.96580100	1.84138400	-0.07476600
H	-0.00708200	-2.97541200	0.01966100
C	2.40334600	-3.22311600	-0.21729100
H	3.47159500	-3.41682500	-0.30089900
H	2.04450400	-3.70086600	0.69964500
H	1.90819600	-3.67720500	-1.08190300
H	-2.17571500	-2.34162100	0.14134100
O	2.38915800	0.74906600	-0.20930600
C	2.92400600	1.43387500	0.93789600
H	2.82631400	0.80927600	1.83105100
H	3.97657600	1.60009400	0.71536400
H	2.42221000	2.38987700	1.08638600

O	0.51431500	2.46010600	-0.26571100
C	-0.36788500	3.57854900	-0.34289700
H	-0.94342300	3.69025600	0.58056800
H	0.28338800	4.44031600	-0.47182100
H	-1.03519900	3.49488700	-1.20513200
O	-3.34177100	-0.02585100	0.11520100
C	-4.25369600	-1.11586500	0.23622600
H	-4.07314000	-1.68048500	1.15570700
H	-5.23803700	-0.65550300	0.28503300
H	-4.20472600	-1.77323600	-0.63695800
N	2.21194900	-1.78594000	-0.17942900
H	3.01399600	-1.18456100	-0.30402800

TI-236

Zero-point correction= 0.265900 (Hartree/Particle)

Thermal correction to Energy= 0.281686

Thermal correction to Enthalpy= 0.282630

Thermal correction to Gibbs Free Energy= 0.222732

Sum of electronic and zero-point Energies= -708.477512

Sum of electronic and thermal Energies= -708.461726

Sum of electronic and thermal Enthalpies= -708.460782

Sum of electronic and thermal Free Energies= -708.520679

C	0.00902400	-1.84561700	-0.02217900
C	1.34878900	-1.61169300	0.05766800
C	2.02366100	-0.36073700	0.04804900
C	-1.09987100	-0.95878100	-0.11558400
C	1.44266500	0.89076100	-0.04066500
C	-1.07173100	0.43033900	-0.06936800

C	0.09303200	1.28745100	-0.10028900
H	-0.25573300	-2.89629400	-0.02074300
H	1.96721500	-2.49822700	0.12372700
H	2.17432300	1.68976200	-0.03927700
C	0.78428100	3.67130100	-0.24131700
H	0.24239000	4.61147300	-0.33021700
H	1.39483400	3.71199300	0.66639800
H	1.43905400	3.56928000	-1.11247200
O	-2.21850800	1.13364800	-0.11592100
C	-3.29401700	0.85577600	0.80109400
H	-3.77761200	1.81551800	0.97880000
H	-3.99666800	0.15273500	0.35868800
H	-2.90227300	0.45773400	1.74000100
O	-2.34187500	-1.44979500	-0.25039300
C	-2.59967300	-2.84914100	-0.30134500
H	-2.31013300	-3.34350900	0.63110400
H	-3.67667800	-2.93408800	-0.43163100
H	-2.09922600	-3.31476100	-1.15564400
O	3.35467500	-0.30175100	0.11858100
C	4.15745100	-1.47709300	0.20894700
H	4.03545700	-2.10776900	-0.67648200
H	5.18245600	-1.11554100	0.25536000
H	3.93144000	-2.04072000	1.11893500
N	-0.18533700	2.59540200	-0.17814300
H	-1.16747500	2.82238100	-0.22774100

TI-237

Zero-point correction= 0.265802 (Hartree/Particle)

Thermal correction to Energy=	0.281426
Thermal correction to Enthalpy=	0.282370
Thermal correction to Gibbs Free Energy=	0.223201
Sum of electronic and zero-point Energies=	-708.470384
Sum of electronic and thermal Energies=	-708.454760
Sum of electronic and thermal Enthalpies=	-708.453816
Sum of electronic and thermal Free Energies=	-708.512985

C	-1.40405200	-1.85874000	-0.19570600
C	-0.19057500	-2.48767500	-0.16117100
C	1.10032600	-1.95421600	-0.00447000
C	-1.66280400	-0.47216600	-0.11339200
C	1.51283800	-0.64352700	0.03431900
C	-0.72410400	0.57436200	-0.09749100
C	0.69830400	0.54076400	-0.19527200
H	-2.26757300	-2.50488000	-0.28663000
H	-0.22559800	-3.57086200	-0.22716600
C	2.63850000	2.10048700	-0.75693500
H	2.59159400	3.10196200	-1.18409000
H	3.28785700	2.11532500	0.11833600
H	3.05460800	1.42351500	-1.50272500
H	1.88067500	-2.69714700	0.10446200
O	-1.22742200	1.83944000	-0.14898600
C	-1.73934500	2.36607500	1.08880300
H	-0.96933800	2.32710300	1.86549700
H	-2.00461600	3.40126100	0.88103200
H	-2.62500800	1.81245000	1.40229800
O	-2.91406300	-0.01587600	-0.09287300
C	-4.03527800	-0.89581500	-0.16286100

H	-4.05040000	-1.58592300	0.68548600
H	-4.90574500	-0.24477800	-0.11885900
H	-4.04285500	-1.44625900	-1.10773200
O	2.77911300	-0.31104100	0.29316200
C	3.75232900	-1.30378700	0.60622000
H	3.92532900	-1.96637000	-0.24700100
H	4.66332000	-0.75182700	0.82788700
H	3.44908300	-1.88196600	1.48414000
N	1.26957500	1.73053100	-0.40737300
H	0.57378900	2.45992900	-0.50600300

TI-245

Zero-point correction= 0.265752 (Hartree/Particle)

Thermal correction to Energy= 0.281480

Thermal correction to Enthalpy= 0.282424

Thermal correction to Gibbs Free Energy= 0.222970

Sum of electronic and zero-point Energies= -708.478378

Sum of electronic and thermal Energies= -708.462650

Sum of electronic and thermal Enthalpies= -708.461705

Sum of electronic and thermal Free Energies= -708.521160

C	1.19617100	0.77865000	-0.03637300
C	1.55095400	-0.58787400	-0.07791700
C	0.64013500	-1.64102900	0.02413300
C	-0.11243200	1.30235400	-0.06019100
C	-0.74238200	-1.68266300	0.09731700
C	-1.36633400	0.73737400	-0.05696500
C	-1.70277000	-0.66311000	0.05134700
H	-1.14583600	-2.68536900	0.17644100

C	-3.57318000	-2.28467400	0.21550800
H	-4.65796800	-2.19554200	0.24360300
H	-3.30172800	-2.90750600	-0.64334800
H	-3.24602900	-2.77784900	1.13658300
H	1.09204900	-2.62639600	0.03539500
H	-0.08060900	2.38533800	-0.08249300
O	-2.47328100	1.48969700	-0.11079600
C	-2.40582600	2.90897000	-0.24200600
H	-3.43977000	3.24034500	-0.30855300
H	-1.93283300	3.35749700	0.63616900
H	-1.87007000	3.18871600	-1.15336100
O	2.09934800	1.75755800	-0.05689300
C	3.38784400	1.68238900	0.57790300
H	4.12276800	1.24251200	-0.09290100
H	3.64230000	2.71875000	0.79453900
H	3.33152300	1.11206800	1.50660500
O	2.86875500	-0.80290500	-0.23219000
C	3.39378700	-2.12227800	-0.30066600
H	2.97091300	-2.67228600	-1.14748900
H	4.46394200	-1.99655400	-0.45240900
H	3.22244500	-2.66753300	0.63324100
N	-3.01194600	-0.95314100	0.10165400
H	-3.64185100	-0.16766500	0.05288200

TI-246

Zero-point correction= 0.266012 (Hartree/Particle)

Thermal correction to Energy= 0.281604

Thermal correction to Enthalpy= 0.282549

Thermal correction to Gibbs Free Energy= 0.223478
 Sum of electronic and zero-point Energies= -708.496698
 Sum of electronic and thermal Energies= -708.481105
 Sum of electronic and thermal Enthalpies= -708.480161
 Sum of electronic and thermal Free Energies= -708.539232

C	1.69628700	-0.69502500	-0.00013400
C	1.71976200	0.67818700	-0.00004000
C	0.61604400	1.55664800	0.00030700
C	0.55749400	-1.56266900	0.00009700
C	-0.75087200	1.26587800	0.00043800
C	-0.77155800	-1.28536500	0.00019000
C	-1.41298500	0.03722700	-0.00012400
H	2.67453000	1.18716800	-0.00016900
H	-1.40518800	2.12522900	0.00082500
C	-3.62095200	1.16042500	-0.00116200
H	-4.65254200	0.81243900	-0.00292900
H	-3.46443100	1.77287500	0.89281200
H	-3.46185100	1.77410500	-0.89382500
H	0.84847300	-2.60608500	0.00016200
O	-1.70280600	-2.25041200	0.00045500
C	-1.33071600	-3.62746700	0.00090900
H	-2.26842400	-4.17867700	0.00124800
H	-0.75818800	-3.87280600	-0.89820900
H	-0.75792700	-3.87213600	0.90004200
O	2.81222600	-1.42498800	-0.00040900
C	4.09075800	-0.79436500	-0.00081000
H	4.22361900	-0.18468800	0.89774800
H	4.81314800	-1.60750100	-0.00112000

H	4.22298900	-0.18455500	-0.89937100
O	1.03254000	2.82229600	0.00053700
C	0.12440400	3.91960600	0.00067200
H	0.75219600	4.80813300	0.00056000
H	-0.49855800	3.91427100	-0.89896200
H	-0.49824800	3.91429600	0.90052100
N	-2.74922900	0.00288200	-0.00079000
H	-3.16667600	-0.91588600	-0.00052700

TI-247

Zero-point correction= 0.266154 (Hartree/Particle)

Thermal correction to Energy= 0.281758

Thermal correction to Enthalpy= 0.282702

Thermal correction to Gibbs Free Energy= 0.222897

Sum of electronic and zero-point Energies= -708.478692

Sum of electronic and thermal Energies= -708.463088

Sum of electronic and thermal Enthalpies= -708.462144

Sum of electronic and thermal Free Energies= -708.521949

C	-2.06061400	-0.37245700	-0.00033800
C	-1.40924900	-1.59281000	-0.00045400
C	-0.03386500	-1.81448500	-0.00022700
C	-1.43982100	0.89644000	-0.00021000
C	1.06997100	-0.97413200	-0.00001000
C	-0.12225700	1.27082200	0.00031900
C	1.08785700	0.45415300	-0.00007900
H	-2.01675000	-2.48902800	-0.00078800
C	3.63364300	0.78302100	-0.00107500
H	4.20099600	1.71344300	-0.00161100

H	3.89319800	0.20996200	0.88785700
H	3.89247600	0.20956600	-0.89004200
H	0.21926000	-2.86808400	-0.00048800
H	-2.16808000	1.69828700	-0.00021800
O	0.21102900	2.57476700	0.00108600
C	-0.77549600	3.60395300	0.00055400
H	-0.21565600	4.53672000	0.00114200
H	-1.39447400	3.54879700	-0.89944800
H	-1.39589700	3.54853100	0.89954300
O	-3.39203800	-0.25613600	-0.00053500
C	-4.21603700	-1.41801400	0.00010000
H	-4.04462900	-2.01831300	0.89893600
H	-5.23824700	-1.04578400	0.00073100
H	-4.04577800	-2.01851700	-0.89881400
O	2.31873300	-1.48365500	-0.00026700
C	2.55013500	-2.88431400	0.00139800
H	2.13971100	-3.35655500	-0.89716800
H	3.63286600	-2.99631600	0.00236900
H	2.13828700	-3.35467600	0.90029300
N	2.22076200	1.16164800	-0.00052100
H	2.04999100	2.15756600	-0.00078200

TI-345

Zero-point correction=	0.264885 (Hartree/Particle)
Thermal correction to Energy=	0.281000
Thermal correction to Enthalpy=	0.281944
Thermal correction to Gibbs Free Energy=	0.221197
Sum of electronic and zero-point Energies=	-708.466709

Sum of electronic and thermal Energies= -708.450594
Sum of electronic and thermal Enthalpies= -708.449650
Sum of electronic and thermal Free Energies= -708.510397

C	0.16802700	0.11153800	1.66366400
C	0.80273000	-0.64087300	0.67438400
C	1.16473500	-0.21514400	-0.63689800
C	-0.09868800	1.51965500	1.61215900
C	0.95065700	0.95855200	-1.28538600
C	-0.06462000	2.37310200	0.50916900
C	0.32120700	2.15550900	-0.81740700
H	1.31041100	0.99362700	-2.31079900
C	-0.44008200	4.43176100	-1.46476400
H	-0.51191900	4.97177700	-2.40753500
H	-1.44879000	4.31605600	-1.05705100
H	0.16393000	5.02590800	-0.77080600
H	1.67937900	-0.96168000	-1.22997800
H	-0.40445000	3.36954600	0.76575200
O	-0.54312200	2.15356500	2.69244900
C	-0.15222500	1.84668400	4.04346300
H	-0.17780000	2.80694100	4.55674400
H	-0.85937900	1.15439100	4.49596900
H	0.85360300	1.42767700	4.07819500
O	-0.16577000	-0.48382200	2.82280100
C	-1.10545500	-1.56939600	2.79715400
H	-0.59142700	-2.52087800	2.66626800
H	-1.60823800	-1.54383500	3.76343000
H	-1.83870400	-1.42399800	1.99892900
O	1.05344300	-1.89518400	1.06335300

C	1.65518000	-2.85420900	0.19768500
H	2.67352500	-2.55954800	-0.07236200
H	1.69323400	-3.77354800	0.77844900
H	1.05043800	-3.01810000	-0.69926300
N	0.16553000	3.13872200	-1.72383100
H	0.51097200	2.97246800	-2.65553300

TI-346

Zero-point correction= 0.265930 (Hartree/Particle)

Thermal correction to Energy= 0.281648

Thermal correction to Enthalpy= 0.282592

Thermal correction to Gibbs Free Energy= 0.223200

Sum of electronic and zero-point Energies= -708.481662

Sum of electronic and thermal Energies= -708.465945

Sum of electronic and thermal Enthalpies= -708.465001

Sum of electronic and thermal Free Energies= -708.524392

C	-0.18894700	0.11420800	1.71377600
C	0.44252100	-0.67717000	0.80129100
C	1.01590300	-0.35822800	-0.46813400
C	-0.33527700	1.56946700	1.64004600
C	0.95335300	0.82528800	-1.17052500
C	-0.12002900	2.35454000	0.53938700
C	0.37108700	2.04814100	-0.76201400
H	0.52783300	-1.73327600	1.02539400
H	1.38613800	0.82898300	-2.16386500
C	-0.19336300	4.37103900	-1.49297300
H	-0.13900100	4.88851900	-2.44952600
H	-1.24159500	4.32923600	-1.18497500

H	0.38059600	4.94620600	-0.75989300
H	-0.36062800	3.39332100	0.72995600
O	-0.82644000	2.23631700	2.68163600
C	-0.45447700	1.96563300	4.04518500
H	-0.42550700	2.94213600	4.52674400
H	-1.20160400	1.33176100	4.51876300
H	0.52958100	1.49753700	4.10311000
O	-0.75864200	-0.37594400	2.81453000
C	-0.76729800	-1.77946600	3.06007300
H	0.25065000	-2.16213100	3.18244500
H	-1.31877000	-1.90592400	3.98909800
H	-1.27814200	-2.30958500	2.25064300
O	1.61376500	-1.44158600	-0.96860400
C	2.24332900	-1.41162900	-2.24554100
H	2.66999700	-2.40323800	-2.37946200
H	1.51132500	-1.21901300	-3.03609500
H	3.04148300	-0.66359300	-2.27096900
N	0.35329200	3.03571300	-1.67282100
H	0.75292200	2.83208600	-2.57552000

TI-347

Zero-point correction= 0.265776 (Hartree/Particle)

Thermal correction to Energy= 0.281450

Thermal correction to Enthalpy= 0.282394

Thermal correction to Gibbs Free Energy= 0.223147

Sum of electronic and zero-point Energies= -708.481110

Sum of electronic and thermal Energies= -708.465437

Sum of electronic and thermal Enthalpies= -708.464492

Sum of electronic and thermal Free Energies= -708.523739

C	-0.31304700	0.13594900	1.78222300
C	0.44789800	-0.47254000	0.81396100
C	0.98655400	0.02284800	-0.39221400
C	-0.66209700	1.53697900	1.79693800
C	0.85014300	1.23743500	-1.00877100
C	-0.48695200	2.44744800	0.76910700
C	0.10473500	2.37123400	-0.50476700
H	0.66421100	-1.52132400	0.97815200
C	-0.62914800	4.68290800	-1.03692800
H	-0.54195700	5.32070300	-1.91495300
H	-1.69125800	4.51589100	-0.83534700
H	-0.17632600	5.20259200	-0.18646800
H	1.57422200	-0.71096700	-0.93128600
H	-0.89660900	3.41518000	1.03364200
O	-1.30658200	2.06636200	2.83338100
C	-1.03996100	1.73000800	4.20704000
H	-1.23364100	2.65050300	4.75588000
H	-1.70921600	0.94002500	4.54133500
H	-0.00003800	1.42961300	4.34400900
O	-0.82294900	-0.52809800	2.82772200
C	-0.60627800	-1.92660800	2.97021300
H	0.45776400	-2.14860700	3.10064200
H	-1.14922300	-2.21282900	3.86864500
H	-1.00727500	-2.47343600	2.11099900
O	1.40161100	1.51911500	-2.20268300
C	2.18807200	0.55096800	-2.89008700
H	1.59113400	-0.33241000	-3.13665600

H	2.51248000	1.03840600	-3.80693200
H	3.06313100	0.26843600	-2.29691400
N	0.05197100	3.43246100	-1.31545100
H	0.54580500	3.33716500	-2.19065800

TI-2345

Zero-point correction= 0.298374 (Hartree/Particle)

Thermal correction to Energy= 0.316962

Thermal correction to Enthalpy= 0.317906

Thermal correction to Gibbs Free Energy= 0.251732

Sum of electronic and zero-point Energies= -822.921047

Sum of electronic and thermal Energies= -822.902459

Sum of electronic and thermal Enthalpies= -822.901515

Sum of electronic and thermal Free Energies= -822.967689

C	-1.25584700	-0.25494500	0.09363100
C	-1.48575900	1.12591900	0.06599000
C	-0.49284900	2.12765500	0.11816000
C	-0.01408100	-0.94726800	0.14313400
C	0.87236100	2.03104700	0.11742600
C	1.29293800	-0.45807600	0.01689500
C	1.72744400	0.90310600	0.03765100
H	1.38454800	2.98550900	0.15536800
C	3.74335000	2.36477800	0.06466300
H	4.81361200	2.17579500	-0.00204500
H	3.46220300	3.01357600	-0.77091300
H	3.54633500	2.88387300	1.00852900
H	-0.86269700	3.14577300	0.15175800
O	2.33098900	-1.31721900	-0.00334100

C	2.36087600	-2.43010300	-0.91639100
H	3.41272500	-2.57582300	-1.16021300
H	1.95266800	-3.32119200	-0.44500100
H	1.79788000	-2.19723700	-1.82300300
O	-0.07532500	-2.28820300	0.23023900
C	-0.75013300	-2.89214600	1.35098400
H	-1.72324600	-3.27177200	1.04226700
H	-0.10797900	-3.71019900	1.67784300
H	-0.87602200	-2.17305500	2.16226500
O	-2.36156700	-1.02711800	0.13691200
C	-2.76849800	-1.59043500	-1.11761300
H	-2.00944400	-2.28322600	-1.49360000
H	-3.69404600	-2.12654400	-0.91535700
H	-2.95707800	-0.79777800	-1.84678600
O	-2.78272000	1.43423400	-0.00927400
C	-3.22112800	2.78819600	-0.04269500
H	-2.81504000	3.31706300	-0.91087800
H	-4.30414100	2.73149900	-0.12958500
H	-2.96096300	3.31263000	0.88202500
N	3.05638400	1.08993300	0.00072000
H	3.60295000	0.24165900	-0.01500000

TI-2346

Zero-point correction= 0.298733 (Hartree/Particle)

Thermal correction to Energy= 0.317001

Thermal correction to Enthalpy= 0.317945

Thermal correction to Gibbs Free Energy= 0.252836

Sum of electronic and zero-point Energies= -822.939995

Sum of electronic and thermal Energies= -822.921727
Sum of electronic and thermal Enthalpies= -822.920783
Sum of electronic and thermal Free Energies= -822.985892

C	-0.95334900	1.31893600	-0.11310000
C	0.29169800	1.88926400	-0.11362100
C	1.56011500	1.26679700	-0.03782500
C	-1.29005200	-0.09732400	-0.05693800
C	1.86837500	-0.08434200	0.05007000
C	-0.44725400	-1.17796200	-0.03852500
C	1.01240000	-1.19310000	0.05255600
H	0.36095600	2.96789200	-0.16630400
H	2.91950900	-0.32454000	0.11087300
C	2.94425700	-2.73394000	0.26462000
H	3.04870100	-3.81485400	0.34246900
H	3.50265300	-2.39650100	-0.61482200
H	3.37703500	-2.28163500	1.16291700
O	-0.95477800	-2.42983500	-0.01340300
C	-1.94508900	-2.84255700	-0.97585600
H	-1.73965600	-3.89505100	-1.16960500
H	-2.94641300	-2.72194600	-0.56750400
H	-1.84973600	-2.26515000	-1.89714700
O	-2.61411000	-0.36638700	-0.08470900
C	-3.25658400	-0.37545500	1.19731800
H	-3.15950700	0.59826600	1.68427900
H	-4.30755700	-0.58151600	1.00188300
H	-2.83246600	-1.16149000	1.83012300
O	-2.06367200	2.04923400	-0.15770500
C	-1.99519300	3.47068600	-0.22445200

H	-3.02986700	3.80452400	-0.26043600
H	-1.50472900	3.88136300	0.66339400
H	-1.47375400	3.79301200	-1.13052300
O	2.52331800	2.18873000	-0.05053700
C	3.90080900	1.83499800	0.02522400
H	4.43923200	2.77959600	-0.00826300
H	4.12168700	1.32185000	0.96617500
H	4.19522100	1.21630800	-0.82805100
N	1.53564800	-2.41965400	0.14372900
H	0.86229900	-3.17249600	0.14845200

TI-2347

Zero-point correction= 0.299342 (Hartree/Particle)

Thermal correction to Energy= 0.317378

Thermal correction to Enthalpy= 0.318322

Thermal correction to Gibbs Free Energy= 0.253820

Sum of electronic and zero-point Energies= -822.922380

Sum of electronic and thermal Energies= -822.904344

Sum of electronic and thermal Enthalpies= -822.903399

Sum of electronic and thermal Free Energies= -822.967901

C	0.19839700	-0.01354200	1.74585800
C	0.84394600	-0.67144700	0.72638900
C	0.97224400	-0.31066300	-0.62233000
C	-0.59824600	1.17623300	1.60835500
C	0.63069800	0.84238200	-1.28170500
C	-0.59559700	2.10463500	0.56418800
C	0.04317900	2.03995700	-0.71991700
H	1.32887800	-1.60516800	0.98244700

C	-0.29870600	4.48877400	-1.33692100
H	0.06779800	5.03162600	-2.20822900
H	-1.37057900	4.65260900	-1.23669500
H	0.21391500	4.87618800	-0.45461300
H	1.47564100	-1.05801700	-1.22374800
O	-1.38790900	3.18803500	0.69406100
C	-1.22811000	4.08205700	1.80564900
H	-1.34815500	5.08839900	1.40035000
H	-1.99082800	3.88844100	2.55754200
H	-0.23631900	3.98017000	2.25284900
O	-1.37261000	1.53891400	2.63540600
C	-2.26013900	0.59573300	3.25870600
H	-1.81157900	0.20020300	4.16809200
H	-3.16346200	1.15887100	3.49172700
H	-2.50539400	-0.21906600	2.57383100
O	0.20120300	-0.45959700	3.00952700
C	0.89996300	-1.65058100	3.34957600
H	0.75702600	-1.77298000	4.42122200
H	0.48364900	-2.51707700	2.82561600
H	1.96849000	-1.55289100	3.13362200
O	0.90174700	1.01727600	-2.59281300
C	1.51586100	-0.01007900	-3.36260200
H	0.89851000	-0.91339800	-3.37265800
H	1.59009300	0.39119700	-4.37119700
H	2.51811000	-0.23494500	-2.98499000
N	0.01711600	3.08209500	-1.55654200
H	0.38614000	2.85849600	-2.46989100

TI-2356

Zero-point correction= 0.298811 (Hartree/Particle)

Thermal correction to Energy= 0.317105

Thermal correction to Enthalpy= 0.318049

Thermal correction to Gibbs Free Energy= 0.252717

Sum of electronic and zero-point Energies= -822.933225

Sum of electronic and thermal Energies= -822.914931

Sum of electronic and thermal Enthalpies= -822.913987

Sum of electronic and thermal Free Energies= -822.979320

C	0.08050000	-1.68849500	-0.01942400
C	1.33131800	-1.14204100	0.06887600
C	1.64171400	0.27204900	0.17275900
C	-1.21345100	-1.10880100	-0.07259800
C	0.76737200	1.31672300	0.01244300
C	-1.54029700	0.24278500	-0.14506000
C	-0.63944600	1.34681100	-0.19235100
H	0.12067100	-2.76983500	-0.05642800
H	1.21369600	2.29839500	0.08742000
C	-0.55274300	3.81825600	-0.50549300
H	-1.30033700	4.57140800	-0.74923900
H	-0.07551800	4.10801400	0.43682900
H	0.19680000	3.81088200	-1.30351200
O	-2.84660100	0.59396500	-0.29043100
C	-3.68536000	0.44320400	0.86768900
H	-3.23544700	0.94254300	1.73154400
H	-4.62941300	0.92224000	0.61296100
H	-3.85225400	-0.61193900	1.08523500
O	-2.28986400	-1.89838500	-0.11084800

C	-2.19058100	-3.31953700	-0.05150100
H	-1.70165300	-3.64640900	0.87063400
H	-3.21948400	-3.67325900	-0.06206000
H	-1.66603100	-3.71490900	-0.92590900
O	2.31943500	-2.04071600	0.16679000
C	3.50087600	-1.94628500	-0.64650400
H	4.30654300	-1.46497200	-0.09445900
H	3.76901100	-2.97535100	-0.88334300
H	3.29923600	-1.40030900	-1.57130300
O	2.93141400	0.46685500	0.44497300
C	3.46294500	1.77847500	0.59701000
H	4.51755100	1.63613200	0.82240700
H	3.36060600	2.35113200	-0.33031300
H	2.97769900	2.30146600	1.42687100
N	-1.22189100	2.53857300	-0.39347600
H	-2.22059000	2.49214800	-0.54194500

TI-2357

Zero-point correction= 0.299022 (Hartree/Particle)

Thermal correction to Energy= 0.317235

Thermal correction to Enthalpy= 0.318179

Thermal correction to Gibbs Free Energy= 0.253245

Sum of electronic and zero-point Energies= -822.933099

Sum of electronic and thermal Energies= -822.914887

Sum of electronic and thermal Enthalpies= -822.913943

Sum of electronic and thermal Free Energies= -822.978877

C	0.72263500	1.81324700	-0.10152000
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C	-0.66111900	1.87412300	-0.07109500
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C	-1.56920600	0.80176900	0.08226100
C	1.54888400	0.69013000	-0.06986500
C	-1.34165700	-0.55180800	0.08459600
C	1.17830100	-0.67831100	-0.10974100
C	-0.10004600	-1.26385600	-0.19436100
H	1.19356300	2.78538600	-0.16064100
C	-1.20224600	-3.47405800	-0.83301600
H	-0.74196600	-4.35166100	-1.28676400
H	-1.80264800	-3.79108400	0.01988900
H	-1.85206400	-3.00512800	-1.57355200
H	-2.59716300	1.09005100	0.24593200
O	2.19745100	-1.57622200	-0.23262700
C	2.88770400	-1.90159400	0.98570800
H	2.18683800	-2.30240200	1.72530200
H	3.61982400	-2.66128400	0.71701500
H	3.39681200	-1.02252600	1.38378900
O	2.87451600	0.82838900	-0.05951100
C	3.48809200	2.11468600	-0.07648200
H	3.19962200	2.70133300	0.80069100
H	4.55762000	1.91765100	-0.04826100
H	3.24202700	2.65334800	-0.99599200
O	-1.11275300	3.13031500	-0.13978400
C	-2.50369600	3.43020100	-0.16731000
H	-2.98350200	3.17311100	0.78242100
H	-2.56123800	4.50673400	-0.31418900
H	-3.00176900	2.92393900	-0.99995800
O	-2.32158100	-1.41228800	0.36467600
C	-3.62842400	-0.96758000	0.71106800

H	-4.09898800	-0.44458500	-0.12738700
H	-4.18787500	-1.87372700	0.93383900
H	-3.60049400	-0.32595500	1.59715900
N	-0.11514900	-2.58786200	-0.43177400
H	0.82105900	-2.94141800	-0.58037600

TI-2367

Zero-point correction= 0.298593 (Hartree/Particle)

Thermal correction to Energy= 0.317273

Thermal correction to Enthalpy= 0.318217

Thermal correction to Gibbs Free Energy= 0.250585

Sum of electronic and zero-point Energies= -822.920479

Sum of electronic and thermal Energies= -822.901799

Sum of electronic and thermal Enthalpies= -822.900854

Sum of electronic and thermal Free Energies= -822.968487

C	-0.59234500	-0.26794500	1.20804800
C	0.24934200	-0.75004100	0.24747600
C	0.86806100	-0.08525500	-0.83430600
C	-1.11953600	1.03112500	1.38469200
C	0.69913100	1.24897900	-1.21802000
C	-0.95022000	2.12377300	0.53685500
C	-0.26333500	2.19453700	-0.72993600
H	-0.91000200	-1.00201100	1.93788100
H	0.48393200	-1.80286500	0.34387100
C	-0.19839700	3.68935100	-2.78765700
H	-0.89917900	4.47936500	-3.05903900
H	0.82010300	4.06116000	-2.90619100
H	-0.34581600	2.84373100	-3.45772700

O	-1.59958200	3.27382500	0.83150300
C	-1.29965900	3.95930700	2.06222500
H	-1.44992900	5.01828000	1.85552500
H	-1.97361100	3.62884200	2.85004000
H	-0.26119000	3.78277500	2.35362400
O	-1.92133400	1.30484000	2.42422400
C	-2.23880800	0.31905700	3.40113100
H	-1.33933600	-0.04703200	3.90559700
H	-2.87447100	0.82945600	4.12191000
H	-2.79516200	-0.51276200	2.95878300
O	1.72753600	-0.73686400	-1.63018800
C	2.09649800	-2.08913800	-1.38252000
H	1.23813600	-2.76035900	-1.48168700
H	2.82605000	-2.32972800	-2.15319000
H	2.55906500	-2.20260600	-0.39710600
O	1.44963400	1.72202700	-2.23046100
C	2.87940600	1.69192600	-2.11467200
H	3.28278500	0.80833300	-2.60714400
H	3.23574100	2.59596500	-2.60918500
H	3.18205100	1.70558000	-1.06390500
N	-0.48904600	3.32804300	-1.40406100
H	-1.10843400	3.95112700	-0.90364400

TI-2456

Zero-point correction= 0.298659 (Hartree/Particle)

Thermal correction to Energy= 0.317030

Thermal correction to Enthalpy= 0.317975

Thermal correction to Gibbs Free Energy= 0.252382

Sum of electronic and zero-point Energies=	-822.937802
Sum of electronic and thermal Energies=	-822.919430
Sum of electronic and thermal Enthalpies=	-822.918486
Sum of electronic and thermal Free Energies=	-822.984078
C	-0.96055700 -1.23871600 -0.08542000
C	-1.44477700 0.06070100 -0.08579700
C	-0.64938600 1.24773700 -0.12056200
C	0.39793200 -1.66976900 0.01567800
C	0.73912000 1.38975700 -0.11388400
C	1.57655300 -0.99415700 0.06364400
C	1.76667600 0.44918900 -0.02829000
H	1.08407000 2.41201900 -0.16346500
C	3.49386400 2.22600200 -0.09696500
H	4.58234400 2.23193000 -0.07350100
H	3.16707500 2.69765600 -1.02955600
H	3.12842000 2.81308400 0.75237100
H	0.45337000 -2.75091900 0.05501100
O	2.75977400 -1.61943400 0.17214700
C	2.82852200 -3.03947700 0.27825400
H	3.88680000 -3.26994900 0.37877600
H	2.28946300 -3.38814400 1.16382900
H	2.43112400 -3.51414400 -0.62355300
O	-1.76191100 -2.30706300 -0.11457300
C	-3.03387100 -2.33764000 -0.78208100
H	-3.01207900 -1.73892200 -1.69302800
H	-3.18598300 -3.38876600 -1.02348900
H	-3.83024800 -1.98729700 -0.12681700
O	-2.78923800 0.24629200 -0.09990100

C	-3.37460000	0.45313200	1.18912700
H	-4.44159900	0.58763200	1.01679500
H	-3.20869600	-0.41826000	1.83229100
H	-2.96622600	1.34997000	1.66307400
O	-1.42654100	2.32694800	-0.15309600
C	-0.89205900	3.64482600	-0.20619800
H	-1.75960000	4.30104500	-0.22662800
H	-0.29015000	3.86402100	0.68132700
H	-0.30397000	3.79344300	-1.11677100
N	3.04304700	0.85176200	-0.01802300
H	3.73338100	0.11981900	0.05784600

TI-2457

Zero-point correction= 0.298737 (Hartree/Particle)

Thermal correction to Energy= 0.317098

Thermal correction to Enthalpy= 0.318042

Thermal correction to Gibbs Free Energy= 0.251985

Sum of electronic and zero-point Energies= -822.928952

Sum of electronic and thermal Energies= -822.910591

Sum of electronic and thermal Enthalpies= -822.909647

Sum of electronic and thermal Free Energies= -822.975704

C	-0.35272200	0.00776500	1.70505000
C	0.50818100	-0.59906600	0.76906400
C	0.86470400	-0.05879400	-0.46773800
C	-0.83581600	1.31338200	1.62416100
C	0.64206000	1.17022800	-1.07608800
C	-0.65207200	2.34557000	0.72124500
C	0.05783400	2.35223700	-0.52525000

C	0.84488000	3.99521200	-2.32053100
H	0.72428500	5.07778100	-2.36082200
H	1.90560700	3.76907300	-2.20620300
H	0.48377400	3.56581300	-3.25451500
H	1.44117500	-0.73596000	-1.08182600
H	-1.45129900	1.54686000	2.48470400
O	-1.20459700	3.55315200	0.95280900
C	-1.95818700	3.82314200	2.13102500
H	-2.24383600	4.87001000	2.05214800
H	-2.85818400	3.20248300	2.17054500
H	-1.35062200	3.67593700	3.02853400
O	-0.71755800	-0.61728500	2.83503300
C	-1.18328200	-1.97489400	2.81727200
H	-0.35928400	-2.67004200	2.97067500
H	-1.89383900	-2.04342900	3.64011900
H	-1.69125000	-2.19919600	1.87574900
O	0.95715300	-1.80245700	1.15593800
C	1.83719400	-2.56012800	0.33855400
H	2.76638900	-2.01440500	0.14424100
H	2.06182200	-3.45796400	0.91093500
H	1.35813400	-2.84622400	-0.60403200
O	1.04091400	1.36865500	-2.34402900
C	1.62148800	0.33309000	-3.12215100
H	0.94535300	-0.52409500	-3.20597700
H	1.77591800	0.76933500	-4.10721700
H	2.58766200	0.01956600	-2.71274000
N	0.07149600	3.53076900	-1.17321800
H	-0.44204500	4.24653700	-0.68136000

TI-3456

Zero-point correction= 0.297552 (Hartree/Particle)

Thermal correction to Energy= 0.316412

Thermal correction to Enthalpy= 0.317356

Thermal correction to Gibbs Free Energy= 0.249976

Sum of electronic and zero-point Energies= -822.925818

Sum of electronic and thermal Energies= -822.906958

Sum of electronic and thermal Enthalpies= -822.906014

Sum of electronic and thermal Free Energies= -822.973393

C	-0.21217400	0.04482700	1.59127600
C	0.27578300	-0.60696700	0.48099500
C	0.57829800	-0.05368500	-0.82568600
C	-0.34230800	1.48384100	1.77447700
C	0.34623300	1.22109800	-1.29764900
C	-0.33620500	2.44658000	0.79968300
C	-0.12778300	2.35536300	-0.60125300
H	0.57543700	1.38257200	-2.34069200
C	-0.12177000	3.67127100	-2.71963800
H	-0.39174100	4.69454800	-2.97600800
H	0.92719800	3.51743900	-2.99374900
H	-0.75377600	2.99417400	-3.30269800
H	-0.53974600	3.43860400	1.19255000
O	-0.62151000	1.96310100	2.98649400
C	0.00270900	1.47256100	4.18510000
H	0.15622900	2.35554400	4.80455600
H	-0.65247400	0.76452100	4.68876000
H	0.96381400	1.00250800	3.96913200

O	-0.56341300	-0.64889300	2.68347900
C	-1.41679400	-1.80095300	2.56921000
H	-0.83052000	-2.71607700	2.49488000
H	-2.01126000	-1.80527200	3.48217100
H	-2.06811400	-1.71085000	1.69771200
O	0.43714800	-1.94759900	0.56536800
C	1.63495600	-2.36967600	1.22887700
H	1.63851800	-2.03890400	2.27280700
H	1.63191100	-3.45761800	1.18491800
H	2.51595200	-1.98430800	0.70832400
O	1.10566600	-0.99163100	-1.60386200
C	1.46708400	-0.71510800	-2.95252200
H	2.22402700	0.07386000	-3.00203800
H	1.88258100	-1.64541900	-3.33345100
H	0.58770200	-0.44009500	-3.54327200
N	-0.32750400	3.49079400	-1.29464100
H	-0.64497200	4.29416000	-0.77553400

TI-23456

Zero-point correction= 0.330394 (Hartree/Particle)

Thermal correction to Energy= 0.351732

Thermal correction to Enthalpy= 0.352676

Thermal correction to Gibbs Free Energy= 0.280586

Sum of electronic and zero-point Energies= -937.383125

Sum of electronic and thermal Energies= -937.361787

Sum of electronic and thermal Enthalpies= -937.360843

Sum of electronic and thermal Free Energies= -937.432932

C	-0.34721000	-1.29691500	-0.02576100
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C	-1.49301600	-0.54224600	-0.13550900
C	-1.58784600	0.89447800	-0.09944500
C	1.03124400	-0.87661400	0.03475600
C	-0.56100500	1.81617500	0.00265800
C	1.56037500	0.39342100	0.02459400
C	0.83534100	1.64759100	0.05417300
H	-0.87713500	2.84894600	0.02655200
C	1.16333400	4.10746100	0.19678500
H	2.03940800	4.75081700	0.26121300
H	0.60245100	4.38359800	-0.70231100
H	0.54183500	4.28507700	1.08067400
O	2.89805700	0.58018600	0.08364700
C	3.76927800	-0.08308200	-0.85241700
H	4.58309900	0.61717500	-1.03955600
H	4.15531900	-1.00662600	-0.42533300
H	3.24093100	-0.29851400	-1.78322200
O	1.92692200	-1.89186100	0.05307500
C	2.19645900	-2.43979700	1.35309400
H	1.28902900	-2.87408800	1.77825300
H	2.94093300	-3.21893300	1.19728800
H	2.60064700	-1.66588300	2.01282600
O	-0.52554000	-2.63251800	0.07131500
C	-0.51327500	-3.34824500	-1.17367300
H	0.45623600	-3.23374400	-1.66580100
H	-0.67560500	-4.39361200	-0.91761000
H	-1.32261500	-2.99344200	-1.81660800
O	-2.65007500	-1.20669100	-0.33083300
C	-3.36494900	-1.57724300	0.85505500

H	-4.25512900	-2.10218000	0.51333000
H	-2.75425200	-2.24185400	1.47185400
H	-3.65810300	-0.68735900	1.41968300
O	-2.85616400	1.28193600	-0.16751200
C	-3.21606000	2.65922900	-0.17803900
H	-4.29984000	2.66947900	-0.27033800
H	-2.92294800	3.14960600	0.75558900
H	-2.77183700	3.17144200	-1.03692600
N	1.61443800	2.73243900	0.13493400
H	2.60489200	2.53931200	0.18075300

TI-23457

Zero-point correction= 0.331742 (Hartree/Particle)

Thermal correction to Energy= 0.352647

Thermal correction to Enthalpy= 0.353591

Thermal correction to Gibbs Free Energy= 0.282476

Sum of electronic and zero-point Energies= -937.375099

Sum of electronic and thermal Energies= -937.354193

Sum of electronic and thermal Enthalpies= -937.353249

Sum of electronic and thermal Free Energies= -937.424365

C	-1.50558300	0.49132500	0.10872700
C	-0.67727200	1.61273100	-0.01219500
C	0.72808400	1.64433200	0.08697600
C	-1.09829100	-0.85107600	0.25959200
C	1.66396300	0.63917300	0.15377000
C	0.18999100	-1.40998100	0.11000700
C	1.45726900	-0.78698500	0.00748300
C	3.90180000	-1.39942800	-0.44526300

H	4.30845600	-2.35660400	-0.77263300
H	4.00858000	-0.68372000	-1.26021400
H	4.47218900	-1.04888600	0.41582600
H	1.14537100	2.63947900	0.13526300
O	0.26977700	-2.76942600	0.15123900
C	-0.22454700	-3.47327000	-1.00120200
H	-0.00196200	-4.52382400	-0.82117700
H	-1.30104900	-3.33646700	-1.10493800
H	0.29223700	-3.13214200	-1.90415000
O	-2.04552700	-1.78270600	0.42364800
C	-3.06096000	-1.63021800	1.43261900
H	-3.99450300	-1.29410300	0.98396700
H	-3.18251200	-2.62109700	1.86944000
H	-2.74518000	-0.92088600	2.19874200
O	-2.84001300	0.72954000	0.11535900
C	-3.47617800	0.59256400	-1.15919500
H	-3.35207700	-0.42389600	-1.54791800
H	-4.53280600	0.79536200	-0.99065100
H	-3.07290600	1.31989800	-1.86979400
O	-1.36736800	2.74121800	-0.19325500
C	-0.71814600	3.99639700	-0.34898000
H	-0.02346900	3.98448300	-1.19515600
H	-1.51689700	4.70822200	-0.54669500
H	-0.19815500	4.29009300	0.56867100
O	2.95684800	0.92295100	0.34349700
C	3.41066900	2.25867500	0.52000900
H	2.93745600	2.72214000	1.39134700
H	4.48221900	2.17542600	0.68950000

H	3.23000600	2.85745300	-0.37862800
N	2.49994200	-1.62797900	-0.11735800
H	2.21087000	-2.59313500	-0.03727600

TI-23567

Zero-point correction= 0.331133 (Hartree/Particle)

Thermal correction to Energy= 0.352296

Thermal correction to Enthalpy= 0.353240

Thermal correction to Gibbs Free Energy= 0.280903

Sum of electronic and zero-point Energies= -937.373279

Sum of electronic and thermal Energies= -937.352116

Sum of electronic and thermal Enthalpies= -937.351172

Sum of electronic and thermal Free Energies= -937.423509

C	-0.95027400	-0.23042300	1.29587800
C	-0.05216400	-0.84104700	0.45552900
C	0.78980800	-0.19618900	-0.52026400
C	-1.29699400	1.12601600	1.44156400
C	0.66636100	1.08739800	-1.02987000
C	-0.87589800	2.21055600	0.66366500
C	-0.06086400	2.21861400	-0.50639200
H	-1.43175400	-0.93463200	1.96189100
C	0.77418200	3.93167100	-2.23524100
H	0.57725400	5.00295200	-2.28108400
H	1.84328100	3.77537500	-2.10347300
H	0.45953000	3.48621200	-3.18085200
O	-1.41635700	3.42588900	0.96590700
C	-0.84042900	4.09659000	2.09926900
H	-1.34170200	5.06130000	2.15919800

H	-1.02252900	3.53075700	3.01406000
H	0.23417800	4.24306800	1.94987200
O	-2.14730300	1.49777500	2.40158200
C	-2.70601100	0.55687200	3.31501000
H	-1.92658400	0.05734700	3.89783100
H	-3.33371400	1.14926000	3.97733900
H	-3.32490900	-0.17839200	2.79284900
O	0.08056200	-2.15263800	0.67953500
C	0.18597000	-3.10684900	-0.38944600
H	1.22970800	-3.34373500	-0.58707200
H	-0.34398100	-3.99043900	-0.03553100
H	-0.28964300	-2.73277700	-1.29875300
O	1.72292100	-1.01677800	-1.03520600
C	3.08879900	-0.57499300	-1.10592100
H	3.68939200	-1.46925100	-0.94491500
H	3.30870400	-0.14160100	-2.08170100
H	3.29423300	0.15895700	-0.32354500
O	1.42108200	1.37383100	-2.12155700
C	1.02384600	0.72006800	-3.33605300
H	1.66798700	1.12791700	-4.11380600
H	1.16440900	-0.36136100	-3.26415200
H	-0.02223200	0.94690500	-3.56251200
N	0.00787200	3.41917500	-1.10515600
H	-0.60657000	4.08421500	-0.65338100

TI-234567

Zero-point correction= 0.362995 (Hartree/Particle)

Thermal correction to Energy= 0.387171

Thermal correction to Enthalpy= 0.388115
 Thermal correction to Gibbs Free Energy= 0.308974
 Sum of electronic and zero-point Energies= -1051.821148
 Sum of electronic and thermal Energies= -1051.796972
 Sum of electronic and thermal Enthalpies= -1051.796028
 Sum of electronic and thermal Free Energies= -1051.875168

C	-0.13766700	-0.29637300	1.37646200
C	0.72571300	-0.74354100	0.39901800
C	1.07799000	-0.08714600	-0.83010600
C	-0.78183800	0.98136100	1.48981400
C	0.77332100	1.20422700	-1.24112300
C	-0.55305700	2.12271500	0.73614900
C	0.19189500	2.27358500	-0.48809500
C	0.97249400	4.12940900	-2.04361100
H	0.98031700	5.20385600	-1.85767000
H	1.99763400	3.76288400	-2.04189500
H	0.53300200	3.94515800	-3.02564300
O	-1.19111800	3.26508100	1.10880400
C	-0.73135800	3.89747400	2.31785100
H	-1.25695600	4.84978200	2.36732300
H	-0.97955800	3.28894100	3.18700700
H	0.34816100	4.07034400	2.26611100
O	-1.59289800	1.17330900	2.54145500
C	-2.69988600	0.28076100	2.76722200
H	-2.45373500	-0.43729500	3.54797100
H	-3.52774900	0.91691900	3.07911700
H	-2.96615400	-0.24828700	1.85033600
O	-0.40610200	-1.17254100	2.37377000

C	0.41360100	-1.02682200	3.54217700
H	0.27619400	-0.03600000	3.98670300
H	0.07778100	-1.79235000	4.23976400
H	1.46334400	-1.19367500	3.28797400
O	1.34070700	-1.92114200	0.62389200
C	0.64251800	-3.09672800	0.19172800
H	1.27721900	-3.93613300	0.47034700
H	-0.32085700	-3.17547200	0.70222300
H	0.50771400	-3.08006300	-0.89296900
O	1.72358300	-0.90819600	-1.66327800
C	2.93164700	-0.50060000	-2.32558200
H	3.56934200	-1.38383900	-2.32913300
H	2.72244900	-0.18037600	-3.34604700
H	3.41909400	0.30858600	-1.77873400
O	1.11248800	1.51905500	-2.52380900
C	0.16269900	1.06954200	-3.49862500
H	0.55431900	1.38598500	-4.46479400
H	0.06843500	-0.02029100	-3.47484400
H	-0.81367900	1.53372700	-3.32508600
N	0.19368300	3.52202500	-0.97152600
H	-0.39541400	4.14176600	-0.43101800

Cartesian Coordination of MeO-TI Free Bases and Their Thermochemical Values (M06-2X/6-31g(d,p))

TI-2

Zero-point correction= 0.185084 (Hartree/Particle)

Thermal correction to Energy= 0.195384

Thermal correction to Enthalpy= 0.196328

Thermal correction to Gibbs Free Energy= 0.149351

Sum of electronic and zero-point Energies= -479.090433

Sum of electronic and thermal Energies= -479.080133

Sum of electronic and thermal Enthalpies= -479.079189

Sum of electronic and thermal Free Energies= -479.126166

C	-0.77292300	0.00532900	1.10980200
C	0.02198900	-0.49614000	0.13411400
C	0.96228800	0.25434900	-0.65293000
C	-0.88437200	1.35602800	1.58658700
C	1.01928800	1.59037900	-0.84422400
C	-0.48855900	2.51215300	0.98595800
C	0.09785400	2.63986300	-0.37818000
H	-1.37613200	-0.71256100	1.66084400
H	0.00451200	-1.56984900	-0.02680300
H	1.82951300	1.96049100	-1.46785100
N	-0.14821100	3.72458400	-1.00890400
C	0.42450700	3.89592700	-2.32994900
H	-0.10714700	4.69963000	-2.84267100
H	1.48015300	4.19358800	-2.26177400
H	0.37333200	2.99011800	-2.94849000
H	1.71993400	-0.33593200	-1.16480100

H	-1.39506200	1.45008800	2.53802700
O	-0.64217200	3.72194600	1.55098400
C	-1.17429600	3.80240500	2.85505400
H	-1.14749100	4.85749300	3.12381400
H	-2.21007700	3.44472700	2.88335600
H	-0.57275400	3.22340000	3.56574600

TI-3

Zero-point correction= 0.184312 (Hartree/Particle)

Thermal correction to Energy= 0.194949

Thermal correction to Enthalpy= 0.195893

Thermal correction to Gibbs Free Energy= 0.147685

Sum of electronic and zero-point Energies= -479.087559

Sum of electronic and thermal Energies= -479.076921

Sum of electronic and thermal Enthalpies= -479.075977

Sum of electronic and thermal Free Energies= -479.124185

C	-0.71390600	0.00643700	1.26781400
C	0.10086300	-0.49521700	0.31770000
C	0.91401500	0.24133800	-0.62484300
C	-0.99253300	1.40017800	1.55533400
C	0.89192800	1.55173100	-0.94376000
C	-0.67510300	2.49927400	0.84161600
C	0.01856600	2.63125900	-0.44395800
H	-1.24099400	-0.69107800	1.91453100
H	0.19027400	-1.57678100	0.26487000
H	1.61668800	1.86931800	-1.68817700
N	-0.11336100	3.77147400	-1.02347800
C	0.55302900	4.00513900	-2.28977600

H	0.18848500	4.94466000	-2.70891300
H	1.64128700	4.10196400	-2.16518900
H	0.37355400	3.21079900	-3.02681900
H	-1.03857700	3.44435300	1.23517500
O	-1.75171800	1.59652900	2.69149200
C	-1.02187400	1.41208900	3.89227000
H	-0.21440900	2.14992500	3.97189100
H	-1.72606100	1.54840200	4.71346300
H	-0.58721200	0.40576300	3.95205100
H	1.64066400	-0.36503500	-1.16154800

TI-4

Zero-point correction= 0.184441 (Hartree/Particle)

Thermal correction to Energy= 0.195102

Thermal correction to Enthalpy= 0.196046

Thermal correction to Gibbs Free Energy= 0.147731

Sum of electronic and zero-point Energies= -479.089575

Sum of electronic and thermal Energies= -479.078915

Sum of electronic and thermal Enthalpies= -479.077971

Sum of electronic and thermal Free Energies= -479.126286

C	-0.58382000	-0.27205600	1.12031500
C	0.18792400	-0.68671900	0.08988200
C	0.55646300	0.06772300	-1.08035900
C	-1.21775300	1.02243200	1.28205900
C	0.44333400	1.38720200	-1.34891500
C	-1.02309200	2.16201300	0.59215200
C	-0.09839000	2.46841800	-0.51051000
H	0.52121100	-1.71858300	0.14012900

H	0.80429500	1.70633600	-2.32210000
N	0.09508100	3.72204600	-0.72212600
C	0.98444300	4.12326100	-1.79468300
H	1.18126100	5.19327500	-1.70705800
H	1.94659800	3.59363100	-1.77772100
H	0.52997500	3.95199000	-2.78096000
H	1.02130600	-0.52982000	-1.86190500
H	-1.95747800	1.05002400	2.07894500
H	-1.59915500	3.03449100	0.88913100
O	-0.88544700	-1.20136300	2.08487700
C	-0.39655000	-0.88311600	3.37895000
H	-0.73385400	-1.67876800	4.04323900
H	0.69891700	-0.84312800	3.37758200
H	-0.78536000	0.07619900	3.73921100

TI-23

Zero-point correction= 0.218141 (Hartree/Particle)

Thermal correction to Energy= 0.230859

Thermal correction to Enthalpy= 0.231803

Thermal correction to Gibbs Free Energy= 0.179775

Sum of electronic and zero-point Energies= -593.526721

Sum of electronic and thermal Energies= -593.514003

Sum of electronic and thermal Enthalpies= -593.513059

Sum of electronic and thermal Free Energies= -593.565087

C	0.60085400	0.04424800	1.81597000
C	1.07066000	-0.73310500	0.81732100
C	0.75817300	-0.62261300	-0.58965200
C	-0.34275600	1.13663000	1.72040400

C	0.25818500	0.44403900	-1.24306600
C	-0.63350500	1.90708300	0.64137700
C	-0.01307300	1.79175800	-0.70966900
H	0.86933700	-0.19946700	2.84060500
H	1.71336800	-1.56286900	1.09837100
H	0.12980100	0.37952300	-2.32020700
N	0.19881400	2.76399000	-1.51110400
C	0.03240800	4.13788100	-1.08058400
H	0.65751900	4.76955500	-1.71591100
H	-1.00804200	4.45765800	-1.20228500
H	0.31703500	4.30829400	-0.03366900
H	0.99486800	-1.49736900	-1.19031800
O	-1.61702800	2.85237100	0.69400100
C	-1.60411900	3.80485300	1.75330800
H	-1.95935800	4.74429400	1.32336100
H	-2.26288100	3.49855300	2.56916000
H	-0.59360600	3.93770300	2.14938800
O	-1.00881200	1.39189200	2.90441400
C	-2.30174400	0.79909000	2.92957300
H	-2.93969900	1.22585700	2.14669500
H	-2.23348400	-0.28596400	2.78925200
H	-2.72605800	1.01310300	3.91180600

TI-24

Zero-point correction= 0.218358 (Hartree/Particle)

Thermal correction to Energy= 0.231081

Thermal correction to Enthalpy= 0.232025

Thermal correction to Gibbs Free Energy= 0.179625

Sum of electronic and zero-point Energies=	-593.539678
Sum of electronic and thermal Energies=	-593.526955
Sum of electronic and thermal Enthalpies=	-593.526011
Sum of electronic and thermal Free Energies=	-593.578411
C	-0.29727900 0.06706900 1.60866000
C	0.02961600 -0.79515100 0.61089100
C	0.02620500 -0.49764100 -0.79929200
C	-0.78206500 1.42345700 1.46806300
C	0.07015400 0.69574500 -1.42642100
C	-0.62522400 2.26339900 0.42032400
C	0.20570000 2.01778100 -0.80000100
H	0.27538000 -1.81723400 0.87158900
H	0.12100000 0.71517900 -2.51095600
N	0.92594300 2.88912800 -1.39143700
C	1.14477100 4.20341000 -0.81821900
H	2.12721900 4.55291000 -1.14462900
H	0.39639700 4.90803400 -1.19562200
H	1.10284500 4.22838400 0.27716200
H	0.03729600 -1.37463600 -1.44274900
H	-1.33290100 1.76225400 2.33833200
O	-1.23163600 3.47154900 0.34517900
C	-2.12257000 3.84215100 1.37654800
H	-2.54810600 4.79900300 1.07668000
H	-2.91966900 3.09887200 1.49083600
H	-1.59756900 3.95738700 2.33185800
O	-0.31785600 -0.28342900 2.92563700
C	0.04012100 -1.60259200 3.27020900
H	1.06557400 -1.83086400 2.95677200

H	-0.03063900	-1.66170400	4.35587500
H	-0.64371600	-2.33133800	2.81867700

TI-25

Zero-point correction= 0.218075 (Hartree/Particle)

Thermal correction to Energy= 0.230916

Thermal correction to Enthalpy= 0.231860

Thermal correction to Gibbs Free Energy= 0.179076

Sum of electronic and zero-point Energies= -593.537972

Sum of electronic and thermal Energies= -593.525132

Sum of electronic and thermal Enthalpies= -593.524188

Sum of electronic and thermal Free Energies= -593.576971

C	-0.21340200	-0.06498600	1.36841800
C	0.18691100	-0.83881900	0.32870000
C	0.20748100	-0.45442500	-1.06916800
C	-0.73207700	1.28038400	1.30639600
C	0.21092200	0.78301100	-1.59368700
C	-0.59354000	2.20900300	0.33130200
C	0.25427900	2.07523600	-0.88783500
H	-0.23540800	-0.50905700	2.35659200
H	0.28508100	0.88054300	-2.67329100
N	0.93393700	3.00447100	-1.43918000
C	1.09169000	4.29991600	-0.80603000
H	2.04381600	4.72171600	-1.13692900
H	0.29310500	4.97669800	-1.12720400
H	1.07581800	4.26443200	0.28954300
H	0.27957300	-1.29906800	-1.74907300
H	-1.31099900	1.56468500	2.17922000

O	-1.23037900	3.41208100	0.33914400
C	-2.12531900	3.68781200	1.39197700
H	-2.56760900	4.65810400	1.16796700
H	-2.91273200	2.92667000	1.45048600
H	-1.60444300	3.73926700	2.35599200
O	0.57910500	-2.13864000	0.46095900
C	0.57458800	-2.70398000	1.75054900
H	-0.43527800	-2.70982700	2.17955700
H	0.92722600	-3.72841100	1.63520800
H	1.24619900	-2.15975700	2.42584800

TI-26

Zero-point correction= 0.217336 (Hartree/Particle)

Thermal correction to Energy= 0.230505

Thermal correction to Enthalpy= 0.231450

Thermal correction to Gibbs Free Energy= 0.177002

Sum of electronic and zero-point Energies= -593.534008

Sum of electronic and thermal Energies= -593.520839

Sum of electronic and thermal Enthalpies= -593.519894

Sum of electronic and thermal Free Energies= -593.574342

C	0.68297200	0.37346800	1.55659700
C	1.21328200	-0.35942000	0.55058200
C	1.00776100	-0.15456700	-0.86837300
C	-0.22495600	1.48766500	1.47355900
C	0.63285900	0.99674200	-1.47238700
C	-0.40159200	2.30619500	0.40722000
C	0.43495800	2.30152700	-0.83542000
H	0.91215500	0.04377800	2.56700400

H	1.83175400	-1.20673500	0.82803000
H	0.59475600	0.99081000	-2.55732000
N	0.85961900	3.34267100	-1.43788600
C	0.68664200	4.66240700	-0.86114000
H	1.51021400	5.29178200	-1.20687900
H	-0.24886400	5.10956800	-1.21327300
H	0.66828100	4.67306000	0.23572900
H	-0.81138000	1.67451100	2.36677000
O	-1.35748200	3.26028800	0.34077700
C	-2.27890400	3.36044400	1.40673200
H	-3.00168900	4.11968300	1.11061000
H	-2.78878100	2.40485800	1.57378100
H	-1.78044400	3.67087900	2.33251300
O	1.29927300	-1.18817400	-1.71896100
C	1.19773400	-2.51171200	-1.23368000
H	0.30340100	-2.64785900	-0.61527200
H	1.12983500	-3.15223600	-2.11391900
H	2.08181200	-2.80666100	-0.65666600

TI-27

Zero-point correction= 0.218250 (Hartree/Particle)

Thermal correction to Energy= 0.231057

Thermal correction to Enthalpy= 0.232001

Thermal correction to Gibbs Free Energy= 0.179445

Sum of electronic and zero-point Energies= -593.536084

Sum of electronic and thermal Energies= -593.523277

Sum of electronic and thermal Enthalpies= -593.522332

Sum of electronic and thermal Free Energies= -593.574888

C	0.23274800	0.25653900	1.72503800
C	0.79597400	-0.53182300	0.77933800
C	0.74864800	-0.37998900	-0.65346700
C	-0.57668400	1.42997500	1.50952700
C	0.53846900	0.76932200	-1.34303200
C	-0.56642700	2.21512300	0.40730200
C	0.41573100	2.11018400	-0.71089300
H	0.32501900	-0.06504900	2.75869400
H	1.30059600	-1.42938700	1.12784400
N	1.07234800	3.07332100	-1.21674300
C	0.99373500	4.39421300	-0.62174800
H	1.94462100	4.90205800	-0.79713300
H	0.20502700	4.97145700	-1.11422400
H	0.78082700	4.38447700	0.45434700
H	0.95630300	-1.28065200	-1.22092600
H	-1.25467300	1.68842900	2.31679500
O	-1.42248500	3.24664300	0.18434200
C	-2.42155900	3.49058200	1.14983900
H	-3.02881400	4.30649800	0.75935100
H	-3.04653400	2.60278700	1.30278300
H	-1.98085500	3.78885300	2.10900100
O	0.49224900	0.86138600	-2.68810600
C	0.62083200	-0.32810600	-3.43479000
H	-0.15235000	-1.05511500	-3.15767800
H	0.50118900	-0.04351500	-4.47945200
H	1.60844700	-0.78128200	-3.28928300

TI-34

Zero-point correction= 0.218015 (Hartree/Particle)

Thermal correction to Energy= 0.230992

Thermal correction to Enthalpy= 0.231936

Thermal correction to Gibbs Free Energy= 0.178596

Sum of electronic and zero-point Energies= -593.534642

Sum of electronic and thermal Energies= -593.521665

Sum of electronic and thermal Enthalpies= -593.520720

Sum of electronic and thermal Free Energies= -593.574061

C	-0.28705200	0.07125700	1.63089600
C	0.46505000	-0.71032400	0.81924000
C	1.29665700	-0.30666600	-0.29134300
C	-0.36380700	1.53990300	1.58015300
C	1.34638500	0.85638900	-0.96850000
C	-0.01105900	2.35736300	0.56865300
C	0.55260800	2.07163200	-0.76068100
H	0.46432100	-1.77609400	1.01523100
H	2.00971100	0.92626400	-1.82578200
N	0.50927500	2.89362800	-1.74767100
C	-0.24980800	4.12040900	-1.60497200
H	-0.37605900	4.57343500	-2.59009100
H	-1.24419000	3.96818600	-1.16465000
H	0.28251300	4.84846800	-0.97565200
H	1.94489900	-1.09764800	-0.66057800
H	-0.18223100	3.40668600	0.79244800
O	-0.92277600	2.13766700	2.67830800
C	-0.13134300	2.06297200	3.85683200
H	-0.69117100	2.58157200	4.63517900
H	0.03725200	1.02570200	4.16021300

H	0.83077500	2.56521000	3.70152800
O	-1.05283100	-0.41461000	2.64112200
C	-1.12041100	-1.81308000	2.81323600
H	-0.14139800	-2.23070500	3.07793800
H	-1.82158000	-1.98106000	3.62959800
H	-1.48762100	-2.30430000	1.90476900

TI-35

Zero-point correction= 0.217234 (Hartree/Particle)

Thermal correction to Energy= 0.230545

Thermal correction to Enthalpy= 0.231490

Thermal correction to Gibbs Free Energy= 0.176895

Sum of electronic and zero-point Energies= -593.534763

Sum of electronic and thermal Energies= -593.521451

Sum of electronic and thermal Enthalpies= -593.520507

Sum of electronic and thermal Free Energies= -593.575101

C	-0.66561900	0.20245900	1.65830300
C	0.03197400	-0.69823300	0.92343000
C	0.99091800	-0.40723900	-0.12658500
C	-0.62656900	1.63955200	1.56423400
C	1.18342200	0.74866500	-0.78994600
C	-0.13803700	2.43383000	0.58217500
C	0.50583000	2.04996800	-0.67372500
H	-1.33188800	-0.21161900	2.40823300
H	1.93138700	0.75258400	-1.57913500
N	0.65539200	2.82433900	-1.69107800
C	0.03095500	4.13149700	-1.65477000
H	0.07277500	4.57226400	-2.65258900

H	-1.01850900	4.09710000	-1.33207900
H	0.56177300	4.81071600	-0.97177400
H	1.61864800	-1.23928200	-0.42837700
H	-0.26028700	3.49667300	0.76392900
O	-1.26152500	2.29856300	2.59210900
C	-0.72156000	2.06234600	3.88214900
H	0.32615900	2.38205300	3.92647900
H	-1.31450300	2.65731900	4.57694700
H	-0.78248100	1.00702600	4.16954200
O	-0.17616100	-1.99830200	1.27307600
C	0.15927900	-3.02965500	0.36338200
H	1.23693000	-3.22640400	0.34985800
H	-0.35424100	-3.92107900	0.72382500
H	-0.18200500	-2.79937900	-0.65128400

TI-36

Zero-point correction= 0.217047 (Hartree/Particle)

Thermal correction to Energy= 0.230355

Thermal correction to Enthalpy= 0.231299

Thermal correction to Gibbs Free Energy= 0.176657

Sum of electronic and zero-point Energies= -593.531958

Sum of electronic and thermal Energies= -593.518650

Sum of electronic and thermal Enthalpies= -593.517706

Sum of electronic and thermal Free Energies= -593.572348

C	-0.74988800	0.02351300	1.22533200
C	0.05570400	-0.48936200	0.27532500
C	0.91987700	0.24088400	-0.63556200
C	-0.98980200	1.41384000	1.55944400

C	0.90081000	1.56277700	-0.92761600
C	-0.65937500	2.51444500	0.85803700
C	0.02863000	2.63416500	-0.43304800
H	-1.32569900	-0.67461100	1.82863900
H	0.06988500	-1.56968300	0.17991900
H	1.64776900	1.85762900	-1.65844700
N	-0.09431900	3.78088900	-1.00445200
C	0.56752900	4.00229600	-2.27378100
H	0.20897500	4.94165600	-2.69892100
H	1.65726200	4.09082900	-2.15260900
H	0.38283100	3.20120400	-3.00264400
H	-1.00290200	3.46397200	1.25872900
O	-1.73484100	1.59396800	2.70741800
C	-0.99438600	1.36755100	3.89425500
H	-0.17191200	2.08764500	3.98147200
H	-1.68562800	1.49649200	4.72759700
H	-0.57838800	0.35163000	3.92387500
O	1.83827000	-0.48094900	-1.34762800
C	2.30690300	-1.71091600	-0.82928000
H	1.59790000	-2.52733200	-1.00748200
H	3.22994200	-1.92951000	-1.36668700
H	2.52002300	-1.64311200	0.24321600

TI-45

Zero-point correction=	0.217416 (Hartree/Particle)
Thermal correction to Energy=	0.230555
Thermal correction to Enthalpy=	0.231499
Thermal correction to Gibbs Free Energy=	0.177687

Sum of electronic and zero-point Energies=	-593.529829
Sum of electronic and thermal Energies=	-593.516691
Sum of electronic and thermal Enthalpies=	-593.515746
Sum of electronic and thermal Free Energies=	-593.569558
C	0.18608800 0.13515600 1.72853000
C	0.73882300 -0.70413000 0.80836300
C	1.32953000 -0.32260500 -0.45590600
C	0.15037500 1.58128200 1.63287400
C	1.31936900 0.84039600 -1.13570500
C	0.34896600 2.41842300 0.59618100
C	0.68244900 2.11920600 -0.80551000
H	1.83125400 0.86756300 -2.09355400
N	0.55336900 2.95041100 -1.77794900
C	-0.04824800 4.24441300 -1.52058900
H	-0.23445400 4.74168100 -2.47420700
H	-1.00100900 4.17667100 -0.97809200
H	0.61939500 4.89371000 -0.93600100
H	1.88155000 -1.13903300 -0.91630800
H	0.24282200 3.47504600 0.82442000
H	-0.12312900 2.03242600 2.58403700
O	-0.31884600 -0.27536300 2.92561400
C	-1.06027300 -1.48249400 3.00194500
H	-0.41011200 -2.34925200 3.12800200
H	-1.71378800 -1.37551500 3.86947200
H	-1.67387500 -1.61545200 2.10295800
O	0.86611700 -2.03335100 1.14333300
C	0.19840100 -2.94055600 0.28046400
H	0.57265300 -2.87905500 -0.74705500

H	0.39115200	-3.93998200	0.67191500
H	-0.88196000	-2.75000300	0.27216800

TI-234

Zero-point correction= 0.250922 (Hartree/Particle)

Thermal correction to Energy= 0.266454

Thermal correction to Enthalpy= 0.267399

Thermal correction to Gibbs Free Energy= 0.208466

Sum of electronic and zero-point Energies= -707.972018

Sum of electronic and thermal Energies= -707.956485

Sum of electronic and thermal Enthalpies= -707.955541

Sum of electronic and thermal Free Energies= -708.014474

C	0.33763500	0.07337500	1.70107600
C	0.72011600	-0.73606900	0.68348100
C	0.41863300	-0.56851200	-0.72028500
C	-0.54113500	1.24459300	1.59637600
C	0.09457600	0.55972100	-1.37715000
C	-0.68891900	2.04980600	0.51738200
C	0.01974100	1.90806500	-0.79194500
H	1.29713100	-1.61988200	0.92843100
H	-0.02667600	0.52944300	-2.45581500
N	0.43756400	2.88241200	-1.50228300
C	0.43803900	4.23130200	-0.97125800
H	1.23149800	4.79230000	-1.47061900
H	-0.51504700	4.72533300	-1.18853200
H	0.60400600	4.28048800	0.11354000
H	0.53574700	-1.46851000	-1.31948300
O	-1.58852500	3.07065100	0.49003000

C	-1.67927900	3.96668500	1.59257900
H	-1.93359800	4.94072500	1.16750500
H	-2.45011200	3.65093200	2.29702500
H	-0.72485800	4.03259500	2.12313300
O	-1.25460800	1.54788300	2.72929400
C	-2.25165500	0.58537200	3.04264600
H	-2.75834800	0.94633700	3.93857700
H	-2.97194600	0.49499000	2.22154900
H	-1.80217400	-0.39140000	3.24984800
O	0.64052400	-0.16427100	3.00565500
C	1.42770000	-1.29449700	3.30628500
H	1.56771200	-1.28489100	4.38656600
H	0.92244600	-2.22184000	3.00940700
H	2.40290300	-1.24213100	2.80824100

TI-235

Zero-point correction= 0.250723 (Hartree/Particle)

Thermal correction to Energy= 0.266294

Thermal correction to Enthalpy= 0.267238

Thermal correction to Gibbs Free Energy= 0.207808

Sum of electronic and zero-point Energies= -707.970938

Sum of electronic and thermal Energies= -707.955367

Sum of electronic and thermal Enthalpies= -707.954423

Sum of electronic and thermal Free Energies= -708.013853

C	-0.02196000	-0.18075800	1.81613700
C	0.34859600	-1.02155900	0.82017000
C	0.11969200	-0.81032800	-0.59598600
C	-0.71388400	1.07637800	1.70400000

C	-0.10816800	0.35868100	-1.22244800
C	-0.76828800	1.93297000	0.64990700
C	-0.11279600	1.72499000	-0.66585900
H	0.14381900	-0.52236800	2.83316600
H	-0.22833800	0.34077600	-2.30231600
N	0.33329200	2.64033400	-1.43927100
C	0.42105700	4.01279100	-0.98019800
H	1.17271900	4.52651100	-1.58398800
H	-0.53622800	4.52751600	-1.11424100
H	0.70380800	4.10111600	0.07745500
H	0.14835900	-1.69982600	-1.21811500
O	-1.54095300	3.06160200	0.69932400
C	-1.35633200	3.96954900	1.78065100
H	-1.47259000	4.97350600	1.36473000
H	-2.10074600	3.80558400	2.56357000
H	-0.35940800	3.86337100	2.21746500
O	-1.37088700	1.44424500	2.86288100
C	-2.76137500	1.15046400	2.80333400
H	-2.92350000	0.07808400	2.64384400
H	-3.18466300	1.44395600	3.76520700
H	-3.24222400	1.71560500	1.99627500
O	0.89597200	-2.20360200	1.22832200
C	1.67495400	-2.94724800	0.31101500
H	2.33836300	-2.30061500	-0.27306300
H	2.27464900	-3.63149700	0.91195600
H	1.05005600	-3.53526900	-0.37095000

TI-236

Zero-point correction=	0.250643 (Hartree/Particle)
Thermal correction to Energy=	0.266153
Thermal correction to Enthalpy=	0.267097
Thermal correction to Gibbs Free Energy=	0.207898
Sum of electronic and zero-point Energies=	-707.969292
Sum of electronic and thermal Energies=	-707.953782
Sum of electronic and thermal Enthalpies=	-707.952838
Sum of electronic and thermal Free Energies=	-708.012037

C	0.81238800	0.24591200	1.62094600
C	1.42505800	-0.38559700	0.59933700
C	1.15950000	-0.20681400	-0.81599200
C	-0.25672800	1.21817600	1.56093600
C	0.58403700	0.86627900	-1.39927100
C	-0.55843600	2.05100400	0.53418300
C	0.17720400	2.12725000	-0.76487700
H	1.08194000	-0.03256400	2.63656600
H	2.17938800	-1.12396100	0.85301200
H	0.53623200	0.86111000	-2.48386500
N	0.35579400	3.19632900	-1.44126500
C	0.01066100	4.49391000	-0.89569600
H	0.62228200	5.24577800	-1.40006100
H	-1.04165200	4.72832500	-1.08885600
H	0.18149600	4.57846900	0.18618500
O	-1.63834600	2.87997400	0.58577900
C	-1.82635500	3.70409700	1.73280900
H	-2.25493600	4.63968700	1.36640900
H	-2.50846400	3.23939700	2.44854700
H	-0.87400500	3.90297400	2.23181400

O	-1.02058000	1.27496200	2.71121400
C	-2.23293400	0.54189700	2.58528200
H	-2.02830200	-0.51155900	2.36147400
H	-2.74632200	0.61753300	3.54505600
H	-2.86150700	0.96398000	1.79212400
O	1.61492100	-1.17397100	-1.67417800
C	1.62486100	-2.51313900	-1.21895000
H	0.72222300	-2.75096300	-0.64508400
H	1.65858000	-3.13786900	-2.11231200
H	2.50754000	-2.73332800	-0.60745100

TI-237

Zero-point correction= 0.251189 (Hartree/Particle)

Thermal correction to Energy= 0.266523

Thermal correction to Enthalpy= 0.267467

Thermal correction to Gibbs Free Energy= 0.209297

Sum of electronic and zero-point Energies= -707.972958

Sum of electronic and thermal Energies= -707.957624

Sum of electronic and thermal Enthalpies= -707.956680

Sum of electronic and thermal Free Energies= -708.014850

C	0.56297900	0.14464800	1.85416100
C	1.19725000	-0.55012300	0.88375800
C	1.06804900	-0.41393400	-0.54510000
C	-0.41861700	1.18670000	1.66669100
C	0.64520800	0.68221900	-1.22428000
C	-0.55266700	2.00012500	0.59041700
C	0.33862000	2.00238900	-0.60188500
H	0.71620300	-0.13800700	2.89169200

H	1.84622000	-1.35891000	1.21010200
N	0.76573100	3.03757400	-1.20633700
C	0.52370500	4.35030100	-0.64286300
H	1.29694500	5.02858000	-1.01002400
H	-0.44834300	4.72951900	-0.97480900
H	0.53575800	4.36212100	0.45537500
H	1.39034600	-1.27420600	-1.12087100
O	-1.57408200	2.90353700	0.48060400
C	-1.84632100	3.77345900	1.57423600
H	-2.19224900	4.71261500	1.13619200
H	-2.62036800	3.36372900	2.22754200
H	-0.94607000	3.95167800	2.16958600
O	-1.29736900	1.33775500	2.72260400
C	-2.52898700	0.66707500	2.48776200
H	-2.36241800	-0.40340700	2.32024200
H	-3.13852700	0.80620400	3.38223200
H	-3.04279500	1.09315000	1.61737400
O	0.53173500	0.74442900	-2.56425500
C	0.79589400	-0.42386600	-3.30974300
H	0.15337700	-1.25237700	-2.98846700
H	0.58256000	-0.17304000	-4.34790200
H	1.84588800	-0.72454400	-3.21419100

TI-245

Zero-point correction= 0.250869 (Hartree/Particle)

Thermal correction to Energy= 0.266466

Thermal correction to Enthalpy= 0.267410

Thermal correction to Gibbs Free Energy= 0.207470

Sum of electronic and zero-point Energies= -707.971957
Sum of electronic and thermal Energies= -707.956361
Sum of electronic and thermal Enthalpies= -707.955417
Sum of electronic and thermal Free Energies= -708.015356

C	0.14002000	0.10804600	1.54146600
C	0.63965600	-0.66173000	0.53340700
C	0.61912400	-0.32716400	-0.87121500
C	-0.51256900	1.39108000	1.39381500
C	0.46371300	0.86391700	-1.48223800
C	-0.48542400	2.27907500	0.37342000
C	0.34182100	2.19040300	-0.86516300
H	0.55384200	0.89967600	-2.56397300
N	0.86974400	3.17110300	-1.48931100
C	0.86963200	4.51382400	-0.94171000
H	1.74856300	5.03371200	-1.33072000
H	-0.01882200	5.05992200	-1.27578300
H	0.88953400	4.55057100	0.15365500
H	0.83555500	-1.16780700	-1.52593000
H	-1.10509600	1.63383200	2.26834000
O	-1.26096700	3.39120700	0.34650000
C	-2.15242900	3.62137500	1.41609900
H	-2.70030000	4.52752500	1.16062800
H	-2.85226500	2.78554600	1.53179700
H	-1.61273200	3.77222100	2.35821900
O	0.14901100	-0.26413900	2.85435700
C	-0.10442500	-1.61358500	3.21172200
H	0.80335200	-2.21768400	3.18363700
H	-0.49969700	-1.58198700	4.22887200

H	-0.85610700	-2.05598000	2.54745100
O	1.26789600	-1.84473600	0.87258700
C	0.69061200	-3.02638300	0.34815900
H	0.86360400	-3.12985300	-0.72895400
H	1.17524300	-3.86086800	0.85774800
H	-0.38987800	-3.05950800	0.53705300

TI-246

Zero-point correction= 0.251365 (Hartree/Particle)

Thermal correction to Energy= 0.266726

Thermal correction to Enthalpy= 0.267670

Thermal correction to Gibbs Free Energy= 0.209225

Sum of electronic and zero-point Energies= -707.989142

Sum of electronic and thermal Energies= -707.973780

Sum of electronic and thermal Enthalpies= -707.972836

Sum of electronic and thermal Free Energies= -708.031281

C	-0.20521600	0.11011800	1.75961900
C	0.43959300	-0.72179500	0.90776600
C	0.69805900	-0.48945200	-0.49824900
C	-0.82556300	1.38269800	1.45113800
C	0.73593900	0.69131100	-1.16039700
C	-0.53407900	2.20124300	0.41875300
C	0.58456500	2.02148700	-0.56302000
H	0.76767700	-1.69476800	1.24982400
H	1.03905800	0.71848900	-2.19932400
N	1.32329800	2.96361800	-1.00563400
C	1.24408700	4.30640700	-0.46359700
H	2.23022600	4.76672500	-0.56311000

H	0.53467600	4.90759000	-1.04210400
H	0.93695700	4.35015200	0.58831800
H	-1.60204900	1.65966200	2.15480600
O	-1.24485400	3.31632400	0.13166300
C	-2.37776500	3.60924100	0.92268000
H	-2.82701400	4.50073100	0.48696400
H	-3.09487200	2.78074600	0.89997800
H	-2.09389800	3.81174100	1.96195800
O	-0.44870400	-0.20717500	3.06123300
C	-0.00807700	-1.46026300	3.53536800
H	1.08013300	-1.55756500	3.44694600
H	-0.29415800	-1.50300800	4.58575800
H	-0.48715800	-2.28170400	2.98967500
O	0.98225200	-1.68154500	-1.09915700
C	1.33433600	-1.67064200	-2.46394600
H	1.52353900	-2.70900500	-2.73537700
H	0.52035600	-1.27282000	-3.08122000
H	2.23844900	-1.07486300	-2.63730500

TI-247

Zero-point correction=	0.251415 (Hartree/Particle)
Thermal correction to Energy=	0.266704
Thermal correction to Enthalpy=	0.267649
Thermal correction to Gibbs Free Energy=	0.209358
Sum of electronic and zero-point Energies=	-707.983032
Sum of electronic and thermal Energies=	-707.967743
Sum of electronic and thermal Enthalpies=	-707.966799
Sum of electronic and thermal Free Energies=	-708.025089

C	-0.25617200	0.12339900	1.61032000
C	0.30670800	-0.67775900	0.67216900
C	0.45594100	-0.40353300	-0.73877000
C	-0.86675800	1.41555600	1.38462300
C	0.51113200	0.80031900	-1.35547400
C	-0.59528500	2.26660000	0.37311000
C	0.49061100	2.10117500	-0.63893600
H	0.64481500	-1.66045400	0.97871100
N	1.31852900	2.99966100	-0.98875000
C	1.34464600	4.27583100	-0.29938900
H	2.36711800	4.65832000	-0.33441700
H	0.69901900	4.98865000	-0.82184600
H	1.01317300	4.22497500	0.74512900
H	0.59527200	-1.28695600	-1.35279900
H	-1.60379100	1.68651500	2.13243500
O	-1.27028300	3.42242600	0.15066800
C	-2.33678200	3.74072300	1.01946300
H	-2.76472000	4.66980300	0.64514100
H	-3.09756300	2.95146000	1.01287500
H	-1.97973000	3.88731500	2.04580100
O	-0.41286200	-0.23707400	2.92102700
C	0.02533500	-1.51712500	3.30899100
H	1.10356000	-1.63650500	3.14630800
H	-0.19256600	-1.60449000	4.37326900
H	-0.50645100	-2.30486100	2.76080700
O	0.66381200	0.97996400	-2.68887100
C	0.75622800	-0.16903100	-3.49768900
H	-0.13826500	-0.79751400	-3.40136700

H	0.84342500	0.18873100	-4.52309200
H	1.64078800	-0.76467000	-3.24157300

TI-345

Zero-point correction= 0.250649 (Hartree/Particle)

Thermal correction to Energy= 0.266401

Thermal correction to Enthalpy= 0.267345

Thermal correction to Gibbs Free Energy= 0.207581

Sum of electronic and zero-point Energies= -707.971812

Sum of electronic and thermal Energies= -707.956059

Sum of electronic and thermal Enthalpies= -707.955115

Sum of electronic and thermal Free Energies= -708.014880

C	0.27702400	-0.02226200	1.65827200
C	1.01600000	-0.70419000	0.73647400
C	1.68272100	-0.13730400	-0.41980900
C	-0.01829400	1.40530600	1.64842000
C	1.44341100	1.02245800	-1.05970800
C	0.03808900	2.28286900	0.61826900
C	0.44990800	2.06558900	-0.76859800
H	2.02634200	1.23648500	-1.95159400
N	0.13798000	2.82514500	-1.75840400
C	-0.81621500	3.89020100	-1.52463900
H	-1.16792600	4.27016500	-2.48580200
H	-1.68664300	3.57052800	-0.93560400
H	-0.34960900	4.73069300	-0.99039200
H	2.45852700	-0.76367700	-0.84806900
H	-0.25635600	3.29366300	0.88374500
O	-0.52575100	1.90855800	2.81424800

C	0.18733000	1.64348100	4.02132500
H	0.27310400	2.59405300	4.55277600
H	-0.35762400	0.92142100	4.63295000
H	1.18538200	1.24825400	3.81606600
O	-0.20215600	-0.73159300	2.72983100
C	-1.60990000	-0.92954100	2.68491800
H	-1.86909900	-1.51387000	3.56873800
H	-2.13973000	0.02939500	2.70792600
H	-1.88995700	-1.48620300	1.78384700
O	1.16156400	-2.03221000	0.99320500
C	1.59214400	-2.89463400	-0.04175700
H	2.67150600	-2.81844100	-0.21517200
H	1.36504100	-3.90360300	0.30287900
H	1.05984700	-2.70073100	-0.97928000

TI-346

Zero-point correction= 0.251618 (Hartree/Particle)

Thermal correction to Energy= 0.266931

Thermal correction to Enthalpy= 0.267875

Thermal correction to Gibbs Free Energy= 0.208950

Sum of electronic and zero-point Energies= -707.984653

Sum of electronic and thermal Energies= -707.969341

Sum of electronic and thermal Enthalpies= -707.968396

Sum of electronic and thermal Free Energies= -708.027322

C	-0.48488400	-0.00929000	1.78252500
C	0.32650300	-0.61896200	0.88807400
C	1.02296300	-0.05111700	-0.24789300
C	-0.86495100	1.41227200	1.80347200

C	0.93283400	1.18018400	-0.80924300
C	-0.60844800	2.34901700	0.87449500
C	0.09103300	2.30655600	-0.41503400
H	0.53234400	-1.67467900	1.00599500
H	1.55687100	1.37079000	-1.67068500
N	-0.05105500	3.37992100	-1.11687900
C	0.60035900	3.46099900	-2.40639400
H	0.27933000	4.37550400	-2.90885300
H	1.69631400	3.50273800	-2.31335200
H	0.35988700	2.61004800	-3.06080600
H	-1.02908100	3.32844200	1.08411300
O	-1.62804700	1.79382700	2.87805000
C	-0.88381300	1.97203500	4.07390800
H	-1.59771300	2.27360900	4.84107700
H	-0.39350300	1.04203000	4.37997100
H	-0.13159200	2.75902500	3.94273500
O	-1.06471600	-0.67237900	2.80845400
C	-0.83324900	-2.05960200	2.93336900
H	0.22992200	-2.27169000	3.09554100
H	-1.40805100	-2.38007100	3.80099700
H	-1.17730400	-2.59738700	2.04289800
O	1.84821100	-1.01330100	-0.74907800
C	2.61879600	-0.72605700	-1.89478500
H	3.17061700	-1.63777600	-2.12076700
H	1.98105600	-0.46116500	-2.74628700
H	3.32374100	0.09177400	-1.70582000

TI-347

Zero-point correction=	0.251154 (Hartree/Particle)
Thermal correction to Energy=	0.266581
Thermal correction to Enthalpy=	0.267525
Thermal correction to Gibbs Free Energy=	0.208810
Sum of electronic and zero-point Energies=	-707.977243
Sum of electronic and thermal Energies=	-707.961815
Sum of electronic and thermal Enthalpies=	-707.960871
Sum of electronic and thermal Free Energies=	-708.019586
C	-0.19228100 -0.00134700 1.72542400
C	0.63415900 -0.51797800 0.78356200
C	0.80953800 -0.08816800 -0.58412700
C	-1.07425000 1.15453900 1.54088500
C	0.55829400 1.12442900 -1.12663100
C	-0.94340800 2.13273200 0.62623700
C	0.12373000 2.33141300 -0.36558900
H	1.18921400 -1.41228600 1.04165300
N	0.50754200 3.53004000 -0.57497100
C	1.57002300 3.82213000 -1.51893400
H	2.06897400 4.73731500 -1.19113300
H	2.31410000 3.02272700 -1.61508300
H	1.15019200 4.00481200 -2.51351400
H	1.21053000 -0.85448000 -1.23912300
H	-1.67702400 2.93287300 0.67627900
O	-2.13380800 1.22323500 2.41204500
C	-1.85328200 1.94842300 3.60114900
H	-2.76936500 1.93971600 4.19290400
H	-1.04557400 1.47394600 4.16671100
H	-1.57891100 2.98370600 3.36536700

O	-0.34618100	-0.53436800	2.96806400
C	0.36495600	-1.70926400	3.27916400
H	1.44860400	-1.54868500	3.22105400
H	0.09019000	-1.96752500	4.30130100
H	0.08723500	-2.52956900	2.60627800
O	0.66891700	1.40122800	-2.45272400
C	1.01623200	0.34960000	-3.32547800
H	0.30229700	-0.47892500	-3.24639900
H	0.98555100	0.76798200	-4.33097200
H	2.02578700	-0.02527500	-3.11688300

TI-2345

Zero-point correction= 0.283621 (Hartree/Particle)

Thermal correction to Energy= 0.301927

Thermal correction to Enthalpy= 0.302871

Thermal correction to Gibbs Free Energy= 0.237813

Sum of electronic and zero-point Energies= -822.411024

Sum of electronic and thermal Energies= -822.392718

Sum of electronic and thermal Enthalpies= -822.391774

Sum of electronic and thermal Free Energies= -822.456832

C	0.32494600	-0.27970900	1.27710900
C	0.74243300	-0.90527900	0.14702400
C	0.53956400	-0.44954200	-1.21254400
C	-0.47298200	0.94435400	1.35344000
C	0.29399600	0.79855700	-1.64877200
C	-0.54779700	1.95148900	0.44884600
C	0.20585100	2.02464200	-0.83725000
H	0.24649800	0.97609800	-2.71926800

N	0.66184600	3.09594500	-1.36125900
C	0.65904100	4.33799700	-0.61407300
H	1.46938100	4.96494600	-0.99323000
H	-0.28452100	4.87195100	-0.76922600
H	0.79638700	4.20357600	0.46746800
H	0.69016500	-1.23100000	-1.95311600
O	-1.41666500	2.99157900	0.59100300
C	-1.49394200	3.68325700	1.83226500
H	-1.70845600	4.72580300	1.58531800
H	-2.28574700	3.27689700	2.46354700
H	-0.54547400	3.62099300	2.37471700
O	-1.21147100	1.06647700	2.50902800
C	-2.29366000	0.14429900	2.58104500
H	-2.79767100	0.33407400	3.52957300
H	-2.99133700	0.30956700	1.75239800
H	-1.92723800	-0.88681500	2.56268100
O	0.53492000	-0.91522400	2.47477400
C	1.38259800	-0.19453500	3.36261300
H	0.95269300	0.78344500	3.60092800
H	1.45504100	-0.79191600	4.27187900
H	2.37758200	-0.07174400	2.92215900
O	1.42914700	-2.09032800	0.24143800
C	0.62546900	-3.20316500	0.61240300
H	-0.18226800	-3.35530100	-0.11435900
H	1.28221200	-4.07389000	0.60568600
H	0.20268500	-3.06596900	1.61106500

TI-2346

Zero-point correction=	0.284202 (Hartree/Particle)
Thermal correction to Energy=	0.302202
Thermal correction to Enthalpy=	0.303146
Thermal correction to Gibbs Free Energy=	0.238884
Sum of electronic and zero-point Energies=	-822.421235
Sum of electronic and thermal Energies=	-822.403234
Sum of electronic and thermal Enthalpies=	-822.402290
Sum of electronic and thermal Free Energies=	-822.466553

C	0.46801000	0.17669700	1.87197400
C	1.06485800	-0.58982400	0.93285500
C	0.94618700	-0.47228000	-0.50970100
C	-0.50081800	1.25598900	1.63676700
C	0.62380100	0.63040100	-1.21914300
C	-0.56274800	2.03616900	0.53497800
C	0.35719900	1.95586300	-0.64581500
H	1.69408000	-1.41559500	1.24048700
H	0.68037000	0.62185200	-2.30028400
N	0.79736900	2.97238600	-1.28076100
C	0.58303300	4.31126900	-0.76843500
H	1.39596000	4.94631900	-1.12911700
H	-0.35917200	4.71980400	-1.14915800
H	0.55739000	4.36928900	0.32832200
O	-1.53641000	2.96582400	0.34689300
C	-1.90470500	3.83829100	1.40946100
H	-2.19380700	4.77976000	0.93628800
H	-2.74040400	3.43436900	1.98289000
H	-1.06305800	4.00816000	2.08732000
O	-1.39684000	1.47904400	2.65226600

C	-2.31886800	0.41347100	2.83548800
H	-2.99904700	0.72664000	3.62854200
H	-2.88401500	0.22939400	1.91463000
H	-1.80328900	-0.50284400	3.14164600
O	0.62317500	-0.02465800	3.20657200
C	1.45178000	-1.08769600	3.62338500
H	1.43697800	-1.07062800	4.71241800
H	1.07114700	-2.05112300	3.26366000
H	2.47920700	-0.95231200	3.26631100
O	1.30636400	-1.65611100	-1.08421800
C	1.35123900	-1.71554400	-2.49226800
H	1.65839900	-2.73046400	-2.74330700
H	0.36690500	-1.51141500	-2.92955100
H	2.07695400	-0.99978100	-2.89602500

TI-2347

Zero-point correction= 0.284290 (Hartree/Particle)

Thermal correction to Energy= 0.302328

Thermal correction to Enthalpy= 0.303272

Thermal correction to Gibbs Free Energy= 0.238988

Sum of electronic and zero-point Energies= -822.416260

Sum of electronic and thermal Energies= -822.398221

Sum of electronic and thermal Enthalpies= -822.397277

Sum of electronic and thermal Free Energies= -822.461561

C	0.42318000	0.18718100	1.74184000
C	0.97945100	-0.54914500	0.75188200
C	0.81320700	-0.39216100	-0.67758800
C	-0.53682400	1.27920200	1.55920000

C	0.52887800	0.75210300	-1.33864800
C	-0.57855500	2.10837700	0.49147600
C	0.36797400	2.06778300	-0.66264200
H	1.61391100	-1.37958200	1.04030300
N	0.93463600	3.08056000	-1.18132000
C	0.80281800	4.37360300	-0.53836700
H	1.68335400	4.97055000	-0.78497900
H	-0.08013700	4.89106300	-0.92770200
H	0.70671200	4.31350300	0.55431900
H	1.02061800	-1.28383900	-1.25867200
O	-1.52147300	3.07578900	0.31820700
C	-1.91134100	3.89031600	1.41768800
H	-2.19164100	4.85532400	0.98893600
H	-2.75804000	3.45774600	1.95270100
H	-1.08383300	4.02281600	2.12127100
O	-1.43045700	1.47973800	2.58065800
C	-2.31561300	0.38794000	2.78827200
H	-3.00232300	0.69535900	3.57798800
H	-2.87944500	0.16832800	1.87449800
H	-1.76883700	-0.50402100	3.10930600
O	0.61759400	-0.05196700	3.07295400
C	1.44191700	-1.13608000	3.42963400
H	1.46390000	-1.15490900	4.51889400
H	1.03817600	-2.08500000	3.05427900
H	2.46072100	-1.00591400	3.04486300
O	0.41535100	0.86686100	-2.67997600
C	0.58113600	-0.30156200	-3.44990500
H	-0.14720800	-1.07093200	-3.16410200

H	0.41744300	-0.00838900	-4.48624100
H	1.59333700	-0.70892600	-3.33906300

TI-2356

Zero-point correction= 0.283933 (Hartree/Particle)

Thermal correction to Energy= 0.301947

Thermal correction to Enthalpy= 0.302891

Thermal correction to Gibbs Free Energy= 0.238769

Sum of electronic and zero-point Energies= -822.415086

Sum of electronic and thermal Energies= -822.397073

Sum of electronic and thermal Enthalpies= -822.396129

Sum of electronic and thermal Free Energies= -822.460250

C	0.37321300	-0.01969200	1.69919600
C	0.98983000	-0.72632600	0.73221700
C	0.91080600	-0.47151700	-0.71200900
C	-0.52273700	1.10836900	1.57561400
C	0.55320600	0.69201600	-1.29739600
C	-0.60638300	1.99983300	0.56076700
C	0.23949400	1.98540500	-0.66647700
H	0.50904200	-0.37846400	2.71594300
H	0.61716000	0.77365600	-2.37582600
N	0.61082100	3.02329200	-1.31412700
C	0.39260300	4.35496800	-0.78544600
H	1.12502900	5.02409400	-1.24337600
H	-0.60769200	4.71888900	-1.04337000
H	0.50275400	4.41853300	0.30541800
O	-1.55981200	2.97755000	0.55175300
C	-1.69665200	3.81133700	1.69826800

H	-1.95984300	4.80393100	1.32501600
H	-2.48242900	3.44530400	2.36348400
H	-0.75885200	3.86378300	2.25857700
O	-1.36877900	1.25439000	2.65836700
C	-2.66636700	0.73397800	2.39718200
H	-2.61255200	-0.33048800	2.14015500
H	-3.24397200	0.85809000	3.31452300
H	-3.14649700	1.28023200	1.57690200
O	1.77127200	-1.78681400	1.10913200
C	1.08732100	-3.03246100	1.14251900
H	0.71624100	-3.30323000	0.14996800
H	1.81270000	-3.77385700	1.47920700
H	0.25096600	-2.99161700	1.85152400
O	1.29723400	-1.57213200	-1.41053000
C	1.35057400	-1.47924500	-2.81713200
H	1.69312900	-2.45127100	-3.17003700
H	0.36265000	-1.26077200	-3.23936800
H	2.05626900	-0.70283100	-3.13417000

TI-2357

Zero-point correction= 0.283747 (Hartree/Particle)

Thermal correction to Energy= 0.301921

Thermal correction to Enthalpy= 0.302865

Thermal correction to Gibbs Free Energy= 0.237963

Sum of electronic and zero-point Energies= -822.417676

Sum of electronic and thermal Energies= -822.399502

Sum of electronic and thermal Enthalpies= -822.398558

Sum of electronic and thermal Free Energies= -822.463460

C	-0.05582600	-0.16733700	1.73697600
C	0.44164400	-0.92559000	0.73509600
C	0.38694200	-0.66754100	-0.68770900
C	-0.77218500	1.07694500	1.59393300
C	0.27347200	0.54137700	-1.28699100
C	-0.65706400	1.97838600	0.58827000
C	0.27029000	1.84966800	-0.56802200
H	0.01019800	-0.56393800	2.74488400
N	0.96674700	2.78633500	-1.07426300
C	1.01193700	4.07663600	-0.41532400
H	1.94113000	4.57522700	-0.69896300
H	0.17383600	4.69739000	-0.74847200
H	0.96570300	4.00602000	0.67974000
H	0.45846600	-1.56016800	-1.29960600
O	-1.43770800	3.10041900	0.51376700
C	-1.55770000	3.92909200	1.66454700
H	-1.65168000	4.95279400	1.29434700
H	-2.43981700	3.66733400	2.25347300
H	-0.67446200	3.84592200	2.30467600
O	-1.64404200	1.35542400	2.62887100
C	-2.98016000	0.99150200	2.30646200
H	-3.04529500	-0.07729800	2.07216200
H	-3.58673600	1.21069100	3.18654800
H	-3.34299100	1.57319900	1.45020900
O	0.96562900	-2.14965800	1.08502700
C	2.33188300	-2.31704000	0.74386500
H	2.95517500	-1.58674400	1.27329700
H	2.60863900	-3.32596500	1.05117300

H	2.49940000	-2.20728900	-0.33381200
O	0.20019000	0.72056300	-2.61803400
C	0.21924000	-0.42413200	-3.44405300
H	-0.61594900	-1.09464400	-3.20977300
H	0.12368900	-0.05884600	-4.46548700
H	1.16307600	-0.97123000	-3.33543200

TI-2367

Zero-point correction= 0.284300 (Hartree/Particle)

Thermal correction to Energy= 0.302222

Thermal correction to Enthalpy= 0.303166

Thermal correction to Gibbs Free Energy= 0.239503

Sum of electronic and zero-point Energies= -822.411634

Sum of electronic and thermal Energies= -822.393712

Sum of electronic and thermal Enthalpies= -822.392768

Sum of electronic and thermal Free Energies= -822.456431

C	0.30653300	-0.03565800	1.97846700
C	0.96676800	-0.82433500	1.09930500
C	1.02573400	-0.72165100	-0.33598100
C	-0.50366700	1.11464800	1.67063300
C	0.79370800	0.39363900	-1.08568100
C	-0.41962300	1.89464800	0.56367900
C	0.59944700	1.74617500	-0.51053700
H	0.29359800	-0.31914400	3.02691900
H	1.45373600	-1.71675300	1.48359400
N	1.22646700	2.71073200	-1.06524400
C	1.08640100	4.05467800	-0.54067600
H	1.97190700	4.62710600	-0.82436100

H	0.20756400	4.54608000	-0.97222100
H	0.98332000	4.08250800	0.55254300
O	-1.29715900	2.91187200	0.31093200
C	-1.60457800	3.83886600	1.34798300
H	-1.77758400	4.79822000	0.85496500
H	-2.49955800	3.53925300	1.89813100
H	-0.77440800	3.92883500	2.05431600
O	-1.45906600	1.41640200	2.62152400
C	-2.72276700	0.84797100	2.30198400
H	-2.64651400	-0.24154300	2.20905300
H	-3.39707700	1.09918700	3.12213300
H	-3.10802600	1.26359100	1.36284400
O	1.36227400	-1.89811400	-0.96303600
C	2.66697900	-1.90985200	-1.52809800
H	3.42537800	-1.74335700	-0.75309500
H	2.80570600	-2.90202200	-1.95954600
H	2.76839700	-1.15129200	-2.30802000
O	0.91465600	0.25844700	-2.42685600
C	0.21872800	1.17053700	-3.26772800
H	0.15211400	0.67778400	-4.23805700
H	-0.79004900	1.35996500	-2.88460900
H	0.75589700	2.11626300	-3.34911700

TI-2456

Zero-point correction= 0.284123 (Hartree/Particle)

Thermal correction to Energy= 0.302135

Thermal correction to Enthalpy= 0.303079

Thermal correction to Gibbs Free Energy= 0.238425

Sum of electronic and zero-point Energies=	-822.417261
Sum of electronic and thermal Energies=	-822.399250
Sum of electronic and thermal Enthalpies=	-822.398305
Sum of electronic and thermal Free Energies=	-822.462960
C	0.10136300 0.14270300 1.50388600
C	0.66384300 -0.61031400 0.51934200
C	0.64504500 -0.27475600 -0.90922400
C	-0.63030700 1.38627100 1.34529800
C	0.51441500 0.94460800 -1.47795300
C	-0.54056000 2.29889400 0.35675900
C	0.40858700 2.23810600 -0.79539000
H	0.61324100 1.03914800 -2.55211500
N	1.01762300 3.23472500 -1.30873900
C	0.96413400 4.54765600 -0.69402700
H	1.89573000 5.06728400 -0.93113800
H	0.13872700 5.12961900 -1.11752400
H	0.83466400 4.52874900 0.39438700
H	-1.30323300 1.56838100 2.17513900
O	-1.33708400 3.39112400 0.27019000
C	-2.31630700 3.58311400 1.26897400
H	-2.86145300 4.48334800 0.98819800
H	-3.00449400 2.73105400 1.31232400
H	-1.85476100 3.72379400 2.25311900
O	0.12099700 -0.19627200 2.82464000
C	0.06586000 -1.55379000 3.23013600
H	1.05101400 -2.02217700 3.20937100
H	-0.31745800 -1.53829700 4.25211500
H	-0.62241900 -2.12429600 2.59584100

O	1.38498100	-1.72640700	0.87097500
C	0.84270200	-3.00045900	0.54029800
H	1.36422000	-3.42200500	-0.32081900
H	0.98061000	-3.65025800	1.41071500
H	-0.22461500	-2.92925300	0.30861800
O	0.86135900	-1.40008500	-1.64686800
C	0.99050300	-1.27235300	-3.04500800
H	1.17621200	-2.27763300	-3.42275000
H	0.07321000	-0.87553300	-3.49506700
H	1.83121200	-0.61964200	-3.30630000

TI-2457

Zero-point correction= 0.284244 (Hartree/Particle)

Thermal correction to Energy= 0.302264

Thermal correction to Enthalpy= 0.303208

Thermal correction to Gibbs Free Energy= 0.238654

Sum of electronic and zero-point Energies= -822.415834

Sum of electronic and thermal Energies= -822.397813

Sum of electronic and thermal Enthalpies= -822.396869

Sum of electronic and thermal Free Energies= -822.461423

C	0.00917500	0.20149600	1.56273400
C	0.75318400	-0.49429700	0.66001000
C	0.89521200	-0.20590800	-0.75185700
C	-0.74363600	1.40482900	1.28548800
C	0.80615400	0.99294600	-1.37273500
C	-0.53967200	2.30391000	0.29901100
C	0.59221800	2.28487100	-0.67023500
N	1.30942100	3.27778600	-1.00691900

C	1.15020400	4.55215300	-0.33230700
H	0.44141500	5.17380200	-0.88838700
H	0.78826100	4.46771200	0.69933400
H	2.11754400	5.05950000	-0.33524400
H	1.17906400	-1.06026400	-1.35574300
H	-1.54527800	1.57027500	1.99638300
O	-1.35146300	3.36623200	0.05504400
C	-2.48308400	3.53181900	0.88162200
H	-3.01361500	4.40253100	0.49769600
H	-3.13475800	2.65124900	0.83781600
H	-2.19037900	3.70953700	1.92337500
O	-0.14079900	-0.18239700	2.86905100
C	-0.36348400	-1.55170400	3.16089000
H	0.57513000	-2.09150100	3.30017900
H	-0.94498300	-1.57524600	4.08515300
H	-0.93951300	-2.03247400	2.36039100
O	1.45807700	-1.58288500	1.13641600
C	1.20051500	-2.82300700	0.50860800
H	1.71285200	-2.91258400	-0.45674900
H	1.58749200	-3.59595100	1.17538900
H	0.12443300	-2.97824800	0.35787400
O	0.96237000	1.17969500	-2.70170500
C	1.20832000	0.04680700	-3.50231600
H	0.40009800	-0.68930300	-3.40813200
H	1.25888500	0.40699600	-4.52911300
H	2.15993900	-0.42852600	-3.23480800

TI-3456

Zero-point correction= 0.284043 (Hartree/Particle)

Thermal correction to Energy= 0.302319

Thermal correction to Enthalpy= 0.303263

Thermal correction to Gibbs Free Energy= 0.237950

Sum of electronic and zero-point Energies= -822.419157

Sum of electronic and thermal Energies= -822.400881

Sum of electronic and thermal Enthalpies= -822.399937

Sum of electronic and thermal Free Energies= -822.465250

C	-0.01404800	-0.14401700	1.39833800
C	0.17781700	-0.87068000	0.27107300
C	0.55504100	-0.36344900	-1.05656400
C	0.03262300	1.31381600	1.53985600
C	0.40225100	0.88989800	-1.53592300
C	-0.03308400	2.24948800	0.57420000
C	-0.14782800	2.08235600	-0.88198900
H	0.65121000	1.08288800	-2.57242000
N	-0.56720600	3.00489200	-1.67344800
C	-1.08200900	4.23357100	-1.10185800
H	-1.60315900	4.79248700	-1.88154200
H	-1.78066900	4.06812600	-0.27083600
H	-0.26970900	4.87408900	-0.72824900
H	0.00330400	3.27044000	0.94246100
O	0.06186500	1.76306100	2.83617500
C	1.27250900	1.47439500	3.52842600
H	1.15578100	1.88541900	4.53137100
H	1.44499300	0.39666800	3.59112000
H	2.11800200	1.96231200	3.03020700
O	-0.25990200	-0.84157700	2.55291800

C	-1.62907500	-0.80344900	2.94469000
H	-1.70007800	-1.36481500	3.87671500
H	-1.95380400	0.22872800	3.11229300
H	-2.25211000	-1.27738700	2.17909900
O	0.00138900	-2.22178400	0.34175600
C	1.13848900	-2.93130500	0.82070700
H	1.37577400	-2.62486400	1.84433600
H	0.86875200	-3.98774700	0.80677800
H	1.99749400	-2.76484600	0.16299100
O	1.05731300	-1.38503000	-1.79972500
C	1.42186900	-1.11971100	-3.13637500
H	2.21018800	-0.35985700	-3.19224500
H	1.79189200	-2.06244700	-3.53764100
H	0.55814500	-0.78439200	-3.72179300

TI-23456

Zero-point correction= 0.317426 (Hartree/Particle)

Thermal correction to Energy= 0.338156

Thermal correction to Enthalpy= 0.339100

Thermal correction to Gibbs Free Energy= 0.269013

Sum of electronic and zero-point Energies= -936.856119

Sum of electronic and thermal Energies= -936.835389

Sum of electronic and thermal Enthalpies= -936.834445

Sum of electronic and thermal Free Energies= -936.904532

C	0.39043300	-0.20559100	1.37053500
C	0.89129900	-0.82619700	0.27670000
C	0.65290200	-0.43215200	-1.11811700
C	-0.48231200	0.97131200	1.40968300

C	0.40798400	0.81966100	-1.55783800
C	-0.51473500	1.97256300	0.50266400
C	0.34338300	2.03030400	-0.72219100
H	0.34427500	1.01611900	-2.62119900
N	0.87727800	3.09511100	-1.17889300
C	0.83759800	4.32054200	-0.40468800
H	1.71038600	4.92017700	-0.67334200
H	-0.05945600	4.89718000	-0.65391500
H	0.84385200	4.15923000	0.68189300
O	-1.39341900	3.00921000	0.55651000
C	-1.64257800	3.65925800	1.79720000
H	-1.88786100	4.69418700	1.54854200
H	-2.47190500	3.19438400	2.33198100
H	-0.75411000	3.63456700	2.43616500
O	-1.29950200	1.04855500	2.51435100
C	-2.28087800	0.01826300	2.56215200
H	-2.88486200	0.21112300	3.44977200
H	-2.91603000	0.05200400	1.67007300
H	-1.80763900	-0.96474300	2.64783700
O	0.61950600	-0.79900300	2.58525500
C	1.37377300	0.00492800	3.48489200
H	0.86162000	0.95127600	3.68633500
H	1.45959100	-0.56617700	4.40972100
H	2.37203800	0.19611100	3.07717900
O	1.69868400	-1.91693700	0.44093400
C	0.99069600	-3.13054800	0.66116600
H	1.74491600	-3.91154000	0.76638000
H	0.39760800	-3.06758000	1.57923000

H	0.34560800	-3.35819500	-0.19366000
O	0.78336500	-1.51049800	-1.93417900
C	0.66061200	-1.29768100	-3.32295700
H	0.79617500	-2.27192600	-3.79123300
H	-0.32924100	-0.90026600	-3.57733400
H	1.42885500	-0.60449900	-3.68482500

TI-23457

Zero-point correction= 0.317229 (Hartree/Particle)

Thermal correction to Energy= 0.338083

Thermal correction to Enthalpy= 0.339027

Thermal correction to Gibbs Free Energy= 0.268409

Sum of electronic and zero-point Energies= -936.856693

Sum of electronic and thermal Energies= -936.835839

Sum of electronic and thermal Enthalpies= -936.834894

Sum of electronic and thermal Free Energies= -936.905513

C	0.36953400	-0.21558700	1.34924700
C	0.94193400	-0.79752500	0.26479900
C	0.86787700	-0.35234800	-1.10918600
C	-0.49505900	0.96094300	1.33543100
C	0.68577600	0.91522800	-1.54716900
C	-0.44144000	1.98725500	0.45443000
C	0.55100300	2.09890200	-0.65195200
N	1.18753800	3.15253800	-0.97017600
C	1.08940200	4.32392900	-0.12204100
H	2.00398700	4.90938200	-0.23798700
H	0.24422300	4.94191300	-0.44224100
H	0.95026800	4.08522100	0.94132800

H	1.07962200	-1.13920400	-1.82412200
O	-1.32520600	3.02663300	0.44224900
C	-1.68612500	3.65128100	1.66762400
H	-1.90128200	4.69390200	1.42234700
H	-2.56557400	3.18170100	2.11126400
H	-0.86360100	3.60394600	2.38864600
O	-1.41205600	1.02531100	2.35927700
C	-2.37809600	-0.01951900	2.32158600
H	-3.05938000	0.16319300	3.15364900
H	-2.93487500	0.00803700	1.37828400
H	-1.90055400	-0.99576800	2.44592300
O	0.49869800	-0.83768500	2.57021600
C	1.20286100	-0.05825000	3.52811800
H	0.68339900	0.88673800	3.71976800
H	1.23336600	-0.64767300	4.44526400
H	2.22368400	0.14007500	3.18391700
O	1.67755100	-1.94870200	0.41787400
C	0.91473400	-3.09732800	0.76461700
H	0.13704100	-3.28423000	0.01342900
H	1.61177300	-3.93653500	0.77467100
H	0.45558500	-2.98436400	1.74976000
O	0.65953900	1.27693700	-2.84354000
C	0.80948600	0.26206500	-3.81304100
H	0.02836400	-0.50062900	-3.70986800
H	0.71925900	0.75357600	-4.78071000
H	1.79235800	-0.21627300	-3.73259000

TI-23567

Zero-point correction=	0.317064 (Hartree/Particle)
Thermal correction to Energy=	0.337733
Thermal correction to Enthalpy=	0.338677
Thermal correction to Gibbs Free Energy=	0.268893
Sum of electronic and zero-point Energies=	-936.854291
Sum of electronic and thermal Energies=	-936.833621
Sum of electronic and thermal Enthalpies=	-936.832677
Sum of electronic and thermal Free Energies=	-936.902461

C	0.32940000	-0.04834200	1.62256400
C	0.92525500	-0.75961500	0.63825000
C	0.86608200	-0.51840800	-0.79385700
C	-0.50236200	1.11676500	1.47031400
C	0.63534500	0.67601100	-1.40552700
C	-0.47591800	2.00859000	0.44945400
C	0.48033500	1.96694200	-0.68948400
H	0.42970700	-0.42440300	2.63652300
N	1.08640400	2.97863900	-1.17930000
C	0.98885700	4.26194000	-0.51214000
H	1.86285200	4.85696100	-0.78439200
H	0.09198100	4.79810300	-0.84083000
H	0.94600900	4.17489300	0.58172200
O	-1.36384800	3.04566000	0.35504800
C	-1.58287300	3.86953900	1.49596400
H	-1.76014000	4.87798200	1.11454000
H	-2.45173900	3.53387500	2.06700200
H	-0.71027700	3.86976300	2.15490100
O	-1.40274300	1.31554000	2.49835700
C	-2.68960100	0.80153000	2.17999900

H	-2.63580200	-0.27142300	1.96156700
H	-3.31952100	0.96567000	3.05569700
H	-3.11217500	1.32583100	1.31411200
O	1.64629200	-1.87502800	0.99466200
C	0.86981900	-3.06636000	1.04062500
H	0.43464000	-3.28097300	0.06034200
H	1.55001700	-3.86880400	1.32903600
H	0.07367400	-2.97584500	1.78960700
O	1.10976900	-1.62142700	-1.57266000
C	2.45236100	-1.69261000	-2.04268100
H	2.52230000	-2.60266500	-2.64031000
H	2.68630800	-0.82450200	-2.66641500
H	3.14597500	-1.75168800	-1.19747800
O	0.70640900	0.67228600	-2.75504100
C	0.00074200	1.66948500	-3.48491800
H	-0.11330100	1.26418600	-4.49065200
H	-0.98836600	1.84590900	-3.04879700
H	0.55810100	2.60638600	-3.50501500

TI-234567

Zero-point correction= 0.349874 (Hartree/Particle)

Thermal correction to Energy= 0.373661

Thermal correction to Enthalpy= 0.374605

Thermal correction to Gibbs Free Energy= 0.297359

Sum of electronic and zero-point Energies= -1051.291902

Sum of electronic and thermal Energies= -1051.268114

Sum of electronic and thermal Enthalpies= -1051.267170

Sum of electronic and thermal Free Energies= -1051.344417

C	0.32100600	-0.21013500	1.39318000
C	0.82256400	-0.84312200	0.30318200
C	0.58039100	-0.48907100	-1.09488500
C	-0.52653800	0.98176200	1.40908800
C	0.38355300	0.77092300	-1.54940100
C	-0.47913300	1.97502300	0.49279000
C	0.47054300	1.96386500	-0.66005500
N	1.22495700	2.93564300	-0.98624100
C	1.27100000	4.11104500	-0.13453800
H	2.24998100	4.58031500	-0.25025500
H	0.50705300	4.82831300	-0.45154600
H	1.10412400	3.88520500	0.92689600
O	-1.28494200	3.07106100	0.46629000
C	-1.65710600	3.69776700	1.68783900
H	-1.88242100	4.73465400	1.43071700
H	-2.53196800	3.22311100	2.13460000
H	-0.83353600	3.66424300	2.40865800
O	-1.36653600	1.09831100	2.49165400
C	-2.34450400	0.06505100	2.56377900
H	-2.96044900	0.28830200	3.43577500
H	-2.96780200	0.06356700	1.66294500
H	-1.86827000	-0.91150100	2.69061200
O	0.54706200	-0.78295100	2.62044300
C	1.31044300	0.03091100	3.50142800
H	0.80575600	0.98468600	3.68882400
H	1.39819000	-0.52312100	4.43660300
H	2.30798700	0.20984600	3.08587100
O	1.62978300	-1.93378200	0.48417700

C	0.91766300	-3.14168200	0.72247100
H	1.66905400	-3.92454800	0.83641400
H	0.32813900	-3.06440800	1.64189500
H	0.26881100	-3.37590100	-0.12743500
O	0.58459900	-1.58065300	-1.91051800
C	1.31708700	-1.50010100	-3.12439700
H	1.64181700	-2.51673100	-3.35421500
H	0.69743900	-1.11341800	-3.93603800
H	2.19574800	-0.85681200	-3.00100800
O	0.00915400	0.93410100	-2.85197900
C	0.72636900	1.87333700	-3.64656700
H	0.44895300	1.65297000	-4.67923700
H	0.45524300	2.90079000	-3.39826300
H	1.80657200	1.75645200	-3.51237300

Cartesian Coordination of MeO-TI Conjugated Acid and Their Thermochemical Values (M06-2X/6-31g(d,p))

TI-2

Zero-point correction= 0.200000 (Hartree/Particle)

Thermal correction to Energy= 0.210400

Thermal correction to Enthalpy= 0.211344

Thermal correction to Gibbs Free Energy= 0.164312

Sum of electronic and zero-point Energies= -479.495181

Sum of electronic and thermal Energies= -479.484782

Sum of electronic and thermal Enthalpies= -479.483837

Sum of electronic and thermal Free Energies= -479.530870

C	-0.08119800	0.21800400	1.62334700
C	0.76309300	-0.34866000	0.70131200
C	1.19079500	0.23028900	-0.50754000
C	-0.71565100	1.47713700	1.59874100
C	0.89885100	1.45629500	-1.05908000
C	-0.67143000	2.48776900	0.66556700
C	0.08089700	2.51220200	-0.58408700
H	-0.30498100	-0.37844100	2.50312500
H	1.13987300	-1.34223900	0.92054500
H	1.37160700	1.64934000	-2.01538000
C	0.61457400	3.88586000	-2.57749200
H	0.33184600	4.88516100	-2.90182000
H	1.70231100	3.84711500	-2.47258900
H	0.29325800	3.16743000	-3.33685700
N	-0.03911600	3.62358700	-1.30337800
H	-0.63937600	4.34095800	-0.91880100

H	1.85857300	-0.38413100	-1.10563600
H	-1.34008600	1.67671200	2.46195600
O	-1.35429000	3.62746700	0.81810600
C	-2.17865800	3.84586900	1.96619000
H	-1.57455300	3.83256500	2.87694800
H	-2.61350300	4.83232000	1.82475300
H	-2.97062800	3.09390500	2.01532300

TI-3

Zero-point correction= 0.199426 (Hartree/Particle)

Thermal correction to Energy= 0.210051

Thermal correction to Enthalpy= 0.210996

Thermal correction to Gibbs Free Energy= 0.163364

Sum of electronic and zero-point Energies= -479.490639

Sum of electronic and thermal Energies= -479.480014

Sum of electronic and thermal Enthalpies= -479.479070

Sum of electronic and thermal Free Energies= -479.526702

C	-0.09768500	0.33753400	1.70111800
C	0.63845500	-0.27256000	0.73334800
C	1.06990100	0.23681100	-0.52778300
C	-0.63004300	1.66821200	1.68757300
C	0.86070900	1.45423100	-1.09550100
C	-0.51472400	2.61969600	0.68635800
C	0.13434400	2.57869700	-0.56592500
H	-0.30718400	-0.25253800	2.58541300
H	0.94385600	-1.29317700	0.94467600
H	1.29826000	1.59829300	-2.07695900
C	0.65862900	3.87441800	-2.63532400

H	0.41904600	4.88281600	-2.96707100
H	1.74672300	3.77418500	-2.59576100
H	0.24826100	3.16645900	-3.36034600
H	-1.01859700	3.55116800	0.93371300
O	-1.33143000	2.11484500	2.72530000
C	-1.57419900	1.30999700	3.88175400
H	-2.15965600	1.94199500	4.54526900
H	-2.15132800	0.41888400	3.62158800
H	-0.63501100	1.03611700	4.36951900
N	0.06484200	3.68343600	-1.31812400
H	-0.44797400	4.46564300	-0.93588600
H	1.65467900	-0.45929600	-1.12263100

TI-4

Zero-point correction= 0.199516 (Hartree/Particle)

Thermal correction to Energy= 0.210125

Thermal correction to Enthalpy= 0.211069

Thermal correction to Gibbs Free Energy= 0.163430

Sum of electronic and zero-point Energies= -479.489994

Sum of electronic and thermal Energies= -479.479385

Sum of electronic and thermal Enthalpies= -479.478441

Sum of electronic and thermal Free Energies= -479.526079

C	-0.23986400	-0.07039000	1.28064900
C	0.79689800	-0.44342200	0.43603800
C	1.35238500	0.28096400	-0.62085800
C	-0.95456800	1.16937100	1.22541100
C	1.06992800	1.52964800	-1.14202100
C	-0.80962400	2.22721700	0.38193000

C	0.09071300	2.45319000	-0.71640700
H	1.21328800	-1.42512100	0.63909400
H	1.68230400	1.83090000	-1.98390100
C	0.76552800	4.05746500	-2.48463200
H	0.42800400	5.04746700	-2.78450900
H	1.82371100	4.11622200	-2.21348500
H	0.64263500	3.37550600	-3.33106700
N	-0.03747100	3.62518800	-1.35045800
H	-0.74678600	4.26367000	-1.02033100
H	2.16051800	-0.23745700	-1.13032600
H	-1.73469100	1.29391500	1.96812200
H	-1.49733100	3.04976900	0.56986000
O	-0.54281900	-0.98513300	2.19232500
C	-1.58358000	-0.78780500	3.15189000
H	-2.55062600	-0.66354400	2.65703200
H	-1.59364800	-1.69658400	3.74851600
H	-1.36239100	0.06939700	3.79363900

TI-23

Zero-point correction= 0.232341 (Hartree/Particle)

Thermal correction to Energy= 0.245682

Thermal correction to Enthalpy= 0.246626

Thermal correction to Gibbs Free Energy= 0.192173

Sum of electronic and zero-point Energies= -593.936934

Sum of electronic and thermal Energies= -593.923593

Sum of electronic and thermal Enthalpies= -593.922649

Sum of electronic and thermal Free Energies= -593.977102

C	1.46398200	1.57557900	0.07638000
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C	0.56559600	2.59037000	0.23482100
C	-0.84915300	2.51998600	0.26070700
C	1.23366100	0.17929900	-0.09193000
C	-1.65931500	1.43272000	0.11734400
C	0.00734300	-0.49338900	-0.10251400
C	-1.31618600	0.05699800	-0.07577500
H	2.50592200	1.87269000	0.08063300
H	0.98876700	3.58280700	0.35500600
H	-2.72380500	1.63279900	0.16679400
C	-3.72567700	-0.53082400	-0.26414200
H	-4.25843700	-1.46306100	-0.44126500
H	-4.06732900	-0.11388800	0.68746000
H	-3.96391000	0.16427300	-1.07448300
H	-1.35911900	3.46773100	0.40662500
O	0.01878500	-1.83790400	-0.27151700
C	0.50789300	-2.63217600	0.82946900
H	0.30284000	-3.66525300	0.55527200
H	1.57902100	-2.48618100	0.96130700
H	-0.03203500	-2.37231000	1.74450400
O	2.26478100	-0.65153900	-0.25389600
C	3.60933100	-0.17637400	-0.34158200
H	3.72069800	0.52694600	-1.17104500
H	3.92581600	0.28206400	0.59937900
H	4.20778100	-1.06370900	-0.53514600
N	-2.30258200	-0.82893100	-0.22718000
H	-2.00151000	-1.77998200	-0.39815700

TI-24

Zero-point correction= 0.232836 (Hartree/Particle)

Thermal correction to Energy= 0.245861

Thermal correction to Enthalpy= 0.246805

Thermal correction to Gibbs Free Energy= 0.193241

Sum of electronic and zero-point Energies= -593.952985

Sum of electronic and thermal Energies= -593.939961

Sum of electronic and thermal Enthalpies= -593.939016

Sum of electronic and thermal Free Energies= -593.992581

C	1.78819700	-0.07338000	-0.00006500
C	1.65553000	-1.45515300	-0.00014000
C	0.45479300	-2.16387200	-0.00007700
C	0.74249800	0.89582000	-0.00002400
C	-0.86809600	-1.75662200	0.00001400
C	-0.61756600	0.76926000	-0.00002400
C	-1.41287300	-0.46109200	-0.00000300
H	2.55942300	-2.05015600	-0.00024600
H	-1.59273700	-2.56191800	0.00005700
C	-3.71710100	-1.35676200	0.00009000
H	-4.70784500	-0.90666900	0.00017100
H	-3.61568700	-1.98059500	-0.89281800
H	-3.61554400	-1.98057400	0.89299700
H	0.57857200	-3.24384200	-0.00010700
H	1.13694000	1.90528200	0.00002300
O	-1.42293900	1.83888100	0.00002800
C	-0.88514800	3.16242300	-0.00003400
H	-1.74806800	3.82395100	-0.00004800
H	-0.28647700	3.33095800	0.89914100
H	-0.28650100	3.33087900	-0.89924000

O	2.97324000	0.53006600	-0.00006400
C	4.17772300	-0.23717000	0.00019100
H	4.23823400	-0.85703400	-0.89854100
H	4.98311700	0.49347900	0.00050100
H	4.23772400	-0.85723700	0.89881500
N	-2.73287200	-0.28682700	0.00000300
H	-3.06120200	0.66897000	-0.00001400

TI-25

Zero-point correction= 0.232570 (Hartree/Particle)

Thermal correction to Energy= 0.245586

Thermal correction to Enthalpy= 0.246530

Thermal correction to Gibbs Free Energy= 0.193310

Sum of electronic and zero-point Energies= -593.948028

Sum of electronic and thermal Energies= -593.935011

Sum of electronic and thermal Enthalpies= -593.934067

Sum of electronic and thermal Free Energies= -593.987287

C	1.55286400	0.95564200	0.00000600
C	2.00176200	-0.35199300	0.00001900
C	1.16851500	-1.50525400	-0.00006800
C	0.22979200	1.42676900	-0.00008400
C	-0.19086000	-1.62518600	-0.00001200
C	-0.98925700	0.78181200	-0.00006600
C	-1.22095900	-0.64104200	0.00003500
H	2.30426700	1.73641300	0.00006900
H	-0.54899600	-2.64854700	0.00002700
C	-2.96778900	-2.40643100	-0.00001800
H	-4.05573300	-2.38755500	-0.00079600

H	-2.62922200	-2.93889800	-0.89330000
H	-2.63038600	-2.93870100	0.89383000
H	1.73238900	-2.43444800	-0.00011700
H	0.16424900	2.50915400	-0.00016100
O	-2.15718900	1.45207200	-0.00008700
C	-2.18176300	2.87796200	0.00007200
H	-3.23489000	3.14957500	0.00016200
H	-1.69957300	3.27198900	0.89930600
H	-1.69968900	3.27218000	-0.89914000
O	3.29513000	-0.68482200	0.00012200
C	4.29210300	0.33166400	-0.00002800
H	5.24364300	-0.19494900	-0.00011200
H	4.21356200	0.95167300	-0.89848500
H	4.21376000	0.95174400	0.89839800
N	-2.49454300	-1.03042900	0.00007700
H	-3.18155400	-0.28828300	0.00035800

TI-26

Zero-point correction= 0.232664 (Hartree/Particle)

Thermal correction to Energy= 0.245769

Thermal correction to Enthalpy= 0.246713

Thermal correction to Gibbs Free Energy= 0.193060

Sum of electronic and zero-point Energies= -593.951819

Sum of electronic and thermal Energies= -593.938714

Sum of electronic and thermal Enthalpies= -593.937770

Sum of electronic and thermal Free Energies= -593.991424

C	0.50428700	-2.17267300	-0.00011100
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C	1.66170500	-1.44681600	-0.00007500
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C	1.76838200	-0.03123600	-0.00014500
C	-0.85109200	-1.76598200	-0.00020800
C	0.73358400	0.90485700	0.00010100
C	-1.38851000	-0.50630400	-0.00009300
C	-0.65832800	0.76469600	-0.00001400
H	0.63727500	-3.25095400	-0.00010500
H	2.58411500	-2.01323500	-0.00005200
H	1.10717000	1.92222900	0.00030900
C	-0.93736700	3.22333400	-0.00001100
H	-1.79593500	3.89174200	-0.00069500
H	-0.33775200	3.42433100	0.89287900
H	-0.33672600	3.42392100	-0.89229200
H	-1.56107800	-2.58396300	-0.00036800
O	-2.70671800	-0.28791200	-0.00005400
C	-3.62872300	-1.37986800	0.00029000
H	-4.61609300	-0.92412200	0.00075000
H	-3.49873700	-1.98763000	-0.89914600
H	-3.49793200	-1.98773400	0.89953800
O	2.96065900	0.55780100	-0.00040800
C	4.17112600	-0.20142700	0.00043200
H	4.24204200	-0.81908600	-0.89874300
H	4.96853200	0.53809800	0.00083800
H	4.24092900	-0.81888800	0.89982600
N	-1.42745600	1.85602800	-0.00004800
H	-2.42553600	1.70250000	0.00030200

TI-27

Zero-point correction= 0.233136 (Hartree/Particle)

Thermal correction to Energy=	0.246041
Thermal correction to Enthalpy=	0.246985
Thermal correction to Gibbs Free Energy=	0.193692
Sum of electronic and zero-point Energies=	-593.938364
Sum of electronic and thermal Energies=	-593.925459
Sum of electronic and thermal Enthalpies=	-593.924515
Sum of electronic and thermal Free Energies=	-593.977808

C	-0.47229000	-0.08906500	1.68409900
C	0.35000600	-0.70448100	0.77293700
C	0.79023200	-0.20415000	-0.45992800
C	-1.03599400	1.19140700	1.59780100
C	0.60902400	1.02685200	-1.06461400
C	-0.86926100	2.18921000	0.65960300
C	-0.02657200	2.20530900	-0.52261700
H	-0.73362300	-0.65466300	2.57243700
H	0.67909100	-1.71104200	1.01021900
C	0.90291700	3.86173800	-2.23310300
H	0.84157400	4.94891000	-2.21538300
H	1.93826500	3.56030800	-2.08336200
H	0.55294300	3.49385200	-3.19674800
H	1.37111000	-0.90930200	-1.04295500
H	-1.68683400	1.44959600	2.42514300
O	-1.49437400	3.37503700	0.79030300
C	-2.41043100	3.61620000	1.85780800
H	-2.79246200	4.62008900	1.68729300
H	-3.23341200	2.89704600	1.82714700
H	-1.89769600	3.57484900	2.82271500
O	1.06197200	1.25984000	-2.30558500

C	1.66493800	0.22256100	-3.07460400
H	0.98098800	-0.62403000	-3.18489800
H	1.86068700	0.66610700	-4.04863900
H	2.60674700	-0.10279200	-2.62314600
N	0.05382100	3.38176400	-1.13849400
H	-0.51384400	4.09489300	-0.69844000

TI-34

Zero-point correction= 0.232313 (Hartree/Particle)

Thermal correction to Energy= 0.245494

Thermal correction to Enthalpy= 0.246438

Thermal correction to Gibbs Free Energy= 0.192911

Sum of electronic and zero-point Energies= -593.939295

Sum of electronic and thermal Energies= -593.926113

Sum of electronic and thermal Enthalpies= -593.925169

Sum of electronic and thermal Free Energies= -593.978696

C	-0.15668500	0.10501900	1.66072700
C	0.46465800	-0.68005900	0.72189100
C	0.99231600	-0.31899400	-0.54156000
C	-0.31230000	1.55565700	1.58832900
C	0.95315600	0.85703300	-1.22957800
C	-0.11417900	2.36378900	0.49166700
C	0.37683100	2.09417600	-0.81267200
H	0.55056800	-1.73362200	0.95830700
H	1.39840300	0.85420300	-2.22111900
C	-0.16311300	4.42550500	-1.49863000
H	-0.09227300	4.96860300	-2.43896900
H	-1.21376500	4.38016900	-1.20005500

H	0.40947800	4.96708700	-0.73975200
H	1.47532200	-1.13879600	-1.06596700
H	-0.37320400	3.39464000	0.70596400
O	-0.80026900	2.20979000	2.63885800
C	-0.40113700	1.93309700	3.99612100
H	-0.35947400	2.90815200	4.47915400
H	-1.14064100	1.29735700	4.47857000
H	0.58199300	1.46033100	4.02503500
O	-0.69835100	-0.38938500	2.77261200
C	-0.68494700	-1.79599000	3.01254700
H	0.34162000	-2.16139600	3.10861900
H	-1.21521000	-1.93374900	3.95202200
H	-1.20539600	-2.32546400	2.20964800
N	0.37203200	3.08804100	-1.70704800
H	0.77482700	2.89264800	-2.61265200

TI-35

Zero-point correction= 0.232192 (Hartree/Particle)

Thermal correction to Energy= 0.245434

Thermal correction to Enthalpy= 0.246379

Thermal correction to Gibbs Free Energy= 0.192631

Sum of electronic and zero-point Energies= -593.945954

Sum of electronic and thermal Energies= -593.932712

Sum of electronic and thermal Enthalpies= -593.931767

Sum of electronic and thermal Free Energies= -593.985515

C	-0.24244300	0.31051600	1.82164300
C	0.08549800	-0.64710100	0.88374500
C	0.44375300	-0.42624100	-0.49104100

C	-0.31657400	1.70991000	1.66579800
C	0.53054400	0.73761300	-1.17653500
C	-0.08091400	2.49182900	0.52665000
C	0.29394400	2.09981400	-0.75725400
H	-0.46968000	-0.10352500	2.79612100
H	0.82725400	0.63578100	-2.21855000
C	0.27850100	4.45694800	-1.52083500
H	0.47424100	4.95920500	-2.46621800
H	-0.74803800	4.67896800	-1.21312400
H	0.97333100	4.84303200	-0.76864200
H	0.68157100	-1.31417900	-1.06474200
H	-0.22012000	3.55051900	0.71071400
O	-0.65724000	2.47142000	2.70313100
C	-0.95389600	1.91163800	3.98264300
H	-1.19869000	2.76293500	4.61331700
H	-1.81333300	1.23865100	3.92205400
H	-0.08359000	1.38934900	4.38903500
O	0.05166700	-1.88564900	1.36940800
C	0.32614800	-3.03056900	0.56039300
H	1.35465900	-3.01089000	0.19012600
H	0.19646300	-3.88152500	1.22506500
H	-0.38361400	-3.10269000	-0.26815100
N	0.46348600	3.02937300	-1.71346900
H	0.73582700	2.71655300	-2.63293800

TI-36

Zero-point correction= 0.232449 (Hartree/Particle)

Thermal correction to Energy= 0.245651

Thermal correction to Enthalpy= 0.246595
 Thermal correction to Gibbs Free Energy= 0.192945
 Sum of electronic and zero-point Energies= -593.943066
 Sum of electronic and thermal Energies= -593.929864
 Sum of electronic and thermal Enthalpies= -593.928920
 Sum of electronic and thermal Free Energies= -593.982570

C	-0.10143700	0.35282800	1.67988600
C	0.63284200	-0.27484000	0.72676000
C	1.08044000	0.21915300	-0.54615700
C	-0.63812600	1.68568500	1.68482800
C	0.84949100	1.46351700	-1.09242400
C	-0.52357500	2.62919700	0.69175900
C	0.13381800	2.56789500	-0.56656300
H	-0.31251300	-0.24070100	2.56181800
H	0.91838600	-1.29283600	0.96433400
H	1.29605700	1.58512900	-2.07235800
C	0.65552000	3.86093500	-2.63137200
H	0.42004200	4.86757300	-2.97151000
H	1.74345700	3.75507500	-2.58916200
H	0.24648500	3.14703600	-3.35196700
H	-1.02152200	3.56611500	0.92892900
O	-1.33744100	2.11864200	2.73750700
C	-1.56525100	1.29929200	3.88306400
H	-2.14640800	1.91954000	4.56170200
H	-2.14318700	0.40864800	3.62091200
H	-0.62196400	1.02113800	4.36162000
O	1.80577900	-0.56634200	-1.34312500
C	2.16745100	-1.89783700	-0.97657900

H	1.27991900	-2.52265800	-0.84299300
H	2.75044100	-2.27157800	-1.81522100
H	2.78377900	-1.90250100	-0.07351000
N	0.06068800	3.67852200	-1.31655000
H	-0.45065500	4.45995800	-0.93361000

TI-45

Zero-point correction= 0.232079 (Hartree/Particle)

Thermal correction to Energy= 0.245420

Thermal correction to Enthalpy= 0.246365

Thermal correction to Gibbs Free Energy= 0.192078

Sum of electronic and zero-point Energies= -593.934038

Sum of electronic and thermal Energies= -593.920697

Sum of electronic and thermal Enthalpies= -593.919752

Sum of electronic and thermal Free Energies= -593.974039

C	-0.49320600	0.11624700	1.81151500
C	0.30527700	-0.55182700	0.86629100
C	0.77778900	0.01296800	-0.33760600
C	-0.79164200	1.50387700	1.79305000
C	0.71314900	1.27734600	-0.87815800
C	-0.52017200	2.50863000	0.90805300
C	0.14726800	2.46225100	-0.34707100
H	1.18897000	1.37345800	-1.84754500
C	0.87868300	3.75980800	-2.33707700
H	0.79002300	4.80110500	-2.64076900
H	1.94139800	3.50516000	-2.28154200
H	0.39315800	3.13634600	-3.09397700
H	1.31529700	-0.68738100	-0.96786200

H	-0.89572300	3.48722200	1.19856800
H	-1.35503100	1.79425000	2.67585500
O	-0.98661200	-0.47627300	2.89493200
C	-1.41199000	-1.85063400	2.93590800
H	-0.57889600	-2.50116000	3.19356000
H	-2.17279900	-1.87629700	3.71406800
H	-1.84360200	-2.14725300	1.97851200
O	0.59908900	-1.81777600	1.19745100
C	1.44050900	-2.62193200	0.37545800
H	2.42531100	-2.16065200	0.25601400
H	1.54287000	-3.56526400	0.90755300
H	0.98095700	-2.80293600	-0.60088500
N	0.23595100	3.60674500	-1.04187200
H	-0.17369600	4.43271700	-0.63052500

TI-234

Zero-point correction= 0.265400 (Hartree/Particle)

Thermal correction to Energy= 0.281194

Thermal correction to Enthalpy= 0.282138

Thermal correction to Gibbs Free Energy= 0.222573

Sum of electronic and zero-point Energies= -708.385452

Sum of electronic and thermal Energies= -708.369658

Sum of electronic and thermal Enthalpies= -708.368714

Sum of electronic and thermal Free Energies= -708.428280

C	1.47003600	-0.69877500	-0.10525300
C	1.05616900	-2.01526300	-0.08318800
C	-0.25256500	-2.50454700	0.01916300
C	0.64467000	0.48776700	0.01440200

C	-1.46156100	-1.85649200	0.08578800
C	-0.73553300	0.58856800	-0.01914100
C	-1.73081000	-0.46956300	0.05003800
H	1.82751300	-2.77034800	-0.16187500
H	-2.33148700	-2.49876800	0.14781700
C	-4.16382400	-0.90143600	0.22333400
H	-5.04566700	-0.26473400	0.25402300
H	-4.24840200	-1.57182800	-0.63688000
H	-4.12832200	-1.49320000	1.14272600
H	-0.32186200	-3.58878400	0.03845700
O	-1.31663500	1.80340900	-0.00812300
C	-0.88079500	2.85267600	-0.89779000
H	-1.78894800	3.37775600	-1.19223700
H	-0.20106200	3.52401100	-0.37803300
H	-0.38698800	2.42828700	-1.77343400
O	1.28801500	1.66807500	0.05367100
C	2.22256800	1.91654900	1.12136500
H	3.23815600	1.87338100	0.73142700
H	1.99757900	2.91581200	1.49506100
H	2.09740700	1.18732600	1.92500400
O	2.75188500	-0.36137000	-0.23188200
C	3.75393800	-1.36884300	-0.36396200
H	4.69247500	-0.82878700	-0.46521900
H	3.78339000	-2.00352300	0.52615900
H	3.57537700	-1.97228300	-1.25823400
N	-2.99391200	-0.04773300	0.10505000
H	-3.12164400	0.95506200	0.09201900

TI-235

Zero-point correction= 0.265209 (Hartree/Particle)

Thermal correction to Energy= 0.281096

Thermal correction to Enthalpy= 0.282040

Thermal correction to Gibbs Free Energy= 0.222079

Sum of electronic and zero-point Energies= -708.388510

Sum of electronic and thermal Energies= -708.372623

Sum of electronic and thermal Enthalpies= -708.371679

Sum of electronic and thermal Free Energies= -708.431640

C	-1.32134000	0.97747700	-0.05740300
C	-2.02042200	-0.21069000	0.04489400
C	-1.46288700	-1.52218800	0.07057800
C	0.06115100	1.21712200	-0.14271300
C	-0.15709000	-1.89825600	-0.00530900
C	1.12147100	0.28724300	-0.12200500
C	1.04561400	-1.12573800	-0.11038200
H	-1.96921100	1.84520900	-0.06935900
H	0.00389200	-2.97032300	0.02976600
C	2.39357700	-3.21997600	-0.21732400
H	3.45877700	-3.42419700	-0.30905400
H	2.03669700	-3.68360900	0.70715500
H	1.88277400	-3.67318400	-1.07283500
H	-2.16866600	-2.34011200	0.15515300
O	2.38622200	0.76911400	-0.22756100
C	2.92052800	1.40631400	0.94906700
H	2.88985400	0.71440000	1.79634700
H	3.95216100	1.65408500	0.70592900
H	2.36408000	2.31480700	1.17854000

O	0.51233300	2.46846100	-0.24943000
C	-0.38091300	3.57749900	-0.34455300
H	-0.97793700	3.67858300	0.56616900
H	0.26158800	4.44750100	-0.46008000
H	-1.02894300	3.48029000	-1.21978500
O	-3.34154300	-0.03147800	0.12057100
C	-4.23985800	-1.13475100	0.22462600
H	-4.05091400	-1.70873200	1.13631400
H	-5.23093100	-0.68957000	0.27573600
H	-4.17384200	-1.77890300	-0.65688800
N	2.21597000	-1.77880000	-0.18833100
H	3.02374500	-1.18775000	-0.33027200

TI-236

Zero-point correction= 0.265269 (Hartree/Particle)

Thermal correction to Energy= 0.281137

Thermal correction to Enthalpy= 0.282082

Thermal correction to Gibbs Free Energy= 0.221999

Sum of electronic and zero-point Energies= -708.390003

Sum of electronic and thermal Energies= -708.374135

Sum of electronic and thermal Enthalpies= -708.373191

Sum of electronic and thermal Free Energies= -708.433273

C	0.00092900	-1.84182500	-0.02041000
C	1.34325600	-1.61577300	0.05543400
C	2.02211400	-0.36578500	0.04552000
C	-1.10342800	-0.94781600	-0.10765600
C	1.44706600	0.88901500	-0.04189200
C	-1.07087800	0.44050000	-0.05855200

C	0.09815000	1.29307400	-0.09657200
H	-0.27247200	-2.89057000	-0.02088600
H	1.95972800	-2.50405200	0.11601300
H	2.18266100	1.68509500	-0.04380700
C	0.81664100	3.66299600	-0.24758100
H	0.28794900	4.61057200	-0.33129700
H	1.43527400	3.68945400	0.65454800
H	1.46067700	3.54583800	-1.12450600
O	-2.21471200	1.14796300	-0.09747600
C	-3.30799100	0.83999400	0.79105200
H	-3.76266400	1.79964400	1.03406100
H	-4.02486800	0.19311400	0.29042400
H	-2.93586300	0.36156000	1.69954200
O	-2.35045200	-1.43263500	-0.24024600
C	-2.60314200	-2.83234800	-0.32093800
H	-2.31058300	-3.34243300	0.60181700
H	-3.67937600	-2.91885300	-0.45540200
H	-2.09422600	-3.27525200	-1.18197800
O	3.35456200	-0.31490800	0.11313900
C	4.14112900	-1.50016400	0.21552700
H	4.01066600	-2.13403600	-0.66629000
H	5.17106500	-1.15415400	0.26409600
H	3.89845200	-2.05421700	1.12671900
N	-0.17065600	2.60126300	-0.17582900
H	-1.15008300	2.84487500	-0.21917200

TI-237

Zero-point correction= 0.266198 (Hartree/Particle)

Thermal correction to Energy=	0.281752
Thermal correction to Enthalpy=	0.282697
Thermal correction to Gibbs Free Energy=	0.223519
Sum of electronic and zero-point Energies=	-708.382629
Sum of electronic and thermal Energies=	-708.367075
Sum of electronic and thermal Enthalpies=	-708.366130

C	-1.41216800	-1.85515100	-0.18159100
C	-0.19943900	-2.48593500	-0.14478000
C	1.09515400	-1.95302200	0.00128500
C	-1.66471300	-0.46523300	-0.11241600
C	1.51140800	-0.64344100	0.02807100
C	-0.72473000	0.57874400	-0.10264600
C	0.69863200	0.54501100	-0.19669100
H	-2.27926300	-2.49785700	-0.26137400
H	-0.23610000	-3.56993600	-0.19801500
C	2.65194100	2.09613500	-0.74219300
H	2.61120600	3.10336200	-1.15468900
H	3.29605900	2.09186700	0.13653500
H	3.06245600	1.42334600	-1.49433900
H	1.87579000	-2.69517300	0.11344700
O	-1.23049400	1.84378300	-0.15283400
C	-1.73240000	2.35655300	1.09652000
H	-0.94431600	2.33546900	1.85574400
H	-2.03077800	3.38392900	0.89523300
H	-2.59483200	1.77578900	1.42436600
O	-2.91661300	-0.00578600	-0.09595100
C	-4.03198000	-0.89283000	-0.17975900
H	-4.05553300	-1.57361300	0.67556900

H	-4.90751700	-0.24805600	-0.16014900
H	-4.01256100	-1.45410600	-1.11772900
O	2.78249500	-0.31360800	0.27435500
C	3.74426400	-1.31657800	0.59399300
H	3.90514400	-1.98540900	-0.25645100
H	4.66168700	-0.77497000	0.81391400
H	3.42850000	-1.88567200	1.47297200
N	1.27593500	1.73142000	-0.40103300
H	0.58958100	2.47046200	-0.50112200

TI-245

Zero-point correction= 0.265681 (Hartree/Particle)

Thermal correction to Energy= 0.281317

Thermal correction to Enthalpy= 0.282261

Thermal correction to Gibbs Free Energy= 0.223359

Sum of electronic and zero-point Energies= -708.390734

Sum of electronic and thermal Energies= -708.375097

Sum of electronic and thermal Enthalpies= -708.374153

Sum of electronic and thermal Free Energies= -708.433055

C	1.19380400	0.78182000	-0.04073600
C	1.55014400	-0.58356800	-0.07867300
C	0.63947900	-1.63877700	0.02121600
C	-0.11576000	1.30588100	-0.06394200
C	-0.74351500	-1.68161700	0.09424800
C	-1.36951400	0.74022400	-0.05668300
C	-1.70614200	-0.66157300	0.05174300
H	-1.14737700	-2.68458600	0.17003500
C	-3.55854400	-2.29419500	0.21567400

H	-4.64370300	-2.21818500	0.24682500
H	-3.27828200	-2.90855400	-0.64578800
H	-3.21886700	-2.78292200	1.13421600
H	1.09293900	-2.62385900	0.02937900
H	-0.08526400	2.38917700	-0.08927900
O	-2.47711800	1.49305900	-0.10964900
C	-2.39675100	2.91265300	-0.23754600
H	-3.42692800	3.25514100	-0.30153700
H	-1.91537400	3.35058400	0.64125000
H	-1.85624900	3.18563800	-1.14776200
O	2.10315500	1.75543100	-0.06741700
C	3.38227700	1.67098200	0.58728800
H	4.12767900	1.25180100	-0.08501600
H	3.62869800	2.70136900	0.83794800
H	3.31146600	1.07060500	1.49580000
O	2.86962700	-0.79656000	-0.23330700
C	3.38559600	-2.12078300	-0.29778000
H	2.95647800	-2.66695000	-1.14368000
H	4.45725200	-2.00564100	-0.44646700
H	3.20242100	-2.66131800	0.63632200
N	-3.01239800	-0.95438200	0.10379200
H	-3.64986900	-0.17334200	0.05535300

TI-246

Zero-point correction= 0.266407 (Hartree/Particle)

Thermal correction to Energy= 0.281797

Thermal correction to Enthalpy= 0.282741

Thermal correction to Gibbs Free Energy= 0.224321

Sum of electronic and zero-point Energies=	-708.407791
Sum of electronic and thermal Energies=	-708.392401
Sum of electronic and thermal Enthalpies=	-708.391457
Sum of electronic and thermal Free Energies=	-708.449877
C	-1.71148300 -0.65593100 0.00009900
C	-1.70515200 0.71706100 0.00005700
C	-0.57768200 1.56789500 -0.00021100
C	-0.59183600 -1.55123000 -0.00003000
C	0.78246800 1.24733400 -0.00027400
C	0.74344500 -1.30592800 -0.00012900
C	1.41682100 0.00211000 0.00002900
H	-2.64680900 1.25020200 0.00018700
H	1.45578700 2.09144500 -0.00053200
C	3.63704900 1.08815500 0.00050000
H	4.66375100 0.72779400 0.00123600
H	3.48240000 1.70152700 -0.89294400
H	3.48132100 1.70206700 0.89337600
H	-0.90794300 -2.58753900 -0.00005400
O	1.65090000 -2.29522900 -0.00028700
C	1.22830800 -3.65803900 -0.00030700
H	2.14309800 -4.24592700 -0.00041000
H	0.64475000 -3.87698000 0.89816100
H	0.64460700 -3.87690100 -0.89870400
O	-2.84471300 -1.35997600 0.00030100
C	-4.10350200 -0.69064400 0.00027400
H	-4.21232000 -0.07564900 -0.89772100
H	-4.85069500 -1.48086800 0.00024700
H	-4.21237600 -0.07566500 0.89827400

O	-0.96270900	2.84450600	-0.00043300
C	-0.02164400	3.91354300	-0.00009100
H	-0.62086400	4.82107800	0.00014900
H	0.60068400	3.88412300	0.89903400
H	0.60073200	3.88464400	-0.89919900
N	2.74990100	-0.05984100	0.00036200
H	3.15600000	-0.98482700	0.00020900

TI-247

Zero-point correction= 0.266186 (Hartree/Particle)

Thermal correction to Energy= 0.281736

Thermal correction to Enthalpy= 0.282680

Thermal correction to Gibbs Free Energy= 0.222485

Sum of electronic and zero-point Energies= -708.391272

Sum of electronic and thermal Energies= -708.375722

Sum of electronic and thermal Enthalpies= -708.374778

Sum of electronic and thermal Free Energies= -708.434973

C	2.06055200	-0.37513300	0.00032100
C	1.40897000	-1.59470700	0.00000800
C	0.03006000	-1.81077500	-0.00016200
C	1.43977200	0.89647100	0.00068700
C	-1.07135200	-0.96893700	-0.00018700
C	0.12371700	1.27479100	0.00022300
C	-1.08988900	0.46097100	-0.00016800
H	2.01453900	-2.49191300	-0.00003200
C	-3.63727500	0.77677500	-0.00098900
H	-4.20682600	1.70496100	-0.00204800
H	-3.88927400	0.20025900	-0.88940400

H	-3.89013500	0.20177300	0.88821400
H	-0.22853600	-2.86319400	-0.00031500
H	2.16937000	1.69796100	0.00106900
O	-0.20594500	2.58093300	0.00015300
C	0.79336000	3.59828000	0.00050800
H	0.24529000	4.53773500	0.00027400
H	1.41168400	3.53070700	0.89972400
H	1.41236600	3.53067700	-0.89823400
O	3.39277100	-0.26007700	0.00057600
C	4.20551400	-1.43004600	-0.00121400
H	4.02227600	-2.02717300	-0.89964000
H	5.23191800	-1.07067300	-0.00196400
H	4.02416400	-2.02865300	0.89661700
O	-2.32335700	-1.47555900	-0.00037200
C	-2.54845100	-2.87857400	0.00134600
H	-2.13082700	-3.34324300	0.90015300
H	-3.63040800	-2.99609300	0.00186100
H	-2.13151200	-3.34535300	-0.89668400
N	-2.22284200	1.16333500	-0.00067400
H	-2.06180900	2.16179900	0.00003000

TI-345

Zero-point correction= 0.264569 (Hartree/Particle)

Thermal correction to Energy= 0.280619

Thermal correction to Enthalpy= 0.281563

Thermal correction to Gibbs Free Energy= 0.221309

Sum of electronic and zero-point Energies= -708.379558

Sum of electronic and thermal Energies= -708.363508

Sum of electronic and thermal Enthalpies= -708.362564

Sum of electronic and thermal Free Energies= -708.422817

C	0.10328600	0.12259600	1.65956000
C	0.75907500	-0.63127500	0.68595400
C	1.12421600	-0.21303200	-0.62617000
C	-0.13942100	1.53718900	1.60393700
C	0.92237200	0.96035800	-1.28364000
C	-0.08102100	2.39197400	0.50701700
C	0.31046400	2.16777000	-0.82057300
H	1.28042400	0.98692600	-2.31010000
C	-0.40933200	4.45666400	-1.45246500
H	-0.45130900	5.01381400	-2.38643300
H	-1.42637200	4.34927800	-1.06450100
H	0.19326000	5.02349900	-0.73531200
H	1.63288200	-0.96841800	-1.21388700
H	-0.40447000	3.39386200	0.76507900
O	-0.58664700	2.16092200	2.69192500
C	-0.12209300	1.86249700	4.02257700
H	-0.08588300	2.82748400	4.52636100
H	-0.81969200	1.19364700	4.52228700
H	0.87098800	1.41219500	3.99582400
O	-0.27555000	-0.45741500	2.80956200
C	-1.07510400	-1.65316400	2.77287800
H	-0.44567200	-2.52883800	2.92199900
H	-1.79026100	-1.55248100	3.58891400
H	-1.60719000	-1.72942000	1.82143800
O	1.02021800	-1.88208000	1.09042300
C	1.63709800	-2.83588600	0.22932500

H	2.64746300	-2.52056100	-0.04620700
H	1.69292100	-3.75106000	0.81483700
H	1.03195200	-3.01131100	-0.66512900
N	0.17823200	3.15569100	-1.72180100
H	0.52149700	2.98583300	-2.65527600

TI-346

Zero-point correction= 0.265606 (Hartree/Particle)

Thermal correction to Energy= 0.281250

Thermal correction to Enthalpy= 0.282194

Thermal correction to Gibbs Free Energy= 0.223211

Sum of electronic and zero-point Energies= -708.393811

Sum of electronic and thermal Energies= -708.378168

Sum of electronic and thermal Enthalpies= -708.377223

Sum of electronic and thermal Free Energies= -708.436206

C	-0.20036900	0.11304100	1.71428200
C	0.43576900	-0.68127000	0.80769100
C	1.01104200	-0.36255500	-0.46311700
C	-0.36167200	1.56708700	1.62915300
C	0.95495600	0.81942800	-1.16831100
C	-0.14148400	2.35223400	0.53040000
C	0.37146000	2.04452700	-0.76442300
H	0.52313100	-1.73662600	1.03547600
H	1.39402200	0.82197000	-2.15880900
C	-0.16951800	4.37245500	-1.48496800
H	-0.08909600	4.90093300	-2.43307000
H	-1.22356900	4.33215600	-1.19851300
H	0.39360800	4.92893500	-0.72990700

H	-0.39569400	3.38921100	0.71489100
O	-0.87692400	2.22236000	2.66831600
C	-0.46710600	1.96916500	4.02598100
H	-0.42644200	2.95025500	4.49724800
H	-1.20000600	1.33610800	4.52224200
H	0.51846900	1.50107300	4.05692300
O	-0.76738500	-0.37197300	2.81997900
C	-0.75458700	-1.77580200	3.06881300
H	0.27105600	-2.13863700	3.18424900
H	-1.30124100	-1.90983500	3.99947100
H	-1.25849100	-2.31183800	2.25946900
O	1.61005800	-1.44673000	-0.96244900
C	2.23652800	-1.41020600	-2.24066400
H	2.66035600	-2.40158300	-2.38285000
H	1.50162100	-1.20760000	-3.02562900
H	3.03429400	-0.66162800	-2.26050000
N	0.37098300	3.03356900	-1.66997800
H	0.78028800	2.83112400	-2.57023500

TI-347

Zero-point correction= 0.266038 (Hartree/Particle)

Thermal correction to Energy= 0.281531

Thermal correction to Enthalpy= 0.282475

Thermal correction to Gibbs Free Energy= 0.223843

Sum of electronic and zero-point Energies= -708.393388

Sum of electronic and thermal Energies= -708.377895

Sum of electronic and thermal Enthalpies= -708.376951

Sum of electronic and thermal Free Energies= -708.435583

C	-0.31455100	0.14367100	1.78457400
C	0.44686900	-0.46798400	0.81946700
C	0.99249000	0.02907900	-0.38556100
C	-0.65798700	1.54747100	1.79761700
C	0.85700800	1.24196000	-1.00596500
C	-0.48634800	2.45597200	0.76859300
C	0.10212400	2.37502000	-0.50910900
H	0.65916200	-1.51749100	0.98503700
C	-0.66575600	4.66959500	-1.04073000
H	-0.61436600	5.29871000	-1.92715200
H	-1.71680400	4.47483600	-0.81082100
H	-0.20442200	5.20487200	-0.20500200
H	1.58311500	-0.70426000	-0.92222600
H	-0.89193000	3.42582200	1.03384700
O	-1.29887200	2.06912300	2.84136000
C	-0.99309800	1.73010300	4.20748800
H	-1.14519400	2.65475200	4.76219000
H	-1.66892800	0.95491800	4.56228400
H	0.04310100	1.40226300	4.30474400
O	-0.83323900	-0.51761500	2.82901100
C	-0.64271300	-1.92332900	2.94450400
H	0.41678900	-2.16458500	3.07575700
H	-1.19851500	-2.21988400	3.83126100
H	-1.04393200	-2.44017700	2.06724600
O	1.41344700	1.52145300	-2.19910700
C	2.21321700	0.54743500	-2.86424500
H	1.61871000	-0.33764800	-3.10841900
H	2.55320500	1.02553800	-3.78022000

H	3.07491200	0.27207700	-2.24950800
N	0.03774600	3.43002700	-1.32288100
H	0.53193400	3.34368600	-2.20026000

TI-2345

Zero-point correction= 0.297915 (Hartree/Particle)

Thermal correction to Energy= 0.316407

Thermal correction to Enthalpy= 0.317351

Thermal correction to Gibbs Free Energy= 0.251832

Sum of electronic and zero-point Energies= -822.823851

Sum of electronic and thermal Energies= -822.805359

Sum of electronic and thermal Enthalpies= -822.804415

Sum of electronic and thermal Free Energies= -822.869934

C	-1.24864400	-0.25191500	0.10654700
C	-1.48330600	1.12680900	0.05921600
C	-0.49011500	2.12986500	0.07753600
C	-0.00733200	-0.94529800	0.12823500
C	0.87662700	2.03160100	0.08394900
C	1.30004000	-0.46012200	-0.00147500
C	1.73501000	0.90286600	0.03469700
H	1.39052300	2.98614500	0.09814900
C	3.73305100	2.37899200	0.10017100
H	4.80637600	2.19896900	0.09803500
H	3.48802000	3.00578500	-0.76277900
H	3.47530700	2.91231700	1.02052900
H	-0.85970800	3.14881200	0.08157400
O	2.33680500	-1.31801200	-0.03912000
C	2.32879700	-2.46865000	-0.90780100

H	3.34960200	-2.56142800	-1.27727300
H	2.04141000	-3.35640800	-0.34864600
H	1.63939900	-2.31427200	-1.73967700
O	-0.07770900	-2.28985100	0.20200100
C	-0.73963300	-2.89091800	1.33453700
H	-1.70158600	-3.29732300	1.02504600
H	-0.08002900	-3.68791900	1.67894500
H	-0.88842100	-2.15830700	2.12947800
O	-2.34934500	-1.03151600	0.18156700
C	-2.78604100	-1.56987500	-1.07647500
H	-2.01012800	-2.21174400	-1.50493500
H	-3.67721100	-2.15494300	-0.85636900
H	-3.03760400	-0.75732000	-1.76324500
O	-2.78351200	1.43166100	-0.00342100
C	-3.21235900	2.78884900	-0.04456900
H	-2.82091400	3.29987400	-0.92982200
H	-4.29754300	2.74223200	-0.10186400
H	-2.91872600	3.32205200	0.86470100
N	3.06189800	1.09406400	0.02676900
H	3.62146400	0.25355100	0.00513800

TI-2346

Zero-point correction= 0.298860 (Hartree/Particle)

Thermal correction to Energy= 0.317121

Thermal correction to Enthalpy= 0.318066

Thermal correction to Gibbs Free Energy= 0.253249

Sum of electronic and zero-point Energies= -822.840172

Sum of electronic and thermal Energies= -822.821911

Sum of electronic and thermal Enthalpies= -822.820967
Sum of electronic and thermal Free Energies= -822.885784

C	1.07070700	-1.16858200	-0.11927000
C	-0.10232900	-1.87233400	-0.10900400
C	-1.43226400	-1.39275000	-0.00534100
C	1.26085000	0.27046700	0.01526500
C	-1.88610500	-0.08471000	0.05804500
C	0.30367200	1.25573000	-0.00426700
C	-1.14986700	1.11140300	0.03264500
H	-0.05305600	-2.94977100	-0.19750000
H	-2.95655900	0.04339300	0.11631900
C	-3.24921400	2.41902700	0.16363000
H	-3.48252600	3.48183500	0.18020600
H	-3.74243900	1.96883600	-0.70352500
H	-3.63891500	1.96274200	1.07940600
O	0.67118300	2.55483000	0.04097700
C	1.68012500	3.06498600	-0.85362800
H	1.36077700	4.07519200	-1.10874600
H	2.64728100	3.08404500	-0.35600100
H	1.73821400	2.44823000	-1.75229700
O	2.53324500	0.70819700	0.05265400
C	3.37872600	0.27355400	1.13365800
H	4.09941800	-0.45266800	0.76123200
H	3.88884200	1.16494800	1.50024600
H	2.78605700	-0.16565500	1.93969200
O	2.25208500	-1.77451800	-0.24897600
C	2.31643400	-3.19071800	-0.39689900
H	3.37427100	-3.42182200	-0.49938400

H	1.90870700	-3.69039100	0.48677500
H	1.77836000	-3.50784800	-1.29466500
O	-2.28831800	-2.41692000	0.01106600
C	-3.69356400	-2.20254100	0.09211700
H	-4.13690300	-3.19575200	0.08544300
H	-3.95516300	-1.68822400	1.02170600
H	-4.04967200	-1.63447000	-0.77257500
N	-1.80915000	2.27179100	0.07680100
H	-1.23124000	3.10094800	0.08860000

TI-2347

Zero-point correction= 0.298703 (Hartree/Particle)

Thermal correction to Energy= 0.316814

Thermal correction to Enthalpy= 0.317758

Thermal correction to Gibbs Free Energy= 0.253235

Sum of electronic and zero-point Energies= -822.826084

Sum of electronic and thermal Energies= -822.807974

Sum of electronic and thermal Enthalpies= -822.807030

Sum of electronic and thermal Free Energies= -822.871553

C	0.20671500	-0.00265600	1.74113300
C	0.85028800	-0.66470600	0.72355000
C	0.97103000	-0.30815600	-0.62998800
C	-0.59637500	1.18424500	1.59831300
C	0.63110300	0.84430600	-1.29146600
C	-0.60107000	2.10566700	0.55144900
C	0.05325300	2.04664500	-0.72708300
H	1.34021600	-1.59464600	0.98386500
C	-0.24990300	4.50491800	-1.28764900

H	0.17531800	5.07034400	-2.11634800
H	-1.32148500	4.69236000	-1.22981500
H	0.22911300	4.83326800	-0.36358300
H	1.47056700	-1.05692600	-1.23329900
O	-1.41340800	3.17870400	0.66691300
C	-1.28481300	4.06897300	1.78756400
H	-1.39118200	5.07799900	1.38478400
H	-2.07002100	3.86966000	2.51412700
H	-0.30712900	3.95814100	2.26291400
O	-1.37349200	1.54356000	2.62648900
C	-2.24114600	0.58356100	3.25664300
H	-1.79383400	0.23055600	4.18374500
H	-3.16929100	1.11842200	3.45621500
H	-2.43705500	-0.25750500	2.58781500
O	0.21291700	-0.44014000	3.00912000
C	0.91704200	-1.63100800	3.34246400
H	0.78825900	-1.75331700	4.41578100
H	0.49447800	-2.49477700	2.81923900
H	1.98138200	-1.53058400	3.10902700
O	0.89706400	1.01633000	-2.60487100
C	1.47693500	-0.03522000	-3.36982000
H	0.84017000	-0.92418600	-3.34941200
H	1.54137400	0.34697400	-4.38623500
H	2.47939600	-0.27426700	-3.00242100
N	0.03822200	3.09670300	-1.54887000
H	0.40033600	2.88959800	-2.47012600

TI-2356

Zero-point correction= 0.298114 (Hartree/Particle)

Thermal correction to Energy= 0.316641

Thermal correction to Enthalpy= 0.317585

Thermal correction to Gibbs Free Energy= 0.251547

Sum of electronic and zero-point Energies= -822.834890

Sum of electronic and thermal Energies= -822.816363

Sum of electronic and thermal Enthalpies= -822.815418

Sum of electronic and thermal Free Energies= -822.881456

C	0.07389700	-1.69959500	-0.02780100
C	1.32506500	-1.15256700	0.05230800
C	1.63487200	0.26227100	0.17480800
C	-1.21879400	-1.11327400	-0.07276300
C	0.76538300	1.31143500	0.01720800
C	-1.54191000	0.23800100	-0.16012400
C	-0.64125700	1.34184600	-0.20411300
H	0.11088300	-2.78133600	-0.06799200
H	1.21221600	2.29191200	0.10595800
C	-0.53196300	3.80730700	-0.52164900
H	-1.26804700	4.56732700	-0.77751300
H	-0.06312500	4.09216300	0.42598100
H	0.22758900	3.78269200	-1.30960200
O	-2.85154500	0.58055600	-0.30921100
C	-3.65427700	0.48820900	0.88170200
H	-3.23619600	1.12484700	1.66806500
H	-4.64372400	0.84434000	0.59995100
H	-3.71440800	-0.54591100	1.22172700
O	-2.29957700	-1.89945400	-0.09441800
C	-2.19264600	-3.31999300	-0.01745600

H	-1.68640100	-3.62761200	0.90170300
H	-3.21921200	-3.67948400	-0.00939900
H	-1.67459000	-3.72051400	-0.89317100
O	2.32082700	-2.04477700	0.12949900
C	3.50578400	-1.90331300	-0.67444200
H	4.31406700	-1.48381300	-0.07799900
H	3.75759000	-2.91182700	-1.00028900
H	3.31353500	-1.27215100	-1.54515500
O	2.92325300	0.45076500	0.46360200
C	3.44147300	1.76352500	0.65203300
H	4.49091900	1.62648600	0.90284500
H	3.35479000	2.34991500	-0.26814000
H	2.92670200	2.26681000	1.47576400
N	-1.21795400	2.53400000	-0.41200400
H	-2.21433500	2.49831900	-0.58276100

TI-2357

Zero-point correction= 0.299126 (Hartree/Particle)

Thermal correction to Energy= 0.317178

Thermal correction to Enthalpy= 0.318123

Thermal correction to Gibbs Free Energy= 0.253651

Sum of electronic and zero-point Energies= -822.833963

Sum of electronic and thermal Energies= -822.815911

Sum of electronic and thermal Enthalpies= -822.814966

Sum of electronic and thermal Free Energies= -822.879438

C	0.75434300	1.80298400	-0.10307800
C	-0.62880000	1.88239100	-0.07217200
C	-1.55446000	0.82300400	0.08042500

C	1.56198000	0.66478400	-0.07403200
C	-1.34642900	-0.53415900	0.07957600
C	1.17063700	-0.69741500	-0.11777400
C	-0.11539100	-1.26632600	-0.20034200
H	1.23937600	2.76863800	-0.15968000
C	-1.26486400	-3.45267800	-0.83258000
H	-0.82311800	-4.33177800	-1.30049000
H	-1.86282800	-3.76564900	0.02318200
H	-1.91010500	-2.95820700	-1.55975200
H	-2.57727600	1.12752400	0.24711100
O	2.18048100	-1.60754800	-0.23365400
C	2.84547900	-1.93199000	1.00038400
H	2.12843800	-2.33937200	1.72025800
H	3.59056700	-2.68483100	0.74811900
H	3.33557100	-1.04773300	1.41027700
O	2.89094100	0.78318100	-0.06256500
C	3.51209300	2.06643000	-0.07886100
H	3.22790400	2.64960200	0.80146000
H	4.58053700	1.86407200	-0.05880400
H	3.25870100	2.60854500	-0.99404200
O	-1.06521000	3.14495000	-0.13767700
C	-2.45418400	3.45477000	-0.16456800
H	-2.93249700	3.19785300	0.78585300
H	-2.50463500	4.53135500	-0.31169400
H	-2.95373300	2.94738200	-0.99510400
O	-2.34016400	-1.38116600	0.35940400
C	-3.63381700	-0.90486500	0.71669200
H	-4.09407900	-0.36732800	-0.11793800

H	-4.21544200	-1.79551400	0.94409900
H	-3.57740900	-0.26315400	1.60098900
N	-0.15551100	-2.58977000	-0.42998800
H	0.77069300	-2.96991800	-0.58000200

TI-2367

Zero-point correction= 0.298456 (Hartree/Particle)

Thermal correction to Energy= 0.316780

Thermal correction to Enthalpy= 0.317725

Thermal correction to Gibbs Free Energy= 0.252298

Sum of electronic and zero-point Energies= -822.822782

Sum of electronic and thermal Energies= -822.804457

Sum of electronic and thermal Enthalpies= -822.803513

Sum of electronic and thermal Free Energies= -822.868940

C	-0.58331300	-0.24856700	1.20747100
C	0.25432000	-0.73377500	0.24205900
C	0.87075100	-0.06668400	-0.83946900
C	-1.10087100	1.05376100	1.38810800
C	0.70107800	1.26762200	-1.22228100
C	-0.92732400	2.15047800	0.54544200
C	-0.26015100	2.21468900	-0.73259100
H	-0.90706800	-0.98204200	1.93555700
H	0.48512300	-1.78815900	0.33204400
C	-0.21816100	3.66413000	-2.81604500
H	-0.92082200	4.44863400	-3.09615000
H	0.80116400	4.02386400	-2.95896100
H	-0.37952200	2.79613300	-3.45381100
O	-1.55764100	3.30653400	0.84869800

C	-1.32883900	3.93500400	2.12625800
H	-1.26872400	5.00455100	1.92649400
H	-2.15847100	3.71701700	2.79544800
H	-0.39117100	3.58308600	2.56148100
O	-1.90395600	1.32984400	2.42994400
C	-2.22086100	0.33388700	3.39706000
H	-1.31821500	-0.04083000	3.88898900
H	-2.85164700	0.83636500	4.12748500
H	-2.77910500	-0.49029400	2.94360600
O	1.72850700	-0.71774400	-1.64122100
C	2.10256600	-2.06678900	-1.37970900
H	1.24473400	-2.73879600	-1.47448600
H	2.83652800	-2.31186100	-2.14470900
H	2.55755100	-2.16555800	-0.38954900
O	1.45245300	1.74341200	-2.23388900
C	2.88428800	1.65871900	-2.14278300
H	3.24697100	0.82879000	-2.74679200
H	3.26381700	2.60533900	-2.52886400
H	3.19720900	1.53097400	-1.10328800
N	-0.48859500	3.34019900	-1.41590600
H	-1.09452500	3.98286500	-0.92289700

TI-2456

Zero-point correction= 0.298512 (Hartree/Particle)

Thermal correction to Energy= 0.316881

Thermal correction to Enthalpy= 0.317825

Thermal correction to Gibbs Free Energy= 0.252181

Sum of electronic and zero-point Energies= -822.839515

Sum of electronic and thermal Energies= -822.821146
Sum of electronic and thermal Enthalpies= -822.820202
Sum of electronic and thermal Free Energies= -822.885846

C	-0.96033900	-1.23651900	-0.08094400
C	-1.44210400	0.06185800	-0.09396700
C	-0.64632700	1.24976700	-0.11049300
C	0.39661900	-1.67269600	0.03116700
C	0.74189700	1.39117700	-0.10680700
C	1.57693600	-0.99791800	0.07195000
C	1.76947600	0.44585900	-0.03475600
H	1.08933400	2.41279100	-0.14814700
C	3.48245400	2.22663700	-0.15152800
H	4.57051200	2.23958200	-0.16255700
H	3.11926500	2.68193500	-1.07838400
H	3.13634800	2.81772800	0.70274200
H	0.44857800	-2.75385700	0.08000000
O	2.75938200	-1.62604600	0.18535000
C	2.80857200	-3.04584500	0.31367800
H	3.86254500	-3.29167100	0.42104200
H	2.25797200	-3.36865900	1.20154600
H	2.40408400	-3.52506000	-0.58230200
O	-1.77612600	-2.29620800	-0.10632800
C	-3.01790000	-2.31311300	-0.83157400
H	-2.95178700	-1.69223000	-1.72555700
H	-3.16158100	-3.35836200	-1.10170400
H	-3.84052000	-1.97023400	-0.20509700
O	-2.78751100	0.24633700	-0.11583300
C	-3.36783900	0.43313700	1.18089000

H	-4.43716700	0.56088100	1.01765500
H	-3.18643600	-0.44606900	1.80880500
H	-2.95882000	1.32787100	1.65822000
O	-1.42528300	2.32945300	-0.12551400
C	-0.88299400	3.64542900	-0.15551600
H	-1.74566800	4.30759200	-0.16413600
H	-0.27712400	3.83993200	0.73474100
H	-0.29221100	3.80194500	-1.06295100
N	3.04373000	0.84838300	-0.04495100
H	3.74216900	0.12228000	0.02673500

TI-2457

Zero-point correction= 0.299050 (Hartree/Particle)

Thermal correction to Energy= 0.317201

Thermal correction to Enthalpy= 0.318145

Thermal correction to Gibbs Free Energy= 0.253125

Sum of electronic and zero-point Energies= -822.830271

Sum of electronic and thermal Energies= -822.812119

Sum of electronic and thermal Enthalpies= -822.811175

Sum of electronic and thermal Free Energies= -822.876195

C	-0.36706300	0.01270000	1.69961300
C	0.50062200	-0.59191800	0.76990000
C	0.84826300	-0.05754600	-0.47391100
C	-0.85539500	1.31812200	1.61571400
C	0.62130900	1.17099600	-1.08187800
C	-0.66570100	2.35281500	0.71695800
C	0.05688500	2.36102600	-0.52345400
C	0.91901600	3.98625800	-2.29161800

H	0.87527000	5.07479200	-2.29358100
H	1.95697700	3.67707800	-2.16783600
H	0.54334300	3.61090000	-3.24314800
H	1.41443500	-0.73930300	-1.09301600
H	-1.47403200	1.54962100	2.47490400
O	-1.21806100	3.56166100	0.94757900
C	-1.98501000	3.81343300	2.12218700
H	-2.27914300	4.85851600	2.05434100
H	-2.87705700	3.18145900	2.14539700
H	-1.38121800	3.65699200	3.02048500
O	-0.73313000	-0.61678900	2.82715500
C	-1.16603800	-1.98652700	2.80160700
H	-0.33562400	-2.65317800	3.02751500
H	-1.93197600	-2.06036200	3.57266500
H	-1.59519900	-2.23866500	1.82879000
O	0.96134800	-1.78959500	1.16576600
C	1.88229900	-2.51795000	0.36488900
H	2.78051700	-1.92549200	0.16366600
H	2.14865700	-3.39328700	0.95333800
H	1.42027000	-2.83970400	-0.57451600
O	0.99610100	1.36485700	-2.36012100
C	1.53765300	0.30999000	-3.14232800
H	0.84804100	-0.53905700	-3.18452200
H	1.66459600	0.72747700	-4.13919400
H	2.51149900	-0.00902900	-2.75667100
N	0.09682900	3.53730100	-1.16874100
H	-0.41785100	4.26506700	-0.69383100

TI-3456

Zero-point correction= 0.298012 (Hartree/Particle)

Thermal correction to Energy= 0.316539

Thermal correction to Enthalpy= 0.317484

Thermal correction to Gibbs Free Energy= 0.251964

Sum of electronic and zero-point Energies= -822.827431

Sum of electronic and thermal Energies= -822.808904

Sum of electronic and thermal Enthalpies= -822.807959

Sum of electronic and thermal Free Energies= -822.873479

C	-0.22262900	0.05076400	1.59039500
C	0.25475600	-0.60131800	0.47761700
C	0.58191900	-0.04503400	-0.82282800
C	-0.34712800	1.49111800	1.77479300
C	0.35768100	1.23052200	-1.29680000
C	-0.34483300	2.45375000	0.80082400
C	-0.13296100	2.36110700	-0.60141500
H	0.60633000	1.39714300	-2.33455700
C	-0.14109500	3.65751200	-2.72600300
H	-0.43619800	4.66988800	-2.99548500
H	0.91021800	3.52106600	-2.99938900
H	-0.75939300	2.95438500	-3.29209900
H	-0.55097200	3.44641400	1.19187100
O	-0.62109100	1.96027700	2.99293700
C	0.03008800	1.45464300	4.17251800
H	0.24844100	2.33316400	4.77852600
H	-0.63750900	0.77857000	4.70321500
H	0.95691500	0.93712800	3.91845500
O	-0.57391800	-0.64472500	2.68339000

C	-1.41312700	-1.80897300	2.56026100
H	-0.81077500	-2.71674200	2.54506800
H	-2.05320700	-1.79291800	3.44146600
H	-2.01496900	-1.75136200	1.65176000
O	0.39915300	-1.94585800	0.55984700
C	1.59181800	-2.36735700	1.23597500
H	1.59908500	-1.99733600	2.26675100
H	1.57051800	-3.45600800	1.22996400
H	2.47536900	-2.01229200	0.69844100
O	1.12426100	-0.98272800	-1.59247600
C	1.50942400	-0.69403300	-2.93258800
H	2.26406700	0.09811500	-2.95786900
H	1.93136900	-1.62032600	-3.31524100
H	0.63877700	-0.41137500	-3.53186300
N	-0.33876100	3.49112000	-1.29670200
H	-0.66244000	4.29600800	-0.78068600

TI-23456

Zero-point correction= 0.331206 (Hartree/Particle)

Thermal correction to Energy= 0.352265

Thermal correction to Enthalpy= 0.353210

Thermal correction to Gibbs Free Energy= 0.281914

Sum of electronic and zero-point Energies= -937.272600

Sum of electronic and thermal Energies= -937.251541

Sum of electronic and thermal Enthalpies= -937.250597

Sum of electronic and thermal Free Energies= -937.321892

C	-0.04609100	-1.30836800	-0.02120100
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C	-1.32550300	-0.82261900	-0.14668100
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C	-1.74038600	0.55568100	-0.06625300
C	1.20702800	-0.60475800	0.11637800
C	-0.94090400	1.67885700	0.01985800
C	1.44641200	0.75256600	0.05373600
C	0.46401700	1.81641900	0.03630400
H	-1.47403300	2.61765100	0.05609400
C	0.22819500	4.28611100	0.11112800
H	0.93460100	5.11366700	0.13522600
H	-0.39792400	4.39171900	-0.78047700
H	-0.40115100	4.34203300	1.00533700
O	2.70845600	1.23055200	0.12218400
C	3.74023400	0.69374400	-0.72806200
H	4.37075500	1.54101300	-0.99630800
H	4.31620500	-0.05649500	-0.19042000
H	3.30250500	0.25153000	-1.62535200
O	2.31231500	-1.37093900	0.21416200
C	2.41527300	-2.30073400	1.31106600
H	2.30330900	-3.31802800	0.93832500
H	3.40738600	-2.15632200	1.73988300
H	1.65192800	-2.10043900	2.06501400
O	0.06697600	-2.65937400	-0.01422500
C	0.33874400	-3.22754200	-1.30642900
H	1.28822400	-2.84538700	-1.69365800
H	0.40473200	-4.30336300	-1.15271400
H	-0.48236600	-2.99713600	-1.98986200
O	-2.30101300	-1.71844700	-0.40623100
C	-2.90534200	-2.30762400	0.75491500
H	-3.64997800	-3.00761200	0.38073800

H	-2.14988000	-2.84047000	1.33824900
H	-3.39161000	-1.53653900	1.35894900
O	-3.06645700	0.64842600	-0.09605000
C	-3.71235000	1.91674500	-0.06895800
H	-4.77648200	1.69756900	-0.11631700
H	-3.48570100	2.45016200	0.85946300
H	-3.42043400	2.51715000	-0.93576500
N	0.98285500	3.04808200	0.07513600
H	1.99174900	3.09011700	0.12411100

TI-23457

Zero-point correction= 0.330995 (Hartree/Particle)

Thermal correction to Energy= 0.352116

Thermal correction to Enthalpy= 0.353060

Thermal correction to Gibbs Free Energy= 0.280810

Sum of electronic and zero-point Energies= -937.267122

Sum of electronic and thermal Energies= -937.246001

Sum of electronic and thermal Enthalpies= -937.245057

Sum of electronic and thermal Free Energies= -937.317307

C	1.51040500	0.48493300	-0.12215700
C	0.68980300	1.60999100	0.00406100
C	-0.71837500	1.64816900	-0.07332300
C	1.09613400	-0.85813100	-0.24566400
C	-1.66041300	0.64776100	-0.13673000
C	-0.19512300	-1.41025600	-0.11608000
C	-1.46264400	-0.78334900	-0.01612600
C	-3.91945400	-1.38559800	0.39554100
H	-4.33386600	-2.34790900	0.69499100

H	-4.03221900	-0.68504600	1.22209700
H	-4.47006900	-1.01303200	-0.46895900
H	-1.13035000	2.64615100	-0.10573400
O	-0.27555500	-2.77051800	-0.16547300
C	0.17660800	-3.46233600	1.01319300
H	-0.02390300	-4.51681400	0.83041200
H	1.24535900	-3.30689100	1.16024000
H	-0.38523100	-3.12087500	1.88875400
O	2.05026900	-1.79251800	-0.37363700
C	3.05950000	-1.66158700	-1.39498200
H	3.99776900	-1.32744000	-0.95406600
H	3.16929900	-2.65765100	-1.82225200
H	2.74233700	-0.95434400	-2.16268200
O	2.84682500	0.71528600	-0.14224600
C	3.47975700	0.57835000	1.13650600
H	3.35648400	-0.44173000	1.51563000
H	4.53549600	0.79058700	0.97457400
H	3.06248400	1.30023300	1.84407400
O	1.38792900	2.73705000	0.17288100
C	0.73647500	3.99108800	0.33412100
H	0.06029400	3.97659000	1.19479600
H	1.53553300	4.70800800	0.50946700
H	0.19356700	4.27213300	-0.57380700
O	-2.95590300	0.94183600	-0.30464100
C	-3.38982300	2.28462000	-0.48510200
H	-2.90890600	2.73297100	-1.35994700
H	-4.46362200	2.22064000	-0.64824700
H	-3.19008600	2.88294100	0.40943500

N	-2.51048900	-1.61769000	0.08648300
H	-2.23255100	-2.58571600	-0.00877300

TI-23567

Zero-point correction= 0.331236 (Hartree/Particle)

Thermal correction to Energy= 0.352312

Thermal correction to Enthalpy= 0.353256

Thermal correction to Gibbs Free Energy= 0.281267

Sum of electronic and zero-point Energies= -937.265001

Sum of electronic and thermal Energies= -937.243925

Sum of electronic and thermal Enthalpies= -937.242980

Sum of electronic and thermal Free Energies= -937.314969

C	-0.94005500	-0.23939400	1.31598100
C	-0.05756600	-0.84612000	0.45720100
C	0.78680500	-0.19373000	-0.51419700
C	-1.28109900	1.11974500	1.46928500
C	0.67176300	1.09423200	-1.00971000
C	-0.88488200	2.20392200	0.67860100
C	-0.07863900	2.21732900	-0.49830900
H	-1.41579400	-0.94603900	1.98412000
C	0.69281300	3.90442100	-2.28157000
H	0.43491700	4.95867800	-2.37642800
H	1.77058200	3.80944000	-2.16181100
H	0.38558200	3.39111200	-3.19465500
O	-1.43497900	3.41443800	0.98560700
C	-0.83724200	4.08532000	2.10964100
H	-1.35174800	5.04117400	2.19365500
H	-0.98463100	3.50377200	3.02054700

H	0.23010200	4.24783600	1.92842600
O	-2.11312300	1.49025900	2.44765400
C	-2.65010200	0.53861400	3.36409400
H	-1.85439900	0.03284700	3.91806800
H	-3.26234300	1.12148800	4.04860300
H	-3.27783600	-0.19092600	2.84496000
O	0.07376300	-2.16289400	0.65312600
C	0.16159300	-3.08280000	-0.44850100
H	1.19845500	-3.36723700	-0.61788200
H	-0.42865700	-3.94824500	-0.14996100
H	-0.25605700	-2.64499200	-1.35790000
O	1.72273500	-1.01219800	-1.03107800
C	3.08597400	-0.55855100	-1.11474500
H	3.69632500	-1.42971300	-0.88013700
H	3.31071000	-0.19868700	-2.11932800
H	3.26800800	0.23630600	-0.38875500
O	1.45491800	1.39355800	-2.08096000
C	1.08013800	0.74649200	-3.30748500
H	1.75010400	1.14483000	-4.06866600
H	1.20116100	-0.33701500	-3.22929200
H	0.04317200	0.98906700	-3.55940800
N	-0.02715300	3.41090900	-1.10898100
H	-0.64315400	4.08036700	-0.66471300

TI-234567

Zero-point correction=	0.363701 (Hartree/Particle)
Thermal correction to Energy=	0.387498
Thermal correction to Enthalpy=	0.388443

Thermal correction to Gibbs Free Energy= 0.311131
Sum of electronic and zero-point Energies= -1051.702554
Sum of electronic and thermal Energies= -1051.678757
Sum of electronic and thermal Enthalpies= -1051.677813
Sum of electronic and thermal Free Energies= -1051.755124

C	-0.08417800	-0.26547200	1.38123600
C	0.76109400	-0.72795300	0.39618600
C	1.09037800	-0.08375300	-0.84337200
C	-0.72264800	1.01464300	1.49373100
C	0.79038700	1.20897200	-1.25418200
C	-0.49540700	2.15674100	0.74124600
C	0.23101700	2.29107200	-0.50163600
C	1.02090200	4.10927400	-2.09156500
H	1.03894600	5.18606100	-1.92500400
H	2.04068700	3.72787900	-2.08293800
H	0.57582100	3.90676300	-3.06721700
O	-1.09850900	3.31356800	1.10323300
C	-0.95143900	3.81380800	2.44707300
H	-0.86327000	4.89621200	2.35382400
H	-1.82505700	3.55114100	3.03925900
H	-0.05141900	3.40316200	2.91008400
O	-1.53548000	1.20011800	2.55079200
C	-2.62809700	0.28545000	2.76629800
H	-2.39797700	-0.37466300	3.60152700
H	-3.49465500	0.90543700	2.99633200
H	-2.82086400	-0.30779700	1.87082200
O	-0.34676100	-1.13310600	2.39018500
C	0.48671600	-0.95191800	3.54591700

H	0.34834100	0.05214800	3.95956200
H	0.16354600	-1.69928500	4.26891800
H	1.53267100	-1.12077200	3.27721100
O	1.36309700	-1.91483500	0.61934800
C	0.62511800	-3.06633600	0.18266200
H	1.23199800	-3.92881800	0.45164500
H	-0.33683000	-3.11107000	0.70019800
H	0.48501000	-3.03293400	-0.90082100
O	1.70695100	-0.91521200	-1.69130800
C	2.89605000	-0.50930000	-2.39212000
H	3.54555800	-1.38342500	-2.38677100
H	2.65522200	-0.22040500	-3.41530100
H	3.37900300	0.32338900	-1.87795200
O	1.10974900	1.51189200	-2.54719600
C	0.14545700	1.03010000	-3.49478000
H	0.49821000	1.35446800	-4.47340300
H	0.08728200	-0.06208700	-3.45989200
H	-0.83786100	1.46582500	-3.29000700
N	0.23789500	3.53068900	-1.00212800
H	-0.30733800	4.17994900	-0.45006300