

1 Cartesian Coordinates and Energies of the Optimized Structures

Cat

Zero-point correction=			0.452500 (Hartree/Particle)
Thermal correction to Energy=			0.485519
Thermal correction to Enthalpy=			0.486463
Thermal correction to Gibbs Free Energy=			0.385122
Sum of electronic and zero-point Energies=			-1971.034627
Sum of electronic and thermal Energies=			-1971.001608
Sum of electronic and thermal Enthalpies=			-1971.000664
Sum of electronic and thermal Free Energies=			-1971.102005
P	-0.01875100	2.29048000	-0.79588600
P	2.30084800	-0.75385800	0.22422000
C	-0.00575600	2.63798000	-2.63918400
H	0.87801900	2.16393000	-3.08751200
H	-0.90393100	2.19461100	-3.10346500
H	0.01350200	3.70590200	-2.86718100
C	1.38860100	3.41820400	-0.27652900
H	2.34328700	3.00919700	-0.65477300
H	1.25721700	4.43467000	-0.64192300
H	1.43934500	3.42687000	0.82418300
C	-1.46640200	3.37570300	-0.31043900
H	-1.54649500	3.42159900	0.77813600
H	-1.37341800	4.38747100	-0.70649900
H	-2.40164800	2.92554600	-0.71102100
C	3.52737400	-0.42140600	-1.14606900
H	3.18895300	-0.87080000	-2.07478300
H	3.61589500	0.65882900	-1.30832500
H	4.52918400	-0.81060500	-0.90367300
C	2.61615000	-2.58351100	0.44583600
H	2.24854800	-3.12480500	-0.43700500
H	3.68108200	-2.81314600	0.57472800
H	2.05724700	-2.93838700	1.31698300
C	3.29237100	-0.11877900	1.65532400
H	4.31412600	-0.52197900	1.68289600
H	3.35088900	0.97535900	1.60735900
H	2.79797100	-0.38424200	2.59510000
Pd	0.01594200	-0.00324000	-0.00754200
P	-1.10647100	-0.11543000	2.13897400
P	-1.16618100	-1.41729300	-1.56959300
C	-2.95047500	0.15818200	2.14370100
H	-3.38048200	0.11132700	3.15328900

H	-3.17954900	1.11720600	1.69611600
H	-3.42604200	-0.62072700	1.53957400
C	-1.03285600	-1.68792000	3.11837000
H	-1.42209000	-2.51284300	2.52600000
H	0.02330100	-1.92222000	3.35923000
H	-1.60171100	-1.63448300	4.06654300
C	-0.63146600	1.08201700	3.49304400
H	-1.21176400	0.92462400	4.40489500
H	0.42386300	0.97376900	3.71413700
H	-0.80074900	2.10497300	3.13426400
C	-2.68400200	-0.73972900	-2.44483100
H	-3.42425900	-0.42072100	-1.68763600
H	-2.39172300	0.16335000	-3.01623700
H	-3.14413700	-1.46432900	-3.11258000
C	-1.90929700	-3.02763900	-0.94837700
H	-2.40631100	-3.60246900	-1.75600300
H	-1.12186200	-3.64969800	-0.50483400
H	-2.64387800	-2.82315100	-0.16644900
C	-0.23763800	-2.07609900	-3.05677500
H	0.61022700	-2.67789000	-2.71043000
H	-0.87168500	-2.68809000	-3.70130700
H	0.16445900	-1.23010800	-3.64499800

R

Zero-point correction=			0.137347 (Hartree/Particle)
Thermal correction to Energy=			0.145707
Thermal correction to Enthalpy=			0.146651
Thermal correction to Gibbs Free Energy=			0.102763
Sum of electronic and zero-point Energies=			-347.671452
Sum of electronic and thermal Energies=			-347.663092
Sum of electronic and thermal Enthalpies=			-347.662148
Sum of electronic and thermal Free Energies=			-347.706037
C	-1.39390500	0.00026900	-0.00000500
C	-2.60031300	0.00036200	-0.00000100
C	0.03421300	0.00011500	-0.00001800
C	0.75098300	-1.20916800	-0.00000300
C	0.75127600	1.20924500	-0.00000300
C	2.14108300	-1.20539600	0.00000500
H	0.20520200	-2.14502700	0.00000100
C	2.14134400	1.20517600	0.00000500
H	0.20577700	2.14526900	0.00000100
C	2.84175900	-0.00019900	0.00000300
H	2.67962900	-2.14651500	0.00001100
H	2.68009600	2.14617700	0.00001100

H	3.92582700	-0.00031000	0.00001000
C	-4.05690800	-0.00007500	0.00000700
H	-4.45150500	-0.51132800	-0.88344000
H	-4.45149600	-0.51059800	0.88388000
H	-4.45071700	1.02036500	-0.00041200

HCOOH

Zero-point correction=			0.033869 (Hartree/Particle)
Thermal correction to Energy=			0.037027
Thermal correction to Enthalpy=			0.037971
Thermal correction to Gibbs Free Energy=			0.009795
Sum of electronic and zero-point Energies=			-189.785611
Sum of electronic and thermal Energies=			-189.782453
Sum of electronic and thermal Enthalpies=			-189.781509
Sum of electronic and thermal Free Energies=			-189.809685
C	0.13601000	0.39808700	-0.00003900
O	1.13450300	-0.26298100	0.00001700
O	-1.11781500	-0.09030800	0.00001000
H	0.09772800	1.49591800	-0.00002300
H	-1.04729600	-1.05813000	0.00004500

PMe3

Zero-point correction=			0.112279 (Hartree/Particle)
Thermal correction to Energy=			0.118971
Thermal correction to Enthalpy=			0.119915
Thermal correction to Gibbs Free Energy=			0.084023
Sum of electronic and zero-point Energies=			-461.051429
Sum of electronic and thermal Energies=			-461.044737
Sum of electronic and thermal Enthalpies=			-461.043793
Sum of electronic and thermal Free Energies=			-461.079686
P	0.00000000	0.00000000	0.60216600
C	0.00000000	1.64083400	-0.27969100
H	-0.88122300	2.21453400	0.01826600
H	0.88122300	2.21453400	0.01826600
H	0.00000000	1.53484100	-1.36921500
C	-1.42100400	-0.82041700	-0.27969100
H	-2.35845400	-0.34410600	0.01826600
H	-1.32921200	-0.76742100	-1.36921500
H	-1.47723200	-1.87042900	0.01826600
C	1.42100400	-0.82041700	-0.27969100
H	1.32921200	-0.76742100	-1.36921500
H	2.35845400	-0.34410600	0.01826600
H	1.47723200	-1.87042900	0.01826600

Pd(PMe₃)₂

Zero-point correction=			0.227510 (Hartree/Particle)
Thermal correction to Energy=			0.244473
Thermal correction to Enthalpy=			0.245417
Thermal correction to Gibbs Free Energy=			0.180763
Sum of electronic and zero-point Energies=			-1048.918508
Sum of electronic and thermal Energies=			-1048.901545
Sum of electronic and thermal Enthalpies=			-1048.900601
Sum of electronic and thermal Free Energies=			-1048.965256
Pd	-0.00001500	0.00598200	0.00081100
P	-2.31739900	-0.00048400	0.00011300
P	2.31727600	-0.00074700	0.00024100
C	-3.16347400	-0.40279000	1.59812900
H	-2.84773300	-1.39235800	1.93367700
H	-2.85934800	0.31953000	2.35801000
H	-4.25359100	-0.38576200	1.50028700
C	-3.15413800	-1.19140300	-1.14579500
H	-2.83862000	-2.20763200	-0.90212300
H	-4.24481800	-1.12707500	-1.07995400
H	-2.84283000	-0.98304900	-2.17111200
C	-3.17160700	1.57885700	-0.45547000
H	-2.86479700	1.87746200	-1.45961600
H	-4.26124600	1.47871800	-0.42616500
H	-2.86420500	2.36652300	0.23496200
C	3.16073300	-0.75960100	1.46448800
H	2.85528700	-0.23154100	2.36973300
H	2.84468600	-1.79980900	1.56288500
H	4.25095500	-0.72096800	1.37470500
C	3.16870000	1.64257000	-0.07934300
H	2.86211500	2.24932300	0.77474900
H	4.25851500	1.54044800	-0.07656200
H	2.85896400	2.16435300	-0.98676700
C	3.15993900	-0.89477900	-1.38621700
H	4.25031800	-0.84683700	-1.30178000
H	2.84466700	-1.93988500	-1.38506300
H	2.85328500	-0.45527500	-2.33721500

Com0

Zero-point correction=			0.365392 (Hartree/Particle)
Thermal correction to Energy=			0.392943
Thermal correction to Enthalpy=			0.393888
Thermal correction to Gibbs Free Energy=			0.297348
Sum of electronic and zero-point Energies=			-1396.592781
Sum of electronic and thermal Energies=			-1396.565229

Sum of electronic and thermal Enthalpies=			-1396.564285
Sum of electronic and thermal Free Energies=			-1396.660825
Pd	2.03434100	0.43546200	0.00085100
C	-3.05169600	-1.51290600	0.01930600
C	-4.39802800	-1.03652500	0.00548000
C	-5.07178500	-0.82369600	-1.21021600
C	-5.07821300	-0.77159600	1.20728600
C	-6.38238200	-0.36020300	-1.21975700
H	-4.55577700	-1.02741600	-2.14080200
C	-6.38877700	-0.30821800	1.18988300
H	-4.56722700	-0.93506200	2.14852400
C	-7.04629800	-0.10031800	-0.02173100
H	-6.88783000	-0.20183000	-2.16594300
H	-6.89921500	-0.10925900	2.12567100
H	-8.06842400	0.26072500	-0.03222300
C	-1.91541400	-1.92213600	0.03108500
P	3.91330600	-0.92166100	-0.00653000
P	0.25882000	1.94417700	0.00018800
C	4.53816300	-1.49094600	-1.65491400
H	3.76104000	-2.07096600	-2.15618600
H	4.75735300	-0.62069100	-2.27620400
H	5.44053100	-2.10346200	-1.56160700
C	3.84196900	-2.53035300	0.91081200
H	3.04689500	-3.15118100	0.49348000
H	4.78928500	-3.07558000	0.85337500
H	3.60194800	-2.33793000	1.95816500
C	5.45301100	-0.18521600	0.71289400
H	5.27003900	0.08708500	1.75392100
H	6.29831200	-0.87899900	0.66460200
H	5.70439000	0.72673400	0.16848400
C	0.72346600	3.73703200	0.01300700
H	1.32348600	3.94883100	0.89988800
H	1.33319800	3.95902100	-0.86471400
H	-0.15922500	4.38426300	0.01187700
C	-0.92628300	1.87319900	1.41969100
H	-0.37932000	2.00462700	2.35520300
H	-1.69850900	2.64481500	1.34168500
H	-1.40397800	0.89202700	1.43754000
C	-0.90821000	1.88854000	-1.43491400
H	-1.68120300	2.65958400	-1.35892800
H	-0.34946600	2.02893500	-2.36210400
H	-1.38584600	0.90775700	-1.46871500
C	-0.54458300	-2.41171000	0.04577400
H	-0.35421700	-3.01056100	0.94157100

H	-0.34564600	-3.03854900	-0.82882100
H	0.17817200	-1.58160100	0.03612000

TS0

Zero-point correction=			0.364993 (Hartree/Particle)
Thermal correction to Energy=			0.391482
Thermal correction to Enthalpy=			0.392426
Thermal correction to Gibbs Free Energy=			0.304162
Sum of electronic and zero-point Energies=			-1396.580715
Sum of electronic and thermal Energies=			-1396.554226
Sum of electronic and thermal Enthalpies=			-1396.553282
Sum of electronic and thermal Free Energies=			-1396.641545
Pd	0.75303600	0.04206800	-0.20817500
C	-1.21578600	-1.65148800	-0.69628300
C	-2.44008200	-1.30836300	-0.04144100
C	-3.63501800	-1.20487300	-0.77623500
C	-2.48439600	-1.09710800	1.34841300
C	-4.83240700	-0.89663300	-0.13896300
H	-3.61132600	-1.37041600	-1.84675600
C	-3.68620400	-0.79620500	1.97876200
H	-1.56412100	-1.16482800	1.91550400
C	-4.86482200	-0.69257500	1.23966500
H	-5.74423000	-0.81933500	-0.72088100
H	-3.70335000	-0.63994400	3.05178900
H	-5.79999700	-0.45574600	1.73416700
C	-0.24662000	-2.06911400	-1.30301100
P	2.89850600	-0.50375400	0.52687800
P	-0.36088500	2.11734700	-0.36167400
C	4.27161100	0.62762900	-0.00805700
H	4.38065900	0.57863200	-1.09351100
H	4.01137400	1.65440900	0.25465800
H	5.22690500	0.36607800	0.45939300
C	3.74654100	-2.14043700	0.24474300
H	3.87408100	-2.30484800	-0.82751500
H	4.72933200	-2.18543100	0.72563600
H	3.12358900	-2.94613100	0.63986200
C	3.08473000	-0.38844900	2.37154400
H	2.42541500	-1.11632600	2.84870900
H	4.11480400	-0.57592500	2.69201700
H	2.78122800	0.60611200	2.70287500
C	0.70135400	3.57006800	-0.82071500
H	1.49553600	3.68229100	-0.08024000
H	1.17053900	3.38234400	-1.78856800
H	0.12639500	4.50057800	-0.87566900

C	-1.16386800	2.77532700	1.17682900
H	-0.42112700	2.83234800	1.97504600
H	-1.59965000	3.76755800	1.02067600
H	-1.94838300	2.08596500	1.49449100
C	-1.74773600	2.35266800	-1.57627900
H	-2.14210300	3.37407900	-1.56127600
H	-1.38685300	2.12572600	-2.58185800
H	-2.55362600	1.65420200	-1.34297900
C	0.73405200	-2.78617900	-2.11568100
H	1.50316100	-3.24204000	-1.48822500
H	0.24542200	-3.57959200	-2.69175600
H	1.23423100	-2.11438900	-2.81734800

M0

Zero-point correction=			0.366151 (Hartree/Particle)
Thermal correction to Energy=			0.392488
Thermal correction to Enthalpy=			0.393433
Thermal correction to Gibbs Free Energy=			0.307351
Sum of electronic and zero-point Energies=			-1396.593143
Sum of electronic and thermal Energies=			-1396.566806
Sum of electronic and thermal Enthalpies=			-1396.565861
Sum of electronic and thermal Free Energies=			-1396.651943
Pd	0.63662700	-0.22835900	-0.03075500
C	-1.21068000	-1.33110700	-0.03216200
C	-2.60536800	-0.96170000	-0.01497400
C	-3.29286400	-0.66589700	-1.20677200
C	-3.31736900	-0.88470900	1.19637200
C	-4.63926600	-0.31657800	-1.18515600
H	-2.75661500	-0.71968000	-2.14725000
C	-4.66345200	-0.53293600	1.21110900
H	-2.80059100	-1.10783100	2.12265300
C	-5.33303500	-0.24545800	0.02242400
H	-5.15016600	-0.09969400	-2.11735700
H	-5.19281300	-0.48481200	2.15687500
H	-6.38152700	0.02960600	0.03659000
C	-0.25519900	-2.15627200	-0.04245500
P	3.00242600	-0.45708200	0.00147700
P	0.02113900	2.09098900	0.01061900
C	4.05724700	0.79069700	-0.87681700
H	3.79098800	0.80621900	-1.93582100
H	3.86174700	1.78263800	-0.46597700
H	5.12439100	0.56756500	-0.78131600
C	3.72267600	-2.02275200	-0.68226500
H	3.44528100	-2.11615500	-1.73424000

H	4.81346700	-2.04713500	-0.59616400
H	3.30169500	-2.87637100	-0.14826800
C	3.77369200	-0.43377300	1.68669700
H	3.33871900	-1.23156600	2.29165500
H	4.85939000	-0.56536000	1.64603800
H	3.54660800	0.51574700	2.17524700
C	1.25871100	3.47526100	0.04063300
H	1.91070300	3.36447900	0.90999900
H	1.87839400	3.43038600	-0.85741500
H	0.77352400	4.45516400	0.08579300
C	-1.03987900	2.55982400	1.45379600
H	-0.47789000	2.41429600	2.37869500
H	-1.37349000	3.60059400	1.39743700
H	-1.91089500	1.90279400	1.48197000
C	-1.04592800	2.63059300	-1.40327700
H	-1.36442800	3.67280600	-1.30261400
H	-0.49401900	2.51408600	-2.33829900
H	-1.92715400	1.98819400	-1.44862700
C	0.19117700	-3.56708600	-0.06272000
H	0.80441800	-3.79944100	0.81318900
H	-0.66257800	-4.25442300	-0.07005800
H	0.80172300	-3.77481700	-0.94605700

M1_{Me-a}

Zero-point correction=			0.400772 (Hartree/Particle)
Thermal correction to Energy=			0.431945
Thermal correction to Enthalpy=			0.432889
Thermal correction to Gibbs Free Energy=			0.332233
Sum of electronic and zero-point Energies=			-1586.394543
Sum of electronic and thermal Energies=			-1586.363371
Sum of electronic and thermal Enthalpies=			-1586.362427
Sum of electronic and thermal Free Energies=			-1586.463083
Pd	0.41043300	-0.33346900	-0.32656800
C	-0.52921800	-2.17707400	0.14448500
C	-1.45795800	-1.32538900	0.06186100
P	2.75738500	-0.77060800	-0.55221000
P	-0.04955800	1.98744700	-0.78325800
C	3.56914700	-1.72993700	0.80519000
H	3.55692800	-1.12254300	1.71128500
H	3.01009900	-2.64841700	0.99106200
H	4.60417400	-1.98296200	0.55601100
C	3.98546000	0.59771700	-0.76475000
H	3.94614900	1.24095100	0.11533100
H	5.00187900	0.20982700	-0.88242000

H	3.72945300	1.19020500	-1.64533800
C	3.14785700	-1.82475700	-2.02597800
H	2.81963100	-1.31560400	-2.93437700
H	4.21846900	-2.03790400	-2.10217400
H	2.60001900	-2.76613600	-1.95375100
C	1.29366800	3.25971500	-0.68193400
H	1.75755400	3.21463900	0.30534900
H	2.06435800	3.04026300	-1.42296500
H	0.91132700	4.27002000	-0.85564100
C	-1.34153600	2.77072500	0.28448500
H	-1.01537300	2.73879000	1.32583600
H	-1.53090200	3.80941900	-0.00253300
H	-2.26763500	2.19857100	0.20919500
C	-0.73421500	2.31730200	-2.47156300
H	-0.96796800	3.37629900	-2.61612600
H	-0.01163800	2.00442700	-3.22785800
H	-1.64309700	1.72851700	-2.60795700
H	0.56218700	0.29778200	1.82790400
C	1.64988900	1.08760800	3.20689300
O	0.48778900	0.60900000	2.77227300
O	2.67848800	1.16090200	2.58274200
H	1.54472500	1.42263100	4.25046600
C	-2.84142500	-0.91231600	0.10299900
C	-3.39688300	-0.35588700	1.26934600
C	-3.67036800	-1.06087400	-1.02356500
C	-4.73385700	0.02628000	1.30654300
H	-2.76722100	-0.22922500	2.14232500
C	-5.00615700	-0.67436800	-0.97988900
H	-3.25406700	-1.48627500	-1.92938400
C	-5.54624000	-0.12851600	0.18366800
H	-5.14377600	0.44729500	2.21841600
H	-5.62879800	-0.80230100	-1.85897200
H	-6.58727600	0.17225400	0.21549500
C	-0.11226000	-3.57224600	0.40699800
H	0.46087900	-3.98079200	-0.43024900
H	0.52708200	-3.62967400	1.29289700
H	-0.98010600	-4.22019600	0.57345800

H₂O

Zero-point correction=	0.021309 (Hartree/Particle)
Thermal correction to Energy=	0.024144
Thermal correction to Enthalpy=	0.025088
Thermal correction to Gibbs Free Energy=	0.003007
Sum of electronic and zero-point Energies=	-76.426139

Sum of electronic and thermal Energies=			-76.423304
Sum of electronic and thermal Enthalpies=			-76.422360
Sum of electronic and thermal Free Energies=			-76.444441
O	0.00000000	0.11873600	0.00000000
H	0.75704900	-0.47481200	0.00000000
H	-0.75704900	-0.47507600	0.00000000

M1_{Me}w-b

Zero-point correction=			0.425620 (Hartree/Particle)
Thermal correction to Energy=			0.459837
Thermal correction to Enthalpy=			0.460782
Thermal correction to Gibbs Free Energy=			0.354400
Sum of electronic and zero-point Energies=			-1662.839813
Sum of electronic and thermal Energies=			-1662.805595
Sum of electronic and thermal Enthalpies=			-1662.804651
Sum of electronic and thermal Free Energies=			-1662.911033
Pd	0.11270000	0.62750000	-0.36880000
C	-1.81220000	1.08470000	0.43440000
C	-3.13910000	0.50930000	0.45800000
C	-3.79520000	0.13200000	-0.72660000
C	-3.81700000	0.32120000	1.67670000
C	-5.07900000	-0.40160000	-0.69440000
H	-3.28570000	0.27870000	-1.67170000
C	-5.09640000	-0.22490000	1.70600000
H	-3.32820000	0.60910000	2.60070000
C	-5.73530000	-0.58880000	0.52190000
H	-5.56940000	-0.67540000	-1.62240000
H	-5.59810000	-0.36330000	2.65770000
H	-6.73270000	-1.01270000	0.54610000
C	-1.00330000	1.99510000	0.78940000
P	0.02900000	-1.47540000	-1.54990000
P	2.34970000	1.49530000	-0.50230000
C	-0.70330000	-1.43420000	-3.25140000
H	-1.72060000	-1.04270000	-3.19890000
H	-0.11690000	-0.76700000	-3.88630000
H	-0.72740000	-2.42940000	-3.70540000
C	-1.01650000	-2.76530000	-0.73530000
H	-2.03470000	-2.38670000	-0.62820000
H	-1.03270000	-3.69770000	-1.30750000
H	-0.62140000	-2.95690000	0.26370000
C	1.58600000	-2.42570000	-1.85900000
H	2.13100000	-2.54760000	-0.92140000
H	1.37720000	-3.40800000	-2.29340000
H	2.22380000	-1.86490000	-2.54460000

C	3.15980000	1.89140000	1.11320000
H	2.50630000	2.53600000	1.70330000
H	3.31790000	0.96110000	1.66050000
H	4.12370000	2.38920000	0.97060000
C	2.42120000	3.13710000	-1.35870000
H	1.75500000	3.83890000	-0.85410000
H	3.43550000	3.54760000	-1.36860000
H	2.07210000	3.02490000	-2.38710000
C	3.72590000	0.59480000	-1.35000000
H	4.64560000	1.18810000	-1.35160000
H	3.90690000	-0.34570000	-0.82760000
H	3.44480000	0.37940000	-2.38290000
C	-0.78450000	3.28630000	1.47970000
H	-0.40620000	4.04470000	0.78800000
H	-1.71350000	3.66470000	1.92130000
H	-0.04520000	3.18810000	2.28080000
H	0.54900000	-0.75300000	1.40070000
O	0.49640000	-1.34960000	2.18000000
O	2.73700000	-2.45620000	3.11740000
O	3.60680000	-1.83050000	1.12910000
H	-0.27870000	-1.04860000	2.66490000
H	1.90640000	-2.01960000	2.77990000
C	3.69250000	-2.36860000	2.20960000
H	4.61040000	-2.85940000	2.56840000

TS1_{ph-f}

Zero-point correction=			0.395947 (Hartree/Particle)
Thermal correction to Energy=			0.426083
Thermal correction to Enthalpy=			0.427027
Thermal correction to Gibbs Free Energy=			0.332372
Sum of electronic and zero-point Energies=			-1586.360693
Sum of electronic and thermal Energies=			-1586.330557
Sum of electronic and thermal Enthalpies=			-1586.329613
Sum of electronic and thermal Free Energies=			-1586.424268
Pd	0.37767500	0.06343200	-0.27343600
C	-0.58521500	-2.01297700	-0.50675000
C	-1.37091500	-0.98622400	-0.30130900
P	2.78140100	0.30297300	-0.77326400
P	-0.19693800	2.10463700	0.66521100
C	3.95672400	0.24217000	0.64220700
H	3.78401000	1.09260500	1.30518900
H	3.78719000	-0.67946000	1.20643400
H	4.99139900	0.27515700	0.28784700
C	3.33044900	1.81665900	-1.69223300

H	3.13382900	2.71268000	-1.09947200
H	4.39952700	1.77903700	-1.91994000
H	2.77351700	1.89891000	-2.62814600
C	3.40391600	-1.04194800	-1.86871000
H	2.84082800	-1.04891100	-2.80425900
H	4.46766900	-0.91224900	-2.08837300
H	3.24086300	-1.98406000	-1.34556300
C	-0.66296400	3.44000700	-0.52003400
H	0.15148600	3.60176300	-1.22794500
H	-1.54650600	3.13267100	-1.08131200
H	-0.87971100	4.37691800	0.00097600
C	1.11218900	2.91871300	1.67976000
H	1.97915700	3.14534700	1.05769800
H	0.74421100	3.84606500	2.12761800
H	1.42946600	2.23866200	2.47201700
C	-1.61760400	2.09562300	1.83812300
H	-1.81914400	3.09960300	2.22205100
H	-2.50685700	1.71325600	1.33640300
H	-1.38592200	1.43131300	2.67246500
O	1.80881100	-2.45452400	0.53529500
H	0.60954800	-2.12871700	0.01828300
C	-2.78943400	-0.68757200	-0.25165800
C	-3.64121500	-1.41486700	0.59985700
C	-3.35309600	0.31971700	-1.05575900
C	-5.00488100	-1.14176800	0.64385200
H	-3.21775600	-2.18902000	1.22885700
C	-4.71816900	0.58009000	-1.01953000
H	-2.70545800	0.87661800	-1.72336400
C	-5.54915900	-0.14550100	-0.16499600
H	-5.64518600	-1.71070700	1.30885800
H	-5.13733100	1.34916200	-1.65907000
H	-6.61239700	0.06322000	-0.13202300
C	-0.87380700	-3.34275700	-1.16201600
H	-0.61307000	-4.16461300	-0.48931900
H	-1.92522300	-3.43273900	-1.44773100
H	-0.25480500	-3.46257400	-2.05592900
C	1.90696000	-2.64899800	1.81352400
H	0.99434600	-3.08087100	2.28647900
O	2.88114200	-2.39714000	2.50522400

TS1_{phw-c}

Zero-point correction=	0.422055 (Hartree/Particle)
Thermal correction to Energy=	0.454701
Thermal correction to Enthalpy=	0.455646

Thermal correction to Gibbs Free Energy=			0.356051
Sum of electronic and zero-point Energies=			-1662.802426
Sum of electronic and thermal Energies=			-1662.769780
Sum of electronic and thermal Enthalpies=			-1662.768836
Sum of electronic and thermal Free Energies=			-1662.868431
Pd	-0.20240000	0.69180000	1.39850000
C	1.80950000	0.63970000	0.21230000
C	1.25050000	1.78660000	0.49870000
P	-1.70240000	-1.27670000	1.63480000
P	-1.14890000	2.25700000	2.84940000
C	-2.98530000	-1.32520000	2.97270000
H	-2.50130000	-1.35880000	3.95060000
H	-3.62320000	-0.44020000	2.92760000
H	-3.61580000	-2.21240000	2.86740000
C	-0.91480000	-2.92550000	1.85830000
H	-0.34170000	-2.93160000	2.78710000
H	-1.67160000	-3.71430000	1.89150000
H	-0.22780000	-3.11430000	1.03390000
C	-2.73560000	-1.52280000	0.12750000
H	-2.06280000	-1.72370000	-0.70920000
H	-3.42490000	-2.36220000	0.25650000
H	-3.30840000	-0.61700000	-0.08240000
C	-0.21670000	3.81260000	3.17510000
H	0.77060000	3.56340000	3.56750000
H	-0.08020000	4.37280000	2.25070000
H	-0.74720000	4.43430000	3.90160000
C	-1.39900000	1.64040000	4.57110000
H	-0.44470000	1.28910000	4.96730000
H	-1.78520000	2.43400000	5.21680000
H	-2.09880000	0.80590000	4.57520000
C	-2.82110000	2.89690000	2.39970000
H	-3.20100000	3.58600000	3.15930000
H	-2.76150000	3.41870000	1.44310000
H	-3.51940000	2.06610000	2.28900000
H	1.83870000	-0.40940000	1.00360000
C	2.46640000	-2.54920000	1.17420000
O	2.36260000	-1.41110000	1.75240000
O	2.01850000	-2.89090000	0.07490000
O	0.07660000	-1.71130000	-1.54420000
H	0.77940000	-2.15640000	-1.02520000
H	0.15620000	-0.78920000	-1.27910000
C	1.44690000	3.19250000	0.19450000
C	2.67930000	3.81300000	0.46550000
C	0.42790000	3.95910000	-0.39860000

C	2.88100000	5.15500000	0.15760000
H	3.47070000	3.23120000	0.92310000
C	0.63830000	5.29560000	-0.71860000
H	-0.52140000	3.48440000	-0.62000000
C	1.86350000	5.90070000	-0.43540000
H	3.83660000	5.61860000	0.37590000
H	-0.15230000	5.86740000	-1.19190000
H	2.02450000	6.94450000	-0.67980000
C	2.80380000	0.32660000	-0.88630000
H	2.46200000	-0.51680000	-1.48810000
H	2.96810000	1.19210000	-1.53290000
H	3.75580000	0.02650000	-0.43870000
H	3.02980000	-3.29660000	1.77130000

M2_{ph-f}

Zero-point correction=			0.402933 (Hartree/Particle)
Thermal correction to Energy=			0.432626
Thermal correction to Enthalpy=			0.433570
Thermal correction to Gibbs Free Energy=			0.341191
Sum of electronic and zero-point Energies=			-1586.404271
Sum of electronic and thermal Energies=			-1586.374578
Sum of electronic and thermal Enthalpies=			-1586.373634
Sum of electronic and thermal Free Energies=			-1586.466013
Pd	0.49403800	0.01989500	-0.47451300
C	-0.38580400	-1.74741100	-1.26718400
C	-1.34054000	-1.04310400	-0.83552800
P	2.86645800	-0.03324300	-0.80760100
P	-0.12815600	2.09620500	0.58778700
C	3.98256200	0.70910600	0.46924800
H	3.76212000	1.77298200	0.57192200
H	3.79504800	0.22965300	1.43192700
H	5.03713600	0.58806900	0.20473300
C	3.43630200	0.83305400	-2.34152200
H	3.14771400	1.88475600	-2.29443000
H	4.52097800	0.76484600	-2.46680100
H	2.94700100	0.38899400	-3.21042100
C	3.66133400	-1.69142800	-1.02328000
H	3.18673500	-2.21753600	-1.85310500
H	4.73427300	-1.60526200	-1.21922000
H	3.51389700	-2.28287400	-0.11752800
C	-1.24497600	3.14578500	-0.44823900
H	-0.72636800	3.43656400	-1.36410600
H	-2.12418400	2.56211900	-0.72664200
H	-1.56400800	4.04686800	0.08395600

C	1.12670500	3.34686900	1.13247400
H	1.72998800	3.65923500	0.27722700
H	0.65315300	4.22999100	1.57158900
H	1.78988100	2.89706500	1.87393400
C	-1.12622400	1.91113300	2.13297600
H	-1.44056300	2.88013600	2.53162900
H	-2.00963200	1.30794800	1.91552100
H	-0.53327900	1.38861800	2.88613200
O	1.42499700	-0.91011700	2.45658400
H	1.10341600	-0.63414200	1.56057600
C	-2.73463200	-0.75049600	-0.59500500
C	-3.35924600	-1.12436300	0.60823700
C	-3.50504600	-0.08290700	-1.56439800
C	-4.70484300	-0.84681300	0.82768300
H	-2.78042100	-1.63969700	1.36589000
C	-4.85017100	0.19142900	-1.33869000
H	-3.03614500	0.21106200	-2.49630700
C	-5.45781800	-0.18650600	-0.14212700
H	-5.16746900	-1.15017500	1.76059700
H	-5.42718700	0.70134200	-2.10265900
H	-6.50572500	0.02926500	0.03178300
C	0.07248500	-2.98841600	-1.93033600
H	0.76225200	-3.54764700	-1.29215600
H	-0.77262000	-3.64202000	-2.17321700
H	0.60507100	-2.76377100	-2.85898200
C	0.86734200	-2.08574400	2.79863800
H	0.17882900	-2.47718700	2.02843800
O	1.09941000	-2.64237000	3.83177200

M2_{phw-c}

Zero-point correction=			0.427906 (Hartree/Particle)
Thermal correction to Energy=			0.459384
Thermal correction to Enthalpy=			0.460328
Thermal correction to Gibbs Free Energy=			0.364950
Sum of electronic and zero-point Energies=			-1662.844469
Sum of electronic and thermal Energies=			-1662.812991
Sum of electronic and thermal Enthalpies=			-1662.812047
Sum of electronic and thermal Free Energies=			-1662.907424
Pd	0.34772100	0.00157900	-0.15231000
C	-1.50937300	2.24700200	0.30324800
C	-1.48193900	0.95152700	-0.03372200
P	2.41929400	-1.17813000	-0.80554200
P	0.08846600	-0.74085700	1.99861800
C	2.94207900	-2.80872400	-0.10349300

H	3.18286400	-2.70642200	0.95644300
H	2.13156900	-3.53274600	-0.20802700
H	3.82450900	-3.19162000	-0.62324600
C	3.96674600	-0.18802400	-0.71284500
H	4.22101900	-0.00596900	0.33285900
H	4.79666500	-0.70161900	-1.20621600
H	3.78749300	0.78032100	-1.18350800
C	2.28003500	-1.56675600	-2.60164000
H	2.01038100	-0.65090500	-3.12826900
H	3.21684600	-1.96767200	-2.99781800
H	1.48191500	-2.29616100	-2.75482900
C	-1.24780500	-0.03345100	3.04089000
H	-1.15860400	1.05230300	3.05282300
H	-2.21947600	-0.29699700	2.62356100
H	-1.17160400	-0.42210700	4.06017100
C	1.60596700	-0.30098500	2.93861100
H	1.83562400	0.74630300	2.72836200
H	1.46663000	-0.46189200	4.01097900
H	2.44397000	-0.90833000	2.59322900
C	-0.13434900	-2.54978900	2.27375300
H	-0.15185100	-2.78094700	3.34244500
H	-1.07698900	-2.86699500	1.82400400
H	0.67594900	-3.10551200	1.80183900
H	-0.58273000	2.68785600	0.66739000
C	2.44904400	2.92503900	0.07708800
O	1.83658200	2.30999100	0.96467300
O	2.40026100	2.73647400	-1.18150200
O	0.67274900	1.14279200	-2.00831500
H	1.40991000	1.83137100	-1.65657900
H	-0.12978400	1.66896900	-2.10547100
C	-2.62694800	0.13537400	-0.49038500
C	-3.81921800	0.06040300	0.25279000
C	-2.55004400	-0.62364900	-1.67352700
C	-4.88503400	-0.73241100	-0.16767300
H	-3.90801500	0.63431000	1.16805800
C	-3.61713700	-1.40802300	-2.09712700
H	-1.64139600	-0.58392300	-2.26387200
C	-4.79022100	-1.47079100	-1.34455300
H	-5.79243000	-0.77035000	0.42579600
H	-3.53380400	-1.97353700	-3.01906800
H	-5.61953100	-2.08691200	-1.67329400
C	-2.68073500	3.19459200	0.20459900
H	-2.38912600	4.09815700	-0.34178500
H	-3.54113100	2.75208200	-0.29897600

H	-3.00189200	3.52763800	1.19940300
H	3.13830500	3.74143500	0.38878500

M2_{ph-c}

Zero-point correction= 0.403290 (Hartree/Particle)

Thermal correction to Energy=	0.432749
Thermal correction to Enthalpy=	0.433694
Thermal correction to Gibbs Free Energy=	0.343008
Sum of electronic and zero-point Energies=	-1586.416654
Sum of electronic and thermal Energies=	-1586.387194
Sum of electronic and thermal Enthalpies=	-1586.386250
Sum of electronic and thermal Free Energies=	-1586.476935

Pd	0.64505200	0.09227000	-0.11538200
C	-1.06292500	-0.59289900	2.19495200
C	-1.09745200	-0.34188000	0.87509700
P	0.26484700	2.41933300	0.05117900
P	1.31111300	-2.18438900	-0.09872700
C	1.40705000	3.15440100	1.29026200
H	1.10722700	2.81921200	2.28510000
H	2.41663100	2.78462600	1.10767500
H	1.38402400	4.24720500	1.25515900
C	-1.37205000	3.11175300	0.52114900
H	-1.65449100	2.72922700	1.50274600
H	-1.33533800	4.20383500	0.55444800
H	-2.12961200	2.79486100	-0.19655500
C	0.66573100	3.28847100	-1.51882000
H	-0.09520700	3.04888100	-2.26427800
H	0.70684600	4.37200600	-1.37947600
H	1.62393900	2.91588200	-1.88101900
C	2.61276600	-2.42082600	1.17821300
H	3.36486900	-1.63900600	1.06324900
H	2.16106300	-2.30627600	2.16564900
H	3.06929500	-3.41192800	1.10493000
C	2.11272200	-2.70814200	-1.66931600
H	2.81951000	-1.93509800	-1.96995600
H	2.62430000	-3.66774300	-1.55773400
H	1.35482500	-2.79443800	-2.45066600
C	0.12308400	-3.54714100	0.24628600
H	0.63795700	-4.51080000	0.28232700
H	-0.37117600	-3.36038900	1.19984400
H	-0.64306800	-3.57729200	-0.52991000
H	-0.10176300	-0.49608700	2.69834900
C	3.54305600	0.74876600	-0.65088600
O	2.44084000	0.54128200	-1.28001000

O	3.73533800	0.72470800	0.56318400
H	4.39106800	0.97195800	-1.33517900
C	-2.18155700	-1.05611500	3.10073300
H	-3.04767700	-1.42123500	2.54755000
H	-1.82739400	-1.86437400	3.75012100
H	-2.52404500	-0.25513900	3.76838700
C	-2.32291000	-0.36789000	0.04103200
C	-2.30445500	-0.90105700	-1.26092500
C	-3.54024000	0.17858700	0.49066000
C	-3.44672500	-0.92826200	-2.05399200
H	-1.36986900	-1.28231100	-1.65479600
C	-4.68306500	0.16116000	-0.30522100
H	-3.58504100	0.63904800	1.46962000
C	-4.64643900	-0.40003400	-1.57952900
H	-3.39757100	-1.35378800	-3.05060700
H	-5.60414600	0.59322800	0.07153300
H	-5.53589000	-0.41391300	-2.19925500

TS1_{ph}'-a

Zero-point correction=			0.396186 (Hartree/Particle)
Thermal correction to Energy=			0.426243
Thermal correction to Enthalpy=			0.427187
Thermal correction to Gibbs Free Energy=			0.332632
Sum of electronic and zero-point Energies=			-1586.349366
Sum of electronic and thermal Energies=			-1586.319308
Sum of electronic and thermal Enthalpies=			-1586.318364
Sum of electronic and thermal Free Energies=			-1586.412919
Pd	0.50272300	-0.30986100	0.19691100
C	-0.74833700	1.56573300	1.30126900
C	-1.29850500	0.58569300	0.62488600
P	2.74012400	0.30653900	-0.64188300
P	0.21612900	-2.61354400	0.39726700
C	2.65112800	1.29926500	-2.19538400
H	2.10324600	0.74740200	-2.96176900
H	2.11494200	2.22104400	-1.96247100
H	3.64977100	1.54205300	-2.57140500
C	3.98115300	-0.99621000	-1.09213000
H	3.56076400	-1.65974500	-1.85126700
H	4.90311400	-0.55545400	-1.48269000
H	4.22481100	-1.59478000	-0.21143100
C	3.73689600	1.41911800	0.44291000

H	3.89506000	0.95313600	1.41768000
H	4.70830700	1.64476700	-0.00758800
H	3.17090200	2.34353000	0.57009300
C	0.34419600	-3.60500300	-1.15890900
H	-0.43824700	-3.29641200	-1.85448500
H	1.31047600	-3.41740300	-1.63007400
H	0.24143900	-4.67622200	-0.96144200
C	-1.36150400	-3.25797000	1.11392100
H	-2.20417600	-2.89899300	0.52083200
H	-1.37825900	-4.35175200	1.14257100
H	-1.47659600	-2.86989300	2.12765400
C	1.46704200	-3.44937600	1.47304800
H	1.29058500	-4.52752300	1.53193500
H	2.46723300	-3.27120500	1.07520000
H	1.42158100	-3.02525100	2.47767200
C	0.25111200	4.22570900	-0.18472700
O	1.26712800	3.52807500	-0.12171400
O	-0.92362800	3.95437900	0.24499400
H	0.31224500	5.22666100	-0.66629200
H	-0.94068600	2.70587900	0.77726700
C	-2.57421000	0.35250900	-0.02452400
C	-2.68046200	-0.41014000	-1.20137600
C	-3.74931100	0.89938800	0.52626900
C	-3.91302400	-0.61513600	-1.80783100
H	-1.77497300	-0.81690200	-1.63616200
C	-4.98198700	0.68927400	-0.08004300
H	-3.67483300	1.49583400	1.42730600
C	-5.06852700	-0.06942300	-1.24657100
H	-3.97622900	-1.19423300	-2.72238800
H	-5.87643600	1.12123700	0.35441700
H	-6.03070200	-0.23149500	-1.71936200
C	0.13416000	1.70987800	2.50708800
H	0.44642700	0.75317600	2.93217300
H	1.01218300	2.30457200	2.24827200
H	-0.41791900	2.26716800	3.27344500

TS1_{ph}'w-a

Zero-point correction=	0.420948 (Hartree/Particle)
Thermal correction to Energy=	0.454081
Thermal correction to Enthalpy=	0.455025
Thermal correction to Gibbs Free Energy=	0.352378
Sum of electronic and zero-point Energies=	-1662.793852
Sum of electronic and thermal Energies=	-1662.760719
Sum of electronic and thermal Enthalpies=	-1662.759775

Sum of electronic and thermal Free Energies=			-1662.862422
Pd	-0.73042400	-0.32056900	-0.09267100
C	1.09811800	1.25532100	-1.26153500
C	1.24031200	0.20583700	-0.50464000
P	-2.90847000	0.52396100	0.71289300
P	-0.56657000	-2.56879000	-0.65285600
C	-2.79549500	1.69618700	2.13426600
H	-2.26480000	1.22900900	2.96598800
H	-2.23365100	2.56817800	1.79215900
H	-3.78870900	2.00867100	2.47178800
C	-4.19635700	-0.67300200	1.30125400
H	-3.79090100	-1.27938700	2.11399700
H	-5.09176800	-0.15571100	1.65879700
H	-4.47899000	-1.34110200	0.48470800
C	-3.85448000	1.52953000	-0.51293800
H	-4.06333400	0.93525400	-1.40478200
H	-4.79807500	1.89000300	-0.09218300
H	-3.22705100	2.37935900	-0.78619200
C	-2.08081200	-3.26090200	-1.45772200
H	-2.93539600	-3.13623400	-0.79081100
H	-2.28516000	-2.71377400	-2.37966500
H	-1.95949000	-4.32301200	-1.69116300
C	-0.32441800	-3.73988000	0.75511000
H	0.62333800	-3.52014300	1.24884500
H	-1.12913300	-3.60870000	1.48037700
H	-0.31504600	-4.77802600	0.40991400
C	0.75125300	-3.11866000	-1.82424000
H	0.64573600	-2.57676400	-2.76573200
H	1.72965800	-2.88014900	-1.40510400
H	0.69287200	-4.19396900	-2.01749500
C	2.42962300	4.10679500	-0.08336800
O	2.86617100	3.09875400	-0.74584400
O	-1.34795400	3.74162400	-0.08906700
H	3.22652300	4.84437600	0.14437100
H	1.98369400	2.19178700	-0.94064100
O	1.28410700	4.33365200	0.30635600
H	-0.38017300	3.80151200	0.07208100
H	-1.60651400	4.66051500	-0.20817400
C	2.36083700	-0.39082200	0.21664400
C	3.64319900	-0.39552000	-0.36189700
C	2.20350900	-0.95886300	1.49296000
C	4.72500900	-0.95186400	0.31254500
H	3.77914400	0.05746600	-1.33605900
C	3.28677700	-1.51312300	2.16505400

H	1.22213400	-0.94242000	1.95327100
C	4.55127100	-1.51545200	1.57540900
H	5.70719400	-0.93969200	-0.14666400
H	3.14899400	-1.93373700	3.15511000
H	5.39625900	-1.94642000	2.10059200
C	0.21206600	1.73786300	-2.36825100
H	-0.39121400	2.58183600	-2.02215900
H	0.84052400	2.10418300	-3.18744400
H	-0.45261200	0.96277900	-2.75889000

M2_{ph}'w-a

Zero-point correction=			0.427238 (Hartree/Particle)
Thermal correction to Energy=			0.459220
Thermal correction to Enthalpy=			0.460164
Thermal correction to Gibbs Free Energy=			0.361187
Sum of electronic and zero-point Energies=			-1662.844593
Sum of electronic and thermal Energies=			-1662.812612
Sum of electronic and thermal Enthalpies=			-1662.811667
Sum of electronic and thermal Free Energies=			-1662.910644
Pd	0.55511800	-0.27338700	0.29658200
C	-1.58271400	-0.51618200	2.37934000
C	-1.37202200	-0.33627000	1.06856300
P	2.83802800	0.31023600	-0.44542300
P	0.24064400	-2.46453900	-0.36420200
C	2.80596600	1.54171500	-1.81495200
H	2.42704100	1.06604400	-2.72215100
H	2.13614200	2.36205200	-1.55435600
H	3.80683400	1.93659900	-2.01082800
C	4.16774100	-0.84758900	-1.01198400
H	3.86952200	-1.35042000	-1.93346700
H	5.09643400	-0.30134500	-1.19855300
H	4.35692500	-1.60631200	-0.25027400
C	3.66816800	1.20893400	0.92720900
H	3.92182400	0.50359900	1.72164900
H	4.57709100	1.71218700	0.58679000
H	2.94962700	1.92845400	1.32034500
C	1.68339600	-3.39517000	-1.04183000
H	2.05652000	-2.89976000	-1.93866500
H	2.48678400	-3.43047100	-0.30505000
H	1.39178200	-4.41698900	-1.29868900
C	-0.99635700	-2.65935400	-1.71118200
H	-1.95488500	-2.25130000	-1.39120600
H	-0.66665000	-2.09839200	-2.58737500
H	-1.11543400	-3.71247200	-1.97987300

C	-0.35728100	-3.62004100	0.93777400
H	0.37906600	-3.67425200	1.74143000
H	-1.28905700	-3.24017900	1.35462100
H	-0.51499600	-4.62005200	0.52531300
C	-0.27303800	4.63604800	-0.13526900
O	-0.69005400	4.72722200	0.99496300
O	0.63016200	1.71730000	0.95033700
H	-0.35606600	5.45799800	-0.86964900
H	-2.59915500	-0.37728400	2.75622600
O	0.32504100	3.58753800	-0.67234000
H	0.42673500	2.80807000	0.03635200
H	-0.06268100	1.83378200	1.60988600
C	-2.48103900	-0.03334500	0.13479800
C	-3.69618100	-0.74005600	0.20161200
C	-2.35671500	0.96127800	-0.85129700
C	-4.74490700	-0.45839100	-0.67085700
H	-3.81190400	-1.52170700	0.94470500
C	-3.40730100	1.24453200	-1.71810800
H	-1.43768000	1.53061200	-0.91531400
C	-4.60553300	0.53564400	-1.63673100
H	-5.67088500	-1.01896400	-0.59641100
H	-3.29020300	2.02873700	-2.45823200
H	-5.42016800	0.75598900	-2.31752200
C	-0.55899700	-0.84980500	3.42787300
H	-0.48846300	-0.05195200	4.17617100
H	-0.83189400	-1.76253800	3.97226900
H	0.43197400	-0.98756100	2.99004000

M2_{phw-e}

Zero-point correction=			0.427783 (Hartree/Particle)
Thermal correction to Energy=			0.460501
Thermal correction to Enthalpy=			0.461446
Thermal correction to Gibbs Free Energy=			0.363078
Sum of electronic and zero-point Energies=			-1662.862325
Sum of electronic and thermal Energies=			-1662.829607
Sum of electronic and thermal Enthalpies=			-1662.828662
Sum of electronic and thermal Free Energies=			-1662.927030
Pd	0.53344100	0.04738400	-0.28878200
C	-0.96972300	-0.34547300	2.19169800
C	-1.13826800	-0.21705100	0.86541600
P	0.27235300	2.39722000	-0.21174300
P	1.01760500	-2.28153100	-0.22217200
C	1.60701600	3.17187400	0.78781800
H	1.62061400	2.70540500	1.77401200

H	2.57087200	2.96523100	0.32191100
H	1.45883300	4.25167100	0.87554500
C	-1.25552800	3.15944400	0.46751800
H	-1.37383900	2.85143600	1.50709700
H	-1.19900400	4.24989600	0.41488100
H	-2.12502500	2.81179400	-0.09145900
C	0.44229700	3.16919200	-1.87298900
H	-0.42183800	2.90219200	-2.48430800
H	0.51585200	4.25815800	-1.80742900
H	1.33529000	2.76217500	-2.34870200
C	-0.19883800	-3.48907800	0.44652100
H	-0.43254800	-3.22624700	1.47843200
H	-1.12384200	-3.44624800	-0.13006200
H	0.20530200	-4.50422400	0.41019400
C	2.52156900	-2.60518100	0.78584100
H	2.38690500	-2.16233800	1.77369500
H	2.71603400	-3.67802200	0.86885200
H	3.37434500	-2.10610300	0.32499900
C	1.44045400	-2.96825500	-1.87753900
H	1.86836700	-3.97123400	-1.79994200
H	0.54247500	-3.00922700	-2.49721600
H	2.15255200	-2.29398300	-2.35449500
H	0.04235600	-0.23157400	2.57677000
C	3.44433800	0.49386500	-1.09986800
O	2.28354100	0.31379700	-1.59552300
O	3.77139600	0.54335800	0.09386300
H	4.23896000	0.61784400	-1.86472100
C	-2.00371100	-0.68394200	3.24139800
H	-2.92967900	-1.07553300	2.81784600
H	-1.60025200	-1.43299800	3.93157500
H	-2.25880800	0.18931300	3.85576000
C	-2.43211500	-0.26167800	0.14593700
C	-2.54412500	-0.86496600	-1.12068500
C	-3.59335000	0.33973400	0.67007000
C	-3.75468200	-0.90960600	-1.80433600
H	-1.65642500	-1.28752300	-1.57620000
C	-4.80457500	0.30340800	-0.01616000
H	-3.53902600	0.85802800	1.61889000
C	-4.89629200	-0.32896000	-1.25393500
H	-3.80448300	-1.39030300	-2.77557200
H	-5.67879100	0.77816500	0.41683300
H	-5.83918600	-0.35657200	-1.78831500
O	2.42894200	0.32578000	2.52937200
H	2.84247200	0.39344100	1.64180800

H	3.16601600	0.41894400	3.14009100
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M2_{ph-c}

Zero-point correction=			0.403290 (Hartree/Particle)
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Thermal correction to Energy=			0.432749
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Thermal correction to Enthalpy=			0.433694
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Thermal correction to Gibbs Free Energy=			0.343008
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Sum of electronic and zero-point Energies=			-1586.416654
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Sum of electronic and thermal Energies=			-1586.387194
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Sum of electronic and thermal Enthalpies=			-1586.386250
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Sum of electronic and thermal Free Energies=			-1586.476935
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Pd	0.64505200	0.09227000	-0.11538200
C	-1.06292500	-0.59289900	2.19495200
C	-1.09745200	-0.34188000	0.87509700
P	0.26484700	2.41933300	0.05117900
P	1.31111300	-2.18438900	-0.09872700
C	1.40705000	3.15440100	1.29026200
H	1.10722700	2.81921200	2.28510000
H	2.41663100	2.78462600	1.10767500
H	1.38402400	4.24720500	1.25515900
C	-1.37205000	3.11175300	0.52114900
H	-1.65449100	2.72922700	1.50274600
H	-1.33533800	4.20383500	0.55444800
H	-2.12961200	2.79486100	-0.19655500
C	0.66573100	3.28847100	-1.51882000
H	-0.09520700	3.04888100	-2.26427800
H	0.70684600	4.37200600	-1.37947600
H	1.62393900	2.91588200	-1.88101900
C	2.61276600	-2.42082600	1.17821300
H	3.36486900	-1.63900600	1.06324900
H	2.16106300	-2.30627600	2.16564900
H	3.06929500	-3.41192800	1.10493000
C	2.11272200	-2.70814200	-1.66931600
H	2.81951000	-1.93509800	-1.96995600
H	2.62430000	-3.66774300	-1.55773400
H	1.35482500	-2.79443800	-2.45066600
C	0.12308400	-3.54714100	0.24628600
H	0.63795700	-4.51080000	0.28232700
H	-0.37117600	-3.36038900	1.19984400
H	-0.64306800	-3.57729200	-0.52991000
H	-0.10176300	-0.49608700	2.69834900
C	3.54305600	0.74876600	-0.65088600
O	2.44084000	0.54128200	-1.28001000
O	3.73533800	0.72470800	0.56318400

H	4.39106800	0.97195800	-1.33517900
C	-2.18155700	-1.05611500	3.10073300
H	-3.04767700	-1.42123500	2.54755000
H	-1.82739400	-1.86437400	3.75012100
H	-2.52404500	-0.25513900	3.76838700
C	-2.32291000	-0.36789000	0.04103200
C	-2.30445500	-0.90105700	-1.26092500
C	-3.54024000	0.17858700	0.49066000
C	-3.44672500	-0.92826200	-2.05399200
H	-1.36986900	-1.28231100	-1.65479600
C	-4.68306500	0.16116000	-0.30522100
H	-3.58504100	0.63904800	1.46962000
C	-4.64643900	-0.40003400	-1.57952900
H	-3.39757100	-1.35378800	-3.05060700
H	-5.60414600	0.59322800	0.07153300
H	-5.53589000	-0.41391300	-2.19925500

Com2_{ph}-a

Zero-point correction=			0.399194 (Hartree/Particle)
Thermal correction to Energy=			0.428925
Thermal correction to Enthalpy=			0.429869
Thermal correction to Gibbs Free Energy=			0.337667
Sum of electronic and zero-point Energies=			-1586.396258
Sum of electronic and thermal Energies=			-1586.366527
Sum of electronic and thermal Enthalpies=			-1586.365583
Sum of electronic and thermal Free Energies=			-1586.457786
Pd	-0.62018400	0.05910200	0.18493400
C	1.49587100	-0.65300000	2.16928700
C	1.30807200	-0.36669400	0.87262200
P	-1.23504800	-2.22981100	0.07889700
P	-0.29606200	2.39624600	0.29172100
C	-2.69911500	-2.58562100	1.13398500
H	-2.46911500	-2.35872700	2.17636400
H	-3.51882400	-1.94919500	0.79789500
H	-2.99281900	-3.63565300	1.04978000
C	-0.02680300	-3.52947300	0.56521000
H	0.31176600	-3.34935400	1.58581300
H	-0.48183800	-4.52122200	0.49921000
H	0.84616100	-3.48679800	-0.08759700
C	-1.79565600	-2.75838400	-1.59129100
H	-0.98681200	-2.63941700	-2.31419400
H	-2.11705800	-3.80345400	-1.58096900
H	-2.63271100	-2.12161700	-1.88039200
C	-0.49227000	3.20520900	-1.34665300

H	0.25704800	2.81706700	-2.03854300
H	-1.48864700	2.96892900	-1.72286100
H	-0.38063500	4.28981300	-1.26293000
C	1.28355700	3.08417400	0.93229800
H	2.10866900	2.76003300	0.29736700
H	1.24687300	4.17668100	0.94891200
H	1.46182300	2.71026700	1.94136300
C	-1.57281700	3.21687100	1.32992300
H	-1.42674300	4.30046900	1.34181800
H	-2.55192600	2.98546100	0.90910600
H	-1.51901100	2.83516100	2.35097300
C	-3.49006200	0.68171700	-0.87575900
O	-3.59561900	1.87734400	-1.00457100
O	-4.07650800	-0.36500600	-1.01181900
H	-2.23672800	0.41207500	-0.38998300
H	0.63245600	-0.59883400	2.83173800
C	2.37554200	-0.32379700	-0.15030100
C	2.19880800	-0.90740700	-1.41828300
C	3.59476100	0.34132200	0.08475300
C	3.19664200	-0.86250300	-2.38616300
H	1.25732100	-1.39361500	-1.64408300
C	4.59097000	0.39641100	-0.88687400
H	3.75481600	0.82806500	1.03916200
C	4.40108200	-0.21006000	-2.12651400
H	3.03005700	-1.33037100	-3.35050100
H	5.51827300	0.91769400	-0.67392700
H	5.17614000	-0.16718200	-2.88319000
C	2.76476400	-1.10716300	2.85524100
H	2.56214400	-1.98458300	3.47977500
H	3.55189900	-1.36977900	2.14787900
H	3.15951200	-0.33543200	3.52801900

TS2_{Ph-a}

Zero-point correction=			0.398272 (Hartree/Particle)
Thermal correction to Energy=			0.427515
Thermal correction to Enthalpy=			0.428460
Thermal correction to Gibbs Free Energy=			0.337094
Sum of electronic and zero-point Energies=			-1586.397023
Sum of electronic and thermal Energies=			-1586.367780
Sum of electronic and thermal Enthalpies=			-1586.366835
Sum of electronic and thermal Free Energies=			-1586.458201
Pd	-0.62118300	0.05353000	0.18197400
C	1.52311400	-0.64176900	2.16654200
C	1.32576800	-0.35518400	0.87044400

P	-1.21082000	-2.23427100	0.07750000
P	-0.32056400	2.38636800	0.28950900
C	-2.65541900	-2.62098100	1.15012000
H	-2.41247400	-2.39694600	2.19021700
H	-3.49221000	-1.99667400	0.83565300
H	-2.93314300	-3.67523900	1.06442600
C	0.01683000	-3.52291900	0.54670800
H	0.37042900	-3.33635100	1.56096200
H	-0.42874100	-4.51961300	0.48960600
H	0.87904300	-3.47232000	-0.11965600
C	-1.78030200	-2.77633100	-1.58646900
H	-0.97852100	-2.64689900	-2.31553700
H	-2.08502800	-3.82634700	-1.57165300
H	-2.62796100	-2.15449300	-1.87541600
C	-0.54029700	3.20927800	-1.34012700
H	0.20524400	2.83137500	-2.04174500
H	-1.53666900	2.97084800	-1.71368600
H	-0.43384100	4.29386100	-1.24925800
C	1.26316700	3.08489900	0.90923500
H	2.08125800	2.76539100	0.26292100
H	1.22101200	4.17721700	0.92868700
H	1.45762200	2.70888500	1.91446400
C	-1.58187000	3.20158800	1.35226600
H	-1.43915700	4.28561800	1.36586900
H	-2.56960600	2.96915100	0.95389400
H	-1.50719800	2.81659400	2.37079400
C	-3.59617300	0.66815400	-0.88160200
O	-3.66645100	1.85717800	-0.98405300
O	-4.12699600	-0.39718600	-0.99634600
H	-2.20787500	0.38247700	-0.37415200
H	0.66152900	-0.59693000	2.83281200
C	2.39563500	-0.30458700	-0.15017600
C	2.22330700	-0.88864100	-1.41893000
C	3.60991200	0.37094600	0.08229400
C	3.21961400	-0.83553900	-2.38806900
H	1.28517900	-1.38205400	-1.64382700
C	4.60423200	0.43559300	-0.89079200
H	3.76716500	0.85920600	1.03648100
C	4.41876400	-0.17257400	-2.13032900
H	3.05582600	-1.30491200	-3.35228500
H	5.52709500	0.96531300	-0.67886700
H	5.19253100	-0.12282600	-2.88797200
C	2.79756900	-1.08541900	2.84994800
H	2.60435500	-1.96478300	3.47502300

H	3.58553500	-1.34146100	2.14091900
H	3.18825000	-0.31092900	3.52220500

M3_{ph-a}

Zero-point correction= 0.398098 (Hartree/Particle)

Thermal correction to Energy=	0.428865
Thermal correction to Enthalpy=	0.429810
Thermal correction to Gibbs Free Energy=	0.330854
Sum of electronic and zero-point Energies=	-1586.407586
Sum of electronic and thermal Energies=	-1586.376818
Sum of electronic and thermal Enthalpies=	-1586.375874
Sum of electronic and thermal Free Energies=	-1586.474829

Pd	-0.55694900	-0.07781500	0.42047300
C	1.93898500	-1.06226600	1.89378700
C	1.52378600	-0.51771300	0.73706800
P	-1.17714200	-2.30274600	0.06951600
P	-0.28554400	2.21705100	0.74688700
C	-2.47831800	-2.88166900	1.24041700
H	-2.10130800	-2.81460500	2.26256300
H	-3.34734800	-2.22892600	1.15346700
H	-2.77135000	-3.91477700	1.03314100
C	0.08269900	-3.64170000	0.19512600
H	0.55771900	-3.60036400	1.17565900
H	-0.37165000	-4.62507000	0.04505100
H	0.86126900	-3.48100100	-0.55195600
C	-1.94288100	-2.63724300	-1.57384800
H	-1.22245500	-2.41925800	-2.36456700
H	-2.25788200	-3.68113800	-1.65822600
H	-2.80519900	-1.98342100	-1.70562700
C	-0.29109700	3.17112200	-0.82892200
H	0.51974100	2.81484900	-1.46634600
H	-1.23855700	3.00246300	-1.34200700
H	-0.16364300	4.24170200	-0.64516300
C	1.23230400	2.83453500	1.58595800
H	2.10579100	2.56391300	0.99253900
H	1.19816800	3.92050100	1.70997300
H	1.32590100	2.35739200	2.56249100
C	-1.62550000	3.02660100	1.71950700
H	-1.44503300	4.09965500	1.83039000
H	-2.57597700	2.86484300	1.21102000
H	-1.68271600	2.56816500	2.70841700
C	-4.25262600	1.08809200	-1.32770800
O	-3.95878800	2.20146800	-1.17860600
O	-4.58649300	-0.00970900	-1.50145800

H	-2.13666700	0.24504600	0.19000300
H	1.19344200	-1.21842500	2.67574300
C	2.43964100	-0.19820400	-0.38093200
C	2.10682700	-0.53576300	-1.70746800
C	3.64123600	0.51444100	-0.19190600
C	2.93802000	-0.21563300	-2.77600000
H	1.17069300	-1.05090800	-1.89158700
C	4.46774500	0.85093000	-1.26187800
H	3.92242700	0.81307100	0.81147600
C	4.12621800	0.48270200	-2.56143300
H	2.65329000	-0.50369600	-3.78285600
H	5.38409700	1.40269600	-1.07800000
H	4.77013300	0.74202200	-3.39432600
C	3.31736900	-1.55956900	2.27274000
H	3.25601900	-2.57245000	2.68905100
H	4.00113900	-1.58688200	1.42327800
H	3.77571100	-0.93655200	3.05204800

M4_{ph}-a

Zero-point correction=			0.385867 (Hartree/Particle)
Thermal correction to Energy=			0.412198
Thermal correction to Enthalpy=			0.413142
Thermal correction to Gibbs Free Energy=			0.326393
Sum of electronic and zero-point Energies=			-1397.774228
Sum of electronic and thermal Energies=			-1397.747897
Sum of electronic and thermal Enthalpies=			-1397.746953
Sum of electronic and thermal Free Energies=			-1397.833702
Pd	-0.85800200	0.68638500	0.13002400
C	0.15518700	-1.17652400	-2.11729200
C	0.41273500	-0.76096700	-0.86431400
P	0.73599200	2.37828600	-0.04685000
P	-2.63862900	-0.80722600	0.32386700
C	1.61402500	2.51481800	-1.66066300
H	2.10334600	1.56683900	-1.88307400
H	0.88710500	2.71251800	-2.45049400
H	2.35550300	3.31855700	-1.64258600
C	2.11611700	2.24155200	1.16576000
H	2.62032600	1.28320000	1.03609100
H	2.83584600	3.05474600	1.03569200
H	1.70884600	2.28004000	2.17753100
C	0.14097400	4.10272100	0.21671900
H	-0.29654900	4.17707500	1.21290000
H	0.95197900	4.82950600	0.11404800
H	-0.64158300	4.32641700	-0.51008500

C	-3.89240600	-0.46291800	1.63084100
H	-3.40704900	-0.47948600	2.60828500
H	-4.29823900	0.53737900	1.47639700
H	-4.70175700	-1.19844600	1.61576600
C	-2.28552900	-2.59663500	0.59350300
H	-1.81959400	-2.73623900	1.57062800
H	-3.20286500	-3.19054700	0.54945000
H	-1.58546000	-2.93829200	-0.16905700
C	-3.65981000	-0.83938700	-1.21070500
H	-4.50280700	-1.52935800	-1.11344500
H	-4.03519900	0.16443300	-1.41516700
H	-3.03424700	-1.15104600	-2.04851400
H	-0.68738800	-0.72070800	-2.64083600
H	-1.80518500	1.76524500	0.87134800
C	1.57625200	-1.24556400	-0.08747700
C	2.88745900	-1.21284600	-0.60295700
C	1.42956700	-1.68217800	1.24355100
C	3.98376800	-1.60828600	0.16158100
H	3.04528300	-0.86489600	-1.61769000
C	2.51954600	-2.09268600	2.00321100
H	0.43817700	-1.68520200	1.68091700
C	3.80769000	-2.05695900	1.46855300
H	4.97955900	-1.56699700	-0.26808400
H	2.36615400	-2.43271900	3.02231600
H	4.65923500	-2.36674900	2.06386700
C	0.85730200	-2.24363100	-2.92990600
H	0.12846500	-2.94967600	-3.34582400
H	1.39092000	-1.81546800	-3.78855800
H	1.57760100	-2.81281100	-2.34061900

M4_{ph}-b

Zero-point correction=			0.385852 (Hartree/Particle)
Thermal correction to Energy=			0.412323
Thermal correction to Enthalpy=			0.413267
Thermal correction to Gibbs Free Energy=			0.327659
Sum of electronic and zero-point Energies=			-1397.772542
Sum of electronic and thermal Energies=			-1397.746072
Sum of electronic and thermal Enthalpies=			-1397.745128
Sum of electronic and thermal Free Energies=			-1397.830735
Pd	-0.60271500	-0.30277600	0.41579400
C	1.65675500	0.31566000	2.31542300
C	1.37977600	-0.13399500	1.08076800
P	-2.81727100	-1.04927700	-0.05264900
P	-0.54496600	1.95992800	-0.52050200

C	-3.15539100	-2.79474500	0.44227400
H	-2.47106100	-3.45546000	-0.09239800
H	-2.95705500	-2.90556400	1.50929500
H	-4.18755500	-3.08733700	0.22785100
C	-3.41095100	-1.05412700	-1.80587700
H	-2.71956100	-1.63501600	-2.41921500
H	-4.41236500	-1.48547500	-1.89096900
H	-3.43105700	-0.03391700	-2.19223700
C	-4.18998300	-0.15543500	0.80773500
H	-4.20454200	0.88919900	0.49204700
H	-5.16361300	-0.60605400	0.59461300
H	-4.01291400	-0.18059800	1.88454700
C	-2.03947200	2.79308000	-1.23700700
H	-2.41528200	2.21532200	-2.08389900
H	-2.82774800	2.84974300	-0.48327900
H	-1.81028400	3.80587700	-1.58051600
C	0.66192300	2.15055600	-1.90277100
H	0.34315300	1.53419600	-2.74586100
H	0.74349900	3.19133000	-2.22900700
H	1.63903100	1.78986900	-1.57981400
C	0.01969500	3.23657700	0.68543700
H	0.18356600	4.20421400	0.20329600
H	-0.73148800	3.34950100	1.47023300
H	0.94291800	2.89147600	1.15197100
H	0.82080700	0.61475600	2.94635700
H	-0.37419000	-1.69723500	1.10559400
C	2.42222800	-0.57723500	0.12569800
C	2.35376500	-1.83870200	-0.49308300
C	3.50187800	0.25423900	-0.22744800
C	3.32929900	-2.25868300	-1.39066300
H	1.51734100	-2.48417800	-0.25278700
C	4.47180900	-0.15954000	-1.13907500
H	3.57725600	1.23801500	0.22317900
C	4.39420500	-1.42092900	-1.72402000
H	3.25555400	-3.24406700	-1.83949400
H	5.29143100	0.50631400	-1.38956000
H	5.14823000	-1.74546200	-2.43256500
C	2.99972800	0.39332800	3.00569400
H	2.95468600	-0.11905200	3.97413000
H	3.79901600	-0.06335800	2.42109700
H	3.28909500	1.43058600	3.21960900

TS3_{Ph}

Zero-point correction=

0.383778 (Hartree/Particle)

Thermal correction to Energy=			0.410366
Thermal correction to Enthalpy=			0.411310
Thermal correction to Gibbs Free Energy=			0.324131
Sum of electronic and zero-point Energies=			-1397.768091
Sum of electronic and thermal Energies=			-1397.741503
Sum of electronic and thermal Enthalpies=			-1397.740559
Sum of electronic and thermal Free Energies=			-1397.827738
Pd	-0.59244100	-0.24638400	0.37856000
C	1.69366500	-0.11619100	2.43280800
C	1.38121200	-0.40749400	1.15796600
P	-2.74942000	-1.13447500	-0.11610300
P	-0.59199300	2.08995700	-0.37351800
C	-2.97607000	-2.93302400	0.25401900
H	-2.24929700	-3.50815000	-0.32262500
H	-2.77268800	-3.10680100	1.31209400
H	-3.98544200	-3.28256700	0.01528100
C	-3.35244900	-1.06547000	-1.86703100
H	-2.63134900	-1.56548500	-2.51660700
H	-4.32901300	-1.54520000	-1.98138400
H	-3.42779500	-0.02454700	-2.18676700
C	-4.19183100	-0.40522200	0.78927700
H	-4.28027600	0.65442200	0.54236900
H	-5.12984500	-0.90942400	0.53802800
H	-4.01950300	-0.48744300	1.86414700
C	-2.13331200	3.02233400	-0.82334900
H	-2.62686000	2.53097100	-1.66496300
H	-2.82266700	3.01841900	0.02385700
H	-1.91900100	4.05935400	-1.09873500
C	0.45890800	2.43074100	-1.85753200
H	0.03674400	1.91842600	-2.72459500
H	0.52531500	3.50164600	-2.07249200
H	1.46019200	2.03051900	-1.69018500
C	0.14382800	3.23353100	0.87892500
H	0.27208400	4.24678900	0.48718900
H	-0.50330500	3.26849700	1.75796100
H	1.10912900	2.83551300	1.19505900
H	0.87234700	0.03288300	3.13092700
H	0.08896200	-1.49998700	1.08116100
C	2.38898100	-0.66574400	0.10269100
C	2.38611800	-1.86462900	-0.63096600
C	3.36816800	0.29009300	-0.22237500
C	3.33100200	-2.10642500	-1.62275500
H	1.62908900	-2.60818600	-0.41036400
C	4.30830400	0.05288100	-1.22310000

H	3.38884600	1.22885900	0.32025900
C	4.29767000	-1.14857400	-1.92799200
H	3.31069600	-3.04667800	-2.16397700
H	5.05294700	0.80900700	-1.44979300
H	5.02917100	-1.33529100	-2.70626200
C	3.06636800	-0.02153400	3.05195500
H	3.12284800	-0.65103200	3.94807400
H	3.85549200	-0.33585300	2.36797600
H	3.29328000	1.00112900	3.37969700

M5_{ph}

Zero-point correction=			0.389773 (Hartree/Particle)
Thermal correction to Energy=			0.416949
Thermal correction to Enthalpy=			0.417893
Thermal correction to Gibbs Free Energy=			0.326357
Sum of electronic and zero-point Energies=			-1397.812725
Sum of electronic and thermal Energies=			-1397.785549
Sum of electronic and thermal Enthalpies=			-1397.784605
Sum of electronic and thermal Free Energies=			-1397.876141
Pd	-1.59295600	0.17868000	-0.01640200
C	2.49610300	-1.56800700	2.18758500
C	2.13942000	-0.74273200	1.19179500
P	-2.07595900	-2.05756800	-0.42070800
P	-1.26840600	2.44310500	0.40731900
C	-0.67373000	-3.23442900	-0.69749600
H	-0.10647500	-2.92026200	-1.57564400
H	0.00129300	-3.20710400	0.15965600
H	-1.02941000	-4.25850000	-0.84774000
C	-3.13287600	-2.42623800	-1.89645600
H	-2.63078700	-2.07028400	-2.79800300
H	-3.33372900	-3.49767500	-1.99603400
H	-4.07902100	-1.88958300	-1.80645600
C	-3.01585800	-2.93981000	0.90965200
H	-3.95457700	-2.41529000	1.09650400
H	-3.23037100	-3.97801100	0.63716500
H	-2.43450800	-2.92449100	1.83337900
C	-2.77050100	3.40092100	0.91414000
H	-3.53038600	3.32196100	0.13466800
H	-3.18219100	2.96866900	1.82795500
H	-2.53902900	4.45667300	1.08714000
C	-0.63872500	3.48673600	-0.98643200
H	-1.32319600	3.40950900	-1.83324400
H	-0.54149100	4.53777800	-0.69687600
H	0.33540000	3.11128900	-1.30494800

C	-0.08805500	2.90929100	1.75545700
H	-0.02442700	3.99456100	1.88198600
H	-0.41561900	2.45781000	2.69380300
H	0.90308600	2.51628900	1.52210600
H	1.72425100	-1.79785300	2.91914500
H	1.09861700	-0.42007600	1.17109300
C	2.93808300	-0.23627000	0.06161700
C	2.26823200	0.07997200	-1.13446200
C	4.32356100	-0.00849700	0.11759500
C	2.95995200	0.56153700	-2.24085600
H	1.19035700	-0.05241000	-1.17941300
C	5.01385400	0.47896300	-0.98916400
H	4.86119100	-0.18160500	1.04074300
C	4.33913000	0.75741000	-2.17587700
H	2.42079900	0.78904000	-3.15425300
H	6.08255300	0.65133600	-0.92012800
H	4.87985000	1.13594300	-3.03614400
C	3.81245800	-2.25451200	2.41883800
H	3.64798400	-3.26582700	2.80281300
H	4.40991400	-2.32977300	1.50888700
H	4.41506900	-1.73044200	3.17154200

(Z)-1-phenylpropene

Zero-point correction= 0.161112 (Hartree/Particle)

Thermal correction to Energy=	0.169267		
Thermal correction to Enthalpy=	0.170211		
Thermal correction to Gibbs Free Energy=	0.127886		
Sum of electronic and zero-point Energies=	-348.891566		
Sum of electronic and thermal Energies=	-348.883410		
Sum of electronic and thermal Enthalpies=	-348.882466		
Sum of electronic and thermal Free Energies=	-348.924791		
C	1.39064000	-1.00261200	-0.38805500
C	2.58020900	-0.45443000	-0.10479100
C	2.87066200	0.87701300	0.52537200
H	3.66847300	0.77468800	1.26758400
H	3.22761200	1.60243000	-0.21616700
H	1.99768100	1.30500900	1.01945200
H	1.40073200	-2.01806100	-0.77843700
C	0.04035600	-0.43788300	-0.20437900
C	-1.01311700	-1.29880600	0.14596900
C	-0.26055200	0.91942400	-0.40169100
C	-2.30536300	-0.82003300	0.32969000
H	-0.80652900	-2.35523800	0.28373400
C	-1.55547700	1.39881300	-0.22330200

H	0.51663900	1.59797800	-0.72954000
C	-2.58209000	0.53444500	0.15012000
H	-3.09890500	-1.50455300	0.60862900
H	-1.76466900	2.45025400	-0.38759000
H	-3.58989800	0.90965600	0.28749600
H	3.45724600	-1.05774800	-0.32875600

TS1_{Me'}-a

Zero-point correction=			0.395608 (Hartree/Particle)
Thermal correction to Energy=			0.425912
Thermal correction to Enthalpy=			0.426857
Thermal correction to Gibbs Free Energy=			0.330908
Sum of electronic and zero-point Energies=			-1586.350959
Sum of electronic and thermal Energies=			-1586.320655
Sum of electronic and thermal Enthalpies=			-1586.319710
Sum of electronic and thermal Free Energies=			-1586.415659
Pd	0.66079700	0.00920000	0.23969000
C	-1.48619800	-0.84511200	1.22649000
C	-0.29310500	-0.89156900	1.78005900
P	2.77618100	-0.93666700	0.10410300
P	0.46031200	2.01794700	-1.17873600
C	3.28885000	-1.45201500	-1.59504900
H	2.59294200	-2.20375000	-1.97132300
H	3.24828900	-0.59073400	-2.26368300
H	4.30190000	-1.86520200	-1.60050800
C	3.15230000	-2.46357300	1.07790000
H	2.47594900	-3.26361300	0.77118400
H	4.18577600	-2.79290900	0.93413800
H	2.98407800	-2.26734700	2.13822300
C	4.17181300	0.16678600	0.60546100
H	4.04746900	0.46115600	1.64908100
H	5.13850700	-0.33169800	0.48695400
H	4.15870000	1.07202600	-0.00374100
C	-1.20689900	2.24034300	-1.93301100
H	-1.43790500	1.40123700	-2.59161400
H	-1.92914500	2.26021600	-1.11542400
H	-1.26423600	3.17425100	-2.50033300
C	1.58375900	2.33588500	-2.61976700
H	1.49348000	1.52319600	-3.34394700
H	1.33891000	3.27922700	-3.11661900
H	2.62105500	2.37881800	-2.27981600
C	0.63548900	3.56489300	-0.19144800
H	0.52328600	4.45364800	-0.81977200
H	-0.14729700	3.55150100	0.56972000

H	1.61233200	3.59045100	0.29579200
C	0.18466800	-0.99516900	3.18182900
H	1.10231500	-0.43457000	3.36405900
H	-0.60094600	-0.62495900	3.84988100
H	0.36173900	-2.04578900	3.44127800
C	-2.75148600	2.01433600	2.21510800
O	-2.02814000	2.38886500	1.29110200
O	-3.00363800	0.81311800	2.59187600
H	-3.27913700	2.77535800	2.83176700
H	-2.23961000	-0.08812200	1.92022200
C	-2.09922000	-1.34802600	-0.00414200
C	-3.31643700	-0.80915500	-0.45574400
C	-1.54771100	-2.43364800	-0.71388900
C	-3.94084000	-1.31761500	-1.58960200
H	-3.76364400	0.00628600	0.09853900
C	-2.18038900	-2.94156800	-1.84195000
H	-0.62503500	-2.87854500	-0.35991600
C	-3.37760000	-2.38305200	-2.29084900
H	-4.87787800	-0.88466900	-1.92251400
H	-1.74227500	-3.78171000	-2.37053600
H	-3.87142100	-2.78246100	-3.16954000

TS1_{Mc}'w-a

Zero-point correction=			0.421676 (Hartree/Particle)
Thermal correction to Energy=			0.454381
Thermal correction to Enthalpy=			0.455325
Thermal correction to Gibbs Free Energy=			0.354439
Sum of electronic and zero-point Energies=			-1662.795215
Sum of electronic and thermal Energies=			-1662.762510
Sum of electronic and thermal Enthalpies=			-1662.761566
Sum of electronic and thermal Free Energies=			-1662.862452
Pd	-0.74601400	-0.18026500	-0.32942300
C	2.09526900	0.42360800	-0.79870300
C	0.99535300	0.22599200	-1.45941900
P	-2.44329400	-1.47654100	1.01667100
P	-1.61467000	1.88309000	-0.88455200
C	-4.18755500	-0.93078300	1.33325100
H	-4.18757200	0.00024300	1.90474200
H	-4.69394500	-0.74742200	0.38300400
H	-4.75328900	-1.68305400	1.89074600
C	-1.90253100	-1.95071600	2.72130900
H	-1.76828500	-1.05536800	3.33161500
H	-2.62581500	-2.61126600	3.20857200
H	-0.94343100	-2.46495800	2.64788500

C	-2.71112200	-3.13395700	0.24492000
H	-1.73678300	-3.60662700	0.11488300
H	-3.35058500	-3.77401900	0.85987500
H	-3.16838900	-3.01203800	-0.73916700
C	-1.87803900	2.92428800	0.61797700
H	-2.50895400	2.38616200	1.32702700
H	-0.91647900	3.11094800	1.09773300
H	-2.35201600	3.87748100	0.36537900
C	-3.30847900	1.84629900	-1.62550400
H	-3.27475400	1.32855000	-2.58583400
H	-3.98443600	1.29889100	-0.96738600
H	-3.69816400	2.85713800	-1.77840800
C	-0.76575400	3.07215800	-2.01485800
H	0.25680500	3.23582200	-1.67534700
H	-0.72030500	2.65508700	-3.02184700
H	-1.30032500	4.02597200	-2.05072400
C	0.75812800	-0.17792500	-2.88790400
H	1.71523000	-0.28686200	-3.40718200
H	0.21844500	-1.12733600	-2.96088000
H	0.16710100	0.56896400	-3.42556500
C	3.61583900	-2.36435800	-1.82784700
O	3.90725900	-1.11112300	-1.97826300
O	0.56242000	-2.14172200	0.39402000
H	4.33912000	-3.01992500	-2.34462800
H	3.16421800	-0.41573900	-1.49267000
C	2.42648800	0.86252700	0.54515200
C	3.11581500	0.01122600	1.43602800
C	2.14408400	2.16935500	0.99363000
C	3.45796900	0.43052400	2.71747200
H	3.39383700	-0.98388500	1.10515600
C	2.50160500	2.58911800	2.27097800
H	1.65877000	2.86117700	0.31508700
C	3.15171900	1.72154100	3.14806400
H	3.98071600	-0.25165900	3.37991300
H	2.27527100	3.60381600	2.58317200
H	3.42976600	2.05054200	4.14272700
O	2.67988700	-2.85858200	-1.20833100
H	1.26054100	-2.36214300	-0.26718100
H	1.06055400	-1.68653400	1.08430900

M2_{Me'}-a

Zero-point correction=	0.403256 (Hartree/Particle)
Thermal correction to Energy=	0.432469
Thermal correction to Enthalpy=	0.433413

Thermal correction to Gibbs Free Energy=			0.343664
Sum of electronic and zero-point Energies=			-1586.409322
Sum of electronic and thermal Energies=			-1586.380109
Sum of electronic and thermal Enthalpies=			-1586.379165
Sum of electronic and thermal Free Energies=			-1586.468914
Pd	-0.64145000	-0.03419600	0.58192400
C	2.17952600	-0.60649000	1.58093500
C	0.90860400	-0.32373500	1.89524900
P	0.18422100	2.06076200	0.09237800
P	-2.66360800	-0.05899900	-0.86136200
C	0.60070900	2.30321800	-1.68533800
H	1.39186500	1.60404700	-1.96033300
H	-0.27177300	2.09530000	-2.30607400
H	0.93742500	3.32659200	-1.87153300
C	1.68719700	2.70258700	0.93346300
H	2.54124500	2.07132000	0.69333200
H	1.88356400	3.72749600	0.60657600
H	1.54136900	2.68649900	2.01373600
C	-1.02549800	3.41202000	0.43564900
H	-1.27110000	3.41425100	1.49909900
H	-0.60866500	4.38557800	0.16345000
H	-1.94334100	3.24748100	-0.12708100
C	-2.45385500	-1.20233700	-2.28949200
H	-1.75525000	-0.75796100	-3.00202400
H	-2.01178500	-2.13191200	-1.92876300
H	-3.40648200	-1.39282000	-2.79180000
C	-3.46361900	1.40691300	-1.66748300
H	-2.75758000	1.91805800	-2.32514300
H	-4.32639400	1.09562400	-2.26288200
H	-3.80560900	2.11372300	-0.90872100
C	-4.08005700	-0.76756000	0.07843200
H	-4.90205400	-1.05083300	-0.58406800
H	-3.72317700	-1.63287600	0.63548200
H	-4.43645700	-0.02763400	0.79848500
C	0.42706700	-0.29631800	3.31971400
H	-0.38174300	-1.01990900	3.45344100
H	1.23554800	-0.54209700	4.01990700
H	0.02526500	0.68569200	3.59671300
C	-1.06709000	-2.98529700	0.66841200
O	-1.36348200	-1.91816100	1.32446700
O	-0.54426000	-3.07021000	-0.43897000
H	-1.35915500	-3.90823300	1.21176500
H	2.86515500	-0.76947200	2.41785400
C	2.82401400	-0.67718000	0.25735400

C	2.16382200	-1.14187000	-0.89373800
C	4.16760100	-0.28021600	0.13107100
C	2.81726500	-1.16295600	-2.12449300
H	1.16055000	-1.54574100	-0.81063500
C	4.81580600	-0.29850000	-1.10037100
H	4.70512200	0.05048100	1.01495500
C	4.13906300	-0.73280100	-2.23929900
H	2.29514100	-1.54613200	-2.99512300
H	5.85080700	0.01923500	-1.16979300
H	4.64362600	-0.75910400	-3.19894300

M2_{Me}'w-a

Zero-point correction=			0.427518 (Hartree/Particle)
Thermal correction to Energy=			0.459120
Thermal correction to Enthalpy=			0.460064
Thermal correction to Gibbs Free Energy=			0.362590
Sum of electronic and zero-point Energies=			-1662.847240
Sum of electronic and thermal Energies=			-1662.815638
Sum of electronic and thermal Enthalpies=			-1662.814694
Sum of electronic and thermal Free Energies=			-1662.912169
Pd	-0.39944300	0.00241900	-0.15927900
C	1.86340100	-1.98793700	-0.51405900
C	0.63496100	-1.60944900	-0.90005000
P	-1.88463500	1.64101700	0.95620900
P	0.71369000	1.36658900	-1.64930300
C	-1.63980500	3.47701900	0.96575400
H	-0.65999200	3.71856800	1.38283200
H	-1.69228100	3.87847800	-0.04830600
H	-2.40596200	3.96835300	1.57164600
C	-1.95024800	1.25143100	2.75214200
H	-1.00742000	1.54463200	3.21896000
H	-2.77575300	1.76965200	3.24692000
H	-2.05622700	0.17085800	2.84998400
C	-3.63965000	1.48680300	0.41784000
H	-3.94841100	0.44414900	0.51237000
H	-4.29578200	2.11895000	1.02279600
H	-3.72808700	1.77946400	-0.63064200
C	1.74830400	2.66657600	-0.85361300
H	1.12757700	3.30115900	-0.22080800
H	2.49952500	2.18435400	-0.22613000
H	2.24581700	3.28592200	-1.60479600
C	-0.40005700	2.32768700	-2.76368800
H	-0.98823300	1.63435600	-3.36746500
H	-1.08918900	2.93422700	-2.17538400

H	0.17423400	2.98056000	-3.42650300
C	1.89255700	0.62355700	-2.84884500
H	2.70224500	0.13751600	-2.30585500
H	1.38516400	-0.13218400	-3.44905000
H	2.29952800	1.39710500	-3.50571000
C	-0.17025600	-2.42057000	-1.87872700
H	0.39700500	-3.28788300	-2.24053200
H	-1.09760500	-2.78312600	-1.42461700
H	-0.46829300	-1.82405700	-2.74928400
C	-4.00102200	-2.85217600	-0.02817200
O	-3.20897200	-3.53987600	-0.63409900
O	-1.31984600	-1.34657200	1.16882900
H	-5.09263600	-3.00446400	-0.11075500
H	2.26628700	-2.89157000	-0.98105300
C	2.80330000	-1.33241200	0.41192700
C	4.18489800	-1.51134500	0.21891500
C	2.39637900	-0.54268600	1.50193500
C	5.11962200	-0.89878000	1.04806800
H	4.52411100	-2.13889600	-0.59949300
C	3.33142900	0.06805900	2.33318000
H	1.33786100	-0.44083700	1.71128100
C	4.69780600	-0.09835500	2.10825400
H	6.17873300	-1.05140600	0.87000800
H	2.99052900	0.66078600	3.17575500
H	5.42309300	0.37350000	2.76165300
O	-3.72703900	-1.86047000	0.79069100
H	-2.68105600	-1.70069100	0.90532400
H	-0.80908700	-2.16203300	1.13156900

M2_{Me}'w-d

Zero-point correction=			0.427674 (Hartree/Particle)
Thermal correction to Energy=			0.459502
Thermal correction to Enthalpy=			0.460447
Thermal correction to Gibbs Free Energy=			0.361714
Sum of electronic and zero-point Energies=			-1662.842672
Sum of electronic and thermal Energies=			-1662.810843
Sum of electronic and thermal Enthalpies=			-1662.809899
Sum of electronic and thermal Free Energies=			-1662.908631
Pd	0.68293800	0.01557600	-0.40918700
C	-2.20339500	0.58978200	-1.17228200
C	-0.91742200	0.61869100	-1.55211900
P	2.71332400	-0.19554500	0.97942500
P	0.16859900	-2.18940500	-0.86107700
C	4.11001600	0.66612000	0.14774500

H	4.41403200	0.11080900	-0.74186900
H	3.74028900	1.64541800	-0.15586100
H	4.96951600	0.77917100	0.81398100
C	3.51766300	-1.74398800	1.60549600
H	3.83312200	-2.37226400	0.76988500
H	4.39611400	-1.51325900	2.21443900
H	2.81294800	-2.31220100	2.21651400
C	2.48802900	0.77471000	2.52630500
H	1.76260800	0.27749500	3.17328500
H	3.43145500	0.89013700	3.06672800
H	2.09871800	1.75267300	2.24427700
C	-0.18757500	-3.20727200	0.63216500
H	0.66165300	-3.17124600	1.31545700
H	-1.05832700	-2.79282500	1.14248000
H	-0.38590800	-4.24756400	0.36042800
C	1.55502600	-3.09922900	-1.67211600
H	1.78310700	-2.62850500	-2.63003400
H	2.44800400	-3.05321500	-1.04849100
H	1.29146300	-4.14656500	-1.84263900
C	-1.24271100	-2.60669400	-1.96234700
H	-2.17011900	-2.25110100	-1.51536600
H	-1.11818700	-2.11222200	-2.92609300
H	-1.29559500	-3.68883900	-2.11020000
C	-0.52134400	1.20153100	-2.88393200
H	-1.40191100	1.41384700	-3.50334900
H	0.01014900	2.14842000	-2.74653300
H	0.14287800	0.53657900	-3.44638300
C	-0.71415900	4.45033300	-0.09561800
O	-0.49164800	3.64703500	0.92033400
O	1.18595800	2.02208500	-0.02939300
H	-1.44624600	5.23326400	0.16582000
H	-2.93865600	0.95722400	-1.89405600
C	-2.79944800	0.08401900	0.07515500
C	-4.09980800	-0.45160700	0.04685200
C	-2.13979400	0.12398000	1.31567000
C	-4.69873900	-0.96469800	1.19348300
H	-4.64224600	-0.46546300	-0.89363000
C	-2.73957200	-0.38635700	2.46384600
H	-1.16825300	0.59866800	1.37632000
C	-4.01772900	-0.94206200	2.40961000
H	-5.70090100	-1.37644300	1.13929300
H	-2.21545600	-0.32730400	3.41210100
H	-4.48520900	-1.33162400	3.30705000
O	-0.20291900	4.38429300	-1.19607500

H	0.19020400	2.91700300	0.61505000
H	1.13139300	2.51683300	-0.85764000

M2_{Me}'-b

Zero-point correction= 0.403469 (Hartree/Particle)

Thermal correction to Energy=	0.432700
Thermal correction to Enthalpy=	0.433644
Thermal correction to Gibbs Free Energy=	0.343229
Sum of electronic and zero-point Energies=	-1586.424842
Sum of electronic and thermal Energies=	-1586.395612
Sum of electronic and thermal Enthalpies=	-1586.394667
Sum of electronic and thermal Free Energies=	-1586.485082

Pd	0.73709000	0.21678200	0.14197700
C	-1.87375200	-0.44801500	1.54592800
C	-0.56133500	-0.17221600	1.65146300
P	1.37295700	-2.09008300	0.12056000
P	0.10281100	2.49993500	0.11844700
C	1.74176100	-2.78866900	-1.54024200
H	0.88230700	-2.65107900	-2.19866800
H	2.60233800	-2.26070000	-1.94678200
H	1.96320700	-3.85660500	-1.45965700
C	0.12851900	-3.28441600	0.77083400
H	-0.79803200	-3.19753800	0.20154500
H	0.50792400	-4.30684100	0.69248900
H	-0.09786300	-3.06117600	1.81323400
C	2.87419200	-2.48135200	1.10584300
H	2.71829300	-2.19355300	2.14709600
H	3.09725800	-3.55099100	1.05939700
H	3.69754400	-1.90328300	0.68899400
C	1.52612700	3.60115800	0.49531400
H	1.84581100	3.45152300	1.52808000
H	2.34654800	3.32488400	-0.16694800
H	1.26588500	4.65261300	0.34698100
C	-1.24399500	3.13660400	1.19593800
H	-0.99100600	2.96914000	2.24409900
H	-1.40093700	4.20578400	1.03063400
H	-2.16598200	2.59537000	0.98111700
C	-0.40141300	3.00933600	-1.57204700
H	-0.52721900	4.09326900	-1.64083500
H	0.37722000	2.67516300	-2.25811900
H	-1.33980500	2.51810100	-1.83453200
C	0.06896800	-0.07523300	3.02086300
H	0.53450000	0.90344600	3.18186800
H	-0.66698700	-0.23652400	3.81851500

H	0.87167400	-0.80942200	3.15193400
C	3.22498600	0.51510200	-1.65910200
O	3.79418300	-0.42384900	-1.10866500
O	2.03810200	0.95779600	-1.44821600
H	3.75721500	1.08164700	-2.45356300
H	-2.41136000	-0.58540800	2.48846300
C	-2.74729000	-0.58988100	0.37170600
C	-4.12819100	-0.76020900	0.58753200
C	-2.30434600	-0.57294800	-0.96428700
C	-5.02186200	-0.89649900	-0.46914700
H	-4.49957500	-0.78352300	1.60734200
C	-3.19770500	-0.70898100	-2.02230100
H	-1.24543500	-0.45278000	-1.16954700
C	-4.56231200	-0.87015300	-1.78444900
H	-6.07950700	-1.02453500	-0.26510000
H	-2.82381800	-0.69298900	-3.04075100
H	-5.25523800	-0.97709800	-2.61134700

Com₃Me'-a

Zero-point correction=			0.398640 (Hartree/Particle)
Thermal correction to Energy=			0.428427
Thermal correction to Enthalpy=			0.429371
Thermal correction to Gibbs Free Energy=			0.336369
Sum of electronic and zero-point Energies=			-1586.402730
Sum of electronic and thermal Energies=			-1586.372943
Sum of electronic and thermal Enthalpies=			-1586.371999
Sum of electronic and thermal Free Energies=			-1586.465000
Pd	0.69957400	0.00036700	0.32452500
C	-2.15772700	-0.00325100	1.47754600
C	-0.83538200	-0.00218000	1.71501600
P	0.77086200	-2.35946100	0.23015800
P	0.76464600	2.36043600	0.23172300
C	0.63034600	-2.98593600	-1.49143700
H	-0.32883900	-2.68431600	-1.91513900
H	1.44055600	-2.54981800	-2.07718700
H	0.70838500	-4.07637200	-1.51447600
C	-0.48439100	-3.33582700	1.15264400
H	-1.48244600	-3.04587900	0.82258700
H	-0.33821000	-4.40618700	0.98525000
H	-0.40775800	-3.12520800	2.22023500
C	2.37951100	-3.04405000	0.79812000
H	2.55167500	-2.77429700	1.84146400
H	2.39673300	-4.13289900	0.69923400
H	3.16588300	-2.60860700	0.17996900

C	2.37168100	3.04911000	0.79934000
H	2.54504600	2.77926200	1.84246100
H	3.15900000	2.61622000	0.18060700
H	2.38581200	4.13806000	0.70106400
C	-0.49273100	3.33292000	1.15539700
H	-0.41494600	3.12186100	2.22281700
H	-0.34945600	4.40375800	0.98856800
H	-1.49018800	3.04053800	0.82569900
C	0.62168200	2.98740700	-1.48948700
H	0.69685600	4.07805700	-1.51202800
H	1.43278400	2.55372200	-2.07581600
H	-0.33689700	2.68345600	-1.91288500
C	-0.32902900	-0.00264600	3.13674200
H	0.29948600	0.87109600	3.34296200
H	-1.15256500	-0.00408900	3.86293100
H	0.30147300	-0.87524600	3.34174600
C	3.17062700	0.00423100	-1.59744400
O	3.46710200	1.15230900	-1.81469200
O	3.47076900	-1.14294100	-1.81449000
H	2.04564200	0.00250500	-0.78627100
H	-2.80596600	-0.00441900	2.35972000
C	-2.91704300	-0.00293200	0.21772300
C	-4.32290000	-0.00275900	0.28646500
C	-2.33780100	-0.00283100	-1.06476300
C	-5.11036100	-0.00239500	-0.85993200
H	-4.79948000	-0.00289600	1.26179200
C	-3.12406400	-0.00247100	-2.21253500
H	-1.25596600	-0.00305100	-1.15672000
C	-4.51562100	-0.00223600	-2.11999200
H	-6.19124200	-0.00224500	-0.76901900
H	-2.64643400	-0.00241900	-3.18678100
H	-5.12570200	-0.00196800	-3.01611200

TS_{Me'}-a

Zero-point correction=			0.398280 (Hartree/Particle)
Thermal correction to Energy=			0.427422
Thermal correction to Enthalpy=			0.428367
Thermal correction to Gibbs Free Energy=			0.336703
Sum of electronic and zero-point Energies=			-1586.402636
Sum of electronic and thermal Energies=			-1586.373494
Sum of electronic and thermal Enthalpies=			-1586.372549
Sum of electronic and thermal Free Energies=			-1586.464213
Pd	-0.74679500	0.00494900	0.37331700
C	2.14758700	-0.00356600	1.47740400

C	0.82800900	-0.00615600	1.73136800
P	-0.75035500	2.36364200	0.23788200
P	-0.71774600	-2.35092100	0.22890400
C	-0.54349700	2.95553500	-1.49008300
H	0.42182700	2.62791600	-1.87902100
H	-1.34245600	2.52691400	-2.09559600
H	-0.59591100	4.04706300	-1.53244400
C	0.51790600	3.31297500	1.17104700
H	1.51076200	2.97226800	0.87596900
H	0.42201000	4.38362300	0.97278100
H	0.40391400	3.13348500	2.24127500
C	-2.34452300	3.12399500	0.75152100
H	-2.55447100	2.87718300	1.79366600
H	-2.31804100	4.21108900	0.63697500
H	-3.13401600	2.71026200	0.12263700
C	-2.29058700	-3.12177100	0.78846300
H	-2.46431900	-2.88376100	1.83936100
H	-3.10234800	-2.70658800	0.18974400
H	-2.26323600	-4.20790000	0.66551800
C	0.58038700	-3.29655900	1.12388100
H	0.51299600	-3.10078900	2.19487100
H	0.46351600	-4.36867600	0.94524500
H	1.56403700	-2.97257900	0.78304000
C	-0.55093400	-2.93358600	-1.50587400
H	-0.56179200	-4.02601700	-1.55124200
H	-1.38817900	-2.53471900	-2.07930800
H	0.38633300	-2.56755700	-1.92783300
C	0.34524400	-0.02112900	3.16166000
H	-0.28607800	-0.89324800	3.36693600
H	1.17907900	-0.03341900	3.87609100
H	-0.27710500	0.85255000	3.38617000
C	-3.20474900	-0.04565900	-1.63272500
O	-3.48213400	-1.19917500	-1.81050600
O	-3.45930800	1.09882400	-1.88240300
H	-2.08594100	-0.02326200	-0.69748800
H	2.81032400	-0.01732500	2.34888400
C	2.88547000	0.00755600	0.20517900
C	4.29205900	-0.02244400	0.24601600
C	2.28170000	0.04545900	-1.06540500
C	5.05670900	-0.01700800	-0.91588400
H	4.78744400	-0.05146400	1.21153600
C	3.04496300	0.05137100	-2.22851000
H	1.19874200	0.07205300	-1.13357300
C	4.43777000	0.01979200	-2.16377700

H	6.13895600	-0.04131700	-0.84657400
H	2.54824200	0.08130900	-3.19274900
H	5.03023500	0.02438500	-3.07164400

M3_{Me}'-a

Zero-point correction=			0.397955 (Hartree/Particle)
Thermal correction to Energy=			0.428572
Thermal correction to Enthalpy=			0.429516
Thermal correction to Gibbs Free Energy=			0.330214
Sum of electronic and zero-point Energies=			-1586.413859
Sum of electronic and thermal Energies=			-1586.383242
Sum of electronic and thermal Enthalpies=			-1586.382298
Sum of electronic and thermal Free Energies=			-1586.481600
Pd	-0.62180400	0.00039000	0.57425700
C	2.45536600	-0.00040500	1.27514400
C	1.17832100	0.00004800	1.70559500
P	-0.74433700	2.32828200	0.45057800
P	-0.74577400	-2.32747600	0.45136300
C	-0.59838500	2.96623800	-1.27084900
H	0.36434900	2.66502400	-1.68693800
H	-1.39332200	2.53256100	-1.87832000
H	-0.67563500	4.05685300	-1.29423500
C	0.49904000	3.34062400	1.35698600
H	1.49955700	3.03923700	1.04540000
H	0.35529200	4.40757000	1.16536300
H	0.41262200	3.15355300	2.42858600
C	-2.34253500	3.05031100	1.01615600
H	-2.51408300	2.78522400	2.06091600
H	-2.34407600	4.13940400	0.91655900
H	-3.14969400	2.62660800	0.41796900
C	-2.34496900	-3.04831500	1.01562700
H	-2.51742900	-2.78265600	2.06009200
H	-3.15125400	-2.62439900	0.41641400
H	-2.34705100	-4.13745100	0.91651400
C	0.49609100	-3.34030000	1.35931100
H	0.40880600	-3.15277800	2.43076200
H	0.35181000	-4.40722300	1.16795700
H	1.49709500	-3.03969800	1.04852600
C	-0.59855600	-2.96612500	-1.26970500
H	-0.67641500	-4.05670400	-1.29277000
H	-1.39269900	-2.53224200	-1.87806800
H	0.36472900	-2.66559900	-1.68501200
C	0.94147200	0.00038100	3.19942300
H	0.35362200	-0.87109300	3.51267200

H	1.87626900	0.00009400	3.77835100
H	0.35435400	0.87245700	3.51238200
C	-3.81158800	-0.00033500	-2.25159400
O	-3.82925700	-1.16098800	-2.26912900
O	-3.82826600	1.16029500	-2.27123500
H	-2.03885400	0.00072900	-0.23442300
H	3.24489200	-0.00051800	2.03603600
C	2.99492800	-0.00075900	-0.09356900
C	4.39184600	-0.00124900	-0.26987500
C	2.20597500	-0.00063000	-1.26027200
C	4.97153500	-0.00159400	-1.53447400
H	5.02863300	-0.00135800	0.60951700
C	2.78393500	-0.00097500	-2.52579300
H	1.12439500	-0.00026200	-1.16197800
C	4.17112800	-0.00145900	-2.67510200
H	6.05241700	-0.00196900	-1.62952600
H	2.14611900	-0.00086400	-3.40419200
H	4.61879700	-0.00172600	-3.66263700

M4_{Me}'-a

Zero-point correction=			0.386237 (Hartree/Particle)
Thermal correction to Energy=			0.412143
Thermal correction to Enthalpy=			0.413087
Thermal correction to Gibbs Free Energy=			0.329187
Sum of electronic and zero-point Energies=			-1397.779066
Sum of electronic and thermal Energies=			-1397.753160
Sum of electronic and thermal Enthalpies=			-1397.752216
Sum of electronic and thermal Free Energies=			-1397.836116
Pd	-1.10083400	0.01314600	-0.15268500
C	1.45289400	-0.08988500	1.72062200
C	0.10908200	-0.06966700	1.60930000
P	-1.14555700	2.33951500	-0.25294900
P	-1.18295700	-2.31459000	-0.32210300
C	-0.47002200	3.01752400	-1.82693100
H	0.58207200	2.74148300	-1.91316400
H	-1.01128600	2.57775200	-2.66510300
H	-0.55938700	4.10699400	-1.86032600
C	-0.23127300	3.31378200	1.01545200
H	0.81321500	3.00025500	1.02175000
H	-0.29554500	4.38667500	0.81351600
H	-0.64658700	3.10851200	2.00321200
C	-2.83420700	3.07414100	-0.18195000
H	-3.30724500	2.80622500	0.76447600
H	-2.79869100	4.16368500	-0.26971500

H	-3.43541100	2.65895300	-0.99141700
C	-2.40974300	-3.01481500	-1.50628800
H	-3.41105200	-2.69060600	-1.21836800
H	-2.20507600	-2.61924900	-2.50193000
H	-2.37167400	-4.10781200	-1.52888700
C	-1.55988000	-3.24689100	1.22317700
H	-2.53031400	-2.93770300	1.61538600
H	-1.57689600	-4.32421900	1.03646100
H	-0.79766900	-3.02147300	1.96962300
C	0.39426400	-3.08959500	-0.86902200
H	0.30218600	-4.17852100	-0.90853900
H	0.66146500	-2.71443900	-1.85776100
H	1.18901500	-2.81110500	-0.17641100
C	-0.69400100	-0.05557200	2.89192000
H	-1.42313500	-0.87232900	2.92838400
H	-0.06363800	-0.12470500	3.79050000
H	-1.28729900	0.86408600	2.97326000
H	1.87693400	-0.12102500	2.73159600
C	2.49146900	-0.05015200	0.67884200
C	3.84352500	-0.10782000	1.06781200
C	2.22978600	0.05872300	-0.70058500
C	4.87671500	-0.06217400	0.13736500
H	4.07926600	-0.18910100	2.12454700
C	3.26140000	0.10404500	-1.63245100
H	1.19780500	0.10468200	-1.03613300
C	4.59377700	0.04422700	-1.22297200
H	5.90659400	-0.10916100	0.47581200
H	3.02405300	0.18658700	-2.68852500
H	5.39607100	0.08055500	-1.95148900
H	-2.06443200	0.10121100	-1.45720200

M4_{Me}'-b

Zero-point correction=			0.385965 (Hartree/Particle)
Thermal correction to Energy=			0.412147
Thermal correction to Enthalpy=			0.413091
Thermal correction to Gibbs Free Energy=			0.328431
Sum of electronic and zero-point Energies=			-1397.778168
Sum of electronic and thermal Energies=			-1397.751987
Sum of electronic and thermal Enthalpies=			-1397.751042
Sum of electronic and thermal Free Energies=			-1397.835702
Pd	0.72230700	-0.00877500	0.63535400
C	-2.18592500	0.40210300	1.60762100
C	-0.87481300	0.63920100	1.79565500
P	2.67951300	-1.15380300	-0.11399400

P	0.30243400	1.78526900	-0.96472100
C	4.08250300	-0.97431100	1.07309300
H	4.39123600	0.07185000	1.11771800
H	3.74194700	-1.26658700	2.06722000
H	4.93945700	-1.58968900	0.78469700
C	3.52904500	-0.84606400	-1.73233500
H	3.84969800	0.19552000	-1.79108900
H	4.40263400	-1.49248400	-1.85733900
H	2.83200100	-1.03576500	-2.55131400
C	2.46070100	-2.98603800	-0.17724600
H	1.70943400	-3.23733700	-0.92850900
H	3.39618800	-3.49800400	-0.42036100
H	2.09466200	-3.33030200	0.79059200
C	1.63510300	2.41444900	-2.08960800
H	2.48880600	2.75105300	-1.49770200
H	1.97009100	1.61528900	-2.75252600
H	1.27744100	3.24911300	-2.69898600
C	-0.28949800	3.36654000	-0.22033000
H	0.49018600	3.78887000	0.41645800
H	-0.55219100	4.09387000	-0.99342800
H	-1.16271500	3.15814100	0.39817200
C	-1.04171600	1.40850800	-2.17120600
H	-1.23197700	2.25998900	-2.83083000
H	-0.76135300	0.54218800	-2.77296100
H	-1.95203700	1.15472800	-1.62765500
C	-0.45186200	1.49614400	2.96552500
H	0.20262000	2.31889000	2.65733800
H	-1.31240700	1.92592000	3.49691100
H	0.12746000	0.90151700	3.67952100
H	-2.88257700	0.89874500	2.29128400
C	-2.86457100	-0.42953400	0.60126900
C	-2.22939200	-1.45295600	-0.12516000
C	-4.23464800	-0.22071100	0.35662600
C	-2.92557000	-2.20736600	-1.06376200
H	-1.18268200	-1.65771600	0.07195200
C	-4.93126300	-0.97300300	-0.58412200
H	-4.75451600	0.55051800	0.91717000
C	-4.27928000	-1.97155600	-1.30527500
H	-2.41119000	-2.99637800	-1.60352900
H	-5.98632900	-0.78236000	-0.75105300
H	-4.81935600	-2.56443000	-2.03519900
H	0.74728100	-1.08590800	1.79340000

TS3_{Me}'

Zero-point correction=			0.384138 (Hartree/Particle)
Thermal correction to Energy=			0.410359
Thermal correction to Enthalpy=			0.411303
Thermal correction to Gibbs Free Energy=			0.325364
Sum of electronic and zero-point Energies=			-1397.773635
Sum of electronic and thermal Energies=			-1397.747415
Sum of electronic and thermal Enthalpies=			-1397.746471
Sum of electronic and thermal Free Energies=			-1397.832409
Pd	0.66759400	-0.00963600	0.56505300
C	-2.26091500	0.39105500	1.56546500
C	-0.94040900	0.49348700	1.82307300
P	2.42734900	-1.50443000	-0.07416200
P	0.77539400	1.99532500	-0.81050500
C	3.52312200	-1.97823800	1.33870800
H	4.03409500	-1.09013000	1.71572900
H	2.90703100	-2.37798600	2.14554500
H	4.26869800	-2.72392800	1.04690300
C	3.69080100	-1.11792600	-1.37769500
H	4.22699600	-0.20531600	-1.10940500
H	4.41279100	-1.93109100	-1.49849500
H	3.18881900	-0.94849300	-2.33278200
C	1.83484400	-3.15837000	-0.65255600
H	1.25161000	-3.03505500	-1.56733600
H	2.66405300	-3.84511900	-0.84687400
H	1.17863200	-3.58590400	0.10687800
C	2.36639400	2.67537200	-1.47632800
H	3.03302000	2.91595300	-0.64538500
H	2.85623500	1.91988000	-2.09376100
H	2.20722700	3.57636600	-2.07615600
C	0.04589300	3.50193700	-0.02778200
H	0.66661200	3.81223800	0.81539700
H	-0.03397800	4.33206800	-0.73538300
H	-0.94450200	3.25154600	0.35625500
C	-0.23647100	1.85645400	-2.35228300
H	-0.26595400	2.80029900	-2.90453300
H	0.18439500	1.08010100	-2.99462600
H	-1.25205700	1.55782100	-2.08736900
C	-0.49750300	1.21382000	3.07687400
H	0.18287800	2.04189100	2.85112700
H	-1.35095700	1.61850800	3.63572700
H	0.05410700	0.53990700	3.74009600
H	-2.93246600	0.88289000	2.27453300
C	-2.97379900	-0.29368200	0.48170900
C	-2.34637200	-1.00530900	-0.55805900

C	-4.38136800	-0.25304800	0.47324000
C	-3.08991100	-1.64053600	-1.54685600
H	-1.26210500	-1.05865700	-0.57646800
C	-5.12505000	-0.88414400	-0.51756000
H	-4.89368300	0.28419100	1.26551200
C	-4.48362400	-1.58421600	-1.53781700
H	-2.57731700	-2.18436300	-2.33412000
H	-6.20845300	-0.83113500	-0.49236600
H	-5.05944100	-2.07772400	-2.31288500
H	-0.04055300	-0.93886900	1.65900100

M5_{Me}'

Zero-point correction=			0.389373 (Hartree/Particle)
Thermal correction to Energy=			0.416669
Thermal correction to Enthalpy=			0.417613
Thermal correction to Gibbs Free Energy=			0.326284
Sum of electronic and zero-point Energies=			-1397.818127
Sum of electronic and thermal Energies=			-1397.790831
Sum of electronic and thermal Enthalpies=			-1397.789887
Sum of electronic and thermal Free Energies=			-1397.881215
Pd	1.49565900	0.06886200	-0.14303100
C	-2.93075000	-0.17095100	1.83119700
C	-1.69738100	-0.13637100	2.35098400
P	1.68917800	-2.24791100	-0.21127500
P	1.36951900	2.39111100	-0.16208600
C	1.18323300	-3.20241000	1.29319400
H	1.78534200	-2.87972400	2.14473900
H	0.13665300	-2.99156300	1.52101000
H	1.30999500	-4.28037400	1.15205700
C	3.38342400	-2.93590300	-0.50524100
H	4.05318800	-2.60186500	0.28923900
H	3.37593600	-4.02999200	-0.53418900
H	3.76951500	-2.55341100	-1.45179300
C	0.72261200	-3.12477000	-1.52446100
H	1.02573300	-2.75066600	-2.50414900
H	0.87843600	-4.20757000	-1.48943600
H	-0.34007600	-2.90994700	-1.39765000
C	2.97230500	3.31858200	-0.20476200
H	3.56740700	3.05551600	0.67163900
H	3.53608400	3.02600200	-1.09239300
H	2.81202300	4.40112900	-0.22009800
C	0.52627700	3.21880100	1.26378200
H	1.05206200	2.96932100	2.18749100
H	0.50466400	4.30674000	1.14629000

H	-0.49610600	2.84559500	1.34722000
C	0.48101500	3.16255600	-1.59125400
H	0.47947900	4.25523100	-1.52698600
H	0.96320800	2.85850900	-2.52216700
H	-0.54924400	2.80289100	-1.61332100
C	-1.40197800	-0.15203900	3.82084300
H	-0.84418900	0.74285500	4.12043100
H	-2.31594100	-0.19943800	4.41830300
H	-0.77372800	-1.00953100	4.08844900
H	-3.77302400	-0.21330200	2.52126100
C	-3.30665700	-0.15568400	0.40879200
C	-2.36748200	-0.11482100	-0.63805300
C	-4.66803800	-0.18149800	0.06746100
C	-2.78259400	-0.09929700	-1.96440500
H	-1.30188200	-0.09349500	-0.42147400
C	-5.08275100	-0.16609500	-1.26167500
H	-5.40959800	-0.21337200	0.85960400
C	-4.14117300	-0.12462200	-2.28597600
H	-2.03803000	-0.06755500	-2.75274600
H	-6.14168900	-0.18639800	-1.49545000
H	-4.45901600	-0.11246400	-3.32257300
H	-0.82832300	-0.09160700	1.69397400

M1_{ph}-Ac-c

Zero-point correction=			0.428306 (Hartree/Particle)
Thermal correction to Energy=			0.461160
Thermal correction to Enthalpy=			0.462105
Thermal correction to Gibbs Free Energy=			0.358337
Sum of electronic and zero-point Energies=			-1625.702952
Sum of electronic and thermal Energies=			-1625.670098
Sum of electronic and thermal Enthalpies=			-1625.669153
Sum of electronic and thermal Free Energies=			-1625.772921
Pd	-0.30192400	-0.66936200	0.17609900
C	1.56179000	-1.11489500	-0.79444800
C	2.91403200	-0.62929100	-0.65229300
C	3.79970700	-1.21418400	0.27097900
C	3.38223400	0.44242500	-1.43408600
C	5.10471700	-0.74922900	0.39851300
H	3.45185900	-2.03977900	0.88109800
C	4.68811900	0.90328600	-1.30053500
H	2.70959400	0.90475300	-2.14717500
C	5.55696500	0.31238900	-0.38402200
H	5.77243800	-1.21960300	1.11246800
H	5.02937500	1.72796700	-1.91718800

H	6.57367300	0.67419500	-0.28137800
C	0.66335100	-1.83476800	-1.31375300
P	-2.61400800	-1.26103300	0.26256300
P	0.17589900	1.00947800	1.84613900
C	-2.98318200	-2.79040700	1.24043400
H	-2.41627000	-3.62742800	0.82878400
H	-2.66405600	-2.64558100	2.27433500
H	-4.04922900	-3.03650000	1.22599200
C	-3.42513600	-1.67355800	-1.35149400
H	-2.89337800	-2.50360500	-1.81985800
H	-4.47690400	-1.94697200	-1.22339200
H	-3.35606700	-0.81284500	-2.01942100
C	-3.85103600	-0.07863700	0.97029200
H	-3.76756100	0.88121700	0.45760300
H	-4.87392200	-0.45627800	0.87874300
H	-3.62796300	0.08959200	2.02527200
C	-1.15331800	1.82103600	2.84630300
H	-1.83653000	2.33004000	2.16491700
H	-1.71014900	1.06598300	3.40541200
H	-0.73884500	2.54762400	3.55180700
C	1.09457800	2.49430200	1.24027700
H	0.43892700	3.05862800	0.57532300
H	1.40697400	3.13916100	2.06732400
H	1.97457200	2.17368100	0.68020300
C	1.31007900	0.39651400	3.17573600
H	1.55456200	1.18201900	3.89728900
H	0.84033000	-0.43754900	3.70124900
H	2.23090300	0.03243600	2.71626500
C	0.28731300	-2.86445100	-2.30772700
H	-0.44444800	-2.47202500	-3.01976000
H	1.16080500	-3.20806800	-2.87333200
H	-0.16715400	-3.73418900	-1.82422500
C	-1.85723000	2.57182600	-1.67723000
O	-2.00166600	2.83894000	-0.50505300
O	-1.29708000	1.43900700	-2.12532000
H	-1.00292900	0.87580100	-1.36302800
C	-2.28170000	3.46768400	-2.81612100
H	-2.75940600	4.36126500	-2.42061700
H	-1.40819500	3.74293400	-3.41172300
H	-2.96862600	2.93329200	-3.47603100

TS1_{ph}-Ac-c

Zero-point correction=

0.423783 (Hartree/Particle)

Thermal correction to Energy=

0.455502

Thermal correction to Enthalpy=			0.456446
Thermal correction to Gibbs Free Energy=			0.357399
Sum of electronic and zero-point Energies=			-1625.669830
Sum of electronic and thermal Energies=			-1625.638111
Sum of electronic and thermal Enthalpies=			-1625.637167
Sum of electronic and thermal Free Energies=			-1625.736214
Pd	-0.31341700	-0.24950800	-0.45652600
C	1.41735700	0.82031100	-0.51709900
C	2.84122500	0.57703400	-0.40528700
C	3.45257600	-0.50456100	-1.06507000
C	3.65242300	1.43987200	0.35569500
C	4.82568100	-0.70464000	-0.98115800
H	2.83413900	-1.16940600	-1.65664500
C	5.02369800	1.22558800	0.45134700
H	3.19051300	2.27280600	0.87256700
C	5.61590400	0.15563800	-0.21781300
H	5.28253400	-1.53366600	-1.51052300
H	5.63255300	1.89797200	1.04566600
H	6.68542100	-0.00688400	-0.14650000
C	0.60008500	1.79754300	-0.82423400
P	-2.64862300	-0.53640600	-1.11449900
P	0.17652400	-2.01361700	0.98921400
C	-3.10327500	-1.81700100	-2.37033000
H	-2.50834200	-1.66574600	-3.27322100
H	-2.87806900	-2.81194600	-1.98075900
H	-4.16456900	-1.77029100	-2.63095500
C	-3.27526400	1.01198100	-1.90156300
H	-2.72445300	1.19074400	-2.82743500
H	-4.34427500	0.94959000	-2.12539100
H	-3.08026900	1.84738500	-1.22672400
C	-3.89368400	-0.82402800	0.21657100
H	-3.65229300	-0.16439100	1.05163900
H	-4.91090000	-0.63402200	-0.13708500
H	-3.83008700	-1.85724700	0.56300600
C	-1.16609700	-3.21492700	1.39591200
H	-2.01932300	-2.66908800	1.79960400
H	-1.48163900	-3.74462800	0.49494700
H	-0.82841000	-3.94447400	2.13764900
C	0.57952500	-1.31470200	2.64310300
H	-0.21090200	-0.61155700	2.91228300
H	0.67649400	-2.09779400	3.40082200
H	1.51686300	-0.75998000	2.57297100
C	1.58987400	-3.15168500	0.65189100
H	1.73884700	-3.84992700	1.48067200

H	1.39504800	-3.71799200	-0.26123400
H	2.50077200	-2.56996100	0.50672200
C	0.83625600	3.04801200	-1.63657700
H	0.52061000	3.92704900	-1.06905700
H	1.88731200	3.15464900	-1.91879400
H	0.23209800	3.02636200	-2.54852700
C	-1.83918600	2.24014200	1.60881600
O	-1.72759500	1.05084000	1.93833900
O	-1.45903000	2.74825700	0.48605100
H	-0.52698000	1.99998400	-0.18900100
C	-2.49027100	3.24099200	2.56220100
H	-2.78898900	2.75116600	3.48862100
H	-1.78954100	4.05137100	2.77784600
H	-3.36345100	3.69145500	2.08276100

TS1_{phW-Ac-c}

Zero-point correction=	0.449570 (Hartree/Particle)
Thermal correction to Energy=	0.483940
Thermal correction to Enthalpy=	0.484885
Thermal correction to Gibbs Free Energy=	0.380547
Sum of electronic and zero-point Energies=	-1702.108436
Sum of electronic and thermal Energies=	-1702.074066
Sum of electronic and thermal Enthalpies=	-1702.073122
Sum of electronic and thermal Free Energies=	-1702.177459

Pd	-1.05721100	-0.05267600	1.51974500
C	0.81215800	0.41666500	0.18409700
C	-0.01215300	1.37418800	0.52537200
P	-1.97112600	-2.34201200	1.84186500
P	-2.24338700	1.22907300	3.06485300
C	-3.10650700	-2.71321000	3.25991100
H	-2.56951200	-2.60765700	4.20445200
H	-3.95638300	-2.02755400	3.26120400
H	-3.48654100	-3.73607800	3.18958600
C	-0.75744500	-3.71629900	2.00509000
H	-0.15959700	-3.56471500	2.90561400
H	-1.27001200	-4.68053500	2.06635400
H	-0.08688600	-3.71239300	1.14569300
C	-2.99635500	-2.87215000	0.40431800
H	-2.35130800	-2.88882700	-0.47726600
H	-3.42170800	-3.86598000	0.57118700
H	-3.80653000	-2.15781100	0.24235600
C	-1.69152800	2.96285100	3.35479400
H	-0.64701200	2.95769400	3.67064700
H	-1.76295100	3.54138600	2.43445700

H	-2.30067800	3.43631000	4.12972400
C	-2.21051600	0.56508900	4.78678800
H	-1.17344600	0.44351100	5.10407500
H	-2.71935300	1.24504700	5.47579600
H	-2.69636300	-0.40886700	4.82478700
C	-4.04898100	1.44480200	2.74768800
H	-4.52746500	2.01863900	3.54636200
H	-4.18812500	1.96823500	1.80032800
H	-4.53089400	0.46914500	2.66957100
H	1.16350000	-0.57459600	0.94655100
C	2.35281500	-2.48871700	1.05522900
O	1.99488300	-1.40873700	1.65320100
O	1.88180800	-2.92547700	-0.00798500
O	-0.38844400	-2.29742500	-1.46866800
H	0.43582900	-2.53641600	-0.99138900
H	-0.53165400	-1.37925200	-1.21784600
C	3.43348700	-3.29204000	1.77234200
H	4.19730000	-2.62875400	2.18125500
H	2.97956900	-3.82794000	2.61178500
H	3.87767400	-4.01842500	1.09246800
C	-0.21934400	2.77842300	0.21987600
C	0.82637100	3.70373700	0.38689600
C	-1.45235800	3.24450000	-0.27062400
C	0.64126700	5.04780800	0.07765900
H	1.77997300	3.35526300	0.76565000
C	-1.62919100	4.58544700	-0.59199300
H	-2.26006500	2.53509300	-0.41204200
C	-0.58488900	5.49375100	-0.41288200
H	1.45771900	5.74808400	0.21492900
H	-2.58112500	4.92451300	-0.98556100
H	-0.72548400	6.54023900	-0.65835400
C	1.76571400	0.37467500	-0.99168000
H	1.61960200	-0.53677600	-1.57330000
H	1.63986000	1.24552000	-1.63971000
H	2.79446600	0.34776700	-0.62070500

M2_{ph}-Ac-c

Zero-point correction=	0.430344 (Hartree/Particle)
Thermal correction to Energy=	0.461862
Thermal correction to Enthalpy=	0.462806
Thermal correction to Gibbs Free Energy=	0.364742
Sum of electronic and zero-point Energies=	-1625.709909
Sum of electronic and thermal Energies=	-1625.678392
Sum of electronic and thermal Enthalpies=	-1625.677448

Sum of electronic and thermal Free Energies=			-1625.775512
Pd	-0.43524100	-0.04806100	0.12956500
C	1.47140500	0.33399000	0.84414400
C	2.49086700	0.42479300	-0.22230000
C	2.32602200	1.31022300	-1.30432100
C	3.63705200	-0.38999300	-0.20716300
C	3.27524200	1.37655800	-2.31866300
H	1.45014500	1.94752800	-1.31636300
C	4.58338300	-0.32386900	-1.22873500
H	3.79084300	-1.07370800	0.62119800
C	4.40601300	0.55894600	-2.29096200
H	3.13372900	2.07467200	-3.13713800
H	5.46180900	-0.95969600	-1.19025900
H	5.14180300	0.61353300	-3.08564900
C	1.66127800	0.61246600	2.13568200
P	-2.71782800	-0.14761100	-0.81365000
P	-0.00298600	-2.28582200	0.49144600
C	-3.09622600	-1.34928000	-2.17509100
H	-2.42617500	-1.15641200	-3.01583500
H	-2.94268500	-2.37874000	-1.84910500
H	-4.12919900	-1.24495900	-2.51850600
C	-3.25737600	1.42749300	-1.60196100
H	-2.49089000	1.77837200	-2.29309500
H	-4.20142800	1.28662400	-2.13526200
H	-3.38639000	2.17083200	-0.81706400
C	-4.06349800	-0.45181900	0.40714300
H	-3.95085200	0.29582500	1.19342400
H	-5.05183900	-0.36508300	-0.05278800
H	-3.96128700	-1.44573400	0.84628800
C	-1.45016400	-3.41756500	0.68557100
H	-2.05264000	-3.09521300	1.53662700
H	-2.07445900	-3.40088200	-0.20690400
H	-1.11354600	-4.44313600	0.85876900
C	0.97041100	-2.74852200	1.98395500
H	0.45733900	-2.38805000	2.87708800
H	1.07962700	-3.83484300	2.04292800
H	1.94961500	-2.27607000	1.94897100
C	0.93915700	-3.06694800	-0.88312900
H	1.15500500	-4.11750000	-0.67019400
H	0.35924400	-2.99725400	-1.80501300
H	1.87385800	-2.52357800	-1.02919700
C	2.91577000	1.16465000	2.76921300
H	3.30990000	0.48440400	3.53454800
H	3.70307800	1.34658300	2.03688500

H	2.69804300	2.11110200	3.27709600
C	-1.29179400	2.69497600	0.69201300
O	-2.15384800	2.16001600	1.39699500
O	-0.50230000	2.07860300	-0.12247500
H	0.82391500	0.48770400	2.82025200
C	-1.09174100	4.20777800	0.72006200
H	-1.86900400	4.68325700	1.31724500
H	-0.11225100	4.43113900	1.15108300
H	-1.09763400	4.60935300	-0.29587100

M2_{ph}w-Ac-c

Zero-point correction=			0.454951 (Hartree/Particle)
Thermal correction to Energy=			0.488431
Thermal correction to Enthalpy=			0.489375
Thermal correction to Gibbs Free Energy=			0.387276
Sum of electronic and zero-point Energies=			-1702.151271
Sum of electronic and thermal Energies=			-1702.117791
Sum of electronic and thermal Enthalpies=			-1702.116846
Sum of electronic and thermal Free Energies=			-1702.218945
Pd	0.22551800	0.26752500	0.09939000
C	-1.18178000	-2.31947700	-0.30787800
C	-1.38756000	-1.03604800	0.01755800
P	2.02278100	1.79135300	0.80159800
P	-0.25534900	0.84796600	-2.07251600
C	2.46339900	3.41569300	0.02900000
H	2.88243300	3.26140200	-0.96637400
H	1.57058400	4.03767900	-0.06322300
H	3.19862900	3.94782100	0.63901400
C	3.67330300	0.98968500	0.95981900
H	4.04862800	0.73174800	-0.03209300
H	4.38843600	1.64836700	1.46048900
H	3.56331100	0.06710000	1.52981700
C	1.63572100	2.28336000	2.53251600
H	1.39515900	1.36824200	3.07449800
H	2.47557600	2.80263400	3.00225200
H	0.75874000	2.93413500	2.53981300
C	-0.13077800	-0.60409800	-3.19212900
H	0.82159100	-1.10376400	-3.00517200
H	-0.92946800	-1.30631100	-2.95634100
H	-0.19984700	-0.29965400	-4.23994900
C	0.88346900	2.04510200	-2.89509600
H	1.90641400	1.66969000	-2.83808700
H	0.61116000	2.17234500	-3.94640500
H	0.83595000	3.01371900	-2.39706500

C	-1.90108800	1.57795700	-2.44935100
H	-2.03256700	1.71170800	-3.52657500
H	-2.68872600	0.93282300	-2.06108900
H	-1.98746400	2.54696800	-1.95389200
H	-0.19787200	-2.59090300	-0.68486000
C	2.83247800	-2.50016400	0.08670800
O	2.29133000	-1.92911100	-0.84910600
O	2.57836600	-2.28339300	1.35968400
O	0.76394500	-0.65229900	1.93740500
H	1.79724000	-1.58522400	1.53890300
H	0.02426300	-1.22093900	2.17483800
C	3.90160500	-3.55731900	-0.11673400
H	4.09616600	-3.69639500	-1.17866500
H	4.81918900	-3.26012700	0.39680600
H	3.57479200	-4.49979200	0.32922200
C	-2.66422300	-0.47697900	0.51627700
C	-3.86893600	-0.65122900	-0.18931800
C	-2.71145700	0.27564700	1.70449100
C	-5.06545000	-0.10815600	0.27480700
H	-3.86183900	-1.22022000	-1.11260800
C	-3.90733000	0.80932500	2.17239600
H	-1.79400300	0.42838800	2.26144200
C	-5.09186900	0.62417000	1.45903800
H	-5.97876100	-0.25955200	-0.29102200
H	-3.91519700	1.37446700	3.09841300
H	-6.02229900	1.04621500	1.82196800
C	-2.14180300	-3.47571100	-0.15803300
H	-1.66698400	-4.28547400	0.40740500
H	-3.06208500	-3.19591900	0.35571500
H	-2.41177100	-3.89925200	-1.13362900

M2_{Ph}-Ac-d

Zero-point correction=			0.430555 (Hartree/Particle)
Thermal correction to Energy=			0.461935
Thermal correction to Enthalpy=			0.462879
Thermal correction to Gibbs Free Energy=			0.366621
Sum of electronic and zero-point Energies=			-1625.721727
Sum of electronic and thermal Energies=			-1625.690347
Sum of electronic and thermal Enthalpies=			-1625.689403
Sum of electronic and thermal Free Energies=			-1625.785661
Pd	0.47800100	0.00773700	-0.02592700
C	-1.43107500	-0.60876100	2.14406000
C	-1.35590700	-0.31070400	0.83576400
P	0.28148700	2.35142500	0.19683000

P	0.94721300	-2.31700000	-0.04303200
C	1.41249900	2.95098600	1.51702100
H	1.01433400	2.64061700	2.48519200
H	2.38661600	2.47583100	1.39418900
H	1.50570600	4.04058400	1.49810300
C	-1.31279200	3.17241200	0.60402900
H	-1.68356400	2.78538500	1.55402000
H	-1.18183600	4.25511100	0.68069000
H	-2.05314000	2.94932500	-0.16507500
C	0.83786700	3.22606200	-1.32154600
H	0.09744500	3.07893400	-2.11023800
H	0.96971500	4.29663700	-1.14401900
H	1.77507200	2.77616400	-1.64879600
C	-0.37319300	-3.58591200	0.14834300
H	-0.92784000	-3.39237300	1.06667300
H	-1.07258600	-3.52473700	-0.68699900
H	0.05594700	-4.59081300	0.18512600
C	2.10715700	-2.69845400	1.33113600
H	1.58259500	-2.56747300	2.27966500
H	2.48220000	-3.72365400	1.26593200
H	2.92920400	-1.98144500	1.30272000
C	1.83932700	-2.86267500	-1.55615600
H	2.26233600	-3.86316500	-1.43337600
H	1.14793300	-2.86696900	-2.40132400
H	2.62778900	-2.14159100	-1.76953500
H	-0.50082100	-0.61196700	2.71064700
C	3.44942800	0.45064600	-0.34957800
O	2.37012300	0.34403700	-1.05107100
O	3.52146500	0.36361400	0.88028400
C	-2.64283300	-1.00568600	2.95643500
H	-3.49924600	-1.26635300	2.33359500
H	-2.40506900	-1.86983000	3.58673900
H	-2.95617000	-0.20578300	3.63951500
C	-2.52178100	-0.19907300	-0.07399500
C	-2.46465500	-0.68735800	-1.39244500
C	-3.71164900	0.44386800	0.31805000
C	-3.54814300	-0.57898300	-2.25782000
H	-1.54446100	-1.14087000	-1.74112400
C	-4.79473500	0.56180300	-0.54968500
H	-3.78015500	0.87297700	1.30990300
C	-4.72352500	0.04405000	-1.84081500
H	-3.47072800	-0.97258300	-3.26574000
H	-5.69553100	1.06591000	-0.21578400
H	-5.56609400	0.13616900	-2.51683700

C	4.71264700	0.74022500	-1.16216200
H	4.89952100	1.81870400	-1.14616900
H	5.57059400	0.25169900	-0.69834900
H	4.60719200	0.42738500	-2.20120400

M4_{ph}-Ac-a

Zero-point correction= 0.414668 (Hartree/Particle)

Thermal correction to Energy=	0.442894
Thermal correction to Enthalpy=	0.443838
Thermal correction to Gibbs Free Energy=	0.355472
Sum of electronic and zero-point Energies=	-1437.062035
Sum of electronic and thermal Energies=	-1437.033808
Sum of electronic and thermal Enthalpies=	-1437.032864
Sum of electronic and thermal Free Energies=	-1437.121230

Pd	0.88140900	0.43887200	-0.10270300
C	-0.60917100	-1.00274100	2.14946800
C	-0.71953700	-0.61910000	0.86343000
P	-0.20808800	2.49220500	0.13556000
P	2.14695300	-1.54890200	-0.18037200
C	-1.80952500	2.58195300	1.03904900
H	-2.55358100	1.97145300	0.52676600
H	-1.67677300	2.17524300	2.04251800
H	-2.16617800	3.61363400	1.10491000
C	-0.61501200	3.31785600	-1.46142500
H	-1.32525800	2.69524500	-2.00849200
H	-1.05322100	4.30678600	-1.30076500
H	0.28889500	3.41406800	-2.06360000
C	0.78988500	3.76206600	1.02748600
H	1.75541000	3.88618500	0.53738900
H	0.27042200	4.72392900	1.05817700
H	0.96752200	3.42060600	2.04903300
C	3.45242900	-1.71258300	-1.47379200
H	2.98427200	-1.73662300	-2.45979100
H	4.11940200	-0.85116600	-1.43936100
H	4.03274300	-2.62826600	-1.33241100
C	1.28790900	-3.17457100	-0.31771400
H	0.80515400	-3.25562000	-1.29301000
H	1.99358900	-4.00151600	-0.19966800
H	0.51533000	-3.23404300	0.44861800
C	3.10846600	-1.74540400	1.38038000
H	3.71643200	-2.65422500	1.36441300
H	3.75638700	-0.87820200	1.51614600
H	2.41463200	-1.79081900	2.22089200
H	0.28230700	-0.68497500	2.69321800

C	-1.91046400	-0.91219500	0.03210300
C	-3.22708200	-0.75933200	0.51362400
C	-1.77291700	-1.28827100	-1.31856600
C	-4.33496900	-0.99912100	-0.29594500
H	-3.37992700	-0.43075000	1.53457100
C	-2.87719900	-1.54142400	-2.12583100
H	-0.77525300	-1.36805000	-1.73447400
C	-4.16890500	-1.40104100	-1.61956700
H	-5.33298000	-0.86897900	0.11023800
H	-2.72970300	-1.83941700	-3.15886400
H	-5.03083100	-1.58987700	-2.24972100
C	-1.52974200	-1.87494200	2.97704300
H	-0.94941500	-2.63386700	3.51525700
H	-2.06246100	-1.29787800	3.74460000
H	-2.27734400	-2.38952700	2.37182000
C	2.49764300	1.47484600	-1.09433200
H	2.34796400	2.55224400	-1.20774100
H	3.43813700	1.34101600	-0.54682300
H	2.62566700	1.05976800	-2.09979000

M4_{Me}-Ac-b

Zero-point correction=			0.414977 (Hartree/Particle)
Thermal correction to Energy=			0.443230
Thermal correction to Enthalpy=			0.444174
Thermal correction to Gibbs Free Energy=			0.355071
Sum of electronic and zero-point Energies=			-1437.059784
Sum of electronic and thermal Energies=			-1437.031532
Sum of electronic and thermal Enthalpies=			-1437.030587
Sum of electronic and thermal Free Energies=			-1437.119691
Pd	0.91788600	-0.46243900	-0.21167900
C	-2.02180000	-0.41790100	0.36906700
C	-3.50166100	-0.38624300	0.30374700
C	-4.23849100	-1.06995600	1.28806100
C	-4.23007600	0.33772900	-0.65636700
C	-5.62878200	-1.06213600	1.29455000
H	-3.70113900	-1.62333500	2.05187400
C	-5.62281400	0.34708700	-0.65204500
H	-3.70158900	0.91993100	-1.40097000
C	-6.33188800	-0.35643200	0.31881400
H	-6.16629300	-1.60760500	2.06321400
H	-6.15617700	0.91726900	-1.40562300
H	-7.41612400	-0.34678200	0.32189100
C	-1.11462000	-0.45014500	-0.62685100
P	0.75557700	1.95396100	0.08975400

P	3.29296500	-0.75314200	0.20893300
C	2.22531600	3.08863600	0.04139900
H	2.96381400	2.78546600	0.78589400
H	2.69276900	3.04014800	-0.94449100
H	1.93641200	4.12452500	0.24051000
C	0.02709100	2.38054900	1.73228700
H	0.68829000	2.03362700	2.52891800
H	-0.12752200	3.45792700	1.83762900
H	-0.92988100	1.86688600	1.83380100
C	-0.37793900	2.84504200	-1.06343200
H	-1.36116000	2.37653700	-1.02283900
H	-0.46779000	3.90097000	-0.79409400
H	0.00036700	2.76773100	-2.08454600
C	4.45291900	0.08468400	-0.96587300
H	4.24167500	-0.25950600	-1.98021700
H	4.29787600	1.16389800	-0.93676700
H	5.49783000	-0.13201700	-0.72615500
C	3.95284500	-2.47733900	0.17003800
H	3.75509500	-2.92389000	-0.80534900
H	5.02887300	-2.49138600	0.36226500
H	3.44446500	-3.08375300	0.92074900
C	3.93228900	-0.17952500	1.85044700
H	5.00808900	-0.34952500	1.94927400
H	3.72950800	0.88460500	1.98136500
H	3.41291700	-0.72022200	2.64425700
C	-1.45964800	-0.54591000	-2.09226700
H	-0.86377800	-1.33444900	-2.56048100
H	-2.51557000	-0.76599800	-2.27883100
H	-1.20849400	0.37938100	-2.62500900
H	-1.64694600	-0.47969300	1.39014200
C	0.70074000	-2.55098500	-0.42836100
H	1.06038500	-3.03941600	0.48169000
H	-0.33448000	-2.84265400	-0.59252700
H	1.30679100	-2.88167900	-1.27791300

TS3Me-Ac

Zero-point correction=	0.414214 (Hartree/Particle)
Thermal correction to Energy=	0.441953
Thermal correction to Enthalpy=	0.442897
Thermal correction to Gibbs Free Energy=	0.354235
Sum of electronic and zero-point Energies=	-1437.034355
Sum of electronic and thermal Energies=	-1437.006616
Sum of electronic and thermal Enthalpies=	-1437.005672
Sum of electronic and thermal Free Energies=	-1437.094334

Pd	0.94636600	-0.35443500	-0.33052800
C	-1.90082300	-0.87998700	0.19048800
C	-3.33818700	-0.61957700	0.27383100
C	-3.99871800	-0.98501300	1.46994900
C	-4.13547700	-0.00926500	-0.72027000
C	-5.35746100	-0.77507800	1.65730600
H	-3.41810100	-1.44991300	2.26067400
C	-5.49843800	0.19916500	-0.53018500
H	-3.69197700	0.31816600	-1.64857100
C	-6.12463600	-0.18141400	0.65446400
H	-5.82238100	-1.07688000	2.59026700
H	-6.07604800	0.67066400	-1.31886200
H	-7.18650800	-0.01552900	0.79602800
C	-1.02012200	-0.80274500	-0.84959100
P	0.68939800	2.03334300	-0.00165000
P	3.24956800	-0.79120800	0.37682300
C	2.10433100	3.23525600	-0.06262300
H	2.88711800	2.91713500	0.62932800
H	2.52735300	3.24791100	-1.06965700
H	1.79293700	4.25010400	0.20277300
C	0.02827700	2.33438900	1.69945600
H	0.75106300	1.99165900	2.44225200
H	-0.19362900	3.39122200	1.87444600
H	-0.88503900	1.74883800	1.82141300
C	-0.56535500	2.94739600	-1.01226200
H	-1.52717700	2.43888000	-0.92813500
H	-0.68087800	3.98112000	-0.67276700
H	-0.26639900	2.94844000	-2.06232300
C	4.60052800	-0.09590100	-0.68517000
H	4.48215100	-0.46817700	-1.70485200
H	4.51568400	0.99209900	-0.71606300
H	5.59546200	-0.36700900	-0.31955700
C	3.74398600	-2.57600900	0.44039700
H	3.58132800	-3.03396400	-0.53758700
H	4.79252000	-2.70533300	0.72378800
H	3.11190500	-3.09948200	1.16075600
C	3.79534700	-0.23046900	2.05823300
H	4.82934900	-0.51714900	2.27191700
H	3.70904400	0.85559100	2.12989100
H	3.14119700	-0.66934700	2.81430600
C	-1.40155600	-0.48702700	-2.27884800
H	-0.58038800	-0.71078100	-2.96129100
H	-2.27915000	-1.05497900	-2.60886100
H	-1.63305400	0.57617200	-2.39494100

H	-1.48429200	-1.22259500	1.13530700
C	0.18397700	-2.39986500	-0.88389200
H	0.13300200	-2.92581700	0.06846000
H	-0.58030900	-2.79940000	-1.54736300
H	1.14386800	-2.58278900	-1.38180800

M5Me-Ac

Zero-point correction= 0.417475 (Hartree/Particle)

Thermal correction to Energy= 0.446154

Thermal correction to Enthalpy= 0.447099

Thermal correction to Gibbs Free Energy= 0.351959

Sum of electronic and zero-point Energies= -1437.113360

Sum of electronic and thermal Energies= -1437.084681

Sum of electronic and thermal Enthalpies= -1437.083737

Sum of electronic and thermal Free Energies= -1437.178876

Pd	-1.69561900	0.11575300	-0.02596700
C	2.38558100	0.21409800	1.04899100
C	2.87523700	-0.52345600	-0.12966500
C	1.96849600	-0.78760700	-1.17307300
C	4.18007100	-1.02988200	-0.25405400
C	2.36262500	-1.48489400	-2.31019500
H	0.94082300	-0.44355700	-1.07539200
C	4.57187500	-1.73187800	-1.39131200
H	4.88554200	-0.90534400	0.55737400
C	3.67014300	-1.95481700	-2.42937200
H	1.64489200	-1.66635200	-3.10319100
H	5.58398200	-2.11610200	-1.46029600
H	3.97824700	-2.50125700	-3.31382400
C	3.03628500	1.06533400	1.86240400
P	-1.43528200	2.31861900	-0.72423300
P	-2.12663300	-2.07974200	0.60087800
C	-2.99449500	3.27826600	-1.00304700
H	-3.59910300	2.77244500	-1.75797100
H	-3.57140300	3.30761200	-0.07697400
H	-2.78840600	4.30159400	-1.33217500
C	-0.56142500	2.59800000	-2.33323200
H	-1.08886400	2.06543600	-3.12684200
H	-0.50762400	3.66102600	-2.58847400
H	0.45018000	2.19260400	-2.27199300
C	-0.50403000	3.47225400	0.38429200
H	0.50603600	3.08678500	0.53443300
H	-0.44737500	4.48237500	-0.03333000
H	-0.99667500	3.51305800	1.35758500
C	-3.41872100	-2.33414900	1.90337900

H	-3.11075900	-1.83011800	2.82131600
H	-4.35691600	-1.88457900	1.57334700
H	-3.58148400	-3.39600100	2.11339700
C	-0.74013100	-3.10223900	1.27911200
H	-0.35509300	-2.63336900	2.18660900
H	-1.06405700	-4.12134300	1.51208400
H	0.07328100	-3.13983000	0.55241300
C	-2.75758600	-3.19108500	-0.73985600
H	-2.96529000	-4.20030900	-0.37044300
H	-3.67109800	-2.76637800	-1.15982600
H	-2.01636100	-3.24747200	-1.53910000
C	4.46758000	1.51072700	1.69638700
H	4.55305000	2.58116900	1.91183900
H	5.13111800	0.99861700	2.40464500
H	4.84783000	1.33365000	0.69069100
H	1.32566600	0.06089900	1.24674800
C	2.32246200	1.67735800	3.04239900
H	1.28878200	1.33521100	3.11527400
H	2.83315400	1.42331800	3.97964900
H	2.32135700	2.77226100	2.97829400

MI_{Me}'-Ac-a

Zero-point correction=			0.428767 (Hartree/Particle)
Thermal correction to Energy=			0.461434
Thermal correction to Enthalpy=			0.462378
Thermal correction to Gibbs Free Energy=			0.360378
Sum of electronic and zero-point Energies=			-1625.701745
Sum of electronic and thermal Energies=			-1625.669078
Sum of electronic and thermal Enthalpies=			-1625.668134
Sum of electronic and thermal Free Energies=			-1625.770135
Pd	-0.56212700	-0.52141900	-0.39099900
C	1.33111400	-0.20414600	-1.34621300
C	0.41892400	0.00533900	-2.19606600
P	-2.93327600	-0.40948400	-0.68005500
P	-0.21388900	-1.22600700	1.89606800
C	-3.87349700	-2.00713500	-0.67985500
H	-3.48945100	-2.65095900	-1.47366600
H	-3.72429800	-2.52254400	0.27060300
H	-4.94464400	-1.84757600	-0.83634600
C	-3.56849200	0.35012000	-2.24603800
H	-3.18355500	-0.21020100	-3.09998800
H	-4.66217600	0.35675100	-2.28472400
H	-3.20173600	1.37544100	-2.32271700
C	-3.88553100	0.56900000	0.57303900

H	-3.49492100	1.58816300	0.59502800
H	-4.95586200	0.59695600	0.34747500
H	-3.74219400	0.13181200	1.56332700
C	1.46458400	-1.88588700	2.30207600
H	1.67295100	-2.75171200	1.67042100
H	2.21654100	-1.12734900	2.08150300
H	1.54142300	-2.17965500	3.35334200
C	-1.27721300	-2.60308300	2.54186000
H	-1.16234600	-3.48041900	1.90183600
H	-1.01331100	-2.87573400	3.56818900
H	-2.32648900	-2.30143100	2.51739400
C	-0.43666000	0.04600500	3.22026900
H	-0.20155500	-0.35592400	4.21041400
H	0.20764800	0.90001000	3.00566500
H	-1.47150600	0.39621500	3.21619600
C	0.03145600	0.41842900	-3.56320400
H	-0.57771100	1.32649300	-3.54187400
H	0.91508400	0.61543100	-4.18080800
H	-0.56272100	-0.35490700	-4.05899900
C	0.03421100	3.34429500	0.86015600
O	0.86788500	2.77080000	1.52274200
O	-0.75413800	2.73802500	-0.04192000
H	-0.52774000	1.77592000	-0.09838800
C	2.72135400	-0.28409700	-0.95631300
C	3.24911100	0.57110400	0.02772100
C	3.58132200	-1.21368500	-1.56733300
C	4.59529500	0.50400400	0.37233600
H	2.59372400	1.28516200	0.51341200
C	4.92419300	-1.28158200	-1.20885000
H	3.18348400	-1.88132400	-2.32291100
C	5.43932400	-0.42285600	-0.23933700
H	4.98630600	1.17832000	1.12686500
H	5.57113900	-2.00681800	-1.69102200
H	6.48637500	-0.47591700	0.03735900
C	-0.24991600	4.82490600	0.93800800
H	-0.03452300	5.29009700	-0.02682600
H	-1.30744200	4.99342100	1.15256000
H	0.36735400	5.27492600	1.71231700

TS1_{Me}'-Ac-a

Zero-point correction=	0.423812 (Hartree/Particle)
Thermal correction to Energy=	0.455614
Thermal correction to Enthalpy=	0.456558
Thermal correction to Gibbs Free Energy=	0.356474

Sum of electronic and zero-point Energies=			-1625.655659
Sum of electronic and thermal Energies=			-1625.623857
Sum of electronic and thermal Enthalpies=			-1625.622913
Sum of electronic and thermal Free Energies=			-1625.722996
Pd	0.76378900	-0.18554400	-0.25780300
C	-1.25596900	0.92731300	-1.24302900
C	-0.19871500	0.48424300	-1.89957100
P	3.03579700	0.18519500	-0.55571000
P	0.32561100	-1.57513700	1.73801800
C	3.84711300	1.06294600	0.85247100
H	3.37165700	2.03473800	0.99521100
H	3.70860200	0.48220200	1.76561400
H	4.91703700	1.20685200	0.67480000
C	3.60880300	1.18893200	-1.99874000
H	3.15744100	2.18121500	-1.94949600
H	4.69811100	1.28979300	-2.01485100
H	3.28056000	0.71411600	-2.92491600
C	4.08357100	-1.32716200	-0.72542700
H	3.77677300	-1.88426700	-1.61240900
H	5.14402600	-1.07228400	-0.81143300
H	3.93940900	-1.97054300	0.14363200
C	-1.12312600	-1.00509900	2.72182700
H	-0.96314500	0.01621100	3.07146100
H	-1.98678800	-1.02247900	2.05464200
H	-1.30220700	-1.66088700	3.57924000
C	1.60579900	-1.86806300	3.04636400
H	1.90777600	-0.91491700	3.48644500
H	1.22498300	-2.51591700	3.84139700
H	2.48813500	-2.33753900	2.60529000
C	-0.18007000	-3.28783400	1.28186100
H	-0.40050500	-3.88786000	2.17002200
H	-1.07862700	-3.20193600	0.66688600
H	0.60990600	-3.77440200	0.70623800
C	0.01182900	0.04335700	-3.30116200
H	0.75317800	-0.75079000	-3.39509200
H	-0.94734600	-0.31030600	-3.69673800
H	0.32645200	0.89066700	-3.92194300
C	-3.41002900	-1.57779400	-1.10100800
O	-2.75167900	-1.71423900	-0.05884900
O	-3.31975100	-0.60193800	-1.93265000
H	-2.26014700	0.26641500	-1.58433600
C	-1.48195600	1.91343900	-0.18327200
C	-2.64675300	1.84809100	0.60041300
C	-0.60097900	2.99406300	0.01860700

C	-2.90574500	2.81417800	1.56632400
H	-3.33208700	1.02478900	0.44519400
C	-0.86969900	3.96053900	0.98083200
H	0.28465100	3.07461000	-0.60101800
C	-2.02083200	3.87399700	1.76383200
H	-3.80793100	2.74326000	2.16414600
H	-0.18342200	4.79007300	1.11530100
H	-2.23116300	4.63063300	2.51140700
C	-4.45307200	-2.62939700	-1.48777500
H	-5.43938700	-2.16070300	-1.53538200
H	-4.23384900	-3.01846000	-2.48505500
H	-4.46707400	-3.44321700	-0.76321800

M2_{Me'}-Ac-a

Zero-point correction=			0.430523 (Hartree/Particle)
Thermal correction to Energy=			0.461685
Thermal correction to Enthalpy=			0.462629
Thermal correction to Gibbs Free Energy=			0.366500
Sum of electronic and zero-point Energies=			-1625.713583
Sum of electronic and thermal Energies=			-1625.682422
Sum of electronic and thermal Enthalpies=			-1625.681477
Sum of electronic and thermal Free Energies=			-1625.777607
Pd	0.47621100	0.03087200	-0.29675400
C	-2.10218500	-1.20904500	-1.29714100
C	-0.85141700	-0.83872200	-1.60089900
P	-0.44679800	2.07120800	-0.81340100
P	2.33468100	0.71404000	1.18743100
C	-1.10588900	2.96682000	0.65564600
H	-1.88288500	2.35643100	1.11860900
H	-0.31266200	3.12641300	1.38586100
H	-1.52791700	3.93323200	0.36692100
C	-1.86331900	2.17868600	-1.98076600
H	-2.70763400	1.62133700	-1.57695800
H	-2.14698900	3.22440400	-2.12822900
H	-1.59198500	1.73707000	-2.93954100
C	0.74025600	3.27223200	-1.55817400
H	1.11495800	2.86727500	-2.49985400
H	0.25619900	4.23384800	-1.74903300
H	1.59067300	3.42730400	-0.89372600
C	2.42624100	-0.39693100	2.65244500
H	1.61875200	-0.14514500	3.34357300
H	2.27216300	-1.41983100	2.31126900
H	3.38468600	-0.30492400	3.17010900
C	2.58231000	2.37397700	1.97410800

H	1.73743600	2.60831900	2.62498100
H	3.49653900	2.38801200	2.57387500
H	2.65874800	3.15249500	1.21252800
C	3.93762400	0.45392700	0.31914300
H	4.78291700	0.49492100	1.01183800
H	3.90280000	-0.50747000	-0.19589900
H	4.05828600	1.22968200	-0.44042700
C	-0.24490600	-1.10366800	-2.95194500
H	0.70097400	-1.64239600	-2.85628800
H	-0.92617400	-1.68445300	-3.58713100
H	-0.00757400	-0.16983700	-3.47720200
C	1.92550100	-2.57379500	-0.48338000
O	1.06712500	-1.95496300	0.26265000
O	2.58370700	-2.06315000	-1.39206200
H	-2.68529400	-1.68588800	-2.09070800
C	-2.84176400	-1.01428400	-0.03805700
C	-4.22827300	-0.78576000	-0.07921200
C	-2.22288100	-1.06289500	1.22372700
C	-4.96139900	-0.56765500	1.08385400
H	-4.73223700	-0.77467700	-1.04102700
C	-2.95800100	-0.84656900	2.38672200
H	-1.17196800	-1.31948200	1.28157900
C	-4.32738900	-0.58824700	2.32505500
H	-6.02927900	-0.38665500	1.02157300
H	-2.46157300	-0.90260000	3.35005100
H	-4.89667300	-0.42629500	3.23368300
C	2.06689300	-4.05916200	-0.16087800
H	3.00052000	-4.44640700	-0.56822200
H	2.01359400	-4.23673800	0.91457100
H	1.23261000	-4.59536400	-0.62271800

MI_{Me}'w-Ac-b

Zero-point correction=			0.453172 (Hartree/Particle)
Thermal correction to Energy=			0.489947
Thermal correction to Enthalpy=			0.490891
Thermal correction to Gibbs Free Energy=			0.374188
Sum of electronic and zero-point Energies=			-1702.133259
Sum of electronic and thermal Energies=			-1702.096484
Sum of electronic and thermal Enthalpies=			-1702.095540
Sum of electronic and thermal Free Energies=			-1702.212243
Pd	2.87520100	-0.23557900	0.19806000
C	-2.49153900	-0.10069300	-1.07963700
C	-1.55202000	0.63754600	-0.88494700
P	1.75929100	-1.51984700	1.79913600

P	4.16398400	0.88491700	-1.36191700
C	1.04827800	-0.67976600	3.28481200
H	1.83673900	-0.11588500	3.78805100
H	0.26482700	0.01815300	2.97975800
H	0.62812800	-1.40868000	3.98588600
C	2.79483300	-2.83352400	2.59761700
H	3.64403000	-2.36749200	3.10083300
H	2.21905000	-3.41318400	3.32623300
H	3.18602500	-3.50514900	1.83127200
C	0.30986500	-2.51869300	1.22698200
H	0.62366500	-3.18224000	0.41891100
H	-0.11322900	-3.11653400	2.04047800
H	-0.45938900	-1.85095700	0.83557800
C	5.93600700	0.35764900	-1.48255500
H	6.41818500	0.49263500	-0.51274600
H	5.97933900	-0.70387800	-1.73266900
H	6.48122000	0.92995500	-2.23990600
C	4.36632500	2.71774500	-1.17282400
H	3.38660700	3.19712500	-1.21668100
H	4.79918300	2.93253900	-0.19399800
H	5.00911600	3.14087800	-1.95137400
C	3.65398000	0.77764500	-3.14063800
H	3.62140700	-0.27093500	-3.44215000
H	2.64920000	1.18875800	-3.25460000
H	4.34126700	1.32025300	-3.79762300
C	-0.40375300	1.48993000	-0.61162000
H	-0.30076100	2.26944300	-1.37274100
H	-0.51277500	1.95144300	0.37375500
H	0.52368600	0.89719300	-0.59356800
C	-4.58724300	2.53472200	0.93751500
O	-4.11203200	2.51799600	-0.30974100
O	-1.39334800	1.63513000	2.48989300
H	-3.42297100	1.82513100	-0.40129200
C	-3.58733100	-0.99076000	-1.30954000
C	-4.50452600	-1.27430800	-0.28206200
C	-3.76313400	-1.59990000	-2.56388800
C	-5.56529400	-2.14408700	-0.50882800
H	-4.37604100	-0.80490900	0.68607800
C	-4.82571400	-2.46931300	-2.78094800
H	-3.05837000	-1.38453700	-3.35789000
C	-5.72987900	-2.74474800	-1.75601400
H	-6.26489900	-2.35518900	0.29221100
H	-4.94844900	-2.93381800	-3.75294300
H	-6.55740900	-3.42357700	-1.92825800

O	-4.16877800	1.82622600	1.83140400
H	-1.38349700	2.25393800	3.22566200
H	-2.33506700	1.49930300	2.29747700
C	-5.70718600	3.52847800	1.09874700
H	-5.36691500	4.52186400	0.79835000
H	-6.53490700	3.25550800	0.44015600
H	-6.04211000	3.54108400	2.13324100

TS1_{Me}'w-Ac-b

Zero-point correction= 0.448468 (Hartree/Particle)

Thermal correction to Energy= 0.483064

Thermal correction to Enthalpy= 0.484008

Thermal correction to Gibbs Free Energy= 0.378347

Sum of electronic and zero-point Energies= -1702.103043

Sum of electronic and thermal Energies= -1702.068447

Sum of electronic and thermal Enthalpies= -1702.067503

Sum of electronic and thermal Free Energies= -1702.173165

Pd	-0.83398100	-0.40867000	-0.50276400
C	1.71985500	0.91699100	-0.62565200
C	0.86192700	0.39335900	-1.44921700
P	-2.13634500	-1.78703800	1.14735400
P	-2.12784300	1.35214800	-1.22632200
C	-2.40245800	-3.55607100	0.67428100
H	-3.05469400	-3.61394000	-0.19967600
H	-1.43573600	-3.98956800	0.41457200
H	-2.84590200	-4.13487300	1.48981100
C	-3.80650100	-1.33702000	1.81512800
H	-4.53866100	-1.31829300	1.00459400
H	-4.14453000	-2.04666800	2.57596800
H	-3.76616300	-0.34078600	2.26096700
C	-1.15078100	-1.96518900	2.69861400
H	-0.99959400	-0.98365200	3.15179200
H	-1.63771300	-2.62726400	3.42070900
H	-0.17281300	-2.36803600	2.43222000
C	-2.63438000	2.47304900	0.14990700
H	-3.16281300	1.89619000	0.91047000
H	-1.74312600	2.90081900	0.61032000
H	-3.28569200	3.27561400	-0.20903800
C	-3.76185000	0.85219700	-1.93308100
H	-3.60319500	0.26521900	-2.83948000
H	-4.29576400	0.22902500	-1.21424400
H	-4.37471200	1.72584300	-2.17500700
C	-1.54674000	2.55905500	-2.49721700
H	-0.59817400	2.99176700	-2.17910800

H	-1.38109500	2.04271500	-3.44416100
H	-2.28224700	3.35446200	-2.65017800
C	1.02301500	-0.09898000	-2.85812300
H	2.07236300	-0.02229600	-3.16033800
H	0.70474300	-1.13994000	-2.97251600
H	0.42682500	0.49329100	-3.55869200
C	4.23843500	-1.21750400	-0.77155100
O	4.09604400	-0.01195500	-1.22677700
O	0.68463500	-2.30995900	-0.19444000
H	3.05170600	0.44457000	-1.00090500
C	1.66385900	1.52278700	0.69781700
C	2.16730300	0.85172800	1.83089800
C	1.19663900	2.83966300	0.87649800
C	2.16284500	1.45710000	3.08248400
H	2.55743400	-0.15295700	1.71385200
C	1.20162200	3.44382500	2.13109600
H	0.85199000	3.39536100	0.01123100
C	1.67765500	2.75572300	3.24566800
H	2.54904800	0.91275600	3.93827500
H	0.83952000	4.46176400	2.23614800
H	1.68489800	3.22741000	4.22181200
O	3.35689300	-1.90457800	-0.24286800
H	0.64020400	-2.86670800	-0.97824500
H	1.63093600	-2.01679800	-0.16540500
C	5.64736800	-1.76202500	-0.92398700
H	5.97854000	-1.65377100	-1.95892200
H	6.32737600	-1.17244600	-0.30376700
H	5.68552100	-2.80681800	-0.62009400

M2_{Me}'w-Ac-b

Zero-point correction=			0.455445 (Hartree/Particle)
Thermal correction to Energy=			0.488767
Thermal correction to Enthalpy=			0.489711
Thermal correction to Gibbs Free Energy=			0.387655
Sum of electronic and zero-point Energies=			-1702.151357
Sum of electronic and thermal Energies=			-1702.118035
Sum of electronic and thermal Enthalpies=			-1702.117090
Sum of electronic and thermal Free Energies=			-1702.219146
Pd	-0.83051700	-0.09296500	-0.57669300
C	1.46657300	1.62484300	-1.60496000
C	0.33059800	0.97360000	-1.89084500
P	-2.09349100	-1.76882600	0.73574500
P	-1.78178400	1.87214900	0.17421900
C	-2.46013300	-3.19696200	-0.36166700

H	-3.25139700	-2.92087500	-1.06201900
H	-1.55505800	-3.40324000	-0.93351000
H	-2.77125900	-4.07578600	0.20905200
C	-3.72206400	-1.48441200	1.57120400
H	-4.46411300	-1.16459700	0.83686000
H	-4.08008300	-2.40056000	2.04876800
H	-3.63289900	-0.70900700	2.33512800
C	-1.09897300	-2.51284200	2.09844600
H	-0.92938600	-1.76475800	2.87598100
H	-1.61789100	-3.37006000	2.53669500
H	-0.12898800	-2.83185800	1.71396800
C	-1.61894300	2.10842500	1.99479300
H	-2.07463100	1.26927300	2.52206400
H	-0.55863300	2.13981800	2.25057000
H	-2.09745000	3.03711800	2.31733000
C	-3.60011400	2.01445200	-0.11213600
H	-3.79834400	1.96821700	-1.18448100
H	-4.12526400	1.18912000	0.36800800
H	-3.98518300	2.95915400	0.28122500
C	-1.18425300	3.48548500	-0.47524500
H	-0.12582500	3.60399300	-0.24634200
H	-1.30304600	3.51481800	-1.55871800
H	-1.75232700	4.30351800	-0.02382000
C	-0.18430200	0.88565200	-3.30477400
H	0.50299800	1.36101000	-4.01595700
H	-0.32483600	-0.15623100	-3.60956800
H	-1.16461100	1.36643600	-3.40708900
C	2.93611800	-3.01009200	-0.29939200
O	3.13568200	-2.71804000	-1.46043900
O	0.12464100	-1.81759400	-1.28074300
H	1.98073900	2.11284600	-2.43816800
C	2.11070600	1.84647300	-0.29854000
C	2.04933200	0.92448400	0.76056100
C	2.83897800	3.03157900	-0.09091000
C	2.65708900	1.19903700	1.98315100
H	1.56039800	-0.02937300	0.60644400
C	3.44253400	3.30757800	1.13242200
H	2.92549900	3.74495600	-0.90483000
C	3.34829300	2.39421000	2.18096900
H	2.60893700	0.46265600	2.77855300
H	3.99296000	4.23290600	1.26493000
H	3.82507600	2.60137400	3.13259900
O	1.77289900	-2.83543700	0.32312700
H	0.75771000	-1.58371100	-1.96956600

H	1.08252800	-2.41785300	-0.34629000
C	3.99407000	-3.60770400	0.60570500
H	4.90254300	-3.79779600	0.03744000
H	4.20929000	-2.91456000	1.42310900
H	3.62660300	-4.53470100	1.05178800

M2_{Me}'-Ac-c

Zero-point correction= 0.430290 (Hartree/Particle)

Thermal correction to Energy=	0.461659
Thermal correction to Enthalpy=	0.462603
Thermal correction to Gibbs Free Energy=	0.364411
Sum of electronic and zero-point Energies=	-1625.730335
Sum of electronic and thermal Energies=	-1625.698967
Sum of electronic and thermal Enthalpies=	-1625.698023
Sum of electronic and thermal Free Energies=	-1625.796214

Pd	0.57759400	0.08908000	0.30060100
C	-2.22323900	-0.35738000	1.40493600
C	-0.90580500	-0.23247800	1.64840500
P	0.95832800	-2.26879300	0.17220000
P	0.20023800	2.42616700	0.35719000
C	1.56249000	-2.86701600	-1.45934500
H	0.88589200	-2.53637100	-2.24900600
H	2.55219000	-2.44603000	-1.62920600
H	1.61637600	-3.95929500	-1.46681800
C	-0.50346000	-3.35181300	0.46759000
H	-1.28887500	-3.11314600	-0.25126700
H	-0.22623000	-4.40439200	0.36518200
H	-0.90274300	-3.17598600	1.46641800
C	2.20579000	-2.91644900	1.35603500
H	1.87947700	-2.73018800	2.38071200
H	2.34708500	-3.99207400	1.21756500
H	3.13717600	-2.38397900	1.16856800
C	1.67004700	3.34650800	0.96881200
H	1.84690700	3.10544700	2.01843700
H	2.53449800	3.02348300	0.38881000
H	1.53590600	4.42657400	0.86442500
C	-1.19801400	3.15145200	1.30493600
H	-1.08572900	2.92236200	2.36581100
H	-1.23624100	4.23605500	1.17338700
H	-2.13312300	2.70779400	0.96164300
C	-0.03526000	3.07424000	-1.34471500
H	-0.04102000	4.16747300	-1.35746400
H	0.78372800	2.69258000	-1.95488600
H	-0.97920100	2.70195100	-1.74625700

C	-0.41007800	-0.27286000	3.07514500
H	0.11612100	0.65000700	3.34452200
H	-1.23218500	-0.41408200	3.78806900
H	0.31337800	-1.08018000	3.23051200
C	3.28790200	0.21161500	-1.11468200
O	3.66785300	-0.73318200	-0.41861500
O	2.10413900	0.72695900	-1.10766100
H	-2.86276600	-0.48756800	2.28274000
C	-2.98749200	-0.33834700	0.14897500
C	-4.39172800	-0.40940300	0.22496400
C	-2.41902800	-0.25644200	-1.13614000
C	-5.18771700	-0.39254000	-0.91513000
H	-4.85999100	-0.47888900	1.20191200
C	-3.21455700	-0.24007100	-2.27760300
H	-1.33937400	-0.20791600	-1.23536900
C	-4.60382700	-0.30654600	-2.17749900
H	-6.26669800	-0.44753700	-0.81768200
H	-2.74447100	-0.17825300	-3.25361100
H	-5.22050400	-0.29414600	-3.06909100
C	4.24460200	0.86036800	-2.11484100
H	5.24120600	0.43149200	-2.01909700
H	3.87394600	0.69871300	-3.13079100
H	4.28775800	1.94056500	-1.95548900

M4_{ph}²-Ac-a

Zero-point correction=			0.414483 (Hartree/Particle)
Thermal correction to Energy=			0.442669
Thermal correction to Enthalpy=			0.443614
Thermal correction to Gibbs Free Energy=			0.355771
Sum of electronic and zero-point Energies=			-1437.066912
Sum of electronic and thermal Energies=			-1437.038725
Sum of electronic and thermal Enthalpies=			-1437.037781
Sum of electronic and thermal Free Energies=			-1437.125623
Pd	-0.79676600	0.44953500	-0.11106100
C	0.60541800	-0.77423500	2.35364400
C	0.70287900	-0.57096200	1.02940700
P	-2.16135900	-1.45458000	-0.21335800
P	0.49484000	2.40540800	-0.12210600
C	-2.45572400	-2.08663700	-1.92196900
H	-2.84110000	-1.28314600	-2.54966700
H	-1.51083100	-2.42966200	-2.34736700
H	-3.16556400	-2.91831800	-1.91820300
C	-3.87231800	-1.18068400	0.41870000
H	-4.31845300	-0.33083600	-0.09826800

H	-4.49737600	-2.06622600	0.27373200
H	-3.82681000	-0.94742500	1.48395800
C	-1.66220000	-2.99071500	0.67217100
H	-1.56061700	-2.78028200	1.73664800
H	-2.39886100	-3.78509300	0.52274000
H	-0.68856800	-3.31955000	0.30694900
C	-0.42191500	3.97963800	0.16416500
H	-1.24209400	4.06301200	-0.54868700
H	-0.84551200	3.96940300	1.17028800
H	0.23795200	4.84557200	0.06291900
C	1.30957100	2.68793800	-1.75076400
H	0.54912300	2.74284000	-2.53089800
H	1.89712300	3.61024700	-1.75040600
H	1.96373700	1.84220500	-1.96879400
C	1.89986200	2.56523700	1.05647800
H	2.41124000	3.52346000	0.92853800
H	1.52690600	2.48572800	2.07838600
H	2.60437500	1.74991100	0.89136400
H	1.37365500	-1.35933200	2.86958300
C	1.89237500	-1.07446100	0.29869500
C	1.79165100	-1.51235300	-1.03579100
C	3.17722800	-1.10829100	0.87950100
C	2.89479900	-1.99289200	-1.73640000
H	0.82480300	-1.46246300	-1.52480900
C	4.28350900	-1.58081900	0.17945800
H	3.30559600	-0.74545400	1.89321700
C	4.15047400	-2.03233100	-1.13289200
H	2.77483200	-2.33071700	-2.76076500
H	5.25721100	-1.58927100	0.65890600
H	5.01321200	-2.39609600	-1.67974400
C	-0.50269100	-0.28627900	3.24686100
H	-1.01053100	-1.11599500	3.75749100
H	-0.11820700	0.36578500	4.04224100
H	-1.24738500	0.27748600	2.67904800
C	-2.30319200	1.50713300	-1.25221300
H	-3.00438400	0.85398100	-1.78024800
H	-2.88685100	2.12735500	-0.56155400
H	-1.86594900	2.16615400	-2.01014300

M4_{Me}'-Ac-b

Zero-point correction=	0.415217 (Hartree/Particle)
Thermal correction to Energy=	0.443191
Thermal correction to Enthalpy=	0.444136
Thermal correction to Gibbs Free Energy=	0.356703

Sum of electronic and zero-point Energies=			-1437.065765
Sum of electronic and thermal Energies=			-1437.037790
Sum of electronic and thermal Enthalpies=			-1437.036846
Sum of electronic and thermal Free Energies=			-1437.124279
Pd	0.65364200	-0.17315900	0.62653100
C	-2.26492700	0.13013800	1.58799000
C	-0.95382900	0.29595100	1.84214200
P	2.68030100	-0.91661800	-0.48307700
P	0.30600600	1.91105000	-0.59776700
C	4.20723500	-0.14656300	0.22157000
H	4.16552800	0.93700900	0.09807900
H	4.24980100	-0.36037900	1.29109700
H	5.11387800	-0.52738700	-0.25710500
C	2.92348500	-0.64727400	-2.30061600
H	2.85596300	0.41542300	-2.53821500
H	3.89484200	-1.02166600	-2.63518500
H	2.13649700	-1.16763800	-2.85051300
C	3.08760900	-2.71352200	-0.36057000
H	2.32115800	-3.29667800	-0.87460600
H	4.06164400	-2.92948400	-0.80782700
H	3.09350700	-3.01990800	0.68565900
C	1.75537300	3.00778600	-0.97121700
H	2.23152800	3.31061000	-0.03628000
H	2.49415900	2.47447400	-1.57139900
H	1.44556600	3.90433100	-1.51554600
C	-0.84698100	3.13754400	0.15681100
H	-0.44620500	3.47453900	1.11450800
H	-0.98526800	4.00144400	-0.49905800
H	-1.80605600	2.65648400	0.34636200
C	-0.44089500	1.68920600	-2.27361400
H	-0.61655800	2.65047600	-2.76480100
H	0.21868200	1.08397200	-2.89808500
H	-1.38693900	1.15618400	-2.16755600
C	-0.53775900	0.90032200	3.16089800
H	-1.40119500	1.19209000	3.77429900
H	0.06460900	0.19072600	3.73827100
H	0.09264600	1.78611400	3.02011700
H	-2.96388700	0.48138300	2.35431800
C	-2.94529100	-0.43262000	0.41170300
C	-2.30367200	-1.19378300	-0.58263200
C	-4.32841700	-0.21720600	0.26242500
C	-3.00653200	-1.69177400	-1.67506800
H	-1.24398400	-1.40058700	-0.47615300
C	-5.03191700	-0.71326300	-0.83034800

H	-4.85390900	0.35279800	1.02274100
C	-4.37429900	-1.45277000	-1.81163700
H	-2.48491000	-2.28249100	-2.42168900
H	-6.09719200	-0.52486800	-0.91437500
H	-4.91960500	-1.84550100	-2.66269600
C	0.69067900	-1.93500200	1.80102600
H	1.61789800	-1.95185900	2.38368200
H	-0.15661100	-1.98918500	2.48104300
H	0.66312300	-2.80461900	1.13995600

TS3_{Me'}-Ac

Zero-point correction=			0.413875 (Hartree/Particle)
Thermal correction to Energy=			0.441707
Thermal correction to Enthalpy=			0.442652
Thermal correction to Gibbs Free Energy=			0.354644
Sum of electronic and zero-point Energies=			-1437.038362
Sum of electronic and thermal Energies=			-1437.010529
Sum of electronic and thermal Enthalpies=			-1437.009585
Sum of electronic and thermal Free Energies=			-1437.097593
Pd	0.64228400	0.03105800	0.60512000
C	-2.28935200	0.63350300	1.28967800
C	-1.00646400	0.59727000	1.75676800
P	2.47650700	-1.41710800	-0.17239100
P	0.76242000	1.95578100	-0.84025300
C	4.20243300	-0.83494600	0.17427000
H	4.37181200	0.12310700	-0.32074600
H	4.32141800	-0.68056900	1.24865500
H	4.95478500	-1.55154600	-0.16872500
C	2.59445900	-1.80728900	-1.98144900
H	2.69589000	-0.87953300	-2.54858500
H	3.44559200	-2.45618600	-2.20850900
H	1.67596100	-2.30030300	-2.30654100
C	2.54125100	-3.12424400	0.54738600
H	1.62069500	-3.65711200	0.30061700
H	3.39652200	-3.69529700	0.17478100
H	2.60687200	-3.05962100	1.63565300
C	2.38285200	2.70241100	-1.35056300
H	2.92633400	3.02995500	-0.46185800
H	2.98954700	1.95039800	-1.85954400
H	2.24787300	3.55698100	-2.02054800
C	-0.15529300	3.46459900	-0.29182100
H	0.36505200	3.92353600	0.55132300
H	-0.24318600	4.19969600	-1.09669400
H	-1.15126700	3.16765600	0.04281500

C	-0.02508900	1.64535600	-2.48712600
H	-0.01726000	2.54124200	-3.11522100
H	0.50552100	0.84284200	-3.00346100
H	-1.05519100	1.32000700	-2.33217200
C	-0.63216100	1.57211500	2.85969000
H	-1.52074300	2.03276300	3.30747700
H	-0.06538500	1.08596800	3.65841100
H	0.00324200	2.37538000	2.47549600
H	-2.95557600	1.34406100	1.78191100
C	-2.94966000	-0.17515000	0.27155600
C	-2.27886100	-1.00629300	-0.65049700
C	-4.35822000	-0.13407600	0.18026500
C	-2.97821800	-1.76742800	-1.58188000
H	-1.19301700	-1.03501300	-0.63648800
C	-5.05432800	-0.88669200	-0.75632600
H	-4.90675000	0.49911000	0.87094600
C	-4.36997400	-1.71666800	-1.64514000
H	-2.42966700	-2.39793200	-2.27487400
H	-6.13732900	-0.82866100	-0.79276000
H	-4.91076400	-2.30468200	-2.37815800
C	-0.37311500	-1.18922800	2.24153300
H	0.61950300	-1.61653900	2.41939400
H	-0.78416700	-0.96949700	3.22376100
H	-1.00686100	-1.90838600	1.72972800

M5_{Me}'-Ac

Zero-point correction=			0.417273 (Hartree/Particle)
Thermal correction to Energy=			0.446036
Thermal correction to Enthalpy=			0.446980
Thermal correction to Gibbs Free Energy=			0.351233
Sum of electronic and zero-point Energies=			-1437.113467
Sum of electronic and thermal Energies=			-1437.084704
Sum of electronic and thermal Enthalpies=			-1437.083760
Sum of electronic and thermal Free Energies=			-1437.179507
Pd	1.66555700	0.35347600	-0.15378700
C	-3.51218100	0.08666200	1.28926600
C	-2.67862100	-0.06140000	2.33402700
P	2.68749000	-1.70666200	0.15922600
P	0.74934300	2.46690200	-0.48443000
C	4.52123900	-1.75877600	-0.09675800
H	4.75178400	-1.43887700	-1.11454000
H	5.00180500	-1.05981800	0.59016400
H	4.92729400	-2.76213600	0.06663400
C	2.14832700	-3.11302000	-0.91926600

H	2.31157900	-2.84767900	-1.96553200
H	2.69652500	-4.03295900	-0.69281000
H	1.07993800	-3.28855800	-0.78089900
C	2.54814400	-2.47881700	1.83659100
H	1.49452500	-2.63004300	2.07795600
H	3.07099400	-3.43890800	1.89035300
H	2.96779900	-1.79969500	2.58111700
C	1.95021700	3.87327200	-0.59201600
H	2.53315900	3.92218700	0.32951400
H	2.64235700	3.69554100	-1.41708000
H	1.44190100	4.83007000	-0.74785500
C	-0.42054400	3.10576100	0.80054300
H	0.09084000	3.14415700	1.76441400
H	-0.79033800	4.10523500	0.55082100
H	-1.26672500	2.42262800	0.89442100
C	-0.24037800	2.72967000	-2.02624400
H	-0.61433700	3.75579700	-2.09795600
H	0.38299800	2.51345900	-2.89591800
H	-1.08444800	2.03775000	-2.03714300
C	-2.91699400	0.70494700	3.61082700
H	-3.77915500	1.37043700	3.53583300
H	-3.08094700	0.02113800	4.45221100
H	-2.04002400	1.31054200	3.86959700
H	-4.37474000	0.73392800	1.43929400
C	-3.46037700	-0.54499900	-0.04239400
C	-2.26441500	-0.79581600	-0.73706900
C	-4.66942000	-0.87312700	-0.68035900
C	-2.28325600	-1.37750600	-2.00300700
H	-1.31011000	-0.50652600	-0.31019400
C	-4.68677900	-1.45993400	-1.94069800
H	-5.60565900	-0.67004400	-0.17004200
C	-3.49055300	-1.71925200	-2.60834200
H	-1.34518400	-1.54855700	-2.51992500
H	-5.63442800	-1.71102800	-2.40480600
H	-3.50092900	-2.17043900	-3.59427300
C	-1.48392600	-0.98017700	2.36199000
H	-0.55460700	-0.43581400	2.15120100
H	-1.37774800	-1.42676900	3.35606300
H	-1.56511300	-1.78341300	1.62904800

Com6_{ph-d}

Zero-point correction=	0.424114 (Hartree/Particle)
Thermal correction to Energy=	0.455317
Thermal correction to Enthalpy=	0.456261

Thermal correction to Gibbs Free Energy=			0.357908
Sum of electronic and zero-point Energies=			-1587.614001
Sum of electronic and thermal Energies=			-1587.582798
Sum of electronic and thermal Enthalpies=			-1587.581854
Sum of electronic and thermal Free Energies=			-1587.680207
Pd	-0.38289000	-0.27822200	-0.04859600
C	0.52591300	-1.62974400	-1.55921200
C	1.38201800	-0.52311200	-1.39469500
P	-2.37303000	-1.38237000	0.66723900
P	-0.00295200	1.84441100	1.05664700
C	-2.08934200	-2.77985400	1.85082200
H	-1.41626600	-3.50885500	1.39611500
H	-1.61129100	-2.39822500	2.75522900
H	-3.02443500	-3.27774300	2.12468200
C	-3.37546700	-2.22175700	-0.64488000
H	-2.75034800	-2.95271000	-1.16119400
H	-4.25337600	-2.72758300	-0.23160600
H	-3.69717500	-1.48109600	-1.37937600
C	-3.70244200	-0.44602400	1.55857300
H	-4.04961800	0.37766300	0.93176500
H	-4.55391100	-1.08476700	1.81276500
H	-3.29176900	-0.01994100	2.47609000
C	1.02184100	1.69171900	2.59264900
H	0.49861100	1.06985600	3.32228000
H	1.96657000	1.20382800	2.34581500
H	1.22807000	2.66858300	3.04042100
C	-1.41463300	2.87817600	1.66171400
H	-2.02626200	2.29958600	2.35685300
H	-1.06408500	3.78430100	2.16532400
H	-2.02810700	3.16012000	0.80478600
C	0.95743000	3.10310100	0.10295300
H	1.16708200	3.99382000	0.70318600
H	1.89976200	2.66247000	-0.22765100
H	0.37413900	3.38955800	-0.77338600
C	-2.48779800	2.12564600	-2.49309100
O	-2.27893300	0.81401000	-2.39375900
O	-2.03584700	2.98134000	-1.77688100
H	-3.15315100	2.33033200	-3.34604900
H	-0.14965700	-1.55544200	-2.40887100
H	1.27980100	0.26355700	-2.13830900
H	-1.66989900	0.60872600	-1.62962700
C	2.69655000	-0.49844700	-0.70812300
C	3.76443900	0.18226900	-1.31773500
C	2.94746600	-1.10590500	0.53545300

C	5.02483800	0.23881600	-0.72853800
H	3.59993800	0.66672500	-2.27498200
C	4.20773500	-1.05618500	1.12280400
H	2.13482000	-1.59294100	1.06100000
C	5.25700900	-0.38593800	0.49425300
H	5.82723400	0.77095500	-1.22835300
H	4.36881000	-1.53424000	2.08337300
H	6.23722900	-0.34518300	0.95549300
C	0.82299900	-3.06063900	-1.16519600
H	1.38063000	-3.56492000	-1.96608100
H	1.41704600	-3.14792200	-0.25703300
H	-0.10081800	-3.62647200	-1.01694100

TS4_{Ph-c}

Zero-point correction=			0.419572 (Hartree/Particle)
Thermal correction to Energy=			0.449680
Thermal correction to Enthalpy=			0.450625
Thermal correction to Gibbs Free Energy=			0.356736
Sum of electronic and zero-point Energies=			-1587.572985
Sum of electronic and thermal Energies=			-1587.542877
Sum of electronic and thermal Enthalpies=			-1587.541932
Sum of electronic and thermal Free Energies=			-1587.635821
Pd	-0.39360700	-0.08995600	-0.17360300
C	0.35111300	-2.22895700	-0.54271100
C	1.29560700	-1.15570700	-0.87334400
P	-2.42280200	0.27207000	1.16008500
P	0.38120200	2.09466700	-0.56672800
C	-2.30361200	1.39496200	2.62998400
H	-1.54480300	1.01552700	3.31755900
H	-2.00428100	2.39685900	2.31517700
H	-3.25737600	1.46525000	3.16081400
C	-3.13217600	-1.24905200	1.92576300
H	-2.40792800	-1.66850300	2.62773600
H	-4.06330800	-1.03334000	2.45780100
H	-3.30318000	-1.98209200	1.13681300
C	-3.86060100	0.98148600	0.24810700
H	-3.97671600	0.43740700	-0.68946300
H	-4.77997800	0.93016100	0.83803400
H	-3.65341100	2.02491300	0.00221700
C	1.41240900	2.86173900	0.75647200
H	0.82856600	2.93842800	1.67574300
H	2.27328800	2.22101100	0.95441400
H	1.76054100	3.85765800	0.46817800
C	-0.90460300	3.38465200	-0.87241400

H	-1.52159100	3.51402300	0.01837800
H	-0.45053000	4.34572900	-1.12976700
H	-1.54936100	3.05936400	-1.69069400
C	1.44871400	2.28793200	-2.05809900
H	1.74915900	3.32972400	-2.20156800
H	2.34134200	1.67092200	-1.94604300
H	0.89944600	1.94677600	-2.93743100
C	-2.80210700	-1.87016300	-1.89424000
O	-2.29935800	-2.52736400	-0.91657100
O	-2.48396300	-0.74241200	-2.28419400
H	-3.62273100	-2.40752300	-2.42155600
H	0.09855900	-2.77257500	-1.45497100
H	1.39277100	-0.98994800	-1.94448500
H	-1.00493300	-1.94513800	-0.54096200
C	2.56434500	-0.87719400	-0.15661000
C	3.73611900	-0.68674700	-0.91038500
C	2.67579200	-0.78497700	1.24316300
C	4.96123300	-0.42650300	-0.30152600
H	3.68264200	-0.75998500	-1.99202800
C	3.89914900	-0.52736500	1.85259000
H	1.78912300	-0.88906600	1.85485300
C	5.05070600	-0.34756200	1.08579900
H	5.84667100	-0.29031600	-0.91295700
H	3.95373100	-0.46211200	2.93402600
H	6.00258100	-0.14770800	1.56442200
C	0.55850500	-3.19630400	0.61773500
H	1.46597200	-3.79246800	0.47273600
H	0.63980100	-2.69895800	1.58359000
H	-0.29113500	-3.88031700	0.66921600

M6_{ph-g}

Zero-point correction=			0.427057 (Hartree/Particle)
Thermal correction to Energy=			0.456817
Thermal correction to Enthalpy=			0.457762
Thermal correction to Gibbs Free Energy=			0.365986
Sum of electronic and zero-point Energies=			-1587.602581
Sum of electronic and thermal Energies=			-1587.572821
Sum of electronic and thermal Enthalpies=			-1587.571877
Sum of electronic and thermal Free Energies=			-1587.663652
Pd	-0.36309000	-0.08256500	0.26827200
C	1.63477900	0.01376700	1.03508500
C	2.44292900	-0.11321600	-0.21423300
C	3.13057200	0.99792200	-0.73723500
C	2.55142200	-1.32989200	-0.91577800

C	3.88699600	0.90734300	-1.90195800
H	3.08990500	1.94350300	-0.20436600
C	3.30833900	-1.41979800	-2.07944200
H	2.00375400	-2.19140500	-0.55582700
C	3.98024100	-0.30542300	-2.58201900
H	4.41434400	1.78060500	-2.27187400
H	3.37285800	-2.36938300	-2.60046700
H	4.57215000	-0.38251800	-3.48726100
C	1.87354900	-1.03088000	2.12711000
P	-0.59529500	2.20424500	0.47320900
P	-2.48320300	-0.54275900	-0.96526500
C	0.49423400	3.17795900	1.60181800
H	0.47394300	2.74377400	2.60265500
H	1.52375900	3.17050200	1.24447100
H	0.14760300	4.21338500	1.65272900
C	-2.25461100	2.69512200	1.11553200
H	-2.39468000	2.25890100	2.10608000
H	-2.34392000	3.78263400	1.18400600
H	-3.04183400	2.31464900	0.46544300
C	-0.44395500	3.15860900	-1.09738900
H	-1.18235600	2.80547700	-1.81761100
H	-0.58798800	4.22953700	-0.93004300
H	0.54811000	2.98767300	-1.51933200
C	-3.26170000	0.65483300	-2.15013600
H	-3.59797000	1.55538600	-1.63285600
H	-2.53365200	0.94524200	-2.91057100
H	-4.12405000	0.20346500	-2.64874500
C	-3.91920200	-1.04524200	0.07382100
H	-4.27093000	-0.18341400	0.64528800
H	-4.74115100	-1.43120700	-0.53586800
H	-3.57707100	-1.79631000	0.78644700
C	-2.22139900	-1.98792200	-2.07855400
H	-3.16249300	-2.32675800	-2.52019100
H	-1.53125600	-1.70087900	-2.87466200
H	-1.75528800	-2.79085000	-1.51042000
C	-0.85607100	-2.83761600	1.23487300
O	-1.66831300	-2.33837300	2.00750900
O	-0.17229400	-2.24737100	0.31659300
H	-0.65342800	-3.92973300	1.27836300
H	1.80053100	0.99885600	1.46820100
H	1.07960500	-0.95799200	2.87594000
H	1.80602000	-2.03501100	1.71065700
C	3.23830700	-0.84752000	2.81364100
H	3.32126900	0.13936800	3.28158600

H	3.38259900	-1.59826100	3.59658400
H	4.05950200	-0.94584600	2.09834400

M6_{ph-e}

Zero-point correction= 0.427271 (Hartree/Particle)

Thermal correction to Energy= 0.457028

Thermal correction to Enthalpy= 0.457972

Thermal correction to Gibbs Free Energy= 0.366715

Sum of electronic and zero-point Energies= -1587.608752

Sum of electronic and thermal Energies= -1587.578995

Sum of electronic and thermal Enthalpies= -1587.578050

Sum of electronic and thermal Free Energies= -1587.669308

Pd	-0.61853600	0.22068800	0.04382000
C	1.16464300	-0.35735100	1.03270100
C	2.33550000	-0.45649800	0.08563200
C	3.55460300	0.17082500	0.39471100
C	2.28333200	-1.18855000	-1.11088900
C	4.66195000	0.07764000	-0.44708700
H	3.63888900	0.73283900	1.31903400
C	3.38573600	-1.28837000	-1.95445700
H	1.35424500	-1.66469700	-1.39205500
C	4.58331900	-0.65319500	-1.62938000
H	5.58742500	0.57408400	-0.17477100
H	3.30673100	-1.85742200	-2.87482700
H	5.44083000	-0.72636900	-2.28872800
C	0.99328000	-1.58302900	1.94741300
P	-0.00887900	2.51210000	0.10000600
P	-1.59555900	-1.98130500	-0.28404000
C	-0.05348500	3.18892000	-1.60739800
H	0.75141800	2.74318700	-2.19449700
H	-1.01020000	2.90544500	-2.04607800
H	0.05678100	4.27670900	-1.60696400
C	1.59290300	3.14064900	0.75705600
H	2.42316900	2.66997300	0.23061100
H	1.65180500	4.22449300	0.62737500
H	1.68124000	2.90936700	1.82025300
C	-1.22750200	3.54705900	1.01182300
H	-1.23211200	3.26651000	2.06648100
H	-0.98076900	4.60853800	0.92183400
H	-2.21877200	3.36460100	0.60080300
C	-2.90716400	-1.97268700	-1.57960600
H	-3.76169600	-1.41618400	-1.20062400
H	-2.53915700	-1.48517900	-2.48279800
H	-3.20916300	-2.99710800	-1.81301300

C	-2.49339300	-2.63252600	1.18452200
H	-3.19341800	-1.85859500	1.49964100
H	-3.03553600	-3.54848700	0.93359700
H	-1.79348900	-2.84155900	1.99421900
C	-0.61354200	-3.44929900	-0.84889700
H	-1.25928400	-4.33096700	-0.88462900
H	-0.22558900	-3.26527700	-1.85270800
H	0.22741900	-3.65561400	-0.18860400
C	-3.52590800	1.04053600	-0.39567400
O	-3.86490800	0.29056300	0.51641000
O	-2.36148700	1.17199200	-0.92293400
H	-4.28750400	1.69965100	-0.86875800
H	1.35331500	0.48702600	1.70245600
H	0.06534600	-1.46728500	2.51556400
H	0.88986000	-2.49220900	1.35082000
C	2.15138200	-1.78024400	2.94061800
H	2.26831500	-0.90429600	3.58675100
H	1.96576000	-2.64474300	3.58535500
H	3.10060400	-1.94373600	2.42473600

TS5_{Ph-a}

Zero-point correction=			0.426900 (Hartree/Particle)
Thermal correction to Energy=			0.455793
Thermal correction to Enthalpy=			0.456737
Thermal correction to Gibbs Free Energy=			0.367623
Sum of electronic and zero-point Energies=			-1587.606864
Sum of electronic and thermal Energies=			-1587.577970
Sum of electronic and thermal Enthalpies=			-1587.577026
Sum of electronic and thermal Free Energies=			-1587.666140
Pd	-0.66155900	-0.03525700	0.00653200
C	1.08959000	0.70570400	0.95671600
C	2.31996700	0.64588600	0.07082500
C	3.62398400	0.54843500	0.58206800
C	2.19883500	0.78964900	-1.32299400
C	4.74183300	0.57693300	-0.25096100
H	3.78442100	0.46308300	1.64986000
C	3.31085000	0.82368100	-2.15889500
H	1.20440300	0.84971000	-1.75285800
C	4.59492900	0.71217500	-1.62786100
H	5.73257100	0.49684400	0.18410500
H	3.17252400	0.92918300	-3.22985500
H	5.46370800	0.73048900	-2.27615200
C	1.20802300	0.15388000	2.39752200
P	-1.63785900	2.12519600	-0.20581900

P	0.13140000	-2.30752200	0.02366300
C	-2.06838300	2.46077700	-1.96117600
H	-1.15471900	2.57643400	-2.54724300
H	-2.61843400	1.59546700	-2.33059500
H	-2.67466600	3.36565700	-2.05668700
C	-0.77723800	3.67162900	0.31368700
H	0.18001500	3.75825200	-0.20404100
H	-1.38787800	4.54693400	0.07758700
H	-0.58568700	3.65656700	1.38808900
C	-3.25667900	2.24569600	0.65952700
H	-3.10652300	2.16540500	1.73749900
H	-3.75738100	3.19087500	0.43308200
H	-3.87411400	1.41058100	0.33097000
C	-0.41770700	-3.27666200	-1.44205000
H	-1.50160300	-3.36774000	-1.40216600
H	-0.13017100	-2.76013100	-2.35908400
H	0.03664800	-4.27125300	-1.43124800
C	-0.45390400	-3.32359900	1.44185600
H	-1.54250900	-3.29587000	1.43558900
H	-0.09865600	-4.35367000	1.34725400
H	-0.08248400	-2.90641000	2.37955700
C	1.94694200	-2.63571800	0.03008000
H	2.12726600	-3.71378500	0.00305500
H	2.41968100	-2.16788000	-0.83387200
H	2.40498100	-2.22084400	0.92746700
C	-3.33581100	-1.45946500	-0.72496500
O	-3.12473800	-2.38995000	0.04763900
O	-2.56483900	-0.47445900	-1.01636100
H	-4.30012200	-1.42397700	-1.27887400
H	0.85897100	1.76850300	1.04486000
H	0.58750000	-0.73658400	2.52075300
H	2.22913700	-0.17776500	2.61093900
C	0.79281800	1.17145300	3.46745600
H	-0.24234900	1.49483700	3.31942400
H	0.86243300	0.74538700	4.47262800
H	1.42997600	2.06094700	3.43659000

M6_{ph}'-a

Zero-point correction=	0.426912 (Hartree/Particle)
Thermal correction to Energy=	0.456569
Thermal correction to Enthalpy=	0.457514
Thermal correction to Gibbs Free Energy=	0.366778
Sum of electronic and zero-point Energies=	-1587.613093
Sum of electronic and thermal Energies=	-1587.583435

	Sum of electronic and thermal Enthalpies=		-1587.582491
	Sum of electronic and thermal Free Energies=		-1587.673227
Pd	0.60885900	0.03830300	-0.03626700
C	-1.04160200	-0.71964200	1.08000700
C	-2.30714400	-0.80200100	0.26537800
C	-3.55522700	-0.37898400	0.74928400
C	-2.28586200	-1.37611300	-1.01967600
C	-4.71726700	-0.51331600	-0.01142300
H	-3.63230100	0.05642100	1.73794800
C	-3.44105500	-1.51607700	-1.77909100
H	-1.33465200	-1.69388600	-1.43311300
C	-4.66971400	-1.08082700	-1.27994400
H	-5.66373400	-0.17376200	0.39621400
H	-3.38330900	-1.96005100	-2.76737900
H	-5.57195100	-1.18418200	-1.87206600
C	-1.16279300	-0.04907800	2.44951900
P	1.71001700	-2.07686600	-0.10068000
P	-0.27016700	2.26190500	-0.20840900
C	2.12686400	-2.52361000	-1.83483200
H	1.21181000	-2.74016600	-2.38947100
H	2.61404300	-1.65831600	-2.28391200
H	2.78605500	-3.39492000	-1.87398900
C	0.94762100	-3.62496400	0.55398400
H	-0.01956000	-3.79777700	0.07819100
H	1.59684300	-4.48259300	0.35986300
H	0.78861500	-3.54298900	1.63077800
C	3.34789600	-2.05417400	0.73793400
H	3.21205800	-1.89560400	1.80914700
H	3.88746100	-2.99172700	0.57797800
H	3.92706300	-1.22421000	0.33501200
C	0.34523700	3.13714100	-1.70723700
H	1.41509900	3.29925500	-1.59434900
H	0.16495000	2.52902500	-2.59455100
H	-0.16383500	4.09861500	-1.81656200
C	0.19967200	3.39733200	1.15988000
H	1.28782600	3.40329700	1.21427900
H	-0.17628500	4.40706300	0.97294300
H	-0.20815100	3.03364900	2.10438500
C	-2.08817100	2.52328700	-0.36092300
H	-2.29751900	3.58092900	-0.54342600
H	-2.48028400	1.92794300	-1.18646400
H	-2.60231300	2.21001100	0.54649000
C	3.20791600	1.48462600	-0.84011200
O	2.99379900	2.36855200	-0.01441500

O	2.44549300	0.50576400	-1.17283700
H	4.16381100	1.49424500	-1.40936900
H	-0.72207000	-1.74837600	1.25772500
H	-1.48280800	0.99357100	2.34522800
H	-1.95942100	-0.54625500	3.02321900
C	0.12198000	-0.09979900	3.28336100
H	0.94228200	0.42468900	2.78620700
H	-0.02947900	0.35575600	4.26634500
H	0.44003000	-1.13453200	3.44866500

M6_{ph}-b

Zero-point correction=			0.426815 (Hartree/Particle)
Thermal correction to Energy=			0.456746
Thermal correction to Enthalpy=			0.457691
Thermal correction to Gibbs Free Energy=			0.365424
Sum of electronic and zero-point Energies=			-1587.606891
Sum of electronic and thermal Energies=			-1587.576959
Sum of electronic and thermal Enthalpies=			-1587.576015
Sum of electronic and thermal Free Energies=			-1587.668282
Pd	0.36215500	0.08326400	0.26196900
C	-1.63343500	0.00173500	1.03445800
C	-2.44808900	0.11398500	-0.21196100
C	-3.14326400	-1.00111400	-0.71605600
C	-2.55706000	1.32212400	-0.92802800
C	-3.90780500	-0.92238400	-1.87628200
H	-3.10328100	-1.93987900	-0.17142300
C	-3.32265800	1.40044200	-2.08670400
H	-2.00257100	2.18546500	-0.58307200
C	-4.00235800	0.28233200	-2.57024700
H	-4.44091300	-1.79831600	-2.23133700
H	-3.38805400	2.34374200	-2.61889800
H	-4.60116100	0.35048200	-3.47166800
C	-1.86477000	1.06225700	2.11322100
P	0.58676500	-2.20128900	0.48640900
P	2.49530700	0.52464500	-0.96397400
C	-0.51272700	-3.17004200	1.60950400
H	-0.50362200	-2.73170500	2.60872100
H	-1.53833700	-3.16544100	1.24106400
H	-0.16506500	-4.20467600	1.66850300
C	2.24045900	-2.68463800	1.14898300
H	2.36397100	-2.25148200	2.14312700
H	2.33742700	-3.77169400	1.21443000
H	3.03273800	-2.29427400	0.51116400
C	0.45047100	-3.16650700	-1.07887200

H	1.19613500	-2.82052900	-1.79489200
H	0.59103800	-4.23618600	-0.90137200
H	-0.53761800	-2.99768300	-1.51092200
C	3.91236200	1.04934500	0.09025300
H	3.55533400	1.80840800	0.78691600
H	4.25708200	0.19728500	0.68041400
H	4.74300200	1.42900900	-0.51164800
C	2.24311700	1.94831900	-2.10678600
H	1.75142000	2.75307700	-1.56311500
H	3.19064600	2.29298900	-2.52962200
H	1.57836500	1.63914700	-2.91618200
C	3.29649100	-0.69116400	-2.11425700
H	4.16396500	-0.24556700	-2.60918700
H	3.62913500	-1.57967200	-1.57423100
H	2.58074000	-0.99974400	-2.87928200
C	0.86020500	2.85985900	1.19037700
O	1.67041400	2.37786000	1.97584000
O	0.18275500	2.25122000	0.27934800
H	0.65387900	3.95194900	1.21284500
H	-1.80000300	-0.97667400	1.48257200
H	-1.06536300	1.00091100	2.85728100
H	-1.80080100	2.06022300	1.68134400
C	-3.22392700	0.88795700	2.81306300
H	-3.30172200	-0.09178800	3.29671100
H	-3.36281300	1.65017700	3.58584800
H	-4.05119800	0.97430000	2.10328200

TS6_{Ph-b}

Zero-point correction=			0.420043 (Hartree/Particle)
Thermal correction to Energy=			0.449896
Thermal correction to Enthalpy=			0.450840
Thermal correction to Gibbs Free Energy=			0.358675
Sum of electronic and zero-point Energies=			-1587.579924
Sum of electronic and thermal Energies=			-1587.550071
Sum of electronic and thermal Enthalpies=			-1587.549127
Sum of electronic and thermal Free Energies=			-1587.641292
Pd	0.49381300	0.20418600	0.34950400
C	-1.26367800	-0.55892800	1.29929800
P	-0.30688200	2.36901300	-0.16002600
P	2.87806500	0.17997100	-0.26188100
C	0.85226000	3.68716700	-0.73996500
H	1.60292100	3.88897800	0.02546200
H	1.36288100	3.35568300	-1.64573800
H	0.31110500	4.61163400	-0.96003500

C	-1.19764400	3.25850100	1.19051200
H	-0.52232400	3.41275800	2.03424800
H	-1.57154100	4.22768700	0.84882000
H	-2.03905300	2.65350800	1.52823700
C	-1.54779300	2.35107600	-1.52267100
H	-2.37030600	1.68623200	-1.25798300
H	-1.93729200	3.35451300	-1.71627800
H	-1.07923000	1.96618900	-2.43024900
C	3.87411300	1.73849200	-0.13785000
H	3.51528400	2.47865400	-0.85382700
H	3.78026600	2.15780800	0.86622500
H	4.93118000	1.54204900	-0.33829200
C	3.26784100	-0.38255100	-1.97324300
H	2.80383300	0.28573300	-2.70148100
H	4.34703500	-0.41192900	-2.14878200
H	2.84748000	-1.38070100	-2.09080300
C	3.88831300	-0.96503400	0.77226300
H	4.94140500	-0.93479400	0.47722700
H	3.80383000	-0.68358100	1.82398200
H	3.48645900	-1.96871000	0.63519200
C	0.92896300	-3.56074100	-1.04186200
O	-0.28403800	-3.64957200	-1.21845600
O	1.55749100	-2.69980800	-0.31954700
H	1.60270800	-4.29151000	-1.54554500
H	-1.36163700	0.02508700	2.21443700
C	-0.34042200	-1.68455800	1.36413700
H	-0.73227600	-2.56792800	0.85535100
H	0.65832500	-1.78556800	0.44117700
C	-2.49799300	-0.57812000	0.48447800
C	-2.62968500	-1.37245500	-0.67038700
C	-3.59438400	0.20947200	0.87512600
C	-3.80910900	-1.35044500	-1.40676000
H	-1.81685500	-2.02232900	-0.98185100
C	-4.77409900	0.22638900	0.13507700
H	-3.52659400	0.80001900	1.78403900
C	-4.88438100	-0.54993000	-1.01611500
H	-3.89101100	-1.97313800	-2.29094500
H	-5.60815200	0.83720400	0.46369700
H	-5.80132200	-0.54338900	-1.59477200
C	0.29730300	-2.01051000	2.71173800
H	0.63331600	-1.10796000	3.22917800
H	-0.41851500	-2.52443200	3.36239300
H	1.15969700	-2.66701200	2.57968100

M7_{ph}-b

Zero-point correction=			0.424013 (Hartree/Particle)
Thermal correction to Energy=			0.455217
Thermal correction to Enthalpy=			0.456161
Thermal correction to Gibbs Free Energy=			0.358726
Sum of electronic and zero-point Energies=			-1587.616793
Sum of electronic and thermal Energies=			-1587.585589
Sum of electronic and thermal Enthalpies=			-1587.584645
Sum of electronic and thermal Free Energies=			-1587.682079
Pd	0.54910000	0.21200000	0.54620000
C	-1.23600000	-0.42920000	1.77820000
P	-0.05740000	2.34390000	-0.39470000
P	2.75510000	-0.53950000	0.02810000
C	1.17030000	3.32630000	-1.37900000
H	2.05910000	3.51210000	-0.77200000
H	1.47150000	2.75160000	-2.25710000
H	0.75790000	4.28540000	-1.70720000
C	-0.56360000	3.60590000	0.86480000
H	0.25950000	3.77900000	1.56110000
H	-0.84420000	4.55600000	0.39990000
H	-1.41250000	3.22250000	1.43330000
C	-1.51390000	2.36830000	-1.53460000
H	-2.37370000	1.92780000	-1.02640000
H	-1.76060000	3.38520000	-1.85470000
H	-1.29460000	1.75610000	-2.41090000
C	4.03250000	-0.02310000	1.26730000
H	4.08540000	1.06670000	1.30420000
H	3.74340000	-0.37960000	2.25760000
H	5.02120000	-0.42070000	1.01920000
C	3.57640000	-0.01000000	-1.54820000
H	3.64660000	1.07940000	-1.57000000
H	4.57960000	-0.43520000	-1.64920000
H	2.96860000	-0.32390000	-2.39870000
C	3.02840000	-2.36820000	-0.03700000
H	4.06530000	-2.61970000	-0.28020000
H	2.77400000	-2.80260000	0.93180000
H	2.35880000	-2.80310000	-0.78090000
C	-0.04870000	-1.92370000	-2.86730000
O	0.12960000	-2.83790000	-2.10580000
O	0.02160000	-0.62400000	-2.57400000
H	-0.29320000	-2.04860000	-3.93310000
H	-1.35870000	0.32600000	2.55240000
C	-0.19540000	-1.34820000	1.95150000
H	-0.23770000	-2.28440000	1.40160000

H	0.20200000	-0.49220000	-1.60420000
C	-2.43670000	-0.62410000	0.93970000
C	-2.54900000	-1.63890000	-0.02840000
C	-3.54790000	0.21620000	1.12790000
C	-3.71430000	-1.79540000	-0.77000000
H	-1.71440000	-2.30460000	-0.21350000
C	-4.71430000	0.05950000	0.38400000
H	-3.49500000	0.99760000	1.88030000
C	-4.80580000	-0.94830000	-0.57320000
H	-3.77130000	-2.58880000	-1.50790000
H	-5.55540000	0.72220000	0.55850000
H	-5.71300000	-1.07640000	-1.15280000
C	0.59970000	-1.40500000	3.23810000
H	0.68430000	-0.41930000	3.70310000
H	0.11430000	-2.07160000	3.96390000
H	1.61120000	-1.78910000	3.08060000

M6_{ph}-al-a

Zero-point correction=			0.426355 (Hartree/Particle)
Thermal correction to Energy=			0.456377
Thermal correction to Enthalpy=			0.457321
Thermal correction to Gibbs Free Energy=			0.364617
Sum of electronic and zero-point Energies=			-1587.597423
Sum of electronic and thermal Energies=			-1587.567401
Sum of electronic and thermal Enthalpies=			-1587.566457
Sum of electronic and thermal Free Energies=			-1587.659161
Pd	0.35705500	0.09018300	0.24354800
C	-1.49306300	0.90892700	0.96530800
P	1.15121400	2.16589500	-0.37692200
P	2.35400000	-1.32197000	-0.39342700
C	2.73044900	2.65862000	0.44055400
H	2.56749700	2.73255900	1.51717000
H	3.49675600	1.90592200	0.26195200
H	3.08202900	3.62334900	0.06491700
C	0.15774200	3.70318600	-0.13900000
H	-0.06246100	3.84710500	0.91962900
H	0.71777200	4.56733300	-0.50545900
H	-0.78707000	3.63899600	-0.67926700
C	1.55577000	2.27449200	-2.17381000
H	0.64529200	2.11950000	-2.75527700
H	1.98309000	3.24844000	-2.42703600
H	2.26463500	1.49143000	-2.44374800
C	4.04525400	-0.67525600	-0.80190700
H	4.00928400	0.00344100	-1.65676000

H	4.45504900	-0.13483000	0.05384700
H	4.72314200	-1.49852900	-1.04324600
C	2.03514700	-2.43641900	-1.83151300
H	1.77467700	-1.85042000	-2.71491900
H	2.91636900	-3.04571700	-2.05114000
H	1.20496700	-3.10093800	-1.58891800
C	2.72316500	-2.51504600	0.95802700
H	3.55847800	-3.16567300	0.68412700
H	2.97061200	-1.97027600	1.87106200
H	1.82621300	-3.10864900	1.14075700
C	-0.71890700	-2.75122200	0.17272400
O	-0.43054100	-3.93518500	0.28142100
O	-0.29623700	-1.80495800	0.95322900
H	-1.39120100	-2.42077300	-0.64743500
H	-1.43547500	1.99107300	0.86066600
C	-1.60156700	0.54464300	2.44412000
H	-2.62046900	0.78596900	2.78335100
H	-1.47342100	-0.53179700	2.57220100
C	-2.56398300	0.39861300	0.06176200
C	-3.35831400	-0.71690400	0.37773000
C	-2.84342600	1.06303900	-1.14795100
C	-4.37441600	-1.14404000	-0.47378800
H	-3.17840000	-1.25724600	1.29741700
C	-3.85273900	0.63606900	-2.00155700
H	-2.25626600	1.93526700	-1.41861000
C	-4.62737300	-0.47557900	-1.66872800
H	-4.96965900	-2.00850500	-0.20017100
H	-4.04225800	1.17412600	-2.92449400
H	-5.41817100	-0.81147500	-2.32987100
C	-0.60039800	1.28308100	3.33799500
H	0.42864000	1.01396400	3.08221900
H	-0.70080400	2.37035300	3.24132000
H	-0.75737300	1.03261500	4.39074500

TS6_{ph}-al-a

Zero-point correction=			0.425066 (Hartree/Particle)
Thermal correction to Energy=			0.454440
Thermal correction to Enthalpy=			0.455384
Thermal correction to Gibbs Free Energy=			0.365061
Sum of electronic and zero-point Energies=			-1587.571785
Sum of electronic and thermal Energies=			-1587.542412
Sum of electronic and thermal Enthalpies=			-1587.541468
Sum of electronic and thermal Free Energies=			-1587.631791
Pd	0.31226900	-0.02430100	0.17688200

C	-1.57490900	0.47319100	1.08959400
P	0.91782000	2.19629100	0.17644200
P	2.34567000	-0.98118800	-0.94059900
C	2.64620000	2.46937500	0.76206600
H	2.72142100	2.15303800	1.80383400
H	3.34431600	1.87344900	0.17533500
H	2.92533500	3.52378700	0.68539500
C	0.02425700	3.47067600	1.16887200
H	-0.00990700	3.17105000	2.21728000
H	0.54256600	4.42953800	1.08667600
H	-0.99847100	3.59390400	0.81257800
C	0.90481400	2.95468700	-1.50373500
H	-0.10718800	2.90079000	-1.90855200
H	1.22748200	3.99910400	-1.47189100
H	1.56301600	2.39492800	-2.16818900
C	3.25703600	-0.05878500	-2.27071700
H	2.58170000	0.13241100	-3.10798100
H	3.62498000	0.90116900	-1.90321700
H	4.11115300	-0.63466400	-2.63790500
C	2.06094700	-2.58918000	-1.79881900
H	1.29757300	-2.47065600	-2.56956200
H	2.98606100	-2.94512100	-2.26058100
H	1.71398800	-3.31926600	-1.06994300
C	3.68554100	-1.39251200	0.25305100
H	4.50674100	-1.92294900	-0.23671600
H	4.07474100	-0.48341400	0.71547400
H	3.23854200	-2.01732400	1.02609400
C	-0.20971700	-2.64374900	0.72393000
O	-1.10021300	-3.43205000	1.01452700
O	0.89789600	-2.37350500	1.25637200
H	-0.43313100	-1.99794200	-0.22732300
H	-1.57045600	1.53246500	1.33374400
C	-1.76042800	-0.32435100	2.37885500
H	-2.76372200	-0.07222700	2.75668700
H	-1.77507500	-1.39791600	2.19388600
C	-2.52679300	0.23151400	-0.02909400
C	-3.06917200	-1.03738300	-0.31261400
C	-2.93222600	1.30835200	-0.84308000
C	-3.96770000	-1.20818000	-1.36167900
H	-2.77428400	-1.90120100	0.27159200
C	-3.82906500	1.13521400	-1.88980500
H	-2.54803200	2.30227100	-0.63383900
C	-4.35253500	-0.12975200	-2.15636400
H	-4.36932600	-2.19631300	-1.55759100

H	-4.12859200	1.98672600	-2.49162600
H	-5.05566600	-0.27057300	-2.96963300
C	-0.72695800	-0.01171800	3.46497500
H	0.26629200	-0.35189000	3.16430900
H	-0.68224400	1.06213700	3.68176500
H	-0.98375100	-0.52395300	4.39584800

M7_{ph}-al-a

Zero-point correction=			0.421537 (Hartree/Particle)
Thermal correction to Energy=			0.452860
Thermal correction to Enthalpy=			0.453804
Thermal correction to Gibbs Free Energy=			0.353000
Sum of electronic and zero-point Energies=			-1587.605576
Sum of electronic and thermal Energies=			-1587.574254
Sum of electronic and thermal Enthalpies=			-1587.573309
Sum of electronic and thermal Free Energies=			-1587.674113
Pd	0.35283900	0.34160100	0.26177800
C	-1.37079800	-0.61978700	1.14577700
P	-0.65473200	2.56444500	0.37086200
P	2.46348600	0.71958700	-0.81389000
C	0.43774000	4.05520700	0.49520200
H	1.06788800	3.97468100	1.38345000
H	1.08565000	4.11492300	-0.37945200
H	-0.15077800	4.97458900	0.56087100
C	-1.83040300	2.92190000	1.75292500
H	-1.31556300	2.80048200	2.70803900
H	-2.22093300	3.94071800	1.68279100
H	-2.66413600	2.22057200	1.72905900
C	-1.67428300	2.97901200	-1.11309100
H	-2.43708100	2.21021200	-1.24717100
H	-2.15303800	3.95790500	-1.01895700
H	-1.03763400	2.97622300	-2.00016300
C	3.07869400	2.33918500	-1.48273300
H	2.37155500	2.73100300	-2.21709600
H	3.17218700	3.06417900	-0.67237900
H	4.05455000	2.22380100	-1.96345400
C	2.68404400	-0.36232900	-2.29414700
H	1.91809300	-0.12712600	-3.03544000
H	3.67324100	-0.23438900	-2.74297300
H	2.55591600	-1.40123700	-1.99086200
C	3.88979700	0.21957100	0.24637500
H	4.84044000	0.31296100	-0.28651300
H	3.91616100	0.84571700	1.14032600
H	3.74992200	-0.81556100	0.55803100

C	2.12923500	-3.97277900	0.25408200
O	1.14595700	-4.53594400	0.49799100
O	3.12019600	-3.41398900	0.01766900
H	0.88705800	-1.14884400	0.24764800
H	-1.86582600	0.16024700	1.73107700
C	-1.06533700	-1.77246600	2.11485800
H	-2.01956300	-2.14898600	2.51778600
H	-0.61020500	-2.61053000	1.58289300
C	-2.27578900	-0.99541000	0.01221700
C	-1.97779900	-2.05000700	-0.87186800
C	-3.48984100	-0.31805600	-0.19985500
C	-2.83788500	-2.39790100	-1.90624100
H	-1.04684900	-2.59000800	-0.74628300
C	-4.35015900	-0.65489700	-1.24439400
H	-3.77711500	0.47460300	0.48482700
C	-4.02937800	-1.69821000	-2.10772600
H	-2.57576400	-3.21870700	-2.56625600
H	-5.27971500	-0.10917800	-1.37224800
H	-4.69631900	-1.96782700	-2.91900400
C	-0.16947800	-1.37161200	3.28870900
H	0.80944300	-1.04077300	2.93040300
H	-0.61002400	-0.54561600	3.85813600
H	-0.02285900	-2.20723700	3.98070900

M6-E

Zero-point correction=			0.426932 (Hartree/Particle)
Thermal correction to Energy=			0.456801
Thermal correction to Enthalpy=			0.457745
Thermal correction to Gibbs Free Energy=			0.365760
Sum of electronic and zero-point Energies=			-1587.607235
Sum of electronic and thermal Energies=			-1587.577366
Sum of electronic and thermal Enthalpies=			-1587.576422
Sum of electronic and thermal Free Energies=			-1587.668407
Pd	0.36174900	-0.08955800	0.29411100
C	-1.86253700	-1.03917800	2.15999700
C	-1.65098400	-0.01201800	1.04523000
P	2.55392100	-0.46311600	-0.85445400
P	0.50259600	2.21425900	0.43550200
C	2.98683400	0.66283800	-2.26730200
H	2.18872600	0.62942700	-3.01229900
H	3.09619800	1.69542600	-1.93100400
H	3.92244300	0.35574700	-2.74292200
C	2.66212000	-2.09759300	-1.70230200
H	1.75580900	-2.27772600	-2.28099500

H	3.53290400	-2.12938700	-2.36285400
H	2.75359900	-2.87171200	-0.94289500
C	4.09670700	-0.44497500	0.15479900
H	3.96346800	-1.17973500	0.94868700
H	4.97099400	-0.69738300	-0.45193100
H	4.24790400	0.53773300	0.60488100
C	0.12342400	3.09513800	-1.13897100
H	0.81305800	2.77014700	-1.91867400
H	-0.88776600	2.83309900	-1.45513500
H	0.19922300	4.17931300	-1.01889200
C	2.17158200	2.86184700	0.88778900
H	2.91984500	2.53410600	0.16745300
H	2.16754600	3.95450800	0.92020400
H	2.45187200	2.47577300	1.86943200
C	-0.53296800	3.14671900	1.64842400
H	-0.23455500	4.19812700	1.66051200
H	-1.58838600	3.08639200	1.38524800
H	-0.40292700	2.72568800	2.64673700
C	0.99003600	-2.92083400	1.01166900
O	0.12492400	-2.23346200	0.35790100
O	2.06163700	-2.54266500	1.48097500
H	0.69054400	-3.98529000	1.12055300
H	-1.83259400	0.97612300	1.46431200
H	-1.73320900	-2.04880700	1.77383200
H	-1.08785500	-0.90315100	2.92167000
C	-2.47571100	-0.17009900	-0.19007800
C	-3.18672400	0.92466300	-0.71643000
C	-2.58452700	-1.39839800	-0.87042700
C	-3.96306500	0.80862300	-1.86602300
H	-3.15006700	1.87800400	-0.19700300
C	-3.36099700	-1.51394500	-2.01881700
H	-2.02243300	-2.24813100	-0.50576400
C	-4.05405700	-0.41485300	-2.52646600
H	-4.50753200	1.67020500	-2.23851100
H	-3.42468400	-2.47216800	-2.52392700
H	-4.66093100	-0.51229300	-3.41974700
C	-3.24593500	-0.90441100	2.82021000
H	-3.36474600	-1.63723900	3.62421000
H	-3.38769100	0.09094600	3.25507700
H	-4.04866900	-1.06733700	2.09610800

TS5-E

Zero-point correction=

0.419209 (Hartree/Particle)

Thermal correction to Energy=

0.449384

Thermal correction to Enthalpy=			0.450328
Thermal correction to Gibbs Free Energy=			0.356333
Sum of electronic and zero-point Energies=			-1587.574720
Sum of electronic and thermal Energies=			-1587.544545
Sum of electronic and thermal Enthalpies=			-1587.543601
Sum of electronic and thermal Free Energies=			-1587.637596
Pd	-0.55805400	-0.34031400	0.42450400
C	0.49413800	1.40052600	1.60143500
C	1.35964600	0.28007800	1.34595500
P	-2.53443200	0.46458900	-0.73257000
P	-0.25208400	-2.65748100	0.21582200
C	-3.93090700	-0.67245700	-1.16318600
H	-3.56850900	-1.47164000	-1.81315100
H	-4.33412500	-1.12541900	-0.25520000
H	-4.73328300	-0.13747000	-1.67946400
C	-2.11567600	1.21964800	-2.36211700
H	-1.59274400	0.49419000	-2.98788500
H	-3.01514100	1.56265000	-2.88222300
H	-1.45751700	2.06999600	-2.17258100
C	-3.41279900	1.85945500	0.09782800
H	-2.70655300	2.68772600	0.18459500
H	-4.28146400	2.18508000	-0.48225100
H	-3.73943700	1.55897200	1.09516700
C	0.61987100	-3.15168600	-1.33377500
H	0.03847100	-2.82524600	-2.19784600
H	1.59021800	-2.65337800	-1.37155500
H	0.76545600	-4.23459100	-1.38658100
C	-1.76760200	-3.71493200	0.16646700
H	-2.40517200	-3.40384000	-0.66214800
H	-1.51464100	-4.77227800	0.04569100
H	-2.33060500	-3.58704300	1.09304300
C	0.74361000	-3.53460600	1.50393400
H	0.82090300	-4.60529300	1.29250500
H	1.74594000	-3.10604600	1.53821000
H	0.27851700	-3.39575600	2.48163400
C	0.42746000	4.20534800	0.01444700
O	-0.41059900	3.50125100	-0.56946400
O	1.24451900	3.84142600	0.92708400
H	0.51115100	5.27895200	-0.25932600
H	1.65547000	-0.30459600	2.21583700
H	0.96541100	2.55359900	1.25723100
H	-0.21572700	1.62473300	0.74075700
C	2.32040600	0.20808800	0.22827100
C	3.39704900	-0.69358000	0.30040200

C	2.21187500	1.01827100	-0.91851200
C	4.32122600	-0.79955100	-0.73405200
H	3.51671700	-1.30357800	1.19068300
C	3.13598500	0.90725600	-1.95120700
H	1.40537600	1.73721500	-0.99769500
C	4.19183900	-0.00133200	-1.86945800
H	5.14844800	-1.49600400	-0.64917700
H	3.03650100	1.54355400	-2.82373500
H	4.91242100	-0.07684000	-2.67596200
C	-0.13399900	1.52061600	2.98674500
H	-0.98215700	2.20831200	2.96735300
H	-0.48554100	0.56371800	3.38568900
H	0.59578300	1.92984900	3.69242000

M7'-E

Zero-point correction=			0.423977 (Hartree/Particle)
Thermal correction to Energy=			0.455658
Thermal correction to Enthalpy=			0.456602
Thermal correction to Gibbs Free Energy=			0.354387
Sum of electronic and zero-point Energies=			-1587.610105
Sum of electronic and thermal Energies=			-1587.578424
Sum of electronic and thermal Enthalpies=			-1587.577480
Sum of electronic and thermal Free Energies=			-1587.679695
Pd	-0.86666400	0.12497700	0.30690400
C	0.90498300	1.30644000	0.88790900
C	1.22465400	-0.05043300	1.09179200
P	-2.35396100	1.75338500	-0.57164800
P	-1.73899800	-2.10797900	0.26062500
C	-3.65882500	1.26150400	-1.79538000
H	-3.18426200	0.80153600	-2.66467100
H	-4.32253900	0.52312900	-1.34148900
H	-4.25355600	2.11833700	-2.12700900
C	-1.58549600	3.17874400	-1.47284000
H	-1.03681500	2.80373900	-2.33915400
H	-2.33286000	3.90385300	-1.80967300
H	-0.86955300	3.67940100	-0.81867600
C	-3.38622600	2.64691100	0.68192900
H	-2.73354200	3.12014800	1.41782900
H	-4.01900700	3.41148100	0.22083300
H	-4.01898100	1.92965200	1.20839700
C	-1.06450900	-3.14842700	-1.11346800
H	-1.34494800	-2.70780000	-2.07224700
H	0.02525400	-3.15544900	-1.05371500
H	-1.43723200	-4.17641700	-1.06908800

C	-3.55799800	-2.43152300	0.08322800
H	-3.91507000	-1.99269200	-0.85065300
H	-3.78601700	-3.50195400	0.08134800
H	-4.09417000	-1.95653400	0.90778500
C	-1.35963500	-3.17472500	1.72825300
H	-1.74629600	-4.19156400	1.60850800
H	-0.27772200	-3.21825200	1.86409100
H	-1.79678800	-2.72995800	2.62462200
C	4.36572900	2.70999300	0.03280900
O	3.60015300	2.90192500	-0.87271600
O	4.19162600	1.85112200	1.04443100
H	5.32881200	3.22698000	0.15472100
H	1.17101900	-0.42150100	2.11326500
H	3.34342400	1.38438100	0.92299000
H	1.27032400	1.79937900	-0.00923500
C	2.01638200	-0.90738900	0.18307600
C	2.52265700	-2.13084500	0.65904100
C	2.31797500	-0.55692900	-1.14715900
C	3.27791200	-2.97192500	-0.15264000
H	2.32301800	-2.41750900	1.68715000
C	3.07558200	-1.39674300	-1.95574700
H	1.95507500	0.37969400	-1.55204400
C	3.55855700	-2.61210900	-1.46931800
H	3.65472400	-3.90728000	0.24769400
H	3.29265900	-1.09777500	-2.97576000
H	4.14916400	-3.26280400	-2.10400200
C	0.65064700	2.23567000	2.05839500
H	-0.01776700	3.05689300	1.78689600
H	0.20093200	1.70462300	2.90095300
H	1.58507100	2.69057800	2.41510000

M8_{ph}-al-a

Zero-point correction=			0.409231 (Hartree/Particle)
Thermal correction to Energy=			0.436040
Thermal correction to Enthalpy=			0.436984
Thermal correction to Gibbs Free Energy=			0.350052
Sum of electronic and zero-point Energies=			-1398.973674
Sum of electronic and thermal Energies=			-1398.946866
Sum of electronic and thermal Enthalpies=			-1398.945922
Sum of electronic and thermal Free Energies=			-1399.032854
Pd	0.50810000	-0.27620000	0.34770000
C	-1.45360000	-0.33860000	1.25190000
P	0.47000000	2.14750000	0.04990000
P	2.57620000	-0.96960000	-0.63570000

C	2.06860000	3.08130000	-0.01050000
H	2.62550000	2.91260000	0.91370000
H	2.67480000	2.72540000	-0.84420000
H	1.89900000	4.15500000	-0.13080000
C	-0.44310000	3.15990000	1.29900000
H	0.00100000	3.00700000	2.28470000
H	-0.40550000	4.22370000	1.04930000
H	-1.48490000	2.84340000	1.34700000
C	-0.32750000	2.68050000	-1.52900000
H	-1.33730000	2.26890000	-1.57430000
H	-0.37140000	3.76980000	-1.61670000
H	0.23640000	2.27610000	-2.37210000
C	3.82420000	0.11640000	-1.48000000
H	3.35170000	0.64620000	-2.31000000
H	4.20980000	0.85520000	-0.77520000
H	4.66300000	-0.46790000	-1.86990000
C	2.30820000	-2.25270000	-1.93680000
H	1.74980000	-1.81640000	-2.76720000
H	3.25410000	-2.65520000	-2.31050000
H	1.70650000	-3.05910000	-1.51680000
C	3.65590000	-1.86040000	0.56920000
H	4.53890000	-2.28700000	0.08480000
H	3.97480000	-1.16920000	1.35190000
H	3.07640000	-2.65530000	1.03980000
H	0.40170000	-1.83340000	0.59530000
H	-1.59280000	0.64190000	1.71720000
C	-1.64210000	-1.38620000	2.36120000
H	-2.67030000	-1.30110000	2.74920000
H	-1.55400000	-2.39510000	1.95020000
C	-2.43480000	-0.46490000	0.12610000
C	-2.54800000	-1.63910000	-0.64290000
C	-3.31230000	0.58650000	-0.19290000
C	-3.47810000	-1.75020000	-1.66920000
H	-1.87540000	-2.46360000	-0.43650000
C	-4.23860000	0.48450000	-1.23070000
H	-3.28370000	1.49490000	0.40190000
C	-4.32810000	-0.68610000	-1.97780000
H	-3.53750000	-2.67150000	-2.24010000
H	-4.90060000	1.31790000	-1.44390000
H	-5.04920000	-0.77270000	-2.78300000
C	-0.66860000	-1.23010000	3.53090000
H	0.36250000	-1.36390000	3.19270000
H	-0.74540000	-0.23240000	3.97740000
H	-0.87350000	-1.96110000	4.31970000

TS7_{ph}-al-a

Zero-point correction=			0.407258 (Hartree/Particle)
Thermal correction to Energy=			0.434243
Thermal correction to Enthalpy=			0.435188
Thermal correction to Gibbs Free Energy=			0.346896
Sum of electronic and zero-point Energies=			-1398.963830
Sum of electronic and thermal Energies=			-1398.936844
Sum of electronic and thermal Enthalpies=			-1398.935900
Sum of electronic and thermal Free Energies=			-1399.024192
Pd	0.53607600	-0.18867200	0.27952500
C	-1.48033200	-0.67888100	1.20137400
P	0.60698800	2.26322300	0.22862100
P	2.52212800	-1.06843100	-0.68821300
C	2.21560300	3.18706900	0.20955200
H	2.79478000	2.92730500	1.09836200
H	2.79372900	2.89300600	-0.66832500
H	2.06500400	4.27059000	0.18836300
C	-0.25213800	3.14195500	1.61622600
H	0.24228700	2.89966100	2.55937200
H	-0.24808600	4.22732700	1.47925900
H	-1.28559000	2.79730200	1.68192700
C	-0.23961200	3.00295300	-1.24196100
H	-1.26257100	2.62554600	-1.29265100
H	-0.25603200	4.09619100	-1.20072700
H	0.27625900	2.68776500	-2.15127000
C	3.83716700	-0.01140500	-1.46494400
H	3.40180300	0.56884900	-2.28149300
H	4.22919000	0.68722200	-0.72306100
H	4.66412100	-0.61039900	-1.85907400
C	2.23146600	-2.28680400	-2.05174500
H	1.70844300	-1.79360900	-2.87335600
H	3.16676200	-2.71429100	-2.42618800
H	1.58991100	-3.08765700	-1.68093300
C	3.55045900	-2.07592500	0.47642500
H	4.41624000	-2.52200000	-0.02266600
H	3.89679400	-1.44309400	1.29592900
H	2.93198800	-2.86711300	0.90316100
H	-0.15723600	-1.56490600	0.58881900
H	-1.49521000	0.22731900	1.81198400
C	-1.77278400	-1.85386800	2.15483100
H	-2.78999900	-1.72725100	2.55404300
H	-1.77878100	-2.80288000	1.60858200
C	-2.46985400	-0.53383300	0.08617500

C	-2.67089600	-1.54621900	-0.86794900
C	-3.26864200	0.61638200	-0.02362000
C	-3.61714600	-1.41312500	-1.87844900
H	-2.06244300	-2.44277300	-0.82137700
C	-4.21232200	0.75757600	-1.03902100
H	-3.15585500	1.40761400	0.71155900
C	-4.39306800	-0.25784800	-1.97511700
H	-3.74698900	-2.21360400	-2.59954300
H	-4.81492800	1.65862900	-1.09125400
H	-5.12807100	-0.15349200	-2.76529700
C	-0.78889600	-1.94517200	3.32245500
H	0.23237600	-2.09220200	2.95963300
H	-0.79743800	-1.02496900	3.91597200
H	-1.04073400	-2.77416600	3.99056100

M9_{ph}-al-a

Zero-point correction=			0.412548 (Hartree/Particle)
Thermal correction to Energy=			0.440614
Thermal correction to Enthalpy=			0.441558
Thermal correction to Gibbs Free Energy=			0.343484
Sum of electronic and zero-point Energies=			-1399.020801
Sum of electronic and thermal Energies=			-1398.992735
Sum of electronic and thermal Enthalpies=			-1398.991791
Sum of electronic and thermal Free Energies=			-1399.089865
Pd	1.60630000	0.23540000	0.00880000
C	-2.84740000	-0.70350000	1.44860000
P	1.16910000	2.45550000	0.55090000
P	2.20130000	-1.93300000	-0.56340000
C	2.59830000	3.43760000	1.20150000
H	2.97560000	2.96750000	2.11150000
H	3.40370000	3.43440000	0.46480000
H	2.31470000	4.47180000	1.42100000
C	-0.11090000	2.80230000	1.84310000
H	0.17150000	2.30860000	2.77480000
H	-0.22360000	3.87560000	2.02500000
H	-1.06920000	2.39190000	1.51970000
C	0.58290000	3.55230000	-0.82070000
H	-0.35470000	3.16000000	-1.21850000
H	0.42650000	4.58090000	-0.48070000
H	1.31940000	3.54860000	-1.62640000
C	2.83020000	-2.18800000	-2.28660000
H	2.05680000	-1.89740000	-2.99990000
H	3.69660000	-1.54530000	-2.45280000
H	3.11350000	-3.22960000	-2.46810000

C	0.91430000	-3.26160000	-0.46450000
H	0.07570000	-3.00300000	-1.11360000
H	1.31210000	-4.23680000	-0.76220000
H	0.53900000	-3.32540000	0.55860000
C	3.56730000	-2.70090000	0.42420000
H	3.80100000	-3.71310000	0.07940000
H	4.46110000	-2.07920000	0.34720000
H	3.27580000	-2.73780000	1.47550000
H	-1.80020000	-0.46580000	1.66310000
H	-3.44860000	-0.22060000	2.22820000
C	-3.04230000	-2.22900000	1.54560000
H	-4.08590000	-2.47320000	1.31800000
H	-2.44010000	-2.71270000	0.76900000
C	-3.22140000	-0.13840000	0.09590000
C	-2.24270000	0.10960000	-0.87340000
C	-4.55850000	0.12020000	-0.22910000
C	-2.59250000	0.59630000	-2.13260000
H	-1.19420000	-0.06370000	-0.63690000
C	-4.91100000	0.60610000	-1.48580000
H	-5.33150000	-0.05650000	0.51320000
C	-3.92750000	0.84440000	-2.44450000
H	-1.81680000	0.78360000	-2.86750000
H	-5.95270000	0.80290000	-1.71550000
H	-4.19980000	1.22430000	-3.42300000
C	-2.66650000	-2.78980000	2.91970000
H	-1.61850000	-2.58310000	3.15810000
H	-3.27820000	-2.34390000	3.71040000
H	-2.81020000	-3.87300000	2.96040000

Com6_{ph}w-b

Zero-point correction=			0.449047 (Hartree/Particle)
Thermal correction to Energy=			0.483242
Thermal correction to Enthalpy=			0.484187
Thermal correction to Gibbs Free Energy=			0.380252
Sum of electronic and zero-point Energies=			-1664.052215
Sum of electronic and thermal Energies=			-1664.018020
Sum of electronic and thermal Enthalpies=			-1664.017076
Sum of electronic and thermal Free Energies=			-1664.121010
Pd	-0.19608000	-0.41633500	-0.01587300
C	0.83699300	-1.78419200	-1.43209800
C	1.60436300	-0.60549800	-1.33719300
P	-2.19694700	-1.54748500	0.69052700
P	0.07790200	1.73243800	1.08230600
C	-3.04994600	-0.97390100	2.22907400

H	-2.34454000	-0.97554700	3.06271100
H	-3.40594000	0.04389500	2.06357400
H	-3.89927100	-1.61700000	2.48055200
C	-2.00293200	-3.35531300	1.05423500
H	-1.24599000	-3.49535500	1.82881100
H	-2.94357200	-3.79995300	1.39323000
H	-1.66482600	-3.87460300	0.15622200
C	-3.62304700	-1.56967100	-0.49000100
H	-3.29127200	-1.91492000	-1.47085400
H	-4.42421400	-2.22332000	-0.13150400
H	-4.01079700	-0.55308700	-0.57666700
C	1.58014100	1.81350600	2.16142100
H	1.48517300	1.08419900	2.96865600
H	2.46469000	1.55512300	1.57774300
H	1.70881400	2.80940300	2.59629400
C	-1.20664800	2.42296200	2.22236100
H	-1.32990700	1.74857400	3.07271400
H	-0.92002300	3.41142000	2.59505400
H	-2.16466000	2.48539600	1.70283100
C	0.36367600	3.17894400	-0.03834700
H	0.56223400	4.09469500	0.52685100
H	1.21780000	2.96747100	-0.68456100
H	-0.51673200	3.32862200	-0.66593500
C	-2.11725300	1.57584000	-2.94830000
O	-1.37864600	0.49136100	-2.80968400
O	-2.56018600	2.27397100	-2.06368600
H	-2.29092700	1.78268900	-4.01412600
H	0.19261400	-1.82431400	-2.30601900
H	1.42293100	0.12077900	-2.12557700
H	-1.16042300	0.30013600	-1.84891600
C	2.90475700	-0.39165700	-0.66966400
C	3.73383600	0.64137000	-1.14814200
C	3.38854300	-1.14587400	0.41610600
C	4.97520800	0.90847000	-0.58058000
H	3.39281800	1.23807900	-1.98849000
C	4.63173700	-0.88144600	0.98217800
H	2.78116000	-1.93423900	0.83730000
C	5.43597000	0.14583200	0.49095600
H	5.58603800	1.71139300	-0.97960800
H	4.97303800	-1.48193400	1.81892000
H	6.40375700	0.34793500	0.93552400
C	1.21450200	-3.15521100	-0.90221100
H	2.18872600	-3.47695700	-1.29204400
H	1.26862200	-3.20854800	0.18600500

H	0.47526100	-3.89356900	-1.22143500
O	-4.00511200	1.77466600	0.34173200
H	-3.44029800	1.95744800	-0.42700500
H	-4.73276500	2.39825700	0.26175100

TS4_{PhW-e}

Zero-point correction= 0.444312 (Hartree/Particle)

Thermal correction to Energy= 0.477495

Thermal correction to Enthalpy= 0.478439

Thermal correction to Gibbs Free Energy= 0.377983

Sum of electronic and zero-point Energies= -1664.021230

Sum of electronic and thermal Energies= -1663.988047

Sum of electronic and thermal Enthalpies= -1663.987103

Sum of electronic and thermal Free Energies= -1664.087559

Pd	0.27383700	-0.10441400	-0.01470200
C	-0.43383600	-2.11086600	0.81279000
C	-1.35713400	-0.99213800	1.00447100
P	2.23673500	-0.02887500	-1.46760300
P	-0.43478700	2.15663800	0.18843800
C	2.20450400	1.15010000	-2.89543900
H	1.29250900	1.00048700	-3.47697100
H	2.21463700	2.17745500	-2.52943200
H	3.06978400	1.00383900	-3.54819400
C	2.61459100	-1.61947500	-2.32561300
H	1.77281700	-1.90135100	-2.96183900
H	3.51493000	-1.53662000	-2.94155300
H	2.75301700	-2.38838000	-1.56518000
C	3.84597500	0.38054200	-0.66332800
H	4.16348100	-0.48084400	-0.07554000
H	4.61550000	0.61298900	-1.40461700
H	3.70883700	1.21675200	0.02323800
C	-1.90041100	2.67116800	-0.80796200
H	-1.66029500	2.60404200	-1.87102700
H	-2.73478400	1.99813200	-0.60621700
H	-2.19734700	3.69737200	-0.57347100
C	0.77741600	3.50252800	-0.15235800
H	1.05285200	3.50627400	-1.20782300
H	0.35582500	4.47881200	0.10390300
H	1.66090600	3.31154500	0.45799800
C	-0.93435300	2.56154900	1.91451800
H	-1.25687500	3.60335600	1.99967100
H	-1.74901100	1.90807600	2.22904500
H	-0.06525900	2.39031100	2.55182300
C	2.80150400	-2.02471600	1.85316000

O	2.23402600	-2.46509300	0.79531800
O	2.51890600	-1.00737300	2.49638600
H	3.64248900	-2.65811400	2.20912400
H	-0.07157700	-2.44088400	1.78732800
H	-1.37224900	-0.62052600	2.02689300
H	0.95748600	-1.86456500	0.57983800
C	-2.66963200	-0.82697800	0.33576400
C	-3.77492500	-0.43044700	1.10919400
C	-2.88354000	-1.02859700	-1.04036400
C	-5.03453600	-0.25210400	0.54314200
H	-3.64134900	-0.27201600	2.17459500
C	-4.14120400	-0.85250200	-1.60652000
H	-2.04934300	-1.29699200	-1.67529300
C	-5.22603600	-0.46488000	-0.81976600
H	-5.86704900	0.04962100	1.16946500
H	-4.27496900	-1.01318700	-2.67089800
H	-6.20519600	-0.32900700	-1.26461700
C	-0.73575800	-3.30221100	-0.09041000
H	-1.62257300	-3.84119200	0.26058500
H	-0.90835200	-3.02330100	-1.12909200
H	0.11107100	-3.99067400	-0.07042900
O	2.36568800	1.73700100	2.17746600
H	2.30146100	0.75942400	2.20939700
H	2.99819500	1.94366300	2.87202700

M6_{ph}w-f

Zero-point correction= 0.450746 (Hartree/Particle)

Thermal correction to Energy=	0.484240
Thermal correction to Enthalpy=	0.485184
Thermal correction to Gibbs Free Energy=	0.384067
Sum of electronic and zero-point Energies=	-1664.045487
Sum of electronic and thermal Energies=	-1664.011992
Sum of electronic and thermal Enthalpies=	-1664.011048
Sum of electronic and thermal Free Energies=	-1664.112165

Pd	-0.35370000	0.00770000	-0.24920000
C	1.76460000	-1.08350000	-2.15730000
C	1.59070000	0.03740000	-1.13200000
P	-2.30280000	-0.50030000	1.21530000
P	-0.45640000	2.31100000	-0.26190000
C	-3.13840000	0.69150000	2.36330000
H	-2.39960000	1.15650000	3.01910000
H	-3.64770000	1.47620000	1.80090000
H	-3.87790000	0.17740000	2.98360000
C	-1.76920000	-1.81500000	2.39260000

H	-1.05250000	-1.38860000	3.09790000
H	-2.62030000	-2.22120000	2.94690000
H	-1.26160000	-2.60830000	1.84210000
C	-3.74130000	-1.25120000	0.34390000
H	-3.38690000	-2.10430000	-0.23330000
H	-4.51190000	-1.57480000	1.04890000
H	-4.16110000	-0.53000000	-0.35910000
C	-0.19620000	3.21740000	1.32200000
H	-0.88810000	2.84440000	2.07760000
H	0.82130000	3.03390000	1.67250000
H	-0.34850000	4.29290000	1.19620000
C	-2.14740000	2.80870000	-0.80180000
H	-2.86960000	2.56970000	-0.02110000
H	-2.19810000	3.87970000	-1.01560000
H	-2.40760000	2.22810000	-1.68920000
C	0.58990000	3.28960000	-1.42460000
H	0.29840000	4.34260000	-1.39060000
H	1.64330000	3.20860000	-1.15790000
H	0.45810000	2.91510000	-2.44090000
C	-0.58230000	-3.12410000	-0.83020000
O	0.12220000	-3.48000000	0.10750000
O	-0.91660000	-1.92290000	-1.15290000
H	-1.01540000	-3.88680000	-1.51290000
H	0.94170000	-1.05270000	-2.87620000
H	1.76120000	0.99110000	-1.63010000
H	1.70860000	-2.05710000	-1.66950000
C	2.43180000	-0.05240000	0.09850000
C	3.23820000	1.02870000	0.50140000
C	2.44400000	-1.21010000	0.90300000
C	4.01630000	0.96740000	1.65360000
H	3.27740000	1.92000000	-0.11740000
C	3.22210000	-1.26740000	2.05560000
H	1.82160000	-2.05770000	0.63590000
C	4.00980000	-0.18300000	2.44090000
H	4.63820000	1.81260000	1.93000000
H	3.21110000	-2.17000000	2.65730000
H	4.61700000	-0.23610000	3.33770000
C	3.10280000	-0.96800000	-2.90830000
H	3.17640000	-0.01760000	-3.44770000
H	3.95030000	-1.02770000	-2.22030000
H	3.20690000	-1.77470000	-3.64030000
O	-2.47510000	-0.22320000	-2.78300000
H	-1.98780000	-0.91360000	-2.29340000
H	-2.09330000	-0.24990000	-3.66500000

M6_{ph}W-1

Zero-point correction=			0.451058 (Hartree/Particle)
Thermal correction to Energy=			0.482783
Thermal correction to Enthalpy=			0.483727
Thermal correction to Gibbs Free Energy=			0.388004
Sum of electronic and zero-point Energies=			-1664.047275
Sum of electronic and thermal Energies=			-1664.015550
Sum of electronic and thermal Enthalpies=			-1664.014606
Sum of electronic and thermal Free Energies=			-1664.110329
Pd	-0.34912200	0.13706300	-0.12280800
C	1.36192500	-0.23715500	1.05471300
C	2.58694500	-0.26833900	0.17503800
C	3.71149300	0.50863400	0.49981800
C	2.68335400	-1.08639300	-0.96190100
C	4.87185500	0.47618900	-0.27167900
H	3.68092500	1.13761000	1.38309500
C	3.83945200	-1.12400300	-1.73557500
H	1.83074900	-1.68423500	-1.25400000
C	4.94178000	-0.34097600	-1.39652000
H	5.72261500	1.08690600	0.01129700
H	3.87786900	-1.76274800	-2.61162600
H	5.84124300	-0.36795800	-2.00108600
C	1.23136800	-1.44068700	2.00134800
P	-0.02803500	2.49631300	0.03923000
P	-1.15767000	-2.16659400	-0.32827500
C	-0.10826300	3.27820800	-1.62104500
H	0.76386900	2.97917700	-2.20569800
H	-1.00618400	2.91216400	-2.11709200
H	-0.13518600	4.36810200	-1.54101700
C	1.46670800	3.27460600	0.78256100
H	2.36200900	2.95998400	0.24588500
H	1.37981100	4.36296000	0.73088300
H	1.56754500	2.98257400	1.82918600
C	-1.39587200	3.28028300	0.98495900
H	-1.28961200	3.01709600	2.03974200
H	-1.35718200	4.36873800	0.88346000
H	-2.36184600	2.90508100	0.64080800
C	-2.48623200	-2.30613100	-1.59758200
H	-3.32856000	-1.69760400	-1.25993800
H	-2.12490400	-1.97538800	-2.57450800
H	-2.80999900	-3.34690000	-1.68334600
C	-2.02415700	-2.81045200	1.16096600
H	-2.87153400	-2.14898000	1.35367100

H	-2.39431800	-3.82192300	0.97161300
H	-1.35762600	-2.82882900	2.02248500
C	-0.06045100	-3.57063100	-0.83174200
H	-0.64166200	-4.49600300	-0.86323000
H	0.34519500	-3.38188000	-1.82780600
H	0.77183800	-3.70216000	-0.14122900
C	-4.57696600	0.50492600	0.59212200
O	-4.37342900	-0.70570700	0.45044300
O	-3.96884800	1.46816000	0.01072400
H	-5.37299800	0.83398100	1.29432200
H	1.43544400	0.64250000	1.69882500
H	0.27524200	-1.36644100	2.52685600
H	1.21259700	-2.37543700	1.43609800
C	2.35836800	-1.52270600	3.04502000
H	2.39005200	-0.61912800	3.66211000
H	2.20393600	-2.37471100	3.71373500
H	3.33644900	-1.63843800	2.57223100
O	-2.06046100	0.83953900	-1.38676800
H	-2.94251300	1.06971200	-0.78107800
H	-2.34401800	0.20333400	-2.04798400

TS5_{ph}W-a

Zero-point correction=			0.450543 (Hartree/Particle)
Thermal correction to Energy=			0.481591
Thermal correction to Enthalpy=			0.482536
Thermal correction to Gibbs Free Energy=			0.387986
Sum of electronic and zero-point Energies=			-1664.042487
Sum of electronic and thermal Energies=			-1664.011439
Sum of electronic and thermal Enthalpies=			-1664.010495
Sum of electronic and thermal Free Energies=			-1664.105044
Pd	-0.29028000	0.11656500	-0.10860900
C	1.41225700	-0.32881600	1.06060400
C	2.61497400	-0.38575800	0.14830800
C	3.77313400	0.34075100	0.47216200
C	2.66449700	-1.18528800	-1.00452300
C	4.92139900	0.27731800	-0.31551500
H	3.77828200	0.95483000	1.36670100
C	3.80803200	-1.25248400	-1.79507700
H	1.78599600	-1.74685500	-1.29265100
C	4.94450300	-0.51971500	-1.45659900
H	5.79890600	0.84939700	-0.03335500
H	3.81001800	-1.87559500	-2.68312700
H	5.83432100	-0.57006500	-2.07377700
C	1.32771000	-1.52871200	2.04555400

P	0.10886500	2.46779200	0.05016800
P	-1.19953400	-2.12959700	-0.26719600
C	0.12702800	3.24896500	-1.61218000
H	1.01550800	2.92278900	-2.15620100
H	-0.75813000	2.90894100	-2.14817500
H	0.12857100	4.33939200	-1.53498600
C	1.59313000	3.19600200	0.86178100
H	2.49951100	2.85257200	0.36258200
H	1.54655000	4.28688200	0.81181100
H	1.63791300	2.89659000	1.91033700
C	-1.27582400	3.29361900	0.93373700
H	-1.23167500	3.01895100	1.98993100
H	-1.19486100	4.38067800	0.84413100
H	-2.23613700	2.95680400	0.53852500
C	-2.40031200	-2.32247700	-1.65094700
H	-3.25193100	-1.66892900	-1.44580300
H	-1.93237000	-2.07046800	-2.60568600
H	-2.75266500	-3.35636000	-1.69848900
C	-2.24399100	-2.57891000	1.18059700
H	-3.10576400	-1.90733200	1.17998100
H	-2.59260100	-3.61157700	1.09030800
H	-1.69074600	-2.46878900	2.11356500
C	-0.12025500	-3.61180100	-0.51143000
H	-0.72635200	-4.52044000	-0.46598100
H	0.35643000	-3.56173800	-1.49219500
H	0.65885700	-3.66526500	0.24770300
C	-4.63827000	0.65708000	0.26107800
O	-4.51088200	-0.55739500	0.07405100
O	-3.89216400	1.59421400	-0.18867700
H	-5.48530900	1.01766800	0.88295400
H	1.52315000	0.56087100	1.68149500
H	0.42590400	-2.12038400	1.89628700
H	2.16666600	-2.20819900	1.85731000
C	1.36286500	-1.08638000	3.51383300
H	0.52506100	-0.41981400	3.74138700
H	1.29922600	-1.94467100	4.18930200
H	2.28883700	-0.55085800	3.74397800
O	-1.92251800	0.86597900	-1.43066100
H	-2.84024000	1.14728400	-0.88722000
H	-2.18873600	0.23602000	-2.10520100

M6_{ph}'w-a

Zero-point correction=

0.450381 (Hartree/Particle)

Thermal correction to Energy=

0.482257

Thermal correction to Enthalpy=			0.483202
Thermal correction to Gibbs Free Energy=			0.386505
Sum of electronic and zero-point Energies=			-1664.051248
Sum of electronic and thermal Energies=			-1664.019372
Sum of electronic and thermal Enthalpies=			-1664.018428
Sum of electronic and thermal Free Energies=			-1664.115124
Pd	-0.30967000	0.17235900	-0.16539400
C	1.35445600	0.53801400	1.10282700
C	2.63821500	0.35095100	0.33754400
C	3.70610900	-0.42407100	0.81597200
C	2.83255300	1.01656100	-0.88779200
C	4.90103400	-0.53706500	0.10428100
H	3.61778300	-0.93929700	1.76446600
C	4.02085200	0.90767300	-1.59897100
H	2.02341300	1.61559600	-1.29165300
C	5.06652300	0.12435900	-1.10748500
H	5.70623500	-1.14278700	0.50646500
H	4.13301300	1.43354200	-2.54115900
H	5.99468200	0.03662500	-1.66064100
C	1.26422000	-0.16991800	2.45387000
P	-1.02490000	2.46157900	-0.09059900
P	-0.00123600	-2.21702700	-0.26101900
C	-1.35853700	3.12222800	-1.77310600
H	-0.41913700	3.22617000	-2.31982200
H	-1.98629300	2.40006600	-2.29379500
H	-1.85662600	4.09400500	-1.72373100
C	-0.00616300	3.79389000	0.67844000
H	0.97140700	3.85152200	0.19592900
H	-0.50879900	4.75911600	0.57728600
H	0.14651900	3.59031100	1.73966800
C	-2.63480500	2.62204300	0.78235400
H	-2.47934900	2.43506000	1.84687300
H	-3.04761100	3.62633200	0.65154500
H	-3.33882000	1.87506500	0.40916300
C	-0.90008000	-2.96325400	-1.68516200
H	-1.96876300	-2.80417500	-1.52170000
H	-0.57439900	-2.51202500	-2.62536500
H	-0.70488100	-4.03804800	-1.72896500
C	-0.71852800	-3.15055000	1.15219600
H	-1.79739900	-2.98011200	1.14641800
H	-0.52105000	-4.22008500	1.03658400
H	-0.29396100	-2.80925000	2.09657500
C	1.68679500	-2.92810400	-0.44816100
H	1.62153200	-4.01099500	-0.58328900

H	2.18371100	-2.48372900	-1.31179800
H	2.29350500	-2.71269400	0.42996600
C	-4.31296000	-1.33624400	0.19077700
O	-3.63358900	-2.34915200	-0.00655000
O	-4.10494600	-0.16109100	-0.27102200
H	-5.21505600	-1.41251600	0.83490800
H	1.25396500	1.60737700	1.29176600
H	1.35776300	-1.25430500	2.33293700
H	2.12644200	0.13245300	3.06695300
C	-0.01231700	0.14462700	3.23969500
H	-0.90544400	-0.17610500	2.69759300
H	-0.00695300	-0.35273600	4.21374700
H	-0.10327200	1.22019700	3.42346900
O	-2.04446900	0.06477000	-1.56448400
H	-2.97891600	-0.08481100	-1.00392800
H	-1.98655800	-0.66962200	-2.18129900

M6_{ph}'w-g

Zero-point correction=			0.452171 (Hartree/Particle)
Thermal correction to Energy=			0.484822
Thermal correction to Enthalpy=			0.485766
Thermal correction to Gibbs Free Energy=			0.388701
Sum of electronic and zero-point Energies=			-1664.058929
Sum of electronic and thermal Energies=			-1664.026278
Sum of electronic and thermal Enthalpies=			-1664.025333
Sum of electronic and thermal Free Energies=			-1664.122398
Pd	0.48418000	-0.02455900	-0.19666400
C	-0.94015100	-0.97530900	1.06889400
C	-2.29103300	-1.01185000	0.41571800
C	-3.43148300	-0.40669800	0.96777500
C	-2.46503400	-1.71899100	-0.78999000
C	-4.67529100	-0.48664700	0.33854700
H	-3.35940500	0.11769300	1.91229700
C	-3.70078000	-1.80410100	-1.41678000
H	-1.60186000	-2.19449800	-1.24446600
C	-4.81928000	-1.18117700	-0.85760200
H	-5.53570000	-0.00896200	0.79548200
H	-3.79554200	-2.35662600	-2.34559900
H	-5.78538800	-1.24446200	-1.34523600
C	-0.89399100	-0.43515400	2.49928300
P	1.90742800	-1.94088400	-0.22658200
P	-0.75624400	2.02512800	-0.44063100
C	2.42188600	-2.33753200	-1.94856500
H	1.55855400	-2.70967700	-2.50388200

H	2.76117700	-1.41913700	-2.42623900
H	3.21353400	-3.09137500	-1.96578700
C	1.37543000	-3.58946900	0.41084600
H	0.47726300	-3.92458100	-0.11148800
H	2.16792700	-4.32708000	0.26039100
H	1.14909100	-3.52957500	1.47648600
C	3.49142700	-1.66485800	0.66818000
H	3.28528900	-1.62323300	1.73921400
H	4.20449900	-2.46928300	0.46754700
H	3.91155900	-0.70241700	0.37600700
C	0.28741800	3.40053900	-1.07445400
H	1.04389400	3.63145700	-0.32454000
H	0.77767800	3.08822800	-1.99536600
H	-0.32824300	4.28457500	-1.26160900
C	-1.57867800	2.82590600	0.99605500
H	-0.81915500	2.98445100	1.76264400
H	-2.00605000	3.78675000	0.69633600
H	-2.37385600	2.19269000	1.38693500
C	-2.08484500	1.91650800	-1.71297700
H	-2.56421500	2.88873400	-1.85797600
H	-1.64402100	1.59169400	-2.65733500
H	-2.83375700	1.18462500	-1.41222700
C	3.02185500	1.40886100	-1.22027300
O	3.36265200	1.66612500	-0.05760000
O	1.97490100	0.80306700	-1.62146600
H	3.69607000	1.72354700	-2.04466100
H	-0.57603800	-2.00289500	1.08703200
H	-1.20640000	0.61077800	2.53114600
H	-1.63219100	-0.99098800	3.09838400
C	0.47285700	-0.54741200	3.18174900
H	1.19933500	0.12097800	2.71599200
H	0.39701300	-0.26925400	4.23725200
H	0.85432100	-1.57387000	3.14438800
O	1.67922800	2.59670200	1.92256400
H	2.29642000	3.04480100	2.50791100
H	2.25204900	2.17010300	1.24926500

M6w-E₁

Zero-point correction=	0.450615 (Hartree/Particle)
Thermal correction to Energy=	0.482736
Thermal correction to Enthalpy=	0.483680
Thermal correction to Gibbs Free Energy=	0.385646
Sum of electronic and zero-point Energies=	-1664.046895
Sum of electronic and thermal Energies=	-1664.014775

Sum of electronic and thermal Enthalpies=			-1664.013831
Sum of electronic and thermal Free Energies=			-1664.111864
Pd	-0.55052100	0.12740200	0.05548700
C	1.54973500	0.78290000	-1.98412300
C	1.22026700	1.19972300	-0.54919200
P	-2.28603300	-1.46952700	0.84731500
P	-1.88867500	1.91833100	-0.52118100
C	-4.06040800	-1.08818900	1.23483200
H	-4.11678600	-0.34274800	2.03096800
H	-4.57388300	-0.69447100	0.35522700
H	-4.58751100	-1.98702500	1.56697900
C	-1.72488700	-2.24626400	2.41706600
H	-1.74577900	-1.50531100	3.21905800
H	-2.35549000	-3.09610400	2.69219700
H	-0.69415500	-2.56304100	2.26202300
C	-2.46070600	-2.89657100	-0.30514500
H	-1.47466700	-3.28316400	-0.56408200
H	-3.06152000	-3.69291100	0.14342900
H	-2.94541900	-2.56104400	-1.22477300
C	-2.90801000	2.61942400	0.84820600
H	-3.52493100	1.83679300	1.28932800
H	-2.24717300	3.00905500	1.62456000
H	-3.55379500	3.42534500	0.48922100
C	-3.15303300	1.47899900	-1.79255400
H	-3.75868400	0.64247400	-1.44357000
H	-3.80670300	2.32723800	-2.01300600
H	-2.64622800	1.16957500	-2.70828600
C	-1.17412900	3.45343800	-1.25444000
H	-1.97493300	4.13639000	-1.54895500
H	-0.53120300	3.95583500	-0.53043200
H	-0.57426900	3.20767300	-2.13180200
C	1.86311100	-3.33027400	-2.01406000
O	0.80095200	-3.33416000	-1.25093600
O	2.78174800	-2.53427100	-1.99423300
H	1.84638800	-4.17512400	-2.72732800
H	0.94924500	2.25444100	-0.52493300
H	1.81836100	-0.27387700	-2.02542700
H	0.64885700	0.88514600	-2.60040700
C	2.26953500	0.98138300	0.48729800
C	2.30926900	1.81663300	1.62073200
C	3.24947600	-0.02671400	0.39078900
C	3.26915600	1.65737400	2.61138000
H	1.56848000	2.60513000	1.71652800
C	4.21434700	-0.18253100	1.38678900

H	3.26421800	-0.69291900	-0.46457400
C	4.23100100	0.65169300	2.50098100
H	3.27268700	2.32047300	3.47023600
H	4.95852300	-0.96493300	1.28317500
H	4.98403800	0.52607700	3.27085700
C	2.67459900	1.62176600	-2.61885200
H	2.85995800	1.30309900	-3.64882300
H	2.41708400	2.68657200	-2.63692000
H	3.60973200	1.51714800	-2.06443000
O	0.59929400	-1.59139200	0.47511300
H	1.46091300	-1.31332500	0.80505700
H	0.78736900	-2.53315400	-0.52327800

TS5w-E₁

Zero-point correction=			0.444220 (Hartree/Particle)
Thermal correction to Energy=			0.477462
Thermal correction to Enthalpy=			0.478406
Thermal correction to Gibbs Free Energy=			0.376600
Sum of electronic and zero-point Energies=			-1664.019701
Sum of electronic and thermal Energies=			-1663.986459
Sum of electronic and thermal Enthalpies=			-1663.985515
Sum of electronic and thermal Free Energies=			-1664.087321
Pd	-0.77865900	-0.17401400	-0.40789200
C	1.34756000	-0.56019200	-1.38885500
C	0.98519000	0.83307600	-1.18918700
P	-1.78622900	-2.16115400	0.57506600
P	-2.24001200	1.64773900	-0.31967700
C	-3.56037100	-2.56819300	0.23803900
H	-4.20364300	-1.75103800	0.56858900
H	-3.70494300	-2.70020400	-0.83630100
H	-3.86183100	-3.48635000	0.75037200
C	-1.72003600	-2.15618500	2.41891300
H	-2.27717900	-1.30473500	2.81425900
H	-2.12632900	-3.08010800	2.84057800
H	-0.67268700	-2.05529700	2.70570800
C	-0.94871800	-3.75694900	0.18240600
H	0.07448000	-3.69301600	0.55933300
H	-1.46363000	-4.60101900	0.65148500
H	-0.92447000	-3.90922800	-0.89834200
C	-1.97583000	2.73478200	1.14659200
H	-2.13419800	2.15617600	2.05834800
H	-0.94516700	3.09280600	1.14816400
H	-2.65840600	3.58953800	1.13945500
C	-4.05234700	1.29771000	-0.21309200

H	-4.26099800	0.72316800	0.69097600
H	-4.63482600	2.22316200	-0.18561400
H	-4.36455700	0.70524500	-1.07492200
C	-2.19712100	2.85782600	-1.71597500
H	-2.91252300	3.67110400	-1.56274400
H	-1.19439800	3.27812800	-1.79982400
H	-2.43252000	2.34546000	-2.65059200
C	4.49150800	-1.77190600	-0.69018600
O	3.94503900	-2.55682900	0.10012200
O	3.98009800	-0.79346500	-1.32072400
H	5.57296700	-1.92045200	-0.89680600
H	0.78819100	1.39756700	-2.09940800
H	2.58831100	-0.67086900	-1.22131100
H	1.12396800	-1.21669300	-0.51087400
C	1.53600900	1.65960000	-0.09654400
C	1.60801300	3.05438100	-0.25708200
C	2.00914400	1.10557400	1.10865500
C	2.11622300	3.87266400	0.74689900
H	1.28119400	3.49630800	-1.19351900
C	2.51383800	1.92784800	2.10981300
H	1.98276800	0.03254000	1.26395600
C	2.56793400	3.31177600	1.93998300
H	2.17147800	4.94493400	0.59318600
H	2.87842200	1.48320200	3.02947500
H	2.96991400	3.94401700	2.72365600
C	1.05942700	-1.18616000	-2.75590400
H	1.15901300	-2.27252100	-2.70500700
H	0.06158400	-0.95668900	-3.14182500
H	1.79350500	-0.83035100	-3.48491500
O	1.72872100	-2.38718800	1.56461700
H	2.10996800	-2.51427800	2.43837200
H	2.51506300	-2.44870000	0.95931700

M7w'-E₁

Zero-point correction=			0.448810 (Hartree/Particle)
Thermal correction to Energy=			0.483504
Thermal correction to Enthalpy=			0.484448
Thermal correction to Gibbs Free Energy=			0.377353
Sum of electronic and zero-point Energies=			-1664.050359
Sum of electronic and thermal Energies=			-1664.015664
Sum of electronic and thermal Enthalpies=			-1664.014720
Sum of electronic and thermal Free Energies=			-1664.121815
Pd	-0.93639900	-0.13757600	-0.44739800
C	1.00319900	-0.89727100	-1.16324800

C	1.07910400	0.51041200	-1.18839000
P	-2.00196500	-2.06897400	0.45370400
P	-2.27430000	1.82827500	-0.20444000
C	-3.65154400	-2.58125100	-0.22223100
H	-4.36017400	-1.75678900	-0.12185300
H	-3.55079700	-2.80953400	-1.28539000
H	-4.04925400	-3.46084400	0.29354700
C	-2.38543300	-1.94812200	2.26306000
H	-3.04736800	-1.09920900	2.44459200
H	-2.85937400	-2.85953200	2.64047200
H	-1.45668500	-1.77759100	2.81041600
C	-1.09082000	-3.67866700	0.41565400
H	-0.11978600	-3.55073000	0.89957700
H	-1.65154100	-4.47251200	0.91947400
H	-0.91968800	-3.97447600	-0.62173700
C	-1.82988600	2.87308200	1.25769700
H	-1.98802200	2.30008200	2.17347600
H	-0.77044700	3.13004900	1.20275800
H	-2.42467000	3.79070600	1.30208200
C	-4.11542000	1.70766200	-0.00190300
H	-4.34491800	1.10349500	0.87843500
H	-4.58268800	2.69086100	0.11156900
H	-4.54442600	1.20985500	-0.87427100
C	-2.17971000	3.07991800	-1.56939400
H	-2.78924600	3.96458900	-1.35985600
H	-1.14016500	3.38582600	-1.69934000
H	-2.51839900	2.62621000	-2.50309000
C	4.85307700	-1.48723200	-0.69045200
O	4.37644300	-2.06181400	0.25739900
O	4.21958300	-0.67393900	-1.52642800
H	5.90782400	-1.57590900	-0.98396300
H	0.96187600	0.99531900	-2.15508900
H	3.28119500	-0.56900600	-1.26518900
H	1.41666700	-1.43770300	-0.31648500
C	1.69107000	1.36930500	-0.15269200
C	1.93697600	2.72462700	-0.43958500
C	2.06973200	0.89761200	1.11996100
C	2.51540300	3.57455300	0.49793200
H	1.67253300	3.11002400	-1.41965800
C	2.65003600	1.74927700	2.05380000
H	1.90534500	-0.14190600	1.37861900
C	2.87470500	3.09363400	1.75572700
H	2.69255900	4.61403500	0.24231800
H	2.93172300	1.35960100	3.02675800

H	3.32752600	3.75178200	2.48843800
C	0.88367900	-1.69779500	-2.44531000
H	0.34763600	-2.63571900	-2.28529500
H	0.35165300	-1.13642200	-3.21730300
H	1.87096300	-1.95969700	-2.85129200
O	2.00531600	-2.72134400	1.78392000
H	2.22416100	-2.39624600	2.66196400
H	2.80858900	-2.56131400	1.26378500

M6_{ph}w-m

Zero-point correction=			0.452168 (Hartree/Particle)
Thermal correction to Energy=			0.484899
Thermal correction to Enthalpy=			0.485843
Thermal correction to Gibbs Free Energy=			0.387961
Sum of electronic and zero-point Energies=			-1664.049623
Sum of electronic and thermal Energies=			-1664.016892
Sum of electronic and thermal Enthalpies=			-1664.015947
Sum of electronic and thermal Free Energies=			-1664.113830
Pd	0.38554500	0.06040200	-0.31426100
C	-1.58730700	0.49287400	-1.06451100
C	-2.52096200	0.07021000	0.01942100
C	-3.01595900	1.02007800	0.93439700
C	-2.95788300	-1.25795600	0.17960000
C	-3.87956700	0.66758100	1.96541000
H	-2.72718100	2.06082200	0.82162500
C	-3.82443300	-1.61347200	1.21041600
H	-2.58639500	-2.01928300	-0.49175200
C	-4.28829600	-0.65749600	2.11356800
H	-4.24366400	1.42838200	2.64785500
H	-4.13886300	-2.64713300	1.30814400
H	-4.96497400	-0.93812000	2.91266700
C	-1.75872600	-0.15285200	-2.44098200
P	0.75915200	2.31354800	0.02719900
P	2.59012000	-0.73195500	0.57964100
C	0.54669500	2.82838400	1.78436700
H	-0.47443900	2.60571300	2.09790500
H	1.22226400	2.25695700	2.42095600
H	0.74292200	3.89638600	1.91203200
C	-0.23517000	3.59348300	-0.86035600
H	-1.27875700	3.56477900	-0.54857000
H	0.16746600	4.58629100	-0.64429000
H	-0.19294100	3.41737400	-1.93652700
C	2.45710900	2.91260300	-0.38165000
H	2.64756600	2.75437400	-1.44465500

H	2.55295400	3.97777100	-0.15572000
H	3.20864600	2.36449000	0.18417300
C	4.00668500	-0.58899100	-0.59333400
H	3.72722400	-1.13516200	-1.49503900
H	4.18815100	0.45341300	-0.85943200
H	4.92046200	-1.01304000	-0.16766000
C	2.66436600	-2.50992300	1.05525700
H	2.54721900	-3.12076600	0.16195100
H	3.63273900	-2.72992800	1.51354900
H	1.86210800	-2.73062400	1.75936400
C	3.24572700	0.03744300	2.13452700
H	4.19648400	-0.41866800	2.42381900
H	3.40082100	1.11146500	2.01998700
H	2.52196000	-0.12519100	2.93592200
O	-0.11207600	-2.01314400	-0.68180400
H	-1.67123700	1.57028400	-1.18776800
H	-0.91449700	0.13429400	-3.07568000
H	-1.71644600	-1.23870200	-2.36289000
C	-3.06913500	0.26695800	-3.13061200
H	-3.11826600	1.35274900	-3.26497400
H	-3.15248800	-0.19380100	-4.11958300
H	-3.94163600	-0.03381600	-2.54476300
O	1.59628500	-2.27805400	-2.13314500
C	0.59501800	-2.66516000	-1.54466700
H	0.20565200	-3.68920700	-1.72298100
H	-0.38210100	-2.33020300	1.15561800
O	-0.38873800	-2.26631300	2.12697400
H	-1.24765300	-1.87677000	2.31879300

M6_{ph}w-al-a

Zero-point correction=			0.451983 (Hartree/Particle)
Thermal correction to Energy=			0.484673
Thermal correction to Enthalpy=			0.485618
Thermal correction to Gibbs Free Energy=			0.387458
Sum of electronic and zero-point Energies=			-1664.043086
Sum of electronic and thermal Energies=			-1664.010395
Sum of electronic and thermal Enthalpies=			-1664.009451
Sum of electronic and thermal Free Energies=			-1664.107611
Pd	-0.29314500	-0.19180100	0.13623100
C	1.57166200	-0.68451900	1.09458500
P	-0.89131200	-2.41870000	-0.00165900
P	-2.42030300	0.76591400	-0.84046900
C	-2.54198500	-2.79764200	0.73271200
H	-2.50492000	-2.60553300	1.80653200

H	-3.31009700	-2.15675700	0.30139900
H	-2.81497000	-3.84309000	0.56627700
C	0.12660100	-3.75213100	0.76794700
H	0.23072900	-3.57422200	1.83901400
H	-0.35640200	-4.72033000	0.61323800
H	1.12306000	-3.78132300	0.32625800
C	-1.03676300	-3.03438700	-1.73406800
H	-0.06505900	-2.95048600	-2.22395700
H	-1.36177100	-4.07800500	-1.75639500
H	-1.74815100	-2.42516400	-2.29034800
C	-3.47214900	-0.14706300	-2.06624800
H	-2.89659000	-0.33743000	-2.97488900
H	-3.81076500	-1.10388300	-1.66505600
H	-4.35238100	0.44492600	-2.33106500
C	-2.20792700	2.38260800	-1.69675600
H	-1.49239200	2.29270500	-2.51572700
H	-3.16618600	2.73025300	-2.09225600
H	-1.83121700	3.10854400	-0.97736900
C	-3.62572700	1.19993000	0.48531300
H	-4.56352600	1.56269000	0.05471500
H	-3.83243900	0.33368500	1.11633400
H	-3.18447000	1.99461800	1.09312700
C	0.74627500	2.67744000	-0.38737800
O	0.70521900	3.89470800	-0.30609700
O	0.19285800	1.86073800	0.46328700
H	1.27715200	2.18722100	-1.22679200
H	1.58524700	-1.76285100	1.23809100
C	1.60099700	0.00538900	2.45578700
H	2.61511100	-0.10099800	2.87011300
H	1.42176800	1.07550900	2.33986500
C	2.64190700	-0.32010400	0.12244600
C	3.37151700	0.87808400	0.20509200
C	2.98589100	-1.21057500	-0.91346800
C	4.38492700	1.17094100	-0.70489600
H	3.14820200	1.58916100	0.98947600
C	3.99317600	-0.91950600	-1.82422700
H	2.45228900	-2.15247500	-0.99843500
C	4.70050000	0.27949600	-1.72647600
H	4.92817300	2.10509700	-0.61313100
H	4.23394700	-1.63024800	-2.60781400
H	5.48894800	0.51063800	-2.43366300
C	0.59846300	-0.56689300	3.46257200
H	-0.43030500	-0.42318600	3.11991500
H	0.75729700	-1.63958900	3.62224800

H	0.69583000	-0.07378200	4.43334100
O	-1.63701000	3.59284000	1.64519500
H	-0.96347700	2.91673200	1.43905700
H	-1.22643500	4.36951100	1.24648500

TS6_{ph}W-a

Zero-point correction= 0.445026 (Hartree/Particle)

Thermal correction to Energy= 0.477769

Thermal correction to Enthalpy= 0.478713

Thermal correction to Gibbs Free Energy= 0.381252

Sum of electronic and zero-point Energies= -1664.025934

Sum of electronic and thermal Energies= -1663.993191

Sum of electronic and thermal Enthalpies= -1663.992247

Sum of electronic and thermal Free Energies= -1664.089708

Pd	0.43516400	0.02901800	-0.51782900
C	-1.35041100	-0.76350700	-1.36765300
C	-2.60523800	-0.68332200	-0.58681700
C	-3.72797100	-0.05825300	-1.15341900
C	-2.73097300	-1.22006400	0.70739400
C	-4.93469600	0.02604900	-0.46248000
H	-3.65549900	0.35375000	-2.15554300
C	-3.93719700	-1.13708100	1.39311200
H	-1.86847900	-1.66576700	1.19089100
C	-5.04605100	-0.51546100	0.81550900
H	-5.78806300	0.50931600	-0.92611900
H	-4.01001000	-1.55314900	2.39216800
H	-5.98328300	-0.45348500	1.35705900
C	-0.45571000	-1.90907100	-1.30928600
P	-0.31491900	2.23543300	-0.07173200
P	2.87024100	0.07627100	-0.17334100
C	-1.65170900	2.29894500	1.18988700
H	-2.50321900	1.70106000	0.86621100
H	-1.24839300	1.87541800	2.11117300
H	-1.97257600	3.33095500	1.36004100
C	-1.04128200	3.15979700	-1.49718200
H	-1.88474200	2.59456100	-1.89698200
H	-1.39089600	4.15033600	-1.19271200
H	-0.29617000	3.27050600	-2.28737200
C	0.87844500	3.46009900	0.62157500
H	1.66714300	3.67708900	-0.09993500
H	0.37030700	4.39323300	0.88099800
H	1.31803600	3.02834000	1.52214400
C	3.74887700	-1.20788900	-1.16984200
H	3.37795200	-2.18637000	-0.86422600

H	3.53043900	-1.06544600	-2.23020900
H	4.83109200	-1.15927100	-1.01749300
C	3.54536400	-0.22351600	1.51831800
H	3.38416800	-1.27126300	1.77267900
H	4.61647800	-0.00686800	1.55956600
H	3.00197100	0.38651800	2.24081000
C	3.79221800	1.60390900	-0.67161000
H	4.87235900	1.43342200	-0.65042100
H	3.50091700	1.90259300	-1.68065100
H	3.55446100	2.41881200	0.01291100
O	0.27871600	-1.91660600	2.22684600
H	-1.42532800	-0.27920100	-2.34146600
H	0.61141900	-1.93451500	-0.34496700
H	-0.85741300	-2.71586200	-0.69562900
C	0.15602800	-2.42297200	-2.60853400
H	0.49360100	-1.59977700	-3.24320700
H	1.01344200	-3.06955400	-2.40924200
H	-0.57596200	-3.00753100	-3.17744200
O	1.36646200	-2.82234500	0.46976900
C	1.01971100	-2.75540900	1.69606700
H	1.45032000	-3.55914500	2.33060000
H	0.48753000	-0.13993000	2.66123300
O	0.66143800	0.75091400	3.02621600
H	0.62164900	0.62162300	3.97851200

TS6_{ph}w-al-a

Zero-point correction=			0.449935 (Hartree/Particle)
Thermal correction to Energy=			0.482531
Thermal correction to Enthalpy=			0.483475
Thermal correction to Gibbs Free Energy=			0.385217
Sum of electronic and zero-point Energies=			-1664.015719
Sum of electronic and thermal Energies=			-1663.983123
Sum of electronic and thermal Enthalpies=			-1663.982179
Sum of electronic and thermal Free Energies=			-1664.080437
Pd	-0.30556800	-0.09403100	0.03214800
C	1.50001900	-0.58803000	1.08550200
P	-1.34542400	-1.95371700	0.92422300
P	-2.18496400	0.76292600	-1.40802200
C	-3.04765000	-1.60691100	1.54302800
H	-2.99241700	-0.88790500	2.36193300
H	-3.65874200	-1.17507700	0.75125000
H	-3.52465000	-2.52359100	1.90021400
C	-0.64865600	-2.89927600	2.34642100
H	-0.47740000	-2.23041600	3.19041300

H	-1.34957400	-3.68327800	2.64460700
H	0.30003500	-3.36353400	2.07590200
C	-1.60715500	-3.28951700	-0.31901000
H	-0.63788400	-3.63762000	-0.67958400
H	-2.15415400	-4.13074200	0.11568000
H	-2.16271200	-2.90008300	-1.17173600
C	-3.27002200	-0.42124800	-2.33928800
H	-2.65999100	-1.01937400	-3.01993100
H	-3.78504200	-1.09877900	-1.65520400
H	-4.02407600	0.11229800	-2.92439500
C	-1.67073300	1.88825900	-2.77699900
H	-0.95459800	1.38423500	-3.42819000
H	-2.53887200	2.19549200	-3.36659300
H	-1.19651900	2.76825700	-2.34579500
C	-3.41122600	1.78941400	-0.49485200
H	-4.15681600	2.21302100	-1.17323700
H	-3.91991200	1.19210000	0.26395100
H	-2.85442300	2.58476900	-0.00024000
C	0.63408500	2.52049300	-0.33158900
O	1.69254000	3.14623100	-0.25620600
O	-0.48189800	2.70030200	0.21772400
H	0.67703100	1.58290400	-1.00991100
H	1.35949900	-1.52024100	1.62609100
C	1.83062400	0.53230500	2.06486100
H	2.84952700	0.33892300	2.43495200
H	1.87916200	1.50543400	1.57947200
C	2.39300800	-0.81926500	-0.07725300
C	3.11963900	0.21437400	-0.70109100
C	2.54943400	-2.12690900	-0.58363200
C	3.95566400	-0.05802100	-1.78002000
H	3.01963400	1.23649300	-0.35650000
C	3.38492600	-2.39473900	-1.65917400
H	2.01704900	-2.94414200	-0.10600100
C	4.09385700	-1.35664800	-2.26588700
H	4.50424900	0.75539100	-2.24171400
H	3.49355400	-3.41187000	-2.02001800
H	4.75103400	-1.56115700	-3.10364100
C	0.88108000	0.63443000	3.26126200
H	-0.14762400	0.79832900	2.92853500
H	0.90870600	-0.26856000	3.88221200
H	1.15478500	1.49103700	3.87850800
O	0.96832500	3.97397800	2.44369200
H	0.16881900	3.67847100	1.98343900
H	1.57117200	4.03016100	1.68834000

M7_{ph}w-al-a

Zero-point correction=			0.450509 (Hartree/Particle)
Thermal correction to Energy=			0.483283
Thermal correction to Enthalpy=			0.484228
Thermal correction to Gibbs Free Energy=			0.386090
Sum of electronic and zero-point Energies=			-1664.028930
Sum of electronic and thermal Energies=			-1663.996155
Sum of electronic and thermal Enthalpies=			-1663.995211
Sum of electronic and thermal Free Energies=			-1664.093348
Pd	0.07120000	-0.18630000	-0.18520000
C	0.71290000	-2.05290000	0.66820000
P	-1.78610000	-1.07780000	-1.31580000
P	0.01920000	2.16910000	-0.85160000
C	-3.10150000	0.12060000	-1.77740000
H	-3.50540000	0.53060000	-0.84890000
H	-2.69210000	0.92170000	-2.39400000
H	-3.89480000	-0.38430000	-2.33640000
C	-2.78300000	-2.40920000	-0.53560000
H	-3.22340000	-1.99590000	0.37180000
H	-3.57370000	-2.73610000	-1.21710000
H	-2.15540000	-3.26170000	-0.27790000
C	-1.29730000	-1.82050000	-2.93500000
H	-0.60690000	-2.64840000	-2.76440000
H	-2.17020000	-2.19070000	-3.48070000
H	-0.78430000	-1.07270000	-3.54190000
C	0.21620000	2.59170000	-2.64040000
H	1.14320000	2.15470000	-3.01680000
H	-0.61410000	2.18070000	-3.21810000
H	0.24590000	3.67450000	-2.78990000
C	1.38640000	3.12140000	-0.06530000
H	2.34490000	2.75700000	-0.43730000
H	1.29330000	4.18850000	-0.28480000
H	1.34920000	2.96170000	1.01440000
C	-1.46440000	3.13300000	-0.34500000
H	-1.32250000	4.19520000	-0.56250000
H	-2.34860000	2.77360000	-0.87100000
H	-1.62330000	2.99070000	0.72640000
C	-0.40100000	1.25450000	2.57230000
O	0.70990000	1.46080000	3.07450000
O	-1.52410000	1.77370000	2.77480000
H	-0.42290000	0.44690000	1.74890000
H	0.43050000	-2.92200000	0.07380000
C	0.40830000	-2.22330000	2.15050000

H	1.05030000	-3.04790000	2.49770000
H	0.72690000	-1.34310000	2.71070000
C	1.98590000	-1.46510000	0.26630000
C	2.46590000	-0.29610000	0.92030000
C	2.70770000	-1.94540000	-0.86160000
C	3.64710000	0.31970000	0.47260000
H	1.98370000	0.09860000	1.81320000
C	3.87320000	-1.33410000	-1.27240000
H	2.34170000	-2.82690000	-1.37730000
C	4.35240000	-0.19510000	-0.60040000
H	4.01210000	1.19270000	1.00110000
H	4.42700000	-1.73640000	-2.11360000
H	5.27680000	0.27160000	-0.92180000
C	-1.04230000	-2.55070000	2.50990000
H	-1.71360000	-1.72840000	2.25410000
H	-1.38970000	-3.45570000	2.00180000
H	-1.12610000	-2.72810000	3.58530000
O	-3.36690000	0.31110000	1.46090000
H	-2.70320000	0.87940000	1.94200000
H	-4.07830000	0.20310000	2.09880000

TS6_{Me}-al-a

Zero-point correction=			0.424913 (Hartree/Particle)
Thermal correction to Energy=			0.454014
Thermal correction to Enthalpy=			0.454958
Thermal correction to Gibbs Free Energy=			0.364930
Sum of electronic and zero-point Energies=			-1587.571166
Sum of electronic and thermal Energies=			-1587.542065
Sum of electronic and thermal Enthalpies=			-1587.541121
Sum of electronic and thermal Free Energies=			-1587.631150
Pd	-0.57167300	-0.14498200	0.58326100
C	1.07091800	-0.85365500	1.74295100
P	0.18015500	2.00940600	0.82543700
P	-2.55653300	0.28392800	-0.91351700
C	0.50290500	2.82296400	-0.79604300
H	1.30020500	2.28109300	-1.30799400
H	-0.39039400	2.78629300	-1.41976000
H	0.80091200	3.86613000	-0.65876000
C	1.71479700	2.43230000	1.75196400
H	2.57328100	1.94189500	1.29211700
H	1.86502600	3.51485500	1.72887900
H	1.63707700	2.10827900	2.79071400
C	-1.04788300	3.11637100	1.64257500
H	-1.20549600	2.77707500	2.66786500

H	-0.69244400	4.15044500	1.65752000
H	-2.00203200	3.07219100	1.11996000
C	-3.50006700	1.88436500	-0.93642200
H	-3.94993600	2.06434200	0.04263100
H	-2.84133000	2.72259200	-1.17262300
H	-4.29828700	1.85555000	-1.68323900
C	-3.94401200	-0.91546500	-0.71917500
H	-4.34161400	-0.86529200	0.29605200
H	-4.74572400	-0.69765500	-1.43026500
H	-3.55791600	-1.91741400	-0.89781300
C	-2.10128100	0.08997800	-2.68750900
H	-2.97529400	0.19519900	-3.33614200
H	-1.35533900	0.83621900	-2.96802100
H	-1.66590200	-0.90216000	-2.80111400
C	-1.15826500	-2.72131300	0.24548300
O	-0.92613200	-3.80213700	0.76133800
O	-1.02706300	-2.28169900	-0.92760200
H	-1.57616200	-1.91125600	0.99768300
H	1.66121600	-0.00646200	2.08348800
C	1.95793600	-1.74177700	0.85825700
H	2.73872800	-2.15931200	1.51352500
H	1.39217800	-2.59738900	0.48703600
C	0.49609500	-1.58556300	2.95111100
H	-0.06490900	-2.47723300	2.66570600
H	1.31817800	-1.91571800	3.60427300
H	-0.15076400	-0.93771900	3.54953100
C	2.62819400	-1.01541100	-0.28786100
C	2.07570300	-1.04368300	-1.57446400
C	3.80977300	-0.29188000	-0.08674000
C	2.68290000	-0.35373000	-2.62312000
H	1.16784300	-1.61445800	-1.74107200
C	4.41731500	0.40165600	-1.13322700
H	4.27028700	-0.28736300	0.89734500
C	3.85205400	0.37559700	-2.40707900
H	2.24740100	-0.39723000	-3.61591300
H	5.33888300	0.94673800	-0.95796900
H	4.32801700	0.90307000	-3.22654700