Supporting Information

Regioselective [2+2] and [4+2] Cycloaddition Reactivity in an asymmetric Niobium(bis-imido) Moiety towards Unsaturated Organic Molecules

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Content

A. General Considerations.

Unless otherwise noted, all reactions were performed using standard Schlenk line techniques or in an MBraun inert atmosphere box under an atmosphere of purified nitrogen (<1 ppm O_2/H_2O). Glassware, cannulae, and aluminiumoxide were stored in an oven at *ca*. 160 ºC. *n*-Pentane, *n*-hexane, Et_2O, THF, toluene, benzene and CH_2Cl_2 were purified by passage through a column of activated alumina, stored over 3 or 4 Å molecular sieves, and degassed prior to use.[1] Deuterated solvents (C_6D_6, C_7D_8) and hexamethyldisiloxane (HMDSO) were dried over sodium/benzophenone, vacuum transferred to a storage flask containing activated molecular sieves, and degassed by three freeze-pump-thaw cycles before being stored in the dry box. *N,N'-bis*-(2,6-diisopropylphenyl)-β-diketiminate (BDI),[2] Li(BDI)·Et_2O,[3] (BDI)pyCl_2Nb(N^{t}Bu)[4] and (BDI)$(Me)_2$Nb(N^{t}Bu)[4] were prepared using literature procedures. For the mono-aza-butadiene part of the described molecules the abbreviation MAD is used. The preparation of (MAD)Nb(N^{t}Bu)(NAr)(THF)[5] and (MAD)Nb(N^{t}Bu)(NAr)(OEt_2)[6] has previously been reported. All other reagents were acquired from commercial sources and used as received. NMR spectra were recorded on Bruker AVQ-400, AVB-400 and DRX-500 spectrometers. Chemical shifts were measured relative to residual solvent peaks, which were assigned relative to an external TMS standard set at 0.00 ppm. ^{1}H and ^{13}C NMR assignments were further confirmed by ^{1}H-^{1}H (COSY, NOESY) or ^{1}H-^{13}C (HSQC and HMBC) correlation experiments where appropriate. NMR multiplicities are abbreviated as follows: s, singlet; d, doublet; t, triplet; qu, quartet; quin, quintet; sex, sextet; sept, septet; m, multiplet; virt, virtual; br, broad. Elemental analyses and High Resolution Mass Spectrometry for complexes which did not pass EA, were determined at the College of Chemistry, University of California, Berkeley. The X-ray structural determinations were performed at CHEXRAY, University of California, Berkeley on Bruker SMART 1000 or SMART APEX diffractometers.

B. Synthesis and characterization of compounds 2-6

(2) (MAD)Nb(N$^{i\mathrm{Pr}}$Ar)(κ^2-*N,O*)(^{t}BuN-C(H)($^{p\text{-}Cl}$Ar)=C(H)-C(Ar)-O): Stirring at room temperature an orange solution of (MAD)Nb(N^{t}Bu)(NAr)(OEt_2) (150 mg, 0.23 mmol) in benzene (5 ml) with (E)-3-(4-chlorophenyl)-1-phenylprop-2-en-1-one (1.1 equiv., 61 mg) overnight resulted in a color change to yellow. After removal of all volatile compounds under reduced pressure, the crude residue was extracted using a minimum amount of hexanes and subsequently filtered at room temperature. Yellow crystalline material was directly obtained from the saturated hexanes solution at room temperature after 24 h in 75% yield (142 mg). Crystals suitable for XRD have been obtained from diethyl ether (-40°C).

^{1}H NMR (400 MHz, C_6D_6, 298K): δ(ppm) 7.45 (d, 2 H, NAr, $^3J_{HH}$ = 8.34 Hz), 7.23-7.00 (m, 11 H, NAr), 6.95-6.90 (m, 2 H, NAr), 6.76 (d, 1 H, *H*C(CMe)Nb , $^4J_{HH}$ = 1.58 Hz), 6.12 (d, 1 H, OC(Ph)=C*H*, $^3J_{HH}$ = 5.30 Hz), 5.07 (d, 1 H, C(Ph)=C-C*H*, $^3J_{HH}$ = 5.30 Hz), 4.46 (br s, 1 H, Nb=NArC*H*Me_2), 4.04 (br s, 1 H, Nb=NArC*H*Me_2), 3.49 (sept, 1 H, NArC*H*Me_2, $^3J_{HH}$ = 7.26 Hz), 2.87 (d, 3 H, CHC(*Me*)Nb, $^4J_{HH}$ = 1.58

Hz), 2.47 (sept, 1 H, NArC*H*Me$_2$, $^3J_{HH}$ = 7.26 Hz), 1.57 (s, 3 H, HC(C(*Me*)NAr), 1.46 (br s, 6 H, Nb=NArCH*Me*$_2$), 1.15 (s, 9 H, NbN^{t}Bu), 1.11 (br s, 3 H, Nb=NArCH*Me*$_2$), 1.04 (br s, 3 H, Nb=NArCH*Me*$_2$), 1.00 (d, 3 H, NArCH*Me*$_2$, $^3J_{HH}$ = 7.26 Hz), 0.97 (d, 3 H, NArCH*Me*$_2$, $^3J_{HH}$ = 7.26 Hz), 0.82 (d, 3 H, NArCH*Me*$_2$, $^3J_{HH}$ = 7.26 Hz), 0.80 (d, 3 H, NArCH*Me*$_2$, $^3J_{HH}$ = 7.26 Hz).

^{13}C {^{1}H} NMR (125 MHz, C_6D_6, 298K): δ(ppm) 185.57 (C_{quart}, (HC(*C*(Me)=NAr)), 167.33 (C_{quart}, NbO-*C*(Ph)=C-C), 152.29 (C_{quart}), 143.94 (C_{quart}), 141.51 (C_{quart}, Ar), 141.36 (C_{quart}), 138.72 (C_{quart}), 137.17 (CH, Ar), 134.04 (C_{quart}), 131.42 (CH, (H*C*(C(Me)NAr), 129.12 (CH, Ar), 127.98 (CH, Ar), 126.64 (CH, Ar), 125.76 (CH, Ar), 124.14 (CH, Ar), 123.71 (CH, Ar), 123.59 (CH, Ar), 97.08 ($C_{(sp2)}$H, OC(Ph)=*C*H), 62.24 (*C*(CH$_3$)$_3$, Nb-N^{t}Bu, C_α), 59.64 ($C_{(sp3)}$H, C(Ph)=C-*C*H), 33.45 (CH$_3$, (HC(C(*Me*)Nb), 33.39 (CH$_3$, Nb-N^{t}Bu, C_β), 29.12 (CH, *C*HMe$_2$ of C=N*Ar*), 28.60 (CH, *C*HMe$_2$ of C=N*Ar*), 25.06 (CH$_3$, CH*Me*$_2$ of C=N*Ar*), 24.81 (CH$_3$, CH*Me*$_2$ of C=N*Ar*), 23.53 (CH$_3$, CH*Me*$_2$ of C=N*Ar*), 23.43 (CH$_3$, CH*Me*$_2$ of C=N*Ar*), 22.53 (CH$_3$, (HC(C(*Me*)=NAr)). *C*$_{quart}$/*C*H of Nb=NAr and *C*H$_3$/*C*H of Nb=NArCHMe$_2$ not observed due to line broadening. Anal. Calcd. for $C_{48}H_{61}ClN_3NbO$; C: 69.93; H: 7.46; N: 5.10. Found: C: 70.16; H: 7.23; N: 5.33.

(3) [(MAD)Nb(N($^{i\text{Pr}}$Ar))(μ_2-O)]$_2$: Heating an orange solution of 150 mg (0.23 mmol) of (MAD)Nb(N^{t}Bu)(NAr)(OEt$_2$) in benzene (5 ml) with 4-bromo-benzaldehyde (1.3 equiv., 55 mg) to 80°C for 14 h resulted in a slow color change to red. The solution was allowed to cool to room temperature and all volatile compounds were removed under reduced pressure. The crude residue was extracted with THF/ hexanes and cooled to -40°C for several days.

^{1}H NMR (400 MHz, C_6D_6, 298K): δ(ppm) 7.12 (d, 1 H, NAr, $^3J_{HH}$ = 8.34 Hz), 7.03-6.93 (m, 4 H, NAr), 6.72 (d, 1 H, *H*C(CMe)Nb , $^4J_{HH}$ = 1.52 Hz), 4.46 (sept, 1 H, Nb=NArC*H*Me$_2$, $^3J_{HH}$ = 7.2 Hz), 3.85 (sept, 1 H, NArC*H*Me$_2$, $^3J_{HH}$ = 7.26 Hz, sept), 3.68 (1 H, Nb=NArC*H*Me$_2$, $^3J_{HH}$ = 7.5 Hz), 3.01 (sept, 1 H, NArC*H*Me$_2$, $^3J_{HH}$ = 7.26 Hz), 2.52 (d, 3 H, CHC(*Me*)Nb, $^4J_{HH}$ = 1.58 Hz), 1.50 (d, 3 H, NArCH*Me*$_2$, $^3J_{HH}$ = 7.26 Hz), 1.45 (d, 3 H, NArCH*Me*$_2$, $^3J_{HH}$ = 7.26 Hz), 1.40 (d, 3 H, NArCH*Me*$_2$, $^3J_{HH}$ = 7.26 Hz), 1.38 (s, 3 H, HC(C(*Me*)NAr), 1.31 (d, 3 H, NArCH*Me*$_2$, $^3J_{HH}$ = 7.26 Hz), 1.12 (d, 3 H, NArCH*Me*$_2$, $^3J_{HH}$ = 7.26 Hz), 0.97 (d, 3 H, NArCH*Me*$_2$, $^3J_{HH}$ = 7.26 Hz), 0.87 (d, 3 H, NArCH*Me*$_2$, $^3J_{HH}$ = 7.26 Hz), 0.83 (d, 3 H, NArCH*Me*$_2$, $^3J_{HH}$ = 7.26 Hz).

^{13}C {^{1}H} NMR (125 MHz, C_6D_6, 298K): δ(ppm) 184.4 (C_{quart}, (HC(*C*(Me)=NAr)),145.1 (C_{quart}), 143.3 (C_{quart}, Ar), 142.1 (C_{quart}), 141.8 (C_{quart}), 140.2 (C_{quart}), 136.01 (CH, (H*C*(C(Me)NAr), 127.7 (CH, Ar), 124.7 (CH, Ar), 123.8 (CH, Ar), 122.8 (CH, Ar), 122.4 (CH, Ar), 122.4 (CH, Ar), 30.4 (CH$_3$, (HC(C(*Me*)Nb), 29.8 (CH, *C*HMe$_2$ of C=N*Ar*), 29.4 (CH, *C*HMe$_2$ of Nb=N*Ar*), 28.6 (CH, *C*HMe$_2$ of C=N*Ar*), 28.4 (CH$_3$, CH*Me*$_2$ of Nb=N*Ar*), 25.6 (CH$_3$, CH*Me*$_2$), 25.5 (CH$_3$, CH*Me*$_2$), 25.0 (CH$_3$, CH*Me*$_2$), 24.3 (CH$_3$, CH*Me*$_2$), 23.9 (CH$_3$, CH*Me*$_2$), 23.5 (CH$_3$, CH*Me*$_2$), 23.3 (CH$_3$, CH*Me*$_2$), 23.0 (CH$_3$, CH*Me*$_2$), 22.0 (CH$_3$, (HC(C(*Me*)=NAr)). Anal. Calcd. for $C_{58}H_{82}N_4Nb_2O_2$; C: 66.15; H: 7.85; N: 5.32. Found: C: 66.06; H: 7.56; N: 5.54.

(4) (κ^2-*N*,*C*)(MAD+PhCCPh+N($^{i\text{Pr}}$Ar))Nb(N^{t}Bu): Heating an orange solution of 150 mg (0.23 mmol) of (MAD)Nb(N^{t}Bu)(NAr)(THF) in benzene (5 ml) with 1,2-diphenylethyne (1.3 equiv., 227 mg) to 80°C for 18 h resulted in a slow color change to red. After removal of all volatile compounds under

reduced pressure, the crude residue was extracted with a minimum amount of hexanes and after filtration cooled to -40°C for 3 days. A red crystalline material suitable for XRD was obtained in 80% yield (140 mg). The analogues reaction using (MAD)Nb(N^{t}Bu)(NAr)(OEt$_2$) was completed within 30 min at room temperature.

^{1}H NMR (400 MHz, C_6D_6, ppm): δ(ppm) 7.25-7.21 (m, 3 H, Ar) ,7.13 (t, 1 H, Ar, $^3J_{HH}$ = 7.14 Hz), 7.05-6.76 (m, 12 H, Ar), 4.49 (s, 1 H, *H*C(C(Me)NAr), 4.07 (sept, 1 H, C*H*Me$_2$, $^3J_{HH}$ = 6.87 Hz), 3.87 (sept, 1 H, C*H*Me$_2$, $^3J_{HH}$ = 6.87 Hz), 3.66 (sept, 1 H, C*H*Me$_2$, $^3J_{HH}$ = 6.87 Hz), 2.99 (s, 3 H, CHC(*Me*)Nb), 2.39 (sept, 1 H, C*H*Me$_2$, $^3J_{HH}$ = 6.69 Hz), 1.85 (s, 3 H, HC(C(*Me*)NAr), 1.54 (d, 3 H, CH*Me*$_2$, $^3J_{HH}$ = 7.02 Hz), 1.51 (d, 3 H, CH*Me*$_2$, $^3J_{HH}$ = 6.73 Hz), 1.51 (d, 3 H, CH*Me*$_2$, $^3J_{HH}$ = 6.80 Hz), 1.27 (d, 3 H, CH*Me*$_2$, $^3J_{HH}$ = 6.64 Hz), 1.11 (s, 9 H, ^{t}Bu), 0.98 (d, 3 H, CH*Me*$_2$, $^3J_{HH}$ = 6.74 Hz), 0.89 (d, 3 H, CH*Me*$_2$, $^3J_{HH}$ = 6.74 Hz), 0.59 (d, 3 H, CH*Me*$_2$, $^3J_{HH}$ = 6.89 Hz).

^{13}C {^{1}H} NMR (125 MHz, C_6D_6, ppm): δ(ppm) 153.59 (C_{quart}, NAr), 145.57 (C_{quart}, NAr), 145.18 (C_{quart}, NAr), 144.52 (C_{quart}, NAr), 143.24 (C_{quart}), 143.06 (C_{quart}, NAr), 141.90 (C_{quart}), 140.34 (C_{quart}), 136.82 (C_{quart}), 131.98 (C_{quart}, ArN*C*MeCHCMe), 130.79 (CH, Ar), 130.15 (CH, Ar), 128.66 (CH, Ar), 128.44 (CH, Ar), 128.14 (CH, Ar), 127.87 (CH, Ar), 127.38 (CH, Ar), 125.91 (CH, Ar), 125.28 (CH, Ar), 124.59 (CH, Ar), 124.07 (CH, NAr), 123.82 (CH, NAr), 123.14 (CH, NAr), 122.97 (CH, NAr), 107.70 (CHC(Me)*C*(Ph)C(Ph)), 97.96 (C_{quart}, Nb*C*MeCH), 84.25 (CH, (H*C*(C(Me)NAr), 67.83 (*C*(CH$_3$)$_3$, Nb=N^{t}Bu, C_α), 33.22 (CH$_3$, Nb=N^{t}Bu, C_β), 30.53 (CH, *C*HMe$_2$ of N*Ar*), 29.35 (CH$_3$, (HC(C(*Me*)Nb)), 28.05 (CH, *C*HMe$_2$ of N*Ar*), 28.03 (CH$_3$, CH*Me*$_2$ of N*Ar*), 27.77 (CH, *C*HMe$_2$ of N*Ar*), 27.62 (CH, *C*HMe$_2$ of N*Ar*), 26.82 (CH$_3$, CH*Me*$_2$ of N*Ar*), 26.25 (CH$_3$, CH*Me*$_2$ of N*Ar*), 24.28 (CH$_3$, CH*Me*$_2$ of N*Ar*), 24.08 (CH$_3$, CH*Me*$_2$ of N*Ar*), 24.00 (CH$_3$, CH*Me*$_2$ of N*Ar*), 23.33 (CH$_3$, (HC(C(*Me*)=NAr)), 22.60 (CH$_3$, CH*Me*$_2$ of N*Ar*), 22.09 (CH$_3$, CH*Me*$_2$ of N*Ar*). Anal. Calcd. for $C_{47}H_{60}N_3Nb$: C: 74.29; H:7.96; N: 5.53. Found: C: 74.16; H: 8.06; N: 5.38.

(5) (κ^2-*N*,*C*)(MAD+EtCCEt+N^{t}Bu)Nb(NAr): Stirring at room temperature an orange solution of (MAD)Nb(N^{t}Bu)(NAr)(OEt$_2$) (150 mg, 0.23 mmol) in benzene (5 ml) with hex-3-yne (1.5 equiv., 29 mg) for 12 h resulted in a slow color change to brownish yellow. After removal of all volatile compounds under reduced pressure, the crude residue was extracted using a minimum amount of HMDSO and subsequently filtered at room temperature. A brownish crystalline material was obtained in 45% yield (69 mg) after 4 weeks. Crystals suitable for XRD have been obtained by re-crystallizing this material using a saturated HMDSO solution after further 4 weeks (-40°C).

^{1}H NMR (400 MHz, C_6D_6, 298K): δ(ppm) 7.22 (dd, 1 H, NAr, $^3J_{HH}$ = 7.72 Hz, $^4J_{HH}$ = 1.63 Hz), 7.17 (dd, 1 H, NAr, $^3J_{HH}$ = 7.72 Hz, $^4J_{HH}$ = 1.41 Hz), 7.12-6.94 (m, 4 H, NAr), 4.48 (sept, 1 H, NArC*H*Me$_2$, $^3J_{HH}$ = 6.81 Hz), 4.27 (s, 1 H, *H*C(C(Me)NAr), 4.07 (sept, 2 H, Nb=NArC*H*Me$_2$, $^3J_{HH}$ = 6.98 Hz), 3.32 (sept, 1 H, NArC*H*Me$_2$, $^3J_{HH}$ = 6.76 Hz), 2.54 (s, 3 H, CHC(*Me*)Nb), 2.06-1.90 (m, 3 H, CH$_2$ of NCEt + C*H*H of NbCMeCEt), 1.86 (s, 3 H, HC(C(*Me*)NAr), 1.53 (d, 3 H, NArCH*Me*$_2$, $^3J_{HH}$ = 7.18 Hz), 1.44 (m, 12 H, Nb-N^{t}Bu + NArCH*Me*$_2$), 1.37 (d, 3 H, NArCH*Me*$_2$, $^3J_{HH}$ = 6.96 Hz), 1.33 (d, 6 H, Nb=NArCHC*Me*$_2$, $^3J_{HH}$ = 6.68 Hz), 1.32 (d, 6 H, Nb=NArCHC*Me*$_2$, $^3J_{HH}$ = 6.73 Hz), 1.12-1.03 (m, 7 H, CH*H* of NbCMeCEt + CH$_3$ of NbCMeCEt + CH$_3$ of NArCH*Me*$_2$), 0.50 (t, 3 H, CH$_3$ of NCEt, $^3J_{HH}$ = 7.40 Hz).

^{13}C {^{1}H} NMR (125 MHz, C_6D_6, 298K): δ(ppm) 153.17 (C_{quart}, NAr), 145.43 (C_{quart}, N*C*EtCEtCMe), 142.88 (C_{quart}), 141.36 (C_{quart}), 140.89 (C_{quart}), 140.44 (C_{quart}), 127.97 (C_{quart}, ArN*C*MeCHCMe), 124.80

(CH, Ar), 123.86 (CH, Ar), 123.57 (CH, Ar), 122.87 (CH, Ar), 121.97 (CH, Ar), 119.22 (C_{quart}, NCEt*C*EtCMe), 97.66 (C_{quart}, Nb*C*MeCH), 85.81 (CH, (H*C*(C(Me)NAr), 58.38 (*C*$(CH_3)_3$, Nb-N*t*Bu, C_α), 33.57 (CH_3, Nb-N*t*Bu, C_β), 29.23 (CH, *C*HMe_2 of NAr), 27.75 (CH, *C*HMe_2 of Nb=NAr), 27.36 (CHC(*Me*)Nb), 27.80 (CH, *C*HMe_2 of NAr), 26.66 (CH_3, CH*Me*$_2$ of N*Ar*), 26.01 (CH_2 of NC*Et*), 25.32 (CH_3, CH*Me*$_2$ of Nb=NAr), 24.74 (CH_3, CH*Me*$_2$ of Nb=NAr), 24.17 (CHH of NbCMeC*Et*), 24.12 (CH_3, CH*Me*$_2$ of NAr), 23.68 (CH_3, CH*Me*$_2$ of NAr), 22.33 (HC(C(*Me*)NAr), 15.63 (CH_3 of NbCMeC*Et*), 12.64 (CH_3 of NC*Et*). Attempts to obtain satisfactory microanalysis data were unsuccessful. Re-crystallization (-40°C in HMDSO, ~4 weeks) or sublimation (decomposition) provided no suitable results. HRMS analysis attempts resulted in a complete decomposition of this compound.

(6) (κ²-*N*,*C*)(MAD+Nor+N*t*Bu)Nb(NAr): Stirring at room temperature an orange solution of (MAD)Nb(N*t*Bu)(NAr)(OEt_2) (150 mg, 0.23 mmol) in benzene (5 ml) with norbornylene (1.5 equiv., 33 mg) for 12 h resulted in a fast color change to yellow (after 3 h over 90% conversion). After removal of all volatile compounds under reduced pressure, the crude residue was extracted with HMDSO and after filtration cooled to -40°C. A yellow crystalline material was obtained in 70% yield (109 mg) after 3 days. Crystals suitable for XRD have been obtained from a saturated HMDSO solution at +5°C after one week.

^{1}H NMR (400 MHz, C_6D_6, 298K): δ(ppm) 7.30 (m, 2 H, NAr), 7.15-7.11 (m, 3 H, NAr), 6.99 (t, 1 H, NAr, $^3J_{HH}$ = 7.61 Hz), 4.39 (s, 1 H, *H*C(C(Me)NAr), 4.11 (sept, 2 H, Nb=NArC*H*Me_2, $^3J_{HH}$ = 6.69 Hz), 3.82 (m, 3 H, NC*H*$_{nor}$ + C*HH* of NArCHMe_2), 2.66 (d, 1 H, NbCMeC*H*$_{nor}$, $^3J_{HH}$ = 9.30 Hz), 2.51 (s, 3 H, CHC(*Me*)Nb), 1.97 (s, 4 H, HC(C(*Me*)NA + C*H*$_{nor}$), 1.83 (d, 1 H, HC*H*$_{nor\ bridge}$, $^3J_{HH}$ = 10.46 Hz), 1.67 (br s, 1 H, C*H* of C*H*$_{nor}$), 1.59 (s, 9 H, CH_3 of NbN*t*Bu), 1.57 (d, 3 H, NArCH*Me*$_2$, $^3J_{HH}$ = 7.05 Hz), 1.50 (d, 3 H, NArCH*Me*$_2$, $^3J_{HH}$ =7.05 Hz), 1.45 (d, 3 H, NArCH*Me*$_2$, $^3J_{HH}$ = 7.05 Hz), 1.32 (m, 1 H, C*H*$_{exo}$ of CH_{2nor}), 1.30 (d, 6 H, Nb=NArCHC*Me*$_2$, $^3J_{HH}$ = 7.05 Hz), 1.24 (d, 6 H, Nb=NArCHC*Me*$_2$, $^3J_{HH}$ = 7.05 Hz), 1.13 (m, 2 H, C*H*$_{exo}$ of CH_{2nor} +), 1.12 (d, 3 H, NArCH*Me*$_2$, $^3J_{HH}$ = 6.91 Hz), 0.91 (m, 2 H, C*H*$_{endo}$ of CH_{2nor}), 0.47 (d, 1 H, *H*CH$_{nor\ bridge}$, $^3J_{HH}$ = 10.46 Hz).

^{13}C {^{1}H} NMR (125 MHz, C_6D_6, 298K): δ(ppm) 153.96 (C_{quart}, NAr), 145.43 (C_{quart}), 141.86 (C_{quart}), 141,59 (C_{quart}), 141.01 (C_{quart}), 140.68 (C_{quart}), 131,19 (C_{quart}, ArN*C*MeCHCMe), 125.38 (CH, Ar), 123.79 (CH, Ar), 123.18 (CH, Ar), 122,83 (CH, Ar), 122.81 (CH, Ar), 98.40 (CH, (H*C*(C(Me)NAr), 95.95 (C_{quart}, Nb*C*MeCH), 72.00 (CH, N*C*H$_{nor}$), 61.16 (CH, NbCMe*C*H$_{nor}$), 58.66 (*C*$(CH_3)_3$, Nb-N*t*Bu, C_α), 44.77 (*C*H$_{nor}$), 39.64 (*C*H$_{nor}$), 36.64 (CH_2, H*C*H$_{nor\ bridge}$) 35.19 (CHC(*Me*)Nb), 34.02 (*C*H_{2nor}), 31.88 (CH_3, Nb-N*t*Bu, C_β), 31.01 (CH, *C*HMe_2 of NAr), 28.84 (CH_3, CH*Me*$_2$ of NAr), 27.95 (CH, *C*HMe_2 of NAr), 27.87 (CH, *C*HMe_2 of Nb=NAr), 27.35 (CH_3, CH*Me*$_2$ of NAr), 26.46 (*C*H_{2nor}), 25.16 (CH_3, CH*Me*$_2$ of NAr), 25.02 (CH_3, CH*Me*$_2$ of Nb=NAr), 24.85 (CH_3, CH*Me*$_2$ of Nb=NAr), 23.59 (CH_3, CH*Me*$_2$ of NAr), 22.61 (HC(C(*Me*)NAr). MS (ES) *m*/*e* calcd for [$C_{40}H_{60}N_3$Nb+H] 676.40, *m*/*e* found 676.40. Attempts to obtain satisfactory microanalysis data on this material were unsuccessful and hampered due to the thermal instability of the compound together with probably traces of HMDSO.

C. X-ray crystallography

X-ray structural determinations were performed on a Bruker SMART 1000 or SMART APEX diffractometer. Both are 3-circle diffractometers that couple a CCD detector[7] with a sealed-tube source of monochromated Mo Ka radiation (λ = 0.71073 Å). A crystal of appropriate size was coated in Paratone-N oil and mounted on a Kapton® loop. The loop was transferred to the diffractometer, centered in the beam, and cooled by a nitrogen flow low-temperature apparatus that had been previously calibrated by a thermocouple placed at the same position as the crystal. Preliminary orientation matrices and cell constants were determined by collection of 60 10 s frames, followed by spot integration and least-squares refinement. The reported cell dimensions were calculated from all reflections with I > 10 σ. The data were corrected for Lorentz and polarization effects; no correction for crystal decay was applied. An empirical absorption correction based on comparison of redundant and equivalent reflections was applied using SADABS.[8] All software used for diffraction data processing and crystal-structure solution and refinement are contained in the APEX2 program suite (Bruker AXS, Madison, WI).[9] Thermal parameters for all non-hydrogen atoms were refined anisotropically. For all structures, R1 = Σ(|Fo| - |Fc|)/Σ(|Fo|); wR2 = [Σ{w(Fo2 - Fc2)2}/Σ{w(Fo2)2}]1/2. Thermal ellipsoid plots were created using the ORTEP-3 software package and POV-ray.[10]

C.1 Ortep view of compounds 2 and 3

C.1.1 Complexes 2 and 3

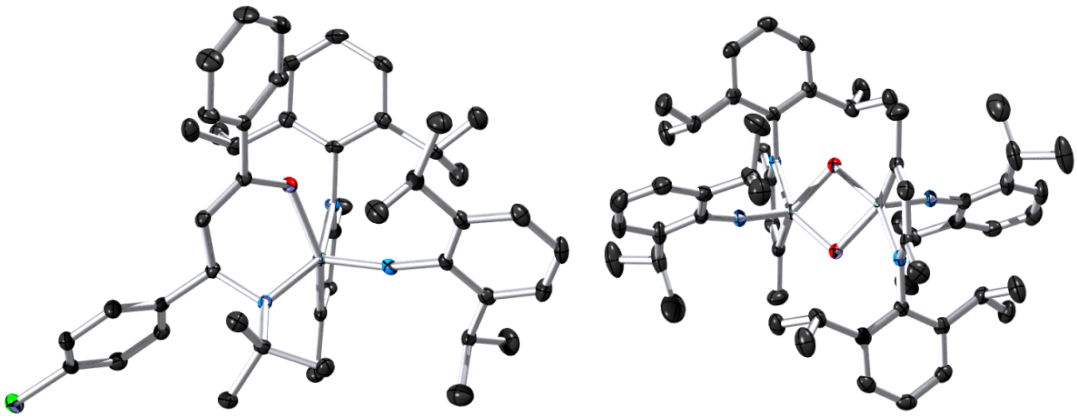


Figure S. 1 Full Ortep diagrams of complexes **2** (left) and **3** (right).

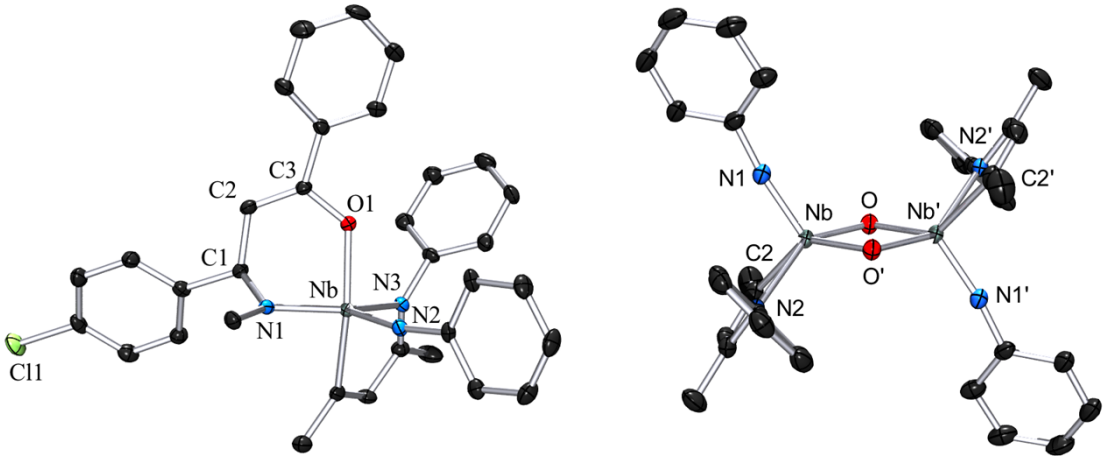


Figure S. 2 Simplified Ortep diagrams of complexes **2** (left) and **3** (right). The hydrogens have been removed, he Aryl group has been truncated to phenyl, and the tbutyl imido to the Cα for clarity.

Table S.1 Selected bond distances of complexes **2** and **3**

	2	**3**
Nb-C2	2.243(2)	2.220(6)
Nb-N1	1.969(2)	2.303(4)
Nb-N2	2.323(2)	1.785(4)
Nb-N3	1.779(3)	-
Nb-O	2.017	1.950 (average)
N1-C1	1.511(3)	-
C1-C2	1.504	-
C3-C4	1.343	-
C4-O	1.346	-

C.1.2 Complexes 4, 5 and 6

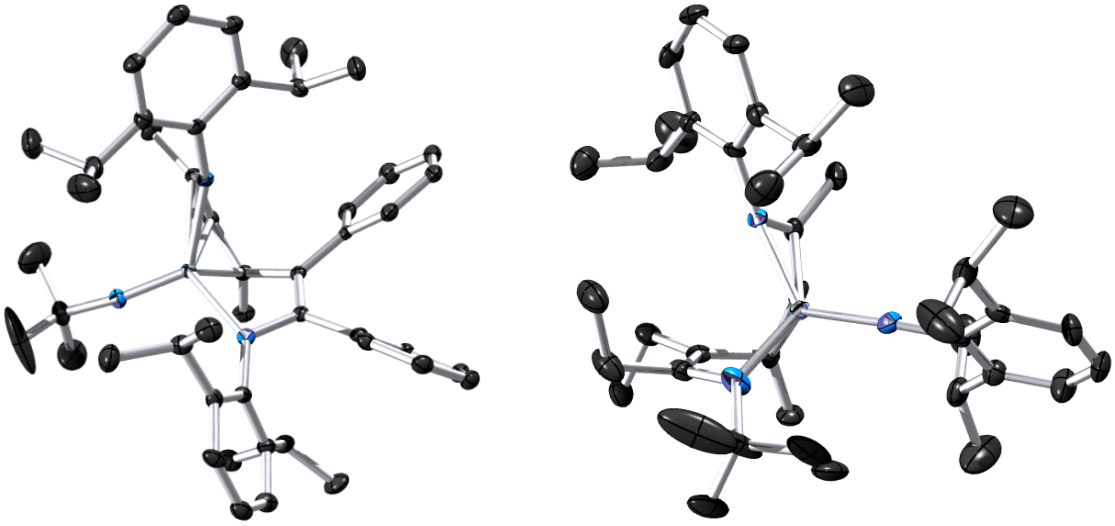


Figure S. 3 Full Ortep diagrams of complexes complexes **4**, **5** and **6**.

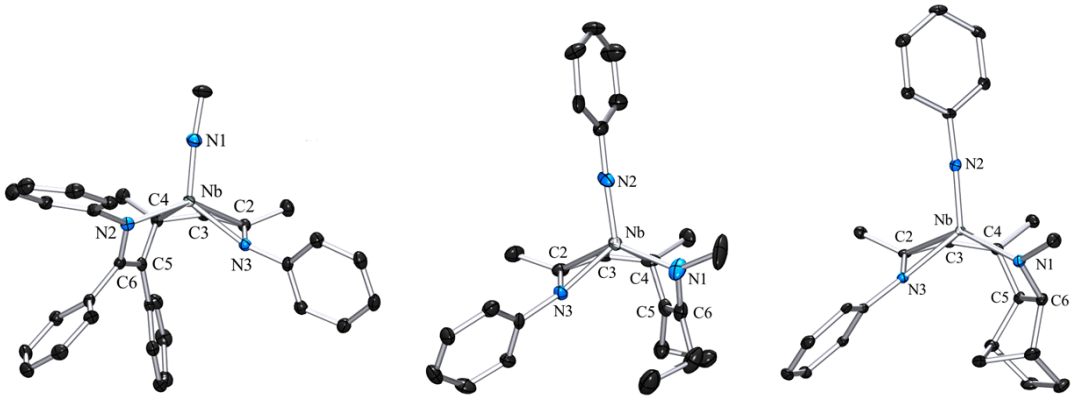


Figure S.4 Simplified Ortep diagrams of complexes **4** (left), **5** (center) and **6** (right). The hydrogens have been removed, he Aryl group has been truncated to phenyl, and the tbutyl imido to the Cα for clarity.

Table S.2 Selected bond distances of complexes **4, 5** and **6**

	4	**5**	**6**
Nb-N1	1.772	2.030	2.014
Nb-N2	2.069	1.807	1.797
Nb-N3	2.099	2.098	2.106
Nb-C2	2.122	2.124	2.172
Nb-C3	2.315	2.335	2.337
Nb-C4	2.400	2.408	2.400
Nb-C5	2.615	2.592	2.849
Nb-C6	2.701	2.606	2.908
C4-C5	1.519	1.511	1.566
C5-C6	1.387	1.336	1.585
C6-N2 (or N1)	1.400	1.430	1.489

C.2 Structural parameters

Table S. 3 Crystallographic parameters for complexes **2** and **3**

Compound	**2**	**½-3**
Formula	$C_{48}H_{61}ClN_3NbO$	$C_{29}H_{41}N_2NbO$
Formula weight (amu)	824.36	526.55
Space Group	P_{-1}	$P2_1/n$
a (Å)	11.3526(7)	11.1260(7)
b (Å)	19.7589(12)	16.7319(11)
c (Å)	20.1301(13)	15.5707(10)
α (°)	96.454(4)°	90°
β (°)	102.126(3)°	108.0600(10)°
γ (°)	91.320(4)°	90°
V (Å^3)	4381.7(5)	2755.8(3)
Z	4	4
ρ_{calcd} (g/cm^3)	1.250	1.269
F_{000}	1744	1112
μ (mm^{-1})	0.373	0.459
T_{min}/T_{max}	0.9224/0.9816	0.8676/0.9452
No. rflns measured	84384	41926
No. indep. rflns	16211	4934
R_{int}	0.0667	0.0257
No. obs. ($I > 2.00\sigma(I)$)	16211	4934
No. variables	999	308
R_1, wR_2	0.0399/0.0779	0.0421/0.0588
R_1 (all data)	0.0649	0.0303
GoF	1.024	1.094
Res. peak/hole (e$^-$/Å^3)	0.504/-0.415	0.519/-0.248

Table S. 4 Crystallographic parameters for complexes **4**, **5** and **6**

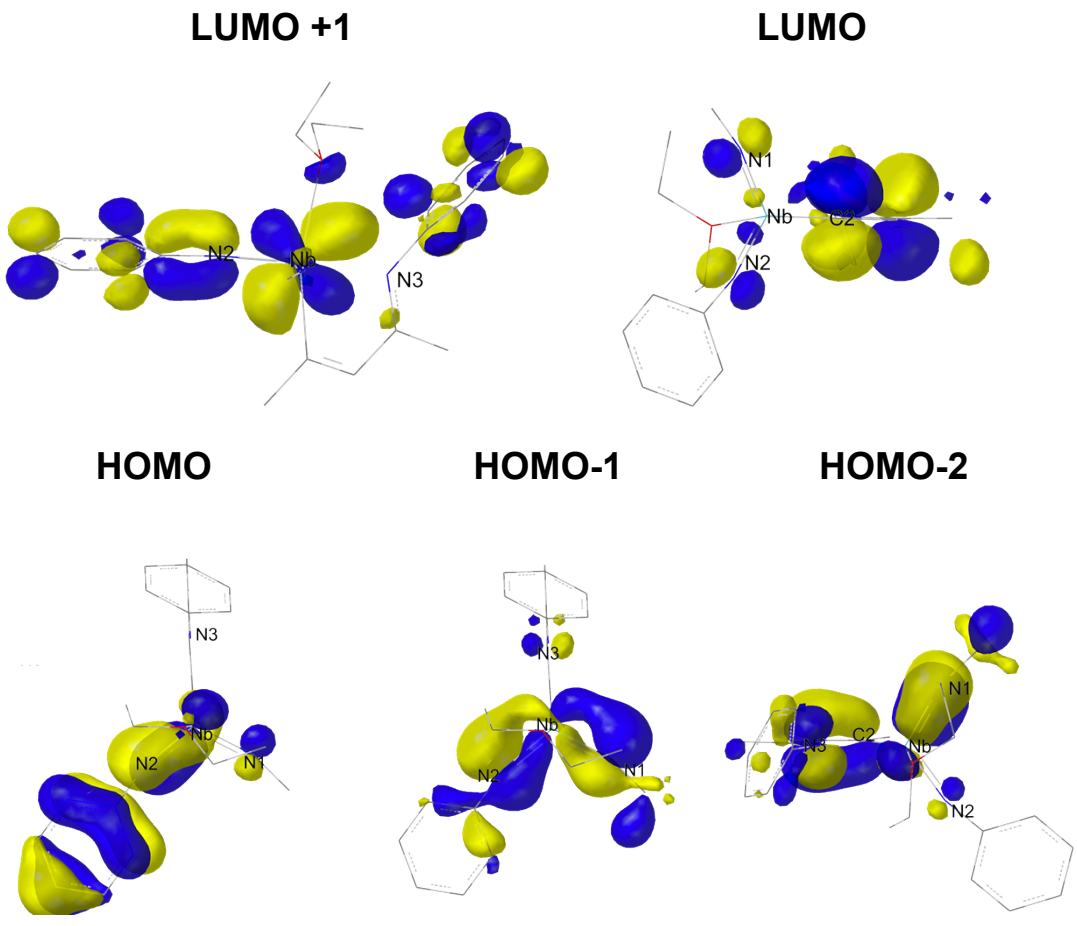
Compound	**4**	**5**	**6**
Formula	$C_{47}H_{60}N_3Nb$	$C_{39}H_{60}N_3Nb$	$C_{40}H_{60}N_3Nb$
Formula weight (amu)	759.89	663.79	675.82
Space Group	P_1	P_{-1}	$C_{2/c}$
a (Å)	10.7140(19)	12.5601(4)	34.020(3)
b (Å)	11.714(2)	35.9930(11)	13.2760(13)
c (Å)	18.976(3)	9.2081(3)	16.2477(16)
α (°)	86.853(10)°	90°	90°
β (°)	76.422(9)°	116.264(2)°	96.893(5)°
γ (°)	65.449(8)°	90°	90°
V (Å^3)	2103.3(7)	3733.0(2)	7285.2(12)
Z	2	4	8
ρ_{calcd} (g/cm^3)	1.200	1.181	1.232
F_{000}	808	1424	2896
μ (mm^{-1})	0.320	0.351	0.361
T_{min}/T_{max}	0.9387/0.9810	0.9691/0.9827	0.9479/0.9822
No. rflns measured	45285	7266	48813
No. indep. rflns	7757	4182	6702
R_{int}	0.0379	0.0491	0.0564
No. obs. ($I > 2.00\sigma(I)$)	7757	4182	6702
No. variables	473	404	410
R_1, wR_2	0.0320/0.0809	0.0477/0.0806	0.0299/0.0638
R_1 (all data)	0.0387	0.0685	0.0417
GoF	1.079	1.017	1.030
Res. peak/hole (e$^-$/Å^3)	0.858/-0.436	0.418/-0.365	0.448/-0.425

D. DFT Calculations

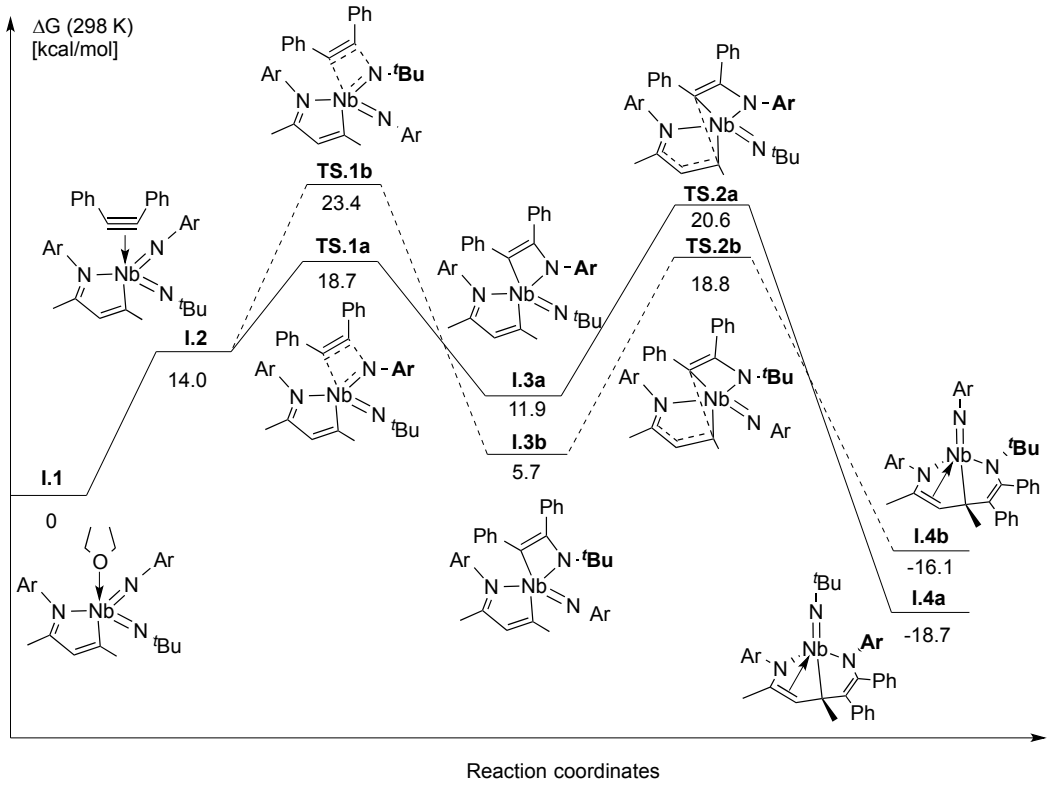
All structures and energies were calculated using the Gaussian09 suite of programs.[11] Self-consistent field computations were performed with tight convergence criteria on ultrafine grids, while geometry optimizations were converged to tight geometric convergence criteria for all compounds. Spin expectation values $<S>^2$ indicated that spin contamination was not significant in any result. Frequencies were calculated analytically at 298.15 K and 1 atm. Structures were considered true minima if they did not exhibit imaginary vibration modes and were considered as transition states when only one imaginary vibration mode was found. Intrinsic Reaction Coordinates (IRC) calculations were performed to ensure the transition state geometries connected the reactants and the products. Optimized geometries were compared using the sum of their electronic and zero-point energies.

The B3LYP hybrid functional was used throughout this computational study.[12][13] For geometry optimizations and frequency calculations, the light atoms (H, C, N and O) were treated with Pople's 6-31G(d,p) double-ζ split-valence basis,[14][15] while the niobium atom was treated with a Stuttgart/Dresden ECPs pseudopotential (SDD).[16][17] In order to reduce the computational time, the system was structurally simplified by replacing 2,6-diisopropylphenyl groups by phenyl and the *tert.*-butyl group by methyl in the case of the diethyl acetylene and norbornene pathways.

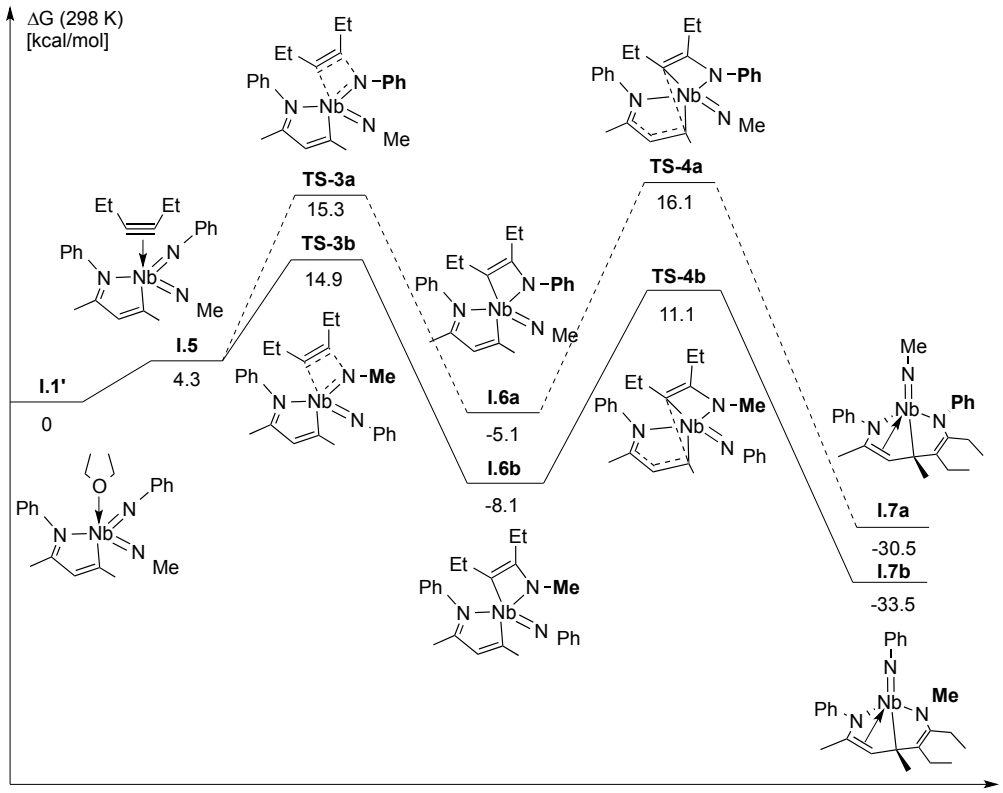
D.1 Frontier orbitals analysis



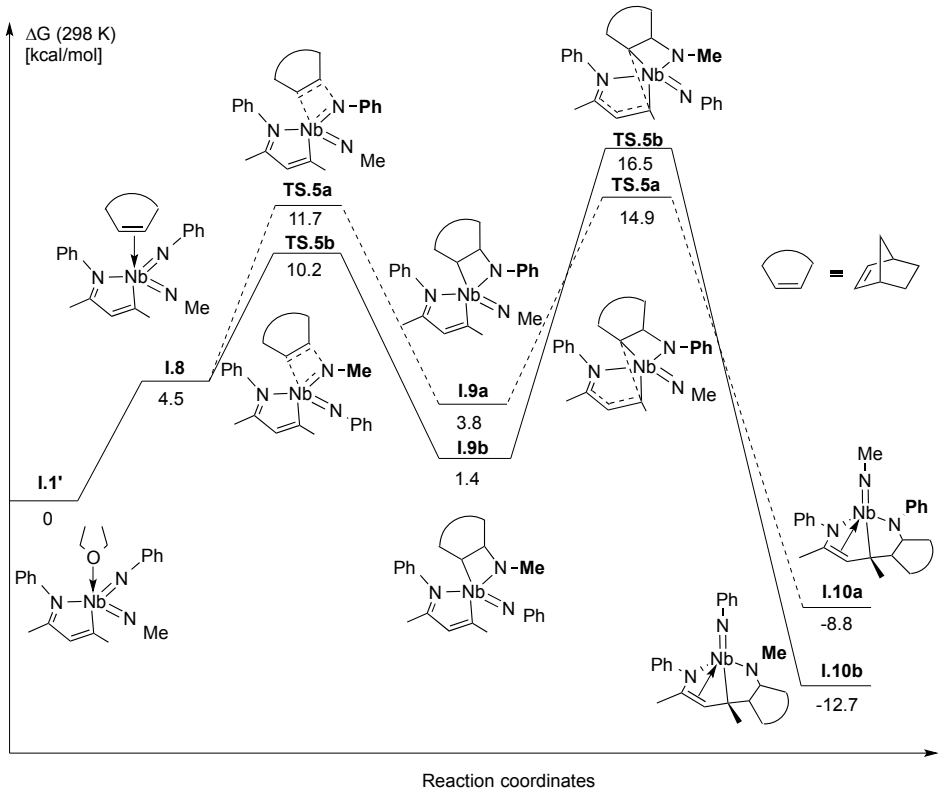
D.2 DFT Analysis on PhCCPh



D.3 DFT Analysis on EtCCEt



D. 4 DFT Analysis on Norbornene



D.5 Atoms coordinate

PhCCPh:
G (a.u.) = -539.310305

C	-1.15907	2.02313	0.00122
C	0.24961	2.00944	0.00105
C	0.94201	3.23626	-0.00057
C	0.24157	4.44007	-0.00201
C	-1.15540	4.44281	-0.00186
C	-1.85145	3.23158	-0.00024
H	-1.69632	1.08017	0.00249
H	2.02726	3.23014	-0.00068
H	0.78762	5.37909	-0.00326
H	-1.69850	5.38340	-0.00299
H	-2.93769	3.22814	-0.00011
C	0.96414	0.77173	0.00257
C	1.57175	-0.28137	0.00376
C	2.28584	-1.51934	0.00513
C	2.64428	-2.14078	-1.20726
C	2.64293	-2.13885	1.21888
C	3.33985	-3.34737	-1.20128
H	2.37111	-1.66679	-2.14455
C	3.33851	-3.34547	1.21557
H	2.36873	-1.66340	2.15513
C	3.68920	-3.95366	0.00783
H	3.61018	-3.81609	-2.14317
H	3.60778	-3.81268	2.15851
H	4.23163	-4.89463	0.00886

Norbornene:
G (a.u.) = -232.367843

C	0.21552	0.33132	-0.10796
C	-0.32188	2.52309	-0.10882
C	0.56903	1.58011	0.73511
H	1.63359	1.84114	0.70447
H	0.23886	1.49957	1.77465
C	0.68972	0.80493	-1.52634
H	1.77018	0.66186	-1.63597
H	0.19935	0.24564	-2.32769
C	0.31759	2.32121	-1.52709
H	1.20909	2.94803	-1.63742
H	-0.37598	2.58911	-2.32874
H	0.63742	-0.62426	0.21143
H	-0.38970	3.56576	0.20963
C	-1.30414	0.43051	-0.11241
H	-1.97919	-0.41223	-0.22048
C	-1.62332	1.73240	-0.11232
H	-2.61159	2.16739	-0.22037

Et_2O:
G (a.u.) = -233.566076

C	1.40488	0.84701	0.15044
H	1.73358	-0.19507	0.08568
H	1.75826	1.37887	-0.73776
H	0.31116	0.86738	0.14796
C	1.94662	1.49926	1.41222
H	1.60227	0.95292	2.30766
H	3.05006	1.46458	1.42156
C	1.94696	3.54808	2.59484
H	3.05042	3.55760	2.62907
H	1.60313	3.04567	3.51585
C	1.40483	4.96680	2.52908
H	0.31110	4.95849	2.51057
H	1.73366	5.54396	3.39909
H	1.75778	5.47021	1.62430
O	1.49741	2.84139	1.45323

EtCCEt:
G (a.u.) = -234.503474

C	-0.00456	0.68393	-0.00026
H	3.04706	1.17247	-0.89145
H	3.04609	1.23018	0.86015
C	-1.46927	0.71371	-0.00214
H	-1.84459	0.14005	-0.86024
H	-1.84564	0.19767	0.89135
C	-2.04626	2.14106	-0.04945
H	-3.14057	2.11227	-0.04915
H	-1.71697	2.72257	0.81640
H	-1.71591	2.66440	-0.95126
C	3.24732	-0.77093	0.04951
H	4.34163	-0.74244	0.04923
H	2.91679	-1.29410	0.95136

H	2.91788	-1.35241	-0.81631
C	1.20595	0.68655	0.00030
C	2.67064	0.65657	0.00209

Intermediate **I.1**:
G (a.u.) = -1741.883925

Nb	8.39063	17.25164	4.75117
O	9.16086	15.05053	5.11246
N	7.48961	17.55628	6.30083
N	10.06582	18.01565	4.64811
N	7.07618	16.20722	2.99087
C	6.99512	18.05306	7.56704
C	11.25545	18.71420	4.67437
C	11.93523	18.99003	5.90249
C	13.15740	19.66660	5.87298
H	13.67510	19.86357	6.80845
C	13.72727	20.09890	4.67818
H	14.67566	20.62898	4.68026
C	13.06347	19.84334	3.48129
H	13.50563	20.18070	2.54682
C	11.84580	19.15897	3.44755
C	7.61354	20.35784	3.85187
H	7.10078	21.00447	3.12535
H	8.68160	20.60378	3.85505
H	7.25108	20.60817	4.85512
C	7.42333	18.89409	3.58047
C	6.63395	18.50497	2.54343
H	6.11184	19.21484	1.89625
C	6.44428	17.09940	2.26055
C	5.51728	16.75608	1.11896
H	5.96311	17.09282	0.17622
H	4.57940	17.30888	1.23396
H	5.30181	15.69100	1.04509
C	6.94059	14.80426	2.71788
C	6.09681	14.02187	3.54996
C	6.03492	12.64167	3.32561
H	5.39284	12.02879	3.94942
C	6.77454	12.03570	2.31253
H	6.71120	10.96242	2.15684
C	7.58121	12.81646	1.49274
H	8.14128	12.34372	0.69068
C	7.68110	14.20432	1.66860
C	8.63840	14.25846	6.21196
H	7.69025	14.73665	6.45322
C	10.48819	14.68541	4.65096
H	10.68219	15.36559	3.82136
H	11.21076	14.92505	5.43816
H	8.43468	13.24905	5.83960
C	9.54049	14.22933	7.43767
H	9.78022	15.24167	7.77027
H	9.01042	13.71945	8.24924
H	10.47307	13.68513	7.26424
C	10.59880	13.23136	4.21493
H	11.57879	13.07778	3.75087
H	10.52407	12.53627	5.05624
H	9.82753	12.97778	3.48305
C	7.66842	17.28949	8.72846
H	7.28508	17.63623	9.69516
H	7.47014	16.21565	8.65095
H	8.75139	17.44268	8.71430
C	7.28594	19.56180	7.71197
H	8.35645	19.75843	7.61496
H	6.76186	20.12707	6.93615
H	6.94965	19.93230	8.68765
C	5.46753	17.82188	7.62533
H	5.23880	16.75366	7.55083
H	5.04575	18.20033	8.56414
H	4.97618	18.33385	6.79233
C	11.18502	18.89516	2.09955
H	10.23976	18.38459	2.30023
C	12.04584	17.96492	1.22237
H	13.01198	18.42202	0.98027
H	12.24926	17.01594	1.72962
H	11.53871	17.74350	0.27546
C	10.85727	20.19834	1.34588
H	10.32989	19.98033	0.40955
H	10.22170	20.85565	1.94689
H	11.76460	20.75745	1.09042
C	11.37036	18.53108	7.23965
H	10.35438	18.17646	7.05011
C	12.18225	17.35138	7.81137
H	11.74371	16.98868	8.74929
H	12.21689	16.51536	7.10472
H	13.21669	17.64697	8.02116
C	11.28312	19.67400	8.26830
H	12.27376	20.04553	8.55318
H	10.71372	20.52124	7.87317
H	10.78903	19.33026	9.18462
C	5.22444	14.66723	4.62725
H	5.76127	15.54079	5.01494
C	4.92043	13.74297	5.81978
H	5.82387	13.28019	6.22756
H	4.44365	14.31834	6.62003
H	4.22756	12.93856	5.54905
C	3.89357	15.18045	4.03614
H	4.05296	15.92030	3.24935
H	3.31486	14.35337	3.60890
H	3.28632	15.65082	4.81722
C	8.55267	15.00133	0.69536
H	8.51916	16.05400	0.98893
C	8.02170	14.89688	-0.75066
H	8.60012	15.54638	-1.41670
H	8.10945	13.87318	-1.13059
H	6.96991	15.18497	-0.82412
C	10.03081	14.56788	0.73003
H	10.61895	15.17069	0.03049
H	10.46593	14.69454	1.72375
H	10.14875	13.51724	0.44326

Intermediate **I.1'**:
G (a.u.) = -1152.553733

Nb	8.26657	17.29618	4.61910
O	8.88640	15.03399	5.00554
N	7.52957	17.75410	6.20783
N	9.99238	17.90830	4.47152
N	6.90607	16.31028	2.90639
C	7.34340	18.38347	7.47935
C	11.19811	18.53931	4.66120
C	11.68584	18.83973	5.95612
C	12.91426	19.47162	6.12888
H	13.26700	19.68977	7.13403
C	13.69187	19.83223	5.02385
H	14.64811	20.32804	5.16324
C	13.22335	19.54715	3.73833
H	13.81785	19.82332	2.87084
C	12.00038	18.90611	3.55480
C	7.63116	20.42505	3.72959
H	7.12797	21.10276	3.02505
H	8.70827	20.63006	3.71077
H	7.30020	20.66891	4.74675
C	7.38267	18.97441	3.44353
C	6.58582	18.61234	2.39968
H	6.09797	19.33816	1.74441
C	6.33341	17.21477	2.13742
C	5.40871	16.86381	0.99495
H	5.97781	16.77379	0.06196
H	4.67682	17.66220	0.85203
H	4.88888	15.91833	1.15709
C	6.69468	14.92381	2.65737
C	5.93884	14.16006	3.55847
C	5.74374	12.79700	3.33507
H	5.14636	12.21971	4.03528
C	6.30697	12.17493	2.21759
H	6.15306	11.11378	2.04612
C	7.06897	12.92933	1.32290
H	7.51266	12.45664	0.45105
C	7.26554	14.29429	1.54106
C	9.04203	14.67913	6.40993
H	9.66971	13.78562	6.46590
C	9.99867	14.60433	4.17203
H	9.87908	15.14957	3.23407
H	10.93111	14.94834	4.63466
H	11.07491	18.56626	6.81169
H	11.63402	18.68001	2.55747
H	6.48635	19.07319	7.45387
H	8.22430	18.95980	7.79995
H	7.12774	17.64146	8.26467
H	5.50389	14.64840	4.42501
H	7.86145	14.88172	0.84817
H	9.56313	15.50211	6.91105
C	7.68485	14.41404	7.03304
H	7.18964	13.57137	6.54236
H	7.81548	14.17242	8.09345
H	7.05095	15.30112	6.95503
C	9.99858	13.10437	3.91400
H	10.82350	12.86452	3.23418
H	10.14935	12.51947	4.82607
H	9.06331	12.78979	3.44564

Intermediate **I.2**:
G (a.u.) = -2047.606902

Nb	8.52920	17.10126	4.73424
N	7.67671	17.55661	6.26580
N	10.20567	17.87020	4.64151

N	7.11002	16.08499	3.00289
C	7.24750	18.28268	7.44432
C	11.39613	18.56186	4.73721
C	12.18108	18.51785	5.93483
C	13.42643	19.15106	5.95777
H	14.02690	19.10019	6.86218
C	13.91803	19.84688	4.85682
H	14.88827	20.33375	4.90125
C	13.14440	19.91798	3.70198
H	13.52071	20.47119	2.84501
C	11.89722	19.29463	3.61103
C	7.80992	20.22010	3.84886
H	7.55826	20.87179	3.00051
H	8.82359	20.44659	4.18918
H	7.14310	20.48370	4.67990
C	7.64247	18.76063	3.53973
C	6.93206	18.39581	2.44032
H	6.51154	19.12382	1.74161
C	6.60902	17.00517	2.20891
C	5.64245	16.72354	1.08204
H	5.51982	15.66305	0.86913
H	5.98128	17.24075	0.17840
H	4.66286	17.14593	1.33299
C	6.62409	14.73584	2.88415
C	5.38924	14.38826	3.48766
C	4.92633	13.07340	3.34371
H	3.97830	12.79550	3.79547
C	5.64936	12.12202	2.63254
H	5.26764	11.11040	2.52546
C	6.86792	12.47480	2.05656
H	7.42743	11.72882	1.50194
C	7.38022	13.77399	2.16822
C	9.08451	14.35396	5.56718
C	10.02049	14.70347	4.84861
C	11.31070	14.53538	4.21501
C	11.87718	15.45254	3.31892
C	12.01603	13.35060	4.51985
C	13.11929	15.19199	2.74025
H	11.34648	16.37136	3.10814
C	13.25455	13.09923	3.93813
H	11.58157	12.63856	5.21425
C	13.81061	14.01876	3.04428
H	13.55034	15.91772	2.05740
H	13.78683	12.18510	4.18456
H	14.77906	13.82302	2.59330
C	8.14639	13.70258	6.43439
C	7.34832	12.65354	5.93778
C	8.10925	14.00783	7.80873
C	6.53126	11.93055	6.80388
H	7.37896	12.41296	4.88152
C	7.28652	13.28031	8.66386
H	8.72729	14.81231	8.18808
C	6.49565	12.24119	8.16484
H	5.92020	11.12327	6.41146
H	7.26544	13.52186	9.72239
H	5.85651	11.67481	8.83599
C	7.42970	17.39761	8.69520
H	8.48628	17.14911	8.83844
H	7.07938	17.92411	9.59044
H	6.86288	16.46793	8.59783
C	5.75048	18.63282	7.28569
H	5.38528	19.18990	8.15661
H	5.59439	19.24648	6.39329
H	5.15451	17.72161	7.18047
C	8.06651	19.57864	7.61979
H	9.13063	19.34926	7.70152
H	7.93023	20.24344	6.76372
H	7.75509	20.11394	8.52469
C	11.71193	17.76938	7.17674
H	10.65963	17.51745	7.02241
C	11.80803	18.62853	8.45275
H	12.84812	18.83679	8.72710
H	11.30024	19.59021	8.33207
H	11.34939	18.10533	9.30002
C	12.48878	16.45105	7.36797
H	12.39931	15.80391	6.49207
H	13.55531	16.64499	7.53168
H	12.11350	15.90162	8.24024
C	11.10786	19.42746	2.31105
H	10.13651	18.95305	2.46732
C	10.85651	20.90263	1.93803
H	11.78983	21.41949	1.68807
H	10.19999	20.97007	1.06277
H	10.38592	21.45100	2.75868
C	11.79540	18.70535	1.13407
H	12.79171	19.11866	0.93991
H	11.91215	17.63483	1.32641
H	11.20554	18.81655	0.21651
C	4.53501	15.38576	4.27207
H	5.02883	16.35968	4.24166
C	3.13266	15.55108	3.65088
H	3.18279	15.81791	2.59108
H	2.54699	14.62856	3.72999
H	2.57762	16.33784	4.17317
C	4.41479	14.99357	5.75741
H	5.39424	14.95749	6.23956
H	3.80012	15.72723	6.29073
H	3.94083	14.01317	5.87723
C	8.69407	14.13848	1.47984
H	9.13453	14.97054	2.03932
C	9.71703	12.98934	1.47300
H	9.42218	12.18622	0.78845
H	10.68981	13.36026	1.13658
H	9.85043	12.55696	2.46786
C	8.46406	14.63038	0.03491
H	7.98581	13.85050	-0.56874
H	7.82982	15.51874	-0.00188
H	9.41991	14.88262	-0.43734

Intermediate **I.3a**:

G (a.u.) = -2047.604754

Nb	8.74691	17.55796	-4.15236
N	7.73504	18.71100	-5.07503
N	10.62417	17.96532	-4.80885
N	7.02786	16.12870	-3.13775
C	8.94832	19.59753	-1.46164
H	8.45523	19.88077	-0.52130
H	10.00124	19.38208	-1.24298
H	8.94956	20.47032	-2.12223
C	8.28380	18.42424	-2.12568
C	7.15421	17.92214	-1.57137
H	6.70491	18.35941	-0.67529
C	6.48359	16.75556	-2.12656
C	5.18372	16.35997	-1.47093
H	4.72278	15.48647	-1.92851
H	5.33494	16.16998	-0.40363
H	4.49455	17.21003	-1.54154
C	6.55362	14.81330	-3.48878
C	5.86466	14.60488	-4.70634
C	5.46999	13.30427	-5.04172
H	4.92780	13.13770	-5.96746
C	5.74740	12.22519	-4.21061
H	5.43944	11.22204	-4.49150
C	6.40733	12.44500	-3.00743
H	6.61055	11.60326	-2.35208
C	6.81191	13.72524	-2.60980
C	9.96936	15.72537	-4.74786
C	11.03933	16.57895	-4.76957
C	12.50026	16.27498	-4.69129
C	13.10299	15.37038	-5.57922
C	13.29546	16.87632	-3.70390
C	14.46544	15.08618	-5.48825
H	12.49767	14.88485	-6.33657
C	14.65583	16.58285	-3.60494
H	12.83654	17.56555	-3.00269
C	15.24711	15.69027	-4.50118
H	14.91594	14.38810	-6.18828
H	15.25301	17.05114	-2.82726
H	16.30732	15.46506	-4.42924
C	10.06982	14.25853	-4.72710
C	11.00791	13.54843	-3.94561
C	9.21974	13.50358	-5.55887
C	11.10205	12.15931	-4.01493
C	9.32125	12.11514	-5.63554
C	10.26478	11.43328	-4.86515
H	11.83456	11.64222	-3.40035
H	8.65327	11.56539	-6.29299
H	10.34241	10.35105	-4.92032
C	7.47346	13.86435	-1.23484
H	7.69367	14.91947	-1.05577
C	6.53630	13.38287	-0.10523
H	5.55498	13.86330	-0.14300
H	6.37310	12.30145	-0.16214
H	6.98243	13.59457	0.87282
C	8.81321	13.11155	-1.14538
H	9.52038	13.46284	-1.89714
H	9.25820	13.25263	-0.15356
H	8.67842	12.03544	-1.29905
C	5.45485	15.76018	-5.61266
H	6.02963	16.64191	-5.31661
C	5.75316	15.49681	-7.09947
H	6.81337	15.28031	-7.26127
H	5.17267	14.65631	-7.49425
H	5.49590	16.37648	-7.69734
C	3.96064	16.09165	-5.41082

H	3.66206	16.94556	-6.02941
H	3.32926	15.24062	-5.68998
H	3.74135	16.33760	-4.36672
H	11.67090	14.09405	-3.28248
H	8.47772	14.02570	-6.15307
C	11.28052	18.90240	-5.67876
C	11.82186	20.09832	-5.13439
C	11.37176	18.67035	-7.08288
C	12.41131	21.03513	-5.99319
C	11.96973	19.64693	-7.88887
C	12.48478	20.82534	-7.36289
H	12.82688	21.94604	-5.57203
H	12.02592	19.47746	-8.95996
H	12.94264	21.56610	-8.01237
C	10.81835	17.43313	-7.79555
H	10.51810	16.70146	-7.04754
C	11.87382	16.75871	-8.69603
H	12.79769	16.55548	-8.14827
H	11.48660	15.80818	-9.08023
H	12.12828	17.37768	-9.56319
C	9.55911	17.77201	-8.61643
H	9.17713	16.87532	-9.11830
H	8.76783	18.16125	-7.97202
H	9.77175	18.52198	-9.38681
C	11.82860	20.42085	-3.64310
H	11.32640	19.60071	-3.12509
C	11.06183	21.72243	-3.33667
H	10.03356	21.68195	-3.70802
H	11.03010	21.90903	-2.25745
H	11.54487	22.58706	-3.80413
C	13.26585	20.52330	-3.09016
H	13.85024	19.62916	-3.32072
H	13.79546	21.38147	-3.51806
H	13.25056	20.65632	-2.00198
C	7.00596	19.78342	-5.72885
C	6.10106	19.24095	-6.85325
H	6.68487	18.69723	-7.60000
H	5.34241	18.56654	-6.44925
H	5.58721	20.06812	-7.35558
C	6.12983	20.48507	-4.66715
H	6.75144	20.89811	-3.86767
H	5.55913	21.30302	-5.12142
H	5.42434	19.77772	-4.22090
C	8.01215	20.79524	-6.31704
H	8.65326	21.20157	-5.53067
H	8.65548	20.32350	-7.06310
H	7.47854	21.62589	-6.79292

Intermediate **I.3b**:
G (a.u.) = -2047.616209

Nb	8.74038	17.59327	-4.42131
N	7.65080	18.51169	-5.53923
N	10.62990	18.04056	-4.89318
N	7.11243	16.25336	-3.09995
C	9.13549	19.89350	-2.04589
H	8.79732	20.27762	-1.07328
H	10.21479	19.70625	-1.98932
H	9.00534	20.68935	-2.78874
C	8.40380	18.64707	-2.46449
C	7.39936	18.16682	-1.69819
H	7.07001	18.66026	-0.77936
C	6.70741	16.93455	-2.05943
C	5.55530	16.54290	-1.16716
H	5.03506	15.64842	-1.50417
H	5.91190	16.38631	-0.14366
H	4.84831	17.37933	-1.12559
C	6.58332	14.92939	-3.31844
C	5.69151	14.69758	-4.39482
C	5.23699	13.39233	-4.61396
H	4.55011	13.19944	-5.43081
C	5.64482	12.33581	-3.80541
H	5.28576	11.32883	-3.99833
C	6.50350	12.58118	-2.74173
H	6.80999	11.75697	-2.10438
C	6.98133	13.86847	-2.46290
C	9.98202	15.79556	-4.96352
C	11.04664	16.64835	-4.83565
C	12.46564	16.28334	-4.51681
C	13.26590	15.61119	-5.45320
C	13.00121	16.55696	-3.24801
C	14.57124	15.23468	-5.13403
H	12.85467	15.37368	-6.42955
C	14.30404	16.17454	-2.92672
H	12.38933	17.07289	-2.51315
C	15.09504	15.51481	-3.87049
H	15.17755	14.71839	-5.87300
H	14.70101	16.39137	-1.93882
H	16.11010	15.21913	-3.62151
C	9.98530	14.32984	-5.04176
C	10.96099	13.47833	-4.47485
C	8.95407	13.71902	-5.78599
C	10.91013	12.09817	-4.66267
C	8.91052	12.34015	-5.98280
C	9.89123	11.51984	-5.42311
H	11.67317	11.47049	-4.20946
H	8.10338	11.90703	-6.56688
H	9.85918	10.44399	-5.57089
C	6.80834	19.05715	-6.49508
C	6.96925	18.75904	-7.88077
C	5.74978	19.92252	-6.07507
C	6.04052	19.27697	-8.79076
C	4.85770	20.41039	-7.03172
C	4.98527	20.08490	-8.38118
H	6.15149	19.04307	-9.84628
H	4.04685	21.06104	-6.71928
H	4.27548	20.47092	-9.10737
C	11.41095	19.09901	-5.59180
C	12.58870	19.58509	-4.71727
H	12.22672	19.91736	-3.73908
H	13.33731	18.80788	-4.56237
H	13.07929	20.43507	-5.20459
C	10.47779	20.29650	-5.83727
H	9.63153	20.02295	-6.46921
H	10.08414	20.68592	-4.89352
H	11.03510	21.10150	-6.32696
C	11.94000	18.58973	-6.94760
H	12.41121	19.41320	-7.49449
H	12.68817	17.80504	-6.82037
H	11.12407	18.19761	-7.55922
C	5.64019	20.35964	-4.61966
H	6.07325	19.56421	-4.00759
C	4.19918	20.58780	-4.13448
H	3.56526	19.71574	-4.32240
H	4.19599	20.78320	-3.05628
H	3.73106	21.45388	-4.61532
C	6.48899	21.62823	-4.38779
H	7.52767	21.46605	-4.68964
H	6.09737	22.46838	-4.97295
H	6.47814	21.91859	-3.33054
C	8.13135	17.92616	-8.41028
H	8.76566	17.66600	-7.55856
C	7.66663	16.60723	-9.05533
H	7.10715	15.99338	-8.34555
H	7.01979	16.78984	-9.92099
H	8.52857	16.02534	-9.40097
C	8.98810	18.73350	-9.40700
H	9.34992	19.66615	-8.96353
H	9.85754	18.14880	-9.72841
H	8.41794	18.99381	-10.30545
C	7.87496	14.04629	-1.23165
H	8.12428	15.10555	-1.13028
C	7.15216	13.60901	0.06134
H	6.18209	14.09824	0.18322
H	6.97645	12.52808	0.06891
H	7.76621	13.84609	0.93726
C	9.20729	13.28548	-1.35743
H	9.76771	13.60365	-2.23691
H	9.82507	13.45707	-0.46831
H	9.04378	12.20591	-1.44505
C	5.17209	15.84223	-5.25960
H	5.96823	16.58883	-5.33957
C	4.79507	15.41595	-6.68840
H	5.58283	14.81846	-7.15714
H	3.87159	14.82607	-6.70979
H	4.62836	16.30292	-7.30664
C	3.96224	16.53607	-4.59825
H	3.60831	17.35904	-5.22797
H	3.13553	15.82862	-4.46479
H	4.21229	16.94884	-3.61766
H	11.75930	13.89735	-3.87486
H	8.18814	14.35338	-6.21970

Intermediate **I.4a**:
G (a.u.) = -2047.651977

C	10.54834	7.37929	3.89549
C	11.04386	7.24961	2.60141
C	10.25160	6.36835	1.63227
C	9.22687	7.08796	0.75722
H	9.69148	7.78684	0.04948
H	8.53659	7.66500	1.37385
H	8.63466	6.36755	0.18456
C	10.91201	5.21622	0.96891
H	10.56217	5.02118	-0.04262
C	11.69355	4.16529	1.49249

C	12.22383	3.12427	0.52745
H	12.22892	3.51362	-0.49257
H	11.62692	2.20811	0.54708
H	13.24751	2.85183	0.79983
C	12.75246	3.07082	3.43804
C	14.01594	3.56792	3.85191
C	14.92310	2.69377	4.46168
H	15.89393	3.07057	4.76981
C	14.60847	1.35760	4.68106
H	15.32304	0.69528	5.16172
C	13.37041	0.87748	4.27255
H	13.12676	-0.16830	4.43685
C	12.42900	1.70267	3.64171
N	9.61683	6.43014	4.34674
N	8.31346	3.96129	2.69799
N	11.81883	3.99347	2.85547
Nb	9.85774	4.81044	3.03796
C	12.28013	7.90001	2.09187
C	12.47870	8.05693	0.70206
C	13.32606	8.35305	2.92807
C	13.62151	8.66438	0.18343
H	11.72829	7.70020	0.00925
C	14.46474	8.96568	2.41077
H	13.25493	8.21916	3.99868
C	14.62190	9.13453	1.03309
H	13.72491	8.77069	-0.89318
H	15.23965	9.30519	3.09314
H	15.51084	9.61234	0.63169
C	10.97651	8.45213	4.84489
C	11.47444	8.14132	6.11889
C	10.87364	9.80215	4.47468
C	11.87083	9.15166	6.99517
H	11.57444	7.10241	6.41099
C	11.25947	10.81301	5.35414
H	10.49554	10.05346	3.48901
C	11.76096	10.49118	6.61728
H	12.26610	8.89194	7.97323
H	11.17161	11.85245	5.05107
H	12.06476	11.27836	7.30131
C	11.11489	1.06207	3.19976
H	10.51460	1.82395	2.69486
C	11.34453	-0.09434	2.20374
H	11.95820	0.21127	1.35168
H	11.85105	-0.93805	2.68431
H	10.38675	-0.46346	1.81982
C	10.29236	0.55522	4.39993
H	10.06511	1.36288	5.09877
H	9.34504	0.12112	4.06091
H	10.83224	-0.22211	4.95147
C	14.43232	5.01483	3.61850
H	13.54720	5.56646	3.29704
C	15.47532	5.11305	2.48684
H	15.10251	4.66249	1.56125
H	15.71435	6.16028	2.27675
H	16.40364	4.59619	2.75727
C	14.95595	5.68843	4.90038
H	15.18105	6.74167	4.70598
H	14.21664	5.64179	5.70693
H	15.87661	5.22052	5.26566
C	8.67069	6.70624	5.39041
C	7.65199	7.68267	5.21970
C	8.72170	5.94668	6.59021
C	6.70923	7.86043	6.23873
C	7.74717	6.16219	7.57296
C	6.74381	7.10828	7.40747
H	5.92305	8.59765	6.10672
H	7.78106	5.57869	8.48836
H	5.99696	7.26009	8.18165
C	7.18201	3.13144	2.33609
C	7.61002	2.09829	1.27185
H	7.99277	2.60438	0.37975
H	8.39656	1.44523	1.66115
H	6.76097	1.47256	0.97377
C	6.66147	2.40498	3.59421
H	6.36601	3.13007	4.35840
H	5.79033	1.78663	3.34948
H	7.43563	1.75701	4.01523
C	6.06388	4.02679	1.76094
H	5.20031	3.42274	1.45958
H	5.73219	4.75238	2.50859
H	6.42428	4.57577	0.88554
C	9.78958	4.89163	6.86729
H	10.55721	4.97870	6.09080
C	7.48954	8.50396	3.94327
H	8.40532	8.40771	3.35800
C	7.28477	10.00645	4.21515
H	7.28790	10.56166	3.27033
H	6.32516	10.20848	4.70260
H	8.07798	10.40947	4.85055
C	6.33457	7.94664	3.08690
H	6.22745	8.51885	2.15768
H	6.50922	6.89961	2.82605
H	5.38344	8.00703	3.62768
C	10.48975	5.09360	8.22626
H	10.87262	6.11212	8.33830
H	9.81067	4.90435	9.06424
H	11.33026	4.39788	8.32505
C	9.20077	3.47024	6.78545
H	8.41427	3.32988	7.53542
H	8.75421	3.27710	5.80470
H	9.97654	2.71874	6.96931

Intermediate **I.4b**:
G (a.u.) = -2047.647248

C	10.43894	7.11614	4.27537
C	11.01921	7.19137	3.01284
C	10.26156	6.55439	1.84999
C	9.26406	7.46636	1.14638
H	9.74990	8.33228	0.67932
H	8.53941	7.85682	1.86563
H	8.71569	6.92833	0.36929
C	10.88996	5.51485	1.02138
H	10.46547	5.42119	0.02326
C	11.66156	4.39900	1.40357
C	11.91659	3.33679	0.34374
H	12.34411	3.77680	-0.56118
H	10.97190	2.85540	0.06853
H	12.59322	2.56490	0.70941
C	12.96936	3.30528	3.18262
C	14.27775	3.40861	2.62262
C	15.26205	2.50193	3.03755
H	16.25347	2.57304	2.59988
C	15.01833	1.53919	4.00678
H	15.79844	0.84597	4.30752
C	13.76754	1.50170	4.61354
H	13.58674	0.77966	5.40230
C	12.73900	2.37022	4.23601
C	7.45263	3.08508	1.74393
C	7.50870	1.65847	1.73072
C	6.49137	0.94288	1.09293
H	6.53881	-0.14278	1.08109
C	5.42097	1.58256	0.47596
H	4.64289	1.00474	-0.01469
C	5.35791	2.97219	0.50156
H	4.51934	3.47462	0.02662
C	6.34507	3.74187	1.12301
N	9.44230	6.14449	4.49037
N	8.44908	3.83543	2.35319
N	11.91053	4.14393	2.74528
Nb	9.88045	4.76234	2.98446
C	8.21537	6.38729	5.32050
C	12.30334	7.87681	2.69625
C	12.53835	8.36174	1.39088
C	13.34055	8.06844	3.63486
C	13.70602	9.04751	1.05955
H	11.79519	8.20921	0.61894
C	14.50321	8.76164	3.30680
H	13.24226	7.67015	4.63510
C	14.69354	9.26736	2.01962
H	13.83836	9.41445	0.04524
H	15.27250	8.89305	4.06294
H	15.60020	9.80946	1.76686
C	10.90936	7.98450	5.40465
C	11.52051	7.44653	6.54819
C	10.75615	9.37574	5.31733
C	11.96994	8.27771	7.57290
H	11.64627	6.37213	6.62906
C	11.19166	10.20802	6.34956
H	10.29893	9.80325	4.43001
C	11.80269	9.66196	7.47924
H	12.44967	7.84498	8.44634
H	11.05905	11.28300	6.26700
H	12.14824	10.30900	8.28032
C	7.33667	5.12731	5.23030
H	7.05811	4.89912	4.20093
H	7.86041	4.25608	5.64088
H	6.42332	5.27329	5.81546
C	8.49930	6.62661	6.82126
H	9.15614	5.85002	7.22344
H	8.94864	7.59811	7.02093
H	7.55113	6.58189	7.36800
C	7.43438	7.58894	4.75081
H	7.14543	7.40571	3.71192
H	6.52211	7.76156	5.33220
H	8.03314	8.50351	4.79006

C	8.63059	0.88169	2.40573
H	9.30505	1.61034	2.86252
C	8.08447	-0.02247	3.52872
H	7.54323	0.56214	4.27991
H	7.39260	-0.77479	3.13486
H	8.89861	-0.55431	4.03141
C	9.45318	0.06052	1.39396
H	9.86450	0.69800	0.60493
H	10.28889	-0.44321	1.89302
H	8.84223	-0.71029	0.91125
C	6.20481	5.25830	1.10715
H	7.07113	5.66898	1.63013
C	6.21586	5.81403	-0.33053
H	6.17760	6.90940	-0.32399
H	7.11767	5.50605	-0.87013
H	5.35332	5.45825	-0.90469
C	4.94117	5.72452	1.85709
H	4.02846	5.36198	1.37136
H	4.93336	5.36050	2.88907
H	4.88915	6.81930	1.88160
C	11.43604	2.33919	5.02525
H	10.62473	2.64830	4.34961
C	11.04659	0.95152	5.56051
H	11.08112	0.19123	4.77517
H	11.70502	0.62784	6.37355
H	10.02960	0.97909	5.96422
C	11.49878	3.35280	6.18672
H	11.73526	4.35556	5.82292
H	10.54474	3.39832	6.72445
H	12.27942	3.06090	6.89806
C	14.72701	4.52706	1.67749
H	13.86511	5.14080	1.41020
C	15.35849	4.00695	0.37017
H	14.69646	3.32436	-0.16866
H	15.59321	4.84616	-0.29375
H	16.29597	3.47383	0.56179
C	15.72306	5.45690	2.40163
H	15.98498	6.30721	1.76369
H	15.29369	5.85355	3.32445
H	16.64644	4.92510	2.65684

Intermediate **I.5**:
G (a.u.) = -1153.383116

Nb	8.73785	17.16951	4.83209
N	7.98803	17.32276	6.47168
N	10.35171	18.04400	4.75138
N	7.55155	16.21088	2.97827
C	7.73889	17.72439	7.82080
C	11.44688	18.81624	5.05210
C	11.99432	18.85402	6.35764
C	13.11231	19.63428	6.64026
H	13.51587	19.64463	7.64982
C	13.71337	20.40677	5.64142
H	14.58264	21.01723	5.86784
C	13.18310	20.38321	4.34837
H	13.64174	20.97933	3.56328
C	12.07300	19.59619	4.05105
C	7.55819	20.22915	4.37326
H	6.93895	20.90306	3.76417
H	8.58346	20.61720	4.40052
H	7.20009	20.26523	5.40972
C	7.55906	18.81260	3.88313
C	6.82125	18.46643	2.79158
H	6.21221	19.18137	2.23371
C	6.82279	17.09735	2.33140
C	5.98294	16.72706	1.13130
H	5.15135	16.08042	1.43178
H	6.56865	16.16591	0.39771
H	5.57235	17.61897	0.65577
C	7.54571	14.85028	2.54809
C	6.57985	13.95729	3.03284
C	6.59960	12.61723	2.64131
H	5.84292	11.93652	3.02154
C	7.58099	12.15315	1.76301
H	7.59459	11.11079	1.45914
C	8.54305	13.04076	1.27581
H	9.30776	12.69077	0.58791
C	8.52908	14.38048	1.66603
C	9.25310	14.58427	5.45637
C	10.19581	14.85946	4.72866
H	5.81756	14.32330	3.71508
H	9.27674	15.07397	1.29176
H	11.66089	19.57024	3.04637
H	11.51934	18.25861	7.13201
H	8.57100	18.30106	8.25135
H	6.83345	18.34689	7.88324
H	7.56654	16.85254	8.47192
C	8.23029	14.01252	6.34781
H	8.26991	14.53552	7.30916
H	7.23552	14.21157	5.93615
C	11.41911	14.97013	3.91417
H	11.32893	15.80722	3.21634
H	11.49632	14.05589	3.31122
C	8.42238	12.49720	6.54076
H	7.65740	12.10866	7.22023
H	8.33640	11.97011	5.58651
H	9.40447	12.27588	6.96831
C	12.68537	15.15235	4.77050
H	12.81015	14.31893	5.46814
H	13.56656	15.19432	4.12307
H	12.63251	16.08217	5.34052

Intermediate **I.6a**:
G (a.u.) = -1153.398129

Nb	8.68654	17.57882	4.23199
N	7.47081	18.41214	5.25129
N	10.48975	18.11453	4.98422
N	7.28723	16.06150	3.09550
C	6.64725	18.95717	6.28605
C	10.94968	19.01003	5.95615
C	11.60422	18.58862	7.13129
C	12.01631	19.52022	8.08293
H	12.51416	19.17315	8.98464
C	11.78691	20.88471	7.89356
H	12.11332	21.60569	8.63698
C	11.13235	21.30981	6.73402
H	10.94749	22.36823	6.57058
C	10.72234	20.38832	5.77386
C	9.10690	19.62059	1.61709
H	8.91069	19.78933	0.54903
H	10.19324	19.59490	1.76955
H	8.74659	20.49482	2.17476
C	8.46515	18.36690	2.14293
C	7.71468	17.58476	1.32770
H	7.53203	17.82801	0.27731
C	7.05000	16.39711	1.85286
C	6.09687	15.67530	0.93202
H	5.40911	15.01922	1.46458
H	6.65682	15.07090	0.20812
H	5.52752	16.41093	0.35621
C	6.68049	14.93173	3.71312
C	5.97225	15.11800	4.90940
C	5.39052	14.02864	5.55653
H	4.83609	14.18762	6.47697
C	5.52315	12.74028	5.03260
H	5.07579	11.89298	5.54339
C	6.24418	12.54900	3.85307
H	6.36474	11.55044	3.44287
C	6.82161	13.63570	3.19495
C	9.99651	15.85435	4.75857
C	11.00626	16.76047	4.85804
H	5.88722	16.12053	5.31485
H	7.39818	13.48105	2.28830
H	10.22935	20.71737	4.86394
H	11.75789	17.52865	7.30550
H	7.26070	19.34508	7.11073
H	6.03355	19.78659	5.90715
H	5.96556	18.20271	6.70659
C	10.17023	14.37637	4.55333
H	11.21471	14.11642	4.32273
H	9.57505	14.04520	3.69269
C	12.49681	16.58812	4.63116
H	12.75801	15.53175	4.74758
H	13.05108	17.13780	5.39981
C	12.94329	17.08904	3.24593
H	14.02722	16.99019	3.12553
H	12.45839	16.51684	2.44768
H	12.68320	18.14347	3.11162
C	9.72062	13.56722	5.78418
H	9.83705	12.49183	5.60958
H	10.31480	13.83576	6.66423
H	8.67020	13.76553	6.01609

Intermediate **I.6b**:
G (a.u.) = -1153.402839

Nb	9.48597	16.37587	4.52487
N	9.65432	16.02787	6.48405
N	10.27665	17.98093	4.20451
N	9.28814	15.65397	2.29040
C	10.05091	16.70183	7.70495
C	11.10469	19.06291	4.00699
C	12.49069	18.99134	4.27694
C	13.31006	20.09972	4.07601
H	14.37231	20.02490	4.29409

C	12.77879	21.29971	3.59521
H	13.42223	22.16023	3.43759
C	11.41071	21.38106	3.31953
H	10.98677	22.30939	2.94544
C	10.57962	20.28272	3.52377
C	6.25218	17.10165	4.91232
H	5.25388	17.10240	4.45288
H	6.48263	18.12423	5.23783
H	6.21178	16.49856	5.82813
C	7.32383	16.59271	3.98948
C	7.01955	16.19082	2.73093
H	6.00341	16.22848	2.32853
C	8.07092	15.74342	1.82086
C	7.67541	15.46670	0.39133
H	8.52886	15.43736	-0.28517
H	6.97212	16.23596	0.05832
H	7.14942	14.50661	0.32442
C	10.39016	15.23315	1.49340
C	10.40766	13.98326	0.85651
C	11.52397	13.58632	0.11929
H	11.52622	12.61433	-0.36573
C	12.63230	14.42760	0.01015
H	13.50009	14.11650	-0.56363
C	12.62027	15.66859	0.65174
H	13.47860	16.32984	0.57603
C	11.51245	16.06931	1.39814
H	9.55419	13.31965	0.95554
H	11.50270	17.02710	1.90751
H	9.51567	20.34080	3.31521
H	12.89967	18.05672	4.64948
H	11.12144	16.55636	7.91500
H	9.86369	17.77325	7.60229
H	9.48729	16.33965	8.57633
C	9.97600	14.63037	6.29072
C	9.71788	13.66382	7.42861
H	10.27427	13.99635	8.31538
H	10.12259	12.68279	7.16301
C	8.22692	13.53614	7.78710
H	7.65795	13.13778	6.94051
H	8.08473	12.86318	8.63905
H	7.79742	14.50842	8.04767
C	10.74179	13.06051	4.42907
H	10.45958	12.23406	5.09964
H	10.19936	12.89100	3.49010
C	10.36477	14.39453	5.00605
C	12.25018	12.96195	4.13307
H	12.55913	13.74320	3.43245
H	12.83566	13.08317	5.05084
H	12.50069	11.98955	3.69456

Intermediate **I.7a**:
G (a.u.) = -1153.438544

C	9.75265	6.77539	4.44746
H	10.33066	7.66648	4.71657
H	8.94655	6.64402	5.17281
H	9.30010	6.96980	3.47127
C	10.64776	5.55135	4.40512
C	10.37818	4.46967	5.26611
H	9.63086	4.68211	6.02731
C	11.16834	3.24619	5.50256
C	10.71690	2.36631	6.65928
H	10.42876	2.97589	7.52175
H	11.53133	1.70745	6.97240
H	9.86121	1.73291	6.38995
C	11.79054	2.54842	4.29429
C	13.15017	2.36153	4.24109
C	15.07102	2.51836	5.80037
C	15.13361	1.15044	6.12587
C	16.24370	0.63156	6.79143
H	16.27128	-0.42707	7.03540
C	17.30553	1.46114	7.15650
H	18.16735	1.05388	7.67639
C	17.24556	2.82229	6.84506
H	18.06520	3.48015	7.12089
C	16.14658	3.34607	6.16839
C	12.08992	6.36317	2.57595
C	13.29884	7.06860	2.44138
C	13.57530	7.78717	1.27993
H	14.51411	8.32821	1.19868
C	12.65334	7.82409	0.23085
H	12.86918	8.38890	-0.67089
C	11.45308	7.12098	0.35438
H	10.73149	7.12974	-0.45817
C	11.17277	6.39131	1.50860
C	13.31317	6.36689	8.14962
N	11.85444	5.59603	3.72596
N	13.94951	3.08222	5.16463
N	13.08790	5.57507	6.97827
Nb	12.73587	4.72453	5.43903
H	12.36336	6.72140	8.57437
H	13.82878	5.78737	8.92784
H	13.92521	7.25264	7.92750
H	14.29853	0.50430	5.87180
H	16.10531	4.40128	5.91359
H	10.25314	5.81850	1.58347
H	14.00820	7.05522	3.26493
C	13.86736	1.64275	3.11246
H	13.20289	0.90073	2.66158
H	14.71130	1.08717	3.53204
C	10.86690	2.18110	3.14822
H	11.43707	2.02803	2.22740
H	10.21327	3.04292	2.95954
C	14.39649	2.60656	2.03430
H	13.58151	3.16493	1.56299
H	15.09018	3.33152	2.47002
H	14.92994	2.05540	1.25318
C	9.98621	0.94506	3.40662
H	9.35198	0.73658	2.53811
H	10.59644	0.05638	3.59999
H	9.32877	1.09212	4.26843

Intermediate **I.7b**:
G (a.u.) = -1153.443400

C	11.68960	7.04168	6.16270
H	11.01111	6.27488	6.54831
H	12.04858	7.63456	7.00999
H	12.54755	6.52836	5.71731
C	10.98749	7.93899	5.12763
H	10.16127	8.47302	5.61326
H	11.67435	8.71250	4.77635
C	10.43059	7.17268	3.94369
C	11.01621	7.15026	2.69764
C	12.41302	7.68537	2.43867
H	12.97086	7.77697	3.37588
H	12.94952	6.93555	1.84256
C	12.45983	9.03065	1.69108
H	11.98863	8.96032	0.70640
H	13.49629	9.35227	1.54053
H	11.94110	9.81505	2.25258
C	10.29693	6.47198	1.53227
C	9.40800	7.34666	0.65909
H	9.98925	8.06770	0.06909
H	8.71057	7.91467	1.28082
H	8.82111	6.73673	-0.03519
C	10.97862	5.35382	0.85074
H	10.67196	5.19103	-0.18015
C	11.71221	4.29124	1.41247
C	12.20661	3.17059	0.51809
H	13.29669	3.08969	0.54790
H	11.90945	3.34121	-0.51905
H	11.80331	2.20684	0.84765
C	12.73547	3.44350	3.49525
C	14.10057	3.56065	3.17359
C	15.06316	2.88193	3.91934
H	16.11200	2.98518	3.65430
C	14.69172	2.08712	5.00576
H	15.44467	1.56181	5.58527
C	13.33953	1.98057	5.34111
H	13.03463	1.36702	6.18446
C	12.36972	2.64746	4.59530
C	7.29519	2.98802	2.00925
C	7.51783	1.59336	1.99192
C	6.50183	0.71712	1.61836
H	6.69332	-0.35275	1.61206
C	5.24358	1.20355	1.25263
H	4.45418	0.51695	0.96137
C	5.01086	2.58169	1.26507
H	4.03602	2.97017	0.98205
C	6.01956	3.46647	1.63814
N	9.34476	6.30609	4.16944
N	8.28971	3.86859	2.38143
N	11.75101	4.15252	2.79197
Nb	9.76012	4.83737	2.82567
C	8.26935	6.66534	5.08270
H	8.61423	6.75030	6.12153
H	7.80139	7.61954	4.80154
H	7.50521	5.88631	5.04574
H	8.49709	1.21969	2.27702
H	5.84571	4.53825	1.64989
H	11.31644	2.55078	4.84583
H	14.39979	4.20480	2.35218

Intermediate **I.8**:
G (a.u.) = -1191.593601

Nb	8.61586	17.20568	4.90362
N	7.86764	17.31666	6.54787
N	10.25018	18.04472	4.84487
N	7.45035	16.25431	3.03067
C	7.62651	17.60126	7.92713
C	11.39097	18.73253	5.17586
C	11.46731	19.52435	6.34754
C	12.63250	20.21602	6.66642
H	12.66630	20.82063	7.56935
C	13.75650	20.13727	5.83784
H	14.66396	20.67741	6.09164
C	13.69846	19.35953	4.67780
H	14.56501	19.29470	4.02446
C	12.53494	18.67033	4.34513
C	7.47637	20.27829	4.42506
H	6.87257	20.95648	3.80533
H	8.50460	20.65773	4.46594
H	7.10278	20.31913	5.45582
C	7.47422	18.86136	3.93635
C	6.76122	18.52362	2.82552
H	6.17511	19.24605	2.25303
C	6.75260	17.15509	2.36693
C	5.94047	16.79828	1.14383
H	5.21775	16.00900	1.37290
H	6.58664	16.41108	0.34938
H	5.40480	17.67001	0.76589
C	7.43217	14.89819	2.58554
C	6.50162	13.99226	3.11616
C	6.50615	12.65777	2.70641
H	5.77795	11.96724	3.12246
C	7.43846	12.21067	1.76769
H	7.44114	11.17186	1.45185
C	8.36724	13.10888	1.23813
H	9.09527	12.77124	0.50592
C	8.36728	14.44474	1.64355
H	5.77871	14.34607	3.84625
H	9.08714	15.14787	1.23317
H	12.47992	18.07464	3.43850
H	10.59155	19.58072	6.98728
H	8.50655	18.02672	8.43379
H	6.80083	18.32010	8.03799
H	7.33109	16.69392	8.47620
C	9.66526	14.27078	6.97251
C	11.39583	14.84628	5.63322
C	10.84496	15.26768	7.01415
H	11.54597	15.06362	7.83057
H	10.53025	16.31177	7.04930
C	10.44833	12.91914	6.81105
H	10.79883	12.57361	7.78890
H	9.82509	12.12737	6.38558
C	11.64355	13.31716	5.88691
H	12.60321	13.17480	6.39393
H	11.67328	12.74139	4.95741
H	8.95510	14.29173	7.80031
H	12.25365	15.39730	5.24713
C	9.09295	14.54458	5.59053
H	8.10397	14.23950	5.26582
C	10.13363	14.89011	4.78547
H	10.12485	14.90409	3.70051

Intermediate **I.9a**:
G (a.u.) = -1191.588517

Nb	9.39180	16.24299	4.45729
N	9.07697	15.63546	6.36940
N	10.63527	17.52101	4.28459
N	8.95526	15.74922	2.19919
C	6.56267	17.96786	4.88554
H	5.58936	18.25571	4.46435
H	7.09424	18.88566	5.16978
H	6.39085	17.42333	5.82176
C	7.39616	17.15742	3.93198
C	6.95204	16.90582	2.67567
H	5.99199	17.26640	2.29693
C	7.80346	16.17326	1.74810
C	7.31512	15.99231	0.33292
H	8.10745	15.69442	-0.35309
H	6.86357	16.92686	-0.01386
H	6.52711	15.23020	0.30177
C	9.86487	15.00125	1.40000
C	9.51518	13.75639	0.85724
C	10.44770	13.02580	0.11900
H	10.16568	12.06165	-0.29447
C	11.73490	13.52599	-0.08290
H	12.45902	12.95563	-0.65684
C	12.08794	14.76153	0.46642
H	13.08925	15.15617	0.31945
C	11.16463	15.49287	1.21208
H	8.51853	13.36014	1.02714
H	11.43408	16.44242	1.66273
C	9.92503	14.11300	4.59785
C	11.27342	13.38172	4.75364
C	10.56401	13.57274	6.89715
C	9.38081	14.20345	6.09605
H	9.23541	13.52936	3.97310
H	8.47837	13.59006	6.24027
C	10.97855	12.43230	5.94187
H	11.85468	11.87684	6.29813
H	10.17061	11.72061	5.73691
C	12.32528	14.32367	5.38458
H	13.31776	13.85802	5.37082
H	12.39337	15.27467	4.84883
C	11.80605	14.49208	6.84946
H	12.54929	14.15171	7.57792
H	11.55884	15.52775	7.09500
H	11.60647	12.90705	3.82695
H	10.28093	13.27570	7.90983
C	8.72432	16.07645	7.64384
C	8.26921	15.20899	8.65800
C	8.78913	17.45692	7.93491
C	7.89324	15.70930	9.90519
H	8.19831	14.14431	8.46698
C	8.41558	17.94412	9.18250
H	9.14967	18.13405	7.16491
C	7.96289	17.07480	10.18082
H	7.54293	15.01866	10.66797
H	8.48114	19.01111	9.37917
H	7.67267	17.45690	11.15475
C	11.62781	18.54830	4.35829
H	12.12199	18.68890	3.38589
H	11.19291	19.51475	4.65056
H	12.40842	18.29720	5.09043

Intermediate **I.9b**:
G (a.u.) = -1191.592790

Nb	9.34498	16.24017	4.41799
N	9.07049	15.71483	6.31857
N	10.49099	17.62275	4.16165
N	8.91628	15.65833	2.17567
C	8.75555	16.12609	7.66663
C	11.31627	18.72454	4.17580
C	12.42958	18.79636	5.04267
C	13.25690	19.91662	5.04080
H	14.10669	19.95220	5.71775
C	13.00635	20.98766	4.17837
H	13.65613	21.85772	4.17988
C	11.91027	20.92509	3.31369
H	11.70366	21.75130	2.63812
C	11.07186	19.81285	3.30842
C	6.41858	17.77423	4.84926
H	5.46017	18.07534	4.40387
H	6.93380	18.68041	5.19398
H	6.21006	17.18373	5.75007
C	7.29055	17.00078	3.89891
C	6.85590	16.70949	2.64851
H	5.87641	17.01382	2.27027
C	7.74297	16.01308	1.72379
C	7.26147	15.79356	0.31197
H	8.06585	15.52249	-0.37107
H	6.76920	16.70318	-0.04588
H	6.50739	14.99749	0.29148
C	9.87019	14.95923	1.38405
C	9.59554	13.69101	0.85236
C	10.57196	13.01014	0.12340
H	10.34872	12.02742	-0.28225
C	11.82802	13.58398	-0.07930
H	12.58630	13.05236	-0.64633
C	12.10596	14.84309	0.45953
H	13.08235	15.29543	0.31182
C	11.13929	15.52628	1.19624
H	8.62334	13.23840	1.02357
H	11.35229	16.49497	1.63686
H	10.21645	19.76189	2.64142
H	12.62569	17.96155	5.70854
H	9.60685	15.99281	8.34985
H	8.47314	17.18226	7.68042
H	7.91531	15.53955	8.07238
C	9.95286	14.13238	4.61931
C	11.31728	13.43748	4.79799
C	10.62676	13.73542	6.93529
C	9.41989	14.28511	6.11125
H	9.27091	13.51621	4.01811
H	8.53666	13.65656	6.31609

C	11.05827	12.55057	6.04291
H	11.95115	12.03589	6.41819
H	10.26390	11.81135	5.88995
C	12.35573	14.43542	5.36036
H	13.35745	13.99017	5.36320
H	12.40032	15.35495	4.77010
C	11.84755	14.67852	6.81844
H	12.60634	14.40200	7.55797
H	11.58029	15.72338	6.99729
H	11.65053	12.91759	3.89612
H	10.35483	13.48888	7.96630

Intermediate **I.10a**:
G (a.u.) = -1191.605200

C	10.46194	6.52087	1.40546
C	9.58362	7.23118	0.38015
H	10.17244	7.91803	-0.24661
H	8.81050	7.82255	0.88029
H	9.07626	6.51860	-0.27619
C	11.21947	5.38983	0.83618
H	10.98974	5.19604	-0.20983
C	11.88513	4.31619	1.45755
C	12.41025	3.18008	0.60006
H	13.50171	3.12525	0.64225
H	12.12217	3.31470	-0.44481
H	12.02550	2.21862	0.95580
C	12.73645	3.41715	3.59133
C	14.12420	3.45464	3.36101
C	14.99371	2.72159	4.16710
H	16.06202	2.76340	3.97278
C	14.50520	1.95198	5.22495
H	15.18628	1.38511	5.85218
C	13.13029	1.92543	5.47064
H	12.73500	1.33378	6.29165
C	12.25273	2.64591	4.66288
N	9.51262	6.40129	4.15601
N	8.44019	3.97242	2.28611
N	11.84428	4.18760	2.83141
Nb	9.87603	4.93351	2.75606
H	11.18176	2.60926	4.84442
H	14.51536	4.08125	2.56533
C	12.53600	7.51883	2.92127
C	11.39106	7.98779	4.82209
C	12.48708	7.00330	4.37796
H	13.43638	7.15510	4.90331
H	12.19853	5.95937	4.48304
C	12.90473	9.00015	3.18447
H	13.96733	9.09053	3.43494
H	12.71652	9.64581	2.32037
C	12.00826	9.35490	4.41989
H	12.60439	9.76776	5.23936
H	11.23949	10.09811	4.17824
H	13.21088	7.00074	2.23644
H	11.07814	7.92771	5.86671
C	11.04070	7.53468	2.45679
H	10.88791	8.49470	1.95253
C	10.24812	7.64395	3.82615
H	9.52461	8.46613	3.75327
C	8.56426	6.45675	5.19295
C	8.19204	7.64404	5.85756
C	7.94071	5.25968	5.61283
C	7.22857	7.62809	6.86859
H	8.64993	8.58932	5.59352
C	6.97675	5.25424	6.61346
H	8.21945	4.32398	5.13317
C	6.60914	6.44181	7.25502
H	6.96572	8.56259	7.35765
H	6.51724	4.31294	6.90335
H	5.86443	6.43652	8.04490
C	7.42666	3.00382	1.98922
H	7.49303	2.12945	2.65230
H	6.42367	3.43679	2.10419
H	7.51717	2.64154	0.95566

Intermediate **I.10b**:
G (a.u.) = -1191.6111

C	10.48182	6.59648	1.46175
C	9.61466	7.37177	0.47341
H	10.21647	8.07170	-0.12603
H	8.85877	7.95905	1.00379
H	9.08692	6.70183	-0.21123
C	11.21538	5.48089	0.82966
H	10.98231	5.35006	-0.22556
C	11.86165	4.36290	1.39002
C	12.37506	3.27129	0.46976
H	13.46870	3.25154	0.45093
H	12.02768	3.43098	-0.55341
H	12.03959	2.28679	0.81055
C	12.70013	3.35072	3.48051
C	14.08553	3.35725	3.23321
C	14.94445	2.57742	4.00612
H	16.01094	2.59572	3.79852
C	14.44860	1.79075	5.04780
H	15.12162	1.18670	5.64847
C	13.07660	1.79466	5.31121
H	12.67539	1.18938	6.11937
C	12.20903	2.56175	4.53640
C	7.38481	3.09334	2.02643
C	7.68950	1.71778	1.92654
C	6.68732	0.78634	1.66614
H	6.94262	-0.26770	1.59428
C	5.36250	1.19741	1.49521
H	4.58438	0.46802	1.29072
C	5.04929	2.55631	1.58872
H	4.02247	2.88706	1.45630
C	6.04293	3.49603	1.85170
N	9.57136	6.31984	4.17100
N	8.36150	4.03389	2.28531
N	11.81707	4.16242	2.75543
Nb	9.86379	4.94771	2.73190
C	8.54997	6.42420	5.20381
H	8.99033	6.59035	6.19761
H	7.86024	7.25969	5.00231
H	7.96511	5.50167	5.24777
H	8.72056	1.40133	2.05652
H	5.80661	4.55322	1.92485
H	11.13953	2.54814	4.72990
H	14.48464	3.99575	2.45126
C	12.58798	7.51023	2.99025
C	11.48083	7.83194	4.94304
C	12.56728	6.88497	4.40490
H	13.52720	6.99701	4.92101
H	12.27852	5.83679	4.43425
C	12.96014	8.96859	3.35831
H	14.02803	9.04288	3.59075
H	12.75141	9.67793	2.55077
C	12.09216	9.22634	4.63729
H	12.70778	9.57230	5.47323
H	11.31970	9.98636	4.47263
H	13.25188	7.04723	2.25679
H	11.18731	7.69538	5.98739
C	11.08598	7.55643	2.55437
H	10.92500	8.54312	2.10757
C	10.32130	7.57063	3.94214
H	9.59536	8.39947	3.96845

Transiton state **TS.1a**:
G (a.u.) = -2047.595757

Nb	0.29421	-0.13789	-0.27923
N	-0.64376	0.50011	1.13456
N	2.23000	0.30980	-0.01793
N	-1.52775	-1.23361	-1.63996
C	0.36072	2.59175	-2.18813
H	0.29107	3.23650	-1.30388
H	-0.08956	3.13153	-3.03406
H	1.43044	2.46354	-2.38977
C	-0.30110	1.26227	-1.93630
C	-1.38552	0.91766	-2.66535
H	-1.81989	1.57910	-3.42019
C	-2.03750	-0.37221	-2.48080
C	-3.26219	-0.62441	-3.32752
H	-3.88651	-1.42843	-2.94015
H	-2.95809	-0.88714	-4.34679
H	-3.84993	0.29524	-3.40170
C	-2.08249	-2.56320	-1.58385
C	-2.85804	-2.94106	-0.45946
C	-3.32013	-4.25985	-0.38301
H	-3.91302	-4.56678	0.47138
C	-3.03868	-5.18670	-1.38268
H	-3.40011	-6.20778	-1.29897
C	-2.30665	-4.79165	-2.49454
H	-2.10588	-5.51237	-3.28156
C	-1.82640	-3.48238	-2.63440
C	1.64321	-1.93715	-0.30823
C	2.65272	-1.01713	-0.43371
C	3.98700	-1.23703	-1.08187
C	4.98403	-1.99571	-0.46177
C	4.23042	-0.72621	-2.36440
C	6.20908	-2.21660	-1.09173
H	4.79679	-2.41932	0.52072
C	5.44649	-0.95846	-3.00839
H	3.44205	-0.15049	-2.84435
C	6.44415	-1.70001	-2.36872
H	6.97517	-2.80099	-0.58989

H	5.61672	-0.55707	-4.00356
H	7.39531	-1.87608	-2.86274
C	1.70508	-3.38726	-0.51265
C	2.67865	-4.06393	-1.28528
C	0.75088	-4.18232	0.15762
C	2.70080	-5.45473	-1.35920
H	3.41148	-3.49624	-1.84597
C	0.78078	-5.57437	0.09163
H	-0.01343	-3.68539	0.74565
C	1.75964	-6.22020	-0.66527
H	3.45900	-5.94424	-1.96511
H	0.03134	-6.15159	0.62539
H	1.78547	-7.30490	-0.72110
C	-3.24428	-1.92374	0.61004
H	-2.39252	-1.25285	0.75614
C	-3.57577	-2.55654	1.97119
H	-3.65254	-1.77088	2.72756
H	-4.53489	-3.08694	1.95533
H	-2.80434	-3.26337	2.29276
C	-4.43479	-1.05539	0.14534
H	-4.15224	-0.36632	-0.65401
H	-5.25460	-1.68471	-0.22007
H	-4.81628	-0.45567	0.97877
C	-1.09391	-3.12805	-3.93158
H	-0.87647	-2.05703	-3.92679
C	0.25713	-3.85195	-4.06372
H	0.14534	-4.93505	-3.95003
H	0.69302	-3.66100	-5.05135
H	0.96285	-3.51496	-3.30546
C	-1.96327	-3.42699	-5.17349
H	-2.96878	-3.00494	-5.09127
H	-1.49124	-3.01714	-6.07312
H	-2.07551	-4.50530	-5.32862
C	-1.27145	0.88989	2.30577
C	-2.05513	2.08127	2.32123
C	-1.18859	0.08241	3.48710
C	-2.69546	2.45789	3.50590
C	-1.85092	0.51362	4.63915
C	-2.59458	1.69248	4.66184
H	-3.28284	3.37246	3.52064
H	-1.79138	-0.08703	5.54091
H	-3.09722	2.00394	5.57324
C	-0.37469	-1.20742	3.51054
H	-0.49809	-1.68449	2.53052
C	-0.81861	-2.21710	4.58129
H	-0.61555	-1.85381	5.59491
H	-1.88427	-2.45179	4.51423
H	-0.25778	-3.15004	4.45919
C	1.12566	-0.90666	3.67482
H	1.71547	-1.82889	3.62384
H	1.46830	-0.24016	2.88470
H	1.31933	-0.42608	4.64118
C	-2.20750	2.95856	1.08587
H	-1.84644	2.38257	0.23100
C	-1.34836	4.23449	1.20078
H	-1.44682	4.85479	0.30175
H	-1.65793	4.84103	2.05979
H	-0.29077	3.99003	1.33543
C	-3.68064	3.31402	0.80742
H	-4.29189	2.41210	0.69759
H	-4.12024	3.91556	1.61038
H	-3.76321	3.89552	-0.11805
C	3.12925	1.29853	0.63983
C	2.24470	2.39061	1.26234
H	1.59183	1.98579	2.03833
H	2.87633	3.16623	1.70719
H	1.61567	2.86256	0.50316
C	3.97845	0.65668	1.76084
H	4.66679	-0.09146	1.36456
H	4.57053	1.43445	2.25414
H	3.34968	0.19654	2.52770
C	4.06855	1.97677	-0.39147
H	4.63443	2.77571	0.09977
H	4.78912	1.26981	-0.81213
H	3.49250	2.42375	-1.20687

Transition state **TS.1b**:

G (a.u.) = -2047.589295

Nb	0.21603	0.10517	-0.48398
N	-0.51577	0.67403	1.06300
N	2.21703	0.36445	-0.47249
N	-1.68904	-1.01021	-1.72524
C	-0.26691	3.00283	-2.03041
H	-0.90227	3.60684	-2.69272
H	0.76348	3.04852	-2.40068
H	-0.25943	3.49244	-1.04931
C	-0.73704	1.57372	-1.91899
C	-1.85936	1.20893	-2.57331
H	-2.43999	1.89827	-3.19086
C	-2.32710	-0.16487	-2.49317
C	-3.53069	-0.51344	-3.34024
H	-4.00425	-1.44827	-3.04471
H	-3.23003	-0.60032	-4.39117
H	-4.25910	0.30124	-3.28898
C	-2.07171	-2.39437	-1.78835
C	-2.87495	-2.93237	-0.75416
C	-3.24003	-4.28024	-0.83507
H	-3.85658	-4.71384	-0.05518
C	-2.82111	-5.08103	-1.89343
H	-3.10140	-6.12985	-1.92796
C	-2.04611	-4.53244	-2.90836
H	-1.72884	-5.16355	-3.73271
C	-1.66413	-3.18474	-2.89149
C	1.32534	-1.80549	-0.41105
C	2.46218	-1.05012	-0.47695
C	3.83941	-1.58441	-0.73051
C	4.45914	-2.46977	0.16614
C	4.51422	-1.24295	-1.91214
C	5.73202	-2.96890	-0.09860
H	3.94272	-2.75284	1.07697
C	5.78689	-1.75235	-2.18175
H	4.03089	-0.58571	-2.62896
C	6.40312	-2.61145	-1.27185
H	6.20160	-3.64237	0.61284
H	6.29259	-1.47881	-3.10378
H	7.39555	-3.00346	-1.47507
C	1.12298	-3.26034	-0.40867
C	1.71814	-4.14743	-1.33181
C	0.32189	-3.83028	0.60363
C	1.53357	-5.52567	-1.23716
H	2.34379	-3.75335	-2.12445
C	0.15752	-5.21083	0.71043
H	-0.15777	-3.17443	1.32282
C	0.76012	-6.06949	-0.21044
H	2.00771	-6.17791	-1.96607
H	-0.45228	-5.61555	1.51403
H	0.62532	-7.14458	-0.13192
C	-3.39459	-2.05332	0.38473
H	-2.63732	-1.28568	0.57933
C	-3.62490	-2.82828	1.69194
H	-3.79909	-2.12521	2.51252
H	-4.50477	-3.47888	1.63126
H	-2.76449	-3.44989	1.94874
C	-4.69787	-1.31639	0.00951
H	-4.56001	-0.62635	-0.82548
H	-5.48194	-2.02965	-0.26977
H	-5.05817	-0.73530	0.86615
C	-0.84128	-2.63185	-4.05862
H	-0.86666	-1.54151	-4.01387
C	0.64082	-3.04414	-3.97117
H	0.74602	-4.13312	-3.92413
H	1.18902	-2.68712	-4.85104
H	1.11584	-2.62930	-3.08044
C	-1.42747	-3.02767	-5.42848
H	-2.49344	-2.78558	-5.49684
H	-0.90441	-2.49393	-6.22934
H	-1.31762	-4.09837	-5.62865
C	3.17086	1.44417	-0.07545
C	2.41441	2.46569	0.80604
H	3.07771	3.30210	1.04921
H	1.54800	2.88460	0.28940
H	2.06134	2.01209	1.73365
C	4.39496	0.99312	0.74731
H	5.18866	0.58260	0.13112
H	4.80141	1.85681	1.28222
H	4.11838	0.24267	1.49285
C	3.65122	2.17747	-1.34737
H	4.40001	2.93565	-1.09132
H	4.10614	1.47836	-2.05426
H	2.81560	2.67575	-1.84828
C	-1.01574	0.97058	2.32121
C	-0.63050	0.20909	3.46665
C	-1.96092	2.02888	2.46698
C	-1.21561	0.50896	4.70045
C	-2.51425	2.27691	3.72602
C	-2.15673	1.52541	4.84098
H	-0.91749	-0.06181	5.57490
H	-3.24001	3.07914	3.83183
H	-2.59924	1.73405	5.81076
C	0.48170	-0.83145	3.40826
H	0.56231	-1.17339	2.37334
C	0.22848	-2.07389	4.28174
H	0.31244	-1.85607	5.35192
H	-0.76441	-2.49722	4.10286
H	0.97359	-2.84473	4.05691

C	1.82905	-0.17984	3.78921
H	2.66035	-0.87631	3.63308
H	2.02091	0.71811	3.19430
H	1.83004	0.11672	4.84439
C	-2.39648	2.88774	1.28896
H	-1.88511	2.51192	0.40258
C	-1.98980	4.36355	1.48509
H	-0.95491	4.45177	1.83197
H	-2.08412	4.91976	0.54540
H	-2.62601	4.86005	2.22697
C	-3.90792	2.76555	1.01312
H	-4.19015	3.37573	0.14765
H	-4.18949	1.72733	0.80304
H	-4.50515	3.10591	1.86624

Transiton state **TS.2a**:
G (a.u.) = -2047.590179

Nb	-0.74154	0.70912	0.47957
N	-1.81550	2.13887	0.81949
N	1.10478	0.73296	1.52080
N	-1.61216	-1.02113	-0.44859
C	1.15713	2.07764	-1.80664
H	1.92169	1.82114	-2.55120
H	1.63528	2.65101	-1.01058
H	0.43431	2.73891	-2.29389
C	0.45144	0.83839	-1.25789
C	-0.48152	0.15042	-2.19705
H	-0.47342	0.44932	-3.24193
C	-1.38221	-0.81433	-1.80854
C	-2.01533	-1.70702	-2.84400
H	-1.40209	-2.61261	-2.93760
H	-2.03053	-1.21702	-3.82066
H	-3.01984	-2.03129	-2.58402
C	-2.64570	-1.91692	0.00841
C	-4.02124	-1.54734	-0.08505
C	-4.97709	-2.36744	0.52671
H	-6.02488	-2.08916	0.45994
C	-4.62540	-3.53605	1.19353
H	-5.38944	-4.15728	1.65253
C	-3.28740	-3.90373	1.25532
H	-3.00762	-4.81845	1.77022
C	-2.28564	-3.11467	0.67527
C	1.43679	-0.19129	-0.62193
C	1.94300	-0.04113	0.68174
C	3.46682	-0.23836	0.72252
C	4.17752	-1.24432	1.40250
C	4.24060	0.66315	-0.03047
C	5.56998	-1.27864	1.43196
H	3.63972	-2.07709	1.84332
C	5.63645	0.62338	-0.02791
H	3.74818	1.42823	-0.61504
C	6.31470	-0.33057	0.72737
H	6.06826	-2.08337	1.96497
H	6.18492	1.35652	-0.61251
H	7.40016	-0.35927	0.74042
C	1.90766	-1.31050	-1.46999
C	2.13717	-1.15820	-2.85372
C	2.17192	-2.58192	-0.91760
C	2.60578	-2.21314	-3.63504
H	1.97553	-0.19497	-3.32178
C	2.64754	-3.63574	-1.69408
H	1.99261	-2.73825	0.14066
C	2.86345	-3.46002	-3.06254
H	2.78167	-2.05460	-4.69570
H	2.84176	-4.59932	-1.23057
H	3.22804	-4.28137	-3.67258
C	-4.52958	-0.30776	-0.82772
H	-3.66638	0.30197	-1.10577
C	-5.32141	-0.66119	-2.10656
H	-5.71666	0.25179	-2.56571
H	-4.72408	-1.17762	-2.85908
H	-6.17478	-1.30446	-1.86527
C	-5.42324	0.57873	0.06007
H	-5.60489	1.54194	-0.42678
H	-6.39820	0.11528	0.24827
H	-4.94759	0.78354	1.01796
C	-0.83666	-3.55464	0.81658
H	-0.23434	-2.88986	0.19513
C	-0.61428	-4.99047	0.30588
H	-1.12159	-5.73278	0.93221
H	-0.98350	-5.10782	-0.71765
H	0.45326	-5.23304	0.30667
C	-0.34480	-3.40510	2.27032
H	0.71269	-3.68157	2.35485
H	-0.45191	-2.37386	2.62535
H	-0.91168	-4.04930	2.95186
C	1.51779	1.64113	2.68358
C	2.06532	0.80771	3.82560
H	2.56519	1.42868	4.57515
H	1.25355	0.26649	4.31640
H	2.80172	0.11043	3.44051
C	2.50502	2.72539	2.20877
H	3.42143	2.31381	1.78706
H	2.02961	3.37329	1.46297
H	2.79043	3.34762	3.06412
C	0.27732	2.36409	3.24907
H	0.32727	2.35020	4.34023
H	0.18205	3.40623	2.92166
H	-0.64138	1.86186	2.96526
C	-2.74763	3.15623	1.02277
C	-3.53119	3.21203	2.21789
C	-2.91706	4.17598	0.03554
C	-4.42947	4.26891	2.39336
C	-3.84174	5.19864	0.26381
C	-4.59424	5.26052	1.43305
H	-5.01536	4.31154	3.30747
H	-3.97498	5.96722	-0.49146
H	-5.30203	6.06922	1.59074
C	-3.40829	2.18330	3.34092
H	-2.76406	1.37317	2.98191
C	-4.75791	1.54033	3.73026
H	-4.58579	0.69893	4.41014
H	-5.40781	2.25228	4.25070
H	-5.30359	1.16321	2.86305
C	-2.77339	2.81593	4.59884
H	-2.96346	2.17638	5.47431
H	-1.70112	2.95229	4.50640
H	-3.21445	3.79764	4.79929
C	-2.17509	4.12958	-1.29285
H	-1.31717	3.46576	-1.16346
C	-1.63080	5.50487	-1.72401
H	-2.43678	6.21678	-1.92918
H	-0.98368	5.94215	-0.95700
H	-1.04742	5.41033	-2.64679
C	-3.06330	3.54011	-2.41761
H	-2.45332	3.06576	-3.19407
H	-3.75662	2.78988	-2.03282
H	-3.65867	4.32698	-2.89544

Transition state **TS.2b**:
G (a.u.) = -2047594038

Nb	-0.60147	0.55638	0.27943
N	-1.82181	1.86481	0.63947
N	1.17880	1.14751	1.04916
N	-1.89366	-0.95384	-0.82990
C	1.01476	1.79955	-2.31259
H	1.32075	1.54838	-3.33709
H	1.90561	1.86139	-1.68485
H	0.56580	2.80065	-2.33801
C	0.01602	0.81646	-1.76294
C	-0.72225	0.02603	-2.63962
H	-0.50659	0.02211	-3.70839
C	-1.66451	-0.91200	-2.14723
C	-2.28322	-1.88825	-3.11925
H	-1.48818	-2.53190	-3.51302
H	-2.72508	-1.36318	-3.97120
H	-3.04010	-2.52116	-2.65805
C	-2.98326	-1.69942	-0.26571
C	-4.33212	-1.35314	-0.55433
C	-5.35486	-2.09497	0.05291
H	-6.38756	-1.84337	-0.17041
C	-5.08613	-3.13016	0.93974
H	-5.89901	-3.68740	1.39650
C	-3.76396	-3.43855	1.24302
H	-3.55228	-4.24085	1.94225
C	-2.70316	-2.74173	0.65588
C	1.35133	-0.64826	-0.42684
C	1.93310	-0.00412	0.62397
C	3.12947	-0.53509	1.35464
C	3.04538	-0.98035	2.68476
C	4.34831	-0.69660	0.67518
C	4.14831	-1.55374	3.31928
H	2.10625	-0.88597	3.22138
C	5.45196	-1.26488	1.31055
H	4.42289	-0.37338	-0.35857
C	5.35786	-1.69412	2.63611
H	4.06009	-1.89469	4.34726
H	6.38659	-1.37437	0.76763
H	6.21707	-2.13804	3.13042
C	1.74442	-1.90816	-1.05621
C	1.87561	-1.98774	-2.46006
C	1.98609	-3.09047	-0.31970
C	2.23130	-3.18060	-3.09003
H	1.71032	-1.09672	-3.05344

C	2.33658	-4.28167	-0.95124
H	1.91471	-3.06200	0.76234
C	2.45852	-4.33673	-2.34193
H	2.33565	-3.20383	-4.17182
H	2.52259	-5.17005	-0.35316
H	2.73348	-5.26560	-2.83341
C	-4.74191	-0.18651	-1.45428
H	-3.83711	0.28920	-1.84039
C	-5.59023	-0.64261	-2.65976
H	-5.80528	0.20913	-3.31433
H	-5.08643	-1.40796	-3.25576
H	-6.55154	-1.05598	-2.33575
C	-5.51056	0.88314	-0.65181
H	-5.75749	1.73703	-1.29171
H	-6.45139	0.48325	-0.25788
H	-4.92066	1.25559	0.18813
C	-1.26931	-3.07105	1.04706
H	-0.62405	-2.78230	0.21407
C	-1.01894	-4.56466	1.31303
H	-1.52623	-4.91846	2.21707
H	-1.35838	-5.17683	0.47231
H	0.05159	-4.74547	1.44911
C	-0.85221	-2.24093	2.27920
H	0.20667	-2.37586	2.51946
H	-1.02877	-1.15914	2.13922
H	-1.44778	-2.51590	3.15719
C	1.76772	2.33143	1.74266
C	-2.74006	2.87301	0.87331
C	-3.40314	2.93064	2.13768
C	-3.03117	3.85384	-0.12119
C	-4.33835	3.94368	2.36448
C	-3.97347	4.84502	0.16622
C	-4.63057	4.89746	1.39285
H	-4.84874	3.98707	3.32316
H	-4.19790	5.59412	-0.58869
H	-5.36107	5.67668	1.59119
C	-2.33521	3.85610	-1.47657
H	-1.68423	2.98055	-1.50814
C	-3.33139	3.72831	-2.64486
H	-3.93335	2.81937	-2.55449
H	-4.01825	4.58103	-2.68868
H	-2.79664	3.68653	-3.60067
C	-1.45305	5.10843	-1.65322
H	-0.71756	5.19501	-0.84747
H	-0.91348	5.07059	-2.60704
H	-2.05422	6.02471	-1.65132
C	-3.12046	1.91708	3.24150
H	-2.33845	1.24702	2.87315
C	-4.35637	1.05220	3.55650
H	-4.12049	0.30834	4.32646
H	-5.18679	1.66224	3.92947
H	-4.70670	0.51981	2.66700
C	-2.58122	2.59312	4.51692
H	-2.32822	1.84104	5.27328
H	-1.68165	3.18033	4.30570
H	-3.32113	3.26897	4.95974
C	1.87061	2.10638	3.26771
H	2.16743	3.03902	3.75987
H	0.89963	1.80435	3.67379
H	2.60963	1.34598	3.52232
C	3.15664	2.67954	1.16634
H	3.51588	3.60755	1.62310
H	3.89690	1.90311	1.36290
H	3.09852	2.83906	0.08501
C	0.83904	3.53442	1.50450
H	0.72675	3.73430	0.43551
H	-0.15490	3.36334	1.92054
H	1.26490	4.42434	1.97949

Transiton state **TS.3a**:
G (a.u.) = -1153.365547

Nb	0.21321	-0.02570	-0.59635
N	-0.83529	0.48355	0.76545
N	1.97677	0.61548	-0.32786
N	-1.47724	-1.08912	-2.05037
C	-1.35980	1.06291	1.96354
C	2.93866	1.28979	0.39729
C	3.00628	1.21096	1.80870
C	3.96780	1.92684	2.51676
H	4.00288	1.85146	3.60048
C	4.87625	2.75119	1.84463
H	5.61895	3.31491	2.40152
C	4.82107	2.84264	0.45151
H	5.52332	3.48007	-0.07921
C	3.87828	2.11008	-0.26679
C	0.25308	2.77570	-2.38491
H	-0.10508	3.32681	-3.26642
H	1.34661	2.71328	-2.43031
H	0.02830	3.37164	-1.49104
C	-0.34638	1.40210	-2.26057
C	-1.22106	0.96536	-3.19928
H	-1.53015	1.57288	-4.05457
C	-1.86788	-0.32623	-3.03807
C	-2.98843	-0.66056	-3.99546
H	-2.57329	-0.97465	-4.96094
H	-3.58344	0.23766	-4.18437
H	-3.63799	-1.45548	-3.63021
C	-2.11887	-2.32852	-1.78342
C	-2.76499	-2.50472	-0.55037
C	-3.37645	-3.72095	-0.24643
H	-3.88215	-3.84125	0.70771
C	-3.33864	-4.78111	-1.15602
H	-3.81113	-5.72826	-0.91346
C	-2.68525	-4.61379	-2.37847
H	-2.64484	-5.43236	-3.09180
C	-2.07769	-3.39690	-2.69298
C	1.06873	-2.13208	-0.30123
C	2.20379	-1.55250	-0.23705
H	-2.77132	-1.67908	0.15434
H	-1.55890	-3.27088	-3.63889
H	3.83684	2.16897	-1.35022
H	2.28624	0.58302	2.32518
H	-0.75735	1.91697	2.30555
H	-2.38584	1.42565	1.80392
H	-1.39657	0.32982	2.78301
C	3.68166	-1.62130	-0.18664
H	4.08050	-0.92005	0.55190
H	3.91806	-2.62966	0.17940
C	0.57879	-3.55202	-0.20513
H	-0.25338	-3.58295	0.50632
H	0.13687	-3.83214	-1.16666
C	1.65023	-4.57407	0.19548
H	1.21513	-5.57703	0.26209
H	2.46218	-4.61124	-0.53849
H	2.08600	-4.33253	1.17066
C	4.35375	-1.38859	-1.54938
H	5.44074	-1.47304	-1.45377
H	4.01361	-2.12549	-2.28356
H	4.11424	-0.39253	-1.92732

Transition state **TS.3b**:
G (a.u.) = -1153.366271

Nb	0.24111400	-0.04630000	0.60183200
N	-0.90052900	0.39994200	-0.74546000
N	1.89604900	0.70321100	0.24730400
N	-1.46862700	-1.12579300	2.05176200
C	0.39228800	2.67933900	2.50025200
H	0.04725500	3.21050000	3.39899500
H	1.48222400	2.57134900	2.55514700
H	0.19930800	3.31784000	1.62874000
C	-0.25771500	1.33405200	2.31986300
C	-1.14115800	0.89170700	3.24771200
H	-1.42168800	1.48001300	4.12614500
C	-1.84242300	-0.36769200	3.04773600
C	-2.99609600	-0.66618800	3.97707000
H	-2.61455200	-0.98699700	4.95418400
H	-3.57003200	0.24953500	4.14741400
H	-3.65887400	-1.44307700	3.59751700
C	-2.16207700	-2.32722900	1.74182800
C	-2.79560000	-2.44230300	0.49467700
C	-3.44704700	-3.62626900	0.14799900
H	-3.94276900	-3.69930300	-0.81603800
C	-3.46314700	-4.71252500	1.02709000
H	-3.96746500	-5.63366400	0.75064500
C	-2.82443000	-4.60450600	2.26390100
H	-2.82748100	-5.44319800	2.95468600
C	-2.17654800	-3.42084700	2.62190600
C	1.12081700	-2.17685200	0.32447900
C	2.23055800	-1.57942400	0.22658200
H	-2.76115700	-1.59734200	-0.18588600
H	-1.66975500	-3.34043700	3.57941500
C	3.70522000	-1.52940800	0.15689700
H	4.03901700	-0.84929800	-0.63126000
H	4.01687500	-2.53668400	-0.15384800
C	0.56412200	-3.56943600	0.27218000
H	-0.29294200	-3.58155800	-0.40855400
H	0.14892600	-3.81509900	1.25449600
C	1.59293800	-4.62773200	-0.14707300
H	1.12911900	-5.61926000	-0.17691600
H	2.43017700	-4.67022300	0.55758600
H	1.99693500	-4.41503600	-1.14219500
C	4.37426900	-1.16977800	1.49383700
H	5.46258400	-1.15061800	1.38085000
H	4.12147100	-1.90560900	2.26302200

H	4.03778900	-0.18971900	1.84012100
C	2.92619000	1.43539200	-0.41630500
H	3.90718700	1.36302100	0.07791000
H	3.04451700	1.14514400	-1.47107700
H	2.64400900	2.49768400	-0.41018700
C	-1.36847400	0.95050000	-1.91511100
C	-1.12139600	0.33575100	-3.16460800
C	-2.13436800	2.13912000	-1.89911000
C	-1.61078400	0.89585000	-4.34196100
H	-0.53773800	-0.58015800	-3.18492500
C	-2.62260200	2.68592000	-3.08305100
H	-2.33554100	2.61081500	-0.94193900
C	-2.36455000	2.07274200	-4.31253300
H	-1.40421300	0.40747800	-5.29115900
H	-3.20942400	3.60039100	-3.04564900
H	-2.74699200	2.50379100	-5.23305200

Transiton state **TS.4a**:
G (a.u.) = -1153.364365

Nb	-0.78715	0.54394	0.49618
N	-2.08793	1.72758	0.93748
N	0.91579	0.99970	1.51573
N	-1.79598	-0.72177	-1.05973
C	-3.04550	2.78965	0.99135
C	1.36252	1.96832	2.42463
C	0.48351	2.43588	3.42161
C	0.87860	3.43468	4.30669
H	0.18314	3.77700	5.06837
C	2.15920	3.99076	4.22802
H	2.46643	4.76572	4.92375
C	3.03627	3.53760	3.24192
H	4.03160	3.96624	3.15990
C	2.64799	2.54021	2.34739
C	0.79509	2.57112	-1.51610
H	1.15826	2.67969	-2.54677
H	1.65239	2.49547	-0.84288
H	0.26397	3.49331	-1.24489
C	-0.13349	1.40225	-1.35654
C	-0.73686	0.82722	-2.46795
H	-0.50143	1.16056	-3.47902
C	-1.60897	-0.28145	-2.30511
C	-2.22352	-0.93835	-3.51841
H	-3.17672	-0.46578	-3.78254
H	-2.41512	-2.00107	-3.35538
H	-1.55754	-0.82303	-4.37708
C	-2.68758	-1.74698	-0.67601
C	-4.02859	-1.79479	-1.09870
C	-4.88558	-2.78185	-0.61420
H	-5.91775	-2.80238	-0.95282
C	-4.43527	-3.72814	0.30959
H	-5.10968	-4.49118	0.68571
C	-3.11092	-3.67804	0.74845
H	-2.74477	-4.40770	1.46512
C	-2.24517	-2.69873	0.26230
C	1.19398	-0.43245	-0.27078
C	1.75510	0.00104	0.88834
H	-4.40085	-1.04095	-1.78370
H	-1.20713	-2.67653	0.58458
H	3.33105	2.21859	1.56869
H	-0.51149	2.00529	3.47996
H	-2.99496	3.42503	0.09504
H	-4.07052	2.39792	1.06433
H	-2.87460	3.43393	1.86616
C	2.96897	-0.54963	1.63297
H	3.07395	-0.03146	2.59055
H	2.77530	-1.60154	1.87744
C	1.66373	-1.45385	-1.25866
H	0.99874	-1.41346	-2.13451
H	2.65783	-1.18029	-1.64225
C	1.71461	-2.91197	-0.76085
H	0.72951	-3.24581	-0.42064
H	2.03238	-3.58452	-1.56585
H	2.41584	-3.03593	0.07032
C	4.29261	-0.45946	0.85667
H	4.53325	0.57464	0.58964
H	5.11794	-0.84927	1.46180
H	4.25855	-1.03833	-0.07004

Transition state **TS.4b**:
G (a.u.) = -1153.372284

Nb	-0.75603	0.48563	-0.48912
N	-2.05115	1.70474	-0.93224
N	0.94055	0.89947	-1.48955
N	-1.79164	-0.74814	1.06411
C	0.99957	2.36947	1.52715
H	1.43730	2.38389	2.53425
H	1.80379	2.30714	0.79120
H	0.49283	3.33070	1.36816
C	0.00126	1.25836	1.35552
C	-0.64128	0.72663	2.47561
H	-0.37857	1.04426	3.48452
C	-1.57896	-0.32041	2.31373
C	-2.23026	-0.94833	3.52295
H	-3.17504	-0.44987	3.76829
H	-2.44863	-2.00679	3.36347
H	-1.57486	-0.84615	4.39124
C	-2.73930	-1.72078	0.67598
C	-4.08192	-1.69238	1.09543
C	-4.99300	-2.62738	0.60684
H	-6.02563	-2.58797	0.94225
C	-4.59617	-3.59605	-0.31835
H	-5.31280	-4.31771	-0.69809
C	-3.27034	-3.62101	-0.75440
H	-2.94522	-4.36882	-1.47226
C	-2.35028	-2.69476	-0.26377
C	1.20565	-0.51571	0.30704
C	1.77531	-0.07211	-0.84726
H	-4.41289	-0.91806	1.77852
H	-1.31190	-2.73383	-0.58312
C	3.07698	-0.53646	-1.47681
H	2.95607	-0.62882	-2.56349
H	3.29816	-1.54211	-1.10602
C	1.74825	-1.51348	1.28078
H	1.34701	-1.27486	2.27669
H	2.84136	-1.41825	1.36875
C	1.40519	-2.98364	0.96910
H	0.32254	-3.13728	0.96164
H	1.83439	-3.65250	1.72391
H	1.79558	-3.28757	-0.00855
C	4.27447	0.38289	-1.16647
H	4.12614	1.39304	-1.55912
H	5.19252	-0.01567	-1.61142
H	4.43003	0.46508	-0.08622
C	1.40583	1.75277	-2.56447
H	0.55995	2.32694	-2.94883
H	2.17008	2.46290	-2.21834
H	1.83827	1.17974	-3.39655
C	-2.99259	2.70967	-0.97705
C	-3.40947	3.37433	0.19858
C	-3.56901	3.09902	-2.20618
C	-4.36144	4.38875	0.13883
H	-2.96886	3.07579	1.14508
C	-4.52197	4.11346	-2.25301
H	-3.25374	2.58894	-3.11175
C	-4.92439	4.76560	-1.08414
H	-4.66765	4.88924	1.05401
H	-4.95379	4.39766	-3.20921
H	-5.66743	5.55660	-1.12542

Transiton state **TS.5a**:
G (a.u.) = -1191.575926

Nb	0.25527	0.12110	0.58767
N	-0.87816	0.57462	-0.72893
N	2.01637	0.77510	0.26322
N	-1.27948	-1.06321	2.04880
C	0.21210	2.88969	2.42788
H	-0.13244	3.39376	3.34222
H	1.30837	2.89911	2.41356
H	-0.09934	3.49300	1.56527
C	-0.30814	1.48524	2.29433
C	-1.12759	0.97201	3.24512
H	-1.44884	1.53807	4.12403
C	-1.69627	-0.35510	3.06701
C	-2.77063	-0.78405	4.03858
H	-2.31731	-1.10719	4.98362
H	-3.40981	0.07266	4.27100
H	-3.38338	-1.60136	3.65907
C	-1.81527	-2.34745	1.75701
C	-2.37695	-2.57294	0.49067
C	-2.88211	-3.82993	0.16074
H	-3.32475	-3.98714	-0.81900
C	-2.82017	-4.88331	1.07704
H	-3.20955	-5.86227	0.81396
C	-2.24788	-4.66796	2.33149
H	-2.18554	-5.48062	3.04988
C	-1.74666	-3.41026	2.67187
H	-2.40533	-1.75069	-0.21727
H	-1.28752	-3.25010	3.64283
C	1.63776	-2.87802	1.32159
C	3.42959	-1.58054	0.83183
C	2.60340	-1.94346	2.08324
H	3.19676	-2.46129	2.84435
H	2.12095	-1.07731	2.54909
C	2.64409	-3.90048	0.71752

H	2.92181	-4.65930	1.45820
H	2.22525	-4.42352	-0.14736
C	3.86765	-3.00143	0.34850
H	4.77048	-3.30979	0.88538
H	4.10547	-3.01780	-0.71991
H	0.83538	-3.33347	1.90206
H	4.24908	-0.86987	0.94875
C	1.17560	-1.96330	0.17224
H	0.61922	-2.40474	-0.65427
C	2.34645	-1.16494	-0.14696
H	2.61975	-0.93721	-1.17279
C	3.06169	1.51757	-0.26390
C	3.16546	1.77340	-1.64911
C	4.04989	2.05409	0.58883
C	4.21544	2.53600	-2.15507
H	2.40006	1.37546	-2.30950
C	5.08807	2.83095	0.07666
H	3.97425	1.85755	1.65417
C	5.18005	3.07163	-1.29625
H	4.27624	2.72375	-3.22387
H	5.83246	3.24451	0.75193
H	5.99307	3.67211	-1.69366
C	-1.45089	1.19027	-1.88759
H	-1.47550	0.49486	-2.73983
H	-2.48759	1.50063	-1.69141
H	-0.89169	2.08374	-2.20163

Transition state **TS.5b**:
G (a.u.) = -1191.578783

Nb	0.26805	0.13372	0.59196
N	-0.91381	0.53059	-0.73669
N	1.93481	0.87389	0.20563
N	-1.27538	-1.06920	2.04490
C	0.27545	2.86154	2.50139
H	-0.09744	3.36246	3.40623
H	1.37133	2.83842	2.54315
H	0.02335	3.48531	1.63445
C	-0.27145	1.47107	2.32586
C	-1.10573	0.95259	3.26107
H	-1.42219	1.50936	4.14773
C	-1.69548	-0.36388	3.06222
C	-2.79066	-0.78298	4.01409
H	-2.35770	-1.08979	4.97408
H	-3.43832	0.07457	4.21928
H	-3.39177	-1.60749	3.63195
C	-1.82606	-2.34289	1.73342
C	-2.40322	-2.54021	0.46917
C	-2.91566	-3.78965	0.12116
H	-3.37117	-3.92553	-0.85578
C	-2.84656	-4.86096	1.01594
H	-3.24247	-5.83326	0.73828
C	-2.26137	-4.67187	2.26876
H	-2.19626	-5.49804	2.97135
C	-1.75266	-3.42240	2.62805
H	-2.44055	-1.70377	-0.22171
H	-1.28702	-3.28005	3.59893
C	3.04632	1.59388	-0.33164
H	2.85800	2.66835	-0.20937
H	3.99595	1.36890	0.17776
H	3.18529	1.41296	-1.40906
C	-1.40501	1.11097	-1.88347
C	-1.29730	0.45929	-3.13361
C	-2.05537	2.36575	-1.84198
C	-1.80653	1.04717	-4.28896
H	-0.80675	-0.50916	-3.17383
C	-2.56473	2.94071	-3.00321
H	-2.15260	2.86590	-0.88310
C	-2.44330	2.29011	-4.23469
H	-1.70780	0.52890	-5.23956
H	-3.06118	3.90623	-2.94663
H	-2.84195	2.74329	-5.13749
C	1.67429	-2.83267	1.39328
C	3.43438	-1.52005	0.83752
C	2.62431	-1.84807	2.10919
H	3.23340	-2.32210	2.88597
H	2.12754	-0.97322	2.54299
C	2.69975	-3.85993	0.82722
H	2.99576	-4.57938	1.59898
H	2.28822	-4.42802	-0.01202
C	3.90278	-2.95294	0.41387
H	4.81334	-3.21764	0.96067
H	4.13723	-3.01144	-0.65367
H	0.87971	-3.27635	1.99259
H	4.24199	-0.79215	0.92557
C	1.20165	-1.98050	0.20366
H	0.58998	-2.42911	-0.57687
C	2.33422	-1.18044	-0.15199
H	2.57772	-0.93044	-1.18005

Transiton state **TS.6a**:
G (a.u.) = -1191.568164

Nb	-0.43522	0.68668	-0.10814
N	-0.94052	2.37302	0.16107
N	0.96848	0.07155	1.29374
N	-2.05020	-0.62633	-0.59187
C	-1.22860	3.72334	0.54103
C	0.99702	0.19460	2.68370
C	2.18994	0.26279	3.43583
C	2.15318	0.38921	4.82530
H	3.09040	0.43621	5.37421
C	0.94123	0.45485	5.51167
H	0.92117	0.55245	6.59269
C	-0.24890	0.38581	4.78009
H	-1.20668	0.43172	5.29206
C	-0.22298	0.25079	3.39671
C	0.44377	1.25459	-3.32024
H	1.08550	0.68566	-4.00904
H	0.97482	2.15477	-3.00364
H	-0.43211	1.57544	-3.89938
C	-0.05587	0.43057	-2.17239
C	-0.56682	-0.88092	-2.42969
H	-0.18273	-1.50345	-3.23934
C	-1.61346	-1.37973	-1.64818
C	-2.22806	-2.72633	-1.93636
H	-3.30249	-2.64346	-2.12204
H	-2.10699	-3.38992	-1.07221
H	-1.75738	-3.19048	-2.80482
C	-3.32882	-0.80433	-0.00486
C	-4.49640	-0.56559	-0.75042
C	-5.75042	-0.69299	-0.15598
H	-6.64368	-0.50306	-0.74462
C	-5.86242	-1.04690	1.19158
H	-6.84090	-1.13938	1.65315
C	-4.70716	-1.27948	1.93863
H	-4.78177	-1.56104	2.98520
C	-3.44818	-1.16601	1.34549
H	-4.40613	-0.26117	-1.78919
H	-2.54975	-1.37624	1.91827
H	-1.15992	0.18807	2.84832
H	3.15154	0.21433	2.93800
H	-2.21246	3.79291	1.02468
H	-0.48021	4.11297	1.24475
H	-1.24326	4.38303	-0.33735
C	4.39517	-0.88881	-0.14545
C	3.01044	-1.21621	0.45760
C	2.51799	-0.76548	-1.71024
C	4.05683	-0.56250	-1.63656
H	4.88335	-0.05318	0.36834
H	5.06622	-1.75055	-0.07020
H	4.35240	0.45088	-1.92726
H	4.56263	-1.25517	-2.31913
C	2.31759	-1.93190	-0.71827
H	1.26622	-2.16471	-0.52446
H	2.82955	-2.85041	-1.02604
C	2.21189	0.11331	0.53563
H	2.85091	0.92931	0.90864
C	1.84292	0.40942	-0.97015
H	2.18857	1.38964	-1.29984
H	3.03980	-1.75678	1.40659
H	2.16618	-0.93908	-2.72848

Transition state **TS.6b**:
G (a.u.) = -1191.566955

Nb	-0.78337	0.77511	-0.11975
N	-1.88143	2.18212	0.29162
N	0.58348	0.78333	1.32236
N	-1.84268	-0.86488	-1.11080
C	0.93725	2.11443	-2.64246
H	1.34067	1.79404	-3.61224
H	1.77277	2.33859	-1.97356
H	0.39373	3.05525	-2.80046
C	-0.00615	1.10925	-2.04922
C	-0.79357	0.30906	-2.90363
H	-0.71408	0.44063	-3.98311
C	-1.70779	-0.66494	-2.44324
C	-2.52313	-1.43648	-3.45542
H	-2.04055	-2.37960	-3.73381
H	-2.63230	-0.84392	-4.36666
H	-3.51573	-1.67939	-3.06790
C	-2.60054	-1.90615	-0.52887
C	-3.46448	-1.59403	0.53614
C	-4.17694	-2.59907	1.18972
H	-4.84374	-2.33686	2.00624

C	-4.04276	-3.93132	0.79402
H	-4.59911	-4.71318	1.30194
C	-3.17967	-4.24989	-0.25695
H	-3.05563	-5.28467	-0.56408
C	-2.45799	-3.25194	-0.91038
H	-3.58233	-0.55352	0.82764
H	-1.76131	-3.51431	-1.69906
C	3.26502	-1.93682	0.78236
C	1.96792	-1.36793	1.41374
C	1.34293	-1.86242	-0.70968
C	2.82070	-2.34010	-0.66279
H	4.07552	-1.19926	0.78326
H	3.61998	-2.80515	1.34646
H	3.43076	-1.87014	-1.44081
H	2.88564	-3.42585	-0.80700
C	0.88728	-2.22099	0.72343
H	-0.13438	-1.90871	0.96200
H	0.97306	-3.28923	0.95088
C	1.72285	0.03675	0.78914
H	2.63215	0.65704	0.87197
C	1.35438	-0.32487	-0.69059
H	2.07364	0.08190	-1.39976
H	1.96952	-1.37118	2.50819
H	0.76701	-2.30246	-1.52945
C	-2.54107	3.37090	0.50909
C	-3.91273	3.38110	0.84776
C	-1.86783	4.61024	0.41295
C	-4.57771	4.58185	1.08160
H	-4.43659	2.43248	0.91888
C	-2.54204	5.80460	0.65176
H	-0.81414	4.60879	0.14962
C	-3.89931	5.80023	0.98697
H	-5.63345	4.56708	1.33964
H	-2.00535	6.74660	0.57391
H	-4.42179	6.73447	1.17011
C	0.69177	1.34177	2.65636
H	-0.18667	1.95522	2.87105
H	0.76389	0.56112	3.42769
H	1.58882	1.97465	2.74327

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