Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting Information

for

Catalyst Free Boron Carbon Bond Cleavage and Facile Formation of Five-membered PNBCC Heterocycles

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Content:

S1. Experimental Section

All manipulations were performed under a dry and oxygen-free atmosphere (N_2) using standard Schlenk techniques and in a dinitrogen filled MBRAUN MB 150-G1 glovebox. All the glassware was oven-dried at 120 ^oC overnight. The solvents used were purified by MBRAUN solvent purification system MB SPS-800. All other chemicals were purchased from Aldrich were used without further purification. ^1H, ^{13}C, ^{31}P, ^{11}B, NMR spectra were recorded in $CDCl_3$ on a Bruker Ascend 400 MHz spectrometer using an internal standard ($SiMe_4$ for ^1H, ^{13}C, Triphenyl phosphate (TPP) for ^{31}P, and $BF_3{\cdot}OEt_2$ for ^{11}B). Mass spectra were recorded using AB Sciex, 4800 plus MALDI TOF/TOF and HRMS. Melting points were recorded in a sealed glass tube on a Stuart SMP-30 melting point apparatus. Fourier transform infrared (FT-IR) spectra were taken on a PerkinElmer spectrophotometer. The phosphine substituted amino-borane [N(2,6-iPr$_2$C$_6$H$_3$)(PPh$_2$)(BCy$_2$)] (**1**) was prepared according to standard literature method.[1]

Synthesis of 2: A toluene solution (30 mL) of **1** (0.300 g, 0.558 mmol) was taken and to this solution dimethyl acetylene dicarboxylate (DMAD) (0.079 g, 0.07 mL, 0.56 mmol) was added under the flow of argon and allowed to stir at room temperature for 12 h. The solution was filtered over celite and reduced to 5 mL. The storage of this solution at 0 °C afforded off-white crystals of **2.** Yield (0.070 g, 23%). Mp. 104 °C.^1H NMR ($CDCl_3$, 400 MHz, ppm): δ 1.06−1.08 (*d*, 12H, *J* = 7.1 Hz, 2(C*H*$_3$)$_2$CH), 0.87-0.99; 1.18-1.77 (*m*, 22H, cyclohexyl), 3.46-3.87 (*br*, 8H, 2(CH$_3$)$_2$*CH* + 2CO$_2$*CH*$_3$), 7.07−7.78 (*m*, 13H, Ph). $^{13}C\{^1H\}$ NMR ($CDCl_3$, 100.613 MHz, ppm): δ 23.68, 28.23, 123.23, 128.04, 131.97, 142.75, 147.08. $^{31}P\{^1H\}$ NMR ($CDCl_3$, 161.976 MHz, ppm): δ 21.61. ^{11}B NMR ($CDCl_3$, 128.387 MHz, ppm): δ 32.31 (*br*). MALDI: Calcd for $C_{42}H_{55}BNO_4P$ (679.68): m/z 679.39. Found: *m/z* 701.16 ([M + Na]$^+$). Anal. Calcd. C, 74.22; H, 8.16; N, 2.06. Found: C, 73.87; H, 7.78; N, 1.59.

Synthesis of 3: A toluene solution (30 mL) of **1** (0.300 g, 0.558 mmol)) was taken in a 100 ml Schlenk flask and to this solution of diethyl acetylene dicarboxylate (DEAD) (0.095 g, 0.56 mmol) was added under the flow of argon and allowed to stir at room temperature for 12 h. The toluene solution was filtered over celite and reduced to 5 mL. Storing this solution at 0 °C afforded off-white crystals of **3**. Yield (0.09 g, 26 %). Mp. 110 °C. ^{1}H NMR ($CDCl_3$, 400 MHz, ppm): δ 1.05-1.07 (*d*, 12H, *J* = 7.23Hz, *(CH_3)$_2$*CH), 1.22-1.35; 1.67-1.76 (*m*, 22H, cyclohexyl), 3.45-3.64; 4.01-4.34 (merged peaks) (12H) (*m*) [6H [2*CH_3*, CO_2Et]), + [2H, 2$(CH_3)_2$C*H* + 4H (2*CH_2*, CO_2Et)], 7.06−7.77 (*m*, 13H, Ph). ^{13}C{^{1}H} NMR ($CDCl_3$, 100.613 MHz, ppm): δ 23.50, 28.16, 123.54, 127.01, 128.51, 131.88, 132.81, 147.33. ^{31}P{^{1}H} NMR ($CDCl_3$, 161.976 MHz, ppm): δ 21.52. ^{11}B NMR ($CDCl_3$, 128.387 MHz, ppm): δ 32.02 (*br*). MALDI: Calcd for $C_{44}H_{59}BNO_4P$ (707.74): *m/z* 707.42. Found: *m/z* 707.49 ($[M]^+$). Anal. Calcd. C, 74.67; H, 8.40; N, 1.98. Found: C, 74.08; H, 8.13; N, 1.78.

Synthesis of 4: A THF solution (20 mL) of **1** (0.30 g, 0.558 mmol)) was taken in a 100 ml Schlenk flask and to this solution acetylene dicarboxylic acid (0.063 g, 0.56 mmol) was added under the flow of argon and allowed to stir at room temperature for 12 h. The THF solution was evaporated under vacuum and the remaining solid residue was extracted with toluene (30 mL). Subsequently, the toluene solution was reduced to 5 mL and kept at 0 °C to yield off-white crystals of **4**. Yield (0.087 g, 27%). Mp. 66 °C. ^{1}H NMR ($CDCl_3$, 400 MHz, ppm): δ 1.06−1.08 (*d*, 12H, *J* = 7.17 Hz, 2*(CH_3)$_2$*CH), 0.91-0.97; 1.18−2.34 (*m*, 22H, cyclohexyl), 3.56-3.66 (*br*, 2H, $(CH_3)_2$C*H*), 4.51 (*s*, 2H, 2COO*H*) 7.07−7.78 (*m*, 13H, Ph). ^{13}C{^{1}H} NMR ($CDCl_3$, 100.613 MHz, ppm): δ 23.34, 28.24, 123.20, 128.31, 131.79, 147.29. ^{31}P{^{1}H} NMR ($CDCl_3$, 161.976 MHz, ppm): δ 22.10. ^{11}B NMR ($CDCl_3$, 128.387 MHz, ppm): δ 33.61 (*br*). MALDI: Calcd for

$C_{40}H_{51}BNO_4P$ (651.63): *m/z* 651.36. Found: *m/z* 674.28 ($[M + Na]^+$). Anal. Calcd. C, 73.73; H, 7.89; N, 2.15. Found: C, 72.29; H, 7.58; N, 1.93.

S2. Table for Crystal Data and Structure Refinement for 1, 2 and 3.

Single crystals of suitable size, were coated with paraffin oil was mounted for all the complexes. Crystal data for all the complexes were collected on a Bruker S9 Smart Apex Duo diffractometer at 100 K using Mo Kα radiation (λ = 0.71073 Å) for Compound **1** and Cu Kα radiation (λ = 1.54178 Å) for Compounds **2** and **3**. Collected data were integrated by using SAINT and then absorption correction was done by multi-scan method using SADABS program All the structures were solved by direct methods and refined by full-matrix least-squares methods against F2 (SHELXL-2014/6). CCDC no. are 1543526 (**1**), 1543527 (**2**), 1543528 (**3**).

Table S[1]. Crystal Data and Structure Refinement for 1, 2 and 3.

	1	**2**	**3**
Chemical formula	$C_{36}H_{49}BNP$	$C_{49}H_{63}BNO_4P$	$C_{44}H_{59}BNO_4P$
Formula weight	537.54 g/mol	771.78 g/mol	707.70 g/mol
Temperature	100(2) K	100(2) K	100(2) K
Wavelength	0.71073 Å	1.54178 Å	1.54178 Å
Crystal system	Monoclinic	Triclinic	Monoclinic
Space group	$P\,2_1/n$	$P\,\bar{1}$	$P\,2_1/c$
Unit cell dimensions	a = 17.885(9) Å	a = 10.6838(12) Å	a = 18.4589(7) Å
	b = 10.312(5) Å	b = 12.1850(12) Å	b = 10.3146(4) Å
	c = 19.369(10) Å	c = 17.8138(18) Å	c = 24.4094(9) Å
	α = 90°	α = 75.008(4)°	α = 90°
	β = 115.481(11)°	β = 76.864(4)°	β = 104.138(2)°
	γ = 90°	γ = 89.922(3)°	γ = 90°
Volume	3225(3) $Å^3$	2177.4(4) $Å^3$	4506.7(3) $Å^3$
Z	4	2	4
Density (calculated)	1.107 g/cm^3	1.177 g/cm^3	1.043 g/cm^3
Absorption coefficient	0.109 mm^{-1}	0.896 mm^{-1}	0.826 mm^{-1}
F(000)	1168	832	1528
Theta range for data collection	2.052 to 26.078°	2.642 to 69.743°	2.468 to 60.015°
Index ranges	-21<=h<=21, -12<=k<=12, -23<=l<=22	-12<=h<=11, -14<=k<=14, -21<=l<=21	-20<=h<=19, -10<=k<=11, -22<=l<=27
Reflections collected	27848	30493	54285

Independent reflections	6302 [R(int) = 0.0646]	8163 [R(int) = 0.0380]	6388 [R(int) = 0.1334]
Coverage of independent reflections	99.9%	99.7%	95.4%
Function minimized	Σ w(Fo^2 - Fc^2)^2	Σ w(Fo^2 - Fc^2)^2	Σ w(Fo^2 - Fc^2)^2
Data / restraints / parameters	6302 / 0 / 356	8163/ 0 / 512	6388 / 0 / 466
Goodness-of-fit on F^2	1.022	1.003	1.039
Δ/σ max	0.002	0.006	0.000
Final R indices	5072 data; [I>2σ(I)] $R1$ = 0.0413, w$R2$ = 0.1033	7080 data[I>2σ(I)], $R1$ = 0.0467, w$R2$ = 0.1156	3553 data[I>2σ(I)], $R1$ = 0.0922, w$R2$ = 0.2031
	all data , $R1$ = 0.0546, w$R2$ = 0.1119	all data , $R1$ = 0.0545, w$R2$ = 0.1210	all data, $R1$ = 0.1683, w$R2$ = 0.2323
Largest diff. peak and hole	0.251 and -0.294 eÅ^{-3}	0.776 and -0.459 eÅ^{-3}	0.295 and -0.338 eÅ^{-3}
R.M.S. deviation from mean	0.042 eÅ^{-3}	0.055 eÅ^{-3}	0.067 eÅ^{-3}

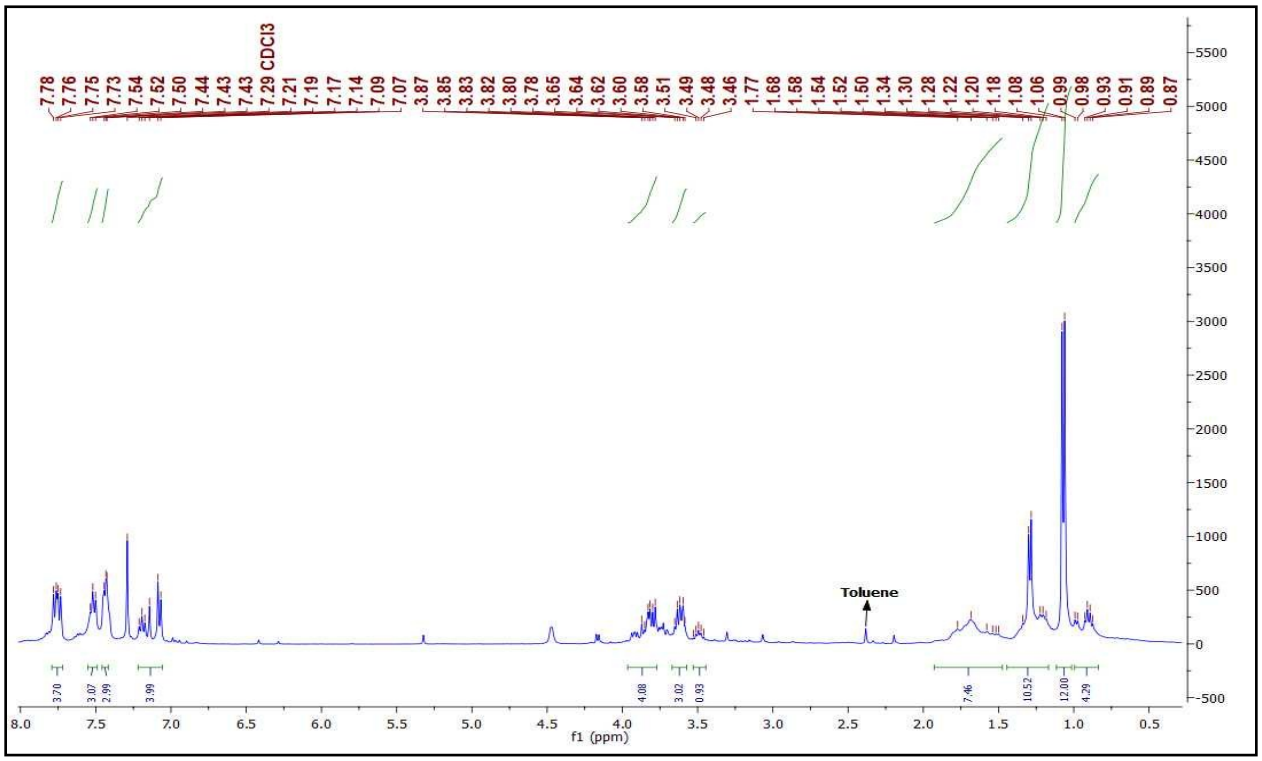
S3. IR Data

Table S[2]. IR Stretching frequencies of key bonds in the five-membered heterocyclic compounds **2-4**.

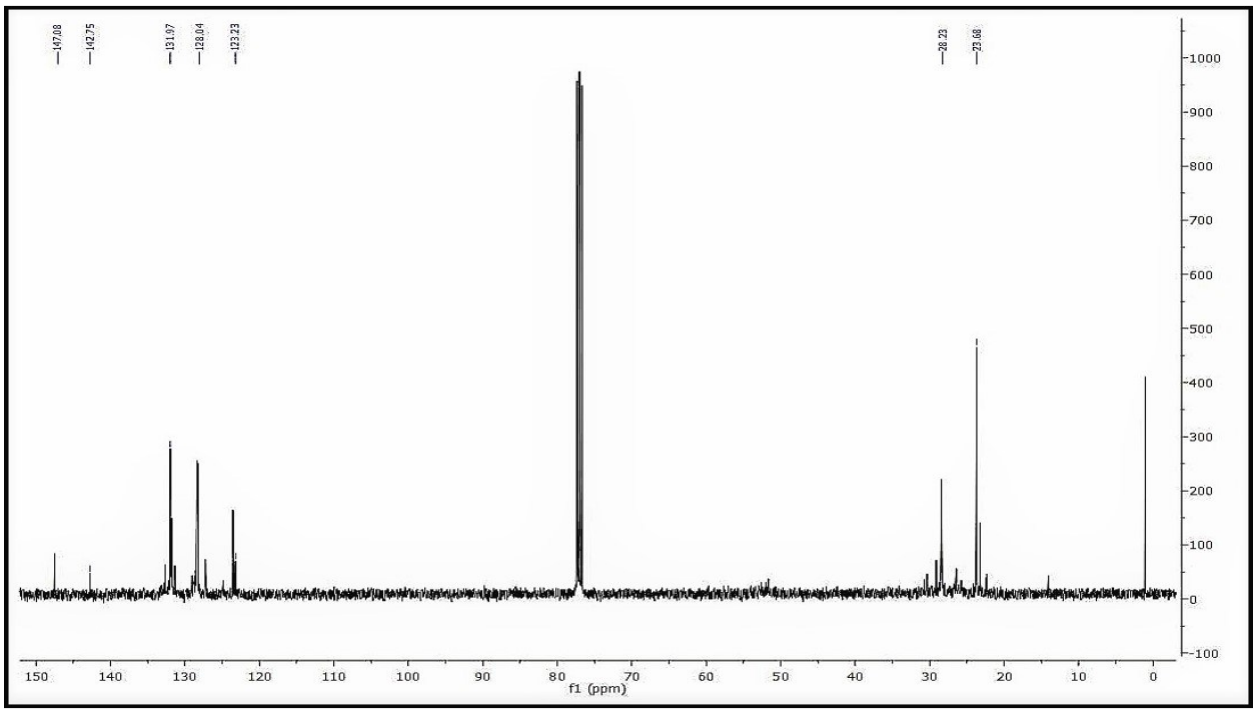
COMPOUND	P=C (cm^{-1})	P-N (cm^{-1})	B-N (cm^{-1})	B-C (cm^{-1})	C=O (cm^{-1})	C-O/O-H (cm^{-1})
1	-	796.01	1438.52	-	-	-
2	1436.02	722.57	1052.37 (*b*)	1201.32	1722.99	1257.48
3	1440.74	751.57	1023.43 (*b*)	1256.81	1718.53	1256.81
4	1448.11	786.05	1007.55 (*b*)	1257.95	1693.65	3743.54 (*b*)

S4. NMR Spectra of 1-4 (in $CDCl_3$)

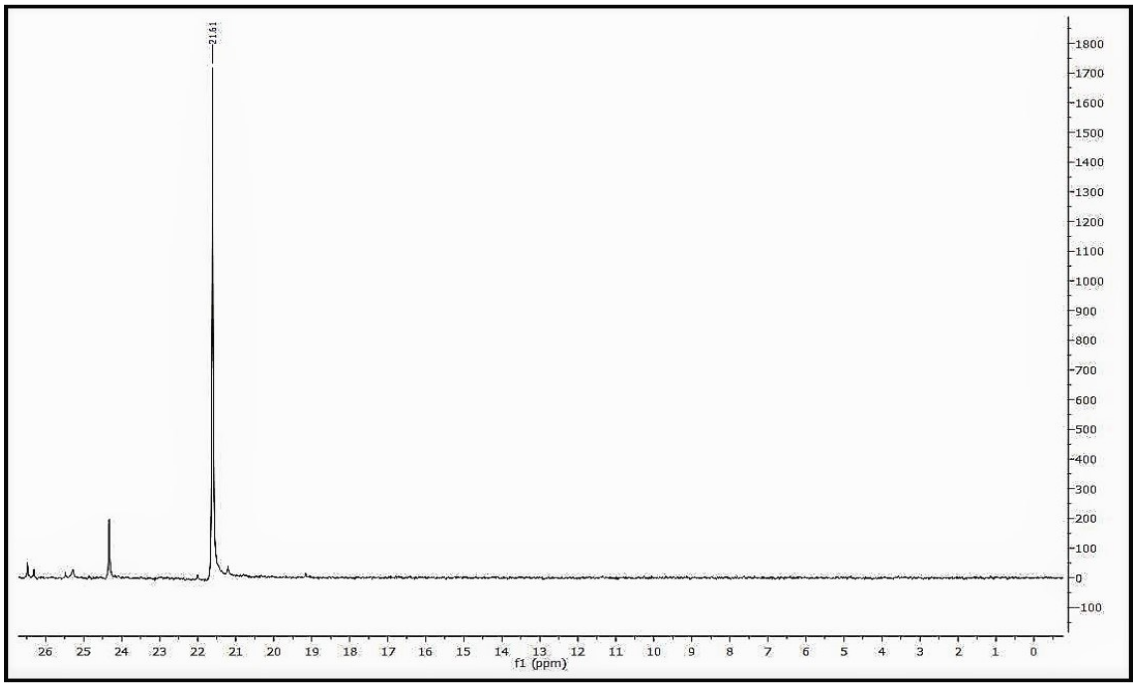
^{1}H NMR spectrum of **2:**



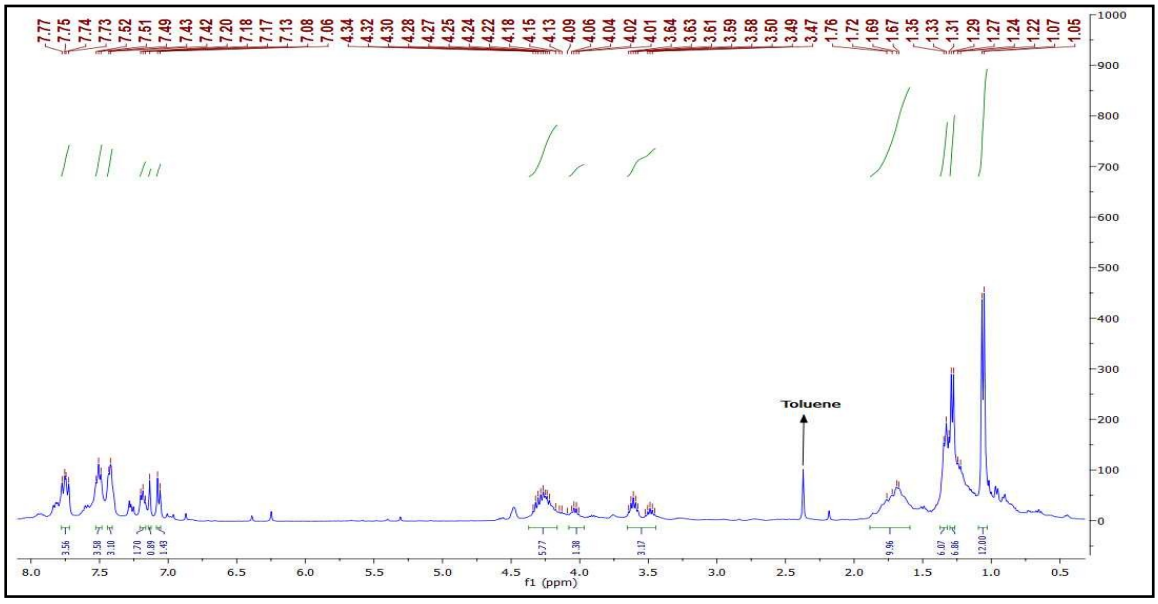
^{13}C NMR spectrum of **2:**



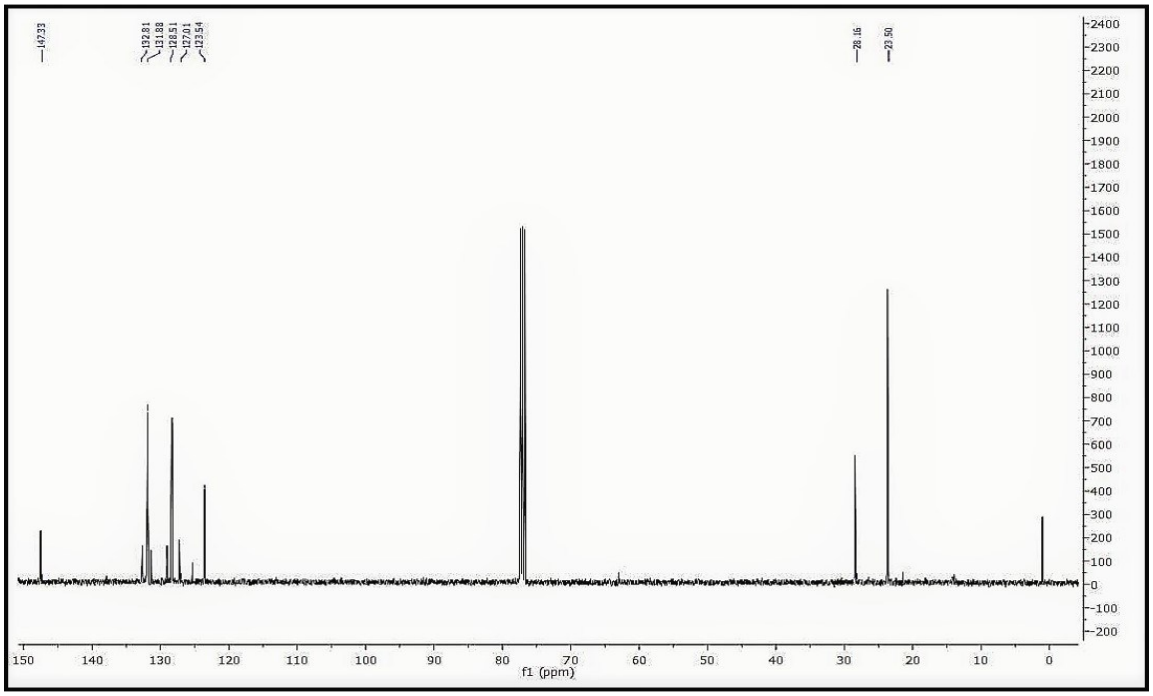
^{31}P NMR spectrum of **2:**



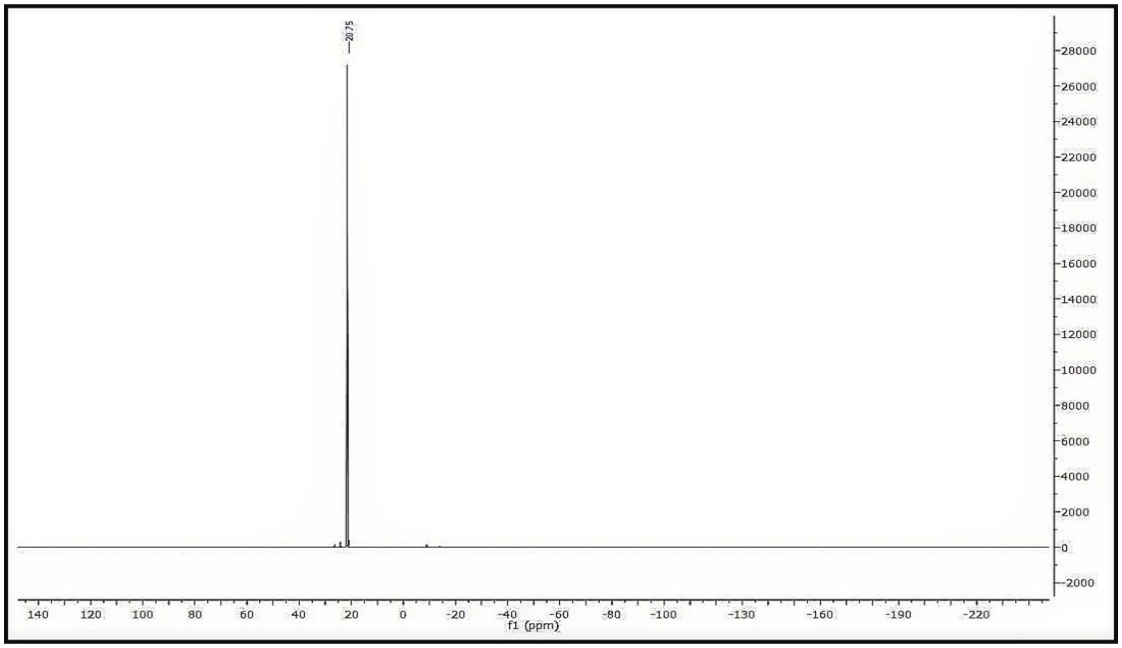
^{1}H NMR spectrum of **3:**



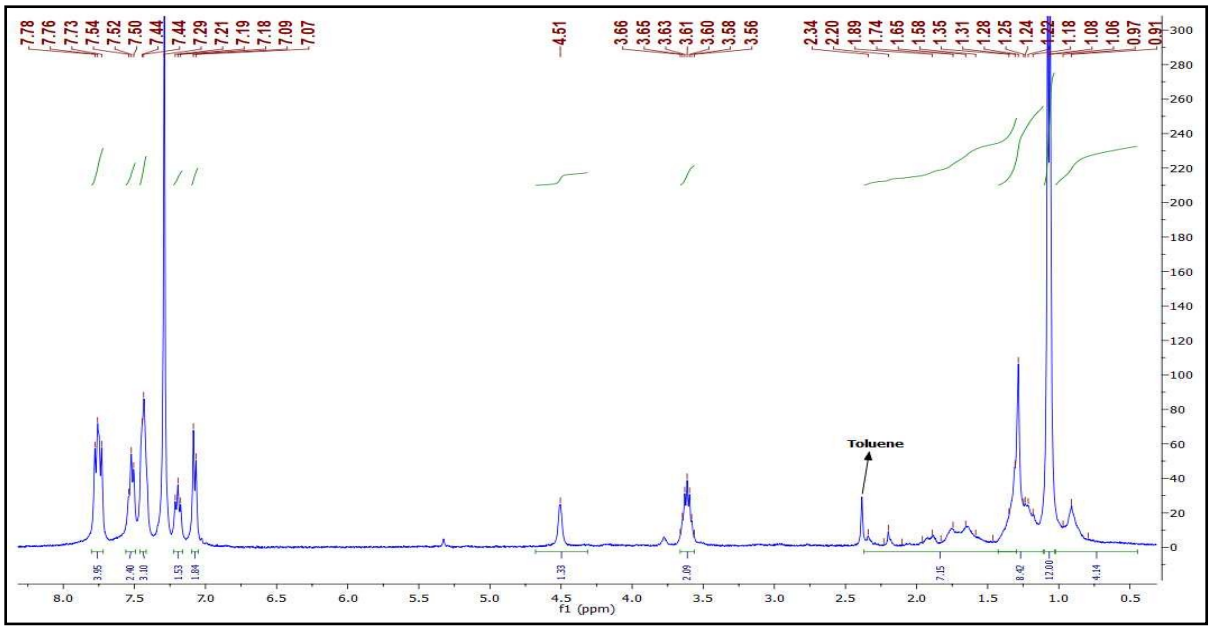
^{13}C NMR spectrum of **3:**



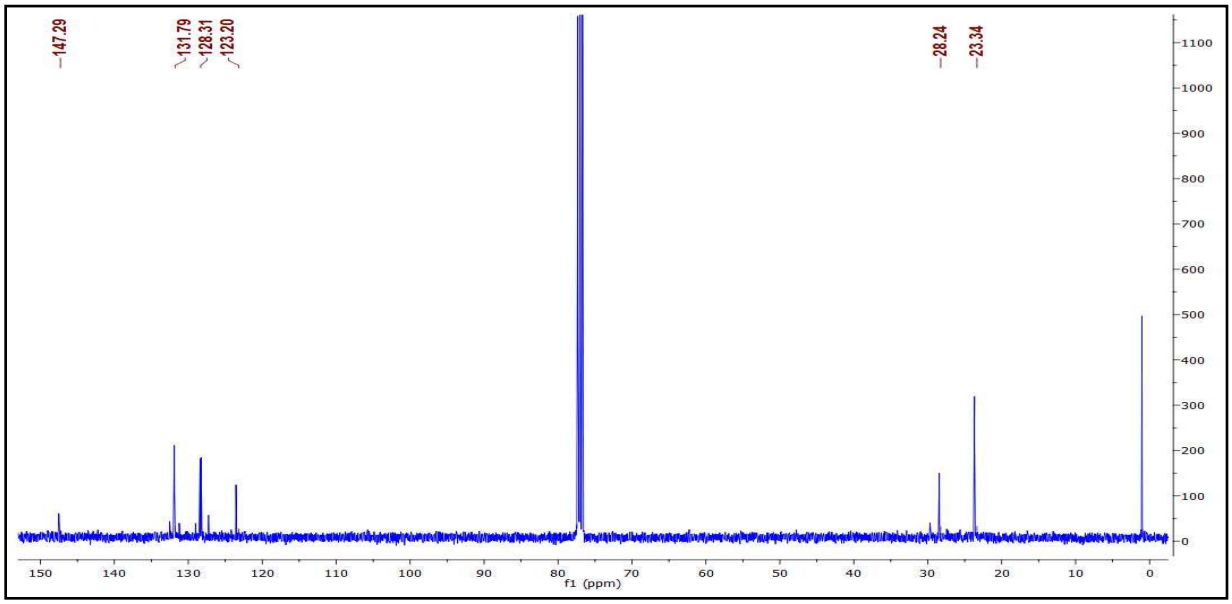
^{31}P NMR spectrum of **3:**



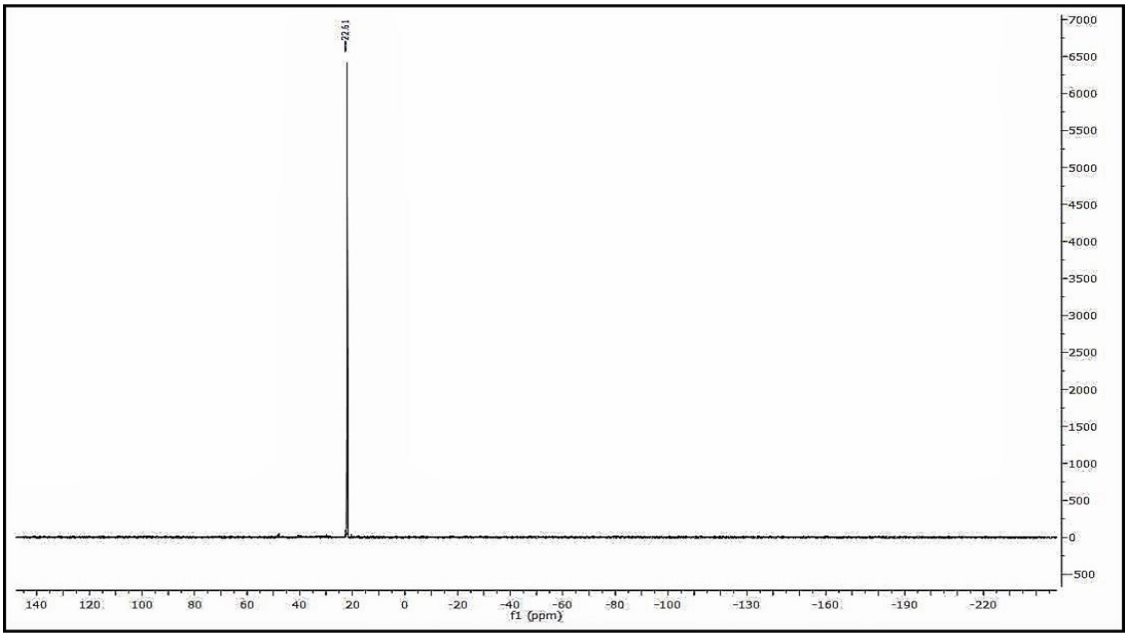
^{1}H NMR spectrum of **4:**



^{13}C NMR spectrum of **4:**



^{31}P NMR spectrum of **4:**



S5. Computational Details

All the calculations were performed at the DFT level of theory using Gaussian 09 program package.[2] We have used the exchange functional of Becke in conjunction with the correlation functional of Perdew (BP86)[3] with the basis set having double ζ-quality augmented with one set of polarization functions (def2-SVP)[4] for the geometry optimization. The single point calculations were performed by using the meta-GGA exchange functional M06[5] with basis set having triple ζ-quality augmented by two sets of polarization functions (def2-TZVPP)[4] The natural bond orbital analysis (NBO)[6] and quantitative analysis of Electrostatic potential (ESP) on the molecular van der Waals surfaces with Multiwfn[7] program have been carried out using M06/def2-TZVPP//BP86/def2-SVP level of theory. We have performed geometry optimization with BP86 (GGA Functional) and single point calculations at the hybrid meta-GGA functional (M06) to get higher accuracy calculation of energetics. Our earlier studies show that optimization at the BP86/def2-SVP level of theory reproduces the experimental geometry quite well and the M06/def2-TZVPP level of theory gives reasonable estimate of the electronic energy[8] The reaction energy (ΔE) and energy of activation ($\Delta E^{\ddagger}$) were calculated by adding electronic energy at the M06/def2-TZVPP level of theory with zero point correction calculated at the BP86/def2-SVP level of theory. ΔG and $\Delta G^{\ddagger}$ (298.5 K and 1atm) represent the free energy of reaction and

free energy of activation calculated by adding electronic energy at the M06/def2-TZVPP level of theory with thermal correction to Gibbs free energy calculated at the BP86/def2-SVP level of theory. All the transition states have been verified by IRC calculations. A. xyz file (Cartesian_coordinate.xyz) with Cartesian coordinates of all calculated molecules along with computed energies is also given below.

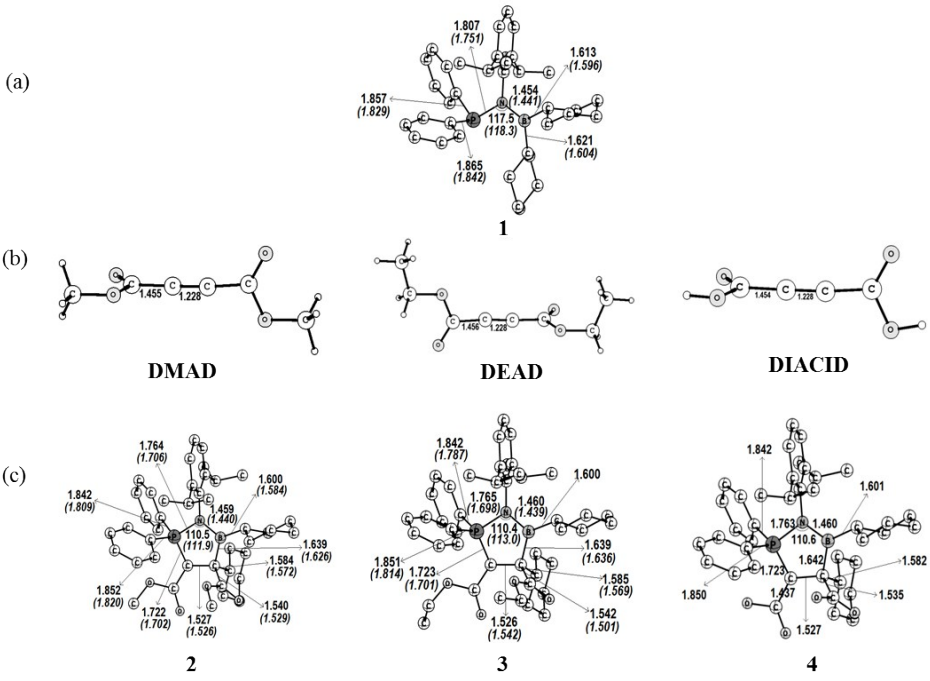


Figure S[1]: Optimized geometries and important geometrical parameters of (a) **1**, (b) alkynes and (c) **2 - 4** at the BP86/def2-SVP level of theory. Experimental values for **1 - 3** are given in parenthesis. Distances are given in angstroms and angles are given in degrees.

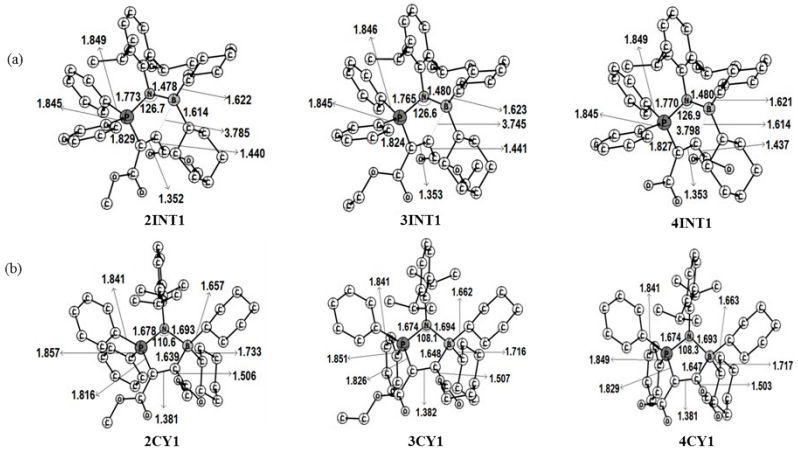


Figure S[2]: Optimized geometries and important geometrical parameters of (a) acyclic intermediates (**2INT1 – 4INT1)** and (b) cyclic intermediates (**2CY1 – 4CY1**) at the BP86/def2-SVP level of theory. Distances are given in angstroms and angles in degrees.

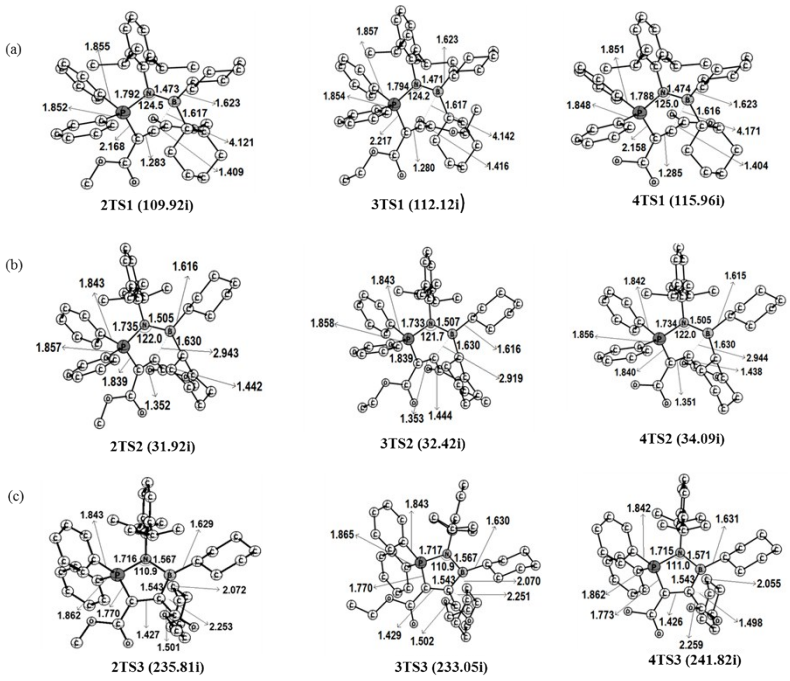
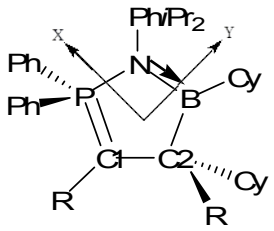


Figure S[3]: Optimized geometries and important geometrical parameters of transition states at the BP86/def2-SVP level of theory. Imaginary frequencies in cm^{-1} are given in parenthesis. Distances are given in angstroms and angles in degrees.

Table S[3]: Charge distribution given by the Natural Population Analysis for **1 – 4**, **INT1** and **CY1** at the M06/def2-TZVPP//BP86/def2-SVP level of theory. p_z atomic orbital occupancy of N,B and C1 atom of are given in parenthesis.

Compound	Atoms				
	N	P	B	C1	C2
1	-1.12 (1.72)	1.07	1.38 (0.26)		
2INT1	-1.17	1.84	1.49	-0.66	-0.13
2CY1	-1.00	1.84	0.69	-0.59	-0.07
2	-1.16 (1.71)	1.85	1.50 (0.22)	-0.77 (1.43)	-0.63
3INT1	-1.17	1.84	1.49	-0.66	-0.15
3CY1	-1.01	1.85	0.69	-0.59	-0.06
3	-1.17 (1.75)	1.86	1.51 (0.22)	-0.77 (1.48)	-0.63
4INT1	-1.17	1.84	1.49	-0.67	-0.14
4CY1	-1.01	1.85	0.69	-0.60	-0.07
4	-1.16 (1.61)	1.85	1.49 (0.24)	-0.78 (1.32)	-0.63



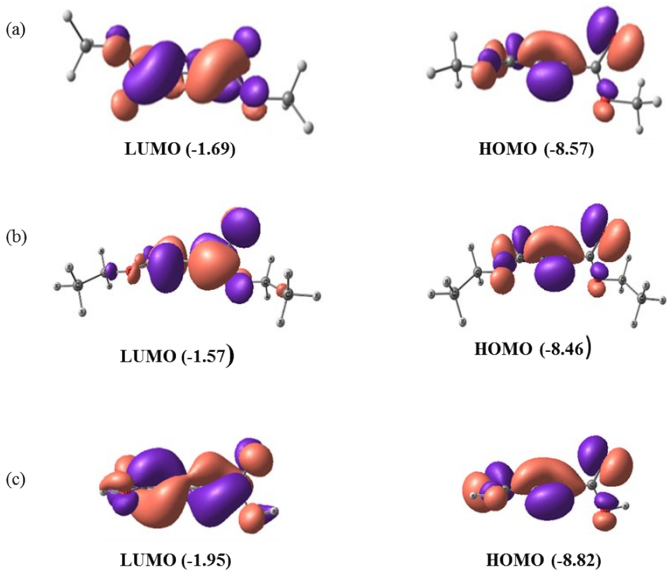


Figure S[4]. HOMO and LUMO of (a) **DMAD** (dimethyl acetylene dicarboxylic acid) and (b) **DEAD (**diethyl acetylene dicarboxylic acid**)** and (c) **DIACID** (acetylene dicarboxylic acid) at the M06/def2-TZVPP//BP86/def2-SVP level of theory. (Energies are given in eV).

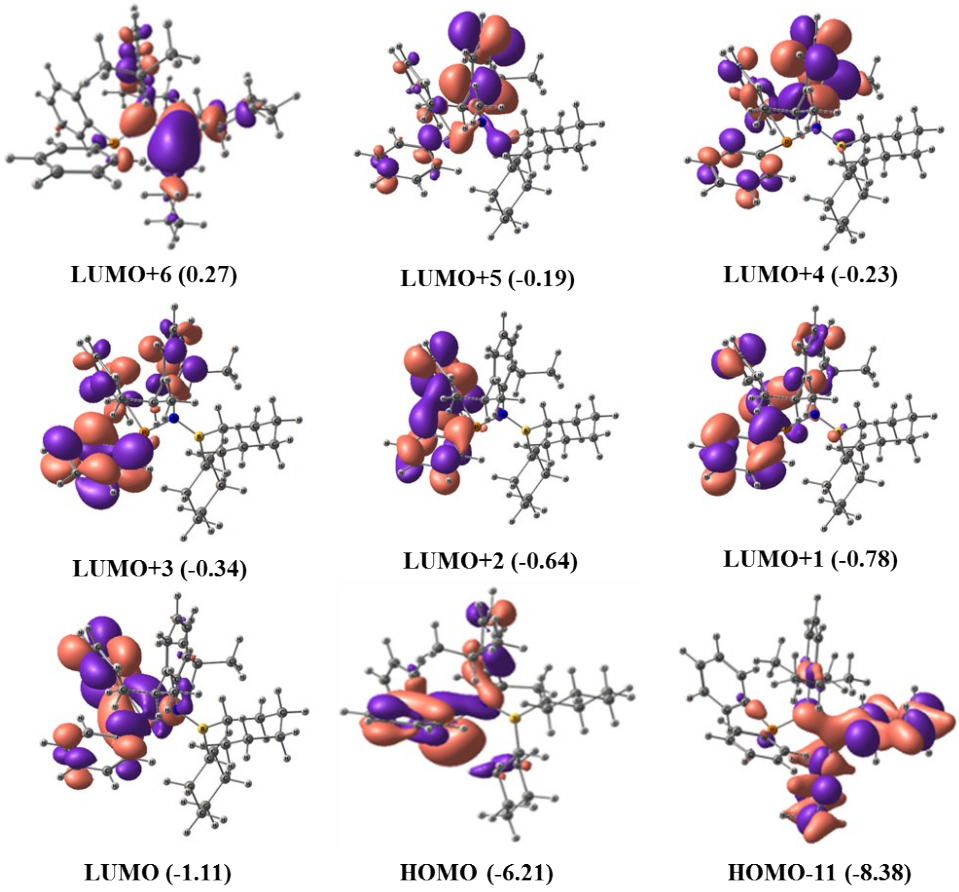


Figure S[5]. Important molecular orbitals of **1** at the M06/def2-TZVPP//BP86/def2-SVP level of theory. (Energies are given in eV).

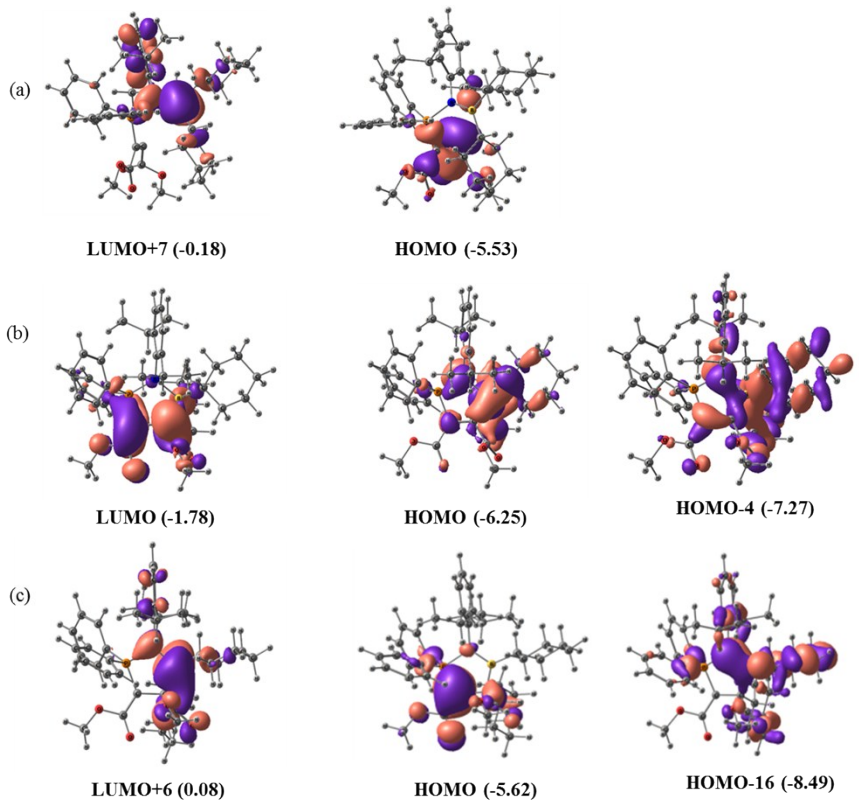


Figure S[6]. Important molecular orbitals of (a) **2INT1** and (b) **2CY1** and (c) **2** at the M06/def2-TZVPP//BP86/def2-SVP level of theory. (Energies are given in eV).

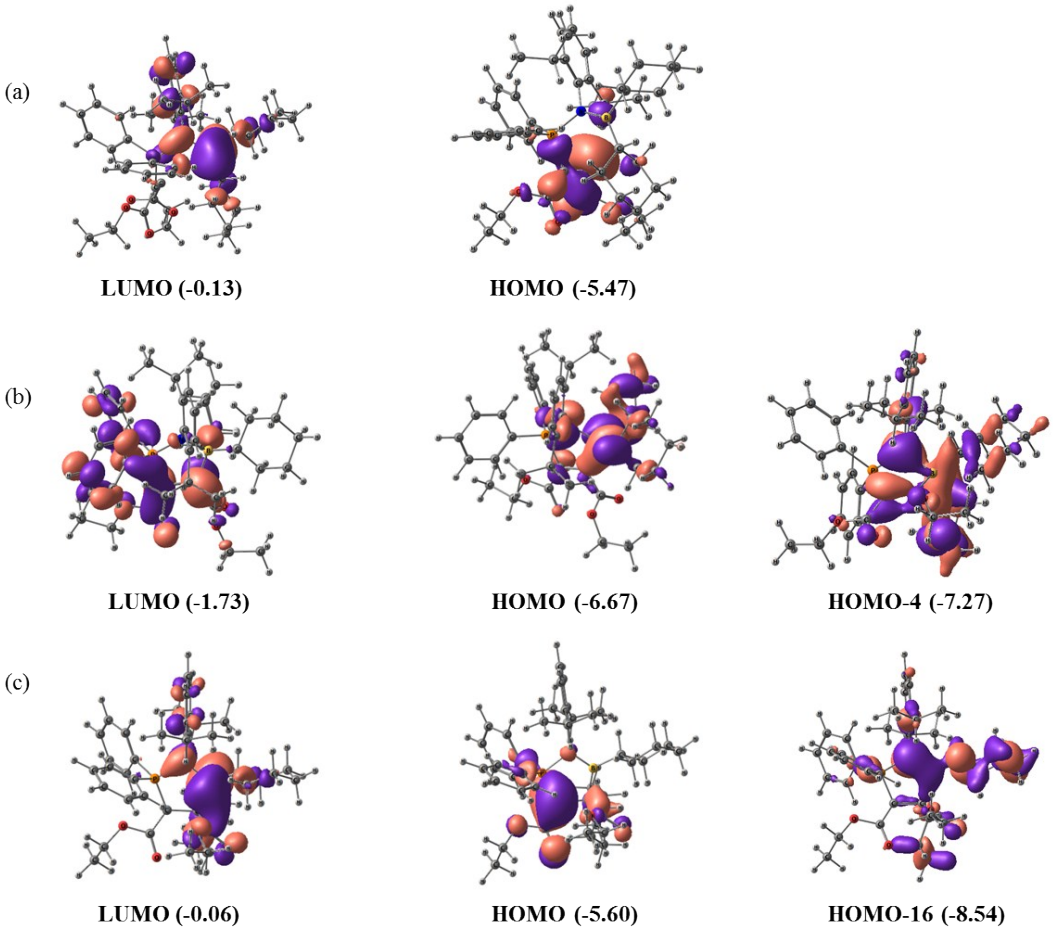


Figure S[7]. Important molecular orbitals of (a) **3INT1** (b) **3CY1** and (c) **3** at the M06/def2-TZVPP//BP86/def2-SVP level of theory. (Energies are given in eV).

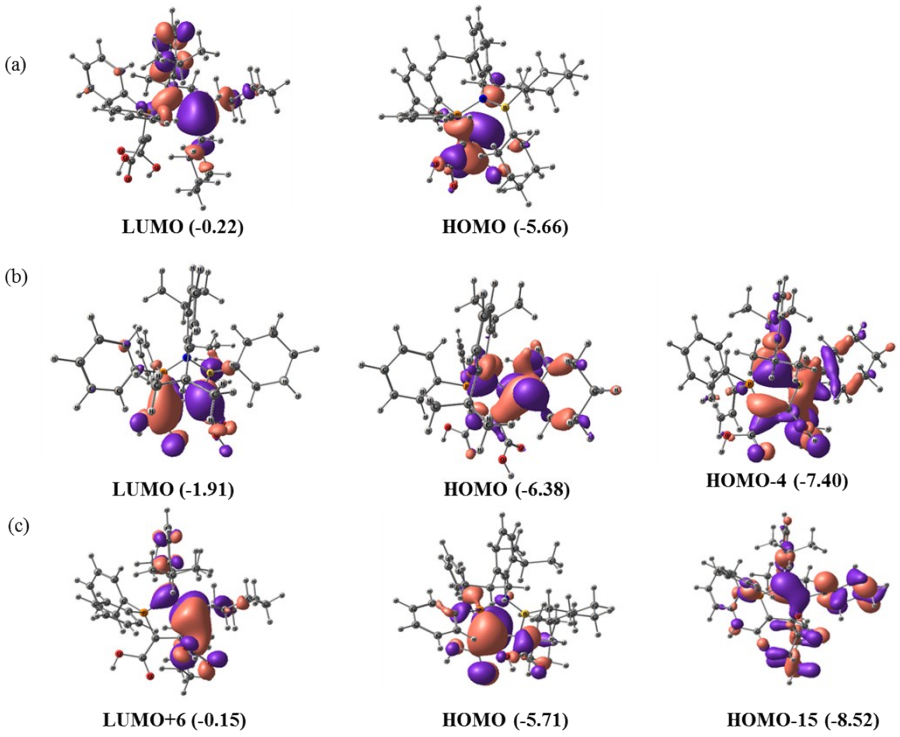
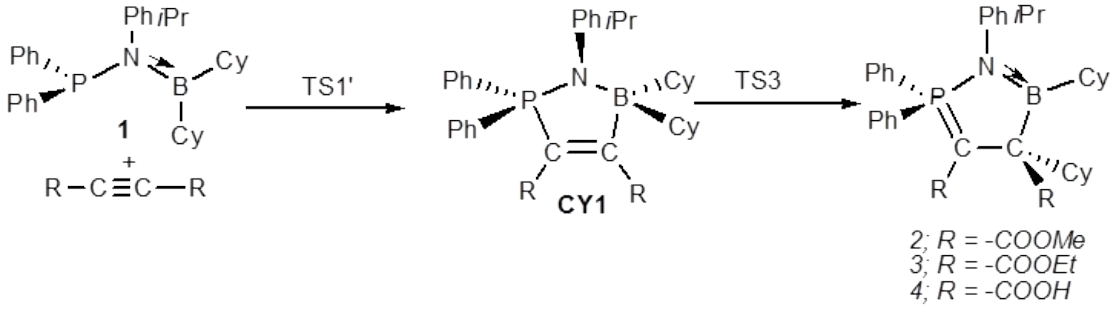


Figure S[8]. Important molecular orbitals of (a) **4INT1** (b) **4CY1** and (c) **4** at the M06/def2-TZVPP//BP86/def2-SVP level of theory. (Energies are given in eV).



Scheme S[1]: Schematic representation of concerted reaction mechanism for the formation of **2**, **3** and **4**.

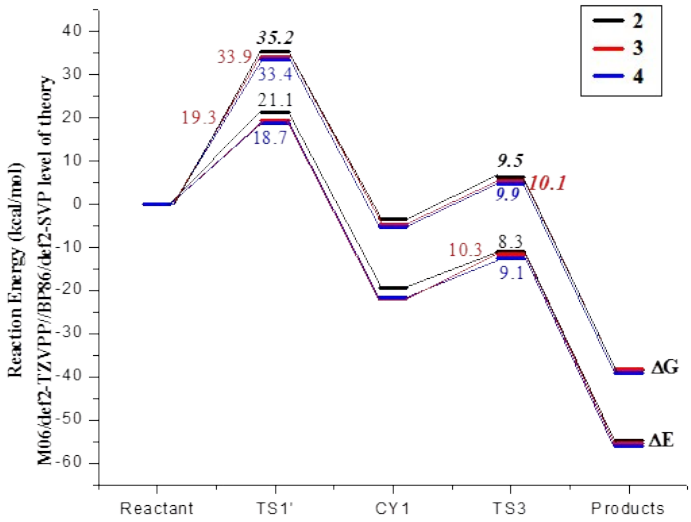


Figure S[9]: Reaction energy profile for the formation of compounds **2 - 4** via concerted mechanism at the M06/Def2-TZVPP//BP86/def2-SVP level of theory (Reactant = 1 + alkyne). Activation energies ($\Delta E^{\ddagger}$) and free energy of activation ($\Delta G^{\ddagger}$, bold and italics) are given in kcal/mol.

Cartesian Coordinates

88

Electronic Energy (BP86) = -1820.430949 a.u.

Zero-point correction (BP86) = 0.750614 a.u.

Thermal correction to Gibbs free Energy (BP86) = 0.680455 a.u.

Electronic Energy (M06) = -1821.7358367 a.u.

1

P	1.081610000	1.174339000	-0.475122000
N	-0.123475000	-0.128094000	-0.134020000
C	-2.139971000	3.904240000	-2.942742000
H	-2.695014000	4.653744000	-3.548684000

H	-1.064135000	4.189532000	-3.002942000
C	-2.592984000	3.957272000	-1.473924000
H	-3.693510000	3.782267000	-1.424977000
H	-2.420446000	4.971534000	-1.051153000
C	-1.873044000	2.897932000	-0.618355000
H	-2.253174000	2.946092000	0.426154000
H	-0.790502000	3.150300000	-0.570277000
C	-2.058559000	1.466127000	-1.192147000
H	-3.165683000	1.320705000	-1.218277000
C	1.500215000	1.904593000	1.188687000
C	2.828695000	2.254942000	1.531399000
H	3.664262000	1.943254000	0.886364000
C	3.101265000	3.001812000	2.691604000
H	4.144332000	3.257466000	2.938967000
C	2.055372000	3.416027000	3.533196000
H	2.270230000	3.998690000	4.443046000
C	0.321700000	-1.470152000	0.217939000
C	0.647068000	-2.371951000	-0.847388000
C	1.061607000	-3.680935000	-0.527058000
H	1.306131000	-4.378680000	-1.343341000
C	1.177339000	-4.110275000	0.799995000
H	1.507062000	-5.136607000	1.027635000
C	0.868568000	-3.219824000	1.833818000
H	0.954350000	-3.556867000	2.879417000
C	0.436758000	-1.900354000	1.575958000
C	0.105802000	-1.017964000	2.780186000
H	-0.296028000	-0.063090000	2.389046000

C	-0.976564000	-1.649721000	3.682351000
H	-1.884446000	-1.925129000	3.109412000
H	-1.278348000	-0.939308000	4.480867000
H	-0.606901000	-2.568743000	4.185113000
C	1.363078000	-0.689201000	3.613550000
H	1.817354000	-1.610056000	4.038443000
H	1.105110000	-0.020150000	4.461049000
H	2.135320000	-0.173111000	3.009229000
C	0.559697000	-1.991357000	-2.330256000
H	0.451847000	-0.889029000	-2.390061000
C	1.827056000	-2.378373000	-3.120854000
H	2.747951000	-1.993773000	-2.641305000
H	1.776471000	-1.963625000	-4.149590000
H	1.929638000	-3.479997000	-3.221570000
C	-0.684709000	-2.612478000	-3.000483000
H	-0.643439000	-3.722391000	-2.969433000
H	-0.750643000	-2.306457000	-4.066124000
H	-1.621620000	-2.300710000	-2.498427000
C	-2.661616000	-0.795892000	0.240337000
H	-2.190899000	-1.688301000	0.712160000
C	-3.711920000	-1.322984000	-0.773428000
H	-4.178099000	-0.465873000	-1.312441000
H	-3.218718000	-1.939913000	-1.554260000
C	-4.826324000	-2.146740000	-0.101428000
H	-5.560735000	-2.488883000	-0.863404000
H	-4.383232000	-3.069256000	0.340628000
C	-5.533284000	-1.347638000	1.004866000

H	-6.309308000	-1.969393000	1.502674000
H	-6.071692000	-0.485362000	0.546822000
C	-4.521648000	-0.822342000	2.035952000
H	-4.075449000	-1.686897000	2.579436000
H	-5.033981000	-0.203475000	2.805377000
C	-3.397409000	-0.007546000	1.367436000
H	-2.674509000	0.335005000	2.140097000
H	-3.843870000	0.917508000	0.934099000
C	-2.322314000	2.495096000	-3.531916000
H	-1.950436000	2.461502000	-4.579919000
H	-3.411189000	2.259270000	-3.581126000
C	-1.611627000	1.425086000	-2.681995000
H	-0.510789000	1.585475000	-2.734254000
H	-1.801899000	0.417636000	-3.113323000
C	2.688790000	0.351599000	-0.909430000
C	3.271845000	0.791639000	-2.120770000
H	2.727284000	1.517537000	-2.747228000
C	4.534477000	0.323542000	-2.527843000
H	4.975004000	0.682191000	-3.471748000
C	5.227174000	-0.602456000	-1.730176000
H	6.215067000	-0.974710000	-2.045794000
C	4.656510000	-1.052737000	-0.524597000
H	5.196553000	-1.778584000	0.104107000
C	3.400924000	-0.576441000	-0.112088000
H	2.975402000	-0.926002000	0.840081000
C	0.455675000	2.350537000	2.034043000
H	-0.590739000	2.124144000	1.777248000

C	0.729541000	3.086986000	3.197714000
H	-0.101628000	3.413731000	3.843255000
B	-1.526246000	0.179590000	-0.361804000

16

Electronic Energy (BP86) = -532.583295 a.u.

Zero-point correction (BP86) = 0.110949 a.u.

Thermal correction to Gibbs free Energy (BP86) = 0.071929 a.u.

Electronic Energy (M06) = -532.9860602 a.u.

DMAD

O	-2.712463000	-0.611100000	0.533818000
O	2.712468000	-0.611043000	-0.533881000
O	-2.567508000	0.985566000	-1.092478000
O	2.567500000	0.985453000	1.092580000
C	-4.145133000	-0.606006000	0.384426000
C	4.145137000	-0.605964000	-0.384478000
C	-2.047521000	0.244228000	-0.276948000
C	2.047519000	0.244198000	0.276971000
C	-0.611771000	0.168653000	-0.054249000
C	0.611771000	0.168646000	0.054252000
H	-4.559213000	0.398464000	0.606786000
H	-4.433072000	-0.885045000	-0.649534000
H	4.559218000	0.398526000	-0.606749000
H	4.433068000	-0.885091000	0.649461000
H	-4.524661000	-1.350248000	1.106999000
H	4.524669000	-1.350143000	-1.107113000

22

Electronic Energy (BP86) = -611.104374 a.u.

Zero-point correction (BP86) = 0.16602 a.u.

Thermal correction to Gibbs free Energy (BP86) = 0.122573 a.u.

Electronic Energy (M06) = -611.5848154 a.u.

DEAD

O	2.706322000	0.377824000	0.060027000
O	-2.737982000	-0.071004000	-0.719755000
O	2.514944000	-1.835742000	-0.472265000
O	-2.552891000	-0.627559000	1.494847000
C	4.148960000	0.285258000	-0.092298000
C	-4.182658000	0.046557000	-0.589498000
C	2.020526000	-0.765596000	-0.160808000
C	-2.059643000	-0.409097000	0.401046000
C	0.590429000	-0.562989000	0.019699000
C	-0.629800000	-0.487121000	0.139995000
H	4.530361000	-0.482240000	0.615045000
H	4.374497000	-0.079711000	-1.117262000
H	-4.538032000	-0.719583000	0.129436000
H	-4.566319000	-0.193480000	-1.600731000
C	-4.589950000	1.447099000	-0.150299000
H	-4.189863000	2.215165000	-0.842874000
H	-5.696651000	1.529848000	-0.143874000
H	-4.225341000	1.663062000	0.873600000
C	4.734338000	1.659780000	0.174845000
H	5.837774000	1.623628000	0.070127000
H	4.342482000	2.407884000	-0.543582000
H	4.494735000	2.003923000	1.201194000

10

Electronic Energy (BP86) = -454.095632 a.u.

Zero-point correction (BP86) = 0.057168 a.u.

Thermal correction to Gibbs free Energy (BP86) = 0.023253 a.u.

Electronic Energy (M06) = -454.4234688 a.u.

DIACID

O	-2.668669000	-0.777917000	-0.781490000
O	2.668601000	0.777966000	-0.781486000
O	-2.650689000	0.845688000	0.816844000
O	2.650759000	-0.845703000	0.816774000
H	-3.635658000	-0.644306000	-0.654390000
H	3.635604000	0.644394000	-0.654446000
C	-2.063742000	0.083234000	0.070153000
C	2.063748000	-0.083189000	0.070202000
C	-0.614029000	-0.003600000	-0.008214000
C	0.614029000	0.003495000	-0.008192000

104

Electronic Energy (BP86) = -2353.083776 a.u.

Zero-point correction (BP86) = 0.866847 a.u.

Thermal correction to Gibbs free Energy (BP86) = 0.783948 a.u.

Electronic Energy (M06) = -2354.8147577 a.u.

2

C	0.281514000	-2.902563000	-1.294569000
C	-2.015476000	-1.052230000	-2.065050000
C	-0.068138000	-1.704919000	-0.580090000
C	1.788754000	-2.291312000	2.158785000
H	1.072415000	-2.967638000	1.666169000
C	1.366316000	2.972254000	-0.000031000

C	0.690761000	2.000088000	0.803420000
C	-2.282006000	1.697958000	-0.308923000
H	-1.826740000	2.578724000	0.206610000
C	-1.450382000	-1.058263000	-0.632177000
C	2.022326000	-1.020191000	1.591266000
C	-2.526452000	-1.759214000	0.295460000
H	-3.502653000	-1.295738000	0.037433000
C	0.560396000	2.208325000	2.216803000
C	2.541469000	-0.429326000	-1.212287000
C	-2.673602000	-3.274676000	0.028373000
H	-1.712164000	-3.778445000	0.271313000
H	-2.855556000	-3.457179000	-1.047388000
C	-2.279702000	-1.530156000	1.798462000
H	-2.233770000	-0.442843000	2.021262000
H	-1.282883000	-1.948764000	2.068324000
C	2.159846000	-0.363852000	-2.572797000
H	1.088541000	-0.392961000	-2.831163000
C	1.963372000	4.081314000	0.638444000
H	2.489776000	4.828498000	0.023684000
C	1.411311000	2.940644000	-1.529020000
H	0.948320000	1.990034000	-1.861745000
C	-2.517318000	2.137752000	-1.790020000
H	-1.554642000	2.292380000	-2.319722000
H	-3.042259000	1.318214000	-2.327118000
C	1.888547000	4.263481000	2.022698000
H	2.367425000	5.134767000	2.497380000
C	2.485726000	-2.687794000	3.312863000

H	2.299580000	-3.682321000	3.748250000
C	-0.292002000	1.323630000	3.128768000
H	-0.530235000	0.397847000	2.571119000
C	1.173292000	3.340462000	2.793263000
H	1.079515000	3.500972000	3.878748000
C	3.913295000	-0.461174000	-0.880897000
H	4.233495000	-0.557756000	0.166009000
C	2.959972000	-0.147127000	2.191908000
H	3.142558000	0.854473000	1.773883000
C	-1.540450000	-0.715204000	-4.356504000
H	-1.809377000	-1.755860000	-4.627895000
H	-0.693281000	-0.365299000	-4.975706000
H	-2.426247000	-0.065989000	-4.513516000
C	3.659245000	-0.553872000	3.341977000
H	4.386433000	0.130252000	3.807429000
C	2.108626000	-4.367847000	-1.787070000
H	1.434764000	-5.249384000	-1.769364000
H	3.093926000	-4.629430000	-1.355990000
H	2.236119000	-4.055279000	-2.846412000
C	2.848183000	2.995988000	-2.086760000
H	3.343342000	3.958151000	-1.835724000
H	2.836113000	2.913205000	-3.193245000
H	3.478888000	2.176010000	-1.692280000
C	0.578894000	4.105837000	-2.113422000
H	-0.451125000	4.126615000	-1.706861000
H	0.510428000	4.020213000	-3.218552000
H	1.047133000	5.086568000	-1.883574000

C	-3.675577000	1.461819000	0.335934000
H	-4.189891000	0.639228000	-0.207548000
H	-3.581147000	1.124528000	1.389159000
C	-3.367457000	-2.171846000	2.681155000
H	-3.127485000	-2.014220000	3.755928000
H	-4.334144000	-1.647291000	2.499419000
C	-4.736077000	3.221999000	-1.168252000
H	-5.319464000	4.168502000	-1.186090000
H	-5.336643000	2.473469000	-1.734453000
C	3.425948000	-1.823656000	3.900968000
H	3.978485000	-2.138804000	4.800494000
C	-3.381471000	3.410276000	-1.872067000
H	-2.834905000	4.258248000	-1.396965000
H	-3.535117000	3.696700000	-2.935919000
C	-3.547625000	-3.668709000	2.381712000
H	-2.627068000	-4.216988000	2.690100000
H	-4.379057000	-4.088113000	2.990030000
C	3.137616000	-0.304673000	-3.577950000
H	2.830111000	-0.257250000	-4.634777000
C	-4.552506000	2.725691000	0.275167000
H	-5.541574000	2.525632000	0.742542000
H	-4.078020000	3.530195000	0.884749000
C	-3.791152000	-3.898960000	0.881884000
H	-4.771036000	-3.450950000	0.595773000
H	-3.872651000	-4.986237000	0.663498000
C	-1.622461000	2.041146000	3.456598000
H	-1.438718000	2.944560000	4.076919000

H -2.298707000 1.371981000 4.029358000

H -2.155302000 2.368753000 2.543152000

C 4.887955000 -0.404379000 -1.893447000

H 5.955224000 -0.436383000 -1.622334000

C 4.503923000 -0.322931000 -3.242150000

H 5.269395000 -0.285542000 -4.033639000

C 0.401525000 0.903490000 4.439948000

H 1.359532000 0.381706000 4.255593000

H -0.256888000 0.214891000 5.009430000

H 0.605064000 1.773718000 5.099774000

P 1.162389000 -0.651855000 0.004231000

O -0.407014000 -3.538854000 -2.092852000

O 1.589834000 -3.305361000 -0.987223000

O -1.089243000 -0.658511000 -2.995046000

O -3.167577000 -1.294761000 -2.380741000

N 0.157228000 0.784358000 0.199967000

B -1.213203000 0.510228000 -0.219229000

110

Electronic Energy (BP86) = -2431.603515 a.u.

Zero-point correction (BP86) = 0.922081 a.u.

Thermal correction to Gibbs free Energy (BP86) = 0.835898 a.u.

Electronic Energy (M06) = -2433.4145794 a.u.

3

C 0.640078000 -2.276495000 0.544910000

C -1.918693000 -0.573293000 -2.537866000

H -1.025400000 0.049680000 -2.706462000

C 1.030531000 -3.968574000 2.271610000

H	1.216299000	-4.226443000	3.325760000
C	-2.720449000	-0.975109000	-3.617288000
H	-2.431569000	-0.695137000	-4.642770000
C	1.275143000	2.627001000	0.901354000
H	2.339378000	2.819994000	0.650368000
C	-4.269608000	-2.045803000	-2.079269000
H	-5.198816000	-2.607329000	-1.892466000
C	0.948732000	-4.990293000	1.319643000
H	1.055023000	-6.044658000	1.620921000
C	1.094733000	-1.570074000	3.019666000
H	0.719379000	-0.601051000	2.639419000
C	-2.425647000	-1.984908000	2.038202000
H	-2.065757000	-2.828809000	1.429845000
C	2.931091000	-0.231535000	-0.317107000
H	3.062147000	-1.278645000	0.049963000
C	1.232533000	2.020731000	2.315163000
H	1.795001000	1.063858000	2.337369000
H	0.177263000	1.771529000	2.572129000
C	0.568536000	4.001595000	0.910988000
H	-0.507470000	3.853797000	1.151772000
H	0.599466000	4.454738000	-0.097905000
C	-2.111035000	-0.652793000	1.679831000
C	-3.895848000	-1.715083000	-3.392297000
H	-4.527952000	-2.022184000	-4.240815000
C	-3.467833000	-1.650305000	-0.993320000
H	-3.792586000	-1.889126000	0.028979000
C	-2.568099000	0.413310000	2.483633000

H	-2.330080000	1.445242000	2.180882000
C	0.887012000	-2.610827000	1.918449000
C	0.752989000	-4.653212000	-0.022596000
H	0.720646000	-5.452276000	-0.780192000
C	-2.277875000	-0.924318000	-1.216048000
C	-3.656896000	-1.171253000	3.979740000
H	-4.265324000	-1.374222000	4.875493000
C	-3.335283000	0.152495000	3.631803000
H	-3.691784000	0.989870000	4.252303000
C	1.143535000	4.347514000	3.362722000
H	0.080806000	4.241733000	3.683054000
H	1.626228000	5.024612000	4.101453000
C	0.484107000	-3.071073000	-1.948210000
H	0.354567000	-1.981763000	-2.109063000
C	0.339585000	-1.873204000	4.329097000
H	0.729643000	-2.782999000	4.833040000
H	-0.745374000	-2.012345000	4.161148000
H	0.468936000	-1.031396000	5.040795000
C	-3.198990000	-2.237977000	3.184935000
H	-3.440085000	-3.276786000	3.461043000
C	4.008093000	0.643018000	0.380418000
H	3.818215000	0.717516000	1.471783000
H	3.943153000	1.679428000	-0.017843000
C	0.606574000	-3.312334000	-0.441878000
C	1.816585000	2.965748000	3.382724000
H	1.729903000	2.502331000	4.390373000
H	2.907620000	3.092375000	3.192490000

C	5.749669000	-0.007713000	-1.361430000
H	6.754898000	-0.457638000	-1.515368000
H	5.795309000	1.016200000	-1.798734000
C	1.185299000	4.952888000	1.951043000
H	2.243316000	5.169659000	1.674743000
H	0.654977000	5.930127000	1.931943000
C	5.429772000	0.102578000	0.138506000
H	6.175428000	0.754386000	0.644293000
H	5.525675000	-0.903006000	0.611280000
C	3.263633000	-0.264690000	-1.843835000
H	2.509994000	-0.855139000	-2.403875000
H	3.212071000	0.771214000	-2.243539000
C	4.676117000	-0.820122000	-2.104689000
H	4.884827000	-0.828148000	-3.197356000
H	4.722158000	-1.883183000	-1.770795000
C	0.927157000	2.208672000	-3.932021000
H	2.007366000	2.032281000	-4.129163000
H	0.784057000	3.307538000	-3.872777000
C	-0.732194000	-3.795210000	-2.562138000
H	-1.680483000	-3.509104000	-2.067185000
H	-0.625875000	-4.898146000	-2.483318000
H	-0.824944000	-3.549920000	-3.640305000
C	2.604253000	-1.416672000	3.319368000
H	3.189701000	-1.182909000	2.409189000
H	3.016269000	-2.355980000	3.746585000
H	2.778306000	-0.605991000	4.057953000
C	1.773461000	-3.511116000	-2.680022000

H	1.904349000	-4.613132000	-2.634802000
H	2.681145000	-3.051007000	-2.243113000
H	1.727220000	-3.227140000	-3.752645000
C	-4.119976000	2.643587000	-1.054131000
H	-4.910833000	1.896791000	-1.277730000
H	-3.757714000	3.084101000	-2.006573000
C	-4.641324000	3.739996000	-0.129704000
H	-3.852855000	4.497324000	0.052789000
H	-4.966384000	3.321139000	0.845310000
H	-5.511756000	4.252682000	-0.591641000
B	1.394963000	0.154673000	-0.093075000
C	0.047578000	1.581019000	-4.999645000
H	-1.024391000	1.779552000	-4.796799000
H	0.201104000	0.483701000	-5.062313000
H	0.295425000	2.014823000	-5.990303000
P	-1.224911000	-0.207972000	0.127248000
N	0.404550000	-0.884469000	0.174118000
O	-1.538546000	3.404040000	-1.307749000
O	0.582282000	1.636151000	-2.648566000
O	-3.050051000	1.896686000	-0.448666000
O	2.059932000	3.071237000	-1.723838000
C	-0.775960000	1.426931000	-0.179586000
C	0.733249000	1.648660000	-0.222392000
C	1.194863000	2.222808000	-1.576551000
C	-1.744492000	2.352098000	-0.700154000

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Electronic Energy (BP86) = -2274.599289 a.u.

Zero-point correction (BP86) = 0.813781 a.u.

Thermal correction to Gibbs free Energy (BP86) = 0.736859 a.u.

Electronic Energy (M06) = -2276.2548008 a.u.

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C	-0.154213000	-2.482746000	-2.266312000
C	-2.047878000	-0.094801000	-2.447160000
C	-0.320051000	-1.493940000	-1.236313000
C	1.270664000	-3.170173000	1.190421000
H	0.461567000	-3.530257000	0.535464000
C	1.818380000	2.496149000	0.745950000
C	0.963596000	1.444479000	1.204737000
C	-1.948345000	2.010978000	0.042076000
H	-1.402990000	2.591880000	0.825258000
C	-1.572165000	-0.632443000	-1.089832000
C	1.756293000	-1.856226000	1.016275000
C	-2.795146000	-1.367240000	-0.407507000
H	-3.661307000	-0.679866000	-0.513755000
C	0.794907000	1.224920000	2.612896000
C	2.485217000	-0.544234000	-1.481286000
C	-3.198860000	-2.689949000	-1.097039000
H	-2.355295000	-3.411209000	-1.022975000
H	-3.366506000	-2.521538000	-2.177690000
C	-2.576609000	-1.619462000	1.094661000
H	-2.341128000	-0.665131000	1.610792000
H	-1.682863000	-2.272458000	1.223360000
C	2.179457000	0.015595000	-2.743937000
H	1.134101000	0.268102000	-2.984841000

C	2.525783000	3.258613000	1.701279000
H	3.188455000	4.065866000	1.351338000
C	1.973770000	2.906087000	-0.720391000
H	1.379910000	2.200414000	-1.335850000
C	-1.959215000	2.914429000	-1.234266000
H	-0.936656000	3.034940000	-1.646728000
H	-2.557431000	2.412460000	-2.024773000
C	2.396612000	3.026550000	3.073618000
H	2.961821000	3.634432000	3.798023000
C	1.835619000	-4.008311000	2.166667000
H	1.452981000	-5.033409000	2.293137000
C	-0.198820000	0.223083000	3.203269000
H	-0.501019000	-0.467531000	2.393212000
C	1.523674000	2.026748000	3.515492000
H	1.396701000	1.859557000	4.596371000
C	3.810908000	-0.944216000	-1.205776000
H	4.061434000	-1.428773000	-0.251952000
C	2.814368000	-1.388527000	1.831842000
H	3.200041000	-0.363655000	1.719685000
H	-1.471217000	0.693949000	-4.048028000
C	3.378223000	-2.234796000	2.802654000
H	4.200060000	-1.864724000	3.435992000
H	1.090617000	-3.736015000	-2.949836000
C	3.438694000	2.844138000	-1.199528000
H	4.073105000	3.573522000	-0.652143000
H	3.502870000	3.097164000	-2.278028000
H	3.880232000	1.838233000	-1.061475000

C	1.413164000	4.329090000	-0.950815000
H	0.377456000	4.437230000	-0.573905000
H	1.411672000	4.575704000	-2.033562000
H	2.034986000	5.093330000	-0.437813000
C	-3.417270000	1.858211000	0.523299000
H	-4.005524000	1.345258000	-0.268786000
H	-3.481267000	1.211920000	1.423778000
C	-3.797229000	-2.268653000	1.771648000
H	-3.579744000	-2.466210000	2.844575000
H	-4.645519000	-1.545651000	1.754516000
C	-4.018578000	4.153870000	-0.402712000
H	-4.437520000	5.152625000	-0.150723000
H	-4.671201000	3.733695000	-1.202122000
C	2.892555000	-3.544665000	2.969203000
H	3.340214000	-4.205124000	3.728869000
C	-2.587514000	4.291284000	-0.948490000
H	-1.960510000	4.836356000	-0.204652000
H	-2.583335000	4.909860000	-1.873023000
C	-4.228817000	-3.561164000	1.059824000
H	-3.434786000	-4.332891000	1.190435000
H	-5.147414000	-3.975647000	1.530497000
C	3.193159000	0.203415000	-3.696096000
H	2.943979000	0.638348000	-4.677114000
C	-4.064874000	3.223596000	0.820350000
H	-5.115331000	3.081084000	1.156295000
H	-3.529528000	3.706203000	1.671454000
C	-4.444442000	-3.311861000	-0.441683000

H	-5.316869000	-2.631761000	-0.580577000
H	-4.708808000	-4.260699000	-0.957735000
C	-1.462006000	0.964203000	3.699159000
H	-1.213390000	1.638950000	4.546123000
H	-2.227000000	0.242846000	4.055850000
H	-1.919686000	1.584851000	2.904984000
C	4.820727000	-0.758155000	-2.166824000
H	5.850033000	-1.080245000	-1.942535000
C	4.516376000	-0.179953000	-3.410293000
H	5.308305000	-0.040919000	-4.163571000
C	0.373700000	-0.638580000	4.346608000
H	1.295285000	-1.170700000	4.043414000
H	-0.373839000	-1.399429000	4.653325000
H	0.605790000	-0.033687000	5.249032000
P	1.041226000	-0.882192000	-0.374668000
O	-0.921856000	-2.741357000	-3.196057000
O	1.045794000	-3.184320000	-2.139762000
O	-1.028171000	0.392583000	-3.224058000
O	-3.205049000	-0.002611000	-2.821130000
N	0.276064000	0.575868000	0.253887000
B	-1.100680000	0.678824000	-0.220947000

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Electronic Energy (BP86) = -2352.991668 a.u.

Zero-point correction (BP86) = 0.864043 a.u.

Thermal correction to Gibbs free Energy (BP86) = 0.779605 a.u.

Electronic Energy (M06) = -2354.716143 a.u.

2INT1

C	3.279487000	0.277579000	1.249292000
C	2.214935000	0.158600000	0.202650000
C	2.239875000	-2.484630000	-1.390409000
H	2.951228000	-1.647017000	-1.452272000
C	-2.732030000	-1.642072000	-0.443726000
C	-1.654601000	-0.886518000	-1.007718000
C	-0.290257000	2.535074000	0.773860000
H	-1.058409000	3.305176000	1.025143000
C	2.325734000	0.620389000	-1.063316000
C	1.027321000	-2.369196000	-0.670177000
C	-2.716629000	1.773230000	-0.138512000
H	-3.271651000	0.949470000	-0.638972000
C	-1.405100000	-0.929048000	-2.416920000
C	0.379007000	-1.545573000	2.039451000
C	-3.436159000	2.053603000	1.220349000
H	-2.892663000	2.861052000	1.762451000
H	-3.393697000	1.162918000	1.883741000
C	-2.874252000	3.028823000	-1.042179000
H	-2.414253000	2.849212000	-2.035855000
H	-2.317876000	3.884763000	-0.597046000
C	-0.386279000	-0.822928000	2.978666000
H	-0.867817000	0.121217000	2.687950000
C	-3.524559000	-2.429726000	-1.307321000
H	-4.354369000	-3.015239000	-0.880700000
C	-3.123983000	-1.646888000	1.038970000
H	-2.516635000	-0.873873000	1.548855000
C	0.527640000	2.400167000	2.084814000

H	-0.148348000	2.093838000	2.913515000
H	1.291485000	1.601460000	2.007737000
C	-3.293495000	-2.475835000	-2.685699000
H	-3.932057000	-3.093543000	-3.337339000
C	2.543206000	-3.677906000	-2.070879000
H	3.492053000	-3.747100000	-2.625315000
C	-0.277107000	-0.160078000	-3.105513000
H	0.463062000	0.158432000	-2.336535000
C	-2.245417000	-1.724509000	-3.225325000
H	-2.060201000	-1.754937000	-4.310090000
C	1.000963000	-2.750754000	2.442790000
H	1.615211000	-3.322110000	1.731469000
C	0.134363000	-3.467853000	-0.649428000
H	-0.809852000	-3.408779000	-0.093094000
C	0.441006000	-4.649311000	-1.340800000
H	-0.272447000	-5.487916000	-1.320053000
C	-2.838399000	-2.999329000	1.728625000
H	-1.760221000	-3.252116000	1.738253000
H	-3.383074000	-3.826535000	1.225462000
H	-3.174921000	-2.971131000	2.786031000
C	-4.612929000	-1.284438000	1.237886000
H	-4.897650000	-0.370696000	0.681559000
H	-4.829589000	-1.113586000	2.313480000
H	-5.281296000	-2.103383000	0.898265000
C	0.539646000	3.197055000	-0.372532000
H	1.306759000	2.489098000	-0.750932000
H	-0.118013000	3.405109000	-1.243357000

C	-4.343285000	3.447247000	-1.230282000
H	-4.399907000	4.347597000	-1.880526000
H	-4.890679000	2.639084000	-1.768475000
C	2.085607000	4.274139000	1.332207000
H	2.576297000	5.222297000	1.643461000
H	2.901873000	3.554224000	1.098182000
C	1.649421000	-4.760183000	-2.051716000
H	1.891662000	-5.690389000	-2.590235000
C	1.224076000	3.717746000	2.476787000
H	0.449264000	4.473042000	2.749094000
H	1.837716000	3.560314000	3.391065000
C	-5.028943000	3.713871000	0.118549000
H	-4.550861000	4.596161000	0.604149000
H	-6.098255000	3.980964000	-0.028403000
C	-0.540202000	-1.298984000	4.291095000
H	-1.144710000	-0.724254000	5.010411000
C	1.232821000	4.494945000	0.073535000
H	1.859952000	4.879516000	-0.759053000
H	0.465404000	5.277928000	0.283171000
C	-4.902686000	2.494630000	1.044429000
H	-5.493935000	1.654023000	0.614102000
H	-5.352311000	2.710594000	2.038766000
C	-0.800625000	1.117208000	-3.794428000
H	-1.539461000	0.875882000	-4.589695000
H	0.038882000	1.671635000	-4.263629000
H	-1.293754000	1.802488000	-3.077634000
C	0.841740000	-3.225428000	3.754265000

H	1.324829000	-4.169683000	4.051774000
C	0.070643000	-2.502750000	4.682575000
H	-0.055048000	-2.878784000	5.710294000
C	0.495398000	-1.019243000	-4.129105000
H	0.786365000	-2.002222000	-3.709255000
H	1.426240000	-0.493916000	-4.427103000
H	-0.089547000	-1.203550000	-5.056481000
P	0.707068000	-0.864620000	0.356546000
O	4.295099000	0.937838000	1.107356000
N	-0.778349000	-0.046863000	-0.161642000
B	-1.182955000	1.337777000	0.160951000
O	3.007725000	-0.419438000	2.391062000
C	3.999466000	-0.325296000	3.425633000
H	4.129514000	0.726771000	3.752072000
H	3.626239000	-0.945651000	4.260833000
H	4.979584000	-0.702140000	3.068173000
C	3.519392000	1.091981000	-1.716095000
O	4.325950000	0.303309000	-2.223212000
O	3.609400000	2.448750000	-1.869447000
C	4.751012000	2.899475000	-2.608443000
H	4.784123000	2.441821000	-3.619285000
H	4.648006000	3.997828000	-2.689448000
H	5.694610000	2.645685000	-2.081605000

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Electronic Energy (BP86) = -2431.512422 a.u.

Zero-point correction (BP86) = 0.918665 a.u.

Thermal correction to Gibbs free Energy (BP86) = 0.829023 a.u.

Electronic Energy (M06) = -2433.314391 a.u.

3INT1

6	-2.975285000	-0.254331000	-1.443495000
6	-1.945745000	0.056859000	-0.400220000
6	-2.091992000	-2.103312000	1.784813000
1	-2.790630000	-1.277433000	1.579923000
6	2.892936000	-1.495471000	0.997895000
6	1.806766000	-0.607193000	1.281337000
6	0.559483000	2.289291000	-1.333443000
1	1.352110000	2.964514000	-1.736052000
6	-2.146112000	0.886450000	0.649178000
6	-0.834230000	-2.174583000	1.140173000
6	2.956861000	1.727355000	-0.229100000
1	3.490948000	1.047989000	0.471103000
6	1.471531000	-0.285909000	2.635247000
6	-0.008585000	-1.980937000	-1.662967000
6	3.674371000	1.623451000	-1.614607000
1	3.130505000	2.254675000	-2.353690000
1	3.623213000	0.585302000	-2.008352000
6	3.143611000	3.169014000	0.321019000
1	2.699942000	3.252522000	1.335147000
1	2.586787000	3.891258000	-0.317978000
6	0.793231000	-1.447310000	-2.694513000
1	1.228938000	-0.442854000	-2.593466000
6	3.600362000	-2.057709000	2.083081000
1	4.437672000	-2.742390000	1.874231000
6	3.386835000	-1.862087000	-0.407532000

1	2.819698000	-1.246422000	-1.132199000
6	-0.261766000	1.904676000	-2.592531000
1	0.382001000	1.355899000	-3.314343000
1	-1.097331000	1.226023000	-2.333076000
6	3.275597000	-1.760141000	3.410397000
1	3.845834000	-2.211644000	4.237985000
6	-2.456816000	-3.086888000	2.721573000
1	-3.438923000	-3.014947000	3.214423000
6	0.351522000	0.679119000	3.028600000
1	-0.314405000	0.837028000	2.150918000
6	2.225379000	-0.875365000	3.672711000
1	1.971152000	-0.631270000	4.715661000
6	-0.559424000	-3.274666000	-1.821853000
1	-1.201196000	-3.699491000	-1.037126000
6	0.038364000	-3.246039000	1.447666000
1	1.016584000	-3.327733000	0.956566000
6	-0.332297000	-4.217250000	2.389832000
1	0.364061000	-5.037869000	2.623127000
6	3.147624000	-3.344664000	-0.768944000
1	2.072413000	-3.607667000	-0.797696000
1	3.649917000	-4.021276000	-0.045015000
1	3.561996000	-3.565045000	-1.774925000
6	4.887593000	-1.537741000	-0.580074000
1	5.130694000	-0.509883000	-0.248779000
1	5.185986000	-1.636709000	-1.645048000
1	5.524391000	-2.235829000	0.003056000
6	-0.272427000	3.205704000	-0.380191000

1	-1.088610000	2.612073000	0.087743000
1	0.355455000	3.555985000	0.467172000
6	4.620008000	3.604051000	0.370869000
1	4.694547000	4.641198000	0.764980000
1	5.172796000	2.956846000	1.090669000
6	-1.705629000	3.983374000	-2.331120000
1	-2.121198000	4.871979000	-2.855224000
1	-2.572700000	3.375823000	-1.988767000
6	-1.582761000	-4.141841000	3.028955000
1	-1.874081000	-4.906824000	3.766451000
6	-0.851351000	3.143627000	-3.293346000
1	-0.019500000	3.772123000	-3.692033000
1	-1.452881000	2.824801000	-4.172542000
6	5.283561000	3.504803000	-1.011336000
1	4.796653000	4.229098000	-1.704922000
1	6.354589000	3.798388000	-0.955980000
6	1.047893000	-2.192011000	-3.858612000
1	1.676657000	-1.760115000	-4.652974000
6	-0.880894000	4.415463000	-1.108894000
1	-1.512659000	4.989970000	-0.397705000
1	-0.066222000	5.104091000	-1.437728000
6	5.144511000	2.085048000	-1.579066000
1	5.739348000	1.385396000	-0.948847000
1	5.580664000	2.026704000	-2.600763000
6	0.922419000	2.055577000	3.431982000
1	1.580569000	1.976388000	4.324752000
1	0.097877000	2.757520000	3.676479000

1	1.520609000	2.511041000	2.618331000
6	-0.296715000	-4.018157000	-2.982953000
1	-0.723777000	-5.028097000	-3.088700000
6	0.506624000	-3.480277000	-4.005061000
1	0.710671000	-4.066298000	-4.915160000
6	-0.539921000	0.134661000	4.164551000
1	-0.901105000	-0.891177000	3.952819000
1	-1.430771000	0.785381000	4.282166000
1	-0.014122000	0.117523000	5.143886000
15	-0.444581000	-0.957587000	-0.191498000
8	-3.765815000	0.558378000	-1.893455000
7	0.992575000	-0.010837000	0.200867000
5	1.418459000	1.254497000	-0.438248000
8	-2.975661000	-1.576943000	-1.790409000
6	-3.957599000	-1.993219000	-2.773750000
1	-4.105101000	-1.164451000	-3.496254000
1	-3.486383000	-2.852210000	-3.293602000
6	-3.410881000	1.460873000	1.033642000
8	-4.273397000	0.784844000	1.611189000
8	-3.523331000	2.812934000	0.840456000
6	-4.740251000	3.424809000	1.321996000
1	-5.581336000	2.714266000	1.184534000
1	-4.897127000	4.300707000	0.659932000
6	-5.275008000	-2.383858000	-2.115312000
1	-5.985629000	-2.755536000	-2.883049000
1	-5.126294000	-3.186215000	-1.364062000
1	-5.735105000	-1.509761000	-1.613462000

6 -4.624564000 3.846228000 2.783333000

1 -5.542746000 4.384677000 3.100618000

1 -4.504972000 2.957671000 3.434796000

1 -3.757433000 4.520943000 2.937874000

98

Electronic Energy (BP86) = -2274.507286 a.u.

Zero-point correction (BP86) = 0.810412 a.u.

Thermal correction to Gibbs free Energy (BP86) = 0.730646 a.u.

Electronic Energy (M06) = -2276.156187 a.u.

4INT1

6 2.870367000 2.001621000 1.257129000

6 2.041714000 1.316334000 0.217811000

6 3.347069000 -1.158663000 -1.080172000

1 3.603644000 -0.098710000 -1.229188000

6 -1.503972000 -2.594969000 -0.246055000

6 -0.863511000 -1.489828000 -0.892650000

6 -1.299200000 2.341777000 0.471090000

1 -2.344469000 2.704609000 0.621141000

6 2.012584000 1.661237000 -1.090196000

6 2.174576000 -1.540923000 -0.386572000

6 -3.065743000 0.458951000 -0.325804000

1 -3.160455000 -0.575709000 -0.722424000

6 -0.546691000 -1.554949000 -2.287327000

6 1.080647000 -0.842841000 2.212607000

6 -3.892964000 0.523764000 0.998541000

1 -3.795909000 1.541564000 1.441594000

1 -3.479946000 -0.175907000 1.757004000

6	-3.736157000	1.397226000	-1.368788000
1	-3.203244000	1.338123000	-2.340390000
1	-3.647016000	2.455711000	-1.034684000
6	0.030128000	-0.448985000	3.067942000
1	-0.806221000	0.148317000	2.677865000
6	-1.798341000	-3.743227000	-1.013612000
1	-2.291180000	-4.598463000	-0.524805000
6	-1.934675000	-2.625998000	1.225919000
1	-1.776012000	-1.612059000	1.641789000
6	-0.584182000	2.740594000	1.788419000
1	-1.094960000	2.257427000	2.650592000
1	0.459744000	2.371895000	1.810084000
6	-1.496200000	-3.817853000	-2.376938000
1	-1.743024000	-4.723801000	-2.953368000
6	4.197599000	-2.141246000	-1.618675000
1	5.105188000	-1.822838000	-2.154713000
6	0.135611000	-0.425734000	-3.060852000
1	0.600774000	0.278130000	-2.335129000
6	-0.882947000	-2.726605000	-2.999047000
1	-0.646421000	-2.779531000	-4.072848000
6	2.155943000	-1.592234000	2.744786000
1	2.995169000	-1.890337000	2.099487000
6	1.876687000	-2.918135000	-0.247061000
1	0.977585000	-3.242117000	0.292695000
6	2.725939000	-3.889729000	-0.797167000
1	2.471275000	-4.955332000	-0.686062000
6	-1.105416000	-3.617111000	2.072425000

1	-0.032953000	-3.344807000	2.117498000
1	-1.183822000	-4.649228000	1.669087000
1	-1.479240000	-3.637346000	3.117419000
6	-3.433744000	-2.969911000	1.374518000
1	-4.071340000	-2.351547000	0.713791000
1	-3.765620000	-2.809605000	2.421962000
1	-3.632695000	-4.034375000	1.130109000
6	-0.783299000	3.168318000	-0.749407000
1	0.237986000	2.832810000	-1.029536000
1	-1.410902000	2.959141000	-1.641944000
6	-5.226202000	1.078422000	-1.586377000
1	-5.656249000	1.777622000	-2.336566000
1	-5.325204000	0.056645000	-2.020762000
6	0.015149000	5.016429000	0.805483000
1	0.005563000	6.112731000	0.991502000
1	1.081726000	4.726920000	0.672286000
6	3.892291000	-3.504682000	-1.482412000
1	4.560799000	-4.269016000	-1.909968000
6	-0.575636000	4.265680000	2.009164000
1	-1.621684000	4.614991000	2.178869000
1	-0.013555000	4.507101000	2.938140000
6	-6.015832000	1.149988000	-0.270452000
1	-6.008855000	2.200117000	0.103653000
1	-7.083010000	0.885128000	-0.435486000
6	0.042400000	-0.811201000	4.424655000
1	-0.787462000	-0.499235000	5.078179000
6	-0.762197000	4.681538000	-0.476708000

1	-0.313847000	5.202785000	-1.349325000
1	-1.808061000	5.059156000	-0.380810000
6	-5.391812000	0.229795000	0.789671000
1	-5.521144000	-0.828992000	0.468062000
1	-5.931519000	0.325775000	1.757638000
6	-0.879880000	0.382337000	-3.895942000
1	-1.379287000	-0.255935000	-4.657216000
1	-0.366026000	1.210335000	-4.427614000
1	-1.671802000	0.831194000	-3.264934000
6	2.162537000	-1.955624000	4.100604000
1	3.002524000	-2.545756000	4.499990000
6	1.106217000	-1.568761000	4.944347000
1	1.112582000	-1.857352000	6.007377000
6	1.273430000	-0.927747000	-3.975182000
1	1.962084000	-1.612525000	-3.442126000
1	1.870523000	-0.063535000	-4.332799000
1	0.891695000	-1.457812000	-4.874610000
15	1.149291000	-0.258464000	0.463864000
8	3.498326000	3.027337000	1.053503000
7	-0.512025000	-0.261254000	-0.147204000
5	-1.520347000	0.809788000	0.014092000
8	2.868968000	1.391240000	2.480206000
6	2.893617000	2.560221000	-1.782534000
8	3.998099000	2.183802000	-2.196611000
8	2.384464000	3.789046000	-2.098213000
1	3.435624000	1.958011000	3.049766000
1	3.090927000	4.217369000	-2.630473000

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Electronic Energy (BP86) = -2353.034583 a.u.

Zero-point correction (BP86) = 0.865368 a.u.

Thermal correction to Gibbs free Energy (BP86) = 0.781834 a.u.

Electronic Energy (M06) = -2354.756707 a.u.

2CY1

C	1.310487000	-2.236135000	-2.263114000
C	-1.605942000	-1.850125000	-2.417717000
C	0.578221000	-1.285446000	-1.396498000
C	2.069871000	-2.348529000	1.434483000
H	1.136451000	-2.802410000	1.074221000
C	-0.448830000	2.920860000	-0.291113000
C	-0.151157000	1.934213000	0.718355000
C	-2.777284000	0.485519000	-0.126503000
H	-2.492970000	1.429817000	-0.626507000
C	-0.797384000	-1.180069000	-1.338274000
C	2.444129000	-1.062100000	0.988989000
C	-1.787996000	-1.765855000	1.058322000
H	-2.902090000	-1.716223000	1.055899000
C	0.098048000	2.369056000	2.063443000
C	2.486995000	1.066919000	-0.942856000
C	-1.488751000	-3.239804000	0.683105000
H	-0.392204000	-3.424054000	0.612370000
H	-1.885012000	-3.467152000	-0.324707000
C	-1.353020000	-1.500326000	2.515476000
H	-1.623204000	-0.470638000	2.815770000
H	-0.243143000	-1.559385000	2.591353000

C	3.044438000	0.836063000	-2.220137000
H	2.752176000	-0.047991000	-2.800330000
C	-0.528504000	4.277222000	0.094064000
H	-0.765798000	5.031514000	-0.672779000
C	-0.657825000	2.639108000	-1.791387000
H	-0.645059000	1.540012000	-1.943794000
C	-3.879088000	-0.149176000	-1.013880000
H	-3.486518000	-0.306006000	-2.039647000
H	-4.143460000	-1.161472000	-0.629774000
C	-0.304867000	4.697114000	1.408973000
H	-0.373756000	5.764234000	1.674386000
C	2.885942000	-3.066900000	2.322139000
H	2.573066000	-4.069239000	2.654629000
C	0.482771000	1.417327000	3.198011000
H	0.470782000	0.392097000	2.781809000
C	0.015377000	3.741773000	2.378081000
H	0.205746000	4.064717000	3.414517000
C	2.881953000	2.217523000	-0.217721000
H	2.447648000	2.434383000	0.768618000
C	3.673416000	-0.521913000	1.432909000
H	4.015930000	0.457519000	1.070004000
C	-2.230680000	-1.629828000	-4.683776000
H	-3.304788000	-1.776596000	-4.449241000
H	-1.793619000	-2.604118000	-4.982884000
H	-2.108753000	-0.886813000	-5.492965000
C	4.488397000	-1.242516000	2.322896000
H	5.442429000	-0.805222000	2.657503000

C	3.432913000	-3.219598000	-2.681244000
H	3.411311000	-3.003155000	-3.769184000
H	3.047103000	-4.247384000	-2.524148000
H	4.461935000	-3.129548000	-2.288538000
C	0.457083000	3.265264000	-2.662805000
H	0.424514000	4.374288000	-2.607981000
H	0.309555000	2.983818000	-3.726880000
H	1.470155000	2.947907000	-2.364731000
C	-2.004973000	3.185449000	-2.326792000
H	-2.874538000	2.864355000	-1.722836000
H	-2.167030000	2.836028000	-3.367805000
H	-2.005727000	4.295770000	-2.351182000
C	-3.382103000	0.911630000	1.237692000
H	-3.662216000	0.008057000	1.825645000
H	-2.621758000	1.451927000	1.840882000
C	-1.965593000	-2.498905000	3.518183000
H	-1.607549000	-2.274983000	4.548142000
H	-3.071928000	-2.361325000	3.537327000
C	-5.720073000	1.085376000	0.263949000
H	-6.621443000	1.728669000	0.156553000
H	-6.054229000	0.165786000	0.798856000
C	4.096025000	-2.513570000	2.775075000
H	4.738184000	-3.077170000	3.470418000
C	-5.165131000	0.697800000	-1.114565000
H	-4.946211000	1.630057000	-1.685786000
H	-5.933198000	0.151067000	-1.705818000
C	-1.648340000	-3.952563000	3.138432000

H	-0.550076000	-4.124037000	3.234824000
H	-2.134474000	-4.659924000	3.846497000
C	3.984119000	1.732650000	-2.756865000
H	4.407252000	1.539773000	-3.755230000
C	-4.640685000	1.789140000	1.099878000
H	-5.036270000	2.052011000	2.106260000
H	-4.370866000	2.754901000	0.612211000
C	-2.084608000	-4.240597000	1.693792000
H	-3.196804000	-4.184579000	1.636588000
H	-1.816644000	-5.280731000	1.402735000
C	-0.529669000	1.470576000	4.363292000
H	-0.497281000	2.450207000	4.886432000
H	-0.300656000	0.685838000	5.114680000
H	-1.570021000	1.314509000	4.014032000
C	3.821000000	3.109867000	-0.761899000
H	4.112535000	4.003292000	-0.187941000
C	4.377927000	2.868469000	-2.029442000
H	5.114572000	3.569445000	-2.452908000
C	1.905110000	1.697395000	3.730148000
H	2.670295000	1.630030000	2.930683000
H	2.180732000	0.958644000	4.512088000
H	1.980454000	2.709022000	4.183691000
P	1.334137000	-0.156121000	-0.191894000
O	0.821271000	-2.946109000	-3.127572000
O	2.646152000	-2.265253000	-1.951099000
O	-1.523929000	-1.098146000	-3.549928000
O	-2.292628000	-2.851156000	-2.323884000

N	-0.086331000	0.517863000	0.393878000
B	-1.415706000	-0.450323000	-0.006694000

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Electronic Energy (BP86) = -2431.555174 a.u.

Zero-point correction (BP86) = 0.920034 a.u.

Thermal correction to Gibbs free Energy (BP86) = 0.833657 a.u.

Electronic Energy (M06) = -2433.359035 a.u.

3CY1

C	-1.660893000	2.806055000	-0.453235000
C	1.223942000	3.021900000	-0.222641000
C	-0.804545000	1.613626000	-0.238413000
C	-2.787853000	0.735369000	2.197690000
H	-2.469993000	1.751399000	1.932592000
C	0.936358000	-1.740056000	-2.255188000
C	0.593913000	-1.951996000	-0.872785000
C	2.828722000	-0.036140000	-0.027357000
H	2.735953000	-0.385094000	-1.078103000
C	0.563310000	1.678256000	-0.048839000
C	-2.382384000	-0.363097000	1.409341000
C	1.361693000	0.529747000	2.227484000
H	2.442151000	0.766563000	2.380288000
C	0.700193000	-3.277214000	-0.327910000
C	-2.365879000	-0.783530000	-1.452061000
C	0.601274000	1.689852000	2.918031000
H	-0.494687000	1.511947000	2.845248000
H	0.803566000	2.651844000	2.407546000
C	1.081131000	-0.769333000	3.016671000

H	1.622473000	-1.624421000	2.572027000
H	-0.003775000	-1.013794000	2.939515000
C	-3.096744000	0.086238000	-2.291533000
H	-3.018331000	1.171698000	-2.159684000
C	1.437400000	-2.824262000	-3.007763000
H	1.714313000	-2.654675000	-4.060610000
C	0.742652000	-0.419898000	-3.018142000
H	0.319136000	0.326089000	-2.317402000
C	3.772397000	1.192909000	-0.065868000
H	3.344143000	1.982150000	-0.714000000
H	3.853840000	1.639941000	0.952177000
C	1.585889000	-4.103078000	-2.462391000
H	1.986669000	-4.928557000	-3.072123000
C	-3.606444000	0.538978000	3.323630000
H	-3.911036000	1.406454000	3.930095000
C	0.260853000	-3.654011000	1.090840000
H	-0.079833000	-2.722279000	1.583406000
C	1.200167000	-4.320230000	-1.136411000
H	1.290107000	-5.331342000	-0.707523000
C	-2.488412000	-2.180591000	-1.641249000
H	-1.907095000	-2.883642000	-1.029794000
C	-2.819089000	-1.658469000	1.766435000
H	-2.528754000	-2.530441000	1.165563000
C	1.868493000	4.605412000	-1.888842000
H	1.387436000	5.322205000	-1.193021000
H	1.466979000	4.771980000	-2.908636000
C	-3.631683000	-1.852470000	2.894258000

H	-3.958958000	-2.869925000	3.160116000
C	-3.905095000	3.629670000	-0.531732000
H	-3.630406000	4.400360000	0.219565000
H	-3.749289000	4.091190000	-1.530871000
C	-0.248870000	-0.599327000	-4.193052000
H	0.202675000	-1.207106000	-5.005905000
H	-0.510404000	0.387523000	-4.629978000
H	-1.186416000	-1.099622000	-3.886863000
C	2.053904000	0.175622000	-3.579517000
H	2.793434000	0.396940000	-2.787418000
H	1.838571000	1.125710000	-4.110824000
H	2.530297000	-0.514568000	-4.308256000
C	3.536330000	-1.191721000	0.724785000
H	3.649352000	-0.926561000	1.801184000
H	2.909209000	-2.105424000	0.691409000
C	1.453648000	-0.652670000	4.508794000
H	1.226979000	-1.606787000	5.036112000
H	2.555496000	-0.504725000	4.596003000
C	5.845197000	-0.284863000	0.184038000
H	6.845648000	-0.521935000	-0.241240000
H	6.020048000	0.028445000	1.239890000
C	-4.026786000	-0.753486000	3.677633000
H	-4.664340000	-0.905516000	4.562920000
C	5.188469000	0.869554000	-0.585613000
H	5.123771000	0.588377000	-1.663209000
H	5.826030000	1.780783000	-0.543357000
C	0.732377000	0.522158000	5.186783000

H	-0.361547000	0.307732000	5.217796000
H	1.059749000	0.626629000	6.245275000
C	-3.940277000	-0.431568000	-3.288975000
H	-4.500736000	0.261518000	-3.936033000
C	4.935168000	-1.521263000	0.168819000
H	5.393255000	-2.351067000	0.752070000
H	4.839017000	-1.892823000	-0.877878000
C	0.968379000	1.825954000	4.409118000
H	2.043825000	2.109598000	4.490267000
H	0.396207000	2.662422000	4.869571000
C	1.408099000	-4.245847000	1.939128000
H	1.746049000	-5.225343000	1.538105000
H	1.070724000	-4.413994000	2.983506000
H	2.289878000	-3.576851000	1.972095000
C	-3.331279000	-2.690914000	-2.642197000
H	-3.406673000	-3.780860000	-2.779910000
C	-4.063800000	-1.819473000	-3.466104000
H	-4.724299000	-2.222586000	-4.249993000
C	-0.912071000	-4.661923000	1.074140000
H	-1.767656000	-4.319922000	0.454703000
H	-1.290894000	-4.839172000	2.103009000
H	-0.596244000	-5.644441000	0.663625000
P	-1.316361000	-0.132097000	-0.086679000
O	-1.261400000	3.946278000	-0.633526000
O	-2.998487000	2.505463000	-0.392106000
O	1.415006000	3.268730000	-1.544523000
O	1.573611000	3.767169000	0.676120000

N	0.197641000	-0.842948000	-0.017031000
B	1.302611000	0.321173000	0.524730000
C	3.385779000	4.738742000	-1.858969000
H	3.870163000	4.004930000	-2.534873000
H	3.676505000	5.756897000	-2.193662000
H	3.774519000	4.589655000	-0.832838000
C	-5.324198000	3.121695000	-0.345791000
H	-6.038388000	3.964515000	-0.444884000
H	-5.585398000	2.357986000	-1.106116000
H	-5.460579000	2.669266000	0.657093000

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Electronic Energy (BP86) = -2274.550695 a.u.

Zero-point correction (BP86) = 0.811174 a.u.

Thermal correction to Gibbs free Energy (BP86) = 0.733091 a.u.

Electronic Energy (M06) = -2276.197287 a.u.

4CY1

C	-1.319895000	1.406527000	-3.124492000
C	1.567751000	1.049402000	-3.042046000
C	-0.640875000	0.842093000	-1.937195000
C	-2.333758000	2.937787000	-0.080507000
H	-1.966269000	3.114656000	-1.099049000
C	0.212784000	-2.841649000	0.029605000
C	0.096215000	-1.697391000	0.895239000
C	2.694278000	-0.559486000	-0.236404000
H	2.367878000	-1.600548000	-0.449283000
C	0.732221000	0.730875000	-1.834308000
C	-2.177828000	1.672484000	0.525454000

C	1.722799000	1.962200000	0.310802000
H	2.835363000	1.976545000	0.218557000
C	0.125899000	-1.896424000	2.317561000
C	-2.736634000	-0.963201000	-0.500639000
C	1.245276000	3.257153000	-0.394179000
H	0.137171000	3.331304000	-0.326082000
H	1.498633000	3.233476000	-1.472313000
C	1.402752000	2.079976000	1.818631000
H	1.752197000	1.185440000	2.365989000
H	0.297464000	2.114316000	1.954137000
C	-3.515220000	-1.069066000	-1.674739000
H	-3.293338000	-0.438580000	-2.544280000
C	0.433495000	-4.111680000	0.604993000
H	0.541146000	-4.983341000	-0.060293000
C	0.054285000	-2.807352000	-1.498625000
H	-0.151643000	-1.762368000	-1.802156000
C	3.794726000	-0.232124000	-1.279789000
H	3.389870000	-0.322324000	-2.306540000
H	4.119431000	0.828316000	-1.167957000
C	0.515634000	-4.296962000	1.988394000
H	0.698312000	-5.298701000	2.409006000
C	-2.973645000	3.981824000	0.609856000
H	-3.086303000	4.963277000	0.123059000
C	-0.115995000	-0.780791000	3.340140000
H	-0.235080000	0.161957000	2.771005000
C	0.341869000	-3.193564000	2.829335000
H	0.376330000	-3.337056000	3.921470000

C	-3.058283000	-1.775412000	0.612707000
H	-2.453474000	-1.736472000	1.528577000
C	-2.681570000	1.472006000	1.830420000
H	-2.585298000	0.494270000	2.321530000
H	2.160668000	0.277379000	-4.647710000
C	-3.313985000	2.518417000	2.519268000
H	-3.695316000	2.346162000	3.538038000
C	-1.138247000	-3.683483000	-1.951631000
H	-0.915500000	-4.762787000	-1.811944000
H	-1.340121000	-3.528358000	-3.032472000
H	-2.066115000	-3.459987000	-1.392184000
C	1.314936000	-3.261329000	-2.269004000
H	2.195215000	-2.628950000	-2.049756000
H	1.128871000	-3.206236000	-3.361485000
H	1.579122000	-4.312778000	-2.026239000
C	3.341911000	-0.616710000	1.170370000
H	3.684103000	0.401057000	1.468638000
H	2.588545000	-0.927877000	1.921454000
C	2.015770000	3.341541000	2.460120000
H	1.751203000	3.388237000	3.540570000
H	3.127413000	3.266707000	2.416019000
C	5.629747000	-1.187621000	0.226762000
H	6.488117000	-1.894085000	0.271957000
H	6.038831000	-0.182060000	0.481905000
C	-3.461122000	3.777768000	1.910793000
H	-3.958566000	4.598613000	2.451199000
C	5.031855000	-1.149686000	-1.186350000

H	4.736940000	-2.185296000	-1.476967000
H	5.797280000	-0.828568000	-1.927603000
C	1.567419000	4.622273000	1.739878000
H	0.472293000	4.762734000	1.896367000
H	2.062634000	5.515568000	2.181638000
C	-4.595314000	-1.966447000	-1.728836000
H	-5.191771000	-2.038091000	-2.651981000
C	4.550992000	-1.568118000	1.250413000
H	4.971788000	-1.565596000	2.280697000
H	4.211996000	-2.612136000	1.055681000
C	1.852757000	4.527359000	0.233491000
H	2.955817000	4.517748000	0.070708000
H	1.473879000	5.432259000	-0.292248000
C	1.059037000	-0.594591000	4.325303000
H	1.191716000	-1.487336000	4.973003000
H	0.870648000	0.273309000	4.991567000
H	2.018300000	-0.416798000	3.801460000
C	-4.138614000	-2.670430000	0.549717000
H	-4.369019000	-3.300469000	1.422974000
C	-4.912205000	-2.767548000	-0.619458000
H	-5.758764000	-3.470662000	-0.666454000
C	-1.407594000	-1.031925000	4.154018000
H	-2.299405000	-1.194644000	3.512821000
H	-1.624373000	-0.169979000	4.820102000
H	-1.311192000	-1.932015000	4.797431000
P	-1.371913000	0.264939000	-0.362703000
O	-0.785468000	1.703004000	-4.181055000

O	-2.665589000	1.616829000	-2.929085000
O	1.592134000	-0.009117000	-3.897412000
O	2.209275000	2.067955000	-3.225335000
N	0.011856000	-0.349315000	0.352130000
B	1.352683000	0.417557000	-0.341263000
H	-2.989891000	2.014572000	-3.767905000

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Electronic Energy (BP86) = -2352.983421 a.u.

Zero-point correction (BP86) = 0.863047 a.u.

Thermal correction to Gibbs free Energy (BP86) = 0.778196 a.u.

Electronic Energy (M06) = -2354.699656 a.u.

2TS1, Number of imaginary frequency = 1(109.9i)

C	3.098455000	2.357002000	-0.202511000
C	2.169289000	1.542586000	-1.031509000
C	3.117016000	-1.403095000	-1.515478000
H	3.256973000	-0.455689000	-2.052629000
C	-1.373268000	-2.560867000	0.432655000
C	-0.879523000	-1.647654000	-0.552818000
C	-1.261249000	2.404420000	-0.114912000
H	-2.261369000	2.800914000	0.184551000
C	1.939910000	1.566963000	-2.293819000
C	2.165626000	-1.519922000	-0.474959000
C	-3.082214000	0.394174000	-0.194326000
H	-3.191082000	-0.704383000	-0.335890000
C	-0.713950000	-2.078506000	-1.909338000
C	1.415318000	-0.169382000	1.970903000
C	-3.714892000	0.747271000	1.190829000

H	-3.605877000	1.841179000	1.372888000
H	-3.165300000	0.247820000	2.017419000
C	-3.938072000	1.073012000	-1.300932000
H	-3.548077000	0.816094000	-2.307412000
H	-3.855081000	2.179941000	-1.211808000
C	0.437406000	0.364299000	2.839785000
H	-0.498009000	0.770004000	2.428899000
C	-1.687582000	-3.878219000	0.031237000
H	-2.070951000	-4.585658000	0.783774000
C	-1.628806000	-2.217323000	1.905265000
H	-1.477412000	-1.127174000	2.025662000
C	-0.281090000	3.071787000	0.883970000
H	-0.535544000	2.773968000	1.923156000
H	0.758084000	2.721901000	0.713650000
C	-1.536983000	-4.305042000	-1.291119000
H	-1.795127000	-5.337317000	-1.576718000
C	3.889292000	-2.514315000	-1.900511000
H	4.621455000	-2.397475000	-2.714638000
C	-0.179401000	-1.169052000	-3.015134000
H	0.446399000	-0.385500000	-2.537708000
C	-1.056242000	-3.404442000	-2.246590000
H	-0.933484000	-3.737102000	-3.288022000
C	2.618531000	-0.668051000	2.530906000
H	3.405897000	-1.068520000	1.875947000
C	2.009597000	-2.776235000	0.161280000
H	1.283928000	-2.895995000	0.975560000
C	2.776570000	-3.881998000	-0.232672000

H	2.631608000	-4.849118000	0.273959000
C	-0.658683000	-2.935993000	2.869008000
H	0.394497000	-2.626018000	2.723090000
H	-0.715438000	-4.038524000	2.745622000
H	-0.919844000	-2.702989000	3.922425000
C	-3.081362000	-2.542305000	2.320674000
H	-3.821237000	-2.130258000	1.607699000
H	-3.300499000	-2.122437000	3.325006000
H	-3.252025000	-3.637741000	2.382112000
C	-1.049791000	2.954946000	-1.562464000
H	-0.084207000	2.595492000	-1.967981000
H	-1.827586000	2.552996000	-2.245000000
C	-5.426481000	0.689144000	-1.221295000
H	-5.992317000	1.195804000	-2.033595000
H	-5.534452000	-0.405444000	-1.401793000
C	-0.050243000	5.105030000	-0.639440000
H	-0.092812000	6.215629000	-0.677608000
H	0.980489000	4.816593000	-0.946231000
C	3.724621000	-3.753861000	-1.263774000
H	4.331535000	-4.621003000	-1.569924000
C	-0.306109000	4.609305000	0.792164000
H	-1.303061000	4.974946000	1.135051000
H	0.441019000	5.039978000	1.494323000
C	-6.025407000	1.039059000	0.149512000
H	-6.019809000	2.146278000	0.279123000
H	-7.090374000	0.724462000	0.207183000
C	0.639145000	0.375951000	4.229813000

H	-0.142243000	0.788022000	4.887917000
C	-1.066472000	4.492769000	-1.615953000
H	-0.856638000	4.825992000	-2.655411000
H	-2.088298000	4.863979000	-1.364341000
C	-5.212185000	0.391730000	1.280662000
H	-5.334171000	-0.714061000	1.224691000
H	-5.611929000	0.696074000	2.273210000
C	-1.319223000	-0.429299000	-3.744696000
H	-1.996931000	-1.145297000	-4.257483000
H	-0.904102000	0.264782000	-4.503842000
H	-1.930895000	0.171712000	-3.044802000
C	2.815260000	-0.657265000	3.920789000
H	3.750367000	-1.064284000	4.338153000
C	1.827698000	-0.136529000	4.777513000
H	1.984993000	-0.130542000	5.867604000
C	0.713442000	-1.901138000	-4.037987000
H	1.463474000	-2.548285000	-3.541099000
H	1.267562000	-1.160123000	-4.649092000
H	0.120034000	-2.534480000	-4.732300000
P	1.238443000	-0.032130000	0.132821000
O	3.457528000	3.489072000	-0.472476000
N	-0.504695000	-0.264922000	-0.209635000
B	-1.512903000	0.808050000	-0.175374000
O	3.535909000	1.675528000	0.893482000
C	4.445338000	2.389362000	1.746525000
H	4.009129000	3.358443000	2.062181000
H	4.616619000	1.737540000	2.622393000

H	5.399769000	2.589651000	1.217763000
C	2.040742000	1.598682000	-3.699348000
O	2.844046000	0.903750000	-4.337614000
O	1.153733000	2.459046000	-4.301947000
C	1.267994000	2.541722000	-5.727487000
H	1.001187000	1.578772000	-6.212725000
H	0.559712000	3.330522000	-6.042474000
H	2.300397000	2.808368000	-6.034456000

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Electronic Energy (BP86) = -2431.503435 a.u.

Zero-point correction (BP86) = 0.91801 a.u.

Thermal correction to Gibbs free Energy (BP86) = 0.828451 a.u.

Electronic Energy (M06) = -2433.297646 a.u.

3TS1, Number of imaginary frequecy = 1 (112.1i)

C	3.165836000	2.318128000	-0.178406000
C	2.189410000	1.589437000	-1.028304000
C	3.125889000	-1.361625000	-1.452375000
H	3.282486000	-0.400082000	-1.958500000
C	-1.411365000	-2.540752000	0.401444000
C	-0.905577000	-1.612538000	-0.563285000
C	-1.269253000	2.431541000	-0.080420000
H	-2.260784000	2.841012000	0.230226000
C	1.921096000	1.653124000	-2.278277000
C	2.140819000	-1.496704000	-0.446361000
C	-3.107538000	0.433522000	-0.166798000
H	-3.221190000	-0.664379000	-0.310387000
C	-0.717238000	-2.023145000	-1.922895000

C	1.363455000	-0.164140000	1.997780000
C	-3.739787000	0.786913000	1.218299000
H	-3.620925000	1.878992000	1.405137000
H	-3.195906000	0.278713000	2.043588000
C	-3.957754000	1.117632000	-1.274260000
H	-3.567554000	0.857384000	-2.280035000
H	-3.867132000	2.223970000	-1.185510000
C	0.375756000	0.365886000	2.858045000
H	-0.549477000	0.784959000	2.437425000
C	-1.712628000	-3.853989000	-0.022544000
H	-2.105849000	-4.573052000	0.713745000
C	-1.689235000	-2.215342000	1.873928000
H	-1.541513000	-1.126401000	2.009272000
C	-0.264091000	3.085099000	0.902923000
H	-0.509275000	2.795780000	1.946656000
H	0.765652000	2.714720000	0.717701000
C	-1.534767000	-4.262824000	-1.347519000
H	-1.780945000	-5.292995000	-1.650796000
C	3.908370000	-2.466104000	-1.836158000
H	4.668225000	-2.335394000	-2.622434000
C	-0.182940000	-1.090493000	-3.009191000
H	0.409961000	-0.290690000	-2.516116000
C	-1.043906000	-3.346870000	-2.283327000
H	-0.902306000	-3.665103000	-3.327167000
C	2.550841000	-0.683811000	2.571444000
H	3.343035000	-1.086752000	1.924083000
C	1.961903000	-2.765111000	0.158459000

H	1.210749000	-2.899351000	0.946973000
C	2.737954000	-3.864988000	-0.234700000
H	2.574222000	-4.842249000	0.246134000
C	-0.731227000	-2.942897000	2.843011000
H	0.323728000	-2.632240000	2.711566000
H	-0.786985000	-4.044384000	2.709791000
H	-1.004567000	-2.718447000	3.895210000
C	-3.147456000	-2.546684000	2.263110000
H	-3.876166000	-2.122113000	1.545782000
H	-3.381420000	-2.143165000	3.270782000
H	-3.319462000	-3.642938000	2.303597000
C	-1.065731000	2.973755000	-1.532725000
H	-0.112797000	2.591044000	-1.948224000
H	-1.860974000	2.586192000	-2.203346000
C	-5.448983000	0.744670000	-1.196480000
H	-6.010176000	1.255184000	-2.009618000
H	-5.564982000	-0.349181000	-1.376481000
C	-0.009781000	5.106129000	-0.631273000
H	-0.029385000	6.217234000	-0.674414000
H	1.010730000	4.794708000	-0.949417000
C	3.719078000	-3.718431000	-1.231874000
H	4.332960000	-4.581109000	-1.536760000
C	-0.259246000	4.622261000	0.805385000
H	-1.244201000	5.010341000	1.158282000
H	0.505263000	5.039718000	1.496631000
C	-6.046345000	1.099940000	0.173643000
H	-6.030550000	2.207088000	0.303262000

H	-7.114275000	0.795278000	0.230037000
C	0.553730000	0.356493000	4.251303000
H	-0.234946000	0.766924000	4.901693000
C	-1.049962000	4.511195000	-1.592937000
H	-0.844268000	4.834384000	-2.636165000
H	-2.060751000	4.905182000	-1.331353000
C	-5.240459000	0.444777000	1.305532000
H	-5.372503000	-0.659726000	1.249061000
H	-5.638840000	0.752289000	2.297665000
C	-1.333579000	-0.385108000	-3.756140000
H	-1.983737000	-1.122707000	-4.274025000
H	-0.930566000	0.315787000	-4.515533000
H	-1.971967000	0.199339000	-3.065748000
C	2.724237000	-0.694243000	3.964833000
H	3.647594000	-1.117423000	4.392164000
C	1.727980000	-0.174818000	4.811921000
H	1.866792000	-0.185188000	5.904492000
C	0.752753000	-1.787566000	-4.018178000
H	1.508287000	-2.420160000	-3.511136000
H	1.300222000	-1.024922000	-4.608806000
H	0.193542000	-2.428913000	-4.733129000
P	1.210157000	-0.007534000	0.156960000
O	3.539476000	3.458587000	-0.392198000
N	-0.533477000	-0.237760000	-0.194783000
B	-1.535850000	0.838383000	-0.147334000
O	3.616405000	1.551717000	0.854010000
C	4.585338000	2.161237000	1.746424000

H	4.357705000	3.243990000	1.822899000
H	4.402730000	1.676537000	2.726482000
C	2.086461000	1.848621000	-3.671439000
O	2.872864000	1.184079000	-4.357178000
O	1.281787000	2.839845000	-4.179689000
C	1.465606000	3.158800000	-5.577385000
H	2.520485000	2.958631000	-5.856360000
H	1.273433000	4.249225000	-5.646260000
C	6.010623000	1.933903000	1.258877000
H	6.730611000	2.345410000	1.996746000
H	6.224662000	0.852832000	1.133641000
H	6.183169000	2.445061000	0.290820000
C	0.513255000	2.374745000	-6.473544000
H	0.628218000	2.701666000	-7.528601000
H	0.732718000	1.289282000	-6.427075000
H	-0.543008000	2.537733000	-6.176278000

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Electronic Energy (BP86) = -2274.499105 a.u.

Zero-point correction (BP86) = 0.809317 a.u.

Thermal correction to Gibbs free Energy (BP86) = 0.729189 a.u.

Electronic Energy (M06) = -2276.139132 a.u.

4TS1, Number of imaginary frequency = 1(115.9i)

C	3.205196000	2.248921000	-0.112574000
C	2.249576000	1.527057000	-0.997147000
C	3.103935000	-1.430620000	-1.641471000
H	3.214402000	-0.482896000	-2.186021000
C	-1.309716000	-2.594406000	0.346043000

C	-0.830787000	-1.660175000	-0.626454000
C	-1.211504000	2.382982000	-0.096775000
H	-2.211715000	2.775515000	0.207428000
C	2.049197000	1.660361000	-2.258981000
C	2.202860000	-1.555889000	-0.557925000
C	-3.031551000	0.373810000	-0.192425000
H	-3.143137000	-0.721739000	-0.353792000
C	-0.677627000	-2.061314000	-1.993712000
C	1.479910000	-0.212009000	1.913591000
C	-3.647818000	0.700627000	1.206837000
H	-3.531802000	1.789946000	1.410362000
H	-3.091391000	0.181468000	2.016641000
C	-3.898942000	1.075716000	-1.275700000
H	-3.522405000	0.836884000	-2.291512000
H	-3.811165000	2.180382000	-1.166568000
C	0.498788000	0.308991000	2.787330000
H	-0.440716000	0.708737000	2.380517000
C	-1.619806000	-3.905592000	-0.078168000
H	-1.991412000	-4.630060000	0.663955000
C	-1.562038000	-2.278126000	1.825568000
H	-1.418558000	-1.189179000	1.965003000
C	-0.228245000	3.039745000	0.905601000
H	-0.471070000	2.725336000	1.942457000
H	0.811565000	2.703374000	0.715785000
C	-1.480866000	-4.304537000	-1.410289000
H	-1.735307000	-5.332566000	-1.713836000
C	3.865215000	-2.536689000	-2.060863000

H	4.557976000	-2.415103000	-2.908040000
C	-0.159984000	-1.124920000	-3.086080000
H	0.490273000	-0.367585000	-2.599562000
C	-1.016875000	-3.382006000	-2.353398000
H	-0.904692000	-3.694042000	-3.402230000
C	2.687910000	-0.706819000	2.467727000
H	3.475790000	-1.097644000	1.808440000
C	2.084714000	-2.811960000	0.086438000
H	1.396447000	-2.936134000	0.932105000
C	2.842569000	-3.911518000	-0.341058000
H	2.729570000	-4.879347000	0.172300000
C	-0.586185000	-3.005724000	2.776517000
H	0.463896000	-2.681979000	2.638340000
H	-0.631543000	-4.106318000	2.632942000
H	-0.850819000	-2.794851000	3.833717000
C	-3.012177000	-2.619159000	2.237229000
H	-3.755315000	-2.198747000	1.532474000
H	-3.232297000	-2.218314000	3.249050000
H	-3.176344000	-3.716483000	2.279361000
C	-0.995416000	2.949086000	-1.536883000
H	-0.025231000	2.595853000	-1.936174000
H	-1.766000000	2.552018000	-2.230353000
C	-5.387359000	0.694575000	-1.185957000
H	-5.960561000	1.218203000	-1.982139000
H	-5.500798000	-0.396043000	-1.386055000
C	-0.005512000	5.092983000	-0.588275000
H	-0.053766000	6.203698000	-0.613528000

H	1.028229000	4.812570000	-0.891621000
C	3.740286000	-3.776493000	-1.415409000
H	4.339665000	-4.638966000	-1.748341000
C	-0.261743000	4.578097000	0.836293000
H	-1.260413000	4.934531000	1.184175000
H	0.484886000	5.000684000	1.543448000
C	-5.969649000	1.020176000	0.197820000
H	-5.959014000	2.124656000	0.348515000
H	-7.034830000	0.707627000	0.261825000
C	0.703440000	0.314192000	4.176591000
H	-0.079303000	0.717003000	4.838669000
C	-1.014867000	4.487385000	-1.575982000
H	-0.800293000	4.829196000	-2.611677000
H	-2.039256000	4.853111000	-1.326980000
C	-5.145446000	0.348530000	1.306582000
H	-5.271947000	-0.755535000	1.230971000
H	-5.532300000	0.635016000	2.309476000
C	-1.306860000	-0.345651000	-3.761311000
H	-2.002765000	-1.035581000	-4.285064000
H	-0.899842000	0.373593000	-4.500950000
H	-1.896338000	0.233669000	-3.025529000
C	2.886364000	-0.702418000	3.857184000
H	3.825598000	-1.103651000	4.270506000
C	1.897059000	-0.193153000	4.718239000
H	2.056934000	-0.191553000	5.807967000
C	0.691597000	-1.836230000	-4.157159000
H	1.444445000	-2.511299000	-3.703712000

H	1.240592000	-1.083360000	-4.757968000
H	0.066492000	-2.435677000	-4.853574000
P	1.289622000	-0.077742000	0.080384000
O	3.427719000	3.445327000	-0.139918000
N	-0.453916000	-0.284126000	-0.257157000
B	-1.462778000	0.788716000	-0.184166000
O	3.858983000	1.399157000	0.732225000
C	2.028555000	1.617060000	-3.662334000
O	2.778820000	0.886763000	-4.331651000
O	1.112784000	2.449068000	-4.261485000
H	4.447924000	1.963481000	1.281595000
H	1.260941000	2.314861000	-5.223191000

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Electronic Energy (BP86) = -2352.985207 a.u.

Zero-point correction (BP86) = 0.864112 a.u.

Thermal correction to Gibbs free Energy (BP86) = 0.780222 a.u.

Electronic Energy (M06) = -2354.709752 a.u.

2TS2, Number of imaginary frequency = 1(31.9i)

C	-2.165490000	2.659277000	0.265740000
C	0.094173000	2.878093000	2.330967000
C	-1.088397000	1.656749000	0.515524000
C	-2.543752000	-0.251856000	2.445696000
H	-2.252321000	0.801645000	2.577711000
C	0.728875000	-3.102316000	-0.677822000
C	0.702368000	-2.009618000	0.248064000
C	1.515219000	1.558435000	-1.622368000
H	2.543791000	1.446193000	-2.047730000

C	-0.032847000	1.837173000	1.340870000
C	-2.075155000	-0.992806000	1.337826000
C	3.004513000	-0.214468000	-0.225106000
H	2.946613000	-1.002959000	0.554216000
C	1.019142000	-2.234988000	1.629978000
C	-2.388040000	-0.452988000	-1.443766000
C	3.742491000	-0.872777000	-1.425993000
H	3.831898000	-0.138464000	-2.260839000
H	3.147049000	-1.720474000	-1.823254000
C	3.894451000	0.924518000	0.348543000
H	3.398264000	1.400398000	1.221167000
H	4.010235000	1.729777000	-0.411825000
C	-3.764424000	-0.633779000	-1.151676000
H	-4.119089000	-0.594170000	-0.113106000
C	1.077243000	-4.387084000	-0.207646000
H	1.096339000	-5.228484000	-0.918335000
C	0.352703000	-2.986755000	-2.158755000
H	0.244013000	-1.908617000	-2.386366000
C	0.603933000	1.570663000	-2.870298000
H	0.628196000	0.579074000	-3.374038000
H	-0.452442000	1.761584000	-2.573453000
C	1.399848000	-4.614695000	1.133222000
H	1.677042000	-5.623924000	1.477538000
C	-3.358966000	-0.874251000	3.408490000
H	-3.724355000	-0.286834000	4.265224000
C	1.007285000	-1.162237000	2.727274000
H	0.596561000	-0.221112000	2.297986000

C	1.364561000	-3.543896000	2.031412000
H	1.615549000	-3.720307000	3.089069000
C	-1.980088000	-0.494509000	-2.793262000
H	-0.925071000	-0.359395000	-3.052819000
C	-2.401425000	-2.364581000	1.224523000
H	-2.041520000	-2.952222000	0.367210000
C	1.240130000	4.774560000	3.146355000
H	0.322338000	5.386598000	3.270617000
H	2.082608000	5.417952000	2.830531000
H	1.469706000	4.292720000	4.119642000
C	-3.196043000	-2.982162000	2.202632000
H	-3.438149000	-4.052540000	2.110539000
C	-4.437953000	2.988795000	-0.334778000
H	-4.700203000	3.562259000	0.577879000
H	-5.292507000	2.366187000	-0.657703000
H	-4.160288000	3.708632000	-1.131272000
C	-1.001783000	-3.677311000	-2.437762000
H	-0.939283000	-4.767293000	-2.231934000
H	-1.297660000	-3.551163000	-3.500278000
H	-1.820269000	-3.260857000	-1.817530000
C	1.424160000	-3.559722000	-3.111144000
H	2.421587000	-3.109199000	-2.938470000
H	1.141627000	-3.364942000	-4.167190000
H	1.529719000	-4.659539000	-3.000861000
C	1.530474000	2.989167000	-1.007230000
H	0.507115000	3.268524000	-0.685853000
H	2.143001000	3.027349000	-0.086872000

C	5.299081000	0.426062000	0.737298000
H	5.907623000	1.271422000	1.127246000
H	5.215178000	-0.306020000	1.573733000
C	1.120899000	4.043316000	-3.275559000
H	1.491627000	4.774918000	-4.026959000
H	0.098290000	4.380640000	-2.988720000
C	-3.689718000	-2.233812000	3.287980000
H	-4.326099000	-2.717394000	4.046252000
C	1.034620000	2.639752000	-3.896152000
H	2.034918000	2.359508000	-4.301847000
H	0.337598000	2.637944000	-4.763569000
C	6.010944000	-0.244075000	-0.448412000
H	6.209545000	0.521104000	-1.234835000
H	7.004597000	-0.636188000	-0.139040000
C	-4.691430000	-0.854518000	-2.181327000
H	-5.754163000	-0.997839000	-1.929028000
C	2.011980000	4.039855000	-2.023015000
H	2.015357000	5.045747000	-1.549646000
H	3.066843000	3.827571000	-2.317793000
C	5.150762000	-1.369376000	-1.046918000
H	5.055231000	-2.193964000	-0.303383000
H	5.651520000	-1.809800000	-1.937550000
C	2.421208000	-0.831843000	3.257170000
H	2.907610000	-1.730524000	3.694985000
H	2.350100000	-0.066274000	4.057826000
H	3.089137000	-0.431780000	2.474178000
C	-2.911879000	-0.711695000	-3.822683000

H	-2.564204000	-0.742729000	-4.867335000
C	-4.271097000	-0.893698000	-3.522624000
H	-5.000688000	-1.068348000	-4.329172000
C	0.137835000	-1.585676000	3.934384000
H	-0.837731000	-2.008644000	3.631688000
H	-0.054314000	-0.706906000	4.583897000
H	0.652865000	-2.347925000	4.558349000
P	-1.234735000	-0.092748000	-0.033130000
O	-2.024946000	3.866139000	0.365820000
O	-3.358340000	2.078599000	-0.070380000
O	1.077395000	3.801030000	2.108002000
O	-0.559484000	2.837289000	3.380607000
N	0.391055000	-0.656487000	-0.252763000
B	1.515573000	0.276216000	-0.615920000

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Electronic Energy (BP86) = -2431.505703 a.u.

Zero-point correction (BP86) = 0.919205 a.u.

Thermal correction to Gibbs free Energy (BP86) = 0.831602 a.u.

Electronic Energy (M06) = -2433.308198 a.u.

3TS2, Number of imaginary frequency = 1(32.4i)

C	-2.214580000	2.642874000	0.226073000
C	0.027907000	2.902746000	2.295380000
C	-1.126045000	1.654731000	0.484735000
C	-2.574346000	-0.260744000	2.419039000
H	-2.291400000	0.795468000	2.548824000
C	0.746151000	-3.086988000	-0.676469000
C	0.699434000	-1.992821000	0.246792000

C	1.484101000	1.575458000	-1.631087000
H	2.515947000	1.468444000	-2.050134000
C	-0.071637000	1.853412000	1.308645000
C	-2.097047000	-1.001198000	1.314596000
C	2.981988000	-0.164453000	-0.199493000
H	2.923939000	-0.947474000	0.585233000
C	1.008957000	-2.211735000	1.631531000
C	-2.401676000	-0.471196000	-1.469142000
C	3.739629000	-0.824345000	-1.387268000
H	3.830162000	-0.095695000	-2.226932000
H	3.157793000	-1.681682000	-1.784066000
C	3.853501000	0.988510000	0.374166000
H	3.342804000	1.465396000	1.237815000
H	3.967922000	1.789117000	-0.391317000
C	-3.778405000	-0.655702000	-1.180835000
H	-4.136493000	-0.610257000	-0.143859000
C	1.107932000	-4.366313000	-0.201739000
H	1.142576000	-5.208690000	-0.910705000
C	0.378340000	-2.978412000	-2.159972000
H	0.255100000	-1.902238000	-2.389387000
C	0.577875000	1.561399000	-2.882213000
H	0.616645000	0.563750000	-3.372781000
H	-0.481754000	1.742802000	-2.591046000
C	1.424720000	-4.587149000	1.141643000
H	1.712828000	-5.591993000	1.489808000
C	-3.388495000	-0.886748000	3.380498000
H	-3.760332000	-0.300291000	4.235131000

C	0.972391000	-1.138357000	2.727991000
H	0.551990000	-0.203837000	2.294078000
C	1.368964000	-3.515305000	2.037549000
H	1.614635000	-3.686764000	3.097263000
C	-1.988805000	-0.521154000	-2.816944000
H	-0.933392000	-0.384383000	-3.073930000
C	-2.413398000	-2.375388000	1.203228000
H	-2.046750000	-2.962600000	0.348421000
C	1.144790000	4.823856000	3.130914000
H	0.177809000	5.355383000	3.267205000
H	1.365438000	4.311881000	4.093178000
C	-3.207502000	-2.996180000	2.179798000
H	-3.442230000	-4.068331000	2.089163000
C	-4.528845000	2.916623000	-0.351403000
H	-5.171921000	2.329354000	-1.038150000
H	-4.144756000	3.810566000	-0.884196000
C	-0.964177000	-3.688607000	-2.447356000
H	-0.888246000	-4.777308000	-2.239210000
H	-1.254128000	-3.568426000	-3.512214000
H	-1.792832000	-3.282430000	-1.833717000
C	1.464958000	-3.535792000	-3.104275000
H	2.453649000	-3.068591000	-2.925767000
H	1.186366000	-3.347502000	-4.162550000
H	1.587732000	-4.633542000	-2.991087000
C	1.481277000	3.013328000	-1.033460000
H	0.454190000	3.284819000	-0.716756000
H	2.092708000	3.068354000	-0.113278000

C	5.259408000	0.508681000	0.781336000
H	5.854878000	1.363508000	1.170876000
H	5.174527000	-0.217840000	1.622499000
C	1.064079000	4.034891000	-3.315461000
H	1.426927000	4.762688000	-4.074374000
H	0.036409000	4.361527000	-3.034558000
C	-3.709932000	-2.248754000	3.261730000
H	-4.345724000	-2.734944000	4.018841000
C	0.998115000	2.623149000	-3.919714000
H	2.003291000	2.351154000	-4.318955000
H	0.303933000	2.601950000	-4.789158000
C	5.990799000	-0.163088000	-0.391473000
H	6.189351000	0.598010000	-1.181867000
H	6.985351000	-0.541899000	-0.068644000
C	-4.701097000	-0.886892000	-2.212141000
H	-5.764124000	-1.032526000	-1.962443000
C	1.952342000	4.057326000	-2.061089000
H	1.942729000	5.069073000	-1.600406000
H	3.010286000	3.854356000	-2.351372000
C	5.149129000	-1.302453000	-0.989706000
H	5.055051000	-2.122248000	-0.240721000
H	5.663948000	-1.744241000	-1.871604000
C	2.375896000	-0.786390000	3.271574000
H	2.873242000	-1.678263000	3.710975000
H	2.284894000	-0.024745000	4.073965000
H	3.043951000	-0.372539000	2.496011000
C	-2.916135000	-0.749427000	-3.848028000

H	-2.564521000	-0.786782000	-4.891145000
C	-4.275771000	-0.934057000	-3.551657000
H	-5.001773000	-1.117014000	-4.359605000
C	0.098074000	-1.574805000	3.926968000
H	-0.867595000	-2.013380000	3.614999000
H	-0.114258000	-0.699287000	4.574606000
H	0.619091000	-2.328666000	4.556111000
P	-1.256652000	-0.098159000	-0.054469000
O	-2.069391000	3.853211000	0.278595000
O	-3.410037000	2.041095000	-0.059790000
O	1.001863000	3.836521000	2.087999000
O	-0.646527000	2.855831000	3.332458000
N	0.375332000	-0.645363000	-0.259911000
B	1.491411000	0.304992000	-0.609668000
C	-5.273110000	3.316577000	0.916586000
H	-6.159585000	3.932185000	0.656401000
H	-5.624144000	2.424516000	1.474627000
H	-4.620086000	3.917017000	1.580554000
C	2.258301000	5.775850000	2.726288000
H	2.393769000	6.555573000	3.504083000
H	3.221010000	5.238332000	2.604571000
H	2.021452000	6.280650000	1.767563000

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Electronic Energy (BP86) = -2274.500681 a.u.

Zero-point correction (BP86) = 0.81049 a.u.

Thermal correction to Gibbs free Energy (BP86) = 0.731604 a.u.

Electronic Energy (M06) = -2276.150377 a.u.

4TS2, Number of imaginary frequency = 1(34.1i)

C	-2.309810000	2.938727000	0.381363000
C	-0.022789000	3.153177000	2.439724000
C	-1.234170000	1.935965000	0.630150000
C	-2.685992000	0.024754000	2.557933000
H	-2.392739000	1.077256000	2.692935000
C	0.597390000	-2.821066000	-0.551921000
C	0.566115000	-1.724942000	0.369811000
C	1.370130000	1.843107000	-1.508174000
H	2.396113000	1.731271000	-1.939884000
C	-0.175533000	2.122191000	1.449337000
C	-2.218074000	-0.714344000	1.448495000
C	2.865921000	0.070365000	-0.116027000
H	2.810445000	-0.718009000	0.663722000
C	0.879354000	-1.944214000	1.753391000
C	-2.524257000	-0.168734000	-1.332893000
C	3.600334000	-0.587859000	-1.319247000
H	3.688525000	0.147234000	-2.153505000
H	3.003035000	-1.434395000	-1.716015000
C	3.758276000	1.209057000	0.454536000
H	3.265308000	1.686652000	1.328083000
H	3.873453000	2.013392000	-0.306864000
C	-3.904149000	-0.326642000	-1.044731000
H	-4.263348000	-0.272063000	-0.008497000
C	0.946523000	-4.103312000	-0.075448000
H	0.969279000	-4.947526000	-0.782625000
C	0.226202000	-2.712597000	-2.034641000

H	0.121554000	-1.635396000	-2.268471000
C	0.451146000	1.858736000	-2.750531000
H	0.475499000	0.869566000	-3.258631000
H	-0.604492000	2.044591000	-2.447658000
C	1.265310000	-4.325136000	1.267277000
H	1.543048000	-5.332551000	1.616377000
C	-3.503462000	-0.598128000	3.518447000
H	-3.868566000	-0.011961000	4.376115000
C	0.863839000	-0.866977000	2.846006000
H	0.449179000	0.070488000	2.413079000
C	1.225730000	-3.250903000	2.161095000
H	1.474083000	-3.422677000	3.220103000
C	-2.110557000	-0.226484000	-2.680265000
H	-1.052254000	-0.110119000	-2.935794000
C	-2.547685000	-2.084997000	1.331056000
H	-2.188766000	-2.671183000	0.472357000
H	0.947430000	4.633055000	3.038266000
C	-3.344037000	-2.703258000	2.307154000
H	-3.588642000	-3.772788000	2.212068000
H	-4.123687000	3.134483000	-0.102339000
C	-1.129318000	-3.400943000	-2.314354000
H	-1.070259000	-4.489813000	-2.101819000
H	-1.421055000	-3.280406000	-3.378648000
H	-1.949091000	-2.978769000	-1.699809000
C	1.298417000	-3.294072000	-2.981083000
H	2.297762000	-2.848826000	-2.805956000
H	1.020938000	-3.100648000	-4.038697000

H	1.397296000	-4.394134000	-2.867642000
C	1.390513000	3.272203000	-0.888581000
H	0.369657000	3.551100000	-0.558781000
H	2.012499000	3.308134000	0.025440000
C	5.162952000	0.708724000	0.840649000
H	5.773254000	1.553353000	1.229306000
H	5.079459000	-0.023120000	1.677331000
C	0.961609000	4.334119000	-3.149440000
H	1.325214000	5.069251000	-3.900809000
H	-0.059175000	4.668773000	-2.853187000
C	-3.836768000	-1.956645000	3.394174000
H	-4.474869000	-2.440774000	4.150614000
C	0.873000000	2.932896000	-3.774783000
H	1.870922000	2.655933000	-4.188514000
H	0.169891000	2.933151000	-4.637211000
C	5.871672000	0.037622000	-0.346415000
H	6.070076000	0.802611000	-1.133042000
H	6.865252000	-0.356008000	-0.038832000
C	-4.829909000	-0.540254000	-2.076870000
H	-5.896066000	-0.662493000	-1.828362000
C	1.862929000	4.327011000	-1.904413000
H	1.869365000	5.330680000	-1.426585000
H	2.915520000	4.116499000	-2.208308000
C	5.008864000	-1.086328000	-0.943651000
H	4.913939000	-1.911312000	-0.200483000
H	5.507029000	-1.526726000	-1.835733000
C	2.277100000	-0.528239000	3.372309000

H	2.768077000	-1.423174000	3.812587000
H	2.204020000	0.240222000	4.169996000
H	2.941786000	-0.128510000	2.586344000
C	-3.041059000	-0.437460000	-3.711726000
H	-2.689842000	-0.481942000	-4.754678000
C	-4.404284000	-0.596151000	-3.415562000
H	-5.133157000	-0.764993000	-4.224003000
C	-0.003517000	-1.287907000	4.055433000
H	-0.976960000	-1.717326000	3.754692000
H	-0.199997000	-0.406233000	4.699650000
H	0.515012000	-2.044004000	4.683898000
P	-1.374057000	0.185331000	0.080115000
O	-2.168697000	4.145380000	0.483703000
O	-3.512430000	2.377998000	0.042813000
O	0.952303000	4.084338000	2.222705000
O	-0.650499000	3.105553000	3.506645000
N	0.253342000	-0.373490000	-0.136216000
B	1.376106000	0.559506000	-0.504019000

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Electronic Energy (BP86) = -2353.023297 a.u.

Zero-point correction (BP86) = 0.864968 a.u.

Thermal correction to Gibbs free Energy (BP86) = 0.783261 a.u.

Electronic Energy (M06) = -2354.743001 a.u.

2TS3, Number of imaginary frequency = 1(235.8i)

C	1.181205000	-2.508504000	-1.875120000
C	-1.751184000	-1.836699000	-2.202827000
C	0.526763000	-1.389588000	-1.215064000

C	2.160329000	-2.225956000	1.484999000
H	1.282129000	-2.750756000	1.083374000
C	-0.352533000	3.028314000	-0.330756000
C	-0.094659000	2.032573000	0.678513000
C	-2.780749000	0.660037000	-0.055599000
H	-2.501105000	1.704398000	-0.311836000
C	-0.887932000	-1.212536000	-1.145394000
C	2.455412000	-0.920056000	1.033412000
C	-1.774470000	-1.966464000	0.784191000
H	-2.865068000	-1.848914000	0.629548000
C	0.157444000	2.440713000	2.027303000
C	2.470850000	1.023796000	-1.084194000
C	-1.391217000	-3.425167000	0.483121000
H	-0.283780000	-3.540517000	0.482528000
H	-1.737622000	-3.724163000	-0.521050000
C	-1.354720000	-1.602423000	2.215879000
H	-1.638303000	-0.569101000	2.480843000
H	-0.247531000	-1.647459000	2.299070000
C	2.942016000	0.685940000	-2.371739000
H	2.583546000	-0.232721000	-2.856655000
C	-0.367609000	4.385536000	0.055506000
H	-0.569364000	5.152961000	-0.708584000
C	-0.611533000	2.735605000	-1.820454000
H	-0.613280000	1.634448000	-1.962767000
C	-3.836560000	0.228510000	-1.106549000
H	-3.386576000	0.250938000	-2.122250000
H	-4.128932000	-0.831035000	-0.937103000

C	-0.131442000	4.786885000	1.375226000
H	-0.151136000	5.855056000	1.644598000
C	2.991170000	-2.871910000	2.413930000
H	2.741943000	-3.891544000	2.747884000
C	0.472500000	1.458252000	3.158307000
H	0.509240000	0.444895000	2.711853000
C	0.132113000	3.815597000	2.346076000
H	0.322082000	4.127683000	3.385752000
C	2.938360000	2.206274000	-0.460532000
H	2.560472000	2.506454000	0.528214000
C	3.629785000	-0.292641000	1.508239000
H	3.924293000	0.697163000	1.132779000
C	-2.017753000	-1.970224000	-4.544745000
H	-3.109595000	-1.785156000	-4.478438000
H	-1.845585000	-3.065299000	-4.588909000
H	-1.596568000	-1.480254000	-5.442083000
C	4.460283000	-0.939250000	2.439927000
H	5.370533000	-0.432179000	2.797263000
C	3.292021000	-3.490545000	-2.384452000
H	3.029216000	-3.636959000	-3.452626000
H	3.077438000	-4.437704000	-1.846272000
H	4.362861000	-3.232502000	-2.283294000
C	0.476168000	3.336502000	-2.740758000
H	0.469331000	4.446360000	-2.691116000
H	0.274900000	3.053895000	-3.795437000
H	1.493728000	2.995926000	-2.486480000
C	-1.974158000	3.286981000	-2.306359000

H	-2.824262000	2.954800000	-1.681890000
H	-2.167521000	2.954050000	-3.347396000
H	-1.976299000	4.397701000	-2.312721000
C	-3.452085000	0.787809000	1.339098000
H	-3.760741000	-0.216353000	1.709423000
H	-2.724102000	1.186406000	2.077134000
C	-1.964172000	-2.573104000	3.257443000
H	-1.627399000	-2.278148000	4.276230000
H	-3.072776000	-2.460701000	3.250745000
C	-5.733164000	1.203869000	0.299274000
H	-6.620639000	1.874273000	0.284064000
H	-6.105407000	0.199227000	0.608053000
C	4.140905000	-2.226832000	2.901831000
H	4.795830000	-2.733806000	3.628238000
C	-5.103999000	1.105400000	-1.098412000
H	-4.848814000	2.133401000	-1.446809000
H	-5.840905000	0.709204000	-1.831443000
C	-1.601506000	-4.034438000	2.960736000
H	-0.503410000	-4.174657000	3.094623000
H	-2.092833000	-4.715694000	3.690051000
C	3.878181000	1.510286000	-3.019170000
H	4.240063000	1.236659000	-4.022882000
C	-4.697341000	1.693526000	1.322308000
H	-5.145198000	1.742219000	2.339557000
H	-4.392567000	2.734945000	1.066534000
C	-1.990990000	-4.398881000	1.522476000
H	-3.101302000	-4.384165000	1.428810000

H	-1.675567000	-5.437318000	1.278687000
C	-0.626286000	1.459035000	4.243498000
H	-0.681016000	2.439059000	4.764093000
H	-0.417998000	0.684589000	5.011467000
H	-1.628673000	1.254622000	3.816932000
C	3.873556000	3.025594000	-1.116115000
H	4.224657000	3.947298000	-0.626056000
C	4.349696000	2.676601000	-2.392325000
H	5.084052000	3.320243000	-2.902207000
C	1.844463000	1.744270000	3.805350000
H	2.661704000	1.756656000	3.057100000
H	2.091228000	0.963324000	4.554833000
H	1.853580000	2.723616000	4.329726000
P	1.331653000	-0.152113000	-0.237631000
O	0.635659000	-3.453439000	-2.436163000
O	2.564004000	-2.397427000	-1.815908000
O	-1.324220000	-1.402733000	-3.424248000
O	-2.727317000	-2.556246000	-2.064218000
N	-0.091106000	0.622171000	0.329531000
B	-1.371194000	-0.153247000	-0.133624000

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Electronic Energy (BP86) = -2431.543060 a.u.

Zero-point correction (BP86) = 0.91946 a.u.

Thermal correction to Gibbs free Energy (BP86) = 0.832699 a.u.

Electronic Energy (M06) = -2433.341999 a.u.

3TS3, Number of imaginary frequency = 1(233.0i)

C	1.501931000	-2.650276000	-0.905521000

C	-1.511496000	-2.620217000	-1.151221000
C	0.676753000	-1.489238000	-0.603947000
C	2.554134000	-1.074123000	2.026638000
H	1.785571000	-1.850051000	1.902794000
C	-0.980148000	2.734515000	-1.205408000
C	-0.504854000	2.228604000	0.057309000
C	-2.908945000	0.278320000	0.130632000
H	-2.842951000	1.197786000	-0.490250000
C	-0.744448000	-1.529649000	-0.458698000
C	2.568005000	0.036847000	1.153762000
C	-1.387852000	-1.688875000	1.692658000
H	-2.487553000	-1.808853000	1.634977000
C	-0.291967000	3.131951000	1.147210000
C	2.143289000	1.103611000	-1.482566000
C	-0.751677000	-3.077919000	1.861725000
H	0.353955000	-3.010906000	1.752689000
H	-1.099947000	-3.766261000	1.072586000
C	-0.969833000	-0.774406000	2.853152000
H	-1.436631000	0.223064000	2.780939000
H	0.127063000	-0.602886000	2.811026000
C	2.631531000	0.423382000	-2.619847000
H	2.440681000	-0.653088000	-2.732039000
C	-1.246625000	4.115837000	-1.316253000
H	-1.614868000	4.509974000	-2.276819000
C	-1.213512000	1.884769000	-2.468892000
H	-0.994165000	0.825087000	-2.219640000
C	-3.910428000	-0.657960000	-0.592922000

H	-3.520651000	-0.914556000	-1.600878000
H	-3.984980000	-1.625786000	-0.050063000
C	-1.052921000	4.999403000	-0.248333000
H	-1.272379000	6.072624000	-0.366542000
C	3.527383000	-1.216428000	3.028119000
H	3.497528000	-2.094278000	3.692814000
C	0.251168000	2.692669000	2.509770000
H	0.465790000	1.607742000	2.442938000
C	-0.574750000	4.503461000	0.968549000
H	-0.415568000	5.196523000	1.810406000
C	2.395620000	2.489814000	-1.341427000
H	1.996692000	3.048861000	-0.482006000
C	3.608281000	0.984264000	1.287464000
H	3.688530000	1.827727000	0.587687000
C	-1.749226000	-3.658965000	-3.289410000
H	-1.834076000	-4.571719000	-2.665499000
H	-0.987623000	-3.830650000	-4.077081000
C	4.580383000	0.843737000	2.293016000
H	5.381796000	1.594474000	2.379980000
C	3.745250000	-3.409514000	-1.264692000
H	3.599976000	-4.169952000	-0.466771000
H	3.482148000	-3.907599000	-2.223667000
C	-0.293021000	2.302930000	-3.639036000
H	-0.522330000	3.336804000	-3.974863000
H	-0.458921000	1.631385000	-4.507459000
H	0.778442000	2.263875000	-3.380290000
C	-2.671117000	1.967485000	-2.983086000

H	-3.420082000	1.716367000	-2.209356000
H	-2.812664000	1.265934000	-3.831453000
H	-2.905111000	2.986374000	-3.358642000
C	-3.526583000	0.775637000	1.465784000
H	-3.618282000	-0.070580000	2.183635000
H	-2.856169000	1.522429000	1.940907000
C	-1.314592000	-1.394323000	4.230179000
H	-0.983637000	-0.702842000	5.036801000
H	-2.421860000	-1.475523000	4.324743000
C	-5.891690000	0.417904000	0.606669000
H	-6.892398000	0.883246000	0.467968000
H	-6.045523000	-0.463505000	1.271832000
C	4.540450000	-0.252365000	3.170872000
H	5.306850000	-0.363503000	3.954412000
C	-5.321570000	-0.054794000	-0.738540000
H	-5.285689000	0.815217000	-1.435231000
H	-6.001486000	-0.796959000	-1.212014000
C	-0.686655000	-2.782770000	4.405628000
H	0.423246000	-2.681323000	4.439169000
H	-0.987600000	-3.228827000	5.379179000
C	3.372605000	1.115840000	-3.592993000
H	3.748301000	0.574757000	-4.475823000
C	-4.923383000	1.398762000	1.284609000
H	-5.323518000	1.725407000	2.270032000
H	-4.838760000	2.320054000	0.662528000
C	-1.081496000	-3.697429000	3.239004000
H	-2.176197000	-3.900168000	3.288578000

H	-0.581602000	-4.687316000	3.325441000
C	-0.781601000	2.902532000	3.638631000
H	-1.006021000	3.980508000	3.786938000
H	-0.394312000	2.506740000	4.601072000
H	-1.740837000	2.391213000	3.422226000
C	3.136852000	3.174584000	-2.319838000
H	3.319786000	4.254422000	-2.203781000
C	3.631780000	2.489231000	-3.443265000
H	4.212968000	3.029304000	-4.207506000
C	1.566038000	3.419142000	2.865762000
H	2.331932000	3.305219000	2.072940000
H	1.994579000	3.010535000	3.804891000
H	1.403020000	4.507194000	3.020183000
P	1.274274000	0.123270000	-0.186205000
O	1.115398000	-3.807343000	-1.041419000
O	2.840180000	-2.309781000	-1.037633000
O	-1.196207000	-2.595298000	-2.478391000
O	-2.335289000	-3.385776000	-0.674612000
N	-0.245298000	0.808664000	0.223691000
B	-1.376252000	-0.275015000	0.180226000
C	-3.097125000	-3.280050000	-3.891039000
H	-3.024964000	-2.341541000	-4.478376000
H	-3.448767000	-4.084818000	-4.570570000
H	-3.857432000	-3.144728000	-3.096479000
C	5.163975000	-2.863940000	-1.277418000
H	5.885554000	-3.690263000	-1.443162000
H	5.303411000	-2.118289000	-2.086762000

H 5.411860000 -2.375045000 -0.313490000

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Electronic Energy (BP86) = -2274.538411 a.u.

Zero-point correction (BP86) = 0.811281 a.u.

Thermal correction to Gibbs free Energy (BP86) = 0.734666 a.u.

Electronic Energy (M06) = -2276.182965 a.u.

4TS3, Number of imaginary frequency = 1(241.8i)

C -0.783478000 2.163675000 -2.706930000

C 1.955757000 0.872206000 -2.802236000

C -0.324539000 1.163431000 -1.756819000

C -1.653334000 2.998084000 0.614191000

H -0.698624000 3.218313000 0.116410000

C -0.248520000 -2.923241000 0.333499000

C -0.266124000 -1.657429000 1.022225000

C 2.594421000 -1.081602000 -0.045043000

H 2.107776000 -2.079573000 -0.008336000

C 1.032802000 0.746483000 -1.628644000

C -2.210618000 1.703200000 0.515119000

C 2.129513000 1.806807000 0.038132000

H 3.175177000 1.457469000 -0.072828000

C -0.534980000 -1.620049000 2.428157000

C -2.671609000 -0.706137000 -0.977246000

C 2.000878000 3.176693000 -0.649404000

H 0.932840000 3.487516000 -0.695530000

H 2.354692000 3.126899000 -1.693799000

C 1.718554000 1.919474000 1.512801000

H 1.824787000 0.957594000 2.043257000

H	0.642560000	2.189383000	1.576975000
C	-3.141396000	-0.640250000	-2.307451000
H	-2.654387000	0.034686000	-3.025322000
C	-0.486037000	-4.096144000	1.081687000
H	-0.472837000	-5.067656000	0.562234000
C	0.006680000	-3.111713000	-1.173708000
H	0.220285000	-2.116492000	-1.616865000
C	3.668561000	-1.168470000	-1.161186000
H	3.179958000	-1.376464000	-2.137267000
H	4.167762000	-0.182305000	-1.284945000
C	-0.742275000	-4.063465000	2.457065000
H	-0.922958000	-4.997705000	3.012438000
C	-2.318462000	4.017102000	1.313641000
H	-1.865558000	5.019458000	1.372167000
C	-0.596952000	-0.323270000	3.239569000
H	-0.445993000	0.514581000	2.530810000
C	-0.765616000	-2.830687000	3.116676000
H	-0.967114000	-2.800484000	4.199574000
C	-3.310775000	-1.570534000	-0.055391000
H	-2.944712000	-1.657918000	0.978395000
C	-3.472747000	1.466840000	1.106818000
H	-3.963513000	0.489306000	1.002000000
H	2.093552000	0.318497000	-4.583118000
C	-4.137127000	2.487292000	1.808531000
H	-5.120055000	2.281379000	2.261060000
C	-1.210633000	-3.714659000	-1.912533000
H	-1.429742000	-4.739976000	-1.544853000

H	-0.989889000	-3.794885000	-2.997610000
H	-2.127866000	-3.113427000	-1.796925000
C	1.215434000	-4.036659000	-1.458219000
H	2.136294000	-3.722737000	-0.932097000
H	1.434326000	-4.049555000	-2.546312000
H	0.997120000	-5.082938000	-1.156221000
C	3.287407000	-0.952730000	1.338318000
H	3.796689000	0.034471000	1.418543000
H	2.530227000	-0.984030000	2.150150000
C	2.540247000	2.999905000	2.256939000
H	2.205295000	3.051821000	3.316821000
H	3.609704000	2.687979000	2.283160000
C	5.400079000	-2.077121000	0.482072000
H	6.139134000	-2.888308000	0.663786000
H	5.973881000	-1.121293000	0.506081000
C	-3.560761000	3.763403000	1.920413000
H	-4.086040000	4.563450000	2.465917000
C	4.743209000	-2.241462000	-0.896338000
H	4.280592000	-3.254288000	-0.952219000
H	5.510508000	-2.211724000	-1.701014000
C	2.427320000	4.370894000	1.578025000
H	1.378559000	4.738984000	1.668298000
H	3.064673000	5.119839000	2.097804000
C	-4.241265000	-1.419441000	-2.705844000
H	-4.600094000	-1.359652000	-3.745472000
C	4.334267000	-2.053609000	1.587939000
H	4.808105000	-1.908363000	2.584018000

H	3.824108000	-3.044161000	1.628158000
C	2.806553000	4.266217000	0.094719000
H	3.892025000	4.028350000	0.010597000
H	2.665698000	5.242657000	-0.419002000
C	0.525136000	-0.253507000	4.298310000
H	0.404733000	-1.044241000	5.069386000
H	0.509126000	0.726547000	4.820049000
H	1.529194000	-0.381809000	3.846715000
C	-4.408699000	-2.347088000	-0.463358000
H	-4.893178000	-3.022682000	0.258996000
C	-4.879050000	-2.269633000	-1.786208000
H	-5.740610000	-2.879166000	-2.101969000
C	-1.968881000	-0.131540000	3.921082000
H	-2.804743000	-0.186613000	3.195547000
H	-2.021637000	0.861105000	4.415469000
H	-2.149737000	-0.900984000	4.701831000
P	-1.300203000	0.418015000	-0.477413000
O	-0.090242000	2.795103000	-3.499215000
O	-2.154399000	2.356642000	-2.657755000
O	1.438179000	0.184502000	-3.862244000
O	3.051036000	1.408455000	-2.859054000
N	-0.020801000	-0.423543000	0.293647000
B	1.362757000	-0.058875000	-0.354474000
H	-2.329457000	3.062892000	-3.316975000

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Electronic Energy (BP86) = -2352.976749 a.u.

Zero-point correction (BP86) = 0.861939 a.u.

Thermal correction to Gibbs free Energy (BP86) = 0.775226 a.u.

Electronic Energy (M06) = -2354.688592 a.u.

2TS1', Number of imaginary frequency = 1(112.5i)

C	-1.676843000	-2.213734000	-2.629586000
C	1.952962000	-1.692209000	-2.690811000
C	-0.560584000	-1.610860000	-1.879679000
C	-3.867850000	0.294855000	-1.030424000
H	-3.736693000	-0.677674000	-1.525579000
C	0.327509000	2.933086000	1.183860000
C	0.067303000	2.077549000	0.061812000
C	1.262303000	-1.559506000	1.226082000
H	0.285218000	-2.021563000	0.952579000
C	0.702020000	-1.543074000	-2.005664000
C	-2.829136000	0.811325000	-0.220602000
C	2.827533000	0.456012000	0.143525000
H	3.138362000	-0.373101000	-0.546923000
C	-0.197073000	2.654587000	-1.223126000
C	-1.973627000	-1.182481000	1.539489000
C	3.028460000	1.754952000	-0.672987000
H	2.799124000	2.640171000	-0.038521000
H	2.319049000	1.795680000	-1.518980000
C	3.883226000	0.420030000	1.287971000
H	3.799175000	-0.507943000	1.887151000
H	3.681031000	1.253844000	1.995620000
C	-2.342511000	-2.540644000	1.420195000
H	-2.187499000	-3.061365000	0.463120000
C	0.371338000	4.329006000	0.983424000

H	0.580163000	4.984612000	1.843899000
C	0.523151000	2.439366000	2.622583000
H	0.575207000	1.332770000	2.597152000
C	2.323920000	-2.623628000	0.843862000
H	2.319097000	-2.794828000	-0.250058000
H	3.343634000	-2.255915000	1.094909000
C	0.158243000	4.897297000	-0.276086000
H	0.206916000	5.989248000	-0.413366000
C	-5.070941000	1.001458000	-1.195925000
H	-5.865602000	0.580854000	-1.832274000
C	-0.571752000	1.870401000	-2.487712000
H	-0.746886000	0.814197000	-2.202992000
C	-0.130771000	4.058311000	-1.356029000
H	-0.314674000	4.502435000	-2.346645000
C	-2.189478000	-0.514043000	2.763462000
H	-1.921599000	0.546366000	2.870660000
C	-3.027969000	2.054354000	0.423942000
H	-2.242643000	2.493652000	1.052261000
C	3.711334000	-3.180140000	-3.233755000
H	3.620756000	-3.013827000	-4.326855000
H	3.980407000	-4.232456000	-3.027833000
H	4.493978000	-2.498298000	-2.841709000
C	-4.230217000	2.760464000	0.249736000
H	-4.362316000	3.730429000	0.754981000
C	-3.715272000	-3.414130000	-2.505220000
H	-4.420688000	-3.744425000	-1.721142000
H	-3.316739000	-4.286363000	-3.062322000

H	-4.221465000	-2.742047000	-3.227813000
C	-0.669096000	2.841812000	3.522523000
H	-0.562307000	2.402516000	4.537007000
H	-1.646272000	2.514222000	3.112480000
H	-0.723928000	3.944902000	3.640395000
C	1.827554000	2.959597000	3.262941000
H	2.004558000	2.465302000	4.241363000
H	1.782532000	4.053099000	3.451797000
H	2.707940000	2.769831000	2.619513000
C	1.230375000	-1.398092000	2.778128000
H	2.184400000	-0.939435000	3.122889000
H	0.426924000	-0.695294000	3.081569000
C	5.324871000	0.554574000	0.762395000
H	6.042929000	0.547822000	1.612475000
H	5.566393000	-0.341450000	0.143914000
C	2.072423000	-3.785808000	3.097504000
H	1.872017000	-4.755963000	3.603559000
H	3.079645000	-3.456352000	3.444660000
C	-5.255061000	2.240073000	-0.559689000
H	-6.194379000	2.799690000	-0.693522000
C	2.098522000	-3.962619000	1.571127000
H	1.129530000	-4.401346000	1.236704000
H	2.884822000	-4.692552000	1.277466000
C	5.509963000	1.819664000	-0.090880000
H	5.401561000	2.717432000	0.562050000
H	6.540806000	1.862374000	-0.506920000
C	-2.922457000	-3.215498000	2.509196000

H	-3.210515000	-4.273584000	2.402956000
C	1.026092000	-2.738699000	3.510226000
H	1.050493000	-2.576048000	4.610653000
H	0.008383000	-3.123899000	3.274387000
C	4.464557000	1.883065000	-1.214500000
H	4.646420000	1.058179000	-1.941123000
H	4.570865000	2.829889000	-1.788349000
C	0.552258000	1.858196000	-3.547846000
H	0.183528000	1.377058000	-4.477744000
H	1.438721000	1.279538000	-3.225802000
H	0.870154000	2.891413000	-3.805023000
C	-2.756290000	-1.196229000	3.852892000
H	-2.915366000	-0.664285000	4.804499000
C	-3.128152000	-2.547056000	3.727919000
H	-3.578736000	-3.077238000	4.581947000
C	-1.872938000	2.404697000	-3.130567000
H	-1.709902000	3.390165000	-3.616762000
H	-2.693804000	2.522222000	-2.397007000
H	-2.214549000	1.706877000	-3.923335000
P	-1.373895000	-0.324235000	-0.004540000
O	-1.718721000	-2.298428000	-3.843849000
O	-2.655447000	-2.724512000	-1.818366000
O	2.453712000	-2.962940000	-2.575695000
O	2.534304000	-0.802411000	-3.308399000
N	0.086903000	0.628605000	0.277385000
B	1.358751000	-0.111524000	0.503725000

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Electronic Energy (BP86) = -2431.496590 a.u.

Zero-point correction (BP86) = 0.917135 a.u.

Thermal correction to Gibbs free Energy (BP86) = 0.826694 a.u.

Electronic Energy (M06) = -2433.290326 a.u.

3TS1', Number of imaginary frequency = 1(115.5i)

C	1.890923000	2.489887000	-1.807466000
C	-1.785456000	2.392342000	-1.904732000
C	0.702424000	1.870248000	-1.195528000
C	3.997124000	-0.309700000	-0.650743000
H	3.939846000	0.785801000	-0.741752000
C	-0.468411000	-3.344875000	0.157560000
C	-0.107051000	-2.170815000	-0.583473000
C	-1.276203000	0.880872000	1.727492000
H	-0.288886000	1.392172000	1.662235000
C	-0.560837000	1.947871000	-1.302030000
C	2.857179000	-1.037592000	-0.230951000
C	-2.817417000	-0.588376000	-0.041825000
H	-3.105098000	0.441026000	-0.384484000
C	0.221075000	-2.279953000	-1.973945000
C	1.935351000	0.448685000	1.936019000
C	-3.003971000	-1.486535000	-1.287430000
H	-2.799179000	-2.548112000	-1.025345000
H	-2.271381000	-1.216001000	-2.069411000
C	-3.898973000	-0.963995000	1.013303000
H	-3.823920000	-0.323828000	1.914518000
H	-3.717073000	-2.002877000	1.366337000
C	2.297359000	1.788811000	2.197943000

H	2.171691000	2.548615000	1.410991000
C	-0.537239000	-4.582286000	-0.516671000
H	-0.821144000	-5.483580000	0.049003000
C	-0.745815000	-3.359370000	1.665846000
H	-0.860721000	-2.309688000	2.001357000
C	-2.318211000	2.029689000	1.710282000
H	-2.270291000	2.572723000	0.745942000
H	-3.349208000	1.617228000	1.785391000
C	-0.259635000	-4.690324000	-1.883314000
H	-0.330934000	-5.664215000	-2.393251000
C	5.205031000	-0.966498000	-0.935755000
H	6.079075000	-0.380595000	-1.261542000
C	0.703568000	-1.126389000	-2.861632000
H	0.889889000	-0.247297000	-2.214962000
C	0.121888000	-3.546058000	-2.589502000
H	0.355456000	-3.629625000	-3.662376000
C	2.121435000	-0.527812000	2.938206000
H	1.864900000	-1.578893000	2.741485000
C	2.958448000	-2.441523000	-0.103439000
H	2.094007000	-3.041776000	0.206601000
C	-3.384444000	4.175809000	-1.998189000
H	-3.472596000	3.829199000	-3.047865000
H	-3.212307000	5.271595000	-1.990562000
C	4.169612000	-3.093712000	-0.394229000
H	4.227017000	-4.189148000	-0.292698000
C	3.955338000	3.631711000	-1.384632000
H	4.742057000	3.465958000	-0.621281000

H	4.266750000	3.166448000	-2.342361000
C	0.437890000	-3.974597000	2.447991000
H	0.257368000	-3.920222000	3.542596000
H	1.399085000	-3.463718000	2.236959000
H	0.574986000	-5.044705000	2.182594000
C	-2.039197000	-4.116299000	2.035629000
H	-2.293740000	-3.947497000	3.102958000
H	-1.928704000	-5.212735000	1.897400000
H	-2.900843000	-3.788055000	1.422273000
C	-1.292942000	0.187093000	3.125595000
H	-2.259061000	-0.348658000	3.264481000
H	-0.502407000	-0.589738000	3.184081000
C	-5.328055000	-0.875111000	0.445589000
H	-6.067041000	-1.176373000	1.221141000
H	-5.551011000	0.189663000	0.200294000
C	-2.129826000	2.325427000	4.234971000
H	-1.940311000	3.054862000	5.053155000
H	-3.149151000	1.911338000	4.417309000
C	5.295065000	-2.363459000	-0.812044000
H	6.239461000	-2.882005000	-1.041354000
C	-2.107410000	3.025032000	2.866457000
H	-1.125704000	3.536329000	2.733536000
H	-2.879643000	3.824741000	2.826518000
C	-5.497789000	-1.728053000	-0.822033000
H	-5.407860000	-2.806006000	-0.550002000
H	-6.519064000	-1.600045000	-1.244296000
C	2.835146000	2.143905000	3.447796000

H	3.118424000	3.190878000	3.640952000
C	-1.102000000	1.183731000	4.283969000
H	-1.160082000	0.648649000	5.257788000
H	-0.075512000	1.611143000	4.223013000
C	-4.426666000	-1.380864000	-1.867547000
H	-4.586018000	-0.341671000	-2.236185000
H	-4.524931000	-2.042856000	-2.755934000
C	-0.344560000	-0.676247000	-3.903444000
H	0.097001000	0.103526000	-4.558088000
H	-1.243672000	-0.227111000	-3.439357000
H	-0.659959000	-1.524835000	-4.548181000
C	2.647192000	-0.165290000	4.189366000
H	2.783706000	-0.934451000	4.966219000
C	3.007342000	1.170286000	4.446472000
H	3.425073000	1.450092000	5.426650000
C	2.032244000	-1.460988000	-3.578243000
H	1.883707000	-2.211614000	-4.383724000
H	2.800660000	-1.856014000	-2.884915000
H	2.436138000	-0.545047000	-4.057187000
P	1.405033000	0.039315000	0.197248000
O	2.039897000	2.640902000	-3.008360000
O	2.800042000	2.910831000	-0.875431000
O	-2.179552000	3.614308000	-1.421251000
O	-2.413895000	1.764888000	-2.755628000
N	-0.092533000	-0.887773000	0.124960000
B	-1.357360000	-0.222488000	0.544272000
C	-4.627321000	3.806369000	-1.197301000

H -4.540685000 4.135376000 -0.141812000

H -5.519592000 4.297642000 -1.639477000

H -4.797528000 2.711266000 -1.213839000

C 3.656258000 5.113838000 -1.569076000

H 3.303552000 5.573414000 -0.623470000

H 4.576767000 5.644793000 -1.889420000

H 2.884942000 5.264889000 -2.349952000

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Electronic Energy (BP86) = -2274.491631 a.u.

Zero-point correction (BP86) = 0.808904 a.u.

Thermal correction to Gibbs free Energy (BP86) = 0.72825 a.u.

Electronic Energy (M06) = -2276.130676 a.u.

4TS3, Number of imaginary frequency = 1(121.4i)

C -1.942741000 0.715034000 3.383455000

C 1.821424000 0.624839000 3.330998000

C -0.721960000 0.725491000 2.561222000

C -4.046351000 -0.301789000 0.489726000

H -3.989004000 0.443174000 1.298499000

C 0.452294000 -2.184005000 -1.993806000

C 0.054145000 -1.815801000 -0.664455000

C 1.405764000 1.924975000 -0.331091000

H 0.485913000 2.326433000 0.148563000

C 0.534398000 0.712805000 2.722030000

C -2.881551000 -0.618414000 -0.252996000

C 2.813437000 -0.433222000 -0.027593000

H 3.183546000 0.137181000 0.864727000

C -0.345147000 -2.825654000 0.267422000

C	-1.857450000	1.966285000	-0.581558000
C	2.934163000	-1.920917000	0.380363000
H	2.662480000	-2.576082000	-0.476269000
H	2.221478000	-2.158201000	1.191318000
C	3.859742000	-0.138882000	-1.144057000
H	3.825265000	0.920995000	-1.468147000
H	3.603048000	-0.738972000	-2.044148000
C	-1.928505000	3.128823000	0.218538000
H	-1.612874000	3.087541000	1.271901000
C	0.455406000	-3.549332000	-2.346908000
H	0.758856000	-3.838009000	-3.364418000
C	0.836597000	-1.168902000	-3.078133000
H	1.199536000	-0.253644000	-2.569773000
C	2.576809000	2.682325000	0.348105000
H	2.607271000	2.450143000	1.431376000
H	3.548223000	2.340384000	-0.072445000
C	0.090016000	-4.545803000	-1.434275000
H	0.111144000	-5.607111000	-1.728733000
C	-5.273411000	-0.918138000	0.200024000
H	-6.166137000	-0.657419000	0.790416000
C	-0.849297000	-2.563599000	1.692338000
H	-1.006594000	-1.473863000	1.807191000
C	-0.304684000	-4.174996000	-0.146599000
H	-0.598347000	-4.955456000	0.572504000
C	-2.302198000	2.025866000	-1.920911000
H	-2.293157000	1.121821000	-2.547874000
C	-2.978720000	-1.569507000	-1.293760000

H	-2.097659000	-1.848381000	-1.884242000
C	-4.211451000	-2.184746000	-1.577332000
H	-4.266434000	-2.923993000	-2.392170000
C	-0.386573000	-0.765332000	-3.929119000
H	-0.107499000	-0.002049000	-4.685940000
H	-1.200113000	-0.342687000	-3.308536000
H	-0.799912000	-1.644795000	-4.467969000
C	1.966058000	-1.654585000	-4.009973000
H	2.337171000	-0.810526000	-4.627663000
H	1.617442000	-2.438891000	-4.714969000
H	2.825428000	-2.068520000	-3.445590000
C	1.314980000	2.341623000	-1.832509000
H	2.204162000	1.950903000	-2.378754000
H	0.430132000	1.870418000	-2.309804000
C	5.293702000	-0.493137000	-0.707061000
H	6.006725000	-0.293945000	-1.537924000
H	5.592826000	0.181671000	0.128657000
C	2.409847000	4.590444000	-1.329433000
H	2.311279000	5.691943000	-1.448666000
H	3.368628000	4.308520000	-1.824352000
C	-5.360197000	-1.866596000	-0.834136000
H	-6.320766000	-2.356232000	-1.059620000
C	2.479283000	4.207543000	0.157281000
H	1.567805000	4.585838000	0.676001000
H	3.343022000	4.708393000	0.647633000
C	5.405418000	-1.953594000	-0.240518000
H	5.241521000	-2.626976000	-1.114471000

H	6.433472000	-2.167768000	0.126608000
C	-2.424959000	4.330321000	-0.316373000
H	-2.481404000	5.226797000	0.321090000
C	1.246416000	3.868669000	-2.027070000
H	1.231462000	4.110784000	-3.112976000
H	0.283265000	4.241806000	-1.611512000
C	4.361436000	-2.271630000	0.841700000
H	4.591100000	-1.694167000	1.766287000
H	4.415780000	-3.345547000	1.126100000
C	0.165573000	-2.962555000	2.786003000
H	-0.294145000	-2.818149000	3.785630000
H	1.081993000	-2.340938000	2.763888000
H	0.457660000	-4.030769000	2.693449000
C	-2.782033000	3.231969000	-2.456987000
H	-3.119145000	3.265832000	-3.505228000
C	-2.847155000	4.386310000	-1.655400000
H	-3.234149000	5.328507000	-2.075007000
C	-2.207666000	-3.249568000	1.963602000
H	-2.098192000	-4.350905000	2.059148000
H	-2.947037000	-3.051076000	1.162565000
H	-2.626118000	-2.878829000	2.922059000
P	-1.397988000	0.369879000	0.267917000
O	-2.150544000	-0.048684000	4.309695000
O	-2.842081000	1.680880000	3.019538000
O	2.322806000	1.844308000	3.708830000
O	2.449015000	-0.419019000	3.513161000
N	0.087214000	-0.392768000	-0.312780000

B	1.390657000	0.311581000	-0.198713000
H	-3.584427000	1.595903000	3.659579000
H	3.209421000	1.639575000	4.082096000

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