

Supporting Information

Mechanistic insights into photocatalytic nitrene transfer reactions of benzoyl azide in the presence of phosphoric acid

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1. Computational methods

Energy barriers of single electron transfer steps, involved in this whole study, by using Marcus-Hush theory¹

Applying the Marcus theory of electron transfer, the free energy barrier of a singlet electron transfer process can be estimated according to the following equation:

$$\Delta G_{MH}^{\ddagger} = \frac{(\Delta G_r + \lambda)^2}{4\lambda} \quad \text{S1}$$

$$\lambda = \lambda_o + \lambda_i \quad \text{S2}$$

ΔG_r is the free energy change of the step, λ is the reorganization energy, which has two components, inner sphere and outer sphere. In addition, the solvent outer-sphere reorganization energy could be λ_o calculated from Equations:

$$\lambda_o = 332 \left(\frac{1}{2a_1} + \frac{1}{2a_2} - \frac{1}{R} \right) \left(\frac{1}{\epsilon_{op}} - \frac{1}{\epsilon} \right) \quad \text{S3}$$

$$R = a_1 + a_2 \quad \text{S4}$$

a_1 and a_2 are the radii of the excited-state photoredox *PC and reactant, respectively. ϵ_{op} and ϵ are the optical dielectric constant and the static dielectric constant of solvent, respectively. The radius of a molecule can be derived by calculating molecular volume via a Monte-Carlo integration as implemented in the Gaussian 09 program. The internal λ_i reorganization energy can be estimated according to the equation:

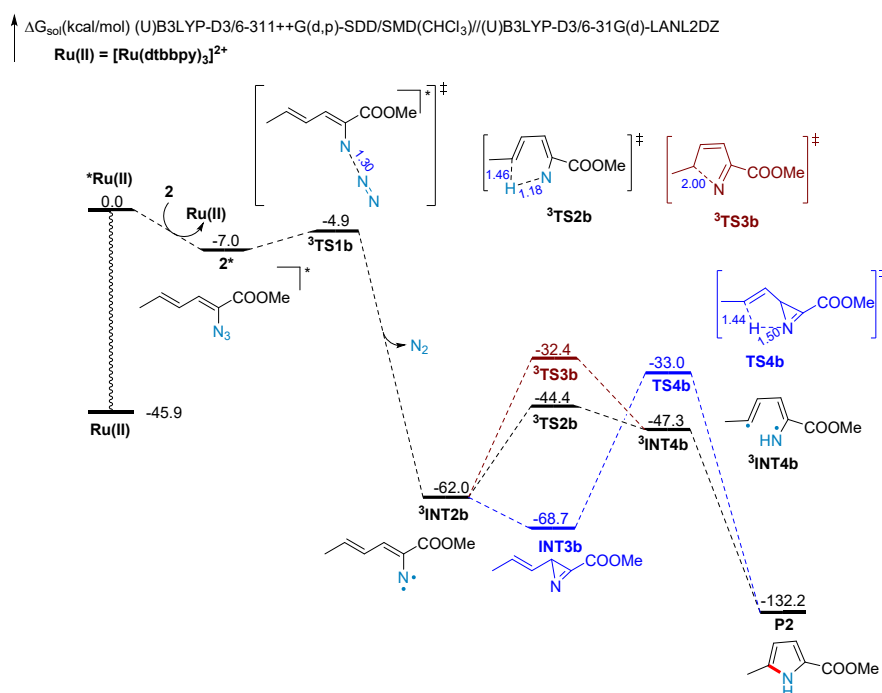
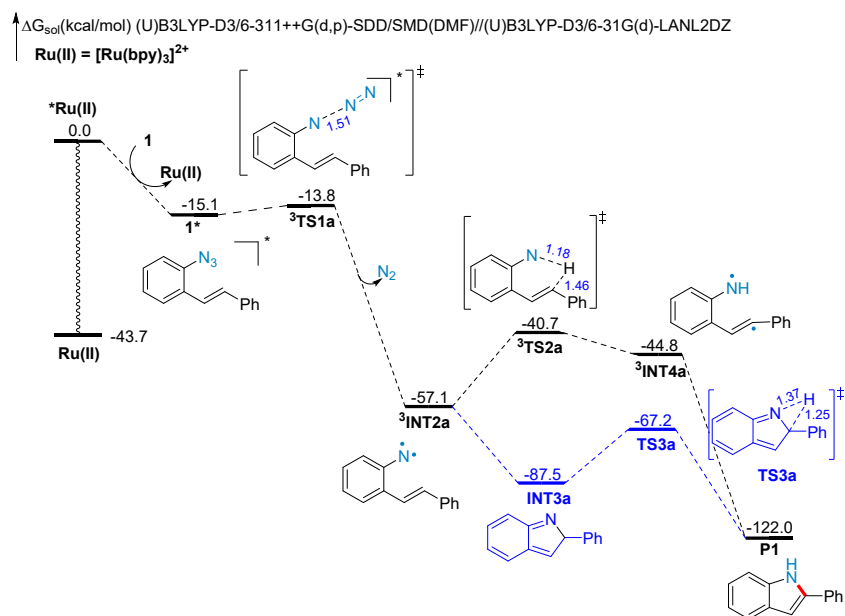
$$\lambda_{i1} = [E^D(Q_R) + E^A(Q_R)] - [E^D(Q) + E^A(Q_P)] \quad \text{S5}$$

$$\lambda_{i2} = [E^{D+}(Q_R) + E^{A-}(Q_R)] - [E^{D+}(Q) + E^{A-}(Q_P)] \quad \text{S6}$$

$$\lambda_i = (\lambda_{i1} + \lambda_{i2})/2 \quad \text{S7}$$

where Q_R and Q_P are the equilibrium geometries of the reactants and products, respectively.

2. Additional computational results



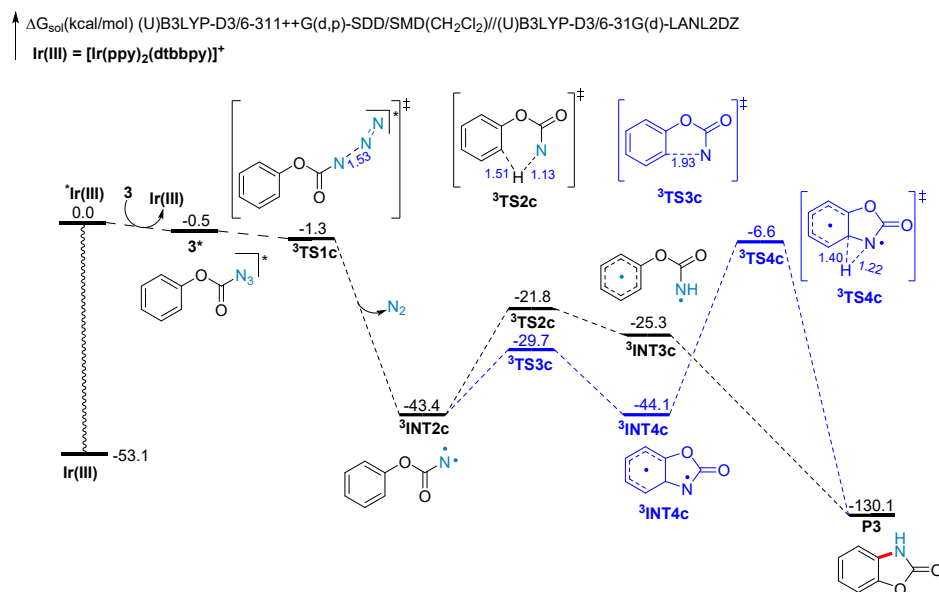


Fig. S3: Energy profiles (in kcal/mol) for the photocatalytic intramolecular cyclization of **3** to form product **P3** via triplet-triplet energy transfer mechanism. Bond lengths are shown in Å.

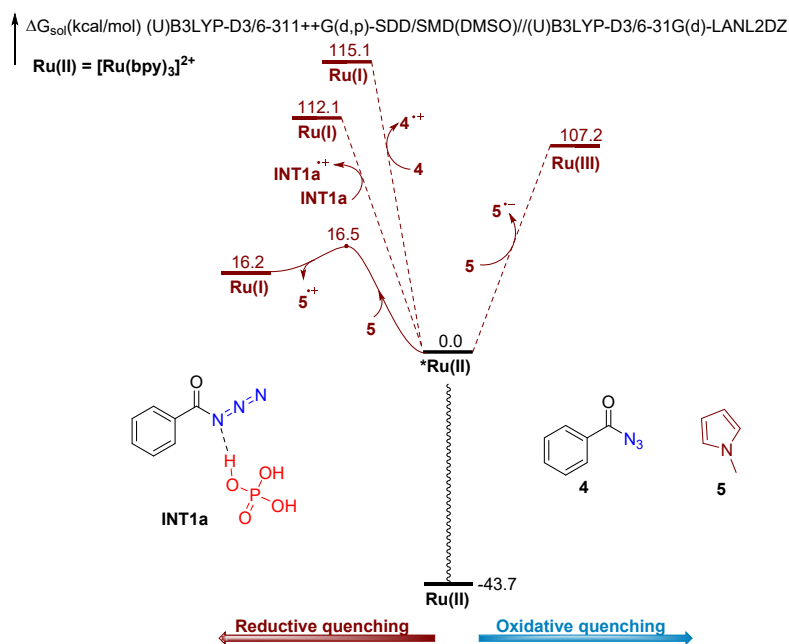


Fig. S4: Energy profiles (in kcal/mol) for the potential oxidative and reductive quenching of the excited $^*\text{Ru(II)}$ photocatalyst via single electron transfer pathway.

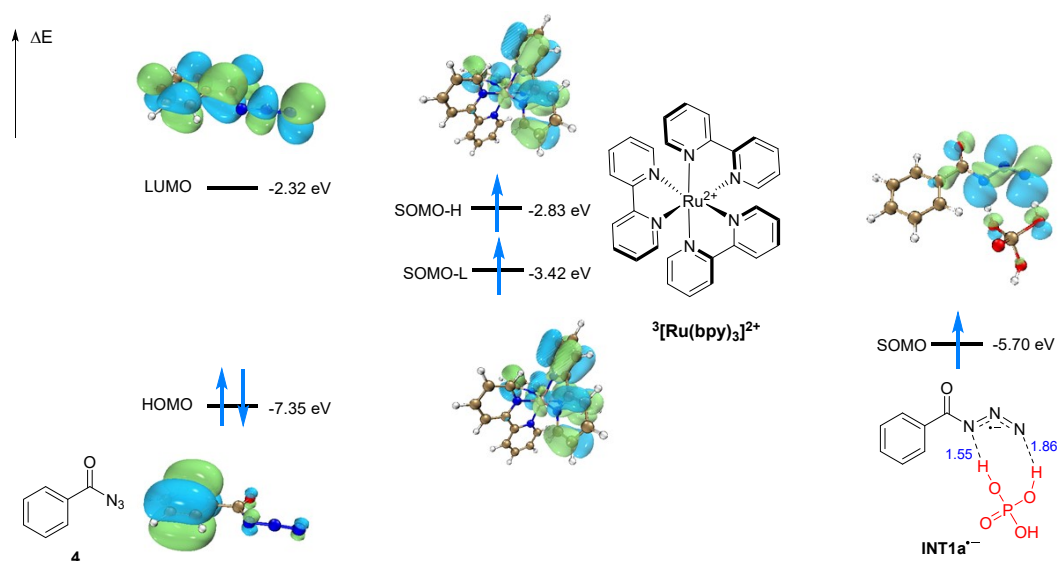


Fig. S8: Frontier molecular orbital analysis (isosurface value = 0.025) for the substrate **4**, the triplet excited state of the photocatalyst, and **INT1a⁻**.

3. Cartesian Coordinates and Energies

1

C 3.64699500 0.03583200 0.00023800
C 2.25556500 0.18992500 -0.00020800
C 1.39903800 -0.93958400 0.00011300
C 2.02515600 -2.20280300 0.00069900
C 3.40515200 -2.35943300 0.00114900
C 4.22395300 -1.22924600 0.00093400
H 4.28035800 0.91834500 -0.00000100
H 1.38855900 -3.08347400 0.00088500
H 3.83924500 -3.35446800 0.00165100
H 5.30523600 -1.32734000 0.00127300
C -0.06246200 -0.92837800 -0.00017400
C -0.92419100 0.11047200 0.00033400
H -0.48140700 -1.93314500 -0.00058800
H -0.53303200 1.12075800 0.00101400
C -2.38548000 0.01403100 0.00011800
C -3.09324200 -1.20332200 -0.00226900
C -3.13179400 1.20654200 0.00237800
C -4.48335500 -1.22139400 -0.00227400
H -2.55319500 -2.14497000 -0.00422900
C -4.52434400 1.18983500 0.00240000
H -2.60272900 2.15628200 0.00418800
C -5.20813200 -0.02580400 0.00007500
H -5.00727600 -2.17335000 -0.00415900
H -5.07510400 2.12635900 0.00420200
H -6.29415700 -0.04463000 0.00004000
N 1.65580900 1.47552900 -0.00105800
N 2.38698900 2.47145600 -0.00135200
N 2.93953700 3.47010100 -0.00121200

Zero-point correction= 0.218765 (Hartree/Particle)

Thermal correction to Energy= 0.232749

Thermal correction to Enthalpy= 0.233694

Thermal correction to Gibbs Free Energy= 0.174152

Sum of electronic and zero-point Energies= -704.137573

Sum of electronic and thermal Energies= -704.123588

Sum of electronic and thermal Enthalpies= -704.122644

Sum of electronic and thermal Free Energies= -704.182185

B3LYP-D3/6-311++G(d,p)/SMD//B3LYP-D3/6-31G(d) energy = -704.5477378

B3LYP-D3/6-311++G(d,p)//B3LYP-D3/6-31G(d) energy = -704.53537

1*

C -3.75969600 0.35987400 -0.00008700
C -2.43552900 -0.19173100 0.00014800
C -1.29529700 0.71496400 0.00051100

C -1.55576500 2.09730400 0.00066800
 C -2.84747300 2.59733000 0.00036100
 C -3.95482400 1.71873500 -0.00002600
 H -4.59648300 -0.32662000 -0.00033300
 H -0.72379200 2.79320500 0.00132300
 H -3.01007700 3.67091800 0.00052000
 H -4.96331300 2.12154300 -0.00014300
 C 0.04043600 0.16054400 0.00090700
 C 1.19927300 0.86521800 -0.00137700
 H 0.07728000 -0.92297100 0.00306400
 H 1.16267200 1.95307800 -0.00385700
 C 2.54682600 0.31109400 -0.00076900
 C 3.64112600 1.19724800 -0.00075500
 C 2.81470700 -1.07315600 -0.00022100
 C 4.95053900 0.72592700 0.00004600
 H 3.45172500 2.26789700 -0.00127400
 C 4.12213700 -1.54265400 0.00054200
 H 1.99465600 -1.78362100 -0.00060500
 C 5.19703900 -0.64753100 0.00072400
 H 5.77812200 1.42947800 0.00012000
 H 4.30735000 -2.61297300 0.00091000
 H 6.21718100 -1.02018200 0.00129100
 N -2.14492900 -1.50195500 0.00010000
 N -3.36676800 -2.32828300 -0.00061600
 N -3.29920500 -3.50244200 -0.00020600
 Zero-point correction= 0.214479 (Hartree/Particle)
 Thermal correction to Energy= 0.229286
 Thermal correction to Enthalpy= 0.230230
 Thermal correction to Gibbs Free Energy= 0.169058
 Sum of electronic and zero-point Energies= -704.088913
 Sum of electronic and thermal Energies= -704.074107
 Sum of electronic and thermal Enthalpies= -704.073162
 Sum of electronic and thermal Free Energies= -704.134334
 B3LYP-D3/6-311++G(d,p)/SMD//B3LYP-D3/6-31G(d) energy = -704.497057
 B3LYP-D3/6-311++G(d,p)//B3LYP-D3/6-31G(d) energy = -704.48194
2
 C 3.40463200 -0.68432900 0.00000400
 C 2.27795700 0.05435500 0.00000800
 H 3.31575300 -1.77176000 -0.00004500
 H 2.34368200 1.14010900 -0.00002300
 C 4.79276900 -0.12818200 0.00000200
 H 5.35526800 -0.46977900 0.87977400
 H 5.35532200 -0.46977900 -0.87972600
 H 4.78817800 0.96627300 0.00002300
 C 0.96012500 -0.52705300 0.00000500

C -0.20283700 0.17610700 -0.00001900
 H 0.87945800 -1.60823200 0.00001700
 C -1.52983100 -0.48893400 -0.00000600
 O -2.58604300 0.11475300 -0.00001500
 O -1.44163400 -1.83565200 0.00002100
 C -2.70282100 -2.52314100 0.00000100
 H -2.45389100 -3.58423400 -0.00005800
 H -3.28090000 -2.26141300 0.88983600
 H -3.28094200 -2.26131900 -0.88977700
 N -0.14380200 1.57874800 -0.00005700
 N -1.16627700 2.28281300 0.00002300
 N -1.94713300 3.11192200 0.00002900
 Zero-point correction= 0.161011 (Hartree/Particle)
 Thermal correction to Energy= 0.173972
 Thermal correction to Enthalpy= 0.174916
 Thermal correction to Gibbs Free Energy= 0.120375
 Sum of electronic and zero-point Energies= -586.654423
 Sum of electronic and thermal Energies= -586.641462
 Sum of electronic and thermal Enthalpies= -586.640518
 Sum of electronic and thermal Free Energies= -586.695059
 B3LYP-D3/6-311++G(d,p)/SMD//B3LYP-D3/6-31G(d) energy = -586.989652
 B3LYP-D3/6-311++G(d,p)//B3LYP-D3/6-31G(d) energy = -586.9829
2*
 C 3.46947100 -0.59671700 -0.15628200
 C 2.22388700 0.01271200 0.04829600
 H 3.50044300 -1.53416000 -0.71001100
 H 2.20780300 0.95001100 0.60457600
 C 4.76443000 -0.03421100 0.32577100
 H 5.28432900 -0.73568300 0.99519400
 H 5.45608700 0.16132400 -0.50730300
 H 4.61897500 0.90508500 0.86962200
 C 1.02496200 -0.47559800 -0.41711100
 C -0.26506900 0.20241600 -0.20704800
 H 0.99124600 -1.41738800 -0.95639000
 C -1.51768600 -0.50288100 -0.00050500
 O -2.60260000 0.05165500 0.14153500
 O -1.35123600 -1.85020100 -0.00411300
 C -2.55669900 -2.60288700 0.18467300
 H -2.25301000 -3.64975500 0.16377700
 H -3.01897200 -2.35488000 1.14406300
 H -3.27125700 -2.39286900 -0.61604500
 N -0.23950000 1.56546700 -0.21796800
 N -1.26725900 2.25900700 -0.02594000
 N -2.02820100 3.09548000 0.13624700
 Zero-point correction= 0.157316 (Hartree/Particle)

Thermal correction to Energy= 0.170859
 Thermal correction to Enthalpy= 0.171804
 Thermal correction to Gibbs Free Energy= 0.114229
 Sum of electronic and zero-point Energies= -586.590808
 Sum of electronic and thermal Energies= -586.577265
 Sum of electronic and thermal Enthalpies= -586.576321
 Sum of electronic and thermal Free Energies= -586.633896
 B3LYP-D3/6-311++G(d,p)/SMD//B3LYP-D3/6-31G(d) energy = -586.9214657
 B3LYP-D3/6-311++G(d,p)//B3LYP-D3/6-31G(d) energy = -586.91524

3

C 2.62405200 0.41459900 1.20920800
 C 1.42354700 -0.29529700 1.21595400
 C 0.84057400 -0.63489000 0.00031600
 C 1.42407600 -0.29719800 -1.21559500
 C 2.62458500 0.41270100 -1.20943500
 C 3.22425200 0.77007000 -0.00026200
 H 3.09019500 0.68796400 2.15105400
 H 0.94018800 -0.58746400 2.14218500
 H 0.94111400 -0.59081500 -2.14157300
 H 3.09114200 0.68458600 -2.15150500
 H 4.15957000 1.32149800 -0.00048800
 O -0.32578900 -1.41346300 0.00063900
 C -1.54666600 -0.84254500 0.00038600
 O -2.56042400 -1.48936100 0.00077200
 N -1.46104200 0.58116100 -0.00042500
 N -2.57124300 1.14858800 -0.00073800
 N -3.51328900 1.77627900 -0.00089500
 Zero-point correction= 0.118083 (Hartree/Particle)

Thermal correction to Energy= 0.127929
 Thermal correction to Enthalpy= 0.128873
 Thermal correction to Gibbs Free Energy= 0.080391
 Sum of electronic and zero-point Energies= -584.308181
 Sum of electronic and thermal Energies= -584.298335
 Sum of electronic and thermal Enthalpies= -584.297391
 Sum of electronic and thermal Free Energies= -584.345873
 B3LYP-D3/6-311++G(d,p)/SMD//B3LYP-D3/6-31G(d) energy = -584.5987968
 B3LYP-D3/6-311++G(d,p)//B3LYP-D3/6-31G(d) energy = -584.58909

3*

C 2.69624700 0.42683100 1.21021700
 C 1.38273800 -0.33368200 1.21557000
 C 0.80957600 -0.65835500 0.00004500
 C 1.38283000 -0.33403100 -1.21550300
 C 2.69636300 0.42643700 -1.21026000
 C 3.28621900 0.76499300 -0.00003700
 H 3.14421400 0.69540300 2.15912900
 H 0.91756700 -0.62919000 2.14709600

H 0.91770600 -0.62974900 -2.14698700
 H 3.14444900 0.69467300 -2.15921000
 H 4.22631000 1.31004000 -0.00008000
 O -0.36399000 -1.42908100 0.00011100
 C -1.57425300 -0.83629100 0.00009700
 O -2.59930800 -1.46574100 0.00015200
 N -1.46536700 0.58593300 -0.00008200
 N -2.56679500 1.17023100 -0.00013800
 N -3.49957800 1.81269100 -0.00018500
 Zero-point correction= 0.109093 (Hartree/Particle)
 Thermal correction to Energy= 0.119875
 Thermal correction to Enthalpy= 0.120819
 Thermal correction to Gibbs Free Energy= 0.070890
 Sum of electronic and zero-point Energies= -584.174640
 Sum of electronic and thermal Energies= -584.163858
 Sum of electronic and thermal Enthalpies= -584.162913
 Sum of electronic and thermal Free Energies= -584.212842
 B3LYP-D3/6-311++G(d,p)/SMD//B3LYP-D3/6-31G(d) energy = -584.511643
 B3LYP-D3/6-311++G(d,p)//B3LYP-D3/6-31G(d) energy = -584.50109

4

C 2.77477900 -0.95859000 -0.00067200
 C 1.40703400 -1.21009600 -0.00033200
 C 0.49825400 -0.14224000 0.00029400
 C 0.96889700 1.17789800 0.00050300
 C 2.33971100 1.42420700 0.00009400
 C 3.24223700 0.35859400 -0.00049900
 H 3.47777000 -1.78623900 -0.00105500
 H 1.01868800 -2.22275900 -0.00047900
 H 0.26067500 1.99857800 0.00109700
 H 2.70447900 2.44699100 0.00020200
 H 4.31085400 0.55417800 -0.00084500
 C -0.94625300 -0.47026200 0.00063900
 O -1.40310600 -1.59651100 0.00093400
 N -1.77372000 0.70439300 0.00041600
 N -2.99627800 0.46826400 0.00074000
 N -4.12365600 0.35652400 -0.00209100
 Zero-point correction= 0.114169 (Hartree/Particle)
 Thermal correction to Energy= 0.122950
 Thermal correction to Enthalpy= 0.123894
 Thermal correction to Gibbs Free Energy= 0.079285
 Sum of electronic and zero-point Energies= -509.098058
 Sum of electronic and thermal Energies= -509.089277
 Sum of electronic and thermal Enthalpies= -509.088333
 Sum of electronic and thermal Free Energies= -509.132942
 B3LYP-D3/6-311++G(d,p)/SMD//B3LYP-D3/6-31G(d) energy = -509.355961

B3LYP-D3/6-311++G(d,p)//B3LYP-D3/6-31G(d) energy = -509.351

4*

C 2.71327400 1.02986700 -0.09136300

C 1.33813800 1.22487700 -0.04407600

C 0.47792700 0.11966200 0.04554400

C 1.00475400 -1.18021500 0.08875900

C 2.38369700 -1.36830700 0.03919100

C 3.23684300 -0.26660400 -0.05021800

H 3.37986400 1.88409700 -0.16094000

H 0.90768500 2.21998300 -0.07599700

H 0.33493000 -2.02903800 0.16820700

H 2.79312300 -2.37322400 0.07422000

H 4.31203600 -0.41678600 -0.08688000

C -0.97742900 0.37542000 0.07741600

O -1.49641300 1.47851400 0.11085300

N -1.77096600 -0.81921700 0.13572500

N -3.03270800 -0.66817800 -0.42967900

N -3.88483300 -0.04422400 0.12296100

Zero-point correction= 0.110331 (Hartree/Particle)

Thermal correction to Energy= 0.119659

Thermal correction to Enthalpy= 0.120604

Thermal correction to Gibbs Free Energy= 0.073534

Sum of electronic and zero-point Energies= -509.014178

Sum of electronic and thermal Energies= -509.004850

Sum of electronic and thermal Enthalpies= -509.003906

Sum of electronic and thermal Free Energies= -509.050976

B3LYP-D3/6-311++G(d,p)/SMD//B3LYP-D3/6-31G(d) energy = -509.266327

B3LYP-D3/6-311++G(d,p)//B3LYP-D3/6-31G(d) energy = -509.26513

4-

C 2.82007900 -0.85268700 0.00002900

C 1.46123500 -1.16651100 -0.00001200

C 0.49093800 -0.15823000 -0.00002700

C 0.91018500 1.17929100 -0.00001300

C 2.26854000 1.49689900 0.00003300

C 3.23053200 0.48264100 -0.00003100

H 3.56266000 -1.64909100 0.00021700

H 1.10559300 -2.19219300 -0.00009000

H 0.14662600 1.94933200 0.00003300

H 2.58058600 2.54001800 -0.00004500

H 4.29025200 0.73149400 -0.00003300

C -0.97791200 -0.57282900 -0.00000400

O -1.23850800 -1.79129900 -0.00002200

N -1.78903800 0.50704600 -0.00001300

N -3.14580800 0.11874000 0.00008100

N -4.06504300 0.87412700 -0.00003100

Zero-point correction= 0.110794 (Hartree/Particle)
 Thermal correction to Energy= 0.119893
 Thermal correction to Enthalpy= 0.120838
 Thermal correction to Gibbs Free Energy= 0.075015
 Sum of electronic and zero-point Energies= -509.127142
 Sum of electronic and thermal Energies= -509.118042
 Sum of electronic and thermal Enthalpies= -509.117098
 Sum of electronic and thermal Free Energies= -509.162921
 B3LYP-D3/6-311++G(d,p)/SMD//B3LYP-D3/6-31G(d) energy = -509.475426
4⁺⁺

C -2.73560400 0.98662100 0.29345500
 C -1.37108800 1.19770300 0.22183600
 C -0.49228900 0.08525300 -0.01901300
 C -0.99593000 -1.20650100 -0.26698200
 C -2.36017500 -1.40489000 -0.18177500
 C -3.23532000 -0.30540000 0.08588200
 H -3.41093800 1.81044400 0.49532400
 H -0.93903300 2.18252700 0.35924900
 H -0.31651500 -2.02662300 -0.46925700
 H -2.77873000 -2.39847100 -0.30504100
 H -4.30598200 -0.48374500 0.11991100
 C 0.95686000 0.37805600 -0.10928500
 O 1.26186600 1.44553500 -0.64069900
 N 1.80066100 -0.60640500 0.34135400
 N 3.04349200 -0.37256200 0.19562800
 N 4.16406600 -0.31152800 0.14597500

Zero-point correction= 0.111966 (Hartree/Particle)
 Thermal correction to Energy= 0.121158
 Thermal correction to Enthalpy= 0.122102
 Thermal correction to Gibbs Free Energy= 0.076022
 Sum of electronic and zero-point Energies= -508.769557
 Sum of electronic and thermal Energies= -508.760365
 Sum of electronic and thermal Enthalpies= -508.759421
 Sum of electronic and thermal Free Energies= -508.805501
 B3LYP-D3/6-311++G(d,p)/SMD//B3LYP-D3/6-31G(d) energy = -509.096
Ru(bpy)₃²⁺

C -1.65136700 2.37736000 -0.57797000
 C 0.11626400 2.24145400 -2.10093800
 C -2.09960000 3.55597200 -1.17976600
 C -0.28195100 3.40897600 -2.74170100
 H 0.98572100 1.68367200 -2.42674000
 C -1.41163100 4.07849100 -2.27164800
 H -2.97625400 4.06655100 -0.80090500
 H 0.28463700 3.78048900 -3.58814100
 C 1.10280300 1.95237000 2.10420300

C 2.66805400 1.12426600 0.57883200
C 2.06394800 2.72562500 2.74492600
H 0.07016000 1.94527000 2.43114600
C 3.67730100 1.88039800 1.18041200
C 3.37609700 2.68851400 2.27346200
H 1.78440300 3.34141800 3.59237000
H 4.69075500 1.84394400 0.80050700
C -2.23825500 -0.02421700 2.10667200
C -2.30907000 1.74448100 0.58052600
C -3.38955500 0.41860200 2.74750700
H -1.71288400 -0.91307800 2.43404400
C -3.46988600 2.23733600 1.18200500
C -4.01707000 1.57130700 2.27540500
H -3.94760800 3.13181400 0.80194300
C -1.23581600 -2.61595300 -0.58020000
C -1.99589600 -1.01550700 -2.10445900
C -2.03464200 -3.59136200 -1.18240300
C -2.80971700 -1.94208300 -2.74587400
H -1.94393600 0.01609900 -2.43055400
C -2.82915600 -3.25488500 -2.27515500
H -2.04166700 -4.60576600 -0.80335000
H -3.41278500 -1.63583100 -3.59323600
C 1.87846000 -1.21835500 -2.10591400
C 2.88480500 0.23854000 -0.58038500
C 3.08771800 -1.45941100 -2.74765100
H 0.95907900 -1.68888500 -2.43239100
C 4.12886900 0.03485300 -1.18290700
C 4.23449700 -0.82040300 -2.27650100
H 5.01097400 0.53550100 -0.80344600
C -0.35934100 -2.87148800 0.57814300
C 1.14179700 -1.93062200 2.10252700
C -0.20879800 -4.12377300 1.17923900
C 1.33133300 -3.14984400 2.74271300
H 1.65216400 -1.03287500 2.42941100
C 0.64263900 -4.26743500 2.27146600
H -0.74764100 -4.98301700 0.79964500
N -1.22428800 -1.33706500 -1.05038700
N -0.54767000 1.73102100 -1.04804500
N 1.39015700 1.16740500 1.05003600
Ru 0.00067400 0.00062800 0.00063500
N 1.77131400 -0.39024200 -1.05109100
N -1.70445800 0.61791700 1.05182600
N 0.31754500 -1.78659500 1.04904700
H 3.12384800 -2.13407200 -3.59560800

H 2.00506400 -3.21594600 3.58960300
 H -3.78116200 -0.13193600 3.59548000
 H -4.91830500 1.94655000 2.74851100
 H -1.75221000 4.99327900 -2.74496700
 H -3.45282400 -4.00559500 -2.74879500
 H 0.76596600 -5.23601100 2.74423600
 H 4.15325400 3.27927000 2.74663700
 H 5.19638000 -0.98481000 -2.75043300
 Zero-point correction= 0.486781 (Hartree/Particle)
 Thermal correction to Energy= 0.515473
 Thermal correction to Enthalpy= 0.516417
 Thermal correction to Gibbs Free Energy= 0.426775
 Sum of electronic and zero-point Energies= -1579.423342
 Sum of electronic and thermal Energies= -1579.394650
 Sum of electronic and thermal Enthalpies= -1579.393706
 Sum of electronic and thermal Free Energies= -1579.483349
 B3LYP-D3/6-311++G(d,p)-SDD/SMD//B3LYP-D3/6-31G(d)-LANL2DZ energy = -1581.55469
³Ru(bpy)₃²⁺
 C 2.64842800 1.15084700 -0.57591000
 C 2.17607800 -0.61458200 -2.06762000
 C 3.87957400 1.36562500 -1.21665000
 C 3.38243200 -0.44673100 -2.72490500
 H 1.46739700 -1.37897700 -2.36285600
 C 4.24786800 0.57164000 -2.29116200
 H 4.54093300 2.15109000 -0.87205100
 H 3.64083400 -1.09339500 -3.55519000
 C 1.74566000 -1.44064400 2.06495700
 C 0.55964500 -2.83286700 0.57492900
 C 2.29389200 -2.52849400 2.72180400
 H 1.97229800 -0.42311400 2.35983800
 C 1.08329300 -3.96781800 1.21536600
 C 1.94715600 -3.81944000 2.28882000
 H 2.97385100 -2.37343600 3.55121900
 H 0.81241000 -4.95845700 0.87134400
 C 0.37675600 2.23123000 2.06592400
 C 2.17454500 1.90029900 0.57484800
 C 1.04553500 3.24925000 2.72306100
 H -0.61780500 1.91920800 2.36115600
 C 2.89646500 2.92045500 1.21559600
 C 2.33686800 3.59402800 2.28974300
 H 3.88976600 3.18096600 0.87122600
 C -2.32177100 1.71757000 -0.57480300
 C -0.55685400 2.19362000 -2.06586300
 C -3.12407800 2.67598000 -1.21521800
 C -1.30607200 3.15420600 -2.72271600

H 0.45978300 1.96353400 -2.36116300
 C -2.62106400 3.39299000 -2.28924600
 H -4.13519400 2.85501600 -0.87070500
 H -0.87544900 3.70230900 -3.55245700
 C -1.62261000 -1.57806600 -2.06514500
 C -0.32747600 -2.86906800 -0.57484900
 C -2.08069200 -2.70696800 -2.72177000
 H -1.93123200 -0.58237600 -2.36014900
 C -0.75734500 -4.04293300 -1.21495800
 C -1.63037200 -3.96541800 -2.28845800
 H -0.40717300 -5.00826400 -0.87055100
 C -2.73325700 0.93190200 0.57585300
 C -2.11916700 -0.78953900 2.06728300
 C -3.97766600 1.04616300 1.21677500
 C -3.33509500 -0.72012900 2.72471100
 H -1.35086400 -1.49400800 2.36240600
 C -4.28027500 0.22477400 2.29120800
 H -4.70052900 1.77553700 0.87242500
 N -1.04758500 1.47981000 -1.03155800
 N 1.80452000 0.16701200 -1.03269200
 N 0.89007200 -1.57923700 1.03109900
 Ru -0.00004500 0.00017700 -0.00020300
 N -0.75859600 -1.64651800 -1.03127900
 N 0.92380400 1.55986400 1.03147800
 N -1.81230000 0.01974700 1.03244800
 H -2.77091500 -2.60777900 -3.55127100
 H -3.54010900 -1.38569600 3.55495900
 H 0.57188100 3.76030900 3.55299500
 H 2.89209600 4.38197100 2.78734100
 H 5.19777500 0.73539400 -2.78875300
 H -3.23837800 4.13352200 -2.78651100
 H -5.24025900 0.31095200 2.78894400
 H 2.35275600 -4.69400000 2.78618100
 H -1.96372900 -4.87013700 -2.78554000
 Zero-point correction= 0.481110 (Hartree/Particle)
 Thermal correction to Energy= 0.510763
 Thermal correction to Enthalpy= 0.511707
 Thermal correction to Gibbs Free Energy= 0.418368
 Sum of electronic and zero-point Energies= -1579.339161
 Sum of electronic and thermal Energies= -1579.309508
 Sum of electronic and thermal Enthalpies= -1579.308564
 Sum of electronic and thermal Free Energies= -1579.401903
 B3LYP-D3/6-311++G(d,p)-SDD/SMD//B3LYP-D3/6-31G(d)-LANL2DZ energy = -1581.4765669
²Ru(bpy)₃³⁺
 C 0.60430300 2.83617200 -0.56346400

C 1.79244500 1.44001700 -2.03253900
C 1.17470600 3.96525900 -1.15308900
C 2.38489700 2.52935900 -2.65980900
H 2.00445500 0.42361900 -2.34101700
C 2.06989900 3.81341500 -2.21154900
H 0.92960600 4.95719200 -0.79381200
H 3.07716500 2.37015900 -3.47917600
C 2.20949400 0.63193600 2.03458600
C 2.66563300 -1.14261200 0.56423700
C 3.44122500 0.48786900 2.66165700
H 1.50106000 1.39078500 2.34350500
C 3.91711600 -1.32763500 1.15363400
C 4.30905100 -0.50924800 2.21260600
H 3.71015300 1.14479900 3.48144700
H 4.58647300 -2.09930300 0.79364500
C -1.65373600 1.59801100 2.03250100
C -0.34274500 2.87958900 0.56350500
C -2.14442900 2.73698500 2.65946600
H -1.95759700 0.60521400 2.34096400
C -0.80786300 4.05613000 1.15278300
C -1.71345100 3.98684400 2.21103200
H -0.47325500 5.02148800 0.79332700
C -2.75866900 -0.89475000 -0.56444900
C -2.14214700 0.83111200 -2.03425700
C -4.02158200 -0.96482400 -1.15434900
C -3.38158900 0.79994100 -2.66190900
H -1.36723000 1.52211100 -2.34271900
C -4.33685800 -0.11397500 -2.21333000
H -4.75866200 -1.67229500 -0.79478100
H -3.58920300 1.47876400 -3.48168600
C 0.35250200 -2.27263300 -2.03257200
C 2.15529000 -1.94084700 -0.56324300
C 1.00031600 -3.33000400 -2.65980300
H -0.63397900 -1.94878200 -2.34107400
C 2.84866200 -2.99881800 -1.15297400
C 2.27008100 -3.69845200 -2.21154100
H 3.83038600 -3.28191700 -0.79358100
C -2.32350500 -1.73629200 0.56306300
C -0.55893300 -2.23095700 2.03300400
C -3.11053700 -2.72673000 1.15250100
C -1.30068000 -3.22479800 2.66009400
H 0.45287500 -1.99847200 2.34186900
C -2.59855400 -3.47603800 2.21135800
H -4.11382200 -2.91931000 0.79275700

N -1.83369200 0.00055300 -1.01931600
 N 0.91819200 1.58762100 -1.01809000
 N 1.82623300 -0.16684400 1.01959500
 Ru -0.00003600 -0.00039200 0.00035800
 N 0.91698700 -1.58898500 -1.01807900
 N -0.76938700 1.66499300 1.01831000
 N -1.05839800 -1.49875300 1.01826800
 H 0.51658700 -3.85028100 -3.47910600
 H -0.86671400 -3.78687600 3.47965600
 H -2.84856700 2.64178600 3.47865000
 H -2.07865800 4.89724900 2.67544600
 H 2.51653400 4.68659600 -2.67626600
 H -5.31632000 -0.16332900 -2.67820700
 H -3.20492900 -4.24699900 2.67592200
 H 5.28012300 -0.64774100 2.67707300
 H 2.80350300 -4.52147700 -2.67628000
 Zero-point correction= 0.487139 (Hartree/Particle)
 Thermal correction to Energy= 0.515932
 Thermal correction to Enthalpy= 0.516876
 Thermal correction to Gibbs Free Energy= 0.426895
 Sum of electronic and zero-point Energies= -1578.979337
 Sum of electronic and thermal Energies= -1578.950544
 Sum of electronic and thermal Enthalpies= -1578.949600
 Sum of electronic and thermal Free Energies= -1579.039581
 B3LYP-D3/6-311++G(d,p)-SDD/SMD//B3LYP-D3/6-31G(d)-LANL2DZ energy = -1581.360493
²Ru(bpy)₃⁺
 C 0.02693700 2.88392800 -0.59364300
 C 1.34668100 1.72593200 -2.15158300
 C 0.30084900 4.09350600 -1.25658000
 C 1.65750000 2.89067400 -2.83496800
 H 1.73131000 0.76284700 -2.46588400
 C 1.11414500 4.10179900 -2.37699600
 H -0.12763700 5.01933000 -0.89183000
 H 2.30648300 2.85234100 -3.70231700
 C 2.00443100 0.87572800 2.15341400
 C 2.80061500 -0.68867400 0.59502700
 C 3.20932300 0.88781400 2.83776700
 H 1.16634000 1.48663300 2.46750300
 C 4.03981900 -0.72343800 1.25891100
 C 4.24844200 0.06168400 2.38003900
 H 3.33227400 1.52541800 3.70568900
 H 4.83088700 -1.36774400 0.89439300
 C -1.76257600 1.29809000 2.15179800
 C -0.80413500 2.76957800 0.59421900
 C -2.37603700 2.33563300 2.83548000

H -1.87325400 0.26685700 2.46575600
 C -1.39419600 3.86025500 1.25743400
 C -2.17951200 3.64855100 2.37784700
 H -1.23134300 4.86743600 0.89294200
 C -2.51113300 -1.41864900 -0.59499700
 C -2.16662000 0.30280400 -2.15318900
 C -3.69528400 -1.78602000 -1.25862500
 C -3.33028400 -0.01033200 -2.83736100
 H -1.52447900 1.11728200 -2.46710900
 C -4.10809700 -1.08605600 -2.37956300
 H -4.28339400 -2.61968800 -0.89404700
 H -3.62083100 0.57069600 -3.70507900
 C 0.82309500 -2.02770200 -2.15293200
 C 2.48485500 -1.46475600 -0.59360300
 C 1.67697100 -2.87841500 -2.83662500
 H -0.20313500 -1.87924700 -2.46768100
 C 3.39595800 -2.30600900 -1.25673900
 C 2.99726600 -3.01357500 -2.37802100
 H 4.41181300 -2.39790300 -0.89151800
 C -1.99739400 -2.08107000 0.59333600
 C -0.24453900 -2.17579600 2.15169700
 C -2.64770300 -3.13693400 1.25653100
 C -0.83718200 -3.22536100 2.83538900
 H 0.70396500 -1.75649700 2.46600100
 C -2.07249100 -3.71115200 2.37736100
 H -3.60139700 -3.49911300 0.89173900
 N -1.75105100 -0.37745900 -1.06771200
 N 0.54910500 1.70539700 -1.06661300
 N 1.78786100 0.10891600 1.06769900
 Ru 0.00001500 -0.00021300 -0.00007300
 N 1.20332600 -1.32766500 -1.06707300
 N -0.98898500 1.49378500 1.06691300
 N -0.80005700 -1.60367400 1.06641600
 H 1.31989800 -3.42057400 -3.70467500
 H -0.34670000 -3.65154200 3.70299600
 H -2.99064000 2.12344700 3.70276600
 H -2.63564600 4.48793000 2.89223300
 H 1.32695800 5.03324500 -2.89112200
 H -5.02089100 -1.36736200 -2.89422900
 H -2.57196200 -4.52549300 2.89173900
 H 5.20314700 0.03671700 2.89494100
 H 3.69794700 -3.66297000 -2.89235600
 Zero-point correction= 0.481980 (Hartree/Particle)
 Thermal correction to Energy= 0.510987

Thermal correction to Enthalpy= 0.511931
 Thermal correction to Gibbs Free Energy= 0.420846
 Sum of electronic and zero-point Energies= -1579.664114
 Sum of electronic and thermal Energies= -1579.635107
 Sum of electronic and thermal Enthalpies= -1579.634163
 Sum of electronic and thermal Free Energies= -1579.725248
 B3LYP-D3/6-311++G(d,p)-SDD/SMD//B3LYP-D3/6-31G(d)-LANL2DZ energy = -1581.657028
Ru(dtbbpy)₃²⁺
 C 1.10154600 2.67612100 -0.58232500
 C 1.94028200 1.13134500 -2.10353900
 C 1.84508000 3.68698400 -1.18454800
 C 2.70055700 2.10405300 -2.74122400
 H 1.95017400 0.10059000 -2.43800200
 C 2.67074100 3.42912200 -2.28864600
 H 1.78693200 4.69305100 -0.79006600
 H 3.31080700 1.81343800 -3.58648200
 C 2.24141500 0.11965500 2.10541400
 C 2.39181600 -1.63038100 0.58270700
 C 3.41079800 -0.27515900 2.74374100
 H 1.68238000 0.98549400 2.44041900
 C 3.56821700 -2.06627400 1.18560300
 C 4.11505600 -1.39781500 2.29074900
 H 3.75976000 0.30228700 3.58996000
 H 4.07309700 -2.93839500 0.79102300
 C -1.22589200 1.88297100 2.10306600
 C 0.21587600 2.88638000 0.58037600
 C -1.46841800 3.09372800 2.74028800
 H -1.69675100 0.96637100 2.43850900
 C 0.00538800 4.12369200 1.18216700
 C -0.84742900 4.26426200 2.28675500
 H 0.50868000 4.99651100 0.78709900
 C -2.86931100 -0.38491700 -0.58282100
 C -1.94949000 1.11036700 -2.10662900
 C -4.11601900 -0.24759700 -1.18633600
 C -3.17145400 1.28108700 -2.74576000
 H -1.06132700 1.63327800 -2.44153300
 C -4.30453500 0.59387200 -2.29251800
 H -4.95857600 -0.80018300 -0.79144600
 H -3.22411100 1.95290700 -3.59264000
 C 0.01211000 -2.24776600 -2.10294500
 C 1.76835600 -2.29258600 -0.58056800
 C 0.47583000 -3.39197300 -2.74059300
 H -0.88571400 -1.74166700 -2.43787100
 C 2.27350400 -3.44127100 -1.18282100
 C 1.63861100 -4.02765800 -2.28746900

H 3.17416700 -3.89313400 -0.78808100
C -2.60933000 -1.25511100 0.58147500
C -1.01997900 -2.00109100 2.10513400
C -3.57627100 -2.05424700 1.18458300
C -1.94792700 -2.81474100 2.74366000
H 0.00933500 -1.95113700 2.44045600
C -3.27225400 -2.86164800 2.29041100
H -4.58386900 -2.05444600 0.78966800
N -1.78587200 0.29726600 -1.05111000
N 1.15178300 1.39653400 -1.04995000
N 1.72967000 -0.53443800 1.05071700
Ru -0.00040700 -0.00067800 0.00019700
N 0.63488500 -1.69716900 -1.04886100
N -0.40300000 1.76563400 1.04892600
N -1.32923500 -1.23096700 1.04993100
H -0.08009000 -3.77546700 -3.58628400
H -1.62334400 -3.40566800 3.59026600
H -2.14349500 3.10826800 3.58607600
C -1.06053000 5.63533800 2.92784200
C 0.30197600 6.17197400 3.42345200
C -1.64338200 6.59661100 1.86651600
C -2.02890600 5.56881700 4.11978300
H 0.74039600 5.50459400 4.17314000
H 1.02145000 6.28679100 2.60590200
H 0.16519200 7.15548200 3.88379200
H -2.60692500 6.23441200 1.49243400
H -1.80138400 7.58413100 2.31125000
H -0.97087100 6.72273300 1.01153000
H -2.15010800 6.56884300 4.54574700
H -3.02273100 5.21823700 3.82003500
H -1.65290300 4.91730000 4.91640500
C 3.47709600 4.55822000 -2.92986800
C 2.50097700 5.64942200 -3.42632900
C 4.42902500 5.15566400 -1.86823100
C 4.31302200 4.06339900 -4.12118700
H 1.80996800 5.24983000 -4.17631000
H 1.90921400 6.07530600 -2.60922500
H 3.06510500 6.46665400 -3.88655100
H 5.12693900 4.39936200 -1.49344000
H 5.01404800 5.96680400 -2.31292500
H 3.88433400 5.57073300 -1.01370300
H 4.87051800 4.90231800 -4.54732400
H 5.04348100 3.30406000 -3.82074900
H 3.68482200 3.64969500 -4.91784700

C -5.68494400 0.72600100 -2.93539200
C -6.14185100 -0.66649100 -3.42756400
C -6.67912100 1.25552200 -1.87645600
C -5.67301700 1.69335300 -4.12995100
H -5.44968200 -1.06787700 -4.17551400
H -6.21578400 -1.38906600 -2.60803400
H -7.13119200 -0.58782800 -3.88901100
H -6.37318600 2.23925700 -1.50468600
H -7.67366300 1.35535200 -2.32240300
H -6.76721500 0.57919000 -1.01972900
H -6.67796600 1.75589700 -4.55697000
H -5.38023000 2.70643500 -3.83268500
H -5.00031900 1.35311400 -4.92504300
C -4.35402100 -3.72936300 2.93309700
C -5.49910200 -2.81539800 3.42657600
C -4.89604000 -4.71633100 1.87374100
C -3.81330400 -4.53287300 4.12678300
H -5.13978700 -2.10104900 4.17506900
H -5.95724200 -2.25069700 2.60776500
H -6.28337800 -3.42379600 3.88774200
H -4.10127200 -5.37134000 1.50111300
H -5.67300400 -5.34513700 2.31969600
H -5.34087600 -4.19827300 1.01763100
H -4.61947500 -5.13608900 4.55387900
H -3.01347100 -5.21973700 3.82856900
H -3.43651300 -3.88026200 4.92213200
C 5.40860800 -1.89824800 2.93303500
C 5.19281800 -3.34729100 3.42671400
C 6.53393800 -1.87186000 1.87329100
C 5.83275100 -1.02726400 4.12651400
H 4.39476400 -3.39487400 4.17536900
H 4.93415100 -4.02708600 2.60806200
H 6.11273300 -3.72025400 3.88776200
H 6.70159000 -0.85571900 1.50060200
H 7.46786900 -2.22841400 2.31893400
H 6.30873600 -2.51659000 1.01726400
H 6.75930300 -1.42177000 4.55319700
H 6.02527800 0.00926300 3.82820500
H 5.07953500 -1.02888700 4.92220400
C 2.21503900 -5.28965200 -2.92883200
C 3.64850600 -4.98844100 -3.42324800
C 2.25604400 -6.41353100 -1.86798600
C 1.37040700 -5.76600300 -4.12156000
H 3.64828700 -4.18969100 -4.17267400

H 4.31192600 -4.68896800 -2.60507600
 H 4.07545400 -5.88495700 -3.88355100
 H 1.25182700 -6.64088800 -1.49461800
 H 2.66728800 -7.32506500 -2.31288300
 H 2.88658700 -6.14951600 -1.01247700
 H 1.81942200 -6.66758600 -4.54783800
 H 0.34741600 -6.01998000 -3.82253000
 H 1.32658400 -5.01457000 -4.91772600
 Zero-point correction= 1.165159 (Hartree/Particle)
 Thermal correction to Energy= 1.227974
 Thermal correction to Enthalpy= 1.228918
 Thermal correction to Gibbs Free Energy= 1.063921
 Sum of electronic and zero-point Energies= -2522.458178
 Sum of electronic and thermal Energies= -2522.395363
 Sum of electronic and thermal Enthalpies= -2522.394418
 Sum of electronic and thermal Free Energies= -2522.559416
 B3LYP-D3/6-311++G(d,p)-SDD/SMD//B3LYP-D3/6-31G(d)-LANL2DZ energy = -2525.496641
³Ru(dtbbpy)₃²⁺
 C -2.91859500 0.49177200 -0.53025300
 C -1.60320900 1.74263300 -2.01071500
 C -4.06642700 1.12496000 -1.01442200
 C -2.71684000 2.37195100 -2.53843900
 H -0.60381400 1.96632400 -2.36634600
 C -4.00086600 2.07603100 -2.03586700
 H -5.02354100 0.88145700 -0.57047200
 H -2.57862600 3.09189100 -3.33395600
 C -0.84130900 2.29242200 1.86979800
 C 1.00848000 2.70240400 0.48541400
 C -0.74839700 3.54905800 2.44027800
 H -1.61035700 1.58917100 2.16799900
 C 1.13568200 3.98047000 1.03772800
 C 0.26798200 4.43860300 2.03142200
 H -1.46469400 3.82824800 3.20128300
 H 1.91851800 4.63267800 0.67205000
 C -1.59209400 -1.75393100 2.00977100
 C -2.91541000 -0.51119400 0.52953100
 C -2.70172900 -2.39018700 2.53759700
 H -0.59128700 -1.97144400 2.36526000
 C -4.05922800 -1.15148400 1.01384900
 C -3.98763900 -2.10215300 2.03526900
 H -5.01789300 -0.91390300 0.57003800
 C 1.02697000 -2.69597300 -0.48548900
 C -0.82512200 -2.29857700 -1.87044900
 C 1.16294500 -3.97319500 -1.03764400
 C -0.72353700 -3.55458200 -2.44084700

H -1.59880900 -1.60053600 -2.16890000
C 0.29865800 -4.43723900 -2.03157800
H 1.95002200 -4.62010000 -0.67165000
H -1.43764500 -3.83862200 -3.20211400
C 2.19238100 0.38520200 -2.06074600
C 1.84450700 2.17368300 -0.58278600
C 3.28551400 1.01070200 -2.63241800
H 1.86269600 -0.59256800 -2.39310800
C 2.96081600 2.82693600 -1.11643000
C 3.70706900 2.27092300 -2.15652400
H 3.25180500 3.78463300 -0.70412700
C 1.85911200 -2.16153700 0.58291900
C 2.19428300 -0.37079400 2.06105000
C 2.97971000 -2.80715700 1.11684900
C 3.29148500 -0.98884300 2.63305400
H 1.85782300 0.60469000 2.39333500
C 3.72181900 -2.24610200 2.15720900
H 3.27739400 -3.76280600 0.70456900
N 0.03130200 -1.85943200 -0.92887200
N -1.68693900 0.81329600 -1.04113100
N 0.01835700 1.85911600 0.92846800
Ru -0.04626900 -0.00039300 -0.00021600
N 1.47143100 0.94349100 -1.07015100
N -1.68171200 -0.82505700 1.04027500
N 1.47749900 -0.93395200 1.07020100
H 3.80729300 0.51165000 -3.43778300
H 3.80956400 -0.48627800 3.43862200
H -2.55894400 -3.10936900 3.33299300
C -5.25631000 -2.78726800 2.54345600
C -6.23022300 -1.70957700 3.07286300
C -5.91358900 -3.55048800 1.37018000
C -4.95963400 -3.78347800 3.67618400
H -5.78527200 -1.14727100 3.90066300
H -6.51958700 -0.99779100 2.29272200
H -7.14402700 -2.18726700 3.43987300
H -5.23983700 -4.31623400 0.97088200
H -6.82426700 -4.04797500 1.71841900
H -6.19436100 -2.88130800 0.55016000
H -5.89441200 -4.24286700 4.00978000
H -4.29746400 -4.59201400 3.34718800
H -4.50812700 -3.29217600 4.54514800
C -5.27380000 2.75340900 -2.54376500
C -6.24157200 1.66984300 -3.07240900
C -5.93503700 3.51310200 -1.37041300

C -4.98351100 3.75099200 -3.67694000
H -5.79365300 1.10986000 -3.90018200
H -6.52648900 0.95664900 -2.29191600
H -7.15829800 2.14204000 -3.43923900
H -5.26564400 4.28296100 -0.97169100
H -6.84882600 4.00506100 -1.71835800
H -6.21140700 2.84251300 -0.55004800
H -5.92114400 4.20467200 -4.01033700
H -4.32607000 4.56359500 -3.34848100
H -4.52939500 3.26209300 -4.54590100
C 0.47194700 -5.84119800 -2.61190100
C 1.88239500 -5.95543600 -3.23457200
C 0.32246000 -6.87401000 -1.47084600
C -0.57268800 -6.14989700 -3.69679500
H 2.01717500 -5.22916000 -4.04324000
H 2.67318000 -5.79359600 -2.49461900
H 2.02077100 -6.95753300 -3.65247200
H -0.66669900 -6.80730100 -1.00531300
H 0.44158000 -7.88565600 -1.87142000
H 1.07731300 -6.73596800 -0.68970800
H -0.40625800 -7.15895400 -4.08440200
H -1.59440500 -6.11583600 -3.30267500
H -0.50017600 -5.45812100 -4.54330600
C 4.93839800 -2.98003700 2.72174600
C 4.48568500 -4.35558000 3.26358500
C 5.96950600 -3.18184100 1.58735200
C 5.60709500 -2.19620200 3.86284900
H 3.74751400 -4.24113000 4.06448600
H 4.04568000 -4.98167300 2.48042100
H 5.34783400 -4.89266900 3.67128200
H 6.30071200 -2.22066700 1.17971800
H 6.84779700 -3.70612100 1.97696800
H 5.56428100 -3.78017100 0.76473200
H 6.46704600 -2.76008000 4.23521400
H 5.97623400 -1.22055700 3.52772700
H 4.92639900 -2.04236700 4.70740400
C 0.43168400 5.84361100 2.61198700
C 1.84081600 5.96681300 3.23594600
C 0.27661200 6.87557400 1.47092100
C -0.61589600 6.14549900 3.69595800
H 1.97945900 5.24141000 4.04474500
H 2.63327000 5.80995900 2.49670700
H 1.97246000 6.96977200 3.65395500
H -0.71162900 6.80250300 1.00439600

H 0.38875700 7.88791700 1.87174700
 H 1.03311900 6.74257100 0.69050800
 H -0.45638900 7.15562200 4.08369800
 H -1.63702000 6.10476500 3.30093200
 H -0.53962600 5.45422800 4.54255200
 C 4.91878700 3.01312400 -2.72071500
 C 4.45682500 4.38540000 -3.26302000
 C 5.94800800 3.22226100 -1.58593200
 C 5.59333600 2.23367900 -3.86137600
 H 3.71970600 4.26571400 -4.06412400
 H 4.01230200 5.00864900 -2.48013900
 H 5.31539800 4.92829600 -3.67057400
 H 6.28566700 2.26347700 -1.17796700
 H 6.82282400 3.75251300 -1.97528600
 H 5.53831200 3.81794600 -0.76360600
 H 6.44954300 2.80338300 -4.23349900
 H 5.96903800 1.26066300 -3.52590700
 H 4.91406200 2.07499700 -4.70618100
 Zero-point correction= 1.159833 (Hartree/Particle)
 Thermal correction to Energy= 1.223486
 Thermal correction to Enthalpy= 1.224431
 Thermal correction to Gibbs Free Energy= 1.056305
 Sum of electronic and zero-point Energies= -2522.373552
 Sum of electronic and thermal Energies= -2522.309899
 Sum of electronic and thermal Enthalpies= -2522.308955
 Sum of electronic and thermal Free Energies= -2522.477080
 B3LYP-D3/6-311++G(d,p)-SDD/SMD//B3LYP-D3/6-31G(d)-LANL2DZ energy = -2525.415898
Ir(ppy)₂(dtbbpy)⁺
 C 1.82811400 1.85359300 2.12377400
 C 0.13432600 0.35431200 2.95987000
 C 1.91482900 2.46676700 3.38368200
 C 0.22322300 0.96409400 4.21277100
 H -0.55937700 -0.47094300 2.82499900
 C 1.11307300 2.02211200 4.42843400
 H 2.60661700 3.28628200 3.55606100
 H -0.40174200 0.61266400 5.02969500
 C -0.76860500 2.59334100 -0.71342800
 C -1.96010800 0.65549100 -0.24356300
 C -1.93791800 3.32488200 -0.88651400
 H 0.20900000 3.05171600 -0.81457400
 C -3.16214500 1.33916400 -0.40393700
 C -3.18231400 2.70203600 -0.73231900
 H -1.86145200 4.37581900 -1.13299100
 H -4.09698600 0.81243800 -0.26281900
 C 3.10401900 1.77221900 -1.28422900

C 2.64425200 2.24368400 0.97813000
C 4.07857300 2.75510900 -1.34626200
H 2.86299100 1.14863100 -2.13535800
C 3.62111300 3.24822800 0.96181700
C 4.33874600 3.50788000 -0.19718300
H 3.81586900 3.81453800 1.86444800
C 2.86150700 -1.99821400 -0.84659100
C 3.11131100 -1.53526800 1.51076100
C 3.88554700 -2.95736000 -0.76324000
C 4.12674600 -2.49038500 1.58678100
H 2.82385600 -0.99304600 2.40547000
C 4.51716500 -3.20445500 0.44944500
H 4.19505800 -3.51475800 -1.64238000
H 4.61891000 -2.67892700 2.53724400
C -0.43867700 -2.54597400 0.63016000
C -1.86236400 -0.77265400 0.12005900
C -1.51264000 -3.40444400 0.82507500
H 0.58534400 -2.87291100 0.75581800
C -2.96689200 -1.59843300 0.30139700
C -2.82399200 -2.94465200 0.66304100
H -3.95818700 -1.18777900 0.16089400
C 2.15547700 -1.70839600 -2.09848400
C 0.47440100 -0.39776200 -3.08645900
C 2.38982100 -2.33245500 -3.33380800
C 0.66428400 -0.98147700 -4.33033800
H -0.26944400 0.37560600 -2.92536300
C 1.64698700 -1.96943800 -4.44906200
H 3.15080500 -3.09893000 -3.41422000
N -0.77212700 1.29083100 -0.40695300
N -0.59788300 -1.25698400 0.28624800
N 2.39952400 1.52841500 -0.16265200
N 1.19665400 -0.74404700 -2.00844400
H -1.30508700 -4.42881200 1.10541600
H 0.06284200 -0.67181900 -5.17749300
H 4.62244700 2.91859100 -2.26946700
C -4.51583900 3.43346100 -0.89455900
C -5.32747300 2.75318600 -2.01995100
C -5.29739100 3.34698900 0.43600200
C -4.32007500 4.91490800 -1.25501600
H -4.79098800 2.79624700 -2.97394400
H -5.53860800 1.70229700 -1.79616500
H -6.28727200 3.26474900 -2.14605100
H -4.73688500 3.81407800 1.25263200
H -6.25531900 3.86813300 0.33750400

H -5.51043500 2.31127300 0.72020700
 H -5.29699500 5.39565800 -1.36239400
 H -3.77188600 5.45510800 -0.47544300
 H -3.78735400 5.03695500 -2.20461000
 C -4.05837500 -3.82466500 0.86171900
 C -4.93099400 -3.21593800 1.98267100
 C -4.86138400 -3.86608200 -0.45805200
 C -3.68230600 -5.26214100 1.25543200
 H -4.38034300 -3.16818900 2.92812200
 H -5.26946700 -2.20425700 1.73567900
 H -5.82061100 -3.83526400 2.13725500
 H -4.26063700 -4.28694800 -1.27139800
 H -5.75015800 -4.49287800 -0.33133700
 H -5.19846600 -2.87040500 -0.76486700
 H -4.59316600 -5.85386200 1.38676300
 H -3.07999900 -5.75224000 0.48262800
 H -3.12983300 -5.29449100 2.20083100
 Ir 0.95727700 0.06489500 0.00390600
 H 5.09781000 4.28368400 -0.20646600
 H 1.17968200 2.49278600 5.40418100
 H 5.30846500 -3.94508500 0.50958800
 H 1.82959100 -2.45188400 -5.40430400
 C 2.45357300 -1.26589300 0.30260300
 C 0.93038500 0.77992000 1.88904400
 Zero-point correction= 0.711762 (Hartree/Particle)
 Thermal correction to Energy= 0.751673
 Thermal correction to Enthalpy= 0.752617
 Thermal correction to Gibbs Free Energy= 0.638386
 Sum of electronic and zero-point Energies= -1871.541463
 Sum of electronic and thermal Energies= -1871.501551
 Sum of electronic and thermal Enthalpies= -1871.500607
 Sum of electronic and thermal Free Energies= -1871.614839
 B3LYP-D3/6-311++G(d,p)-SDD/SMD//B3LYP-D3/6-31G(d)-LANL2DZ energy = -1872.489588
³Ir(ppy)₂(dtbbpy)⁺
 C 2.39395300 1.42622300 2.15098000
 C 0.66967300 -0.03438600 3.08284600
 C 2.75030900 1.82555900 3.43888100
 C 1.03601000 0.36825200 4.36116700
 H -0.13411700 -0.74921700 2.94814800
 C 2.07446600 1.29517400 4.54062200
 H 3.54698500 2.54465400 3.60155200
 H 0.51840100 -0.03216100 5.22757400
 C -0.50619200 2.68997400 -0.52247900
 C -1.85643000 0.78940300 -0.03336000
 C -1.60260800 3.50093800 -0.65586100

H 0.50058900 3.07384500 -0.64880600
C -3.00138700 1.61382200 -0.15430800
C -2.91737900 2.95424300 -0.46932700
H -1.45617700 4.54551200 -0.89264400
H -3.97261500 1.16413300 0.01404700
C 3.02275500 1.72431900 -1.41271000
C 3.03523500 1.91631300 0.93124300
C 4.07065500 2.62641700 -1.53819500
H 2.56257900 1.24636400 -2.26876000
C 4.09016000 2.83081700 0.85912400
C 4.60977100 3.18996000 -0.37960600
H 4.50007900 3.25281400 1.76883800
C 2.38492100 -2.12840700 -1.40061900
C 3.30937100 -1.82234800 0.81301700
C 3.29836800 -3.16894300 -1.63078300
C 4.20869000 -2.86396000 0.57811800
H 3.32468000 -1.31661600 1.77219600
C 4.20472400 -3.54041400 -0.64410500
H 3.31189600 -3.68980100 -2.58288400
H 4.91480400 -3.14838800 1.35336500
C -0.55301500 -2.51170500 0.75103800
C -1.86646400 -0.59448000 0.29169000
C -1.67073600 -3.29193500 0.95514200
H 0.44769100 -2.91614500 0.84351200
C -3.02875600 -1.37881600 0.49116500
C -2.96627000 -2.71925900 0.82195700
H -3.99295200 -0.89950800 0.37432900
C 1.42400300 -1.68085100 -2.41436400
C -0.24306000 -0.10399200 -2.89777400
C 1.23346000 -2.27483400 -3.66923900
C -0.47296700 -0.65024600 -4.15294600
H -0.79782300 0.75296000 -2.53732800
C 0.28234400 -1.75907600 -4.54071700
H 1.82080700 -3.13904800 -3.95368300
N -0.59410800 1.36919800 -0.23146800
N -0.62355700 -1.20362800 0.43249000
N 2.51580500 1.39032800 -0.21517100
N 0.68055500 -0.60025900 -2.05888500
H -1.53525200 -4.33290400 1.21353300
H -1.22515100 -0.21832600 -4.80314100
H 4.45377000 2.87461000 -2.52122600
C -4.18636800 3.80327600 -0.59638000
C -5.09632400 3.19996800 -1.68962100
C -4.93435600 3.80020200 0.75592400

C -3.87306200 5.26052100 -0.97566200
 H -4.58740400 3.18742500 -2.65977300
 H -5.39403100 2.17387500 -1.45099000
 H -6.00915300 3.79721200 -1.79153700
 H -4.30700300 4.21718400 1.55108900
 H -5.84386200 4.40707900 0.68437100
 H -5.22888000 2.78888600 1.05414000
 H -4.80694500 5.82470200 -1.06237200
 H -3.25854100 5.75608800 -0.21612700
 H -3.35567900 5.32852200 -1.93911200
 C -4.25288000 -3.52680600 1.02737600
 C -5.07467900 -2.89053600 2.17013000
 C -5.07877900 -3.50341300 -0.27787300
 C -3.96307000 -4.99192000 1.39375900
 H -4.50702300 -2.88957900 3.10702800
 H -5.35380300 -1.85638900 1.94387100
 H -5.99772700 -3.45830700 2.33122500
 H -4.51356300 -3.94393200 -1.10646800
 H -6.00173800 -4.07972000 -0.14975200
 H -5.35819300 -2.48423700 -0.56400700
 H -4.90718400 -5.52826600 1.53155700
 H -3.40364800 -5.50596100 0.60442800
 H -3.39773800 -5.07350800 2.32862800
 Ir 0.97129500 0.02915300 0.07482800
 H 5.42960400 3.89819000 -0.44171500
 H 2.35551100 1.60615800 5.54182900
 H 4.90772900 -4.34646200 -0.82824300
 H 0.12889600 -2.21866300 -5.51212400
 C 2.37112500 -1.44740500 -0.15957700
 C 1.33839000 0.47713200 1.94881100
 Zero-point correction= 0.708769 (Hartree/Particle)
 Thermal correction to Energy= 0.749229
 Thermal correction to Enthalpy= 0.750173
 Thermal correction to Gibbs Free Energy= 0.633362
 Sum of electronic and zero-point Energies= -1871.456985
 Sum of electronic and thermal Energies= -1871.416526
 Sum of electronic and thermal Enthalpies= -1871.415582
 Sum of electronic and thermal Free Energies= -1871.532392
 B3LYP-D3/6-311++G(d,p)-SDD/SMD//B3LYP-D3/6-31G(d)-LANL2DZ energy = -1872.400019
³TS1a
 C 3.69338600 0.04719800 0.00002100
 C 2.26656200 0.23253700 -0.00008400
 C 1.41105000 -0.95322400 0.00002300
 C 2.04995800 -2.21012400 0.00015800
 C 3.42769100 -2.35098800 0.00022700

C 4.25343600 -1.20526200 0.00016500
 H 4.31365600 0.93366700 -0.00002300
 H 1.42433600 -3.09847400 0.00022300
 H 3.87147000 -3.34185400 0.00034000
 H 5.33379600 -1.31524100 0.00023500
 C -0.03327900 -0.96150400 0.00000000
 C -0.90547400 0.08131800 0.00000500
 H -0.44677400 -1.96850900 0.00002400
 H -0.50225000 1.08721800 0.00005100
 C -2.35892600 -0.02139400 -0.00000800
 C -3.06334400 -1.24288700 -0.00039200
 C -3.10727100 1.17233500 0.00037500
 C -4.45240400 -1.26346700 -0.00036100
 H -2.52057100 -2.18277900 -0.00074600
 C -4.49867000 1.15137700 0.00041000
 H -2.57830300 2.12163700 0.00065600
 C -5.17810100 -0.06757300 0.00004500
 H -4.97594700 -2.21539100 -0.00066700
 H -5.05298300 2.08548400 0.00071700
 H -6.26403400 -0.08887100 0.00006400
 N 1.66000700 1.42263900 -0.00026600
 N 2.66445300 2.55733000 -0.00046700
 N 2.29981600 3.66761200 0.00010800
 Zero-point correction= 0.213828 (Hartree/Particle)
 Thermal correction to Energy= 0.228130
 Thermal correction to Enthalpy= 0.229074
 Thermal correction to Gibbs Free Energy= 0.169028
 Sum of electronic and zero-point Energies= -704.088728
 Sum of electronic and thermal Energies= -704.074426
 Sum of electronic and thermal Enthalpies= -704.073482
 Sum of electronic and thermal Free Energies= -704.133528
 B3LYP-D3/6-311++G(d,p)/SMD//B3LYP-D3/6-31G(d) energy = -704.4949641
³INT2a
 C 3.86453900 1.04848800 0.00003800
 C 2.42293000 0.96484500 -0.00000900
 C 1.79984300 -0.35898500 0.00001400
 C 2.65428600 -1.47338000 0.00006200
 C 4.03935700 -1.35721000 0.00009900
 C 4.64479500 -0.08354600 0.00009000
 H 4.30372000 2.04028100 0.00002700
 H 2.20334600 -2.46245700 0.00007400
 H 4.65546600 -2.25112000 0.00013800
 H 5.72727100 0.00387700 0.00012100
 C 0.37318600 -0.57869200 -0.00000800
 C -0.60679400 0.35865400 -0.00000900

H 0.09166500 -1.63023300 -0.00000400
 H -0.31480500 1.40640100 0.00003300
 C -2.04416100 0.11153500 -0.00003600
 C -2.61636200 -1.17644500 -0.00034600
 C -2.91328600 1.21930600 0.00025600
 C -3.99598000 -1.34301700 -0.00033800
 H -1.97694700 -2.05359800 -0.00061700
 C -4.29516500 1.05222900 0.00026500
 H -2.48770300 2.21938100 0.00048400
 C -4.84373800 -0.23073000 -0.00002900
 H -4.41585100 -2.34510100 -0.00058400
 H -4.94404500 1.92345500 0.00049900
 H -5.92146500 -0.36579800 -0.00002700
 N 1.73980600 2.08522900 -0.00006200
 Zero-point correction= 0.206370 (Hartree/Particle)
 Thermal correction to Energy= 0.218467
 Thermal correction to Enthalpy= 0.219411
 Thermal correction to Gibbs Free Energy= 0.165273
 Sum of electronic and zero-point Energies= -594.621298
 Sum of electronic and thermal Energies= -594.609201
 Sum of electronic and thermal Enthalpies= -594.608257
 Sum of electronic and thermal Free Energies= -594.662394
 B3LYP-D3/6-311++G(d,p)/SMD//B3LYP-D3/6-31G(d) energy = -594.9927073
³TS2a
 C 3.56571300 1.21821900 0.24945600
 C 2.17189200 0.86706400 0.15923100
 C 1.83105200 -0.52922700 -0.11754800
 C 2.86438700 -1.45828400 -0.27596800
 C 4.19955300 -1.07720800 -0.17684800
 C 4.54608500 0.26791800 0.08571100
 H 3.80300700 2.25701000 0.45297900
 H 2.61197300 -2.49593200 -0.47899600
 H 4.98191600 -1.81977800 -0.30224000
 H 5.59268700 0.54828200 0.15995900
 C 0.43803000 -0.88127200 -0.22504400
 C -0.52335200 0.04572300 -0.05742600
 H 0.19580900 -1.91677200 -0.47909300
 H 0.22122100 1.27646600 0.16883600
 C -1.96028600 0.00300600 -0.02525000
 C -2.64834200 -1.16287400 0.37800500
 C -2.71491400 1.13938100 -0.38038000
 C -4.03801400 -1.19254100 0.39712300
 H -2.07752800 -2.03470700 0.68334300
 C -4.10521700 1.10319000 -0.35910200
 H -2.19290400 2.04416800 -0.67741300

C -4.77238000 -0.06180600 0.02738800
 H -4.55291100 -2.09729100 0.70835000
 H -4.67146300 1.98626300 -0.64104700
 H -5.85802500 -0.08678100 0.04901400
 N 1.26014000 1.80733500 0.32574600
 Zero-point correction= 0.200458 (Hartree/Particle)
 Thermal correction to Energy= 0.212015
 Thermal correction to Enthalpy= 0.212960
 Thermal correction to Gibbs Free Energy= 0.160496
 Sum of electronic and zero-point Energies= -594.592845
 Sum of electronic and thermal Energies= -594.581288
 Sum of electronic and thermal Enthalpies= -594.580344
 Sum of electronic and thermal Free Energies= -594.632807
 B3LYP-D3/6-311++G(d,p)/SMD//B3LYP-D3/6-31G(d) energy = -594.9618203
³INT4a

C 3.40344600 1.37033900 0.00088500
 C 2.05380700 0.86660300 0.00019700
 C 1.87415300 -0.57665400 -0.00036900
 C 3.00761000 -1.39679900 -0.00063100
 C 4.29630300 -0.86908500 -0.00017100
 C 4.49110300 0.52846900 0.00064300
 H 3.53862800 2.44957100 0.00156900
 H 2.86930400 -2.47505000 -0.00115900
 H 5.15359200 -1.53559500 -0.00044500
 H 5.49835800 0.93490800 0.00111900
 C 0.55265300 -1.18921400 -0.00068400
 C -0.61238600 -0.57261000 -0.00062100
 H 0.56538000 -2.28676600 -0.00110500
 H 1.26926200 2.62808000 0.00056300
 C -1.96691100 -0.31840000 -0.00030300
 C -2.68576700 -0.15864900 1.22406400
 C -2.68607500 -0.15692100 -1.22423600
 C -4.04072300 0.12717200 1.21141700
 H -2.14923200 -0.26562500 2.16116300
 C -4.04103300 0.12888100 -1.21081000
 H -2.14980000 -0.26254200 -2.16163200
 C -4.73178400 0.27261100 0.00049400
 H -4.57104300 0.23995600 2.15330000
 H -4.57162800 0.24300000 -2.15237600
 H -5.79384800 0.49830400 0.00076300
 N 0.97923500 1.64247100 -0.00014600
 Zero-point correction= 0.204529 (Hartree/Particle)
 Thermal correction to Energy= 0.216996
 Thermal correction to Enthalpy= 0.217940
 Thermal correction to Gibbs Free Energy= 0.162544

Sum of electronic and zero-point Energies= -594.593243
 Sum of electronic and thermal Energies= -594.580776
 Sum of electronic and thermal Enthalpies= -594.579832
 Sum of electronic and thermal Free Energies= -594.635228
 B3LYP-D3/6-311++G(d,p)/SMD//B3LYP-D3/6-31G(d) energy = -594.9704071

P1

C 2.98370100 1.41977300 0.26623300
 C 1.83467800 0.64087800 0.11073200
 C 1.89208100 -0.76068300 -0.13791300
 C 3.15031900 -1.37658700 -0.25275700
 C 4.29463800 -0.60494500 -0.10270600
 C 4.21258800 0.77838000 0.15778300
 H 2.92076500 2.48685700 0.46141900
 H 3.22294000 -2.44248700 -0.45092400
 H 5.27210300 -1.07143800 -0.18549400
 H 5.12599500 1.35475600 0.27274000
 C 0.53839500 -1.22337100 -0.21441600
 C -0.29145300 -0.13788300 -0.02368700
 H 0.21246500 -2.23011700 -0.43508600
 H 0.15013800 1.87842200 0.48103600
 C -1.74970900 -0.05484900 -0.01289500
 C -2.52115000 -1.18249600 0.31765800
 C -2.41602400 1.14124500 -0.33039900
 C -3.91068300 -1.11575900 0.32465600
 H -2.01878700 -2.10583300 0.58893600
 C -3.80736800 1.20831400 -0.31201200
 H -1.84255700 2.01492700 -0.62792400
 C -4.56169400 0.08081400 0.01426300
 H -4.48890400 -1.99789200 0.58504000
 H -4.30309900 2.14143000 -0.56478100
 H -5.64642900 0.13284300 0.02645300
 N 0.50078000 0.99450500 0.14590500

Zero-point correction= 0.211332 (Hartree/Particle)

Thermal correction to Energy= 0.222282

Thermal correction to Enthalpy= 0.223226

Thermal correction to Gibbs Free Energy= 0.173929

Sum of electronic and zero-point Energies= -594.723047

Sum of electronic and thermal Energies= -594.712097

Sum of electronic and thermal Enthalpies= -594.711153

Sum of electronic and thermal Free Energies= -594.760450

B3LYP-D3/6-311++G(d,p)/SMD//B3LYP-D3/6-31G(d) energy = -595.1048762

INT3a

C 2.84398900 -1.31733100 -0.50364600
 C 1.67564800 -0.47061100 -0.57100800
 C 1.69564900 0.83554400 0.13092600
 C 2.86287500 1.23426500 0.87271600

C 3.92868300 0.39102800 0.90485100
 C 3.91534100 -0.88611700 0.21311100
 H 2.83621500 -2.27161800 -1.02002600
 H 2.88117200 2.18864000 1.39117600
 H 4.82351300 0.66451900 1.45646800
 H 4.80392100 -1.50811500 0.28122400
 C 0.48742700 1.40371800 -0.10882600
 C -0.29261200 0.44333700 -0.97679900
 H 0.10879900 2.35471900 0.24575700
 H -0.44631000 0.91061400 -1.96450600
 C -1.66040000 0.10800800 -0.39718300
 C -1.87411700 -1.08411100 0.29912300
 C -2.70803600 1.02677200 -0.51850800
 C -3.11920100 -1.34942200 0.87001400
 H -1.06535600 -1.80248700 0.37243600
 C -3.95173500 0.76227300 0.05317500
 H -2.55058700 1.95304100 -1.06705100
 C -4.16047900 -0.42832700 0.75142800
 H -3.27615100 -2.28173300 1.40568800
 H -4.75843900 1.48253500 -0.05214100
 H -5.13012300 -0.63870100 1.19386000
 N 0.55930800 -0.72365200 -1.19415900
 Zero-point correction= 0.209840 (Hartree/Particle)
 Thermal correction to Energy= 0.220826
 Thermal correction to Enthalpy= 0.221770
 Thermal correction to Gibbs Free Energy= 0.171067
 Sum of electronic and zero-point Energies= -594.669165
 Sum of electronic and thermal Energies= -594.658179
 Sum of electronic and thermal Enthalpies= -594.657235
 Sum of electronic and thermal Free Energies= -594.707938
 B3LYP-D3/6-311++G(d,p)/SMD//B3LYP-D3/6-31G(d) energy = -595.047002
TS3a
 C -2.97640000 -1.43442500 0.17042800
 C -1.79990500 -0.64673900 0.14571200
 C -1.86644700 0.77530500 -0.06415600
 C -3.12832600 1.39120700 -0.28604500
 C -4.25176700 0.59906000 -0.29221000
 C -4.17826300 -0.80828700 -0.06506200
 H -2.90871500 -2.50325200 0.34665400
 H -3.19782600 2.46274200 -0.45012400
 H -5.22534700 1.04807900 -0.46829700
 H -5.09612700 -1.38897100 -0.07898800
 C -0.55617000 1.25790900 0.03550900
 C 0.28112100 0.14216100 0.29401200
 H -0.22563500 2.28081400 -0.08425200

C 1.74882200 0.04986900 0.11448400
 C 2.55284200 1.18801900 0.26438300
 C 2.35049300 -1.17547800 -0.20053400
 C 3.93194500 1.10513200 0.09003700
 H 2.09785600 2.13967900 0.52399400
 C 3.73179800 -1.25532600 -0.36934000
 H 1.72338400 -2.05250300 -0.31437100
 C 4.52723100 -0.11761200 -0.22730500
 H 4.54313000 1.99573400 0.20627500
 H 4.18689900 -2.20993700 -0.61828800
 H 5.60320100 -0.18197100 -0.36167400
 N -0.52624300 -1.08936600 0.32271900
 H -0.01895800 -0.38962000 1.38056100
 Zero-point correction= 0.206009 (Hartree/Particle)
 Thermal correction to Energy= 0.216700
 Thermal correction to Enthalpy= 0.217644
 Thermal correction to Gibbs Free Energy= 0.168572
 Sum of electronic and zero-point Energies= -594.638074
 Sum of electronic and thermal Energies= -594.627384
 Sum of electronic and thermal Enthalpies= -594.626439
 Sum of electronic and thermal Free Energies= -594.675512
 B3LYP-D3/6-311++G(d,p)/SMD//B3LYP-D3/6-31G(d) energy = -595.0121062
³TS1b
 C 3.45753200 -0.66375400 -0.12100600
 C 2.24648200 0.00469400 0.04796900
 H 3.43744900 -1.67671100 -0.52161800
 H 2.27654200 1.02449900 0.43036100
 C 4.79039000 -0.08118200 0.21105900
 H 5.31638300 -0.68549600 0.96493700
 H 5.44795500 -0.05263500 -0.67021100
 H 4.69998200 0.93871400 0.59888100
 C 1.00842500 -0.53719900 -0.24097900
 C -0.25192100 0.20053600 -0.11622500
 H 0.93158900 -1.56214600 -0.58818000
 C -1.54987300 -0.48161700 0.01451100
 O -2.62184900 0.10123700 0.05558800
 O -1.41943300 -1.82803000 0.03397200
 C -2.65632000 -2.55172900 0.12119400
 H -3.19845600 -2.27331600 1.02861500
 H -3.28553300 -2.33955800 -0.74726200
 H -2.37623500 -3.60474600 0.14636500
 N -0.19004200 1.52603200 -0.15908600
 N -1.25820800 2.26569900 -0.18521300
 N -1.86428000 3.16644800 0.22179700
 Zero-point correction= 0.156080 (Hartree/Particle)

Thermal correction to Energy= 0.169185
 Thermal correction to Enthalpy= 0.170129
 Thermal correction to Gibbs Free Energy= 0.114438
 Sum of electronic and zero-point Energies= -586.588334
 Sum of electronic and thermal Energies= -586.575229
 Sum of electronic and thermal Enthalpies= -586.574285
 Sum of electronic and thermal Free Energies= -586.629976
 B3LYP-D3/6-311++G(d,p)/SMD//B3LYP-D3/6-31G(d) energy = -586.9183429
³INT2b
 C -3.06244600 -0.71181300 0.00002300
 C -2.05467800 0.20802600 -0.00000300
 H -2.79822600 -1.76985900 0.00004700
 H -2.30707800 1.26722500 -0.00002500
 C -4.51855800 -0.37959400 0.00001200
 H -5.02097900 -0.80589700 -0.87948000
 H -5.02100800 -0.80596000 0.87945500
 H -4.68652900 0.70178000 0.00004500
 C -0.68511900 -0.14205400 -0.00000900
 C 0.37193700 0.81877100 -0.00004600
 H -0.40530400 -1.18964500 0.00001800
 C 1.82177600 0.35857200 -0.00000900
 O 2.77384300 1.10219200 0.00006900
 O 1.91418600 -0.98862400 -0.00004000
 C 3.25758700 -1.50114000 0.00000300
 H 3.15483500 -2.58612500 -0.00009100
 H 3.79348500 -1.16152700 -0.88971900
 H 3.79337000 -1.16167400 0.88985300
 N 0.17288700 2.09979100 -0.00002300
 Zero-point correction= 0.148285 (Hartree/Particle)
 Thermal correction to Energy= 0.159645
 Thermal correction to Enthalpy= 0.160589
 Thermal correction to Gibbs Free Energy= 0.108904
 Sum of electronic and zero-point Energies= -477.138037
 Sum of electronic and thermal Energies= -477.126677
 Sum of electronic and thermal Enthalpies= -477.125733
 Sum of electronic and thermal Free Energies= -477.177418
 B3LYP-D3/6-311++G(d,p)/SMD//B3LYP-D3/6-31G(d) energy = -477.4359944
³TS2b
 C 2.72019400 -0.01628900 -0.00002400
 C 1.93202000 -1.12916500 0.00009800
 H 1.75015000 1.07574800 -0.00006300
 H 2.37650100 -2.12785400 0.00018200
 C 4.18516700 0.17107800 -0.00007900
 H 4.51189600 0.73957700 -0.88102700
 H 4.51193800 0.73981000 0.88070200
 H 4.71576100 -0.79279100 0.00003200

C 0.52931700 -1.00888200 0.00011600
 C -0.06539500 0.30618000 0.00002200
 H -0.11267800 -1.87965600 0.00019900
 C -1.57450200 0.45538300 0.00003200
 O -2.16712900 1.50730000 0.00014100
 O -2.18526000 -0.75284800 -0.00009800
 C -3.62052700 -0.70213000 -0.00009500
 H -3.94984800 -1.74121300 -0.00020800
 H -3.98306800 -0.18050200 0.88930700
 H -3.98306400 -0.18031000 -0.88938700
 N 0.62055500 1.40778900 -0.00007100
 Zero-point correction= 0.142762 (Hartree/Particle)
 Thermal correction to Energy= 0.153429
 Thermal correction to Enthalpy= 0.154373
 Thermal correction to Gibbs Free Energy= 0.104577
 Sum of electronic and zero-point Energies= -477.107149
 Sum of electronic and thermal Energies= -477.096482
 Sum of electronic and thermal Enthalpies= -477.095537
 Sum of electronic and thermal Free Energies= -477.145334
 B3LYP-D3/6-311++G(d,p)/SMD//B3LYP-D3/6-31G(d) energy = -477.4036136
³TS3b
 C 2.48544100 0.08189000 -0.41138900
 C 1.92572700 1.22698800 0.17513100
 H 2.19314800 -0.14216000 -1.43674700
 H 2.44051100 1.74899100 0.98070800
 C 3.81410400 -0.48280100 -0.00310500
 H 3.78391500 -1.57516600 -0.06165600
 H 4.60654100 -0.13861200 -0.68022100
 H 4.07824600 -0.19770300 1.01939700
 C 0.46942400 1.24078900 0.10607900
 C -0.00547000 -0.06302900 0.04901600
 H -0.16280400 2.10712800 0.25894400
 C -1.45291300 -0.43524500 0.05373500
 O -1.88176400 -1.55974300 0.18658700
 O -2.23527900 0.65669200 -0.12210800
 C -3.64611200 0.39165000 -0.12678300
 H -3.90188400 -0.30190300 -0.93201400
 H -3.95754300 -0.04315500 0.82669100
 H -4.12454900 1.35846800 -0.28406800
 N 0.91993700 -1.05041800 0.10528900
 Zero-point correction= 0.147590 (Hartree/Particle)
 Thermal correction to Energy= 0.157973
 Thermal correction to Enthalpy= 0.158917
 Thermal correction to Gibbs Free Energy= 0.110204
 Sum of electronic and zero-point Energies= -477.092398

Sum of electronic and thermal Energies= -477.082015
 Sum of electronic and thermal Enthalpies= -477.081071
 Sum of electronic and thermal Free Energies= -477.129784
 B3LYP-D3/6-311++G(d,p)/SMD//B3LYP-D3/6-31G(d) energy = -477.3900854

3INT4b

C -2.88093900 -0.03854800 -0.00004300
 C -1.97994500 -1.04895300 -0.00020100
 H 0.12308000 2.25957800 -0.00011100
 H -2.36032100 -2.07855200 -0.00033300
 C -4.34301800 0.08290700 0.00034500
 H -4.69359400 0.63573800 0.88232700
 H -4.69402500 0.63721000 -0.88053100
 H -4.83808400 -0.90292300 -0.00034200
 C -0.57818300 -0.90188700 -0.00026200
 C 0.08922100 0.36501100 -0.00018700
 H 0.03509500 -1.79429900 -0.00035000
 C 1.60574100 0.40526400 -0.00001900
 O 2.23762400 1.44208200 0.00006700
 O 2.17527000 -0.81446400 0.00004700
 C 3.61275100 -0.81809600 0.00022800
 H 3.90206000 -1.86883400 0.00010900
 H 3.99384900 -0.31065300 -0.88946900
 H 3.99362100 -0.31092200 0.89017600
 N -0.55980000 1.49121800 -0.00022100
 Zero-point correction= 0.148326 (Hartree/Particle)

Thermal correction to Energy= 0.159598
 Thermal correction to Enthalpy= 0.160542
 Thermal correction to Gibbs Free Energy= 0.109590
 Sum of electronic and zero-point Energies= -477.112041
 Sum of electronic and thermal Energies= -477.100769
 Sum of electronic and thermal Enthalpies= -477.099825
 Sum of electronic and thermal Free Energies= -477.150777
 B3LYP-D3/6-311++G(d,p)/SMD//B3LYP-D3/6-31G(d) energy = -477.4132621

P2

C -2.25387500 0.02832000 0.00040600
 C -1.95079400 -1.33037100 0.00047400
 H -0.93055300 1.70506800 0.00016200
 H -2.68050600 -2.12882200 0.00065900
 C -3.57244700 0.72992800 -0.00027600
 H -3.69562300 1.36983000 0.88289700
 H -3.69774100 1.36433200 -0.88714800
 H -4.38420500 -0.00202800 0.00295800
 C -0.54311300 -1.46418500 -0.00015600
 C -0.00986200 -0.18256500 -0.00031800
 H 0.03240100 -2.37838800 -0.00064700
 C 1.34033900 0.35091700 -0.00005000

O 1.59905400 1.54588500 0.00017800
 O 2.28091600 -0.62176000 -0.00038500
 C 3.63455800 -0.15065500 0.00018900
 H 4.25526700 -1.04711400 0.00112600
 H 3.83366100 0.45348300 -0.88921400
 H 3.83254600 0.45463400 0.88905000
 N -1.06769200 0.70395300 0.00002700
 Zero-point correction= 0.154262 (Hartree/Particle)
 Thermal correction to Energy= 0.164290
 Thermal correction to Enthalpy= 0.165234
 Thermal correction to Gibbs Free Energy= 0.118411
 Sum of electronic and zero-point Energies= -477.250672
 Sum of electronic and thermal Energies= -477.240643
 Sum of electronic and thermal Enthalpies= -477.239699
 Sum of electronic and thermal Free Energies= -477.286523
 B3LYP-D3/6-311++G(d,p)/SMD//B3LYP-D3/6-31G(d) energy = -477.5573178
INT3b
 C -3.07511400 -0.29054600 -0.34141600
 C -1.92243300 0.13737000 0.18552700
 H -3.25465800 -0.12925800 -1.40564500
 H -1.71909900 -0.00876800 1.24650900
 C -4.16142600 -0.98976500 0.41853100
 H -5.10743700 -0.43541300 0.35676000
 H -4.35602900 -1.98903400 0.00618300
 H -3.90216900 -1.10311000 1.47623500
 C -0.86908800 0.80824300 -0.59303900
 C 0.50818800 0.89400900 -0.13978900
 H -1.08182200 0.97322500 -1.64896600
 C 1.85005500 0.29872100 0.09185400
 O 2.79684600 0.90617700 0.53463700
 O 1.84749000 -0.99582600 -0.26598100
 C 3.10120600 -1.67797200 -0.07860800
 H 2.92662400 -2.70165300 -0.40756100
 H 3.88270800 -1.20433800 -0.67799100
 H 3.39282900 -1.65190500 0.97429900
 N -0.07485100 1.98387000 0.09608100
 Zero-point correction= 0.150438 (Hartree/Particle)
 Thermal correction to Energy= 0.161605
 Thermal correction to Enthalpy= 0.162550
 Thermal correction to Gibbs Free Energy= 0.112028
 Sum of electronic and zero-point Energies= -477.147585
 Sum of electronic and thermal Energies= -477.136417
 Sum of electronic and thermal Enthalpies= -477.135473
 Sum of electronic and thermal Free Energies= -477.185994
 B3LYP-D3/6-311++G(d,p)/SMD//B3LYP-D3/6-31G(d) energy = -477.4497889
TS4b

C -2.47594300 -0.29252700 0.18720500
 C -1.89691300 -0.21966400 -1.00171800
 H -1.78655400 0.74631200 0.90335100
 H -2.12001700 -0.83338500 -1.87214900
 C -3.58793900 -1.10207400 0.74299400
 H -3.27513900 -1.64812400 1.64169400
 H -4.42609400 -0.45886600 1.04000800
 H -3.96284700 -1.82870900 0.01018400
 C -0.84957400 0.85943000 -1.10197800
 C 0.26600900 0.85983800 -0.18773700
 H -0.84743500 1.51276600 -1.97207800
 C 1.53507000 0.29076000 0.31090200
 O 2.02254200 0.55322200 1.38723000
 O 2.06259200 -0.54194500 -0.60347100
 C 3.30344800 -1.15744000 -0.21429200
 H 3.58799500 -1.79277500 -1.05228200
 H 4.06355100 -0.39425800 -0.02901100
 H 3.16427900 -1.75052600 0.69311200
 N -0.69196500 1.56105900 0.27926200
 Zero-point correction= 0.144495 (Hartree/Particle)
 Thermal correction to Energy= 0.155157
 Thermal correction to Enthalpy= 0.156102
 Thermal correction to Gibbs Free Energy= 0.105379
 Sum of electronic and zero-point Energies= -477.090577
 Sum of electronic and thermal Energies= -477.079914
 Sum of electronic and thermal Enthalpies= -477.078970
 Sum of electronic and thermal Free Energies= -477.129692
 B3LYP-D3/6-311++G(d,p)/SMD//B3LYP-D3/6-31G(d) energy = -477.3862529
³TS1c
 C -3.17525600 -1.01784800 -0.37767000
 C -1.83792300 -1.31732900 -0.12773900
 C -0.96988100 -0.28792100 0.22663000
 C -1.40208100 1.03091900 0.34974500
 C -2.74530300 1.31166400 0.09455600
 C -3.63138400 0.29750800 -0.26947700
 H -3.85897500 -1.81393000 -0.65626300
 H -1.45670500 -2.33018400 -0.20089300
 H -0.71243300 1.81531800 0.62853100
 H -3.09608000 2.33534300 0.18407200
 H -4.67348700 0.53017800 -0.46590500
 O 0.33946200 -0.69869700 0.52033200
 C 1.39945100 0.05543600 0.17942000
 O 1.40319200 1.15145600 -0.33150900
 N 2.56544200 -0.63031800 0.61370900
 N 3.63787400 -0.46499100 -0.44262800

N 4.37249900 0.43911200 -0.37864200
 Zero-point correction= 0.112874 (Hartree/Particle)
 Thermal correction to Energy= 0.123231
 Thermal correction to Enthalpy= 0.124175
 Thermal correction to Gibbs Free Energy= 0.073094
 Sum of electronic and zero-point Energies= -584.228778
 Sum of electronic and thermal Energies= -584.218420
 Sum of electronic and thermal Enthalpies= -584.217476
 Sum of electronic and thermal Free Energies= -584.268557
 B3LYP-D3/6-311++G(d,p)/SMD//B3LYP-D3/6-31G(d) energy = -584.5089

³INT2c

C 2.12177600 -1.20983800 0.09156700
 C 0.77408400 -1.21625300 -0.26845700
 C 0.12230100 0.00045400 -0.43826700
 C 0.77458400 1.21674000 -0.26740400
 C 2.12227600 1.20945600 0.09260200
 C 2.79537500 -0.00040800 0.27299200
 H 2.64371400 -2.15174400 0.22992000
 H 0.23046800 -2.14267500 -0.42152400
 H 0.23133600 2.14351200 -0.41965200
 H 2.64460600 2.15102600 0.23176400
 H 3.84429100 -0.00074500 0.55306500
 O -1.22363100 0.00094400 -0.85414600
 C -2.16370700 -0.00003500 0.11980000
 O -3.35503000 0.00014900 -0.13603100
 N -1.74932400 -0.00125800 1.44726300

Zero-point correction= 0.105700 (Hartree/Particle)
 Thermal correction to Energy= 0.113003
 Thermal correction to Enthalpy= 0.113947
 Thermal correction to Gibbs Free Energy= 0.071921
 Sum of electronic and zero-point Energies= -474.758262
 Sum of electronic and thermal Energies= -474.750960
 Sum of electronic and thermal Enthalpies= -474.750016
 Sum of electronic and thermal Free Energies= -474.792042
 B3LYP-D3/6-311++G(d,p)/SMD//B3LYP-D3/6-31G(d) energy = -475.0067589

³TS3c

C 2.36574500 0.85777500 -0.30116500
 C 1.10424800 1.42427900 -0.04688100
 C 0.08880500 0.59264500 0.36054900
 C 0.25062600 -0.82580100 0.52656800
 C 1.53597600 -1.36970600 0.21107000
 C 2.55741200 -0.53292400 -0.20513700
 H 3.18527400 1.49655900 -0.61391000
 H 0.90736000 2.47765900 -0.21434500
 H -0.31209800 -1.31290100 1.32571400

H 1.70677900 -2.43287500 0.34250400
 H 3.53472800 -0.95084300 -0.42748200
 O -1.23257700 0.98672600 0.38125300
 C -2.00718700 -0.04970900 -0.15131100
 O -3.21159700 0.02931100 -0.18436000
 N -1.26320000 -1.14074900 -0.62139700
 Zero-point correction= 0.104859 (Hartree/Particle)
 Thermal correction to Energy= 0.112021
 Thermal correction to Enthalpy= 0.112965
 Thermal correction to Gibbs Free Energy= 0.071694
 Sum of electronic and zero-point Energies= -474.734273
 Sum of electronic and thermal Energies= -474.727111
 Sum of electronic and thermal Enthalpies= -474.726167
 Sum of electronic and thermal Free Energies= -474.767438
 B3LYP-D3/6-311++G(d,p)/SMD//B3LYP-D3/6-31G(d) energy = -474.9658379
³TS2c
 C -2.50809300 -0.92979000 -0.00001000
 C -1.18457300 -1.37116800 -0.00002900
 C -0.16100100 -0.42115300 -0.00001400
 C -0.48974400 0.92277300 0.00002400
 C -1.78938700 1.38616400 0.00004300
 C -2.81783600 0.43347000 0.00002500
 H -3.30887100 -1.66293100 -0.00002200
 H 0.87438700 1.57183900 -0.00003200
 H -2.01358200 2.44877100 0.00007300
 H -3.85356400 0.75983300 0.00003800
 O 1.14394400 -0.87088000 -0.00002900
 C 2.20008400 0.01167600 -0.00000600
 O 3.33041600 -0.44883400 0.00009900
 N 1.99181900 1.38215800 -0.00011000
 H -0.93268400 -2.42674000 -0.00005300
 Zero-point correction= 0.099820 (Hartree/Particle)
 Thermal correction to Energy= 0.107437
 Thermal correction to Enthalpy= 0.108381
 Thermal correction to Gibbs Free Energy= 0.065323
 Sum of electronic and zero-point Energies= -474.720179
 Sum of electronic and thermal Energies= -474.712562
 Sum of electronic and thermal Enthalpies= -474.711618
 Sum of electronic and thermal Free Energies= -474.754676
 B3LYP-D3/6-311++G(d,p)/SMD//B3LYP-D3/6-31G(d) energy = -474.9847452
³INT3c
 C 2.44651100 -0.94976000 0.30572900
 C 1.10697100 -1.31519200 0.16181300
 C 0.16988100 -0.34574100 -0.20437800
 C 0.61049100 0.94109700 -0.42266400
 C 1.91715500 1.34489100 -0.27432100

C 2.85639100 0.36927900 0.09527400
 H 3.17480600 -1.70358400 0.58848000
 H 0.77333400 -2.33572600 0.32457400
 H -2.58309300 1.41820500 1.31889800
 H 2.21810900 2.37465000 -0.44540300
 H 3.90072500 0.64376100 0.21434600
 O -1.14593400 -0.76996900 -0.39210200
 C -2.17323500 -0.01244200 0.04849000
 O -3.32590600 -0.37359100 -0.14611600
 N -1.90202200 1.22262500 0.57788500
 Zero-point correction= 0.104567 (Hartree/Particle)
 Thermal correction to Energy= 0.112906
 Thermal correction to Enthalpy= 0.113850
 Thermal correction to Gibbs Free Energy= 0.069284
 Sum of electronic and zero-point Energies= -474.721799
 Sum of electronic and thermal Energies= -474.713461
 Sum of electronic and thermal Enthalpies= -474.712516
 Sum of electronic and thermal Free Energies= -474.757083
 B3LYP-D3/6-311++G(d,p)/SMD//B3LYP-D3/6-31G(d) energy = -474.97541
³INT4c
 C 2.43943600 0.76701800 -0.12909000
 C 1.20399000 1.45820400 0.00619700
 C 0.09364200 0.71055700 0.22925500
 C 0.09453500 -0.77155200 0.45077000
 C 1.35643400 -1.42730400 -0.01981800
 C 2.46869400 -0.65244900 -0.21077200
 H 3.35263900 1.33236000 -0.27775500
 H 1.13602200 2.53059700 -0.14360000
 H -0.02828600 -0.97734000 1.54827200
 H 1.37613200 -2.50788200 -0.10785400
 H 3.41020200 -1.13505200 -0.45930000
 O -1.21511300 1.11051400 0.12548100
 C -1.97893100 -0.04162700 -0.10261300
 O -3.17030300 0.00284700 -0.26193900
 N -1.17573900 -1.20095000 -0.11595500
 Zero-point correction= 0.105501 (Hartree/Particle)
 Thermal correction to Energy= 0.112778
 Thermal correction to Enthalpy= 0.113722
 Thermal correction to Gibbs Free Energy= 0.072409
 Sum of electronic and zero-point Energies= -474.757738
 Sum of electronic and thermal Energies= -474.750461
 Sum of electronic and thermal Enthalpies= -474.749517
 Sum of electronic and thermal Free Energies= -474.790831
 B3LYP-D3/6-311++G(d,p)/SMD//B3LYP-D3/6-31G(d) energy = -475.0083716
³TS4c
 C 2.47359100 0.76733000 -0.04715900

C 1.22648700 1.47573900 0.02220100
 C 0.10653100 0.72679000 0.14191000
 C 0.12339100 -0.74976100 0.26921200
 C 1.38787200 -1.44610900 -0.01852800
 C 2.49972300 -0.67549500 -0.14647900
 H 3.40213300 1.32151900 -0.11296600
 H 1.18220400 2.55506200 -0.06845300
 H -0.80935900 -1.40515700 1.07683800
 H 1.40572200 -2.52656500 -0.09814200
 H 3.45613300 -1.15323200 -0.34062300
 O -1.19663200 1.12208600 0.06153600
 C -2.00156400 -0.04147100 -0.07560100
 O -3.19313600 0.03809500 -0.17204200
 N -1.20212400 -1.20217300 -0.06370700
 Zero-point correction= 0.099701 (Hartree/Particle)
 Thermal correction to Energy= 0.107156
 Thermal correction to Enthalpy= 0.108100
 Thermal correction to Gibbs Free Energy= 0.066562
 Sum of electronic and zero-point Energies= -474.690982
 Sum of electronic and thermal Energies= -474.683527
 Sum of electronic and thermal Enthalpies= -474.682583
 Sum of electronic and thermal Free Energies= -474.724121
 B3LYP-D3/6-311++G(d,p)/SMD//B3LYP-D3/6-31G(d) energy = -474.9428637

P3

C 2.49879600 -0.72613600 -0.00002600
 C 1.28567000 -1.43104100 0.00010700
 C 0.13100200 -0.67483700 0.00002000
 C 0.14792800 0.72478100 -0.00002800
 C 1.34424400 1.42689800 -0.00007400
 C 2.52520000 0.67134400 -0.00007500
 H 3.43209700 -1.27998900 -0.00008700
 H 1.24721600 -2.51445800 0.00014600
 H -1.56932400 2.03719700 -0.00053200
 H 1.36805800 2.51175200 -0.00005700
 H 3.47998000 1.18780500 -0.00011600
 O -1.17309400 -1.12141300 -0.00004900
 C -2.01591600 -0.01056300 -0.00002300
 O -3.21635900 -0.07135200 -0.00014000
 N -1.19199200 1.10244900 0.00039400
 Zero-point correction= 0.110806 (Hartree/Particle)
 Thermal correction to Energy= 0.117750
 Thermal correction to Enthalpy= 0.118694
 Thermal correction to Gibbs Free Energy= 0.079269
 Sum of electronic and zero-point Energies= -474.890635
 Sum of electronic and thermal Energies= -474.883692

Sum of electronic and thermal Enthalpies= -474.882748
 Sum of electronic and thermal Free Energies= -474.922173
 B3LYP-D3/6-311++G(d,p)/SMD//B3LYP-D3/6-31G(d) energy = -475.1523867
H₃PO₄
 P 0.00001300 -0.00009300 0.11818500
 O 1.30987400 -0.60659800 -0.59603200
 H 2.10617600 -0.38684000 -0.08473900
 O -0.12915000 1.43836300 -0.59445800
 H -0.71842800 2.01738400 -0.08329200
 O -1.18069800 -0.83035200 -0.59615000
 H -1.38845100 -1.63030300 -0.08554300
 O 0.00003700 -0.00126800 1.59673900
 Zero-point correction= 0.048227 (Hartree/Particle)
 Thermal correction to Energy= 0.054522
 Thermal correction to Enthalpy= 0.055466
 Thermal correction to Gibbs Free Energy= 0.018636
 Sum of electronic and zero-point Energies= -644.093180
 Sum of electronic and thermal Energies= -644.086885
 Sum of electronic and thermal Enthalpies= -644.085941
 Sum of electronic and thermal Free Energies= -644.122771
 B3LYP-D3/6-311++G(d,p)/SMD//B3LYP-D3/6-31G(d) energy = -644.310954
INT1a
 C 4.21376700 -0.97907000 -0.20773000
 C 3.51617200 0.22293900 -0.21013500
 C 2.13103200 0.22873000 0.01810300
 C 1.45266600 -0.97289700 0.27104100
 C 2.16218000 -2.17182100 0.27986200
 C 3.53634700 -2.17812300 0.03565900
 H 5.28362200 -0.98480400 -0.39335600
 H 4.01990500 1.16648800 -0.39040000
 H 0.39101900 -0.98630300 0.49014100
 H 1.63505400 -3.09852500 0.48385700
 H 4.08332600 -3.11678200 0.03964700
 C 1.44984400 1.53907400 0.00859400
 O 1.99213900 2.62263200 0.05428000
 N 0.00819500 1.41157700 -0.08700500
 N -0.60994600 2.49175800 0.03922000
 N -1.24380000 3.41999200 0.15129000
 P -2.51634800 -0.85457200 0.01013100
 O -3.82295800 -1.58642600 -0.58478000
 H -3.77675100 -2.53596700 -0.38671900
 O -1.74639400 -0.42454700 -1.31601500
 H -0.99107400 0.16422300 -1.08074100
 O -3.06741000 0.57624100 0.53500700
 H -3.31754500 0.51596000 1.47200300
 O -1.78482000 -1.65064900 1.02609600

Zero-point correction= 0.164142 (Hartree/Particle)
 Thermal correction to Energy= 0.180675
 Thermal correction to Enthalpy= 0.181620
 Thermal correction to Gibbs Free Energy= 0.117114
 Sum of electronic and zero-point Energies= -1153.208801
 Sum of electronic and thermal Energies= -1153.192268
 Sum of electronic and thermal Enthalpies= -1153.191323
 Sum of electronic and thermal Free Energies= -1153.255829
 B3LYP-D3/6-311++G(d,p)/SMD//B3LYP-D3/6-31G(d) energy = -1153.6793141
INT1a*

C -4.23151500 -1.01482100 0.14535600
 C -3.57398300 0.18027100 0.11661700
 C -2.08917800 0.21799400 -0.02956300
 C -1.38684600 -1.03103300 -0.25851000
 C -2.07420600 -2.19857300 -0.22666200
 C -3.52214200 -2.23379600 -0.00130700
 H -5.30963100 -1.03628200 0.27463900
 H -4.08228100 1.13076600 0.21565100
 H -0.32301500 -1.03478400 -0.46367800
 H -1.54686400 -3.13383800 -0.38827800
 H -4.03941300 -3.18604900 0.02027800
 C -1.46234300 1.49275700 0.04023400
 O -2.08461700 2.57330000 0.06249300
 N -0.01639200 1.44739700 0.06134100
 N 0.54272200 2.55605900 -0.06669500
 N 1.13126700 3.51966100 -0.17413800
 P 2.54068100 -0.83812200 -0.00677500
 O 3.83717200 -1.54977300 0.63512400
 H 3.79839400 -2.50286300 0.45410900
 O 1.77789900 -0.31663400 1.28729400
 H 1.04637700 0.29308400 1.01664000
 O 3.10227700 0.54696400 -0.63013600
 H 3.30348000 0.43211200 -1.57362400
 O 1.80237300 -1.69497400 -0.96910500

Zero-point correction= 0.158418 (Hartree/Particle)
 Thermal correction to Energy= 0.175861
 Thermal correction to Enthalpy= 0.176805
 Thermal correction to Gibbs Free Energy= 0.109169
 Sum of electronic and zero-point Energies= -1153.094920
 Sum of electronic and thermal Energies= -1153.077477
 Sum of electronic and thermal Enthalpies= -1153.076533
 Sum of electronic and thermal Free Energies= -1153.144169
 B3LYP-D3/6-311++G(d,p)/SMD//B3LYP-D3/6-31G(d) energy = -1153.561
INT1a⁻
 C 4.22655400 -0.89654100 0.29031300

C 3.49461400 0.28808900 0.27691000
 C 2.12876000 0.28042300 -0.03250700
 C 1.50502800 -0.93381100 -0.35290100
 C 2.24260100 -2.11859700 -0.34496200
 C 3.59988800 -2.10665100 -0.01995100
 H 5.28546500 -0.87871900 0.53962400
 H 3.95641100 1.24503400 0.49791500
 H 0.45488200 -0.96525800 -0.61971100
 H 1.74631400 -3.05206600 -0.59758800
 H 4.16900700 -3.03394500 -0.01259500
 C 1.40817400 1.61020500 -0.03652200
 O 2.05042900 2.66291300 -0.07350600
 N 0.04761900 1.46542100 0.00607800
 N -0.63266300 2.66788100 -0.09453800
 N -1.81602200 2.78208900 -0.10158100
 P -2.47544200 -0.84734500 -0.01143800
 O -1.51946900 -0.28050000 1.11332700
 H -0.80597400 0.37140800 0.70443400
 O -3.60975900 -1.66043200 0.83887400
 H -3.52867900 -2.58697300 0.56427300
 O -3.31334300 0.40798900 -0.56640500
 H -2.86730100 1.27212900 -0.36441600
 O -1.87095000 -1.73095500 -1.04883500
 Zero-point correction= 0.161359 (Hartree/Particle)
 Thermal correction to Energy= 0.177127
 Thermal correction to Enthalpy= 0.178071
 Thermal correction to Gibbs Free Energy= 0.115759
 Sum of electronic and zero-point Energies= -1153.283592
 Sum of electronic and thermal Energies= -1153.267824
 Sum of electronic and thermal Enthalpies= -1153.266880
 Sum of electronic and thermal Free Energies= -1153.329193
 B3LYP-D3/6-311++G(d,p)/SMD//B3LYP-D3/6-31G(d) energy = -1153.8173834
INT1a⁺⁺
 C -1.40735400 2.79286300 -0.72004000
 C -0.12444600 2.22054000 -0.94121000
 C 0.44704800 1.39143100 0.00582200
 C -0.25367000 1.13580500 1.21380500
 C -1.53315600 1.75269600 1.44045500
 C -2.10206200 2.56242500 0.47057800
 H -1.84125000 3.42261400 -1.49032600
 H 0.42512000 2.44295600 -1.85002000
 H 0.24537400 0.63103800 2.03049000
 H -2.04356000 1.54901100 2.37428500
 H -3.07509900 3.01236100 0.63298200
 C 1.81107800 0.85372700 -0.26627800

O 2.57148000 1.32987300 -1.07532500
 N 2.09896000 -0.31099800 0.52153900
 N 3.30249300 -0.68963100 0.41613000
 N 4.35612600 -1.08248600 0.38431200
 P -1.28323900 -1.60861900 -0.11198500
 O 0.16625900 -2.23284100 -0.28904500
 H 0.87528800 -1.68179800 0.12919000
 O -1.65807500 -0.72645800 -1.38436700
 H -1.73605600 -1.22973200 -2.21486800
 O -2.26212100 -2.85200200 -0.23123800
 H -2.01110700 -3.63013300 0.29811300
 O -1.43226800 -0.77634100 1.14213400
 Zero-point correction= 0.162925 (Hartree/Particle)
 Thermal correction to Energy= 0.179256
 Thermal correction to Enthalpy= 0.180200
 Thermal correction to Gibbs Free Energy= 0.116983
 Sum of electronic and zero-point Energies= -1152.900270
 Sum of electronic and thermal Energies= -1152.883938
 Sum of electronic and thermal Enthalpies= -1152.882994
 Sum of electronic and thermal Free Energies= -1152.946211
 B3LYP-D3/6-311++G(d,p)/SMD//B3LYP-D3/6-31G(d) energy = -1153.426
INT1b
 C -3.99253000 -1.50774900 -0.45538600
 C -2.73689400 -1.03258100 -0.81549400
 C -2.22883100 0.12781900 -0.21220300
 C -2.98496300 0.80620000 0.75475700
 C -4.24143300 0.32524500 1.11102400
 C -4.74539200 -0.82913100 0.50726900
 H -4.38579000 -2.40609400 -0.92125000
 H -2.13315700 -1.54234300 -1.55801700
 H -2.58157400 1.69738600 1.22145500
 H -4.82712500 0.84794700 1.86096100
 H -5.72602500 -1.20219800 0.78866500
 C -0.89055700 0.58770900 -0.62305100
 O -0.19751100 0.02012000 -1.45811400
 N -0.49382100 1.79006900 0.02443500
 N 0.66139900 2.16708100 -0.21477800
 N 1.69627100 2.60158800 -0.36968300
 P 2.68416200 -0.66817000 0.30769800
 O 2.26592400 -1.15213300 -1.15066400
 H 1.37264500 -0.79996300 -1.37248800
 O 3.47039300 -1.97496800 0.81379900
 H 4.02863700 -1.76802300 1.58052300
 O 3.91640700 0.37543500 0.14414700
 H 3.58011200 1.28742200 0.19069300

O 1.58060000 -0.12693200 1.13991500
 Zero-point correction= 0.164478 (Hartree/Particle)
 Thermal correction to Energy= 0.180771
 Thermal correction to Enthalpy= 0.181715
 Thermal correction to Gibbs Free Energy= 0.117064
 Sum of electronic and zero-point Energies= -1153.213665
 Sum of electronic and thermal Energies= -1153.197371
 Sum of electronic and thermal Enthalpies= -1153.196427
 Sum of electronic and thermal Free Energies= -1153.261078
 B3LYP-D3/6-311++G(d,p)/SMD//B3LYP-D3/6-31G(d) energy = -1153.681135
INT1b*

C 3.87313600 -1.51481700 0.52531000
 C 2.66122700 -1.01091500 0.88851600
 C 2.12404800 0.20557400 0.21859900
 C 2.91012700 0.82006800 -0.83787000
 C 4.11105900 0.29367200 -1.17457300
 C 4.63931300 -0.89415100 -0.49943400
 H 4.26173600 -2.40137100 1.01722000
 H 2.04813200 -1.45864900 1.65983900
 H 2.50864600 1.69191800 -1.33925400
 H 4.70405600 0.74730200 -1.96302000
 H 5.60366200 -1.29274300 -0.79212600
 C 0.85504700 0.69515500 0.64221400
 O 0.18192000 0.14572300 1.54670400
 N 0.43160400 1.86881100 -0.04226800
 N -0.72771400 2.22815800 0.17913900
 N -1.77982900 2.64020000 0.32412000
 P -2.56310000 -0.72574100 -0.31145900
 O -2.12290000 -1.22433900 1.13429100
 H -1.26747000 -0.79339400 1.38461200
 O -3.36801200 -2.02691300 -0.80839200
 H -3.96964000 -1.79880300 -1.53500600
 O -3.78591100 0.32628200 -0.13345100
 H -3.44177500 1.23699500 -0.18150700
 O -1.46922200 -0.19235800 -1.16195200
 Zero-point correction= 0.159093 (Hartree/Particle)
 Thermal correction to Energy= 0.176170
 Thermal correction to Enthalpy= 0.177114
 Thermal correction to Gibbs Free Energy= 0.110383
 Sum of electronic and zero-point Energies= -1153.100775
 Sum of electronic and thermal Energies= -1153.083698
 Sum of electronic and thermal Enthalpies= -1153.082754
 Sum of electronic and thermal Free Energies= -1153.149485
 B3LYP-D3/6-311++G(d,p)/SMD//B3LYP-D3/6-31G(d) energy = -1153.68049
INT1c

C 1.02891300 -2.78202900 0.16032100
 C 0.76645400 -1.41622600 0.15502200
 C 1.82435100 -0.50562200 0.00940100
 C 3.14248800 -0.97332800 -0.12632900
 C 3.39402000 -2.34099200 -0.12608900
 C 2.33824800 -3.24621500 0.01743200
 H 0.20388000 -3.47688900 0.28070500
 H -0.25330800 -1.07298500 0.27862500
 H 3.95517700 -0.26421300 -0.23457900
 H 4.41179800 -2.70286100 -0.23603800
 H 2.53939000 -4.31389700 0.02064600
 C 1.51731600 0.93432700 0.00757700
 O 0.39346800 1.42943400 -0.00576800
 N 2.67940200 1.75241500 0.03569100
 N 2.44669600 2.97952900 0.02496600
 N 2.35342900 4.10680400 0.02157900
 P -2.95107600 -0.07361600 0.01136200
 O -3.43292400 1.08132600 1.03231900
 H -3.75185300 0.68059300 1.85769800
 O -4.26958800 -0.35567500 -0.87705100
 H -4.27052300 -1.28402300 -1.16104100
 O -2.02541400 0.71886100 -1.00332100
 H -1.14637300 0.96328200 -0.61680100
 O -2.39672600 -1.28838300 0.66390700
 Zero-point correction= 0.164198 (Hartree/Particle)
 Thermal correction to Energy= 0.180746
 Thermal correction to Enthalpy= 0.181691
 Thermal correction to Gibbs Free Energy= 0.116179
 Sum of electronic and zero-point Energies= -1153.213152
 Sum of electronic and thermal Energies= -1153.196604
 Sum of electronic and thermal Enthalpies= -1153.195659
 Sum of electronic and thermal Free Energies= -1153.261171
 B3LYP-D3/6-311++G(d,p)/SMD//B3LYP-D3/6-31G(d) energy = -1153.68049
INT1c*
 C 1.01335000 -2.79509700 0.17144900
 C 0.73823700 -1.45823600 0.22230600
 C 1.83499800 -0.46042300 0.05319900
 C 3.18849700 -0.94804800 -0.11866900
 C 3.42281800 -2.28274600 -0.16356600
 C 2.33489400 -3.25898700 -0.02660500
 H 0.20026700 -3.50375600 0.29443300
 H -0.27253300 -1.11115900 0.39408200
 H 3.99148800 -0.22866300 -0.22129300
 H 4.43468700 -2.65204000 -0.30314300
 H 2.56005600 -4.31839700 -0.06724100

C 1.50888300 0.92977800 0.06898600
 O 0.34392700 1.38635400 0.18559700
 N 2.63940900 1.78557800 -0.03926600
 N 2.38261100 3.00343000 -0.02577100
 N 2.26451500 4.13391500 -0.02206600
 P -2.92114100 -0.08264100 -0.00805500
 O -3.44697400 1.07039700 0.99288600
 H -3.77340300 0.66933900 1.81499800
 O -4.20301600 -0.37559300 -0.94696600
 H -4.20104900 -1.31226000 -1.20151200
 O -1.95779600 0.70495500 -0.98636400
 H -1.10063000 0.97046100 -0.55224100
 O -2.39584000 -1.29759000 0.67107900
 Zero-point correction= 0.158426 (Hartree/Particle)
 Thermal correction to Energy= 0.175906
 Thermal correction to Enthalpy= 0.176850
 Thermal correction to Gibbs Free Energy= 0.108751
 Sum of electronic and zero-point Energies= -1153.100411
 Sum of electronic and thermal Energies= -1153.082932
 Sum of electronic and thermal Enthalpies= -1153.081987
 Sum of electronic and thermal Free Energies= -1153.150086
 B3LYP-D3/6-311++G(d,p)/SMD//B3LYP-D3/6-31G(d) energy = -1153.5652066
INT1d
 C 2.28763000 -2.39508600 0.28144200
 C 1.39236000 -1.33995900 0.41475400
 C 1.81709700 -0.02856400 0.14356400
 C 3.13964400 0.21109100 -0.26633800
 C 4.02982300 -0.84988700 -0.38972900
 C 3.60499700 -2.15246800 -0.11575300
 H 1.95568700 -3.40860800 0.48295200
 H 0.36521200 -1.53044100 0.69593500
 H 3.45946500 1.22468100 -0.47891800
 H 5.05317300 -0.66326700 -0.70000000
 H 4.30102900 -2.98029300 -0.21601100
 C 0.85903600 1.07555000 0.29391300
 O -0.25020700 0.98722200 0.82619000
 N 1.32594600 2.30029200 -0.23782500
 N 0.52801900 3.25544100 -0.11557600
 N -0.11558200 4.18372700 -0.06552400
 P -2.70096000 -0.79018800 -0.11937900
 O -2.88503200 0.81157900 -0.14425400
 H -2.05490300 1.26348400 0.10415200
 O -3.92778500 -1.54825300 -0.40662600
 O -1.48313600 -1.06569900 -1.17561400
 H -1.85199800 -1.48426000 -1.97048700

O -2.00001800 -1.11143000 1.29446300
 H -1.29605400 -0.45611800 1.48115600
 Zero-point correction= 0.164807 (Hartree/Particle)
 Thermal correction to Energy= 0.181076
 Thermal correction to Enthalpy= 0.182020
 Thermal correction to Gibbs Free Energy= 0.117937
 Sum of electronic and zero-point Energies= -1153.208792
 Sum of electronic and thermal Energies= -1153.192524
 Sum of electronic and thermal Enthalpies= -1153.191579
 Sum of electronic and thermal Free Energies= -1153.255662
 B3LYP-D3/6-311++G(d,p)/SMD//B3LYP-D3/6-31G(d) energy = -1153.6781965
INT1d*
 C 2.31227700 -2.27331900 0.60104600
 C 1.37621300 -1.27696100 0.70399100
 C 1.65429200 0.08131000 0.14478900
 C 2.88216600 0.27342600 -0.58547700
 C 3.78412000 -0.73864800 -0.67323200
 C 3.53141900 -2.05126000 -0.06373700
 H 2.09560700 -3.25245700 1.01661000
 H 0.41112400 -1.46080900 1.15131100
 H 3.07739500 1.24054700 -1.03151400
 H 4.71991900 -0.58599100 -1.20272900
 H 4.27250100 -2.83589900 -0.16060000
 C 0.72584200 1.14436000 0.36709700
 O -0.34351500 1.03732000 1.02912500
 N 1.10299600 2.36627300 -0.24113400
 N 0.30398300 3.30797200 -0.07824300
 N -0.35255800 4.23198500 0.00635200
 P -2.46988500 -0.91361300 -0.19810500
 O -2.73519000 0.66944100 -0.30737500
 H -1.99929100 1.16878400 0.10838500
 O -3.59180200 -1.75981000 -0.63405300
 O -1.10061900 -1.15464300 -1.06813200
 H -1.33703600 -1.61859300 -1.88781400
 O -1.95653300 -1.14638700 1.31007400
 H -1.34958800 -0.41579300 1.56512400
 Zero-point correction= 0.159716 (Hartree/Particle)
 Thermal correction to Energy= 0.176652
 Thermal correction to Enthalpy= 0.177596
 Thermal correction to Gibbs Free Energy= 0.111815
 Sum of electronic and zero-point Energies= -1153.097535
 Sum of electronic and thermal Energies= -1153.080599
 Sum of electronic and thermal Enthalpies= -1153.079655
 Sum of electronic and thermal Free Energies= -1153.145435
 B3LYP-D3/6-311++G(d,p)/SMD//B3LYP-D3/6-31G(d) energy = -1153.564

5

C -0.17437000 -1.12060500 -0.01540900

C -1.49089900 -0.71219800 0.01712000

C -1.49095800 0.71213800 0.01688500

C -0.17444500 1.12060600 -0.01525700

N 0.62516500 0.00002600 -0.04229300

H 0.26565400 -2.10779400 -0.02442200

H -2.35538100 -1.36204200 0.02385400

H -2.35548100 1.36192400 0.02341800

H 0.26554900 2.10780800 -0.02413000

C 2.07203900 -0.00000700 0.02811500

H 2.46252500 0.88903300 -0.47421900

H 2.42950100 -0.00464300 1.06527000

H 2.46327800 -0.88406700 -0.48244900

Zero-point correction= 0.110748 (Hartree/Particle)

Thermal correction to Energy= 0.116325

Thermal correction to Enthalpy= 0.117270

Thermal correction to Gibbs Free Energy= 0.081735

Sum of electronic and zero-point Energies= -249.385234

Sum of electronic and thermal Energies= -249.379657

Sum of electronic and thermal Enthalpies= -249.378713

Sum of electronic and thermal Free Energies= -249.414247

B3LYP-D3/6-311++G(d,p)/SMD//B3LYP-D3/6-31G(d) energy = -249.575927

5⁺

C -0.16084300 -1.10283500 -0.00635400

C -1.53525000 -0.68592700 0.00669100

C -1.53525500 0.68587600 0.00669300

C -0.16069800 1.10286800 -0.00635100

N 0.64206900 0.00014400 -0.01636500

H 0.25851800 -2.10134000 -0.01008800

H -2.38382600 -1.35593700 0.00978500

H -2.38381700 1.35590800 0.00979000

H 0.25853100 2.10142500 -0.01007800

C 2.11470700 -0.00013000 0.01246800

H 2.47697600 0.89196200 -0.49923500

H 2.46601900 -0.00699200 1.04681300

H 2.47715300 -0.88514600 -0.51131700

Zero-point correction= 0.109791 (Hartree/Particle)

Thermal correction to Energy= 0.114727

Thermal correction to Enthalpy= 0.115672

Thermal correction to Gibbs Free Energy= 0.081099

Sum of electronic and zero-point Energies= -249.106914

Sum of electronic and thermal Energies= -249.101978

Sum of electronic and thermal Enthalpies= -249.101034

Sum of electronic and thermal Free Energies= -249.135606

B3LYP-D3/6-311++G(d,p)/SMD//B3LYP-D3/6-31G(d) energy = -249.372382
5⁻
 C -0.14109400 -1.16669800 -0.03859100
 C -1.47448000 -0.69839900 0.09546300
 C -1.47446800 0.69842000 0.09519100
 C -0.14109600 1.16663600 -0.03849600
 N 0.66845300 0.00003500 -0.34900600
 H 0.12855400 -2.09777700 -0.55836600
 H -2.34026500 -1.33999300 0.25775000
 H -2.34027500 1.34008300 0.25707200
 H 0.12885600 2.09794900 -0.55761800
 C 2.00163800 -0.00002200 0.21418400
 H 2.55528900 0.88992300 -0.12478200
 H 2.01043900 -0.00010500 1.32739000
 H 2.55523600 -0.88995200 -0.12490400
 Zero-point correction= 0.104023 (Hartree/Particle)
 Thermal correction to Energy= 0.109861
 Thermal correction to Enthalpy= 0.110805
 Thermal correction to Gibbs Free Energy= 0.074661
 Sum of electronic and zero-point Energies= -249.293040
 Sum of electronic and thermal Energies= -249.287201
 Sum of electronic and thermal Enthalpies= -249.286257
 Sum of electronic and thermal Free Energies= -249.322402
 B3LYP-D3/6-311++G(d,p)/SMD//B3LYP-D3/6-31G(d) energy = -249.591
TS1'
 C 4.42201500 -0.70485700 -0.13059800
 C 3.62336000 0.43057700 -0.08703700
 C 2.23017600 0.29921300 0.03335900
 C 1.63826500 -0.97154900 0.13044600
 C 2.45291600 -2.10151900 0.09188400
 C 3.83586100 -1.97217700 -0.04352800
 H 5.49858800 -0.60687100 -0.23104900
 H 4.05265200 1.42486200 -0.14809300
 H 0.56678500 -1.10479500 0.27219900
 H 1.99838300 -3.08362600 0.17492800
 H 4.46194200 -2.85938100 -0.07597300
 C 1.44499900 1.54486000 0.07566500
 O 1.85759600 2.66581300 0.28064100
 N 0.05092600 1.34220200 -0.17297600
 N -0.78578000 2.33401500 -0.05013500
 N -1.90925400 2.48937700 -0.19743000
 P -2.54184000 -0.77460800 0.00071800
 O -3.32285700 0.05162400 1.16421500
 H -3.57786200 -0.54613000 1.88584300
 O -3.75596800 -1.60033100 -0.70415800
 H -3.41634100 -2.46941300 -0.97212800

O -2.07742000 0.33273700 -0.98200600
 H -0.58474600 0.55075200 -0.59000200
 O -1.48242600 -1.69893400 0.51582600
 Zero-point correction= 0.161693 (Hartree/Particle)
 Thermal correction to Energy= 0.177263
 Thermal correction to Enthalpy= 0.178207
 Thermal correction to Gibbs Free Energy= 0.116448
 Sum of electronic and zero-point Energies= -1153.152467
 Sum of electronic and thermal Energies= -1153.136897
 Sum of electronic and thermal Enthalpies= -1153.135953
 Sum of electronic and thermal Free Energies= -1153.197712
 B3LYP-D3/6-311++G(d,p)/SMD//B3LYP-D3/6-31G(d) energy = -1153.620777
INT1a⁺

C 4.22655400 -0.89654100 0.29031300
 C 3.49461400 0.28808900 0.27691000
 C 2.12876000 0.28042300 -0.03250700
 C 1.50502800 -0.93381100 -0.35290100
 C 2.24260100 -2.11859700 -0.34496200
 C 3.59988800 -2.10665100 -0.01995100
 H 5.28546500 -0.87871900 0.53962400
 H 3.95641100 1.24503400 0.49791500
 H 0.45488200 -0.96525800 -0.61971100
 H 1.74631400 -3.05206600 -0.59758800
 H 4.16900700 -3.03394500 -0.01259500
 C 1.40817400 1.61020500 -0.03652200
 O 2.05042900 2.66291300 -0.07350600
 N 0.04761900 1.46542100 0.00607800
 N -0.63266300 2.66788100 -0.09453800
 N -1.81602200 2.78208900 -0.10158100
 P -2.47544200 -0.84734500 -0.01143800
 O -1.51946900 -0.28050000 1.11332700
 H -0.80597400 0.37140800 0.70443400
 O -3.60975900 -1.66043200 0.83887400
 H -3.52867900 -2.58697300 0.56427300
 O -3.31334300 0.40798900 -0.56640500
 H -2.86730100 1.27212900 -0.36441600
 O -1.87095000 -1.73095500 -1.04883500
 Zero-point correction= 0.161359 (Hartree/Particle)
 Thermal correction to Energy= 0.177127
 Thermal correction to Enthalpy= 0.178071
 Thermal correction to Gibbs Free Energy= 0.115759
 Sum of electronic and zero-point Energies= -1153.283592
 Sum of electronic and thermal Energies= -1153.267824
 Sum of electronic and thermal Enthalpies= -1153.266880
 Sum of electronic and thermal Free Energies= -1153.329193

B3LYP-D3/6-311++G(d,p)/SMD//B3LYP-D3/6-31G(d) energy = -1153.8173834

²TS1

C 4.16557400 -0.96842600 0.29441400
C 3.47212000 0.23830500 0.27016300
C 2.10472000 0.26798700 -0.03347000
C 1.43926400 -0.92768200 -0.33893000
C 2.14074600 -2.13405700 -0.32055300
C 3.49841000 -2.16100600 -0.00030200
H 5.22523300 -0.98160600 0.53980700
H 3.96734400 1.18127900 0.47820300
H 0.38760800 -0.93989900 -0.60256300
H 1.61193400 -3.05220300 -0.56139100
H 4.03796000 -3.10559400 0.01564100
C 1.43438700 1.61797700 -0.05570900
O 2.09337000 2.65108700 -0.16223400
N 0.06758000 1.54411300 0.04753400
N -0.60094600 2.74966100 -0.07478000
N -1.78343000 2.85682100 -0.01088200
P -2.43057500 -0.85155600 -0.00000400
O -1.51070000 -0.24295600 1.09367100
H -0.66901000 0.57051100 0.58792900
O -3.56413900 -1.72190700 0.81163100
H -3.48951400 -2.62172600 0.45804800
O -3.31995900 0.37809800 -0.58607200
H -2.94413100 1.23604200 -0.29189800
O -1.82139200 -1.71010000 -1.06330700

Zero-point correction= 0.157834 (Hartree/Particle)

Thermal correction to Energy= 0.173449

Thermal correction to Enthalpy= 0.174394

Thermal correction to Gibbs Free Energy= 0.112697

Sum of electronic and zero-point Energies= -1153.283739

Sum of electronic and thermal Energies= -1153.268124

Sum of electronic and thermal Enthalpies= -1153.267179

Sum of electronic and thermal Free Energies= -1153.328876

B3LYP-D3/6-311++G(d,p)/SMD//B3LYP-D3/6-31G(d) energy = -1153.813049

²INT2

C 4.10895700 -1.05353100 0.25745000
C 3.46089500 0.17725000 0.22702900
C 2.08433900 0.24800000 -0.02830100
C 1.36187600 -0.92705300 -0.27821300
C 2.02033700 -2.15711900 -0.25425500
C 3.38650300 -2.22662600 0.01733300
H 5.17548100 -1.10096200 0.46499800
H 3.99929200 1.10457700 0.39371500
H 0.30079200 -0.91908400 -0.50292600
H 1.44571200 -3.05704300 -0.45342100

H 3.89149300 -3.18995500 0.03805600
 C 1.47119500 1.61832000 -0.06552400
 O 2.14470200 2.62861700 -0.23404100
 N 0.10309800 1.62634700 0.10061300
 N -0.55303300 2.83770900 -0.04347000
 N -1.73226500 2.94150400 0.06957700
 P -2.39166500 -0.85076500 0.00745400
 O -1.53575200 -0.15964300 1.06477500
 H -0.50370800 0.81826600 0.47709600
 O -3.54273800 -1.73650200 0.80145600
 H -3.53630700 -2.59660900 0.35401900
 O -3.29402200 0.33305000 -0.69739900
 H -3.05273700 1.17647700 -0.27262100
 O -1.76397300 -1.73909300 -1.02864900
 Zero-point correction= 0.162161 (Hartree/Particle)
 Thermal correction to Energy= 0.178281
 Thermal correction to Enthalpy= 0.179225
 Thermal correction to Gibbs Free Energy= 0.116068
 Sum of electronic and zero-point Energies= -1153.285744
 Sum of electronic and thermal Energies= -1153.269624
 Sum of electronic and thermal Enthalpies= -1153.268680
 Sum of electronic and thermal Free Energies= -1153.331837
 B3LYP-D3/6-311++G(d,p)/SMD//B3LYP-D3/6-31G(d) energy = -1153.8214987
²TS2
 C 4.15533200 -0.98413700 0.25728700
 C 3.46938900 0.22651600 0.21979100
 C 2.09622800 0.25530200 -0.05671900
 C 1.41247000 -0.94273700 -0.30807300
 C 2.10665700 -2.15242800 -0.26890200
 C 3.47266400 -2.17945000 0.01317200
 H 5.22066000 -0.99791800 0.47680700
 H 3.97158700 1.17108000 0.40075200
 H 0.35135400 -0.96823100 -0.53246800
 H 1.56035400 -3.07127000 -0.46217600
 H 4.00658100 -3.12694900 0.04240200
 C 1.43484200 1.61819800 -0.07259500
 O 2.09772600 2.64832100 0.01808500
 N 0.08153300 1.55633200 -0.27386800
 N -0.68129300 3.04151700 0.01579700
 N -1.82380300 3.07216500 0.02733200
 P -2.38014600 -0.91321900 0.03474200
 O -1.56779600 -0.05252500 0.99562900
 H -0.53346300 0.85167100 0.25541100
 O -3.47887900 -1.75731100 0.94228900
 H -3.44880100 -2.65738000 0.58307700

O -3.34889000 0.13571000 -0.79694300
 H -3.19600300 1.01504100 -0.41259800
 O -1.72099000 -1.88112600 -0.90417500
 Zero-point correction= 0.159186 (Hartree/Particle)
 Thermal correction to Energy= 0.175736
 Thermal correction to Enthalpy= 0.176680
 Thermal correction to Gibbs Free Energy= 0.111870
 Sum of electronic and zero-point Energies= -1153.279192
 Sum of electronic and thermal Energies= -1153.262642
 Sum of electronic and thermal Enthalpies= -1153.261698
 Sum of electronic and thermal Free Energies= -1153.326508
 B3LYP-D3/6-311++G(d,p)/SMD//B3LYP-D3/6-31G(d) energy = -1153.813049
²INT3
 C -4.05558700 -0.80722800 0.14665500
 C -3.37384800 0.40594300 0.12488400
 C -1.98176500 0.42791500 -0.02748600
 C -1.27133400 -0.77175100 -0.16618800
 C -1.96180800 -1.98414000 -0.14993700
 C -3.34799900 -2.00595000 0.01079800
 H -5.13628900 -0.82246000 0.26853600
 H -3.89443200 1.35367100 0.21936000
 H -0.19562800 -0.75068500 -0.31656000
 H -1.40849900 -2.91230600 -0.26336900
 H -3.87944800 -2.95492900 0.02824800
 C -1.29952800 1.77014200 -0.04307700
 O -1.93774500 2.81663500 -0.18081400
 N 0.04982400 1.77638000 0.19754000
 P 2.66955800 -0.36718300 -0.07523800
 O 1.66248200 0.14435300 -1.10403000
 H 0.67607900 1.28649800 -0.52499800
 O 3.91651300 0.73434500 -0.10600000
 H 4.69067300 0.25866400 0.23281900
 O 2.00341300 -0.10837900 1.41509900
 H 1.45359400 0.69730300 1.38571300
 O 3.23696500 -1.74848700 -0.10648600
 Zero-point correction= 0.151777 (Hartree/Particle)
 Thermal correction to Energy= 0.165904
 Thermal correction to Enthalpy= 0.166849
 Thermal correction to Gibbs Free Energy= 0.107575
 Sum of electronic and zero-point Energies= -1043.787195
 Sum of electronic and thermal Energies= -1043.773067
 Sum of electronic and thermal Enthalpies= -1043.772123
 Sum of electronic and thermal Free Energies= -1043.831396
 B3LYP-D3/6-311++G(d,p)/SMD//B3LYP-D3/6-31G(d) energy = -1044.2931965
²TS3
 C 4.56042900 -1.19716900 -0.17574800

C 3.62800600 -0.25638000 -0.60351600
 C 2.25515200 -0.46818500 -0.41493200
 C 1.82493500 -1.64556600 0.21658100
 C 2.76454500 -2.58416600 0.64758300
 C 4.12936100 -2.36789300 0.45402300
 H 5.62274500 -1.01964600 -0.33024700
 H 3.93267600 0.66642900 -1.08584400
 H 0.76760600 -1.84354200 0.37845700
 H 2.42067000 -3.49181900 1.13731600
 H 4.85386300 -3.10622600 0.79114600
 C 1.30832200 0.61467100 -0.89257600
 O 1.79307400 1.69497400 -1.28565100
 N -0.02542400 0.36426000 -0.89516100
 P -2.79384200 -1.53805500 -0.12224300
 O -1.38055600 -1.75631100 0.38559100
 H -0.28100900 -0.50304600 -0.39957300
 O -3.46978900 -0.39956200 0.90982100
 H -4.41657200 -0.60737900 0.91604600
 O -2.69560100 -0.66305900 -1.52742700
 H -1.79229100 -0.30617900 -1.63949300
 O -3.80208700 -2.62857100 -0.29784200
 C -1.06783800 1.62125600 0.35529800
 C -0.60530700 1.15629900 1.62609100
 C 0.34973500 2.07295300 2.07838400
 C 0.40479800 3.11213900 1.14783100
 N -0.51821300 2.87637400 0.15971200
 H -2.00380900 1.35706500 -0.11306600
 H -0.91731100 0.21294700 2.04933200
 H 0.94854000 2.00519400 2.97666700
 H 1.04239100 3.98374200 1.10362600
 C -0.58640600 3.57609600 -1.10901200
 H -0.33533300 4.62977700 -0.95299900
 H 0.12143500 3.11555400 -1.80498300
 H -1.60522300 3.50941700 -1.50057700
 Zero-point correction= 0.267008 (Hartree/Particle)
 Thermal correction to Energy= 0.286975
 Thermal correction to Enthalpy= 0.287919
 Thermal correction to Gibbs Free Energy= 0.215581
 Sum of electronic and zero-point Energies= -1293.191528
 Sum of electronic and thermal Energies= -1293.171561
 Sum of electronic and thermal Enthalpies= -1293.170617
 Sum of electronic and thermal Free Energies= -1293.242955
 B3LYP-D3/6-311++G(d,p)/SMD//B3LYP-D3/6-31G(d) energy = -1293.8828743
²TS3'
 C -4.11016000 -2.18784800 0.04807800

C -3.39257200 -1.08974800 0.51434300
 C -2.00741900 -1.00172300 0.31880300
 C -1.34282800 -2.03901900 -0.35403900
 C -2.06845800 -3.13582200 -0.82298600
 C -3.44745900 -3.21751500 -0.62495100
 H -5.18514900 -2.24266900 0.20755500
 H -3.87915000 -0.27153500 1.03464300
 H -0.26812700 -2.00328900 -0.52267200
 H -1.54489400 -3.93216800 -1.34609400
 H -4.00326500 -4.07797000 -0.99159900
 C -1.31162000 0.23998700 0.85381800
 O -2.01275900 1.15607300 1.32262200
 N 0.04156400 0.24212500 0.83715800
 P 3.05268100 -1.13215100 0.00686700
 O 1.74248600 -1.30347500 -0.74486800
 H 0.48544100 -0.39318600 0.14958400
 O 3.64772200 0.35387100 -0.49649000
 H 4.60856200 0.28750400 -0.38598400
 O 2.68718700 -0.81736200 1.58986600
 H 1.76032400 -0.51311800 1.65921500
 O 4.18201600 -2.11040000 -0.04144900
 C 0.01184400 2.95905800 0.66193400
 C 0.90045300 1.92914700 0.25227900
 C 0.75620100 1.84747600 -1.19899100
 C -0.27621700 2.65962600 -1.54752600
 N -0.72557200 3.35359400 -0.41521400
 H -0.24627400 3.28418900 1.65695500
 H 1.82619100 1.68658500 0.75460800
 H 1.33394900 1.18050400 -1.82115300
 H -0.75025900 2.84038500 -2.50283800
 C -2.04309600 3.94336000 -0.29904200
 H -2.33900000 4.37189100 -1.26130200
 H -2.76420000 3.18035400 0.01645700
 H -2.02153100 4.74321700 0.44825100
 Zero-point correction= 0.266328 (Hartree/Particle)
 Thermal correction to Energy= 0.286446
 Thermal correction to Enthalpy= 0.287390
 Thermal correction to Gibbs Free Energy= 0.213877
 Sum of electronic and zero-point Energies= -1293.177283
 Sum of electronic and thermal Energies= -1293.157164
 Sum of electronic and thermal Enthalpies= -1293.156220
 Sum of electronic and thermal Free Energies= -1293.229733
 B3LYP-D3/6-311++G(d,p)/SMD//B3LYP-D3/6-31G(d) energy = -1293.8703116
2INT4
 C -4.33282600 1.44342100 0.41636500

C -2.99703500 1.82968600 0.36121300
 C -2.00903600 0.93221000 -0.06596900
 C -2.37713400 -0.37101300 -0.43255400
 C -3.71816400 -0.75482600 -0.36840200
 C -4.69787500 0.14499800 0.05099600
 H -5.08969600 2.15130700 0.74694800
 H -2.67989800 2.82685600 0.64729400
 H -1.63734500 -1.09971500 -0.75845900
 H -3.99057400 -1.76971000 -0.64574100
 H -5.74005100 -0.16329900 0.09722100
 C -0.58909300 1.45750100 -0.07668500
 O -0.34204800 2.58014600 0.37120300
 N 0.36378700 0.62195500 -0.56744400
 P 0.75289300 -2.81878300 -0.11638400
 O 0.18870100 -2.02260800 -1.28089600
 H 0.14828800 -0.31971900 -0.94135300
 O 2.34985500 -2.32664800 -0.00305400
 H 2.81483000 -3.03244600 0.47251300
 O 0.11786000 -2.17215700 1.27662200
 H -0.02917900 -1.22302700 1.13229200
 O 0.69772900 -4.30531900 -0.00196700
 C 1.78000100 0.98741900 -0.69522600
 C 2.07947500 2.19274400 -1.55326100
 C 2.71597000 3.15002400 -0.78372800
 C 2.87855300 2.65175000 0.51130100
 N 2.42044300 1.35592400 0.58038500
 H 2.23746700 0.06171400 -1.07108000
 H 1.78038700 2.25606900 -2.59076700
 H 3.04059000 4.13093200 -1.11052600
 H 3.30504300 3.12609000 1.38520100
 C 2.08756500 0.66930200 1.80422300
 H 2.84471300 0.90325800 2.56177600
 H 1.10333100 0.97091900 2.19533500
 H 2.08989500 -0.40923800 1.62961900
 Zero-point correction= 0.267651 (Hartree/Particle)
 Thermal correction to Energy= 0.287963
 Thermal correction to Enthalpy= 0.288907
 Thermal correction to Gibbs Free Energy= 0.216435
 Sum of electronic and zero-point Energies= -1293.219252
 Sum of electronic and thermal Energies= -1293.198940
 Sum of electronic and thermal Enthalpies= -1293.197996
 Sum of electronic and thermal Free Energies= -1293.270469
 B3LYP-D3/6-311++G(d,p)/SMD//B3LYP-D3/6-31G(d) energy = -1293.9075528
²TS4
 C -4.79583700 -0.29609700 0.17448900

C -3.70558600 0.55585200 0.11223700
 C -2.38164500 0.03915200 0.05923400
 C -2.20991600 -1.37460000 0.08311400
 C -3.31636700 -2.20852500 0.14926200
 C -4.61826100 -1.68863600 0.19784600
 H -5.80052400 0.12225600 0.20704500
 H -3.83702600 1.63309800 0.09993400
 H -1.21475900 -1.80515400 0.02155600
 H -3.16263200 -3.28530300 0.15726500
 H -5.47659900 -2.35334300 0.25451800
 C -1.27077700 0.93528200 0.03458500
 O -1.38849200 2.23375100 0.02703100
 N 0.04573300 0.48540200 -0.09322400
 P 2.07053900 -2.22804700 -0.20414800
 O 0.94443000 -1.84588200 -1.14846400
 H 0.21387800 -0.41132700 -0.60515200
 O 3.33729000 -1.18577000 -0.58954400
 H 4.14116400 -1.67905400 -0.36372100
 O 1.64702800 -1.68290500 1.30123800
 H 1.02298900 -0.93990400 1.19127300
 O 2.64466700 -3.60045400 -0.07622700
 C 0.88655600 1.56571500 -0.57371400
 C 0.02623000 2.73828600 -1.03461200
 C 0.62996500 3.93171900 -0.53244500
 C 1.57565600 3.54695200 0.39102900
 N 1.73492500 2.20324900 0.45193300
 H 1.53542200 1.15383100 -1.35677700
 H -0.47255600 2.67951600 -1.99525200
 H 0.31599300 4.94658700 -0.73013200
 H 2.19530300 4.18121300 1.01696300
 C 2.65469000 1.45821400 1.28048700
 H 3.40037800 2.14637600 1.69298400
 H 2.13697000 0.95972300 2.10935900
 H 3.15166400 0.68183200 0.69003600
 Zero-point correction= 0.267104 (Hartree/Particle)
 Thermal correction to Energy= 0.286472
 Thermal correction to Enthalpy= 0.287417
 Thermal correction to Gibbs Free Energy= 0.216289
 Sum of electronic and zero-point Energies= -1293.176031
 Sum of electronic and thermal Energies= -1293.156662
 Sum of electronic and thermal Enthalpies= -1293.155718
 Sum of electronic and thermal Free Energies= -1293.226846
 B3LYP-D3/6-311++G(d,p)/SMD//B3LYP-D3/6-31G(d) energy = -1293.8653217
INT5
 C 4.91736700 0.62926900 0.06007300

C 3.90956500 -0.30621000 -0.14806100
 C 2.56329100 0.08088700 -0.08525300
 C 2.23008900 1.41401400 0.20140500
 C 3.24746200 2.34374500 0.41207600
 C 4.58661400 1.95773200 0.33953300
 H 5.95880300 0.32543200 0.00535800
 H 4.13988300 -1.34417100 -0.36170500
 H 1.19583900 1.73693800 0.27599300
 H 2.98769400 3.37428500 0.63493300
 H 5.37252200 2.69008800 0.50284700
 C 1.54201800 -0.97960600 -0.31520200
 O 1.83927700 -2.17902200 -0.37982800
 N 0.24597600 -0.57609500 -0.48595800
 P -2.39123800 1.91151700 -0.23591000
 O -0.98335100 1.64565300 0.25830400
 H -0.10224600 0.40001900 -0.34371100
 O -2.79247700 0.55094900 -1.14701900
 H -3.26351400 0.88517500 -1.92702300
 O -3.35749100 1.69075900 1.08846800
 H -4.13379900 2.26185700 0.97578000
 O -2.82479700 3.11105800 -1.00617000
 C -0.77694700 -1.55457600 -0.52731900
 C -0.44196200 -2.87740100 -1.13490600
 C -0.90084200 -3.87958700 -0.33813700
 C -1.40691800 -3.27235400 0.85427200
 N -1.30966900 -1.97028000 0.81856600
 H -1.64960300 -1.09340800 -1.02589400
 H 0.00038600 -2.96405400 -2.11673500
 H -0.85593300 -4.94452700 -0.51450900
 H -1.84485900 -3.77296900 1.71200300
 C -1.77962800 -1.00431800 1.80740400
 H -1.84518800 -1.49942100 2.77800400
 H -1.08313500 -0.16525800 1.83817300
 H -2.75237500 -0.60287000 1.51153700
 Zero-point correction= 0.270911 (Hartree/Particle)
 Thermal correction to Energy= 0.290788
 Thermal correction to Enthalpy= 0.291732
 Thermal correction to Gibbs Free Energy= 0.220653
 Sum of electronic and zero-point Energies= -1293.154340
 Sum of electronic and thermal Energies= -1293.134462
 Sum of electronic and thermal Enthalpies= -1293.133518
 Sum of electronic and thermal Free Energies= -1293.204598
 B3LYP-D3/6-311++G(d,p)/SMD//B3LYP-D3/6-31G(d) energy = -1293.7888556
TS5
 C -5.01107700 -0.24200600 -0.13346600

C -3.91275500 0.59575300 -0.30015600
 C -2.61297700 0.10067200 -0.13248200
 C -2.42180100 -1.24250500 0.22520600
 C -3.52704800 -2.07497100 0.39848200
 C -4.81936000 -1.58101100 0.21544400
 H -6.01571300 0.14716000 -0.27250300
 H -4.03405700 1.64187600 -0.55959200
 H -1.42801800 -1.64764300 0.39183400
 H -3.37537600 -3.11260400 0.68150700
 H -5.67565900 -2.23638500 0.34906800
 C -1.48701700 1.06970000 -0.31693500
 O -1.65782400 2.28519900 -0.33680100
 N -0.23507100 0.51795900 -0.47633200
 P 2.32645700 -1.77093700 -0.16016100
 O 0.93691700 -1.84861800 0.41008300
 H -0.05912200 -0.47604400 -0.30471400
 O 3.36603700 -2.27258700 0.99416100
 H 4.27604200 -2.06314600 0.72687800
 O 2.52719600 -2.82930400 -1.38515200
 H 2.01353200 -3.63220200 -1.19822800
 O 2.83453100 -0.42597100 -0.70095200
 C 0.91049000 1.34374200 -0.41052000
 C 1.16641800 2.44793600 -1.30779300
 C 1.80960300 3.44661800 -0.61424400
 C 1.84569900 3.04943700 0.74407900
 N 1.26186900 1.87146800 0.89373500
 H 1.88068100 0.55592000 -0.63135900
 H 0.95467900 2.40634100 -2.36722300
 H 2.22332900 4.36557700 -1.00407800
 H 2.29997000 3.55895200 1.58536800
 C 1.03820800 1.12683300 2.12421500
 H 1.76388000 1.44003600 2.87720100
 H 0.02334800 1.31999600 2.48616900
 H 1.14288700 0.05931000 1.91857700
 Zero-point correction= 0.266652 (Hartree/Particle)
 Thermal correction to Energy= 0.286141
 Thermal correction to Enthalpy= 0.287085
 Thermal correction to Gibbs Free Energy= 0.216147
 Sum of electronic and zero-point Energies= -1293.165769
 Sum of electronic and thermal Energies= -1293.146279
 Sum of electronic and thermal Enthalpies= -1293.145335
 Sum of electronic and thermal Free Energies= -1293.216273
 B3LYP-D3/6-311++G(d,p)/SMD//B3LYP-D3/6-31G(d) energy = -1293.7877845
TS5'
 C 2.01067600 4.04338000 0.39957800

C 2.32121900 2.71303600 0.14289600
 C 1.28999300 1.79026400 -0.09802600
 C -0.04918700 2.20607300 -0.07720900
 C -0.34941500 3.53862100 0.18956400
 C 0.67448900 4.45713200 0.42467200
 H 2.80713900 4.75833100 0.58362000
 H 3.35062600 2.37259700 0.12699500
 H -0.87974500 1.53028200 -0.24513500
 H -1.39278000 3.83507700 0.21711600
 H 0.43555700 5.49677900 0.63152200
 C 1.64746500 0.38633000 -0.34923400
 O 2.86415500 -0.00044800 -0.27694200
 N 0.73135000 -0.52420600 -0.67203500
 P -2.92145100 -0.23632500 -0.13036800
 O -1.77570200 -0.82609400 -0.94068500
 H -0.34310700 -0.43289400 -0.75827600
 O -4.33030500 -0.73894100 -0.80910200
 H -4.82177500 0.06352900 -1.04487900
 O -2.89936900 -1.09282600 1.28363600
 H -3.46507100 -0.63105200 1.92328000
 O -3.00096200 1.23705800 0.14315600
 C 1.25979200 -1.85435100 -0.78604200
 C 2.78277500 -1.78162200 -0.84043000
 C 3.27674700 -2.68627600 0.12363800
 C 2.18805100 -3.14656500 0.85381100
 N 1.01502200 -2.69600800 0.40331600
 H 0.81623000 -2.35560800 -1.65326600
 H 3.28469600 -1.55976400 -1.77373500
 H 4.30976000 -2.94243100 0.30161800
 H 2.20612800 -3.83228000 1.69478500
 C -0.31770600 -2.95936100 0.92776200
 H -0.98577900 -3.25329100 0.11516400
 H -0.24637100 -3.76406100 1.66329400
 H -0.75027800 -2.06880600 1.38808200
 Zero-point correction= 0.269339 (Hartree/Particle)
 Thermal correction to Energy= 0.288697
 Thermal correction to Enthalpy= 0.289641
 Thermal correction to Gibbs Free Energy= 0.218932
 Sum of electronic and zero-point Energies= -1293.148020
 Sum of electronic and thermal Energies= -1293.128662
 Sum of electronic and thermal Enthalpies= -1293.127718
 Sum of electronic and thermal Free Energies= -1293.198427
 B3LYP-D3/6-311++G(d,p)/SMD//B3LYP-D3/6-31G(d) energy = -1293.7721873
INT6
 C -5.11360700 0.03929600 -0.04359500

C -3.98117600 0.84661500 -0.09138100
 C -2.70267700 0.27472900 -0.11676500
 C -2.57025100 -1.12090100 -0.07354900
 C -3.70753800 -1.92593600 -0.01991900
 C -4.97882600 -1.35052500 -0.00910700
 H -6.10113900 0.49180300 -0.03135700
 H -4.05788800 1.92827700 -0.10903900
 H -1.59264300 -1.59298100 -0.06198200
 H -3.59805300 -3.00604100 0.01767900
 H -5.86162300 -1.98272400 0.03059700
 C -1.53987400 1.21955300 -0.16505800
 O -1.66255700 2.41733700 0.08024000
 N -0.32895900 0.65783200 -0.48924900
 P 2.09485800 -1.82440800 0.04526800
 O 0.79810600 -1.95679100 -0.66548000
 H -0.25562000 -0.32893400 -0.72861600
 O 1.88191200 -1.16286400 1.50675000
 H 2.72618600 -0.89687400 1.90730900
 O 2.85162800 -3.22206400 0.30230900
 H 2.26708600 -3.95847400 0.05997500
 O 3.28038400 -0.99407900 -0.61946900
 C 0.87427000 1.36735500 -0.54146500
 C 1.78539300 1.46921000 -1.58362700
 C 2.91993500 2.17609500 -1.08106900
 C 2.65812200 2.47495200 0.24238600
 N 1.42059700 1.97413500 0.56818400
 H 2.99092200 -0.08778800 -0.89807400
 H 1.62092200 1.10935500 -2.58975700
 H 3.80644200 2.45571100 -1.63301400
 H 3.23648700 3.02273300 0.97192400
 C 0.79431700 2.03147500 1.87962100
 H 1.51153200 2.45121900 2.58766300
 H -0.10257300 2.65216200 1.83541300
 H 0.52131900 1.02108400 2.19609100
 Zero-point correction= 0.269708 (Hartree/Particle)
 Thermal correction to Energy= 0.290271
 Thermal correction to Enthalpy= 0.291215
 Thermal correction to Gibbs Free Energy= 0.218301
 Sum of electronic and zero-point Energies= -1293.189911
 Sum of electronic and thermal Energies= -1293.169348
 Sum of electronic and thermal Enthalpies= -1293.168404
 Sum of electronic and thermal Free Energies= -1293.241318
 B3LYP-D3/6-311++G(d,p)/SMD//B3LYP-D3/6-31G(d) energy = -1293.8110029
P4
 C -4.05298200 -0.57575400 0.73969900

C -2.68781800 -0.80994600 0.87528000
 C -1.76654300 -0.08821500 0.10585500
 C -2.23431800 0.85113600 -0.82318300
 C -3.60266300 1.07893600 -0.96399400
 C -4.51334100 0.37144800 -0.17829700
 H -4.76017100 -1.13328100 1.34700600
 H -2.30754300 -1.54883100 1.57227700
 H -1.53859300 1.38014000 -1.46843100
 H -3.95700900 1.80163700 -1.69329500
 H -5.57910400 0.55129800 -0.28710700
 C -0.31363800 -0.38893000 0.31492900
 O 0.07129000 -1.45175100 0.78682500
 N 0.55996800 0.60668800 -0.08025500
 H 0.17135700 1.52497100 -0.24336900
 C 1.94943400 0.54745900 0.12667300
 C 2.76790300 1.38329800 0.86155300
 C 4.10135100 0.92854700 0.67378200
 C 4.04724700 -0.16706200 -0.16230000
 N 2.73510700 -0.38963600 -0.51081300
 H 2.43446100 2.21500200 1.46705600
 H 4.99662000 1.35130100 1.10798800
 H 4.82650000 -0.81627200 -0.53428300
 C 2.25281100 -1.46828600 -1.35332300
 H 3.09462100 -1.86996500 -1.92102000
 H 1.79208900 -2.25408700 -0.74991000
 H 1.50626900 -1.08305100 -2.05407200
 Zero-point correction= 0.219739 (Hartree/Particle)
 Thermal correction to Energy= 0.232700
 Thermal correction to Enthalpy= 0.233644
 Thermal correction to Gibbs Free Energy= 0.179172
 Sum of electronic and zero-point Energies= -649.063840
 Sum of electronic and thermal Energies= -649.050879
 Sum of electronic and thermal Enthalpies= -649.049935
 Sum of electronic and thermal Free Energies= -649.104407
 B3LYP-D3/6-311++G(d,p)/SMD//B3LYP-D3/6-31G(d) energy = -649.482824
6
 C 1.89964600 -1.20618200 -0.03036200
 C 0.50589100 -1.20628100 0.02654600
 C -0.20672700 -0.00116900 0.07216400
 C 0.50517000 1.20509700 0.05150000
 C 1.89888800 1.20703200 -0.00535000
 C 2.59978400 0.00092800 -0.04723500
 H 2.43882500 -2.14916500 -0.05844900
 H -0.04015200 -2.14562600 0.04477000
 H -0.04145100 2.14353200 0.08920500

H 2.43752500 2.15070300 -0.01383800
 H 3.68530000 0.00173700 -0.09099000
 C -1.70066000 -0.00195200 0.10964000
 C -2.36525100 -0.02220200 1.26794700
 H -3.45221600 -0.02295900 1.29898500
 H -1.84495800 -0.03866300 2.22131300
 C -2.38947600 0.02115000 -1.23211000
 H -2.09354500 -0.84758100 -1.83477900
 H -3.47908900 0.01919500 -1.12826800
 H -2.09382700 0.91030000 -1.80438100
 Zero-point correction= 0.161715 (Hartree/Particle)
 Thermal correction to Energy= 0.169103
 Thermal correction to Enthalpy= 0.170047
 Thermal correction to Gibbs Free Energy= 0.129955
 Sum of electronic and zero-point Energies= -348.832619
 Sum of electronic and thermal Energies= -348.825231
 Sum of electronic and thermal Enthalpies= -348.824287
 Sum of electronic and thermal Free Energies= -348.864379
 B3LYP-D3/6-311++G(d,p)/SMD//B3LYP-D3/6-31G(d) energy = -349.093362
²TS6
 C -4.65624900 1.96737900 -0.88358000
 C -3.63599000 1.96545700 0.06365800
 C -2.66456300 0.95642600 0.06172000
 C -2.72758000 -0.06353100 -0.89976600
 C -3.75271600 -0.05540500 -1.84701700
 C -4.71657600 0.95381700 -1.84370100
 H -5.40427400 2.75717900 -0.87544700
 H -3.56059600 2.73792500 0.82170300
 H -1.98504700 -0.85876400 -0.92210600
 H -3.79433600 -0.84757200 -2.59001200
 H -5.51254300 0.95141000 -2.58520100
 C -1.58446300 1.03172100 1.12694600
 O -1.59029600 1.96615400 1.93874800
 N -0.71958300 -0.01440500 1.16693400
 P 0.17908000 -3.04804500 0.12207600
 O 0.00096200 -1.83104200 -0.77766700
 H -0.45482200 -0.47300900 0.27260900
 O 1.63811800 -2.75433000 0.90471800
 H 1.94736600 -3.61524500 1.22593800
 O -0.89116400 -2.92142800 1.36631200
 H -0.98630800 -1.97327600 1.59797900
 O 0.18478600 -4.45492900 -0.37646300
 C 4.12986700 2.22046700 -1.53234800
 C 3.35514300 2.37057500 -0.38642200
 C 2.52702400 1.32513400 0.07822100

C 2.48554700 0.12833800 -0.67126700
 C 3.25220300 -0.00743400 -1.82379000
 C 4.08331900 1.02798600 -2.25873200
 H 4.76837400 3.03717000 -1.86162400
 H 3.40409600 3.30279700 0.16767100
 H 1.81529900 -0.68043000 -0.40249500
 H 3.17996900 -0.93174800 -2.38991600
 H 4.67987700 0.91303400 -3.16064800
 C 1.73570500 1.49686900 1.29666800
 C 1.23289400 0.41273700 2.00822800
 H 0.78768700 0.59287400 2.97940300
 H 1.56106300 -0.60132200 1.80358800
 C 1.44632900 2.88941000 1.79623600
 H 1.20114900 3.56605100 0.96973000
 H 0.59120100 2.87032400 2.47364100
 H 2.31410300 3.31903000 2.32001200
 Zero-point correction= 0.317530 (Hartree/Particle)
 Thermal correction to Energy= 0.340252
 Thermal correction to Enthalpy= 0.341196
 Thermal correction to Gibbs Free Energy= 0.262140
 Sum of electronic and zero-point Energies= -1392.648210
 Sum of electronic and thermal Energies= -1392.625488
 Sum of electronic and thermal Enthalpies= -1392.624543
 Sum of electronic and thermal Free Energies= -1392.703599
 B3LYP-D3/6-311++G(d,p)/SMD//B3LYP-D3/6-31G(d) energy = -1393.4086823
²TS6'
 C 5.20603800 -0.21348200 0.52209000
 C 4.10713600 -1.06795500 0.54379300
 C 2.84771500 -0.61384700 0.12888000
 C 2.70416600 0.70410400 -0.32409700
 C 3.80817900 1.55701900 -0.34436600
 C 5.05735100 1.10558400 0.08165900
 H 6.17903500 -0.57274100 0.85066100
 H 4.19562900 -2.09774700 0.87394100
 H 1.74762900 1.07166200 -0.68096600
 H 3.66879000 2.57969300 -0.68252500
 H 5.91374000 1.77643200 0.07296200
 C 1.69601700 -1.60466600 0.20430500
 O 1.94676500 -2.81552600 0.26307700
 N 0.46183900 -1.04755100 0.31838700
 P -0.62251800 2.28292000 -0.16196600
 O -0.38854600 1.08370500 -1.09301000
 H 0.23622600 -0.20932400 -0.28197700
 O -2.18417700 2.77796200 -0.33768600
 H -2.75003200 1.99411100 -0.23830500

O -0.69941400 1.65176900 1.37353000
 H -0.34715900 0.74438000 1.36394900
 O 0.27491300 3.47150100 -0.22892900
 C -3.52751800 -0.38224200 1.73007000
 C -2.47424600 -1.16977900 1.27640000
 C -2.24820900 -1.35446600 -0.09549900
 C -3.10018900 -0.71006000 -1.00078700
 C -4.16717400 0.06765500 -0.54963000
 C -4.38615900 0.23577800 0.81905000
 H -3.66129900 -0.22526900 2.79664600
 H -1.77603500 -1.60332600 1.98443300
 H -2.92095800 -0.79794400 -2.06569300
 H -4.81374600 0.56085800 -1.27086500
 H -5.20061900 0.86308300 1.17102400
 C -1.12614000 -2.21557100 -0.57445800
 C -0.88960900 -3.41622500 0.06202500
 H -0.13003600 -4.09493400 -0.30213700
 H -1.35792400 -3.64996000 1.01262700
 C -0.65179500 -2.02784200 -2.00233500
 H -0.52524600 -0.96656200 -2.22975400
 H 0.29851500 -2.54846800 -2.14660200
 H -1.38132400 -2.45418400 -2.70509800
 Zero-point correction= 0.316020 (Hartree/Particle)
 Thermal correction to Energy= 0.338840
 Thermal correction to Enthalpy= 0.339784
 Thermal correction to Gibbs Free Energy= 0.261339
 Sum of electronic and zero-point Energies= -1392.630618
 Sum of electronic and thermal Energies= -1392.607798
 Sum of electronic and thermal Enthalpies= -1392.606854
 Sum of electronic and thermal Free Energies= -1392.685299
 B3LYP-D3/6-311++G(d,p)/SMD//B3LYP-D3/6-31G(d) energy = -1393.3919239
INT7
 C -4.71710400 -2.03126300 0.90682400
 C -3.58105600 -2.17118800 0.11486800
 C -2.60246700 -1.16901400 0.08707100
 C -2.77754900 -0.01208800 0.86087400
 C -3.92035300 0.12347700 1.65046800
 C -4.88963000 -0.87965900 1.67883900
 H -5.46866800 -2.81731400 0.92210500
 H -3.42218900 -3.04964300 -0.50132000
 H -2.04003600 0.78700900 0.85839400
 H -4.04923400 1.02542900 2.24268000
 H -5.77703100 -0.76468400 2.29728000
 C -1.41332600 -1.41129200 -0.80891200
 O -1.39211500 -2.38967600 -1.56841100

N -0.41411800 -0.49617400 -0.75546000
 P -0.26062700 2.91322000 -0.30769200
 O -0.14119500 1.79529800 0.71818000
 H -0.36840900 0.24242500 -0.02897400
 O 1.13227800 2.77390300 -1.22405300
 H 1.25208400 3.62456500 -1.67383300
 O -1.41781200 2.45341800 -1.39977500
 H -1.35828100 1.48845400 -1.51706700
 O -0.47781600 4.34731200 0.03942200
 C 4.81752300 -1.46723500 1.32682900
 C 3.87489400 -1.91986800 0.41468100
 C 2.79104400 -1.09637500 -0.00752300
 C 2.71186100 0.20893500 0.56087900
 C 3.65738700 0.64309300 1.47888000
 C 4.72025000 -0.18047000 1.86906800
 H 5.63723800 -2.12059000 1.61926300
 H 3.97805000 -2.91751900 0.00004700
 H 1.88787900 0.87186900 0.32291300
 H 3.55365200 1.63917200 1.90105200
 H 5.45652800 0.17069500 2.58786300
 C 1.83482500 -1.56778600 -0.95768500
 C 0.80433200 -0.64302500 -1.56193700
 H 0.50139300 -1.03144000 -2.53856800
 H 1.20533100 0.36442400 -1.69802600
 C 1.81642900 -3.00014500 -1.41344800
 H 2.01834900 -3.69919200 -0.59242100
 H 0.83558300 -3.24071200 -1.83013900
 H 2.57691100 -3.19664000 -2.18920900
 Zero-point correction= 0.320997 (Hartree/Particle)
 Thermal correction to Energy= 0.343822
 Thermal correction to Enthalpy= 0.344767
 Thermal correction to Gibbs Free Energy= 0.265385
 Sum of electronic and zero-point Energies= -1392.699491
 Sum of electronic and thermal Energies= -1392.676666
 Sum of electronic and thermal Enthalpies= -1392.675722
 Sum of electronic and thermal Free Energies= -1392.755103
 B3LYP-D3/6-311++G(d,p)/SMD//B3LYP-D3/6-31G(d) energy = -1393.4585623
INT7'
 C -5.10165500 -0.07588200 -0.70280300
 C -4.06754200 -0.99198300 -0.52994200
 C -2.81156000 -0.56824300 -0.07676700
 C -2.60795300 0.78499300 0.22682100
 C -3.64801000 1.69901300 0.05589000
 C -4.89206600 1.27548500 -0.41304700
 H -6.07112700 -0.41313500 -1.06313700

H -4.20438100 -2.04827500 -0.73723900
 H -1.65541200 1.13306900 0.61617000
 H -3.47002200 2.74488000 0.28956100
 H -5.69774800 1.99351900 -0.54983100
 C -1.74430100 -1.62355800 0.07465300
 O -2.05287400 -2.82343100 0.10557000
 N -0.46857000 -1.16977400 0.12255800
 P 0.87018700 2.40284200 0.39556800
 O 0.45111700 1.14421200 1.16037700
 H -0.26473200 -0.17352700 0.34078100
 O 2.53040300 2.42219900 0.50094100
 H 2.77573000 1.56356100 0.88080900
 O 0.65563300 2.10133800 -1.22017400
 H 1.15366400 1.29710100 -1.44043600
 O 0.29180300 3.74099500 0.69615000
 C 3.03752400 -0.37791500 -2.00276500
 C 1.92169500 -0.98079200 -1.42433300
 C 1.92416100 -1.36755700 -0.07550500
 C 3.08500800 -1.14920900 0.67083500
 C 4.20523100 -0.54442800 0.09414100
 C 4.18624600 -0.15026400 -1.24230100
 H 3.00387100 -0.06930100 -3.04456200
 H 1.01836100 -1.13099800 -2.00808700
 H 3.11435300 -1.42559500 1.71851100
 H 5.08941400 -0.36601600 0.70125900
 H 5.04846200 0.34154800 -1.68313700
 C 0.66501300 -2.03616800 0.50881000
 C 0.57116800 -3.40466600 -0.09865300
 H 0.35531900 -4.26797800 0.51859800
 H 0.49904000 -3.50832900 -1.17539600
 C 0.69107500 -2.11902100 2.04442400
 H 0.78829900 -1.11361600 2.46262800
 H -0.25521500 -2.55562800 2.37680700
 H 1.50644700 -2.75682800 2.40561900
 Zero-point correction= 0.318037 (Hartree/Particle)
 Thermal correction to Energy= 0.341240
 Thermal correction to Enthalpy= 0.342184
 Thermal correction to Gibbs Free Energy= 0.262714
 Sum of electronic and zero-point Energies= -1392.667157
 Sum of electronic and thermal Energies= -1392.643953
 Sum of electronic and thermal Enthalpies= -1392.643009
 Sum of electronic and thermal Free Energies= -1392.722479
 B3LYP-D3/6-311++G(d,p)/SMD//B3LYP-D3/6-31G(d) energy = -1393.4300467
2TS7
 C -4.85497700 -1.88252200 0.81538900

C -3.68161100 -2.06119400 0.08717600
 C -2.68480200 -1.07610900 0.07482300
 C -2.88936000 0.10091200 0.80696100
 C -4.06658000 0.28045600 1.53438700
 C -5.05225100 -0.70702300 1.54363600
 H -5.61721300 -2.65884200 0.81500700
 H -3.50291400 -2.96015800 -0.49258800
 H -2.14125700 0.88203500 0.81777800
 H -4.20967800 1.20181500 2.09309600
 H -5.96798600 -0.56158000 2.11258600
 C -1.44964300 -1.36689400 -0.75366300
 O -1.43213500 -2.40909600 -1.43693100
 N -0.45769800 -0.44851700 -0.72286200
 P -0.21428800 2.85359100 -0.30604800
 O -0.02844600 1.76361300 0.79771900
 H -0.22380600 0.60632500 0.27786100
 O 1.26684500 2.88565400 -1.04845900
 H 1.36417100 3.75926800 -1.45799000
 O -1.19036700 2.19973600 -1.42395500
 H -1.09538200 1.21123500 -1.39972900
 O -0.62964800 4.23026100 0.06724900
 C 4.85667000 -1.52382100 1.28530300
 C 3.81249200 -2.00492000 0.50826700
 C 2.80343000 -1.13935300 -0.00817700
 C 2.91650100 0.24145300 0.32575000
 C 3.96120500 0.70806600 1.10951700
 C 4.94546800 -0.16169200 1.59497800
 H 5.61090500 -2.21562900 1.65554300
 H 3.77143300 -3.06437700 0.27848000
 H 2.16420500 0.94638000 0.00195300
 H 4.00029000 1.76730600 1.35076200
 H 5.76125500 0.21252700 2.20852000
 C 1.74538600 -1.64683200 -0.82232500
 C 0.75355600 -0.73725800 -1.51118000
 H 0.44923000 -1.20608300 -2.45489300
 H 1.21587200 0.22589300 -1.74664500
 C 1.59638000 -3.12675300 -1.04733600
 H 1.65786900 -3.69408800 -0.10853600
 H 0.62801900 -3.33503100 -1.50413200
 H 2.39200100 -3.52166200 -1.70232900
 Zero-point correction= 0.315187 (Hartree/Particle)
 Thermal correction to Energy= 0.337439
 Thermal correction to Enthalpy= 0.338383
 Thermal correction to Gibbs Free Energy= 0.260148

Sum of electronic and zero-point Energies= -1392.680421
 Sum of electronic and thermal Energies= -1392.658169
 Sum of electronic and thermal Enthalpies= -1392.657225
 Sum of electronic and thermal Free Energies= -1392.735460
 B3LYP-D3/6-311++G(d,p)/SMD//B3LYP-D3/6-31G(d) energy = -1393.4268948
2TS7'
 C -2.76487200 3.65466500 0.13006900
 C -2.41740400 2.46748100 -0.49648300
 C -1.07519500 2.01482600 -0.49078300
 C -0.09588300 2.80311600 0.16649400
 C -0.46280400 3.99031900 0.78617300
 C -1.79175200 4.43319000 0.77213900
 H -3.80289500 3.98125900 0.12209100
 H -3.16391100 1.85809000 -0.99486900
 H 0.93113100 2.45616900 0.22884100
 H 0.29773700 4.57478500 1.29866000
 H -2.06625600 5.36624800 1.25779900
 C -0.73307400 0.80090800 -1.18042300
 O -1.62747300 0.04579600 -1.75721700
 N 0.52418200 0.25185100 -1.17020300
 P 3.52673300 -0.12807500 0.38850200
 O 2.26794500 0.57759700 0.87426500
 H 1.12521300 0.45732200 -0.33805200
 O 3.11772800 -1.75035100 0.35673800
 H 3.95290000 -2.23527300 0.44136600
 O 3.66122900 0.20823100 -1.23148200
 H 2.79520200 0.50983000 -1.55663000
 O 4.86932600 0.00474600 1.02464700
 C -3.17184700 -2.87957900 1.45171800
 C -2.69259000 -2.63097300 0.17186600
 C -1.49728000 -1.90626300 -0.04030100
 C -0.80427900 -1.44074600 1.10496100
 C -1.29458600 -1.69165000 2.38288400
 C -2.47874200 -2.40715600 2.57163700
 H -4.09316600 -3.44429300 1.57838500
 H -3.25358400 -3.00584900 -0.67777700
 H 0.13169300 -0.90128600 1.01512700
 H -0.73561300 -1.32296900 3.23879100
 H -2.85586600 -2.59736400 3.57331300
 C -1.01970200 -1.59420600 -1.39259600
 C 0.43860700 -1.17140600 -1.53654200
 H 0.75563300 -1.30875300 -2.57749000
 H 1.11576700 -1.74132400 -0.89558100
 C -1.60072000 -2.36105400 -2.55344100
 H -2.69142100 -2.28706400 -2.57915400

H -1.21912200 -1.95443100 -3.49358100
 H -1.33102700 -3.42392000 -2.49719800
 Zero-point correction= 0.319578 (Hartree/Particle)
 Thermal correction to Energy= 0.341577
 Thermal correction to Enthalpy= 0.342521
 Thermal correction to Gibbs Free Energy= 0.264599
 Sum of electronic and zero-point Energies= -1392.657142
 Sum of electronic and thermal Energies= -1392.635143
 Sum of electronic and thermal Enthalpies= -1392.634198
 Sum of electronic and thermal Free Energies= -1392.712120
 B3LYP-D3/6-311++G(d,p)/SMD//B3LYP-D3/6-31G(d) energy = -1393.417458
INT8
 C -5.16831100 -0.45724400 0.89584500
 C -4.17967600 -0.99209400 0.07743400
 C -2.91697400 -0.38495600 0.00231700
 C -2.65578700 0.77586700 0.74686700
 C -3.65481100 1.30693200 1.56184500
 C -4.90631700 0.69528700 1.64134400
 H -6.14233700 -0.93488900 0.95208100
 H -4.36085900 -1.88069100 -0.51699700
 H -1.69317000 1.27659600 0.69689300
 H -3.45052600 2.20794700 2.13268700
 H -5.67847800 1.11698100 2.27916600
 C -1.92343000 -1.02609000 -0.90778800
 O -2.22919900 -1.95760000 -1.66038500
 N -0.63366100 -0.54553800 -0.87140900
 P 1.15958500 2.39471600 -0.45619800
 O 0.42511100 1.48576000 0.51904500
 H -0.31724600 0.24357900 -0.25272000
 O 0.20535200 3.70960900 -0.67559600
 H 0.46908800 4.13780800 -1.50609300
 O 2.47919600 2.98433900 0.33860600
 H 2.23727100 3.10672800 1.27093900
 O 1.63368400 1.86846200 -1.78340100
 C 3.34126000 -2.20599900 2.00159600
 C 2.33418500 -2.54128300 1.11699600
 C 2.00907400 -1.68264200 0.02938200
 C 2.74632300 -0.47872200 -0.12351000
 C 3.75626100 -0.15215200 0.77189000
 C 4.05418500 -1.00858400 1.83083600
 H 3.57327000 -2.86324700 2.83355600
 H 1.77705500 -3.45569900 1.27799100
 H 2.53074900 0.21163500 -0.93278600
 H 4.28133700 0.78826000 0.64682500
 H 4.83910900 -0.74762600 2.53532500

C 0.97308400 -2.01807900 -0.89735500
 C 0.37507400 -1.00153400 -1.82305800
 H -0.10638800 -1.46063900 -2.68651200
 H 1.00203400 -0.15544800 -2.10724800
 C 0.37025600 -3.37243500 -0.98678000
 H 0.60994600 -4.04415500 -0.16449800
 H -0.71507900 -3.29144300 -1.12842500
 H 0.74655200 -3.81984800 -1.92068000
 Zero-point correction= 0.322532 (Hartree/Particle)
 Thermal correction to Energy= 0.344986
 Thermal correction to Enthalpy= 0.345930
 Thermal correction to Gibbs Free Energy= 0.268658
 Sum of electronic and zero-point Energies= -1392.597454
 Sum of electronic and thermal Energies= -1392.575000
 Sum of electronic and thermal Enthalpies= -1392.574056
 Sum of electronic and thermal Free Energies= -1392.651328
 B3LYP-D3/6-311++G(d,p)/SMD//B3LYP-D3/6-31G(d) energy = -1393.2987179
TS8
 C -3.43069500 -3.16614900 0.87881800
 C -2.23854400 -2.85883200 0.23221700
 C -1.96833700 -1.53435600 -0.14325600
 C -2.88707600 -0.51238900 0.14648800
 C -4.07248800 -0.83257600 0.80308000
 C -4.34891800 -2.15266100 1.16428200
 H -3.64215600 -4.19210700 1.16487900
 H -1.50908400 -3.63054000 0.01287200
 H -2.67040600 0.52129600 -0.11051200
 H -4.77939600 -0.04308500 1.03872900
 H -5.27762900 -2.39189800 1.67475600
 C -0.69149500 -1.24415800 -0.81708900
 O 0.22640000 -2.14659000 -0.86757900
 N -0.43243100 -0.07531100 -1.37020000
 P -0.62019400 2.92924300 0.01519100
 O -1.58376200 2.22192600 -0.93580200
 H -1.01340000 0.82005500 -1.25988700
 O 0.74217000 3.16949300 -0.91634500
 H 1.45173200 3.46563100 -0.32317500
 O -1.18927500 4.44245900 0.25866800
 H -1.74336800 4.68563100 -0.50033900
 O -0.19471200 2.32986600 1.31726600
 C 4.13115900 -1.38181800 1.55504100
 C 3.52574800 -1.61474400 0.32565100
 C 2.41603500 -0.84773500 -0.08219500
 C 1.92615500 0.14803100 0.78613300
 C 2.52625800 0.36746200 2.02025900

C 3.63147000 -0.39193400 2.40715300
 H 4.99115500 -1.97451800 1.85204600
 H 3.92631900 -2.38912100 -0.31847000
 H 1.06615900 0.76337200 0.54887500
 H 2.11003000 1.13774100 2.66130100
 H 4.10477400 -0.21758600 3.36940900
 C 1.76251100 -1.08191900 -1.37662500
 C 0.89707400 0.03339200 -1.95451800
 H 0.83254200 -0.07079600 -3.04378500
 H 1.29401000 1.02617300 -1.72392500
 C 2.40015600 -1.99712000 -2.37945900
 H 2.70258100 -2.94551000 -1.93400700
 H 1.71147400 -2.20021300 -3.20130700
 H 3.29394700 -1.50818300 -2.78946800
 Zero-point correction= 0.322359 (Hartree/Particle)
 Thermal correction to Energy= 0.343801
 Thermal correction to Enthalpy= 0.344746
 Thermal correction to Gibbs Free Energy= 0.270387
 Sum of electronic and zero-point Energies= -1392.615853
 Sum of electronic and thermal Energies= -1392.594411
 Sum of electronic and thermal Enthalpies= -1392.593466
 Sum of electronic and thermal Free Energies= -1392.667825
 B3LYP-D3/6-311++G(d,p)/SMD//B3LYP-D3/6-31G(d) energy = -1393.3146737
TS8'
 C -4.87748600 -1.52842400 0.88118600
 C -3.74860400 -1.80539200 0.11646300
 C -2.68859500 -0.88954100 0.05344900
 C -2.77805000 0.31325300 0.76885500
 C -3.91112800 0.58756400 1.53294600
 C -4.96132600 -0.32910800 1.59236000
 H -5.69260200 -2.24560700 0.92253300
 H -3.66233900 -2.72795900 -0.44643800
 H -1.98054400 1.04279100 0.73820700
 H -3.96999200 1.52396100 2.07970400
 H -5.84265600 -0.10947100 2.18882300
 C -1.51318000 -1.27039900 -0.79670600
 O -1.51708200 -2.35021000 -1.41906500
 N -0.48898000 -0.36960400 -0.87665100
 P 0.24452300 2.84279600 -0.27812400
 O 0.36412400 1.65295100 0.73453100
 H -0.08038700 0.59594400 0.15757100
 O 1.53085800 2.54174000 -1.29107400
 H 1.73164400 3.35152800 -1.78779900
 O -1.03596100 2.52108300 -1.22265900
 H -1.09535300 1.55691200 -1.39727300

O 0.25170300 4.23681300 0.21027200
 C 4.14249600 -1.85681400 1.72762500
 C 3.23861000 -2.28217400 0.77530300
 C 2.54294500 -1.34080300 -0.04174800
 C 2.82066500 0.04408500 0.14298900
 C 3.72887700 0.45824200 1.10512800
 C 4.38682200 -0.48368100 1.89693200
 H 4.65795700 -2.58098400 2.34999400
 H 3.04757100 -3.34217000 0.66771600
 H 2.33075900 0.79783000 -0.45442800
 H 3.90888400 1.51900400 1.24057700
 H 5.09401300 -0.15496300 2.65315800
 C 1.59296700 -1.76529100 -1.00981400
 C 0.66741800 -0.76011000 -1.72900400
 H 0.29924300 -1.23140000 -2.64401800
 H 1.20584500 0.15149400 -1.98941000
 C 1.29060700 -3.17160300 -1.30878000
 H 1.88003600 -3.91948800 -0.78239700
 H 0.20180000 -3.29414700 -1.13285800
 H 1.37376500 -3.32583600 -2.39438600
 Zero-point correction= 0.316694 (Hartree/Particle)
 Thermal correction to Energy= 0.338536
 Thermal correction to Enthalpy= 0.339480
 Thermal correction to Gibbs Free Energy= 0.264069
 Sum of electronic and zero-point Energies= -1392.568141
 Sum of electronic and thermal Energies= -1392.546299
 Sum of electronic and thermal Enthalpies= -1392.545355
 Sum of electronic and thermal Free Energies= -1392.620766
 B3LYP-D3/6-311++G(d,p)/SMD//B3LYP-D3/6-31G(d) energy = -1393.2683288
INT9
 C -2.44507200 3.21347600 -1.48596900
 C -1.32186000 2.71146400 -0.84472800
 C -1.46160200 1.65223500 0.07239600
 C -2.72533400 1.09607900 0.33333500
 C -3.83856900 1.59417700 -0.33451300
 C -3.70256400 2.65182500 -1.23304300
 H -2.34457800 4.03254800 -2.19122600
 H -0.33824300 3.12129600 -1.04460300
 H -2.83984700 0.25393800 1.00546100
 H -4.80284200 1.12756500 -0.16888500
 C -0.27529300 1.10745500 0.70129000
 O 0.91386800 1.50331500 0.29493800
 N -0.22932500 0.23138700 1.67878400
 P -2.12541100 -2.21182400 0.06491300
 O -1.95317800 -1.94055800 1.55261300

H -1.00519500 -0.40735000 1.85442000
 O -0.74529200 -1.56913100 -0.66135200
 H -1.02003000 -1.33510700 -1.56273900
 O -1.91239500 -3.82642500 -0.14380500
 H -1.65135900 -4.18942300 0.71692700
 O -3.28762900 -1.71755600 -0.73146500
 C 5.15866900 -0.00470300 -0.87338700
 C 4.28977600 0.56757000 0.05710700
 C 2.94428000 0.19001800 0.09437200
 C 2.47460800 -0.76680900 -0.81897200
 C 3.34299900 -1.33015600 -1.75002800
 C 4.68741600 -0.95273500 -1.77956400
 H 6.20282300 0.29369500 -0.88691500
 H 4.67568400 1.30415900 0.75303700
 H 1.43201000 -1.07553600 -0.80432900
 H 2.96740000 -2.06992600 -2.45072300
 H 5.36349400 -1.39774500 -2.50389300
 C 1.97326800 0.78816000 1.08926300
 C 1.13155900 -0.26693400 1.85449000
 H 1.39952600 -0.30681800 2.91288100
 H 1.19991000 -1.26825300 1.42435400
 C 2.54405400 1.83955500 2.03015800
 H 2.96724200 2.67749300 1.47126200
 H 1.75161600 2.21974900 2.68171600
 H 3.32433100 1.40112800 2.65932500
 H -4.57649800 3.03501200 -1.75193900
 Zero-point correction= 0.325023 (Hartree/Particle)
 Thermal correction to Energy= 0.346800
 Thermal correction to Enthalpy= 0.347744
 Thermal correction to Gibbs Free Energy= 0.272508
 Sum of electronic and zero-point Energies= -1392.621042
 Sum of electronic and thermal Energies= -1392.599265
 Sum of electronic and thermal Enthalpies= -1392.598321
 Sum of electronic and thermal Free Energies= -1392.673558
 B3LYP-D3/6-311++G(d,p)/SMD//B3LYP-D3/6-31G(d) energy = -1393.3254482
TS9
 C -1.97821200 3.27050200 -1.61585000
 C -0.90966400 2.72503800 -0.91372900
 C -1.15114000 1.77230600 0.09061100
 C -2.46392200 1.37679600 0.38574200
 C -3.52445300 1.90968100 -0.33861300
 C -3.28455800 2.85936000 -1.33258900
 H -1.79389000 4.00625300 -2.39280300
 H 0.10969800 3.01623300 -1.13955400
 H -2.65995100 0.63818300 1.15181400

H -4.52945900 1.55730400 -0.13649300
 C -0.02278600 1.16077600 0.78380600
 O 1.19765000 1.63771700 0.52569900
 N -0.06867200 0.16926800 1.61795500
 P -2.42618200 -2.05008400 0.12749600
 O -1.85027500 -1.84781600 1.55921200
 H -1.04122700 -0.78250100 1.63588400
 O -1.18085000 -1.57114400 -0.85448200
 H -1.58131200 -1.18366800 -1.64956500
 O -2.48826700 -3.66757500 -0.04237100
 H -1.91751400 -4.07548400 0.62799700
 O -3.68652100 -1.40325900 -0.31740600
 C 4.91932500 -0.58875200 -1.17110500
 C 4.29503900 0.11607900 -0.13953100
 C 2.91701600 0.00506200 0.06370900
 C 2.16821800 -0.82468000 -0.78668100
 C 2.79178900 -1.52245200 -1.81689400
 C 4.17019700 -1.40770300 -2.01306100
 H 5.99202100 -0.49367700 -1.31293500
 H 4.89678000 0.74773200 0.50464600
 H 1.09542200 -0.93787800 -0.65390000
 H 2.19673900 -2.16072700 -2.46340800
 H 4.65560600 -1.95578100 -2.81546100
 C 2.19937200 0.74755500 1.17750600
 C 1.28603500 -0.18642000 2.02896800
 H 1.41243500 -0.01443700 3.10375300
 H 1.47110900 -1.24350800 1.82447400
 C 3.07076500 1.64857100 2.03660500
 H 3.59593500 2.38908100 1.42815000
 H 2.44589500 2.17693700 2.76197200
 H 3.80848000 1.05435600 2.58482300
 H -4.11535700 3.27427200 -1.89610000
 Zero-point correction= 0.319104 (Hartree/Particle)
 Thermal correction to Energy= 0.340532
 Thermal correction to Enthalpy= 0.341476
 Thermal correction to Gibbs Free Energy= 0.267125
 Sum of electronic and zero-point Energies= -1392.627162
 Sum of electronic and thermal Energies= -1392.605734
 Sum of electronic and thermal Enthalpies= -1392.604790
 Sum of electronic and thermal Free Energies= -1392.679141
 B3LYP-D3/6-311++G(d,p)/SMD//B3LYP-D3/6-31G(d) energy = -1393.3177108
INT10
 C -1.20364800 4.44925700 -0.27897900
 C -0.41642800 3.40526300 0.19886300
 C -0.92584300 2.09840500 0.21879000

C -2.22743400 1.84442600 -0.24353300
 C -3.00460800 2.89333200 -0.72256200
 C -2.49640900 4.19490400 -0.74061000
 H -0.80829100 5.46042800 -0.29221700
 H 0.58834500 3.59172900 0.56071100
 H -2.62311400 0.83593100 -0.23364500
 H -4.00861400 2.69303500 -1.08310600
 C -0.09513200 0.99787400 0.71269900
 O 1.15511000 1.30612500 1.11600600
 N -0.44104400 -0.24310400 0.79155400
 P -2.66669400 -2.42201900 -0.31307300
 O -1.80445200 -1.53516800 -1.33693200
 H -1.15439400 -0.99222400 -0.83269900
 O -1.52449900 -3.43865700 0.27302100
 H -1.93997000 -4.28959300 0.48724700
 O -2.98337700 -1.43261700 0.91849200
 H -2.16275300 -0.92388200 1.13682900
 O -3.84999900 -3.09598200 -0.87208000
 C 0.68803400 -0.97431600 1.38133600
 C 1.86631000 0.03876000 1.33611800
 H 0.88738900 -1.88566000 0.81460000
 H 0.43505300 -1.26354200 2.40923800
 C 2.62500800 0.17007000 2.65082200
 H 3.14717800 -0.76421500 2.87762300
 H 3.36855800 0.96904000 2.58388100
 H 1.93252200 0.39248700 3.46839500
 C 2.79547100 -0.20969100 0.15641300
 C 2.96366500 0.72954600 -0.86352100
 C 3.50437100 -1.41650500 0.09341800
 C 3.82506600 0.46508900 -1.93007800
 H 2.41833000 1.66516000 -0.82533700
 C 4.36526200 -1.67894800 -0.96936300
 H 3.37916700 -2.16132200 0.87557800
 C 4.52834300 -0.73666300 -1.98677100
 H 3.94166100 1.20252100 -2.71907900
 H 4.90462400 -2.62099200 -1.00535800
 H 5.19599500 -0.94155900 -2.81842900
 H -3.10840900 5.01024600 -1.11533700
 Zero-point correction= 0.323550 (Hartree/Particle)
 Thermal correction to Energy= 0.345578
 Thermal correction to Enthalpy= 0.346522
 Thermal correction to Gibbs Free Energy= 0.268315
 Sum of electronic and zero-point Energies= -1392.633909
 Sum of electronic and thermal Energies= -1392.611882

Sum of electronic and thermal Enthalpies= -1392.610938
Sum of electronic and thermal Free Energies= -1392.689145
B3LYP-D3/6-311++G(d,p)/SMD//B3LYP-D3/6-31G(d) energy = -1393.327

P5

C -3.88817300 1.40409600 0.95475200
C -2.62761000 0.81101400 0.90778700
C -2.32973200 -0.11915500 -0.09633700
C -3.30254600 -0.45115500 -1.05028600
C -4.55817700 0.14441300 -0.99832100
C -4.85411200 1.07337000 0.00373900
H -4.11590400 2.12465900 1.73506600
H -1.87204500 1.05925500 1.64455900
H -3.05145100 -1.17370900 -1.81912700
H -5.30909400 -0.11418200 -1.73939900
C -1.00683900 -0.75394600 -0.16722400
O -0.10655000 -0.36431600 0.78726900
N -0.63575100 -1.62228700 -1.02694700
C 0.74681500 -1.97028600 -0.70628000
C 1.14595200 -1.05224200 0.49894900
H 1.39114000 -1.80445900 -1.57560800
H 0.81181500 -3.03414900 -0.44319500
C 1.52351300 -1.83915900 1.75249900
H 2.44944700 -2.39964700 1.58966200
H 1.67541100 -1.16218500 2.59819100
H 0.72658600 -2.54677600 2.00264800
C 2.20635500 -0.02810400 0.12969000
C 1.94049900 1.34321800 0.13934300
C 3.48558800 -0.46708100 -0.23751300
C 2.93554900 2.25861600 -0.20874300
H 0.95139700 1.68784600 0.41676400
C 4.47891900 0.44591800 -0.58450600
H 3.70717000 -1.53138200 -0.25886900
C 4.20687100 1.81538600 -0.56997300
H 2.71231200 3.32196200 -0.19827200
H 5.46465300 0.08781400 -0.86826900
H 4.97978400 2.52889600 -0.84107300
H -5.83579400 1.53718600 0.04193300

Zero-point correction= 0.272489 (Hartree/Particle)

Thermal correction to Energy= 0.287133

Thermal correction to Enthalpy= 0.288078

Thermal correction to Gibbs Free Energy= 0.228132

Sum of electronic and zero-point Energies= -748.513144

Sum of electronic and thermal Energies= -748.498500

Sum of electronic and thermal Enthalpies= -748.497556

Sum of electronic and thermal Free Energies= -748.557502

B3LYP-D3/6-311++G(d,p)/SMD//B3LYP-D3/6-31G(d) energy = -748.9926
N₂
N 0.00000000 0.00000000 0.55274800
N 0.00000000 0.00000000 -0.55274800
Zero-point correction= 0.005598 (Hartree/Particle)
Thermal correction to Energy= 0.007959
Thermal correction to Enthalpy= 0.008903
Thermal correction to Gibbs Free Energy= -0.012851
Sum of electronic and zero-point Energies= -109.519283
Sum of electronic and thermal Energies= -109.516922
Sum of electronic and thermal Enthalpies= -109.515978
Sum of electronic and thermal Free Energies= -109.537733
B3LYP-D3/6-311++G(d,p)/SMD//B3LYP-D3/6-31G(d) energy = -109.5541899

4. References

- 1 R. A. Marcus, Chemical and Electrochemical Electron-Transfer Theory. *Annu. Rev. Phys. Chem.* **1964**, *15*, 155–196.