Supporting Information

σ-Vinyl endo-palladacycle formation *via* regiospecific functionalisation of an unreactive NHC-tethered C(sp^2) – H Bond

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1. General Considerations

Where stated, manipulations were performed under an atmosphere of dry nitrogen by means of standard Schlenk line or Glovebox techniques. Anhydrous solvents were prepared by passing the solvent over activated alumina to remove water, copper catalyst to remove oxygen and molecular sieves to remove any remaining water, *via* the Dow-Grubbs solvent system. Deuterated chloroform and acetonitrile were dried over CaH_2, cannula filtered or distilled, and then freeze-pump-thaw degassed prior to use. All other reagents and solvents were used as supplied.

^{1}H and ^{13}C NMR spectra were recorded on a Bruker DPX300 spectrometer. The values of chemical shifts are given in ppm and values for coupling constants (*J*) in Hz. Assignment of some ^{1}H NMR spectra was aided by the use of 2D $^{1}H^{1}H$ COSY experiments and the assignment of some $^{13}C\{^{1}H\}$ NMR spectra was aided by $^{13}C\{^{1}H\}$ dept 135 experiments. Mass spectra were collected on a Bruker Daltonics (micro TOF) instrument operating in the electrospray mode. Microanalyses were performed using a Carlo Erba Elemental Analyser MOD 1106 spectrometer.

2. Preparation of imidazolium salts

Imidazolium bromide salts were prepared according to literature procedure.[1] Bromide anions were exchanged for hexafluorophosphate anions through reaction of the bromide salts (2.0 mmol) with ammonium hexafluorophosphate (6.0 mmol) in water (40 mL). After 2 hours at room temperature, the precipitated imidazolium hexafluorophosphate salts were isolated *via* vacuum filtration and washed with water (3 x 30 mL) followed by aliquots of cold diethyl ether (3 x 30 mL) and dried *in vacuo*.

Typical analytical data

1-Allyl-3-(2-(4-methoxy)pyridyl)imidazolium hexafluorophosphate (1a): Yield: 0.72 g, 2.00 mmol, quantitative. ^{1}H NMR (300 MHz, CD_3CN) δ 9.28 (s, 1H, NC*H*N), 8.39 (d, *J* = 6.0 Hz, 1H, pyr*H*), 8.10 (br t, *J* = 3.9, 1.8 Hz, 1H, im*H*), 7.56 (br t, *J* = 3.9, 1.8 Hz, 1H, im*H*), 7.26 (d, *J* = 2.1 Hz, 1H, pyr*H*), 7.11 (dd, *J* = 5.7, 2.1 Hz, 1H, pyr*H*), 6.16 – 6.02 (ddt, *J* = 17.7, 12.6, 6.3 Hz, 1H,

C*H*=CH_2), 5.50 (d, *J* = 17.7 Hz, 1H, CH=CHH_{trans}), 5.45 (d, *J* = 12.6 Hz, 1H, CH=CHH_{cis}), 4.88 (d, *J* = 6.3 Hz, 2H, NCH_2), 3.98 (s, 3H, OCH_3) ppm. $^{13}C\{^1H\}$ NMR (75 MHz, CD_3CN): δ 169.7, 151.3, 149.0, 135.4, 131.4, 124.2, 122.5, 120.6, 112.6, 101.4, 57.5, 53.3 ppm. HRMS (ESI^+): Calcd for $C_{12}H_{14}N_3O$ $[M\text{-}PF_6]^+$: 216.1131. Found: 216.1149.

3. Preparation of palladium complexes

***Bis*[1-allyl-3-(2-(4-methoxy)pyridyl)imidazole-2-ylidene]palladium(II) dihexafluorophosphate (2a):** 1-Allyl-3-(4-methoxy)pyridyl imidazolium hexafluorophosphate (0.25 g, 0.69 mmol) and palladium acetate (77.7 mg, 0.35 mmol) were charged to a flame-dried ampoule under an inert atmosphere and stirred in anhydrous acetonitrile (20 mL) at 80 ˚C for 48 hours. After this time, the mixture was cooled to room temperature, filtered through a celite plug and solvents removed *in vacuo* to give a crude yellow residue. The crude product was dissolved in acetone and purified *via* flash chromatography on silica gel (saturated acetone solution of NH_4PF_6 as eluent) to afford a pale yellow residue. Dissolution of the residue in acetonitrile followed by dropwise addition to cold diethyl ether delivered the pure title compound as an off-yellow solid. Yield: 0.32 g, 0.35 mmol, 50 %. Decomposition T: 209-211 ˚C. ^1H NMR (300 MHz, CD_3CN): δ 7.95 (br d, *J* = 2.1 Hz, 1H, im*H*), 7.82 (br d, *J* = 2.1 Hz, 1H, im*H*), 7.77 (br d, *J* = 16.5 Hz, 2H, pyr*H*), 7.76 (br d, *J* = 16.5 Hz, 2H, pyr*H*), 7.26 (d, *J* = 2.1 Hz, 1H, im*H*), 7.25 (d, *J* = 2.1 Hz, 1H, im*H*), 7.19 (d, *J* = 2.7 Hz, 1H, pyr*H*), 7.08 (d, *J* = 2.7 Hz, 1H, pyr*H*), 6.64 (br m, 2H, C*H*CH_2), 5.91 (br d, *J* = 9.0 Hz, 2H, CH=CH_{cis}), 5.47 (br dd, *J* = 3.3, 9.0 Hz, 2H, CH=CH_{trans}), 4.58 (br d, *J* = 2.7 Hz, 4H, NCH_2), 3.47 (br s, 6H, OCH_3) ppm. $^{13}C\{^1H\}$ NMR (75 MHz, CD_3CN): δ 170.8, 152.7, 151.1, 151.0, 132.5, 125.4, 121.8, 119.8, 111.5, 101.6, 57.8, 54.6 ppm. HRMS (ESI^+): Calcd for $C_{24}H_{26}N_6O_2ClPd$ $[M\text{-}2PF_6\text{+}Cl]^+$: 573.0834. Found: 573.0836. Anal. Calcd for $C_{24}H_{26}N_6O_2P_2F_{12}Pd$: C, 34.86; H, 3.17; N, 10.29. Found: C, 34.90; H, 3.15; N, 10.65.

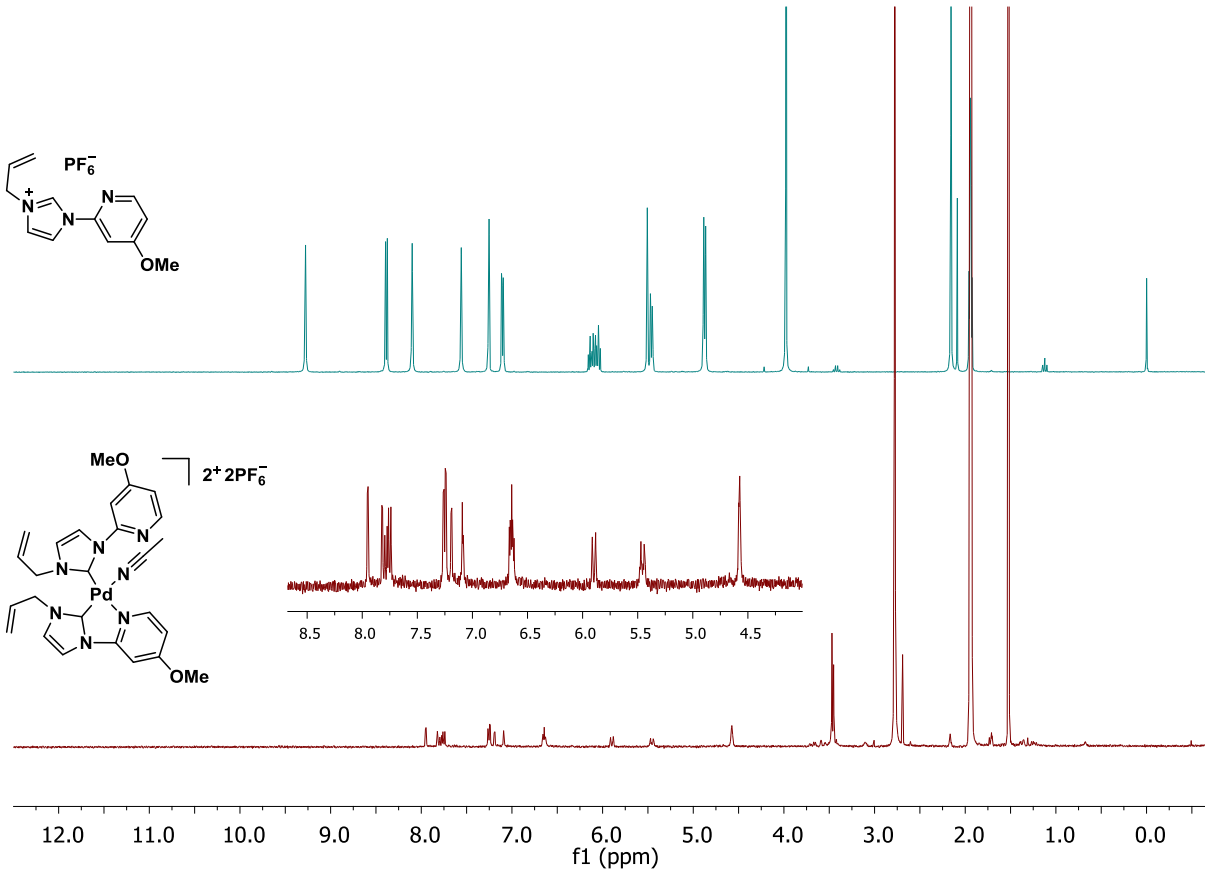


Figure S1. ^{1}H NMR (300 MHz, CD_3CN) spectrum of imidazolium **1a** (top) and *bis*-NHC Pd^{II} complex **2a** (bottom).

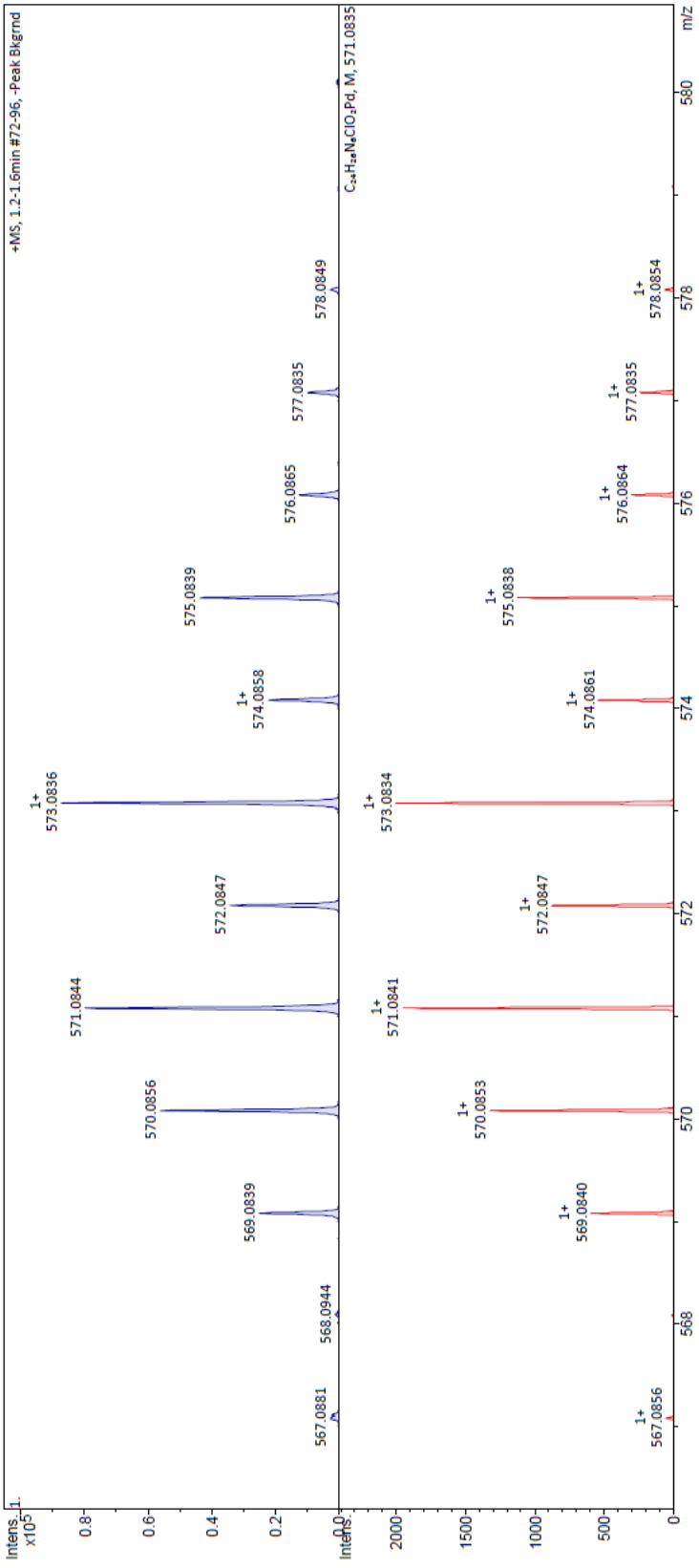


Figure S2. Simulated (bottom in red) and measured (top in blue) ESI MS isotope pattern for [**2a**-$2PF_6$+Cl]$^+$.

Palladacycle (3a): To a stirred solution of palladium acetate (0.25 g, 1.10 mmol, 0.11M) in anhydrous acetonitrile (10 mL) at 80 ˚C was added 1-allyl-3-(4-methoxy)pyridyl imidazolium hexafluorophosphate (0.22 g, 0.60 mmol, 0.03M) in anhydrous acetonitrile (20 mL) dropwise, under an inert atmosphere, and over one hour to maintain high dilution. The reaction mixture was controlled at 80 ˚C for 24 hours. After this time, cold diethyl ether (40 mL) was added to the mixture in a single portion, upon which a pale yellow solid precipitated from solution which was collected *via* vacuum filtration. Reprecipitation of the crude solid from acetonitrile (20 mL) with cold diethyl ether (50 mL), followed by repeated washing with cold pentane (3 x 20 mL) delivered the spectroscopically pure title compound as an off-yellow solid. Yield: 0.25 g, 0.49 mmol, 82 %. Decomposition T: 284-286 ˚C. ^{1}H NMR (300 MHz, CD_3CN): δ 8.27 (d, *J* = 6.3 Hz, 1H, im*H*), 7.89 (d, *J* = 2.1 Hz, 1H, pyr*H*), 7.42 (d, *J* = 2.1 Hz, 1H, pyr*H*), 7.23 (d, *J* = 2.1 Hz, 1H, pyr*H*), 7.07 (dd, *J* = 9.3, 6.3 Hz, 1H, im*H*), 6.63 (dt, *J* = 9.0, 3.9, 1.8 Hz, 1H, CH_2CHCH_{cis}), 6.02 (dt, *J* = 9.0, 3.9, 1.8 Hz, 1H, $CH_2CH_{cis}CH$), 5.03 (m, 2H, CH_2), 4.03 (s, 3H, OCH_3) ppm. $^{13}C\{^{1}H\}$ NMR (75 MHz, CD_3CN): δ 171.1, 155.8, 152.7, 152.5, 126.3, 124.6, 122.7, 118.8, 110.9, 98.6, 58.0, 56.2. HRMS (ESI^+): Calcd for $C_{12}H_{12}N_3OPd$ [M-MeCN-PF_6]$^+$: 320.0015. Found 320.0016. Anal. Calcd for $C_{14}H_{15}N_4OPF_6Pd(^1/_3C_5H_{12})$: C, 35.24; H, 3.55; N, 10.60. Found: C, 35.50; H, 3.20; N, 11.00.

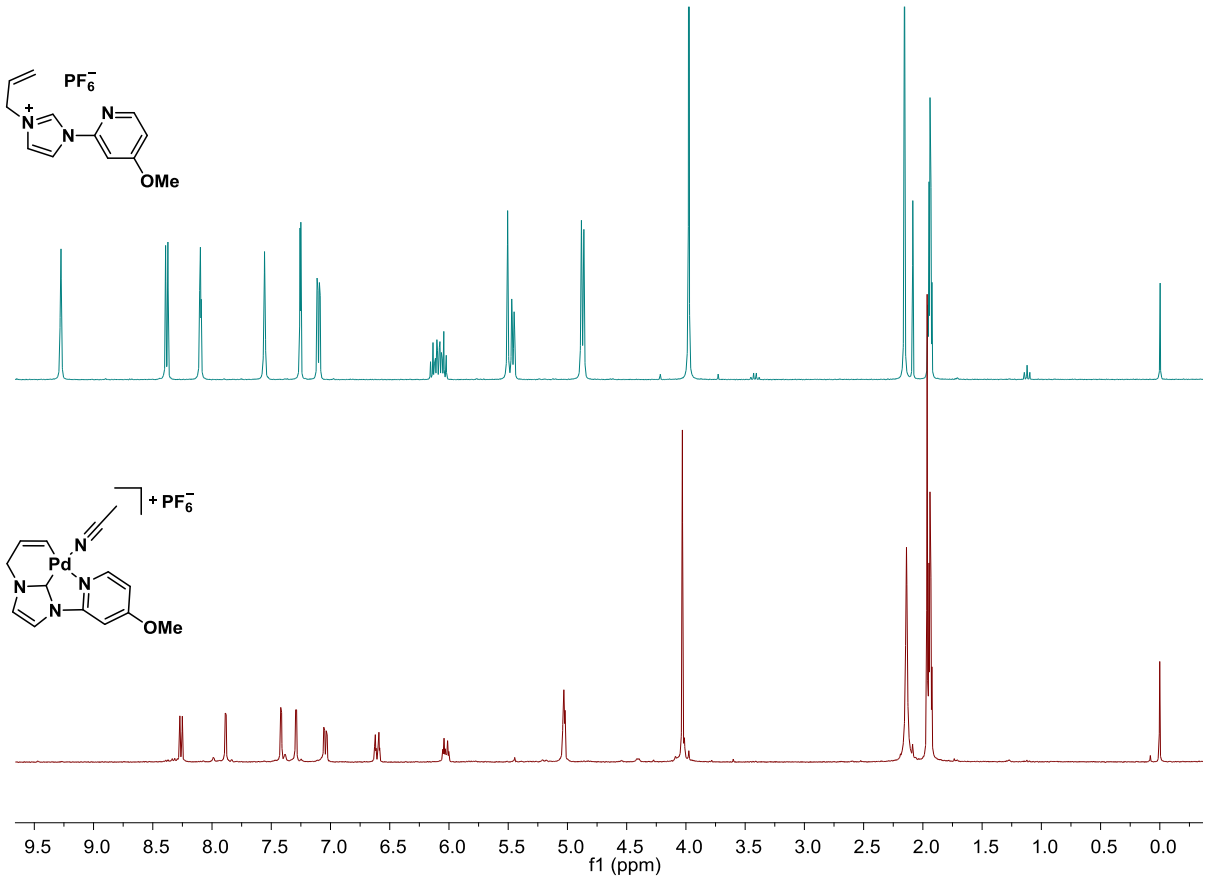


Figure S3. ^{1}H NMR (300 MHz, CD_3CN) spectrum of imidazolium **1a** (top) and palladacycle **3a** (bottom).

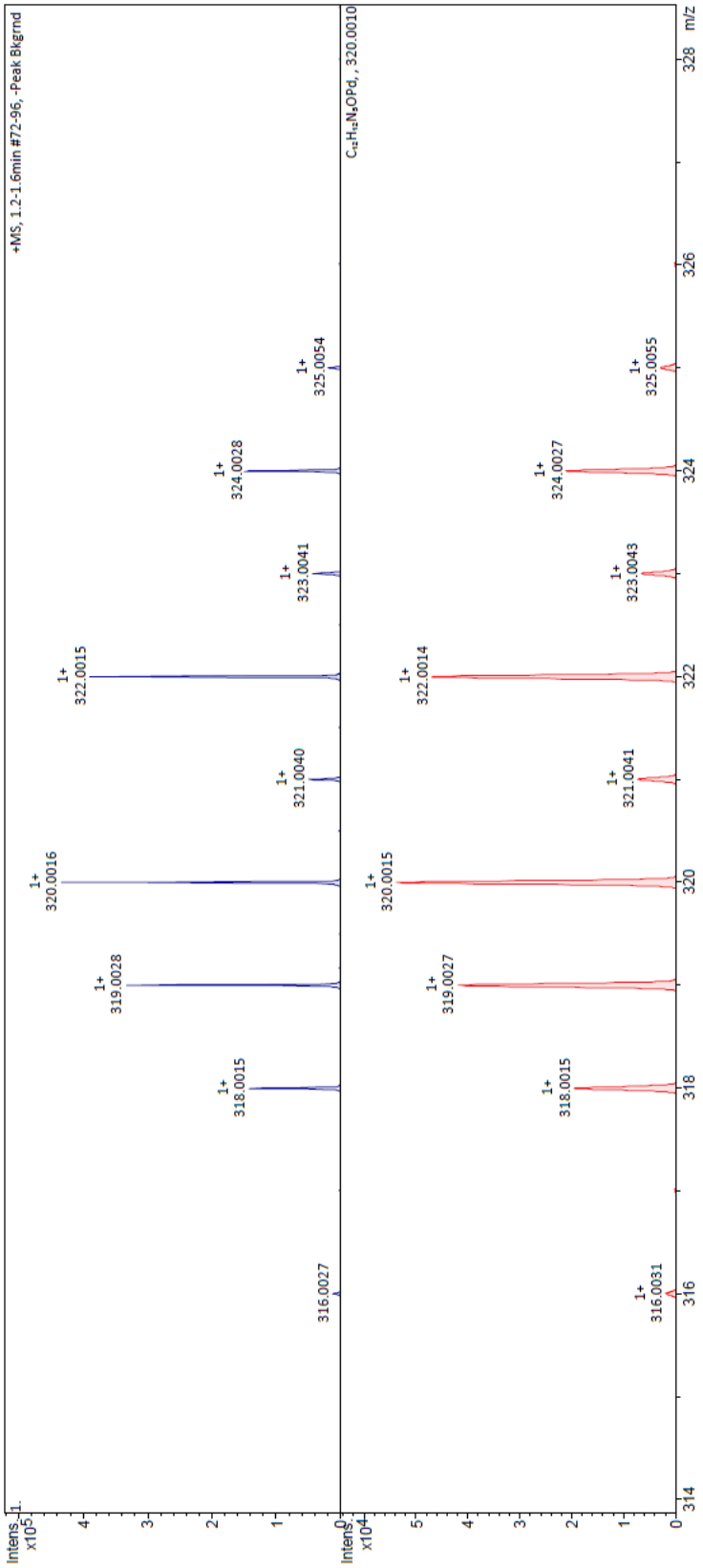


Figure S4. Simulated (bottom in red) and measured (top in blue) ESI MS isotope pattern for [**3a**-MeCN-PF_6]$^+$.

Palladacycle (3·SbF_6): To a stirred solution of palladium acetate (0.25 g, 1.10 mmol, 0.11M) in anhydrous acetonitrile (10 mL) at 80 ˚C was added 1-allyl-3-(4-methoxy)pyridyl imidazolium hexafluoroantimonate (0.27 g, 0.60 mmol, 0.03M) in anhydrous acetonitrile (20 mL) dropwise, under an inert atmosphere, and over one hour to maintain high dilution. The reaction mixture was controlled at 80 ˚C for 24 hours. After this time, cold diethyl ether (40 mL) was added to the mixture in a single portion, upon which a pale yellow solid precipitated from solution which was collected *via* vacuum filtration. Reprecipitation of the crude solid from acetonitrile (20 mL) with cold diethyl ether (50 mL), followed by repeated washing with cold pentane (3 x 20 mL) delivered the title compound as an off-yellow solid. Yield: 0.26 g, 0.44 mmol, 74 %. ^{1}H NMR (500 MHz, CD_3CN): δ 8.26 (d, *J* = 6.5 Hz, 1H, im*H*), 7.88 (d, *J* = 2.0 Hz, 1H, pyr*H*), 7.41 (d, *J* = 2.0 Hz, 1H, pyr*H*), 7.29 (d, *J* = 2.0 Hz, 1H, pyr*H*), 7.10 (dd, *J* = 6.5, 2.5 Hz, 1H, im*H*), 6.61 (dt, *J* = 8.5, 3.5, 1.5 Hz, 1H, CH_2CHCH_{cis}), 6.03 (dt, *J* = 8.5, 3.5, 1.5 Hz, 1H, $CH_2CH_{cis}CH$), 5.03 (m, 2H, CH_2), 4.03 (s, 3H, OCH_3) ppm. $^{13}C\{^{1}H\}$ NMR (125 MHz, CD_3CN): δ 171.0, 155.8, 152.9, 152.5, 126.3, 124.6, 122.8, 118.5, 110.9, 98.6, 58.1, 56.2. HRMS (ESI^+): Calcd for $C_{12}H_{12}N_3OPd$ $[M\text{-}MeCN\text{-}SbF_6]^+$: 320.0015. Found 320.0024.

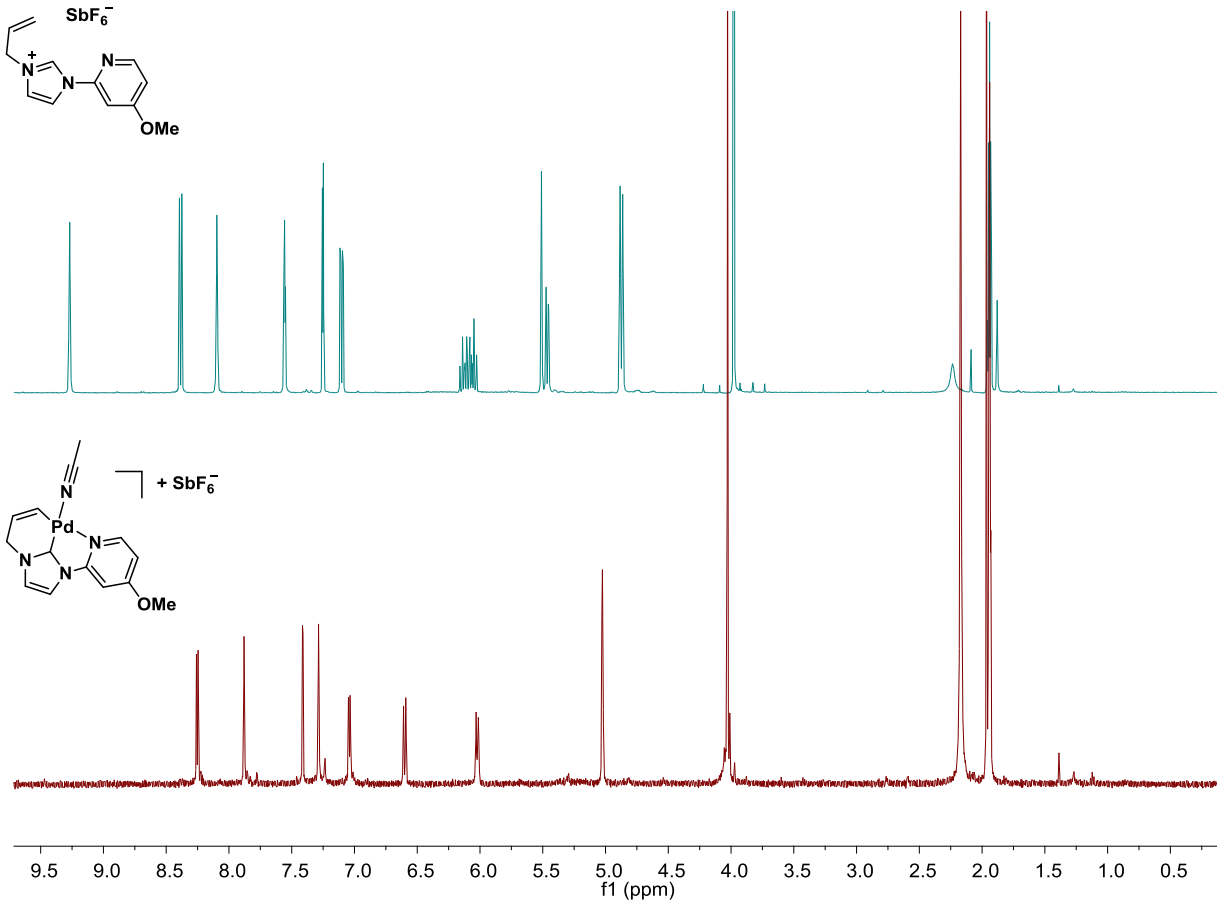


Figure S5. ^{1}H NMR (500 MHz, CD_3CN) spectrum of imidazolium **1·SbF$_6$** (top) and palladacycle **3·SbF$_6$** (bottom).

Reaction of palladium acetate with imidazolium salts 1b-1e under high dilution conditions

Reactions were performed using identical reaction conditions to those for the synthesis of palladacycle **3a**. Using ^{1}H NMR spectroscopy and mass spectrometry, only *bis*-NHC complexes **2b-2e** were observed, with no evidence of palladacycle formation.

***Bis*[1-allyl-3-(2-(4-dimethylamino)pyridyl)imidazole-2-ylidene]palladium(II) dihexafluorophosphate (2b):** ^{1}H NMR (400 MHz, d_6-DMSO): δ (ppm) 8.20 (br s, 2H, im*H*), 8.07 (br d, *J* = 4.8 Hz, 2H, py*H*), 7.32 (br d, *J* = 4.8 Hz, 2H, py*H*), 7.02 (br s, 2H, im*H*), 6.57 (br s, 2H, py*H*), 6.07 (br m, 2H, C*H*=CH$_2$), 5.56 (br m, 4H, CH=C*H*$_2$), 4.97 (br s, 4H, NC*H*$_2$), 3.14 (s, 12H, N(C*H*$_3$)$_2$). HR-MS (ESI$^+$): *m/z* 643.0952 [$C_{26}H_{32}N_8PdBr]^+$, calcd. [M – MeCN – 2PF$_6$ + Br]$^+$ 643.0942.

***Bis*[1-allyl-3-(2-(4-methyl)pyridyl)imidazole-2-ylidene]palladium(II) dihexafluorophosphate (2c):** . ^{1}H NMR (300 MHz, d_6-DMSO): δ (ppm) 7.64 – 7.54 (br m, 4H, im*H*), 7.27 – 7.10 (br m, 2H, py*H*), 6.97 – 6.67 (br m, 4H, py*H*), 5.67 – 3.19 (br m, 6H, CH_2=C*H*), 2.50 (br s, 6H, CH_3), 1.25 – 0.98 (br m, 4H, CH_2). HR-MS (ESI$^+$): *m/z* 252.0623 $[C_{24}H_{26}N_6Pd]^{2+}$, calcd. [M – MeCN – 2PF_6]$^{2+}$ 252.0621.

***Bis*[1-allyl-3-(2-pyridyl)imidazole-2-ylidene]palladium(II) dihexafluorophosphate (2d):** ^{1}H NMR (300 MHz, CD_3CN): δ (ppm) 9.24 (br d, *J* = 6.0 Hz, 2H, im*H*), 7.98 (t, *J* = 6.0 Hz, 2H, pyr*H*), 7.66 (d, *J* = 6.0 Hz, 2H, pyr*H*), 7.46 (t, *J* = 6.0 Hz, 2H, pyr*H*), 7.30 (d, *J* = 6.0 Hz, 2H, pyr*H*), 7.01 (br s, 2H, im*H*), 6.13 – 6.01 (m, 2H, C=C*H*), 5.83 – 5.78 (m, 2H, C=CH_{trans}), 5.39 – 5.14 (m, 4H, NCH_2), 4.99 (br s, 2H, C=CH_{cis}). HR-MS (ESI$^+$): *m/z* 238.0471 $[C_{22}H_{22}N_6Pd]^{2+}$, calcd. [M – 2PF_6]$^{2+}$ 238.0465.

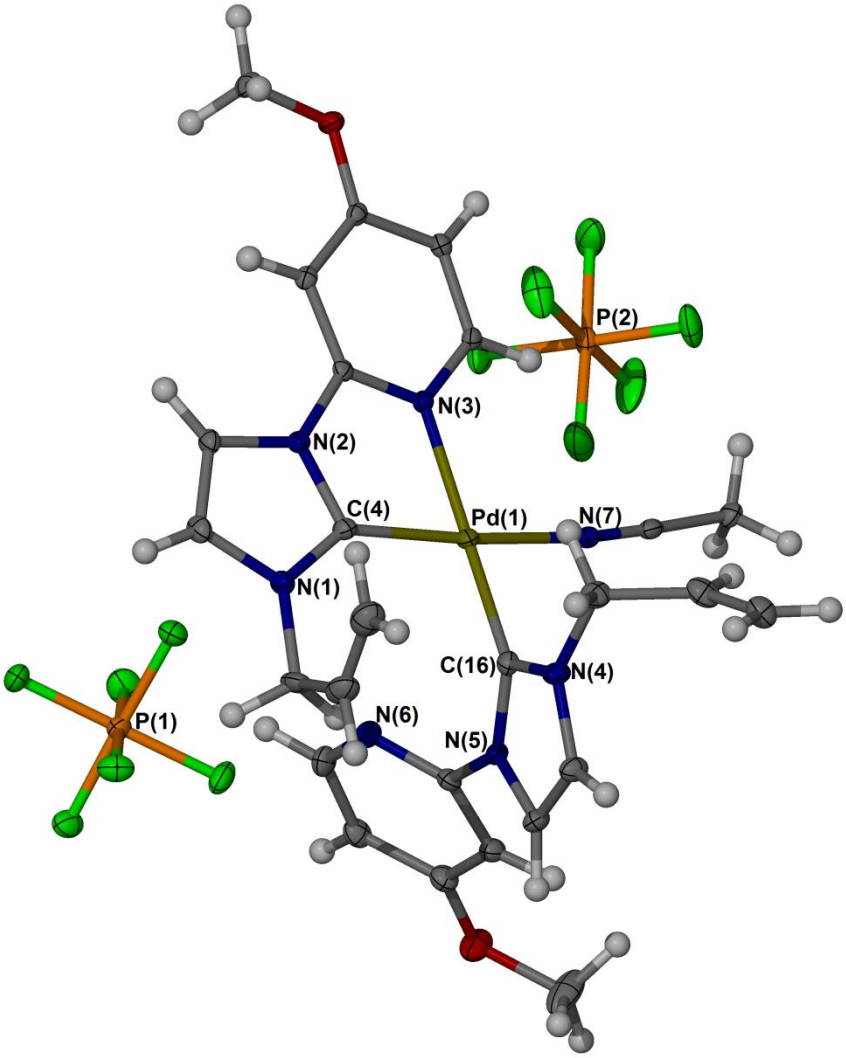
***Bis*[1-allyl-3-(2-(5-nitro)pyridyl)imidazole-2-ylidene]palladium(II) dihexafluorophosphate (2e):** ^{1}H NMR (400 MHz, CD_3CN): δ (ppm) 9.29 (br d, *J* = 2.4 Hz, 2H, im*H*), 8.96 (br dd, *J* = 9.0, 2.1 Hz, 2H, py*H*), 8.13 (d, *J* = 3.3 Hz, 2H, py*H*), 8.12 (d, *J* = 3.3 Hz, 2H, py*H*), 7.48 (br d, *J* = 2.4 Hz, 2H, im*H*), 5.83 (ddt, *J* = 21.9, 10.2, 5.1 Hz, 2H, C*H*=CH_2), 5.16 (br d, *J* = 10.2, 2H, HC=CH_{cis}), 5.00 (br d, *J* = 21.9 Hz, 2H, HC=CH_{trans}), 4.44 (br s, 4H, NCH_2). HR-MS (ESI$^+$): *m/z* 585.0634 $[C_{22}H_{21}N_8O_5Pd]^+$, calcd. [M – MeCN – 2PF_6 + OH]$^+$.

4. Crystallographic details

X-Ray diffraction data were collected on an Agilent SuperNova diffractometer fitted with an Atlas CCD detector with Mo Kα radiation (λ = 0.7107 Å) (complex **2**) or Cu Kα radiation (λ = 1.5418 Å) (complex **3**). Crystals were mounted under oil on nylon fibres. Data sets were corrected for absorption using a multiscan method, and the structures were solved by direct methods using SHELXS-97 and refined by full-matrix least squares on F2using ShelXL-97, interfaced through the program Olex2.[2] Molecular graphics for all structures were generated using POV-RAY in the X-Seed program.

Crystallographic details for 2a

Formula	$C_{26}H_{29}F_{12}N_7O_2P_2Pd$	
Formula weight	867.9	
Size	0.33 x 0.26 x 0.11 mm	
Crystal morphology	Brown irregular	
Temperature	100.0(5) K	
Wavelength	0.71073 Å [Mo-K_α]	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 17.4924(7) Å	α = 90°
	b = 9.5762(5) Å	β = 98.995(4)°
	c = 20.1833(9) Å	γ = 90°
Volume	3339.3(3) Å^3	
Z	4	
Density (calculated)	1.726 Mg/m^3	
Absorption coefficient	0.757 mm^{-1}	
F(000)	1736	
Data collection range	$3.29 \le \theta \le 26.37°$	
Index ranges	$-21 \le h \le 13$, $-11 \le k \le 11$, $-24 \le l \le 25$	
Reflections collected	13373	
Independent reflections	6764 [R(int) = 0.0426]	
Observed reflections	5509 [$I > 2\sigma(I)$]	
Absorption correction	analytical	
Max. and min. transmission	0.927 and 0.841	
Refinement method	Full	
Data / restraints / parameters	6764 / 0 / 454	
Goodness of fit	1.031	
Final R indices [$I > 2\sigma(I)$]	R_1 = 0.0514, wR_2 = 0.113	
R indices (all data)	R_1 = 0.0657, wR_2 = 0.1228	
Largest diff. peak and hole	2.43 and -0.934e.Å^{-3}	

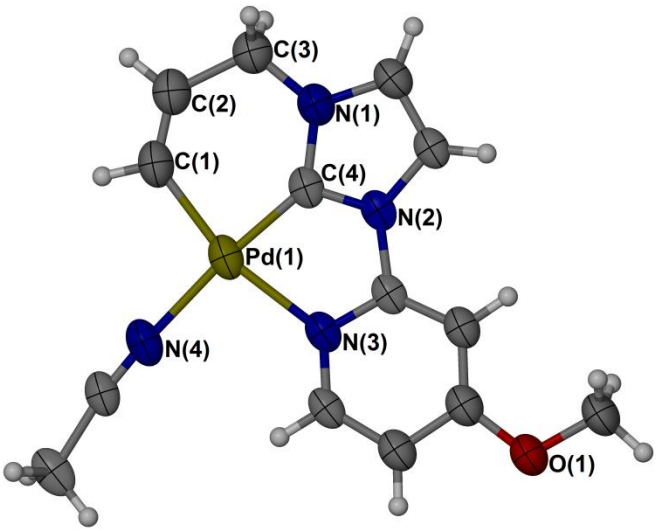


Crystallographic details for 3a

Note: Crystals were weakly diffracting, resulting in limited high angle data. All non-hydrogen atoms were refined anisotropically, however the anisotropic displacement parameters were heavily restrained using the SIMU, DELU and ISOR commands. The structure was solved in the P21/m space group, with the entire molecule lying on the mirror plane.

Empirical formula	$C_{14}H_{15}F_6N_4OPPd$
Formula weight	506.67
Temperature/K	100.2(7)
Crystal system	monoclinic
Space group	$P2_1/m$
a/Å	12.097(3)

b/Å	6.8619(13)
c/Å	21.461(3)
α/°	90.00
β/°	91.882(17)
γ/°	90.00
Volume/Å^3	1780.4(6)
Z	4
ρ_{calc}g/cm^3	1.890
μ/mm^{-1}	9.960
F(000)	1000.0
Crystal size/mm^3	0.11 × 0.06 × 0.03
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	7.32 to 110.2
Index ranges	-9 ≤ h ≤ 12, -7 ≤ k ≤ 5, -21 ≤ l ≤ 22
Reflections collected	6445
Independent reflections	2419 [R_{int} = 0.0685, R_{sigma} = 0.0681]
Data/restraints/parameters	2419/712/327
Goodness-of-fit on F^2	1.073
Final R indexes [I>=2σ (I)]	R_1 = 0.1449, wR_2 = 0.3606
Final R indexes [all data]	R_1 = 0.1697, wR_2 = 0.3755
Largest diff. peak/hole / e Å^{-3}	1.59/-1.20

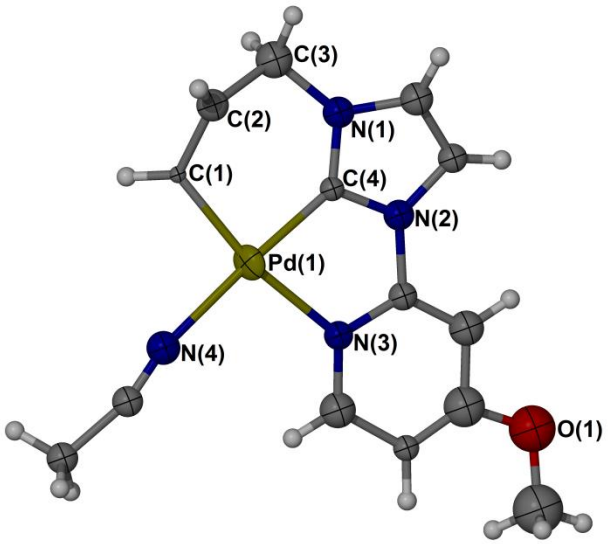


Crystallographic details for 3·SbF_6

Note: A number of different crystals were examined, all of which showed similar problems which appear intractable for these crystals. Extensive twinning was observed, and the data refined with the twin law (-1 0 0, 0 -1 0, 0 0 1) with concurrent racemic twin refinement. Pd and Sb atoms were refined anisotropically, though attempted anisotropic refinement of lighter elements led to nonsensical anisotropic displacement parameters which did not improve markedly through the use of restraints. Bond distances were restrained through the use of DFIX and SADI commands. The structure was solved in the P21 space group. Analysis using the PLATON program[3] suggested a change of space group to P21/m, similar to the PF_6 structure. However, attempted solution in the P21/m space group led to a structure which did not refine satisfactorily resulting in nonsensical geometric parameters.

Empirical formula	$C_{14}H_{15}F_6N_4OPdSb$
Formula weight	597.45
Temperature/K	119.99(18)
Crystal system	monoclinic
Space group	$P2_1$
a/Å	13.0668(11)
b/Å	6.8152(4)
c/Å	21.0073(18)
α/°	90.00
β/°	90.568(8)
γ/°	90.00
Volume/$Å^3$	1870.7(3)
Z	4
$\rho_{calc}g/cm^3$	2.121
μ/mm^{-1}	2.474
F(000)	1144.0
Crystal size/mm^3	0.09 × 0.04 × 0.03
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	6.28 to 50.04
Index ranges	$-15 \leq h \leq 15$, $-8 \leq k \leq 8$, $-25 \leq l \leq 25$
Reflections collected	12591
Independent reflections	6225 [R_{int} = 0.0535, R_{sigma} = 0.0728]

Data/restraints/parameters	6225/87/241
Goodness-of-fit on F^2	1.071
Final R indexes [I>=2σ (I)]	R_1 = 0.1189, wR_2 = 0.3056
Final R indexes [all data]	R_1 = 0.1393, wR_2 = 0.3264
Largest diff. peak/hole / e $Å^{-3}$	2.79/-2.17
Flack parameter	0.00



5. Computational details

Gaussian 09[4] was used to fully optimize all the structures reported in this paper at the M06 level of density functional theory (DFT)[5] in acetonitrile using the CPCM solvation model.[6-8] The effective-core potential of Hay and Wadt with a double-ξ valence basis set (LANL2DZ)[9, 10] was chosen to describe Pd. The 6-31G(d) basis set was used for other atoms.[11] A polarization function was also added for Pd (ξf = 1.472).[12] This basis set combination will be referred to as BS1. Frequency calculations were carried out at the same level of theory as those for the structural optimization. Transition structures were located using the Berny algorithm. Intrinsic reaction coordinate (IRC)[13] calculations were used to confirm the connectivity between transition structures and minima. To further refine the energies obtained from the M06/BS1 calculations, we carried out single-point

energy calculations for all of the structures with a larger basis set (BS2) in acetonitrile using the CPCM solvation model at M06 level. To estimate the corresponding Gibbs energies, ΔG, the entropy corrections were calculated at the M06/BS1 level, adjusted by the method proposed by Whitesides et al[14] and finally added to the single-point energies. BS2 utilizes the def2-QZVP basis set on all atoms. We have used the Gibbs free energies obtained from the M06/BS2//M06/BS1 calculations in acetonitrile throughout the paper unless otherwise stated.

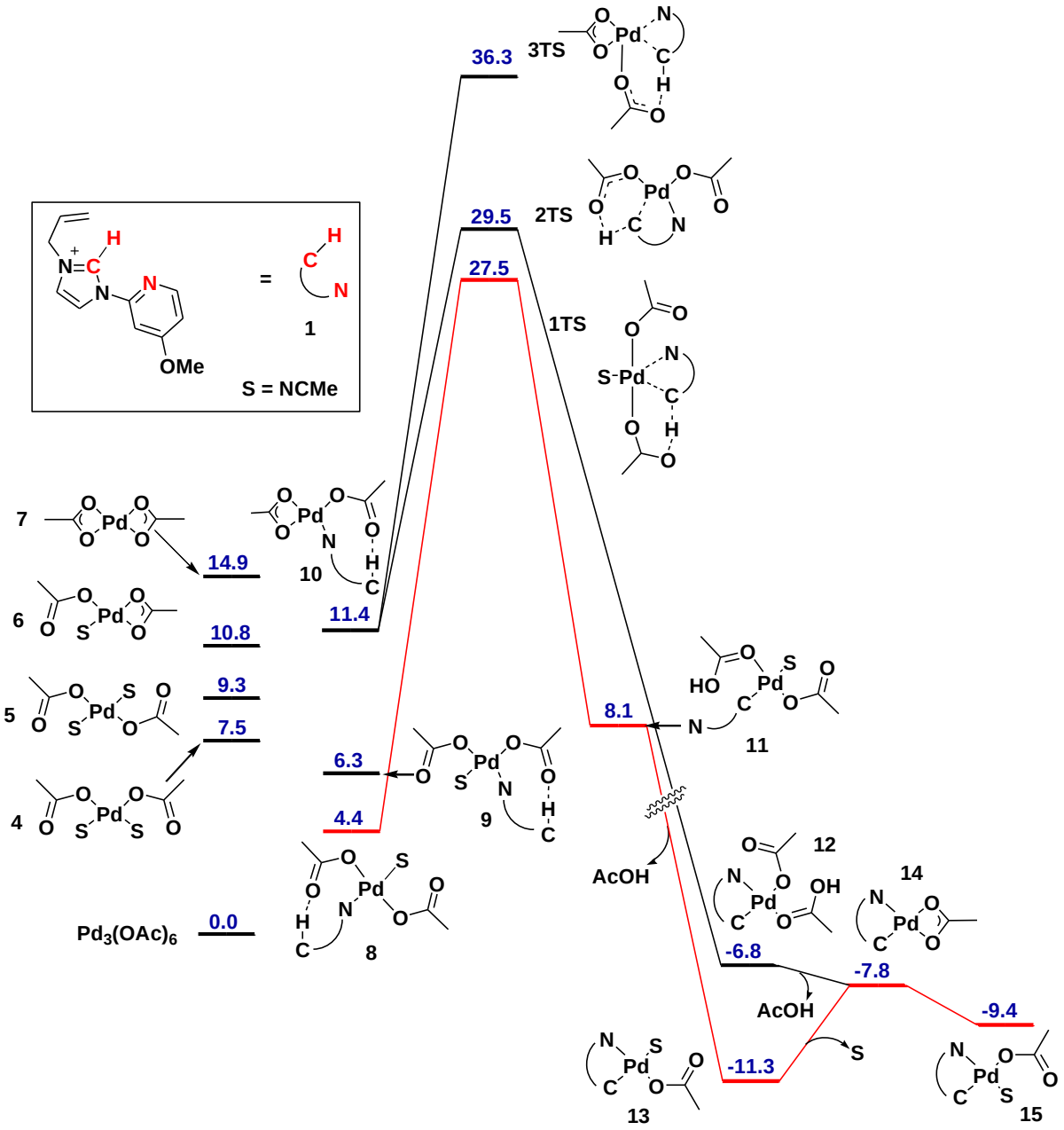


Figure S6. DFT investigations into imidazolium deprotonation. ΔG values are calculated in kcalmol^{-1}. Palladium complexes **11-15** are cationic.

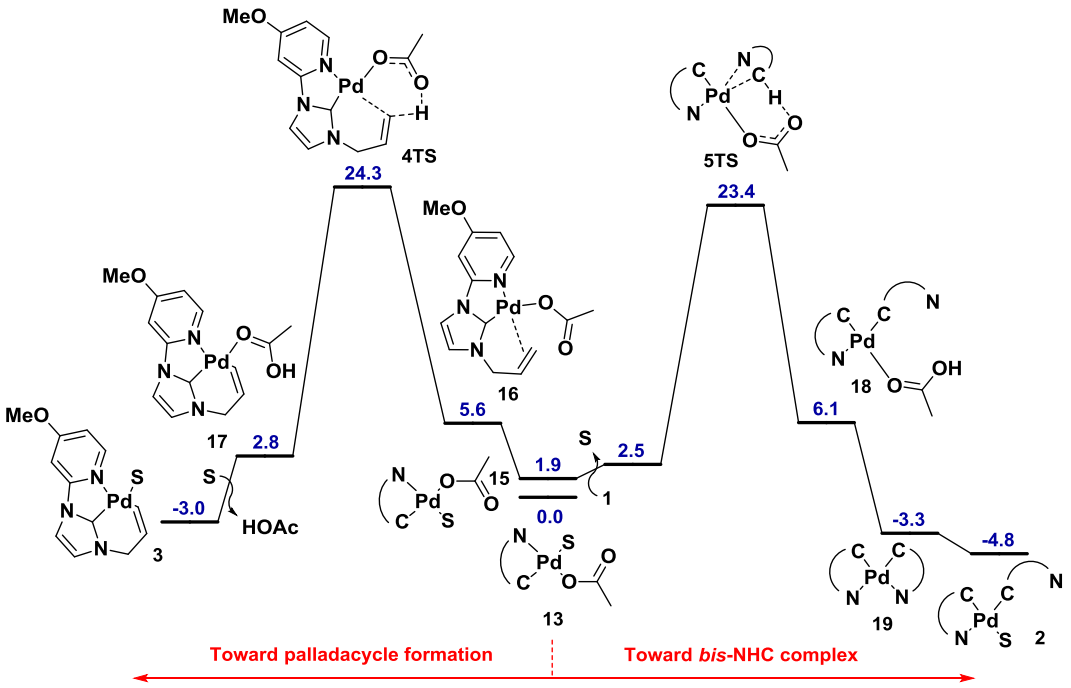


Figure S7. DFT analysis of competitive energy pathways for palladacyclisation versus *bis*-NHC formation. ΔG values are calculated in kcalmol^{-1}. Palladium complexes are cationic.

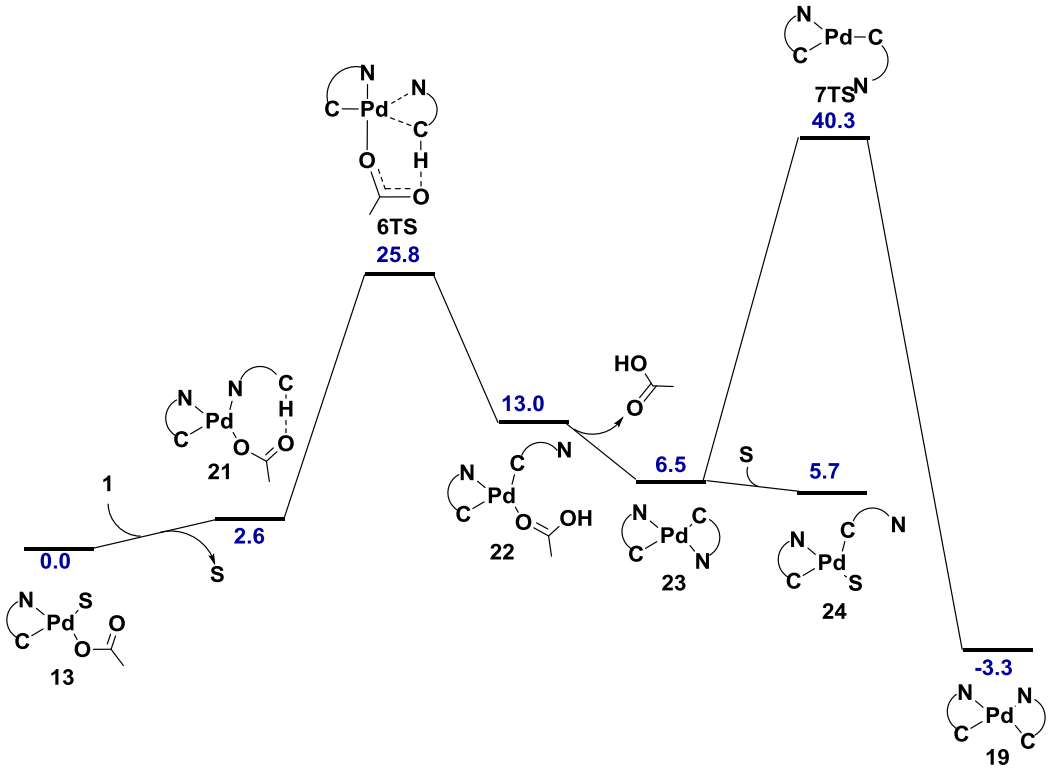


Figure S8. DFT analysis of *bis*-NHC formation starting from complex **13.** ΔG values are calculated in kcalmol^{-1}. Palladium complexes are cationic.

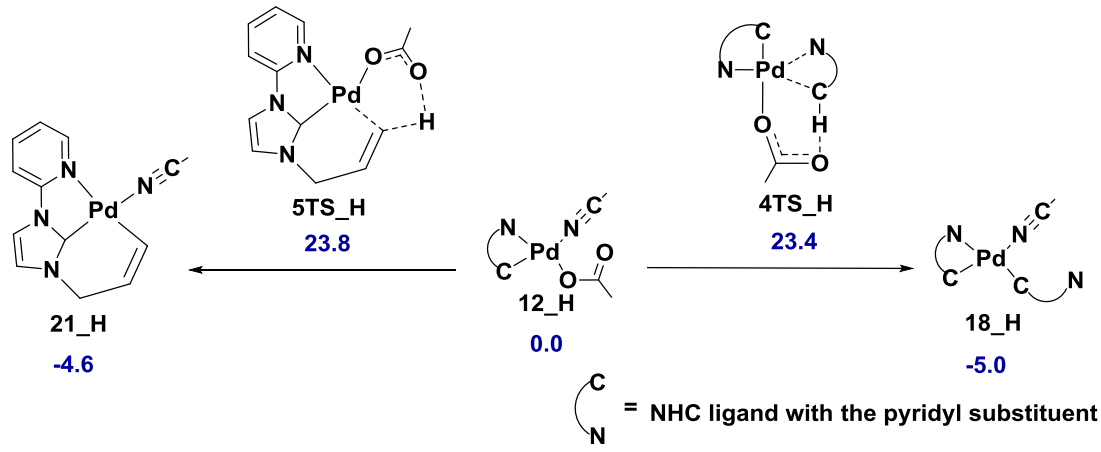


Figure S9. DFT analysis of competitive energy pathways for palladacyclisation versus *bis*-NHC formation with unsubstituted *N*-pyridyl substituent. ΔG values are calculated in kcalmol^{-1}. Palladium complexes are cationic.

Discussion of Figure S9: DFT calculations show that the energies of 5TS_H and 4TS_H are comparable. The same is true for the energies of the products 18_H and 21_H. Based on these findings it is not possible to provide an explanation for the absence of palladacycle formation under kinetic control when the *para*-methoxypyridyl substituent is exchanged for varying pyridyl substituents (*i.e.* imidazolium salts **1b**-**1e**). This discrepancy can be related to either the calculation error or the reaction condition (an unknown reason) which sometimes can switch off one reaction in favour of the other when two reactions are competitive.

The error in calculations can be related to the estimation of entropy effects. The translational contribution to the entropy is suppressed upon going from the gas phase to a solvent, leading to an inadequate estimation of the Gibbs free energy changes especially where the number of reactants is different from that of product.

For the transformation 12_H + NHC → 4TS_H → 18_H, the two reactant molecules are transformed to one molecule. This type of calculation suffers from the error in the entropy and should be corrected. Indeed, the entropy contribution is overestimated in this case. The formulation developed by Whitesides and co-workers was used to reduce the error.[14] Although the entropy effects have been

corrected based on this formulation, the formulation is not always adequate, and there is currently no reliable methodology for estimating the real error.

In contrast, for the transformation 12_H → 5TS_H → 21_H, the error in the entropy is negligible as the number of molecules remains constant during the course of the reaction.

We expect that for the transformation 12_H + NHC → 4TS_H → 18_H the real error should be larger than what the Whitesides formulation predicts, and 4TS_H should actually be much lower in energy than 5TS_H.

Table S1. Cartesian coordinates and total energies in acetonitrile for all of the calculated structures

1
E (M06/BS1) = -704.486438 au
H(M06/BS1) = -704.223589 au
G(M06/BS1) = -704.281833 au
E(M06/BS2//M06/BS1) = -704.8208629 au

C	2.38061200	2.21643900	0.08504500
C	0.99061100	0.44519400	-0.08204700
C	3.49331100	1.40276000	0.15268400
H	2.49086400	3.29923500	0.12661100
C	2.01331600	-0.48978900	-0.02145500
H	4.49519800	1.81169300	0.24865300
H	1.82065300	-1.55606000	-0.06079900
N	-0.37013900	0.00159300	-0.20290800
C	-1.41879900	0.83644900	-0.19437700
C	-0.84392500	-1.29413600	-0.33300500
C	-2.19535800	-1.21592800	-0.39959700
H	-0.19485500	-2.15596700	-0.36988400
H	-2.94954100	-1.98417800	-0.50169200
N	-2.53027500	0.12113900	-0.31341600
N	1.12726600	1.75662900	-0.03301000
C	3.31182200	0.01461900	0.09946600
C	-3.90586900	0.65393900	-0.34503200
H	-3.81651900	1.73991100	-0.22622200
H	-4.31842300	0.45049300	-1.34017300
C	-4.73820100	0.03374900	0.72827300
H	-4.41135200	0.20963300	1.75435100
C	-5.82270900	-0.68979500	0.46627600
H	-6.42699800	-1.12014800	1.26150800
H	-6.15420100	-0.87066300	-0.55646500
O	4.41008100	-0.73896800	0.17199900
C	4.26716400	-2.15255500	0.14574200
H	5.27538300	-2.55906700	0.23818900
H	3.65446900	-2.49962000	0.98745200
H	3.82396300	-2.48608000	-0.80118000
H	-1.34911000	1.91136100	-0.10283600

MeCN

E (M06/BS1) = -132.6602251 au

H(M06/BS1) = -132.610263 au

G(M06/BS1) = -132.638715 au

E(M06/BS2//M06/BS1) = -132.7298634 au

N	-1.43686000	0.00003500	-0.00003500
C	-0.27553900	-0.00014700	0.00003400
C	1.17486000	0.00004000	-0.00007300
H	1.55368200	0.95333800	-0.38248000
H	1.55376600	-0.14506200	1.01690000
H	1.55464800	-0.80787800	-0.63394000

$Pd_3(OAc)_6$

E (M06/BS1) = -1750.589062 au

H(M06/BS1) = -1750.238731 au

G(M06/BS1) = -1750.340807 au

E(M06/BS2//M06/BS1) = -1754.851947 au

Pd	-1.19539300	1.35646700	-0.00123100
O	-0.44151200	2.26360900	-1.66681600
O	-0.20216000	2.64861900	1.25422400
C	0.88481100	2.46174600	1.86644300
O	1.72794800	1.54175200	1.66185600
Pd	1.77210100	0.35564600	0.00204100
C	0.78608200	2.48783300	-1.87207500
O	1.76520400	1.98390400	-1.25689200
O	-2.19518800	0.72696600	1.66256900
O	-2.60476000	0.53330700	-1.25392600
C	-2.55583300	-0.56869600	-1.86575000
O	-1.74778300	-1.52002100	-1.66174000
Pd	-0.57611900	-1.71108300	-0.00116900
C	-2.57281400	-0.46266500	1.86631300
O	-2.19116500	-1.49793800	1.25514800
O	0.46723600	-2.26546500	1.66322300
O	0.83867900	-2.51438600	-1.26000700
C	1.68504300	-1.99629200	1.87267300
C	1.77218700	-1.92314700	-1.86833800
O	2.39310600	-1.15009100	1.26129600
O	2.19640200	-0.75031700	-1.65960600
C	1.10989900	3.48720500	-2.94672400
H	1.20999900	4.47648900	-2.48315100
H	2.05852600	3.23900900	-3.43009000
H	0.30402200	3.53483200	-3.68377500
C	-3.58907200	-0.79195400	-2.93411400
H	-4.47418900	-1.24738800	-2.47298000
H	-3.88700700	0.15692500	-3.38772700
H	-3.21048200	-1.47957100	-3.69521500
C	-3.61039200	-0.65637300	2.93610800
H	-3.52859600	-1.65262500	3.37832000
H	-3.51479800	0.11446600	3.70566000
H	-4.60333100	-0.56037700	2.47972600
C	2.36960000	-2.79339300	2.94717400
H	3.13421000	-2.19071400	3.44460400

H	1.64257400	-3.16716700	3.67284300
H	2.86342700	-3.65452700	2.48006300
C	2.47958300	-2.70686200	-2.93806300
H	3.28733800	-3.28338500	-2.47045100
H	1.79267900	-3.40825000	-3.41898500
H	2.92307600	-2.03493000	-3.67760300
C	1.23185900	3.45666500	2.93826900
H	0.32604100	3.84551000	3.41088600
H	1.89094800	3.00454800	3.68416300
H	1.76468900	4.29581200	2.47410800

7

E (M06/BS1) = -583.487004 au

H(M06/BS1) = -583.374176 au

G(M06/BS1) = -583.420218 au

E(M06/BS2//M06/BS1) = -584.9152203 au

Pd	0.00000400	-0.00001700	-0.00951100
O	1.76417700	-1.08387600	-0.01037000
C	2.43666900	-0.00009000	-0.00452000
O	1.76421400	1.08373900	-0.01045000
C	3.91784500	-0.00001200	0.03670900
H	4.24662600	0.00644700	1.08327400
H	4.31126700	-0.90219300	-0.44042300
H	4.31134200	0.89645600	-0.45107800
O	-1.76409600	1.08392400	-0.01029700
C	-2.43667000	0.00020800	-0.00446100
O	-1.76430200	-1.08368800	-0.01036900
C	-3.91785800	0.00007400	0.03664600
H	-4.24678200	-0.01756000	1.08303200
H	-4.31111400	0.90710300	-0.43129500
H	-4.31137600	-0.89133300	-0.46037400

6

E (M06/BS1) = -716.1635926 au

H(M06/BS1) = -715.996691 au

G(M06/BS1) = -716.059105 au

E(M06/BS2//M06/BS1) = -717.6612122 au

Pd	-0.34247200	0.11766100	-0.18549300
O	1.62224600	-1.44836100	1.41749800
C	1.66301100	-1.81590700	0.24934900
O	0.94988700	-1.32097300	-0.72591300
C	2.55964200	-2.94036500	-0.21888900
H	1.94748400	-3.79673700	-0.52601900
H	3.14646800	-2.63150300	-1.09069900
H	3.22803700	-3.24800700	0.58998500
N	1.20506100	1.41413700	-0.08233700
O	-2.11969500	-0.92163500	-0.19806100
C	-2.76447700	0.14351200	0.09380200
O	-2.08795400	1.21346500	0.22553900
C	-4.23382200	0.11533900	0.29634100
H	-4.44799000	-0.21060300	1.32173200
H	-4.65902300	1.11254400	0.15269200

H	-4.69624400	-0.60142500	-0.38907400
C	2.10540200	2.13440900	-0.00922800
C	3.22667900	3.04040000	0.08399000
H	2.87881000	4.07340400	-0.01668500
H	3.71959900	2.92148400	1.05426500
H	3.94666500	2.82519300	-0.71182800

5

E (M06/BS1) = -848.842010 au

H(M06/BS1) = -848.625729 au

G(M06/BS1) = -848.695633 au

E(M06/BS2//M06/BS1) = -850.4098366 au

Pd	-0.00139800	0.00702400	-0.00539600
O	2.31087800	1.28684100	-1.34889300
C	2.40083500	1.48387600	-0.14015600
O	1.55828900	1.06283000	0.75747200
C	3.53758000	2.28161000	0.46094600
H	3.15215500	3.22244200	0.87198100
H	4.00061900	1.73230500	1.28802800
H	4.28840200	2.50408000	-0.30250200
N	-1.13378500	1.67877900	-0.01515300
O	-1.56140700	-1.04885900	-0.76563600
C	-2.38957900	-1.48928800	0.13533300
O	-2.28949700	-1.30551300	1.34578500
C	-3.51418600	-2.31433300	-0.45081700
H	-3.18764000	-3.35960900	-0.52200900
H	-4.38838600	-2.27600200	0.20619000
H	-3.78300100	-1.97877500	-1.45688800
C	-1.79221400	2.62790000	-0.01863100
C	-2.61714300	3.81376700	-0.02287600
H	-2.21596400	4.54909800	0.68179700
H	-2.63363000	4.25075100	-1.02625500
H	-3.63940700	3.55561000	0.27139900
N	1.12812200	-1.66685400	0.00883600
C	1.77796600	-2.62162400	0.02524800
C	2.59077900	-3.81562500	0.04660000
H	3.54182100	-3.62618000	-0.46136000
H	2.79099900	-4.10987500	1.08179800
H	2.06764100	-4.63052300	-0.46345700

4

E (M06/BS1) = -848.8426212 au

H(M06/BS1) = -848.623375 au

G(M06/BS1) = -848.698593 au

E(M06/BS2//M06/BS1) = -850.4104197 au

Pd	-0.00637700	0.09794700	0.00007500
O	-2.06214000	-1.20300400	-1.66801900
C	-2.08152700	-1.70257100	-0.54731200
O	-1.32399700	-1.34765400	0.45060700
C	-3.00445700	-2.84684700	-0.19153000
H	-2.42347200	-3.77544100	-0.13228900
H	-3.46857500	-2.68952600	0.78766700

H	-3.77586200	-2.96181400	-0.95821200
N	-1.44734700	1.51429300	0.34071200
O	1.31648800	-1.34379100	-0.44975800
C	2.07621600	-1.69117300	0.54772600
O	2.03915800	-1.20526000	1.67460100
C	3.07623000	-2.76742600	0.18683800
H	4.05401800	-2.29942300	0.01745600
H	3.18353700	-3.46306500	1.02538800
H	2.79242400	-3.31253800	-0.71765500
C	-2.28217200	2.29121500	0.52465700
C	-3.32708600	3.26302000	0.75145100
H	-2.89625700	4.18936900	1.14452400
H	-3.84275600	3.47932900	-0.18971400
H	-4.05037900	2.86992400	1.47307700
N	1.43256600	1.51551100	-0.34261000
C	2.27061200	2.28877400	-0.52746500
C	3.32089900	3.25472900	-0.75469500
H	2.94270300	4.08186600	-1.36363300
H	3.67656300	3.64843200	0.20291300
H	4.15648100	2.77804200	-1.27713900

10

E (M06/BS1) = -1288.006619 au

H(M06/BS1) = -1287.625755 au

G(M06/BS1) = -1287.709122 au

E(M06/BS2//M06/BS1) = -1289.763701 au

Pd	0.51453300	1.12841100	-0.65710400
O	-0.05812700	1.67276400	2.25513900
C	-0.23472000	2.69303600	1.58946700
O	-0.08544400	2.79325800	0.30080400
C	-0.65571500	3.99545200	2.22588500
H	0.11469900	4.75746100	2.06051100
H	-1.57877600	4.36140800	1.76247500
H	-0.80974900	3.85955300	3.29951400
C	-2.45998700	1.15816100	-0.80098600
C	-1.65503000	-0.84982100	-0.01574600
C	-3.74898600	0.68163600	-0.80202400
H	-2.22721100	2.17485400	-1.10458200
C	-2.90995300	-1.42045200	0.02658400
H	-4.57686300	1.31098200	-1.11430800
H	-3.02737700	-2.43125500	0.40548500
N	-0.52249200	-1.60258900	0.39526900
C	0.41456400	-1.14453400	1.24443100
C	-0.11989100	-2.83152800	-0.10762300
C	1.08412900	-3.09865500	0.45368800
H	-0.71832900	-3.37566800	-0.82473900
H	1.75487600	-3.93840900	0.33261500
N	1.38719300	-2.04467000	1.29709400
N	-1.40795000	0.39830500	-0.43284000
C	-3.99455800	-0.63770100	-0.39318900
C	2.65566300	-1.88901400	2.03491200
H	2.45324400	-1.20921600	2.86976100
H	2.91221300	-2.87110400	2.44658100
C	3.72796500	-1.37464700	1.12809800

H	3.62393500	-0.33770100	0.79654400
C	4.76213000	-2.11862800	0.74560100
H	5.53986700	-1.72733800	0.09289600
H	4.87651000	-3.14907300	1.08330500
O	-5.25343200	-1.04726200	-0.41428800
C	-5.55118200	-2.37937000	-0.00207400
H	-6.62949600	-2.49198000	-0.11832900
H	-5.03390500	-3.10705700	-0.63843800
H	-5.27645500	-2.53006800	1.04864500
H	0.35498700	-0.19078200	1.78130700
O	2.52644100	1.48187900	-1.09343900
C	2.59550800	0.35174600	-1.68109600
O	1.53824100	-0.36368600	-1.70263300
C	3.85050800	-0.11454600	-2.32099000
H	3.95094100	-1.19797300	-2.19869300
H	3.81341000	0.10495900	-3.39513900
H	4.71360100	0.40177000	-1.88958000

9

E (M06/BS1) = -1420.686287 au

H(M06/BS1) = -1420.253841 au

G(M06/BS1) = -1420.350332 au

E(M06/BS2//M06/BS1) = -1422.512172 au

Pd	-0.65273800	-0.85199900	-0.38147800
O	0.02527500	-1.41528700	2.50252400
C	-0.06020900	-2.47011200	1.87005700
O	-0.32670300	-2.57391000	0.60448200
C	0.12410600	-3.80831200	2.54363800
H	-0.85354700	-4.29181700	2.66025000
H	0.74529400	-4.46952600	1.93084800
H	0.57408000	-3.67716700	3.53142300
C	2.19624400	-1.56326900	-0.91573500
C	2.05815700	0.52780100	0.02026000
C	3.56422100	-1.47045000	-1.01523200
H	1.66335600	-2.45275500	-1.24071000
C	3.42413600	0.71964600	-0.02482400
H	4.14998100	-2.28455300	-1.43123400
H	3.84781500	1.63315900	0.38097200
N	1.22812900	1.55976900	0.53930200
C	0.22804200	1.36336600	1.41676200
C	1.18320800	2.87083600	0.08460800
C	0.12565000	3.45446700	0.69936800
H	1.89158200	3.24702400	-0.64068200
H	-0.28016700	4.45448100	0.62077100
N	-0.44362300	2.50300500	1.52724800
N	1.43099700	-0.56893000	-0.42030100
C	4.20790700	-0.30642300	-0.57002300
C	-1.73369800	2.65818500	2.22749400
H	-1.74235400	1.92431400	3.04102500
H	-1.75061600	3.66168500	2.66600900
C	-2.85382400	2.45209200	1.25607800
H	-2.96202200	1.44117200	0.85231900
C	-3.66956300	3.43442900	0.88253100
H	-4.47777000	3.26694100	0.17364300

H	-3.56607000	4.44374800	1.28212400
O	5.52711300	-0.26967400	-0.68294200
C	6.22622400	0.89155400	-0.24037400
H	7.28145700	0.69223800	-0.43000600
H	5.91060200	1.77471800	-0.80864700
H	6.06946800	1.05377800	0.83275000
H	0.03264400	0.41749000	1.94012800
O	-2.54246300	-2.41166200	-2.00969900
C	-3.15714700	-1.91372200	-1.07064100
O	-2.64031000	-1.13467300	-0.16467000
C	-4.62785100	-2.17957300	-0.84149300
H	-4.74168100	-2.90219600	-0.02402500
H	-5.15368300	-1.26565600	-0.54669700
H	-5.07966500	-2.59800900	-1.74532300
C	-1.68180300	3.04943500	-2.67853000
H	-2.27043100	2.83515900	-3.57626000
H	-2.27200000	3.67872300	-2.00273500
H	-0.77083200	3.58618600	-2.96390300
N	-1.05385000	0.83509900	-1.46881800
C	-1.33618700	1.81702500	-2.00954800

8

E (M06/BS1) = -1420.686621 au

H(M06/BS1) = -1420.254035 au

G(M06/BS1) = -1420.351692 au

E(M06/BS2//M06/BS1) = -1422.514161 au

Pd	0.65397600	-0.94578500	0.49331700
O	0.34373200	-1.70727900	-2.41288800
C	0.33943400	-2.72274500	-1.71209200
O	0.45826400	-2.75176500	-0.42145500
C	0.21876500	-4.09542200	-2.32986300
H	1.21533500	-4.55008900	-2.39185500
H	-0.40523300	-4.75102700	-1.71450800
H	-0.19292300	-4.02014100	-3.34021300
C	-2.23020800	-1.55401900	0.65498300
C	-1.88880700	0.49767200	-0.32132900
C	-3.59256900	-1.37727400	0.64255200
H	-1.78185600	-2.46171100	1.04921200
C	-3.24111800	0.76917700	-0.38908700
H	-4.25846100	-2.14106300	1.03255000
H	-3.57914300	1.69010900	-0.85466200
N	-0.96558300	1.45783100	-0.80983600
C	0.10924900	1.16941400	-1.56238700
C	-0.91661400	2.79341800	-0.43972100
C	0.21272700	3.30307800	-0.98662400
H	-1.67446900	3.23782000	0.19074200
H	0.64138100	4.29501900	-0.94188400
N	0.82549400	2.27879100	-1.68548100
N	-1.36978600	-0.62195600	0.19456100
C	-4.12567200	-0.18889400	0.12209800
C	2.14653100	2.36674300	-2.33302300
H	2.21230700	1.51539600	-3.02026100

H	2.16624900	3.28842100	-2.92508100
C	3.22561000	2.34700300	-1.29890700
H	3.28980300	1.43929200	-0.69333000
C	4.06230900	3.36268000	-1.10950200
H	4.84654500	3.32252600	-0.35697700
H	4.00191000	4.27084800	-1.70978000
O	-5.44460200	-0.06747900	0.13583400
C	-6.03178300	1.12813100	-0.37167400
H	-7.10711500	1.01302800	-0.23179100
H	-5.67870800	2.00205900	0.18876900
H	-5.81129600	1.24657400	-1.43919800
H	0.32447400	0.18231900	-1.99203200
O	-0.24463900	0.07044000	3.16296000
C	0.31329900	0.97824000	2.55319600
O	0.84870100	0.87408800	1.37042300
C	0.47336300	2.36141600	3.14374700
H	1.47189500	2.44903500	3.59017900
H	0.38757300	3.13577900	2.37379500
H	-0.27142700	2.52417100	3.92819300
C	5.16457000	-1.75810000	1.19054200
H	5.29094800	-2.65501800	1.80517900
H	5.66186800	-1.91147100	0.22740800
H	5.62518500	-0.90598700	1.70028100
N	2.63362500	-1.30220600	0.80909700
C	3.75831500	-1.50402600	0.97964700

3TS

E (M06/BS1) = -1287.963174 au

H(M06/BS1) = -1287.587144 au

G(M06/BS1) = -1287.670430 au

E(M06/BS2//M06/BS1) = -1289.719277 au

Pd	-0.79077700	-1.02496200	-0.48963000
O	0.06230800	-1.50675500	2.53109900
C	-0.00411600	-2.60138600	1.84860300
O	-0.30604300	-2.66025400	0.63705800
C	0.30044000	-3.84855700	2.59972200
H	1.27812800	-3.75188900	3.08365500
H	-0.44639300	-3.97934800	3.39113700
H	0.29019700	-4.71323900	1.93437600
C	2.45084000	-1.22248600	-1.05900400
C	1.77621000	0.71943100	-0.04394700
C	3.76165600	-0.80354400	-1.08949100
H	2.15737400	-2.19194500	-1.45714600
C	3.06029700	1.23755800	-0.00946300
H	4.54527200	-1.42441700	-1.51381900
H	3.24959100	2.19534100	0.46548500
N	0.68667300	1.43855600	0.49969900
C	-0.38689600	0.79259800	1.04096900
C	0.49450400	2.81264800	0.47610400
C	-0.73495500	3.02433800	1.00301700
H	1.22237800	3.50042100	0.06772400
H	-1.29179400	3.93838800	1.16342700
N	-1.24542500	1.78251200	1.34227800
N	1.45777500	-0.46414200	-0.56485800

C	4.08147100	0.45848800	-0.56360900
C	-2.59498800	1.56455600	1.86895500
H	-2.64687300	0.49950100	2.13117500
H	-2.71974500	2.15119500	2.78780700
C	-3.61742000	1.93351900	0.84356800
H	-3.49034600	1.45997200	-0.13366600
C	-4.61392900	2.78348700	1.07125700
H	-5.35126600	3.01794300	0.30677900
H	-4.73734000	3.26927600	2.03963800
O	5.36080800	0.81800600	-0.61552900
C	5.73572500	2.08862700	-0.09591100
H	6.80940300	2.17680300	-0.26701300
H	5.21204200	2.89643000	-0.62206600
H	5.53015000	2.14634800	0.98004700
H	-0.16761000	-0.67989200	1.95273100
O	-2.59999300	-1.51119900	-1.68332800
C	-2.46439200	-0.36667500	-2.18840400
O	-1.47387800	0.35255100	-1.76996800
C	-3.38408400	0.17730200	-3.21725700
H	-3.32977400	-0.44096300	-4.12067000
H	-4.41453300	0.13134600	-2.84699400
H	-3.12408300	1.21026100	-3.46474200

2TS

E (M06/BS1) = -1287.968135 au

H(M06/BS1) = -1287.594467 au

G(M06/BS1) = -1287.678423 au

E(M06/BS2//M06/BS1) = -1289.727207 au

Pd	-0.46287500	0.86569000	-0.02641000
O	-1.00060200	2.97384000	1.88139800
C	-0.51065100	3.49784700	0.88818800
O	-0.12023200	2.85017500	-0.17926000
C	-0.26846200	4.98439100	0.78006600
H	0.81039200	5.18096100	0.78330800
H	-0.66800300	5.37427700	-0.16213000
H	-0.73138600	5.50174100	1.62462000
C	2.50739100	1.38137400	-0.31881700
C	1.89032400	-0.81744200	0.01479900
C	3.81545600	1.01192800	-0.51986600
H	2.17052900	2.41388900	-0.37209300
C	3.16670200	-1.29414200	-0.19328000
H	4.57881200	1.75395400	-0.73318200
H	3.37043300	-2.35958300	-0.15896200
N	0.81828000	-1.67270600	0.37041000
C	-0.49530000	-1.29555100	0.22897100
C	0.91162300	-2.75313200	1.21045500
C	-0.35998500	-3.06638600	1.58452300
H	1.85919900	-3.17653000	1.51360100
H	-0.72563000	-3.84878200	2.23618900
N	-1.19680000	-2.16175400	0.99171100
N	1.55046200	0.47515300	-0.04152300
C	4.16576500	-0.34719700	-0.46350100
C	-2.66969300	-2.21903400	1.11485600
H	-2.87641700	-2.25431800	2.19176900

H	-3.06931800	-1.27714200	0.72988300
C	-3.22577900	-3.40928000	0.39993900
H	-2.90811100	-4.38609700	0.76979500
C	-4.08352300	-3.31648000	-0.61075300
H	-4.49432300	-4.20324800	-1.08807800
H	-4.41184600	-2.35277800	-0.99851000
O	5.43703500	-0.64338400	-0.68106800
C	5.84371500	-2.00981700	-0.64563300
H	6.91453500	-2.00617500	-0.85079000
H	5.65911500	-2.44329400	0.34446800
H	5.32284000	-2.58815700	-1.41791800
H	-1.16168800	-0.92763000	-0.79635300
O	-2.31041500	-0.69934300	-1.64754600
C	-2.91278600	0.34271300	-1.26948500
O	-2.45402200	1.17167200	-0.41329000
C	-4.28570500	0.63357500	-1.79911800
H	-5.01929500	0.43271800	-1.00781100
H	-4.37060600	1.69185500	-2.06365400
H	-4.50923000	0.00386500	-2.66340700

1TS

E (M06/BS1) = -1420.645438 au

H(M06/BS1) = -1420.216426 au

G(M06/BS1) = -1420.316295 au

E(M06/BS2//M06/BS1) = -1422.470524 au

Pd	-0.88994900	-0.70249500	-0.12276200
O	-0.02316200	-1.15478900	2.91670400
C	-0.40729000	-2.24935900	2.34253900
O	-0.79217000	-2.32635700	1.15904700
C	-0.37878600	-3.46457400	3.20151200
H	0.61425700	-3.57565100	3.64947900
H	-1.09599000	-3.33799100	4.02074200
H	-0.63519500	-4.35247000	2.62126800
C	2.20046800	-1.70307400	-0.79639000
C	2.07163300	0.39817900	0.10351500
C	3.56882000	-1.61460600	-0.92441100
H	1.65835900	-2.59380000	-1.11011800
C	3.44179000	0.59593900	0.03744100
H	4.15416600	-2.42735200	-1.34448700
H	3.88415900	1.50876300	0.42452000
N	1.21291300	1.39175200	0.62993700
C	0.03562900	1.04957200	1.22518500
C	1.32578900	2.76520500	0.48081500
C	0.18950000	3.28973900	1.00102700
H	2.17485700	3.23876900	0.00695300
H	-0.14429600	4.31563900	1.08755200
N	-0.57039900	2.22665900	1.45649900
N	1.45114500	-0.70586700	-0.30162600
C	4.21137500	-0.43943500	-0.50360100
C	-1.92072600	2.35580000	2.01041100
H	-2.17597900	1.36721900	2.41474500
H	-1.89527600	3.07128000	2.84196800
C	-2.88332300	2.78607800	0.95076000
H	-2.92117200	2.14765800	0.06437500

C	-3.64269200	3.87278800	1.05299100
H	-4.34422300	4.15669400	0.27148100
H	-3.59870300	4.51774100	1.93126100
O	5.53542500	-0.40392300	-0.63848500
C	6.23269200	0.76360700	-0.22156200
H	7.28740600	0.56979700	-0.42216800
H	5.90553300	1.64054900	-0.79402400
H	6.09057800	0.94193000	0.85161700
H	-0.06849600	-0.35303000	2.26772000
O	-0.41257700	-0.55764400	-3.04808100
C	-0.70915300	0.54853200	-2.62143800
O	-1.00334500	0.82763300	-1.37360900
C	-0.79614700	1.77768300	-3.49517900
H	-0.32337800	1.57995400	-4.46124700
H	-1.84887700	2.03711800	-3.65964200
H	-0.31775700	2.63515500	-3.00985700
N	-2.73430600	-1.40907400	-0.82360000
C	-3.75037000	-1.76089300	-1.24843400
C	-5.01862700	-2.20644000	-1.77985100
H	-5.33622800	-3.11905600	-1.26559600
H	-5.77792100	-1.43137100	-1.63452300
H	-4.92052000	-2.41485000	-2.85003200

11

E (M06/BS1) = -1420.679732 au

H(M06/BS1) = -1420.247838 au

G(M06/BS1) = -1420.347527 au

E(M06/BS2//M06/BS1) = -1422.505566 au

Pd	0.92809600	-0.58558900	-0.12819000
O	0.21910700	-1.89100800	-2.97867000
C	-0.83586400	-1.83675300	-2.19748700
O	-0.82045900	-1.36313600	-1.05683100
C	-2.06807600	-2.40999100	-2.79510000
H	-2.22156600	-2.00061600	-3.79872100
H	-1.94567800	-3.49474100	-2.89697600
H	-2.92789300	-2.19537700	-2.15808900
C	-2.43770400	-0.91627700	2.14600500
C	-1.99930000	0.80579500	0.75063300
C	-3.79036900	-0.86120100	1.87810700
H	-2.04900800	-1.65801200	2.84298000
C	-3.33058000	0.96806600	0.38586100
H	-4.49348200	-1.54651200	2.34357100
H	-3.61684500	1.70954000	-0.35401600
N	-1.02246000	1.65241500	0.14052300
C	0.20303100	1.24621700	-0.27751700
C	-1.19789600	3.00121600	-0.14396600
C	-0.06054000	3.42094900	-0.73951400
H	-2.09573800	3.53461700	0.13558300
H	0.23998100	4.39339600	-1.10648300
N	0.78495100	2.32613100	-0.82116500
N	-1.53301600	-0.08644300	1.60595500
C	-4.25755600	0.10928700	0.98147800
C	2.11590000	2.39503400	-1.44381700
H	2.48747500	1.36775500	-1.51265600

H	1.98527200	2.78888800	-2.45975100
C	3.02956300	3.26294200	-0.64260500
H	3.22542700	2.92571300	0.37690200
C	3.57570400	4.37737300	-1.12067600
H	4.24689100	4.98908700	-0.52167200
H	3.37769800	4.71709800	-2.13795600
O	-5.57246600	0.13094800	0.74893600
C	-6.08241100	1.10296500	-0.15208700
H	-7.16249400	0.95080700	-0.18042400
H	-5.86489200	2.11903200	0.20138900
H	-5.66689000	0.96275100	-1.15823300
H	0.99723000	-1.50365000	-2.52454400
O	2.09859800	-0.60995100	2.62908500
C	2.83913400	0.01305900	1.87874500
O	2.62045000	0.24382600	0.61292600
C	4.12772900	0.63820900	2.36573200
H	4.54934200	0.03369400	3.17445600
H	4.85838900	0.75471500	1.55981600
H	3.90582700	1.63439100	2.76992800
N	1.73737000	-2.54046200	0.00020900
C	2.18958200	-3.60206200	0.07112600
C	2.75454800	-4.92864300	0.16010200
H	2.18014000	-5.61952600	-0.46505100
H	3.79382700	-4.91396400	-0.18338500
H	2.72546400	-5.27601600	1.19772700

12

E (M06/BS1) = -1288.031974 au

H(M06/BS1) = -1287.651486 au

G(M06/BS1) = -1287.736865 au

E(M06/BS2//M06/BS1) = -1289.790375 au

Pd	0.59247700	0.33243400	0.03041200
O	0.28169700	2.80316400	-1.62976100
C	0.81455300	3.14774600	-0.58433900
O	0.98192100	2.34628400	0.44864800
C	1.34719400	4.53756100	-0.35130900
H	0.91290100	4.96444200	0.55975200
H	2.43351400	4.49265100	-0.19899600
H	1.12837300	5.18252300	-1.20602000
C	-2.07990300	1.62325200	0.59577200
C	-2.14471600	-0.60755000	-0.01967800
C	-3.44991200	1.67500300	0.66658700
H	-1.45444200	2.48021800	0.82818700
C	-3.52257100	-0.65423100	0.01720400
H	-3.96217900	2.58952800	0.94894300
H	-4.04755800	-1.57453500	-0.21541300
N	-1.33606600	-1.70707500	-0.32535000
C	0.01949200	-1.53231900	-0.32499800
C	-1.66094000	-3.02467500	-0.61729400
C	-0.48251500	-3.65996400	-0.80081100
H	-2.67753100	-3.38663800	-0.66986400
H	-0.26561300	-4.69173300	-1.04412400
N	0.53482000	-2.72700900	-0.62398500
N	-1.42848600	0.49737100	0.24708800

C	-4.19698100	0.52419500	0.36325700
C	1.96769000	-3.06449500	-0.63833000
H	2.10066100	-3.81892600	-1.42376000
H	2.51728400	-2.16278900	-0.92473900
C	2.40283600	-3.57173200	0.69975400
H	1.88827000	-4.46201600	1.06855000
C	3.36479000	-2.99682000	1.41497900
H	3.68041500	-3.39305700	2.37746100
H	3.88257200	-2.10806300	1.05404700
O	-5.51484100	0.64039900	0.43281500
C	-6.32677500	-0.49071700	0.12812600
H	-7.35810600	-0.15207300	0.23207800
H	-6.15224300	-0.82852100	-0.90042200
H	-6.13472700	-1.30737400	0.83417500
H	2.52390700	2.09894900	0.82306800
O	3.49319300	1.81492600	0.77875000
C	3.61058700	0.68966000	0.13974900
O	2.65463300	-0.00055600	-0.25865800
C	5.01322400	0.24781700	-0.08880300
H	5.04032600	-0.65474700	-0.70325200
H	5.57647200	1.05139600	-0.57527100
H	5.49275200	0.05567900	0.87881500

13

E (M06/BS1) = -1191.727522 au

H(M06/BS1) = -1191.364706 au

G(M06/BS1) = -1191.449885 au

E(M06/BS2//M06/BS1) = -1193.441289 au

C	-2.30413300	1.69635000	-0.09913400
C	-2.05989600	-0.59310200	0.05650100
C	-3.67305100	1.58635000	-0.09156400
H	-1.81202300	2.66259900	-0.16517500
C	-3.42256100	-0.81246700	0.06886400
H	-4.30682500	2.46584100	-0.14880400
H	-3.82004800	-1.81934900	0.13913000
N	-1.11528800	-1.62500700	0.13788400
C	0.21127800	-1.29737600	0.15324700
C	-1.27850400	-2.99880800	0.24671500
C	-0.03126400	-3.51172200	0.33112300
H	-2.24459800	-3.48201000	0.25945200
H	0.30743500	-4.53438400	0.42798100
N	0.86856900	-2.45237000	0.28523700
N	-1.49493800	0.62240900	-0.02614200
C	-4.25534000	0.31102400	-0.00708500
C	2.33159600	-2.62579600	0.34717400
H	2.71955100	-1.80364400	0.95631200
H	2.51150400	-3.56316800	0.88518500
C	2.94323900	-2.65733700	-1.01595000
H	2.90886000	-1.71795100	-1.57096800
C	3.51041700	-3.74877500	-1.52156300
H	3.96149300	-3.75389600	-2.51156800
H	3.55231100	-4.68196100	-0.95860400
Pd	0.58420600	0.62095300	-0.06180200
O	2.79106200	1.04134200	1.87575200

C	3.27819000	0.72353500	0.79454000
O	2.59679100	0.40153000	-0.26736300
C	4.77143800	0.63410100	0.57281600
H	5.31142000	0.93785300	1.47359300
H	5.04864500	-0.39558000	0.31215400
H	5.07022800	1.26813100	-0.26953700
N	0.83947300	2.70338600	-0.32101300
C	1.04596000	3.83051400	-0.47536600
C	1.30281700	5.23850900	-0.67100300
H	0.72663400	5.60532000	-1.52640800
H	1.01233000	5.79869300	0.22346500
H	2.36871900	5.39810100	-0.86240600
O	-5.58020300	0.26290500	-0.00478000
C	-6.22377000	-1.00617100	0.06988200
H	-5.95611100	-1.62807900	-0.79293600
H	-5.96336400	-1.52053400	1.00275800
H	-7.29406800	-0.79791900	0.05343700

14

E (M06/BS1) = -1059.049047 au

H(M06/BS1) = -1058.738314 au

G(M06/BS1) = -1058.810666 au

E(M06/BS2//M06/BS1) = -1060.694657 au

C	-2.04016700	-1.87566300	0.20868600
C	-1.81299900	0.40996500	-0.06317800
C	-3.40692300	-1.76221400	0.28459200
H	-1.53614100	-2.83639700	0.28437800
C	-3.17246600	0.63078800	-0.00176000
H	-4.03595100	-2.63575500	0.42390900
H	-3.57199500	1.63528300	-0.09502500
N	-0.86041900	1.42035700	-0.23891600
C	0.44465000	1.03763500	-0.31301600
C	-0.96400200	2.80129200	-0.35094800
C	0.30234900	3.25534400	-0.49488400
H	-1.90722900	3.32766300	-0.32031600
H	0.68674500	4.26009800	-0.61025700
N	1.15174700	2.15308700	-0.48264700
N	-1.24517700	-0.80380500	0.03658600
C	-3.99518800	-0.49011000	0.17796900
C	2.62137200	2.21805100	-0.54212000
H	2.95813600	1.25692300	-0.94814600
H	2.88523600	3.00899300	-1.25325000
C	3.19410800	2.48025700	0.81294600
H	3.01815500	1.70262500	1.56059700
C	3.87749100	3.58082500	1.11164900
H	4.29505700	3.74419200	2.10275800
H	4.05416500	4.35932600	0.36877400
Pd	0.81042000	-0.86745500	-0.09670200
O	-5.31695100	-0.44286200	0.25636300
C	-5.97092400	0.81968300	0.15843800
H	-7.03671700	0.61019100	0.25497700
H	-5.65223800	1.48589400	0.96898100
H	-5.77445600	1.28482700	-0.81499500
O	1.60631600	-2.86816400	0.12165900

C	2.76362200	-2.37512900	-0.02555100
O	2.86435100	-1.10842800	-0.20151200
C	3.98295500	-3.22626500	0.00931100
H	3.87325700	-4.05444800	-0.69927200
H	4.87466500	-2.64281200	-0.23391100
H	4.09393500	-3.66228100	1.00905000

15

E (M06/BS1) = -1191.725924 au

H(M06/BS1) = -1191.363679 au

G(M06/BS1) = -1191.445752 au

E(M06/BS2//M06/BS1) = -1193.440917 au

C	-2.28366600	1.48317600	-0.41113200
C	-1.94074800	-0.76136000	0.04384000
C	-3.64390900	1.29947400	-0.45030700
H	-1.81427200	2.44865700	-0.58474300
C	-3.29039900	-1.04636900	0.02520200
H	-4.31611500	2.12763700	-0.65222400
H	-3.64224200	-2.05732100	0.19988600
N	-0.94684900	-1.71939200	0.27797500
C	0.35938700	-1.31369500	0.28674900
C	-1.03962700	-3.08245900	0.52761600
C	0.22998200	-3.51252200	0.69390900
H	-1.97861400	-3.61503200	0.56979400
H	0.62401500	-4.49824200	0.90213900
N	1.06962300	-2.41219500	0.55625800
N	-1.43618500	0.46662100	-0.16196000
C	-4.16897400	0.01561700	-0.22760700
C	2.53454900	-2.49579200	0.63909800
H	2.88160000	-1.52331500	1.00437200
H	2.77433300	-3.24534100	1.40194900
C	3.13069500	-2.85601300	-0.68306400
H	2.90467000	-2.18054800	-1.51219400
C	3.89301100	-3.92989700	-0.86566000
H	4.32918800	-4.16291800	-1.83441800
H	4.11793500	-4.61422200	-0.04723700
Pd	0.60060100	0.62702600	-0.10209600
O	1.04543100	3.03895400	1.54575200
C	0.76331400	3.41849600	0.40986400
O	0.51256100	2.63387900	-0.59533500
C	0.64952100	4.88620100	0.06331100
H	0.96258400	5.50675500	0.90751200
H	1.25694700	5.12379200	-0.81719600
H	-0.39137700	5.12346600	-0.19066700
N	2.64149700	0.71805800	-0.11746100
C	3.78886200	0.82997900	-0.19462600
C	5.22584400	0.93748000	-0.28402200
H	5.50119100	1.54683800	-1.15069000
H	5.62203900	1.40346900	0.62384300
H	5.66142100	-0.06162000	-0.39463800
O	-5.48853600	-0.10012200	-0.27721800
C	-6.07961100	-1.37932100	-0.06538900
H	-5.74083600	-2.09433700	-0.82460300
H	-5.84615000	-1.75354800	0.93855600

H	-7.15559000	-1.22869300	-0.15900400

16

E (M06/BS1) = -1059.047875 au

H(M06/BS1) = -1058.737036 au

G(M06/BS1) = -1058.808569 au

E(M06/BS2//M06/BS1) = -1060.692214 au

C	-1.35182500	-1.78788500	-0.39356600
C	-1.68870800	0.46698400	-0.00140200
C	-2.70304500	-2.03266100	-0.32438000
H	-0.62527700	-2.57475900	-0.58596700
C	-3.05603600	0.32841200	0.08641600
H	-3.10222700	-3.03362500	-0.45647000
H	-3.68669600	1.19070900	0.27757600
N	-1.00773800	1.69223300	0.13784600
C	0.33247100	1.62442500	0.02254100
C	-1.36637700	3.01874000	0.37830200
C	-0.21278100	3.73765200	0.40150800
H	-2.39131000	3.33625500	0.50690900
H	-0.05050200	4.79478700	0.55519200
N	0.82989100	2.84297000	0.17168000
N	-0.84083100	-0.55547900	-0.23442300
C	-3.57967700	-0.96264800	-0.08130400
C	2.29042800	2.91600700	0.11379500
H	2.59754500	3.81514200	-0.42921000
H	2.68881300	2.96319800	1.13398200
C	2.76819900	1.66446500	-0.61135900
H	2.77108700	1.71833200	-1.70117900
C	3.37080800	0.60053900	0.01357700
H	3.88280700	-0.16580800	-0.56442600
H	3.51689900	0.59207200	1.09401100
Pd	1.22185200	-0.04032100	-0.27820600
O	-4.87126300	-1.25518500	-0.02796300
C	-5.80752000	-0.20607300	0.20401200
H	-6.79174700	-0.67477000	0.17742900
H	-5.64301000	0.25059900	1.18734100
H	-5.74033600	0.55459200	-0.58287400
O	1.91253300	-1.98006200	-0.64668800
C	2.16755400	-2.57849300	0.47307000
O	2.07488200	-2.04275400	1.58187000
C	2.58709300	-4.02195300	0.31961700
H	3.48079500	-4.08981100	-0.31166800
H	2.79164700	-4.47412400	1.29398700
H	1.79437100	-4.58716700	-0.18559300

4TS

E (M06/BS1) = -1059.015331 au

H(M06/BS1) = -1058.710572 au

G(M06/BS1) = -1058.780619 au

E(M06/BS2//M06/BS1) = -1060.657918 au

C	-1.51604700	-1.96122500	-0.30075000
C	-1.81930600	0.30813500	0.00271800
C	-2.87005300	-2.18795200	-0.22792700

H	-0.80038800	-2.76668500	-0.44900900
C	-3.19134500	0.19056300	0.08906800
H	-3.28188000	-3.18833400	-0.31975800
H	-3.81282300	1.06793200	0.23587600
N	-1.13776500	1.53520200	0.11010800
C	0.20960400	1.51561500	-0.06543700
C	-1.54272700	2.81403600	0.48025100
C	-0.41761700	3.56570600	0.53163400
H	-2.57450800	3.07665500	0.66570000
H	-0.27794700	4.61118200	0.76968500
N	0.65383500	2.74048700	0.19340800
N	-0.98715800	-0.73101800	-0.18462800
C	-3.73223900	-1.09715100	-0.02847600
C	2.06961000	3.11337400	0.18793400
H	2.14108800	4.11816400	-0.24067200
H	2.41598400	3.18500600	1.23052400
C	2.94227400	2.16622500	-0.58320600
H	3.71119500	2.67650300	-1.16790900
C	2.88947400	0.81851200	-0.63909400
H	3.57862500	0.34713600	-1.34730500
H	2.95019000	0.02125500	0.37094500
Pd	1.05684500	-0.19302700	-0.32489400
O	-5.02936100	-1.37005800	0.03427800
C	-5.94744800	-0.30000000	0.23631700
H	-6.93766300	-0.75645300	0.25669400
H	-5.75446200	0.20249900	1.19189600
H	-5.89129600	0.42152500	-0.58761600
O	1.95271700	-2.10927100	-0.30137800
C	2.95911400	-2.16093400	0.47288700
O	3.48129400	-1.15704300	1.03635300
C	3.58542500	-3.50796600	0.69914000
H	4.37360600	-3.65735800	-0.04948200
H	4.04720800	-3.55842500	1.68901200
H	2.84632200	-4.30471500	0.57994200

17

E (M06/BS1) = -1059.053458 au

H(M06/BS1) = -1058.742409 au

G(M06/BS1) = -1058.814597 au

E(M06/BS2//M06/BS1) = -1060.696247 au

C	-1.42041200	-2.02724800	-0.28183600
C	-1.80593900	0.21928500	-0.00352600
C	-2.76367800	-2.31314200	-0.20137200
H	-0.68163900	-2.81278100	-0.42854800
C	-3.17624400	0.04958600	0.08823200
H	-3.13376200	-3.33091500	-0.28090000
H	-3.83492100	0.89972700	0.23079100
N	-1.20024600	1.49092200	0.09096200
C	0.15476700	1.59012000	-0.02009400
C	-1.74627000	2.75283400	0.30544800
C	-0.70586600	3.61663500	0.32234700
H	-2.80571400	2.92725600	0.42600100
H	-0.68007500	4.68915900	0.45838500
N	0.45614200	2.87661700	0.11997900

N	-0.93144600	-0.77942300	-0.18517100
C	-3.66799300	-1.25644700	-0.01302300
C	1.80849200	3.42838300	0.07839900
H	1.82296300	4.20694100	-0.69743100
H	1.98531400	3.94171900	1.03479000
C	2.88691900	2.42543600	-0.17951500
H	3.86949900	2.90271700	-0.24480000
C	2.79822700	1.10201700	-0.33441400
H	3.72061800	0.54454500	-0.53392900
H	2.72004100	-0.89514800	1.47592100
Pd	1.16055600	-0.02776300	-0.29851100
O	-4.95577300	-1.58174000	0.05838300
C	-5.91405900	-0.54726100	0.24791700
H	-6.88482900	-1.04287400	0.29108300
H	-5.73227300	-0.01429200	1.18933600
H	-5.89847100	0.15762400	-0.59236100
O	2.24025500	-1.90937500	-0.55298600
C	2.97130900	-2.36949200	0.32554200
O	3.20719400	-1.74979100	1.46466200
C	3.66048500	-3.67961100	0.18111100
H	4.28678900	-3.65703200	-0.71700000
H	4.27055200	-3.91460800	1.05521000
H	2.90733100	-4.46105100	0.03278300

3

E (M06/BS1) = -962.7565037 au

H(M06/BS1) = -962.464188 au

G(M06/BS1) = -962.532778 au

E(M06/BS2//M06/BS1) = -964.3516295 au

C	-1.36568000	2.02579900	-0.00391300
C	-1.62511700	-0.25379200	-0.00353600
C	-2.72656200	2.22694100	-0.00223500
H	-0.67324800	2.86505500	-0.00437000
C	-3.00702800	-0.17161000	-0.00187100
H	-3.15307800	3.22552800	-0.00163400
H	-3.62023600	-1.06662500	-0.00136200
N	-0.95264800	-1.49406000	-0.00472600
C	0.41118600	-1.51296000	-0.00211900
C	-1.44240100	-2.79658100	-0.00802200
C	-0.35926500	-3.60631100	-0.00593900
H	-2.49592300	-3.03591300	-0.01116800
H	-0.28368400	-4.68509200	-0.00640900
N	0.76993900	-2.79260400	-0.00204600
N	-0.80451700	0.80490400	-0.00403300
C	-3.57322900	1.10786000	-0.00050400
C	2.15072400	-3.27065300	0.00204800
H	2.27187800	-3.91995600	0.88119400
H	2.27833400	-3.91717100	-0.87802500
C	3.18536600	-2.19146700	0.00763400
H	4.19719000	-2.60855500	0.01190800
C	3.03701300	-0.86443100	0.00762700
H	3.93815100	-0.24444100	0.01187700
Pd	1.34477500	0.18288700	0.00126900
O	-4.88164700	1.34939300	0.00274700

C	-5.77807500	0.24464100	0.01002700
H	-6.78113200	0.67296400	0.02023800
H	-5.64960000	-0.36828300	-0.89037000
H	-5.63206200	-0.37048000	0.90663500
N	2.33566600	2.05694300	-0.00025100
C	2.88263300	3.07628800	-0.00135400
C	3.56568700	4.35012200	-0.00315200
H	2.84644600	5.15894000	-0.16647800
H	4.06556900	4.50580100	0.95840000
H	4.31433000	4.37090200	-0.80155500

18

E (M06/BS1) = -1763.562543 au

H(M06/BS1) = -1762.986435 au

G(M06/BS1) = -1763.092515 au

E(M06/BS2//M06/BS1) = -1765.537545 au

C	-2.86180400	-1.94068100	-0.73643500
C	-2.73564800	0.36990200	-0.78232300
C	-4.22346100	-1.89737500	-0.56595500
H	-2.31189900	-2.87549700	-0.80744100
C	-4.09766800	0.51933400	-0.61477600
H	-4.80843900	-2.80818400	-0.48523500
H	-4.54577100	1.50680000	-0.57206400
N	-1.84723500	1.44442500	-0.90971900
C	-0.50402000	1.18799600	-0.97590600
C	-2.10124100	2.79833100	-1.07365800
C	-0.89582400	3.37962400	-1.25328100
H	-3.09585400	3.22032400	-1.05581500
H	-0.62617100	4.41285000	-1.42461500
N	0.06912600	2.37874900	-1.18986600
N	-2.12010000	-0.82131400	-0.84079200
C	-4.86438300	-0.64856800	-0.49525200
C	1.49371900	2.61768100	-1.47439700
H	2.04233300	1.76654600	-1.05397200
H	1.63439000	2.59138200	-2.56247600
C	1.95351800	3.91942100	-0.90686800
H	1.77763900	4.07585700	0.15998000
C	2.55154200	4.85383100	-1.63992900
H	2.90665300	5.78302200	-1.20056100
H	2.71981100	4.71848600	-2.70831200
Pd	-0.06559000	-0.76287900	-0.82118300
O	-6.17598200	-0.66417600	-0.31461600
C	-6.87637200	0.57431100	-0.22655500
H	-7.92374100	0.31340500	-0.07194800
H	-6.51574400	1.16473200	0.62471300
H	-6.77234400	1.14545500	-1.15659600
O	0.03066200	-2.92186900	1.38363000
C	0.09400400	-3.45712500	0.27034000
O	0.08933600	-2.83103400	-0.85947400
C	0.12573000	-4.96055100	0.14218200
H	-0.89816600	-5.32403500	-0.01739200
H	0.72523200	-5.27367300	-0.71791200
H	0.51027200	-5.41411800	1.06005000
C	2.76667700	-1.27637400	-1.57170000

C	2.67493700	-0.23799600	0.47514400
C	4.13788700	-1.34123000	-1.52155300
H	2.21883300	-1.67352800	-2.42151300
C	4.04629800	-0.26320800	0.62853200
H	4.70366700	-1.79048600	-2.33204400
H	4.48782400	0.12235800	1.54240800
N	1.88363000	0.37500400	1.48557000
C	0.79213000	-0.16963800	2.04971100
C	2.05166500	1.66547900	1.97247900
C	1.02323700	1.89040500	2.82686400
H	2.88215900	2.28672300	1.66340700
H	0.76630700	2.76112800	3.41430300
N	0.26355200	0.73590100	2.86455500
N	2.02217900	-0.71086000	-0.59619500
C	4.81054000	-0.82305800	-0.40499800
C	-1.00845000	0.55582500	3.59487700
H	-0.97343100	-0.43809400	4.05484600
H	-1.02353100	1.30274800	4.39477800
C	-2.17518600	0.70973300	2.67108900
H	-2.31640100	-0.09017400	1.93582900
C	-3.01407600	1.73967600	2.73152800
H	-3.86768600	1.82339800	2.06069100
H	-2.89070500	2.53375900	3.46789400
O	6.12977000	-0.91318600	-0.40343200
C	6.85664000	-0.40874600	0.71615400
H	7.90858100	-0.58387900	0.48906100
H	6.67951900	0.66600800	0.84066400
H	6.58264500	-0.94931500	1.62980400
H	0.43046100	-1.19476700	1.86826200

5TS

E (M06/BS1) = -1763.528488 au

H(M06/BS1) = -1762.954641 au

G(M06/BS1) = -1763.061336 au

E(M06/BS2//M06/BS1) = -1765.501418 au

C	-2.94038800	-2.29590000	0.11036800
C	-3.10701700	-0.13826800	-0.69396200
C	-4.30629900	-2.43931900	0.09737800
H	-2.28076900	-3.09748100	0.43112500
C	-4.48616700	-0.17817900	-0.74030200
H	-4.77524300	-3.36617600	0.41324600
H	-5.05613400	0.68161100	-1.07593800
N	-2.34808600	0.97261900	-1.08019100
C	-0.98552400	0.91869300	-0.95879500
C	-2.73902200	2.17987900	-1.64119100
C	-1.60109600	2.87095100	-1.86325800
H	-3.77102000	2.43447400	-1.83415900
H	-1.43697800	3.85279300	-2.28671500
N	-0.53474600	2.08215800	-1.44163400
N	-2.34010200	-1.15635500	-0.28121400
C	-5.10532100	-1.36503000	-0.32922900
C	0.86263100	2.51730700	-1.59060100
H	1.48318800	1.70513700	-1.20098700
H	1.07098200	2.60612600	-2.66431400

C	1.09262900	3.81535500	-0.88752900
H	0.83749300	3.84193700	0.17545400
C	1.57319200	4.89159700	-1.50333200
H	1.75016300	5.82296300	-0.97044900
H	1.82036300	4.87749600	-2.56510500
Pd	-0.29265100	-0.73509700	-0.17231200
O	-6.41673800	-1.55858900	-0.31044800
C	-7.27605600	-0.50029000	-0.72526500
H	-8.29112400	-0.88687400	-0.62803600
H	-7.15256600	0.37617900	-0.07790600
H	-7.08319900	-0.23060100	-1.77061200
O	1.03572700	-2.17189900	2.47034200
C	0.62297900	-3.03852500	1.58988700
O	0.11237000	-2.72382400	0.50282000
C	0.80910600	-4.46047600	1.98200900
H	1.87839500	-4.66113200	2.11389100
H	0.32353800	-4.63924800	2.94759800
H	0.39593700	-5.12599900	1.22255100
C	2.31456400	-1.61258500	-1.84540500
C	2.86344500	-0.21907300	-0.10999900
C	3.63603500	-1.90924300	-2.08489400
H	1.52079800	-2.05198300	-2.44587600
C	4.22096700	-0.45482200	-0.25051700
H	3.92902600	-2.58577500	-2.88232800
H	4.92958600	-0.00634100	0.43873800
N	2.37471400	0.65541000	0.88921100
C	1.12889800	0.48419000	1.42218200
C	2.98727700	1.80511900	1.37253200
C	2.09098400	2.37419300	2.21295100
H	3.96918300	2.12789000	1.05390300
H	2.14150000	3.28804500	2.79173100
N	0.97479500	1.55271300	2.22540300
N	1.91915000	-0.75815800	-0.88320500
C	4.62024900	-1.31811100	-1.27634100
C	-0.26521800	1.86473400	2.94585600
H	-0.84317300	0.93278700	2.97826400
H	-0.00648700	2.15081500	3.97258700
C	-1.01026900	2.95958700	2.24968500
H	-1.39516700	2.71939100	1.25334100
C	-1.18978000	4.16916800	2.77275600
H	-1.73019600	4.94969700	2.24188700
H	-0.80722100	4.42080300	3.76244400
O	5.88148700	-1.64184500	-1.54071700
C	6.91414200	-1.07567500	-0.74090200
H	7.85049800	-1.46859400	-1.13925300
H	6.91163900	0.01843800	-0.81812200
H	6.80458800	-1.37906300	0.30749800
H	0.90187400	-1.23399600	2.12284800

19

E (M06/BS1) = -1763.556446 au

H(M06/BS1) = -1762.979683 au

G(M06/BS1) = -1763.087775 au

E(M06/BS2//M06/BS1) = -1765.53054 au

C	-3.17366700	-0.06418100	-1.65143100
C	-2.91313300	-0.84839200	0.50007500
C	-4.45583500	-0.55125800	-1.71665900
H	-2.71869900	0.44517300	-2.49737800
C	-4.18907500	-1.37543700	0.54070400
H	-5.05816700	-0.43438200	-2.61215700
H	-4.54774800	-1.90010700	1.41955800
N	-2.00106500	-0.97357700	1.56175000
C	-0.72190200	-0.50768300	1.42035700
C	-2.16045900	-1.58915200	2.79450200
C	-0.96362100	-1.50226000	3.41176700
H	-3.09042400	-2.02929700	3.12298400
H	-0.63923100	-1.85025100	4.38274800
N	-0.08940200	-0.84688700	2.55119500
N	-2.40483500	-0.19461700	-0.55362200
C	-4.98709600	-1.21672400	-0.59948400
C	1.32101900	-0.57443600	2.89103000
H	1.87379400	-0.56891300	1.94480400
H	1.38457500	0.42470900	3.34176000
C	1.87485000	-1.61038800	3.81187100
H	1.89322800	-2.63426500	3.43363000
C	2.35203900	-1.31867400	5.01838200
H	2.78431800	-2.08209600	5.66102900
H	2.33798200	-0.29991800	5.40602000
Pd	-0.41458200	0.47298300	-0.27446400
O	-6.22911500	-1.66567100	-0.71207800
C	-6.81599400	-2.35480300	0.38852400
H	-7.82591200	-2.61699700	0.07166300
H	-6.25412000	-3.26798600	0.61915800
H	-6.86373100	-1.70667400	1.27182800
C	1.32484200	-2.12571800	-2.50522600
C	2.53112800	-0.76241600	-1.15492900
C	2.36970200	-3.01654900	-2.63275300
H	0.37877600	-2.31282000	-3.01153300
C	3.65078800	-1.58485300	-1.18139400
H	2.28423100	-3.91649800	-3.23525200
H	4.53775700	-1.34807600	-0.60301400
N	2.56626200	0.43590900	-0.37798400
C	1.46036700	1.04153800	0.13144300
C	3.70970900	1.11588800	0.02702000
C	3.29453300	2.15130500	0.78822300
H	4.70195000	0.82872500	-0.28952000
H	3.84450000	2.94106500	1.28267900
N	1.91092300	2.08421700	0.84577000
N	1.38994900	-0.99634100	-1.78385000
C	3.56612800	-2.74542900	-1.95508400
C	1.09371500	3.04751800	1.59726500
H	0.07170500	2.64586300	1.60848500
H	1.46153100	3.06682100	2.63134200
C	1.16788800	4.40815400	0.98450500
H	0.79603400	4.49932600	-0.03832000
C	1.66100200	5.46229500	1.62770200
H	1.70005400	6.44709300	1.16775700
H	2.03915200	5.37964700	2.64708100
O	4.54881700	-3.63726900	-2.09024600
C	5.78073100	-3.39608700	-1.42392500

H	6.43118400	-4.23290300	-1.68255100
H	6.23463900	-2.45799800	-1.76792600
H	5.63972100	-3.36506700	-0.33598700
O	-0.35877500	1.73500700	-2.06342200
C	-0.93719700	2.81751200	-2.17739800
C	-0.79388000	3.68786800	-3.37232500
H	-1.77738200	4.02285400	-3.71665900
H	-0.22316200	4.58179200	-3.09182500
H	-0.26839000	3.15599600	-4.16690200
O	-1.73073500	3.32055600	-1.25155700
H	-1.78122100	2.72021100	-0.47914900

20

E (M06/BS1) = -1534.586892 au

H(M06/BS1) = -1534.079363 au

G(M06/BS1) = -1534.174000 au

E(M06/BS2//M06/BS1) = -1536.449200 au

C	-1.74046000	-2.71798800	-0.50353800
C	-2.88207700	-0.79891700	0.03231700
C	-2.90809900	-3.38906800	-0.77160800
H	-0.77974500	-3.20612900	-0.64285000
C	-4.11302900	-1.37134800	-0.22175200
H	-2.89930600	-4.42240100	-1.10398900
H	-5.02293600	-0.78647400	-0.13781800
N	-2.74171200	0.54132900	0.42846500
C	-1.49431300	1.09506600	0.47908700
C	-3.68484500	1.40456300	0.97036800
C	-3.00067900	2.49668700	1.37157200
H	-4.73648800	1.16604300	1.03533100
H	-3.33274500	3.40425000	1.85777200
N	-1.65917600	2.28637500	1.07092300
N	-1.70932900	-1.44205700	-0.07371800
C	-4.12948000	-2.71355800	-0.61986900
C	-0.60165300	3.19976900	1.53443800
H	0.34761400	2.78290300	1.17929200
H	-0.75938700	4.17861400	1.06407100
C	-0.62014500	3.31027200	3.02457800
H	-0.44786400	2.38320900	3.57493000
C	-0.82693200	4.46033600	3.65901200
H	-0.81908700	4.52345500	4.74465500
H	-1.00369800	5.38776900	3.11351900
Pd	-0.00000600	-0.14467500	0.00022800
O	-5.22848700	-3.40380700	-0.88835400
C	-6.49437800	-2.76210900	-0.76031100
H	-7.23957300	-3.52691800	-0.98134900
H	-6.64079000	-2.39039400	0.26086400
H	-6.58612200	-1.93966200	-1.47981200
C	1.74099600	-2.71779700	0.50393800
C	2.88218000	-0.79865600	-0.03240600
C	2.90879500	-3.38870800	0.77173800
H	0.78039700	-3.20608500	0.64353400
C	4.11328400	-1.37087100	0.22143300
H	2.90019600	-4.42202400	1.10417300
H	5.02308000	-0.78588200	0.13716000

N	2.74158400	0.54156000	-0.42866700
C	1.49414600	1.09518600	-0.47891100
C	3.68444700	1.40461600	-0.97133700
C	3.00007100	2.49661800	-1.37248000
H	4.73607300	1.16612100	-1.03667600
H	3.33190600	3.40408900	-1.85901000
N	1.65870700	2.28635400	-1.07120000
N	1.70954900	-1.44188700	0.07407000
C	4.13004000	-2.71302800	0.61968400
C	0.60105900	3.19993700	-1.53412600
H	-0.34811200	2.78294100	-1.17886800
H	0.75897500	4.17860900	-1.06346100
C	0.61912400	3.31102900	-3.02422300
H	0.44595500	2.38435500	-3.57494100
C	0.82661100	4.46120400	-3.65823300
H	0.81852400	4.52478900	-4.74384700
H	1.00424800	5.38827300	-3.11240100
O	5.22922500	-3.40305800	0.88803800
C	6.49496000	-2.76112900	0.75969900
H	7.24036100	-3.52579200	0.98056600
H	6.64110100	-2.38938100	-0.26150300
H	6.58669200	-1.93866000	1.47918200

2

E (M06/BS1) = -1667.262605 au

H(M06/BS1) = -1666.704203 au

G(M06/BS1) = -1666.812531 au

E(M06/BS2//M06/BS1) = -1669.190530 au

C	-3.36674200	0.46166800	-1.52338400
C	-3.03369800	-0.90761200	0.29748700
C	-4.65121800	0.00230700	-1.68307900
H	-2.94836500	1.20906900	-2.19183100
C	-4.30961400	-1.43245100	0.23026400
H	-5.28643000	0.37302000	-2.48155800
H	-4.64427500	-2.17692100	0.94434200
N	-2.09699300	-1.30771400	1.26609700
C	-0.85507300	-0.73249200	1.29188500
C	-2.20548800	-2.28255000	2.24751400
C	-1.01424200	-2.30524100	2.88155000
H	-3.10125300	-2.86303600	2.41259700
H	-0.65999600	-2.91285800	3.70320500
N	-0.20485400	-1.34231700	2.29120800
N	-2.55580900	0.01845500	-0.54442100
C	-5.14486300	-0.96341100	-0.79167300
C	1.20916700	-1.17839400	2.65019200
H	1.47870700	-0.13840400	2.43317800
H	1.29585400	-1.31558000	3.73405600
C	2.05671600	-2.15690900	1.90141700
H	1.86576700	-2.22441900	0.82621600
C	2.99869100	-2.90349000	2.46860200
H	3.61322600	-3.58096500	1.87903300
H	3.19852800	-2.86018700	3.53921400
Pd	-0.58122600	0.65238500	-0.11337400
O	-6.39148300	-1.37028700	-0.98786300

C	-6.94644300	-2.34742400	-0.11182700
H	-7.96180800	-2.52326600	-0.46883400
H	-6.37384800	-3.28154500	-0.15736700
H	-6.97813500	-1.97258200	0.91817200
C	1.68889700	-1.59731300	-2.57866700
C	2.60609500	-0.31805700	-0.95228400
C	2.80609800	-2.40268800	-2.65486500
H	0.83231000	-1.79008600	-3.22308700
C	3.78465800	-1.05601200	-0.91781200
H	2.86180400	-3.23854300	-3.34669200
H	4.56259800	-0.83885800	-0.19262700
N	2.45152800	0.76997700	-0.03833100
C	1.26089100	1.21353200	0.44208400
C	3.49288800	1.50168400	0.52549800
C	2.92808200	2.40791100	1.35202700
H	4.52748900	1.33836300	0.26034200
H	3.36344900	3.18190400	1.96995000
N	1.55779000	2.20922800	1.29247200
N	1.57417800	-0.55124200	-1.74527500
C	3.88720000	-2.12948200	-1.80553400
C	0.58750700	3.01364300	2.04923000
H	-0.36617700	2.47058800	2.00632100
H	0.91894000	3.03963700	3.09472500
C	0.47521700	4.39167100	1.48248800
H	0.11395600	4.46036800	0.45355200
C	0.79238900	5.48497900	2.16961200
H	0.69291100	6.47945100	1.74026800
H	1.15600400	5.42619200	3.19592600
O	4.94409400	-2.93910300	-1.89431900
C	6.05256800	-2.70167500	-1.03765400
H	6.79260700	-3.46459000	-1.28404800
H	6.47969000	-1.70602200	-1.21304700
H	5.76312500	-2.80132000	0.01645500
N	-0.49599600	2.17979300	-1.56933100
C	-0.40999200	3.03287100	-2.34467900
C	-0.30159600	4.10474900	-3.30611200
H	-1.29786900	4.39778600	-3.65223500
H	0.18440900	4.96854700	-2.84049300
H	0.29482900	3.77752800	-4.16369900

21

E (M06/BS1) = -1763.564176 au

H(M06/BS1) = -1762.987257 au

G(M06/BS1) = -1763.093101 au

E(M06/BS2//M06/BS1) = -1765.538472 au

C	0.71674800	-1.91773000	-1.41751700
C	2.40920600	-0.45232400	-0.86546300
C	1.61792100	-2.91700200	-1.69003300
H	-0.35050300	-2.07215100	-1.55015300
C	3.39530000	-1.38593400	-1.11241900
H	1.28640100	-3.89275600	-2.03158100
H	4.44172200	-1.12904000	-0.98703200
N	2.68165100	0.85881400	-0.45336000
C	1.63182300	1.68890200	-0.17912400

C	3.88816700	1.52031200	-0.26522300
C	3.56250200	2.76943600	0.13374300
H	4.85113700	1.05771600	-0.42601300
H	4.18704300	3.61453800	0.38995700
N	2.17566500	2.85005300	0.19334400
N	1.09216000	-0.69769400	-0.98642900
C	2.98909100	-2.66159200	-1.52532600
C	1.44679100	4.07542100	0.57322200
H	0.63180300	3.76592800	1.23512700
H	2.14600600	4.68538300	1.15546800
C	0.94691300	4.81425000	-0.62567800
H	0.16387200	4.31165800	-1.19637400
C	1.40254300	6.01356400	-0.97548400
H	1.01575800	6.53990100	-1.84556100
H	2.17714000	6.52125300	-0.39986100
Pd	-0.15150800	0.87646300	-0.42120300
O	3.81489500	-3.66266400	-1.78801000
C	5.21868600	-3.45886400	-1.64368500
H	5.68389400	-4.41360300	-1.89086600
H	5.57175800	-2.68645600	-2.33733400
H	5.46687300	-3.18525200	-0.61117300
O	-1.61763200	1.77759200	2.07828800
C	-1.74457900	2.62195200	1.18953300
O	-1.19594600	2.56544800	0.01450100
C	-2.57574400	3.86587100	1.38553900
H	-2.91834500	3.94029600	2.42071100
H	-1.99369400	4.75620200	1.11794000
H	-3.44417100	3.83624000	0.71637900
C	-2.95872000	0.54796900	-1.49243900
C	-2.56156500	-1.11726600	0.02560200
C	-4.24280000	0.10516000	-1.70360300
H	-2.57508800	1.42298100	-2.01054200
C	-3.83320100	-1.64108100	-0.09945500
H	-4.90258200	0.61308200	-2.40059500
H	-4.12674800	-2.48745200	0.51367900
N	-1.64364300	-1.75164500	0.91192600
C	-0.88194000	-1.11405000	1.81832900
C	-1.31663700	-3.10166400	0.91211600
C	-0.32733700	-3.25743000	1.82454400
H	-1.79759000	-3.80573100	0.24656900
H	0.23133900	-4.13347700	2.12553500
N	-0.08129200	-2.01414800	2.37706800
N	-2.09742000	-0.06093500	-0.64937700
C	-4.70511500	-1.01770600	-1.00176600
C	1.01182100	-1.72209100	3.32412800
H	0.77540200	-0.76117900	3.79437800
H	0.99264700	-2.49877500	4.09620900
C	2.31436500	-1.69622700	2.59115300
H	2.44610500	-0.87063400	1.88667600
C	3.26229100	-2.61289300	2.75997900
H	4.20294700	-2.57065900	2.21513500
H	3.13904100	-3.43586300	3.46447200
O	-5.95171200	-1.39945600	-1.23351800
C	-6.46803100	-2.53144200	-0.53656500
H	-7.49114000	-2.65682700	-0.89215000
H	-5.88396600	-3.42972000	-0.76979300

H	-6.47312900	-2.35117400	0.54489700
H	-0.96226000	-0.04543400	2.05431400

6TS

E (M06/BS1) = -1763.524304 au

H(M06/BS1) = -1762.950302 au

G(M06/BS1) = -1763.056231 au

E(M06/BS2//M06/BS1) = -1765.498496 au

C	0.88946800	-2.08156100	-0.89409700
C	2.59008700	-0.51471000	-0.87479600
C	1.73951800	-3.04975800	-1.36341800
H	-0.15913000	-2.29619100	-0.71089800
C	3.52214000	-1.41871700	-1.34277000
H	1.38379400	-4.05624500	-1.55954900
H	4.54837400	-1.10954600	-1.51054800
N	2.88143700	0.82067300	-0.59869900
C	1.87372200	1.61329100	-0.12713900
C	4.05939600	1.54900600	-0.71530900
C	3.75789000	2.79918700	-0.30476600
H	4.98726100	1.12328000	-1.06895600
H	4.37053100	3.68812600	-0.23644800
N	2.41612000	2.81857100	0.06609300
N	1.30068300	-0.82221700	-0.63766300
C	3.08853000	-2.72644500	-1.59175800
C	1.72504100	4.03889100	0.52110300
H	0.98689700	3.72768100	1.26592900
H	2.47748300	4.65827900	1.02141400
C	1.09748600	4.76350000	-0.62505800
H	0.29848700	4.23229800	-1.14705800
C	1.47056700	5.98392000	-0.99890600
H	0.99094700	6.49920400	-1.82826500
H	2.26656800	6.52013200	-0.48134500
Pd	0.13527800	0.70152400	0.07591200
O	3.86310300	-3.70160500	-2.03809000
C	5.24187800	-3.43303900	-2.28478900
H	5.66632300	-4.37115700	-2.64369600
H	5.35497000	-2.65988200	-3.05391700
H	5.74754000	-3.12810100	-1.36096300
O	-2.00175200	1.58455100	2.32182600
C	-1.66352000	2.56067600	1.54229000
O	-0.84838500	2.45656800	0.60344800
C	-2.31861600	3.86709400	1.81407100
H	-2.31793400	4.07021000	2.88935700
H	-1.81064200	4.66666300	1.26934300
H	-3.36434400	3.81459100	1.48756800
C	-2.59643600	0.74558700	-1.85435000
C	-2.70791100	-0.92243300	-0.29891800
C	-3.86079000	0.45987800	-2.31829000
H	-2.00757500	1.55243900	-2.28827400
C	-3.99022100	-1.29501700	-0.66752100
H	-4.30964500	1.02329100	-3.13117800
H	-4.50951500	-2.08207200	-0.12958500
N	-2.03130200	-1.58237300	0.75723400
C	-1.08124900	-0.92872000	1.48826500

C	-2.14360800	-2.91341100	1.13518200
C	-1.22593100	-3.09706600	2.11510200
H	-2.82692700	-3.60513200	0.66167300
H	-0.95939600	-3.97942200	2.68245300
N	-0.59774800	-1.87864200	2.31000300
N	-2.00429400	0.05310000	-0.86666900
C	-4.57922200	-0.58835900	-1.72126600
C	0.48018500	-1.65887800	3.28199800
H	0.71805100	-0.58858400	3.22808700
H	0.09458700	-1.87644000	4.28606500
C	1.66659900	-2.51080700	2.96650200
H	2.13552900	-2.34337700	1.99317600
C	2.14516100	-3.42867300	3.80137400
H	3.01746700	-4.02920400	3.55316800
H	1.68546400	-3.60640100	4.77412900
O	-5.79702100	-0.82475200	-2.20180300
C	-6.56453600	-1.87824900	-1.63102000
H	-7.49845400	-1.90642000	-2.19392700
H	-6.04504000	-2.83927800	-1.73181900
H	-6.77885500	-1.67699600	-0.57409300
H	-1.54120700	0.71515500	2.04076400

22

E (M06/BS1) = -1763.542953 au

H(M06/BS1) = -1762.966661 au

G(M06/BS1) = -1763.075080 au

E(M06/BS2//M06/BS1) = -1765.518714 au

C	2.31450900	-1.51772900	-0.95360800
C	2.96860000	0.64617400	-0.47263200
C	3.50801400	-1.78281300	-1.57478500
H	1.53392100	-2.27098600	-0.89434800
C	4.20160100	0.47408400	-1.07032600
H	3.70216800	-2.75407000	-2.01927300
H	4.91303400	1.29217100	-1.10437700
N	2.55766900	1.86579100	0.07885900
C	1.30295000	1.95256700	0.60951300
C	3.19746900	3.09904400	0.12751500
C	2.31512000	3.94776800	0.69954800
H	4.20180200	3.26448200	-0.23412200
H	2.39680600	5.00035800	0.93410600
N	1.16591300	3.22295400	0.99482400
N	2.03679000	-0.32342600	-0.38826100
C	4.48510000	-0.77557000	-1.63434200
C	-0.06820000	3.80570400	1.54558500
H	-0.45997300	3.08613700	2.27358300
H	0.21375400	4.71458500	2.08818000
C	-1.05587900	4.09460700	0.46120700
H	-1.37207100	3.23125800	-0.13016100
C	-1.53926000	5.30917900	0.22027600
H	-2.27123000	5.48623100	-0.56472000
H	-1.22955700	6.17402600	0.80751000
Pd	0.26469500	0.21288900	0.52775400
O	5.61985900	-1.08647400	-2.24038700
C	6.64313300	-0.09917900	-2.34562800

H	7.47001800	-0.58417200	-2.86531300
H	6.29354000	0.76022900	-2.93005800
H	6.97280500	0.22589700	-1.35181300
O	-1.42774900	-0.01057400	3.37867800
C	-2.01954700	0.71618400	2.46134700
O	-1.52487200	0.96443200	1.35506000
C	-3.36039100	1.22412900	2.84275000
H	-3.38904700	1.47667200	3.90595000
H	-3.61822600	2.08950600	2.22795200
H	-4.09851400	0.43223900	2.66244900
C	-2.14437200	0.88900500	-2.51649200
C	-2.34910500	-0.96416100	-1.23192400
C	-3.49178200	0.89977000	-2.81310200
H	-1.48731900	1.65537600	-2.92607000
C	-3.72044800	-1.05918200	-1.43364700
H	-3.92937600	1.65888200	-3.45555100
H	-4.30501700	-1.83008500	-0.94124200
N	-1.70875100	-1.92472000	-0.39100200
C	-0.62993900	-1.64656500	0.38545300
C	-2.08754900	-3.25299500	-0.24149700
C	-1.22413100	-3.80232500	0.64103300
H	-2.90257700	-3.69114600	-0.80012300
H	-1.14243600	-4.80788900	1.03133800
N	-0.33963000	-2.80178100	1.01337400
N	-1.55547700	-0.03606100	-1.74292800
C	-4.30667800	-0.09883800	-2.26275000
C	0.71182600	-2.98552600	2.02547900
H	1.31016800	-2.06372000	2.02383300
H	0.23163700	-3.07714200	3.00892300
C	1.55133600	-4.18628200	1.73417500
H	2.09617800	-4.18292300	0.78721200
C	1.65555300	-5.21372900	2.57221500
H	2.28760500	-6.07038000	2.34991500
H	1.11665300	-5.23183700	3.51984500
O	-5.60543100	-0.04920300	-2.56431000
C	-6.46656500	-1.03958500	-2.02002100
H	-7.46132400	-0.82212000	-2.41205100
H	-6.16043500	-2.04459100	-2.33726500
H	-6.48573700	-0.98430600	-0.92417400
H	-0.54143900	-0.29274300	3.07473200

23

E (M06/BS1) = -1534.568849 au

H(M06/BS1) = -1534.061699 au

G(M06/BS1) = -1534.156975 au

E(M06/BS2//M06/BS1) = -1536.432499 au

C	2.64131100	-1.30325100	-1.05770600
C	2.81187400	0.68886300	0.08774300
C	4.00563700	-1.42431600	-1.13509600
H	1.98769900	-2.02258100	-1.54080900
C	4.19208400	0.64499300	0.09326500
H	4.46654400	-2.25360300	-1.66249200
H	4.76718700	1.45424200	0.52979100
N	2.08980000	1.81805700	0.50238100

C	0.73903300	1.84906800	0.26780800
C	2.57065400	3.08580800	0.80794500
C	1.50371200	3.90817800	0.75081200
H	3.60685100	3.29399600	1.03112800
H	1.42146400	4.97511400	0.90650600
N	0.39765500	3.13746600	0.40266100
N	2.03336900	-0.28674100	-0.41159900
C	4.81007300	-0.45456400	-0.51413100
C	-0.90475000	3.74102000	0.07066800
H	-1.48786100	2.95667800	-0.42552100
H	-1.41263300	4.03241900	0.99935800
C	-0.73257600	4.92064500	-0.82965600
H	-0.24556000	4.72780300	-1.78746600
C	-1.15956100	6.13866900	-0.50951600
H	-1.05188400	6.97859800	-1.19188700
H	-1.64456100	6.33891600	0.44617400
Pd	-0.00079000	-0.05736000	-0.02852300
O	6.11943300	-0.63829300	-0.57966300
C	6.98472100	0.32250400	0.02124500
H	7.99707700	-0.05003100	-0.13793200
H	6.87165300	1.30077100	-0.46085200
H	6.78690800	0.40358300	1.09664600
C	-2.69858200	1.16649700	0.90368400
C	-2.79887200	-0.81620300	-0.26477200
C	-4.06479200	1.29095300	0.89291700
C	-4.17539300	-0.76893200	-0.36136300
H	-4.55722200	2.11651100	1.39723600
H	-4.72173400	-1.57181800	-0.84409400
N	-2.05132300	-1.94519300	-0.63605300
C	-0.71660900	-1.96077000	-0.32783200
C	-2.50151900	-3.22272100	-0.94748000
C	-1.43034300	-4.03255000	-0.81873600
H	-3.52105900	-3.44433300	-1.22780800
H	-1.33304300	-5.09898000	-0.97026300
N	-0.35211800	-3.24507600	-0.42096800
N	-2.05182700	0.15375600	0.29234700
C	-4.82896700	0.32843500	0.21301300
C	0.90964000	-3.82286800	0.07920500
H	1.39573700	-4.34686600	-0.75433200
H	1.54291200	-2.98781300	0.39201200
C	0.66191500	-4.73193900	1.24247800
H	0.10777000	-5.65140500	1.04584900
C	1.11053100	-4.46555800	2.46534400
H	0.93839000	-5.14653200	3.29586400
H	1.67807500	-3.55997600	2.68191300
O	-6.13940300	0.51554100	0.19365800
C	-6.96477400	-0.43754100	-0.47240000
H	-7.98523700	-0.06640900	-0.37307100
H	-6.69822200	-0.50569000	-1.53377100
H	-6.88216600	-1.42139800	0.00440200
H	-2.07653900	1.87694800	1.43752000

24

E (M06/BS1) = -1667.250888 au

H(M06/BS1) = -1666.692614 au
G(M06/BS1) = -1666.794802 au
E(M06/BS2//M06/BS1) = -1669.179825 au

N	1.54792000	0.68124700	-1.45927000
C	2.62932200	0.94683500	-1.76869200
C	3.97126800	1.31157900	-2.15498900
H	4.12311100	1.10612900	-3.21944500
H	4.12654800	2.37985400	-1.96784000
H	4.69630900	0.73465700	-1.57089600
C	-2.43078000	-1.40649600	0.86314500
C	-2.91850500	0.79612800	0.36870300
C	-3.64692500	-1.58119700	1.47270300
H	-1.70686500	-2.21492200	0.81507700
C	-4.16403500	0.71968300	0.95886800
H	-3.91874400	-2.53403200	1.91623000
H	-4.81348300	1.58780300	0.98224800
N	-2.42176300	1.97737200	-0.19641800
C	-1.16652600	1.97155100	-0.73213200
C	-2.98266300	3.24714100	-0.27117000
C	-2.05018000	4.02616900	-0.86230700
H	-3.97425400	3.48379700	0.08600500
H	-2.06530400	5.07653800	-1.11953400
N	-0.95103100	3.22277000	-1.14407000
N	-2.05792800	-0.23822200	0.29753500
C	-4.54572800	-0.50316900	1.52280800
C	0.31176300	3.70904900	-1.71645600
H	0.66547700	2.92932600	-2.40169400
H	0.08260800	4.59861800	-2.31335300
C	1.31118700	4.00875700	-0.64444700
H	1.49368000	3.20419500	0.07451000
C	1.96463600	5.16327200	-0.55679600
H	2.70724200	5.34030800	0.21794800
H	1.78841700	5.97371400	-1.26422700
Pd	-0.24403300	0.16188800	-0.61508400
O	-5.70640900	-0.72521400	2.11914700
C	-6.65318400	0.33702000	2.21273900
H	-7.52001500	-0.08350700	2.72344200
H	-6.24587400	1.16797300	2.80087000
H	-6.94623500	0.68457000	1.21505700
C	2.25145200	0.74470200	2.41108800
C	2.30619500	-1.12879300	1.14373400
C	3.62679300	0.77708600	2.51999200
H	1.64756400	1.51363800	2.89156000
C	3.69276500	-1.21680300	1.17467600
H	4.13771300	1.56001900	3.07374800
H	4.21052700	-1.99763100	0.62540900
N	1.58197000	-2.07575700	0.35750000
C	0.52326300	-1.74074300	-0.42095700
C	1.89277100	-3.42112400	0.20541400
C	1.00067600	-3.92258900	-0.67787400
H	2.68739300	-3.89692700	0.76337700
H	0.86484000	-4.92200600	-1.06908100
N	0.17178100	-2.87508400	-1.05184000
N	1.57493500	-0.20103700	1.74024800
C	4.37343000	-0.23056800	1.89439900

C	-0.87173500	-2.98953600	-2.08160700
H	-1.40512600	-2.02940400	-2.08903000
H	-0.38008200	-3.10493300	-3.05625400
C	-1.78820500	-4.13728700	-1.80983900
H	-2.34692100	-4.10606300	-0.87146300
C	-1.94097200	-5.15297700	-2.65484000
H	-2.62851700	-5.97021700	-2.44923600
H	-1.38863200	-5.19877100	-3.59377100
O	5.70043200	-0.16036200	2.01521600
C	6.49191400	-1.14698900	1.36799200
H	7.52946000	-0.90000900	1.59845800
H	6.26142000	-2.14981800	1.74932000
H	6.34189100	-1.11837300	0.28082600

7TS

E (M06/BS1) = -1534.513749 au

H(M06/BS1) = -1534.008915 au

G(M06/BS1) = -1534.104766 au

E(M06/BS2//M06/BS1) = -1536.375806 au

C	2.97473100	1.10974400	1.06845500
C	3.09847100	-0.94938200	0.00161100
C	4.27637100	0.99455100	1.49068100
H	2.36051000	1.97477900	1.30695700
C	4.40697200	-1.15342800	0.37116400
H	4.74125900	1.77540000	2.08413500
H	4.93219000	-2.05378500	0.06931800
N	2.31981900	-1.82105400	-0.76026100
C	1.06564600	-1.38546800	-1.03037800
C	2.51123700	-3.07412300	-1.32740000
C	1.34568200	-3.38116600	-1.94584800
H	3.43836900	-3.62304300	-1.24592200
H	1.05704500	-4.25584700	-2.51282000
N	0.46489900	-2.31821900	-1.76131000
N	2.39120900	0.14756200	0.33171300
C	5.01647500	-0.14927000	1.14055700
C	-0.93143100	-2.24582800	-2.23379200
H	-1.10922600	-1.19867700	-2.51646000
H	-0.99896800	-2.85514400	-3.14139700
C	-1.88504200	-2.69986500	-1.17688000
H	-1.78496900	-2.20355100	-0.20694700
C	-2.82409200	-3.61798300	-1.38036500
H	-3.52735400	-3.89372500	-0.59656400
H	-2.93611400	-4.12068800	-2.34116500
Pd	0.45876300	0.30616100	-0.33362200
O	6.26491000	-0.19814600	1.57038700
C	7.06911000	-1.32894000	1.23711100
H	8.04095400	-1.14777000	1.69687100
H	6.63276700	-2.24738000	1.64695000
H	7.18445100	-1.41305300	0.15014200
C	-2.15734000	-1.33074900	2.22962100
C	-2.75329900	0.41952600	0.91925800
C	-3.42396100	-1.87610600	2.17504500
H	-1.37134000	-1.82875500	2.79623400
C	-4.06026900	-0.02837400	0.76925200

H	-3.67143000	-2.80084000	2.68926200
H	-4.76262700	0.50903500	0.13979200
N	-2.36068100	1.62780000	0.26365100
C	-1.12846700	1.82024300	-0.29290100
C	-3.16801200	2.73440500	0.08672700
C	-2.42095200	3.64821700	-0.58482700
H	-4.17798600	2.79028000	0.46910400
H	-2.65034000	4.65742600	-0.90171700
N	-1.19662400	3.06243900	-0.81764500
N	-1.80667200	-0.18869800	1.61701900
C	-4.40495800	-1.21504000	1.42321400
C	-0.07349700	3.75518200	-1.45910800
H	0.65148500	2.97696000	-1.73022500
H	-0.43900300	4.22113900	-2.38256200
C	0.51720100	4.77064800	-0.53528700
H	0.90503100	4.38188600	0.40986000
C	0.57148100	6.06895700	-0.81658800
H	1.01324400	6.78634600	-0.12843900
H	0.18006200	6.46369900	-1.75473400
O	-5.60827400	-1.78828900	1.37107700
C	-6.62896500	-1.15626800	0.61026800
H	-7.51897400	-1.77630300	0.72740500
H	-6.83343300	-0.14702500	0.98929900
H	-6.35400600	-1.10900100	-0.45118500

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