Ring Expansion of Alumoles with Organic Azides: Selective Formation of Six-Membered Aluminum-Nitrogen Heterocycles

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Methods and Materials

All manipulations were performed either under an atmosphere of dry argon or in vacuo using standard Schlenk line or glovebox techniques. Deuterated solvents were dried over molecular sieves and degassed by three freeze-pump-thaw cycles prior to use. All other solvents were distilled and degassed from appropriate drying agents. Solvents (both deuterated and non-deuterated) were stored under argon over activated 4 Å molecular sieves. NMR spectra were acquired on a Bruker Avance 500 NMR spectrometer (^{1}H: 500.1 MHz, ^{13}C{^{1}H}: 125.8 MHz). Chemical shifts (δ) are given in ppm and internally referenced to the carbon nuclei (^{13}C{^{1}H}) or residual protons (^{1}H) of the solvent. Microanalyses (C, H, N) were performed on an Elementar vario MICRO cube elemental analyzer. High resolution mass spectrometry was performed on a Thermo Scientific Exactive Plus spectrometer using a LIFDI 700 source from Linden CMS. $Li_2C_4Et_4$,[1] (η^5-1,2,4-*t*$Bu_3C_5H_2$)$AlBr_2$,[2] *t*$BuAlCl_2$,[3] $MesN_3$,[4] (2,6-$Ph_2C_6H_3$)N_3[5] were synthesized according to literature procedures.

Synthetic Procedures

Synthesis of 1-(*tert*-butyl)-2,3,4,5-tetraethylalumole (1)

A solution of *tert*-butylaluminum dichloride (91.3 mg, 0.374 mmol, 1.05 equiv) in benzene (6 mL) was added to a benzene solution (6 mL) of 1,4-dilithio-1,2,3,4-tetraethylbutadiene (63.5 mg, 0.357 mmol, 1 equiv). The reaction mixture was stirred for 5 min at ambient temperature. Filtration over Celite and evaporation gave a yellow oil. Recrystallization from pentane and evaporation *in vacuo* afforded a colorless solid (5.00 mg, 0.0213 mmol, 6% yield) from which crystals were selected for X-ray diffraction.

^{1}H NMR (500.1 MHz, C_6D_6): δ = 2.47−2.18 (m, 8H, CH_2CH$_3$), 1.17 (t, $^{3}J_{HH}$ = 7.5 Hz, 6H, CH$_2$CH_3), 1.08 (s, 9 H, C(CH_3)$_3$), 1.03 (t, $^{3}J_{HH}$ = 7.7 Hz, 6H, CH$_2$CH_3) ppm.

^{13}C{^{1}H} NMR (125.8 MHz, C_6D_6): δ = 142.2 (*C*(CH$_2$CH$_3$), 127.3 (*C*(CH$_2$CH$_3$), 31.7 (C(*C*H$_3$)$_3$), 25.9 (*C*H$_2$CH$_3$), 24.1 (*C*H$_2$CH$_3$), 17.2 (CH$_2$*C*H$_3$), 15.0 (CH$_2$*C*H$_3$) ppm.

Elemental analysis: Calculated for [$C_{16}H_{29}Al$] = 248.39: C 77.37, H 11.77; found: C 77.32, H 12.21.

Synthesis of 1-(η^5-1,2,4-tris(*tert*-butyl)cyclopentadienyl)-2,3,4,5-tetraethylalumole (2)

A solution of 1,2,4-tris(*tert*-butyl)cyclopentadienylaluminum dibromide (0.500 g, 1.19 mmol, 1 equiv) in benzene (6 mL) was added to a benzene solution (6 mL) of 1,4-dilithio(1,2,3,4-tetraethyl)butadiene

(0.212 g, 1.19 mmol, 1 equiv). The reaction mixture was stirred for 5 min at ambient temperature. Filtration over Celite and evaporation gave a yellow oil. Recrystallization in hexane and evaporation *in vacuo* afforded a colorless solid (0.175 g, 0.412 mmol, 30% yield) from which suitable crystals for X-ray diffraction were obtained.

^{1}H NMR (500.1 MHz, C_6D_6): δ = 6.60 (s, 2H, Cp-*H*), 2.38 (q, $^3J_{HH}$ = 7.5 Hz, 4H, C*H*$_2$CH$_3$), 2.31 (q, $^3J_{HH}$ = 7.5 Hz, 4H, C*H*$_2$CH$_3$), 1.47 (s, 18H, C(C*H*$_3$)$_3$), 1.31 (s, 9H, C(C*H*$_3$)$_3$), 1.15 (t, $^3J_{HH}$ = 7.5 Hz, 6H, CH$_2$C*H*$_3$), 1.01 (t, $^3J_{HH}$ = 7.5 Hz, 6H, CH$_2$C*H*$_3$) ppm.
^{13}C{^{1}H} NMR (125.8 MHz, C_6D_6): δ = 158.9 (*C*(CH$_2$CH$_3$), 135.7 (*C*(CH$_2$CH$_3$), 129.7 (*C*(Cp)-C(CH$_3$)$_3$), 124.7 (*C*(Cp)-C(CH$_3$)$_3$), 109.1 (*C*(Cp)-H), 33.9 (*C*(CH$_3$)$_3$), 33.7 (C(*C*H$_3$)$_3$), 32.1 (C(*C*H$_3$)$_3$), 31.9 (*C*(CH$_3$)$_3$), 23.3 (*C*H$_2$CH$_3$), 22.0 (*C*H$_2$CH$_3$), 16.7 (CH$_2$*C*H$_3$), 15.6 (CH$_2$*C*H$_3$) ppm.
Elemental analysis: Calculated for [$C_{29}H_{49}Al$] = 424.69: C 82.02, H 11.63; found: C 81.76, H 11.44.

Synthesis of 2-DMAP

A solution of 4-(dimethylamino)pyridine (11.2 mg, 0.0928 mmol, 1 equiv) in 0.3 mL C_6D_6 was slowly added to a solution of **2** (39.4 mg, 0.0928 mmol, 1 equiv) in 0.3 mL C_6D_6. The product immediately precipitated from the reaction mixture as a colorless solid, which was collected and dried under vacuum (90%, 45.8 mg, 0.0839 mmol).

^{1}H NMR (500.1 MHz, THF-d_8): δ = 7.83 (d, $^3J_{HH}$ = 7.4 Hz, 2H, o-C*H*), 6.69 (s, 2H, Cp-*H*), 6.50 (d, $^3J_{HH}$ = 7.4 Hz, 2H, m-C*H*), 3.02 (s, 6H, N-(C*H*$_3$)$_2$), 2.39 (q, $^3J_{HH}$ = 7.5 Hz, 4H, C*H*$_2$CH$_3$), 2.25 (q, $^3J_{HH}$ = 7.5 Hz, 4H, C*H*$_2$CH$_3$), 1.31 (s, 18H, C(C*H*$_3$)$_3$), 1.05 (s, 9H, C(C*H*$_3$)$_3$), 0.91 (t, $^3J_{HH}$ = 7.4 Hz, 6H, CH$_2$C*H*$_3$), 0.84 (t, $^3J_{HH}$ = 7.5 Hz, 6H, CH$_2$C*H*$_3$) ppm.
^{13}C{^{1}H} NMR (125.8 MHz, THF-d_8): δ = 156.7 (*p*-*C*(py)), 153.5 (*C*(CH$_2$CH$_3$), 149.6 (*C*(CH$_2$CH$_3$), 148.1 (*m*-*C*H(py)), 140.4 (*C*(Cp)-C(CH$_3$)$_3$), 130.3 (*C*(Cp)-H), 106.2 (*o*-*C*H(py)), 96.1 (*C*(Cp)-C(CH$_3$)$_3$), 38.9 (N(*C*H$_3$)$_2$), 35.5 (*C*(CH$_3$)$_3$), 34.7 (*C*(CH$_3$)$_3$), 33.6 (C(*C*H$_3$)$_3$), 30.5 (C(*C*H$_3$)$_3$), 25.9 (*C*H$_2$CH$_3$), 21.4 (*C*H$_2$CH$_3$), 16.8 (CH$_2$*C*H$_3$), 15.3 (CH$_2$*C*H$_3$) ppm.
Elemental analysis: Calculated for [$C_{36}H_{59}AlN$] = 546.86: C 79.07, H 10.88, N 5.12; found: C 78.93, H 10.97, N 5.12.

Synthesis of 3

A solution of azidotrimethylsilane (8.14 mg, 0.0706 mmol, 1 equiv) in C_6D_6 (0.3 mL) was added to a solution of **2** (30.0 mg, 0.0706 mmol, 1 equiv) in C_6D_6 (0.3 mL) and heated for 24 h at 60 °C.

Evaporation gave a colorless solid. Recrystallization in pentane and evaporation *in vacuo* afforded colorless crystals suitable for X-ray diffraction in 61% yield (22.0 mg, 0.0430 mmol).

^{1}H NMR (500.1 MHz, C_6D_6): δ = 6.25 (s, 2H, Cp-*H*), 2.51–1.99 (m, 8H, C*H*$_2$CH$_3$), 1.48 (s, 18H, C(C*H*$_3$)$_3$), 1.31 (s, 9H, C(C*H*$_3$)$_3$), 1.26 (t, $^{3}J_{HH}$ = 7.5 Hz, 3H, CH$_2$C*H*$_3$), 1.06 (t, $^{3}J_{HH}$ = 7.4 Hz, 3H, CH$_2$C*H*$_3$), 1.03 (t, $^{3}J_{HH}$ = 7.5 Hz, 3H, CH$_2$C*H*$_3$), 0.98 (t, $^{3}J_{HH}$ = 7.4 Hz, 3H, CH$_2$C*H*$_3$), 0.28 (s, 9H, Si−C*H*$_3$) ppm.

^{13}C{^{1}H} NMR (125.8 MHz, C_6D_6): δ = 156.3 (*C*(CH$_2$CH$_3$), 149.4 (*C*(Cp)-C(CH$_3$)$_3$), 142.2 (*C*(CH$_2$CH$_3$), 144.4 (*C*(CH$_2$CH$_3$), 125.0 (*C*(CH$_2$CH$_3$), 109.7 (*C*(Cp)-H), 104.7 (*C*(Cp)-H), 34.8 (*C*(CH$_3$)$_3$), 33.5 (C(*C*H$_3$)$_3$), 33.0 (C(*C*H$_3$)$_3$), 31.8 (C(*C*H$_3$)$_3$), 31.2 (*C*H$_2$CH$_3$), 26.1 (*C*H$_2$CH$_3$), 23.7 (*C*H$_2$CH$_3$), 22.4 (*C*H$_2$CH$_3$), 16.9 (CH$_2$*C*H$_3$), 16.0 (CH$_2$*C*H$_3$), 15.7 (CH$_2$*C*H$_3$), 14.4 (CH$_2$*C*H$_3$), 3.4 (Si−*C*H$_3$) ppm.

Elemental analysis: [$C_{32}H_{58}AlNSi$] = 511.89: C 75.23, H 11.25, N 2.74; found: C 74.29, H 11.66, N 2.63.

Synthesis of 4

A solution of 2,4,6-trimethylphenyl azide (21.0 mg, 7.97 mmol, 1 equiv) in C_6D_6 (0.3 mL) was added to a solution of **2** (7.97 mg, 0.0495 mmol, 1 equiv) in C_6D_6 (0.3 mL) to afford an orange solution. Evaporation gave an orange oil. Recrystallization from toluene and evaporation *in vacuo* afforded an orange solid in 31% yield (9.00 mg, 0.0154 mmol).

^{1}H NMR (500.1 MHz, C_6D_6): δ = 6.78−6.76 (m, 2H, C*H*-mesityl), 6.42 (br. s, 2H, Cp-*H*), 2.62–2.53 (m, 2H, C*H*$_2$CH$_3$), 2.57 (q, $^{3}J_{HH}$ = 7.2 Hz, 4H, C*H*$_2$CH$_3$), 2.33 (s, 6H, C*H*$_3$-mesityl), 2.29–2.17 (m, 2H, C*H*$_2$CH$_3$), 2.11 (s, 3H, C*H*$_3$-mesityl), 1.54 (s, 18H, C(C*H*$_3$)$_3$), 1.26 (t, $^{3}J_{HH}$ = 7.5 Hz, 3H, CH$_2$C*H*$_3$), 1.25 (s, 9H, C(C*H*$_3$)$_3$), 1.11 (t, $^{3}J_{HH}$ = 7.5 Hz, 3H, CH$_2$C*H*$_3$), 1.02 (t, $^{3}J_{HH}$ = 7.5 Hz, 3H, CH$_2$C*H*$_3$), 0.89 (t, $^{3}J_{HH}$ = 7.5 Hz, 3H, CH$_2$C*H*$_3$) ppm.

^{13}C{^{1}H} NMR (125.8 MHz, C_6D_6): δ = 156.0 (*C*(CH$_2$CH$_3$), 155.0 (*C*(CH$_2$CH$_3$), 142.7 (N*C*-mesityl), 141.6 (*C*(CH$_2$CH$_3$), 135.8 (*C*(CH$_3$)-mesityl), 134.8 (*C*C(CH$_3$)$_3$-Cp), 134.5 (*C*(CH$_2$CH$_3$), 133.0 (*C*(CH$_3$)-mesityl), 129.6 (*C*H-mesityl), 34.4 (*C*(CH$_3$)$_3$-Cp), 33.8 (C(*C*H$_3$)$_3$-Cp), 32.6 (*C*(CH$_3$)$_3$Cp), 32.0 (C(*C*H$_3$)$_3$-Cp), 28.1 (CH$_2$*C*H$_3$), 26.0 (CH$_2$*C*H$_3$), 23.5 (CH$_2$*C*H$_3$), 23.3 (CH$_2$*C*H$_3$), 20.9 (*C*H$_3$-mesityl), 19.6 (*C*H$_3$-mesityl), 16.4 (*C*H$_2$CH$_3$), 14.1 (*C*H$_2$CH$_3$), 14.5 (*C*H$_2$CH$_3$), 13.3 (*C*H$_2$CH$_3$) ppm.

LIFDI MS (m/z) calculated for [$C_{38}H_{60}AlN_3$ –H^{+}] = 586.4636; found: 586.4669

Synthesis of 5

A solution of 2,6-diphenylphenyl azide (19.2 mg, 0.0706 mmol, 1 eq.) in C_6D_6 (0.3 mL) was added to a solution of **2** (30.0 mg, 0.07064 mmol, 1 eq.) in C_6D_6 (0.3 mL) to afford an orange solution. Evaporation gave an orange oil. Recrystallization in pentane and evaporation *in vacuo* afforded a yellow solid in 73% yield (49.17 mg, 0.05172 mmol).

^{1}H NMR (500.1 MHz, C_6D_6): δ = 7.48 (d, $^3J_{HH}$ = 7.2 Hz, 2H, *o*-C_6H_5), 7.26−7.22 (m, 4H, *m*-C_6H_5, 2H, *m*-C_6H_3), 7.11 (dd, $^3J_{HH}$ = 7.5 Hz, $^3J_{HH}$ = 7.5 Hz, 2H, *p*-C_6H_5), 7.11 (dd, $^3J_{HH}$ = 7.7 Hz, $^3J_{HH}$ = 7.7 Hz, 1H, *p*-C_6H_3), 6.22 (br. s, 2H, Cp-*H*), 2.51−2.41 (m, 2H, CH_2CH$_3$), 2.28−2.04 (m, 6H, CH_2CH$_3$), 1.25 (br. s, 18H, C(CH_3)$_3$), 1.19 (s, 9H, C(CH_3)$_3$), 1.14 (t, $^3J_{HH}$ = 7.3 Hz, 3H, CH$_2$CH_3), 0.99−0.94 (m, 6H, CH$_2$CH_3), 0.79 (t, $^3J_{HH}$ = 7.4 Hz, 3H, CH$_2$CH_3) ppm.

^{13}C{^{1}H} NMR (125.8 MHz, C_6D_6): δ = 156.50 (*C*(CH$_2$CH$_3$), 147.37 (*C*(CH$_2$CH$_3$), 146.97 (N−*C*$_6$H$_3$), 142.46 (*C*(CH$_2$CH$_3$), 141.96 (C−*C*$_6$H$_5$), 137.76 (C−*C*$_6$H$_3$), 131.41 (*m*-*C*$_6$H$_3$), 131.10 (*o*-*C*$_6$H$_5$), 129.83 (*C*(CH$_2$CH$_3$), 128.26 (*m*-*C*$_6$H$_5$), 126.82 (*p*-*C*$_6$H$_5$), 125.47 (*p*-*C*$_6$H$_3$), 123.82 (*C*(CH$_3$)$_3$), 33.75 (C(*C*H$_3$)$_3$), 33.67 (C(*C*H$_3$)$_3$), 32.30 (C(*C*H$_3$)$_3$), 26.25 (CH$_2$*C*H$_3$), 26.07 (CH$_2$*C*H$_3$), 23.51 (CH$_2$*C*H$_3$), 22.91 (CH$_2$*C*H$_3$), 16.14 (*C*H$_2$CH$_3$), 15.47 (*C*H$_2$CH$_3$), 15.31 (*C*H$_2$CH$_3$) ppm.

Elemental analysis: [$C_{47}H_{62}AlN_3$] = 696.02: C 81.11, H 8.98, N 6.04; found: C 80.81, H 9.19, N 6.30.

NMR Spectra

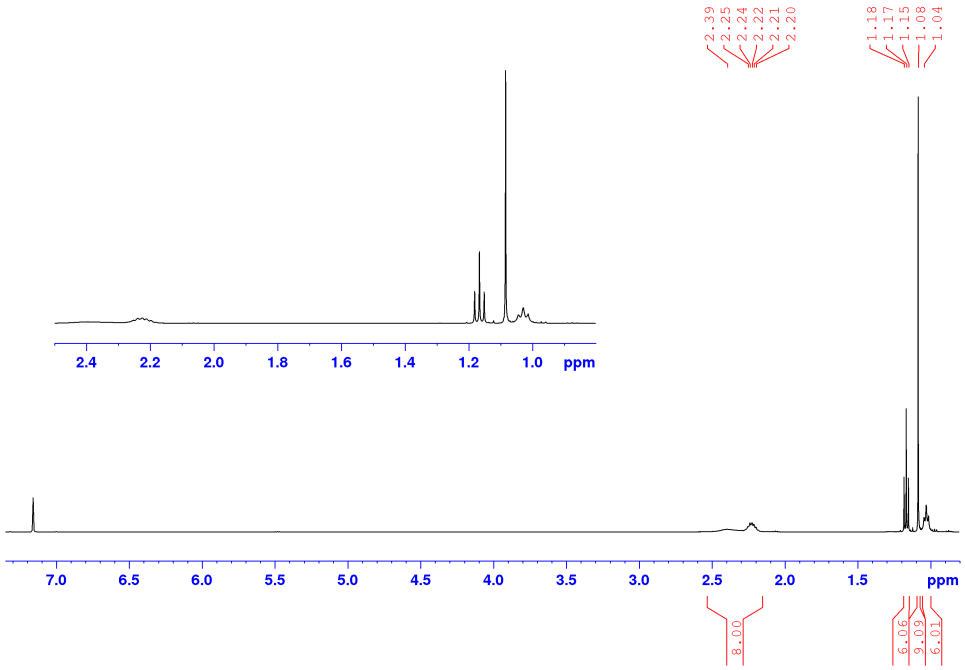


Figure S1. ^{1}H NMR spectrum of **1** in d_6-benzene.

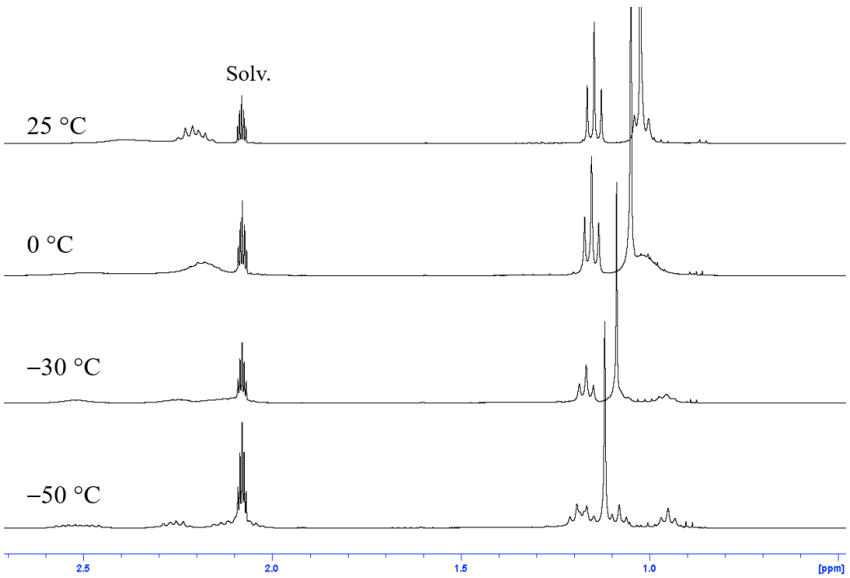


Figure S2. Variable-temperature ^{1}H NMR spectra of **1** in d_8-toluene.

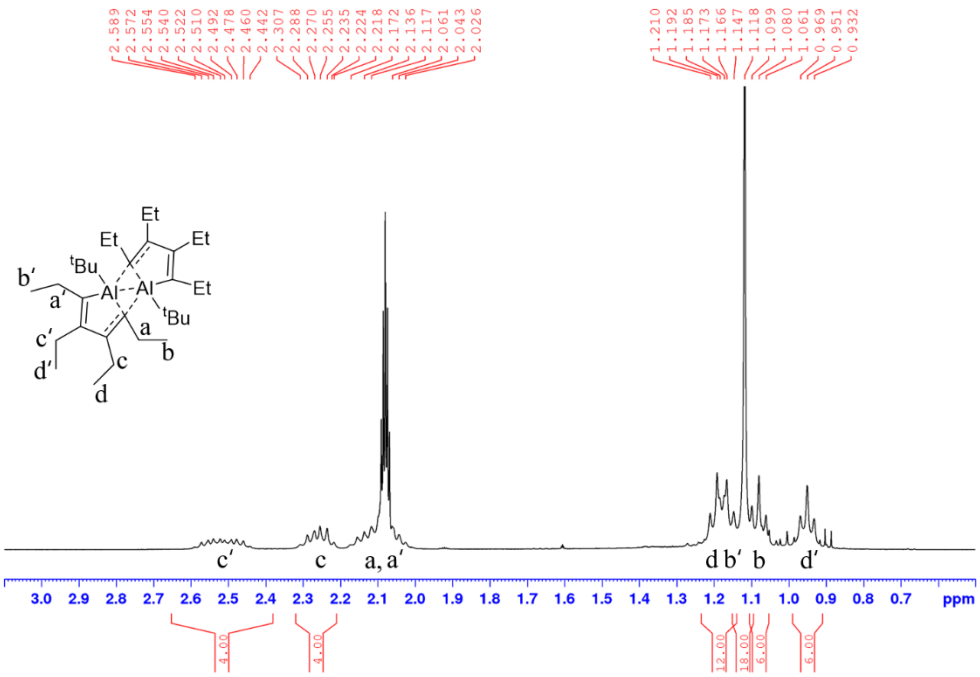


Figure S3. Expanded view of the ^{1}H NMR spectrum of **1** in d_8-toluene at −50 °C.

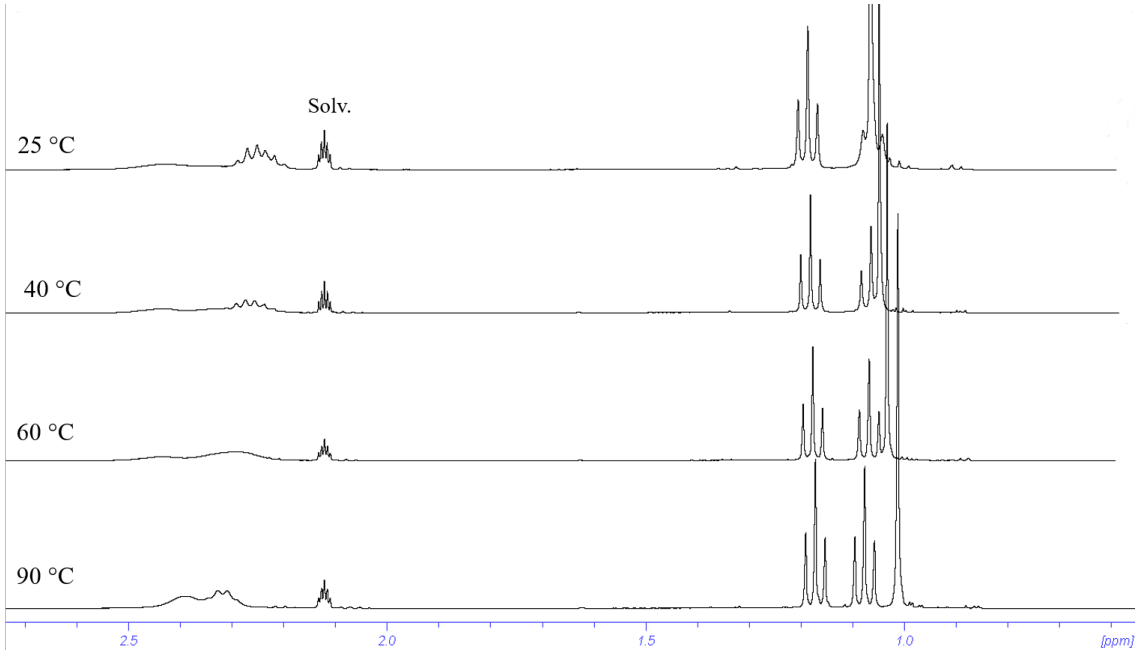


Figure S4. Variable-temperature ^{1}H NMR spectra of **1** in d_8-toluene between 25 and 90 °C.

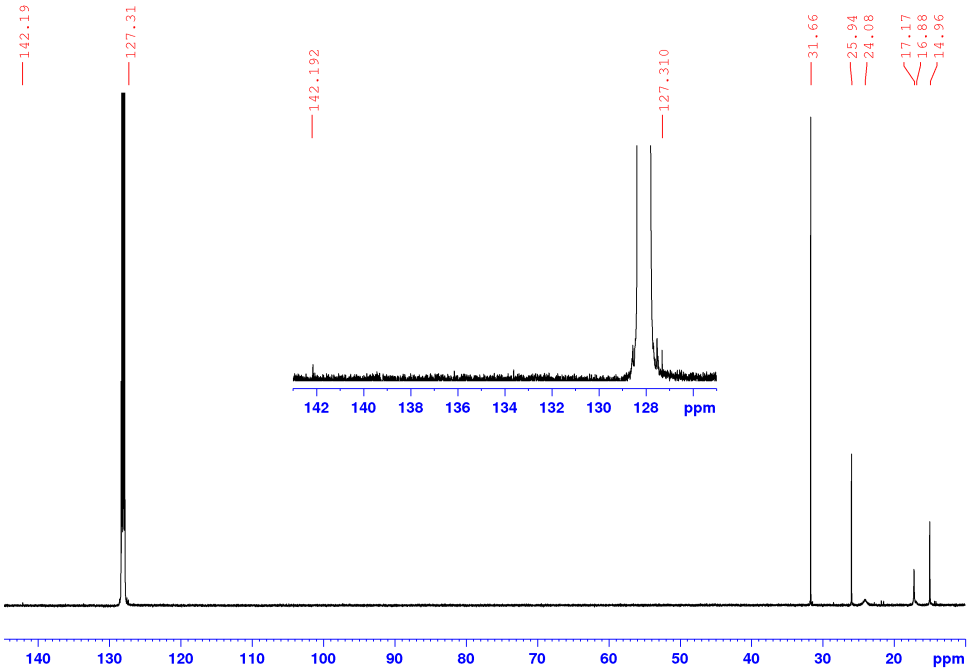


Figure S5. $^{13}C\{^{1}H\}$ NMR spectrum of **1** in d_6-benzene.

Diffusion coefficient of **1**, as determined by ^{1}H DOSY NMR: $D = 8.736 \cdot 10^{-10}\ \frac{m^2}{s}$

According to the relation $= \frac{k_B \cdot T}{6\pi \cdot \eta \cdot r_o}$, the calculated hydrodynamic radius at 25 °C is 4.02 Å.

The experimental hydrodynamic radius of the dimer, estimated from its solid-state structure, is 5.68 Å.

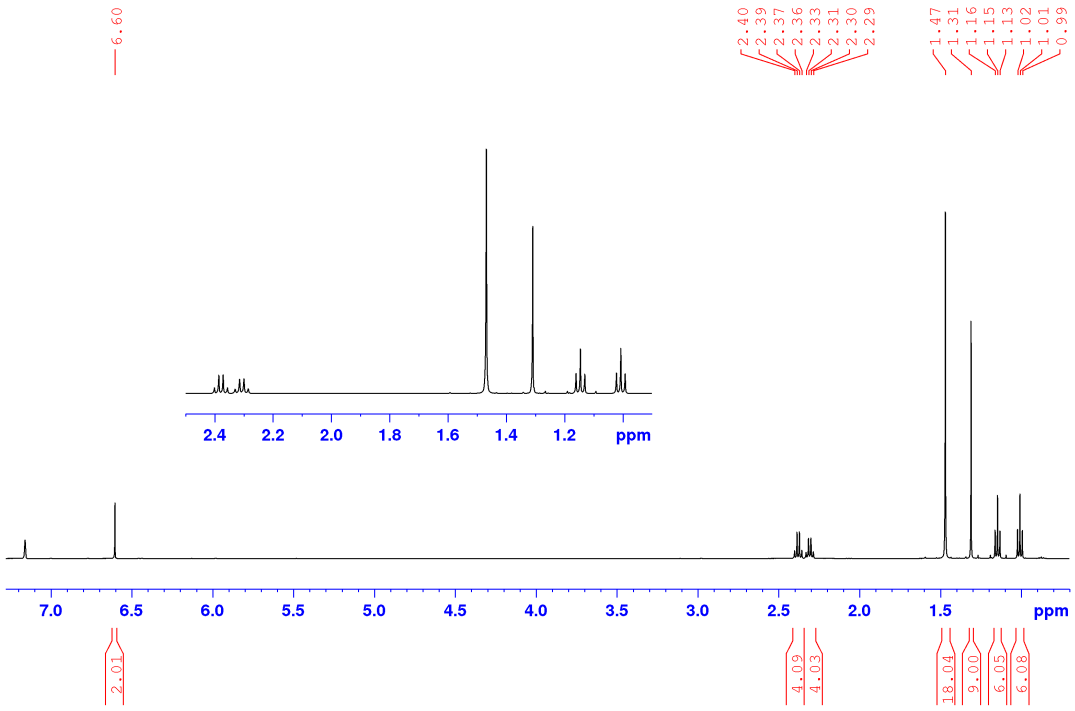


Figure S6. ^{1}H NMR spectrum of **2** in d_6-benzene.

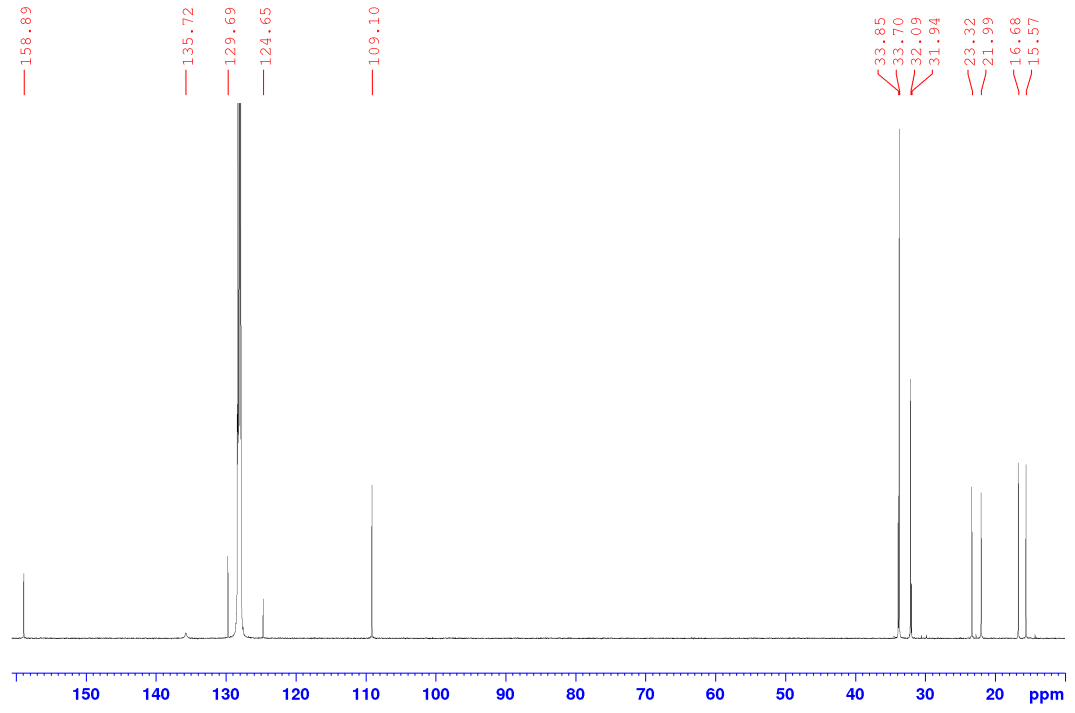


Figure S7. ^{13}C{^{1}H} NMR spectrum of **2** in d_6-benzene.

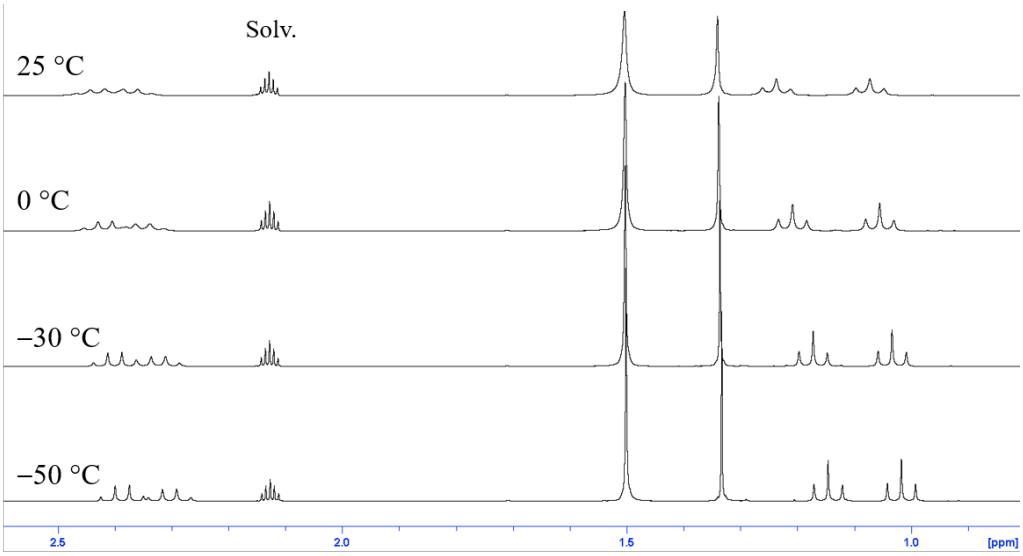


Figure S8. Variable-temperature ^{1}H NMR spectra of **2** in d_8-toluene.

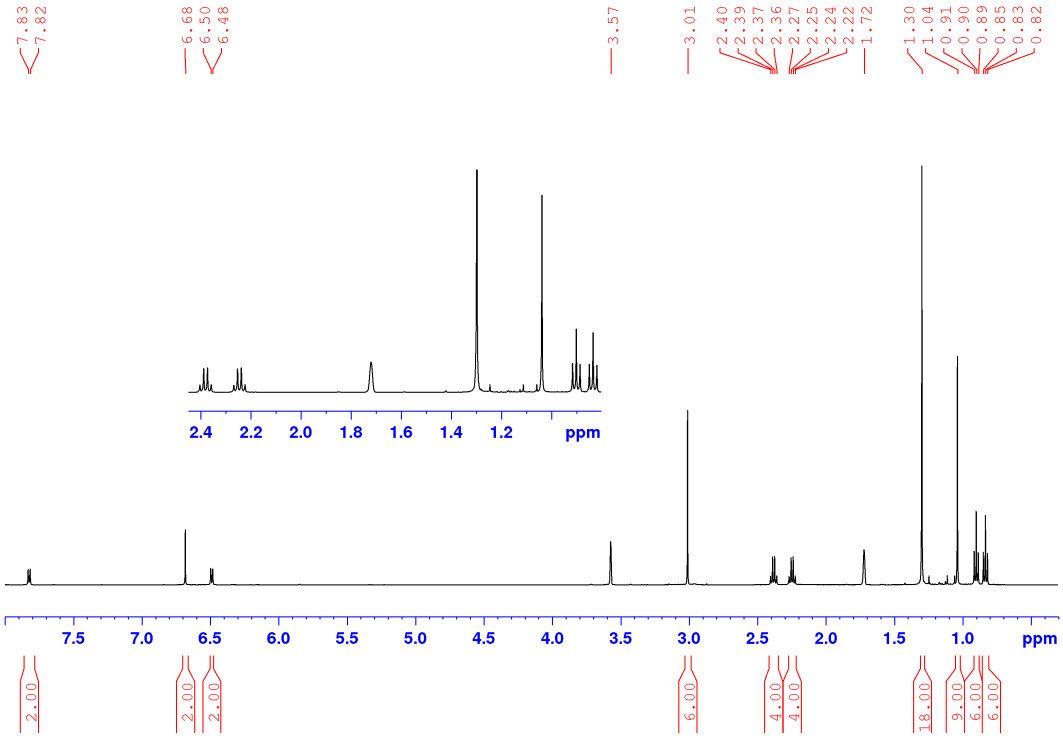


Figure S9. ^{1}H NMR spectrum of **2-DMAP** in d_8-thf.

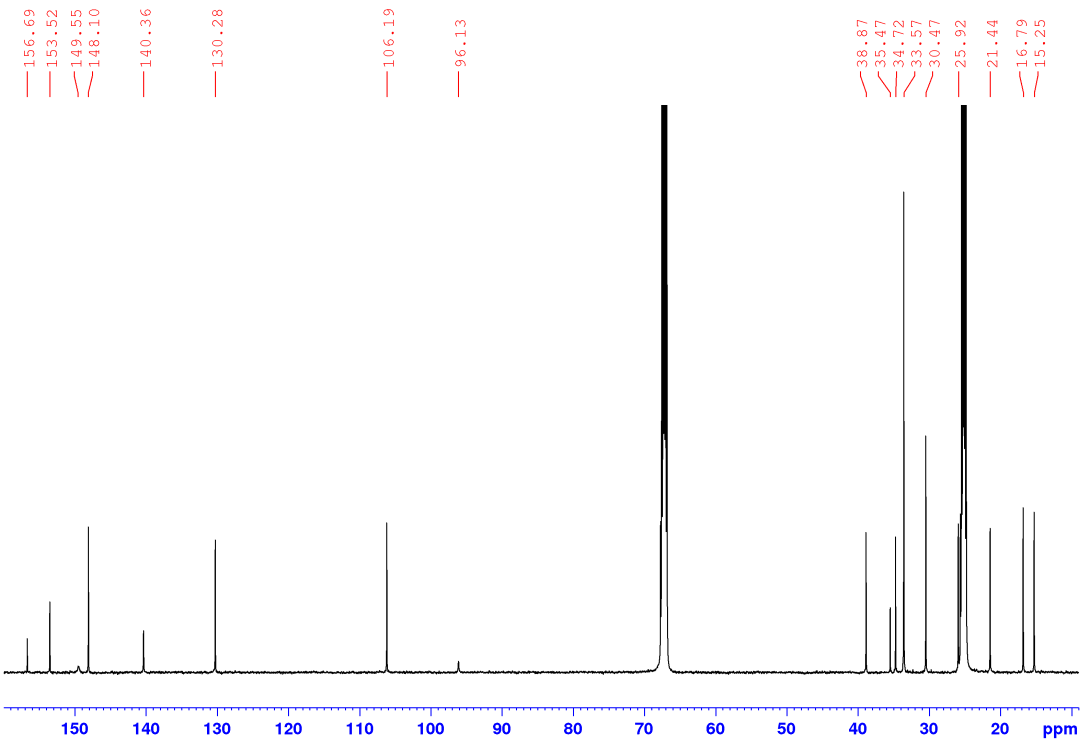


Figure 10. $^{13}C\{^{1}H\}$ NMR spectrum of **2-DMAP** in d_8-thf.

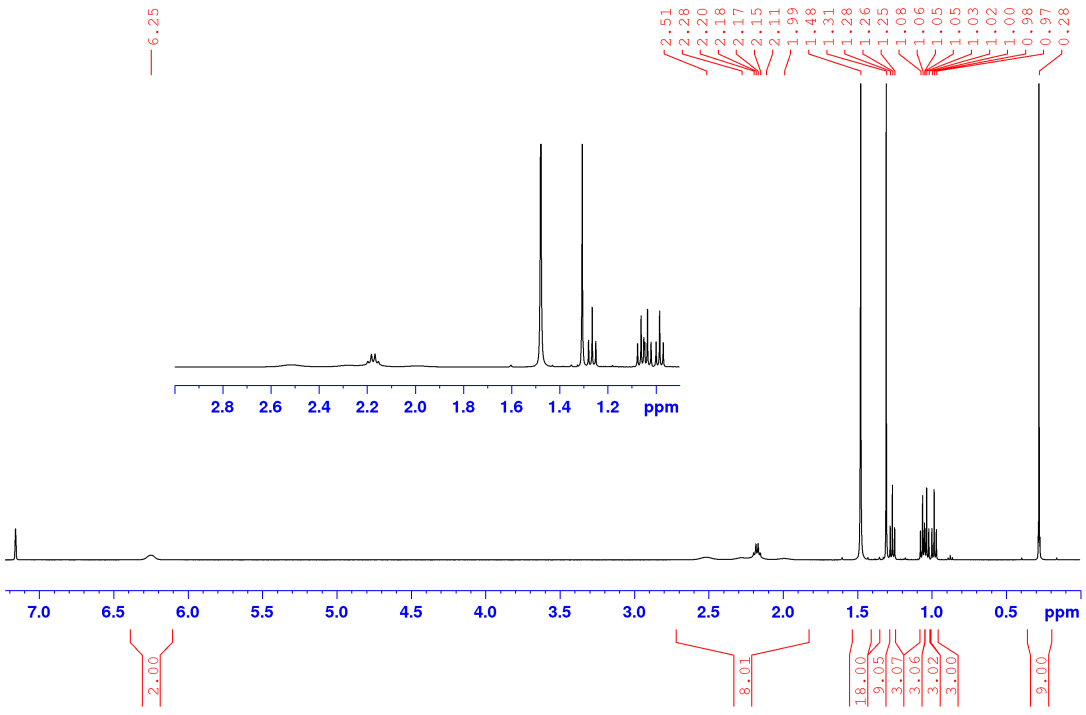


Figure S11. ^{1}H NMR spectrum of **3** in d_6-benzene.

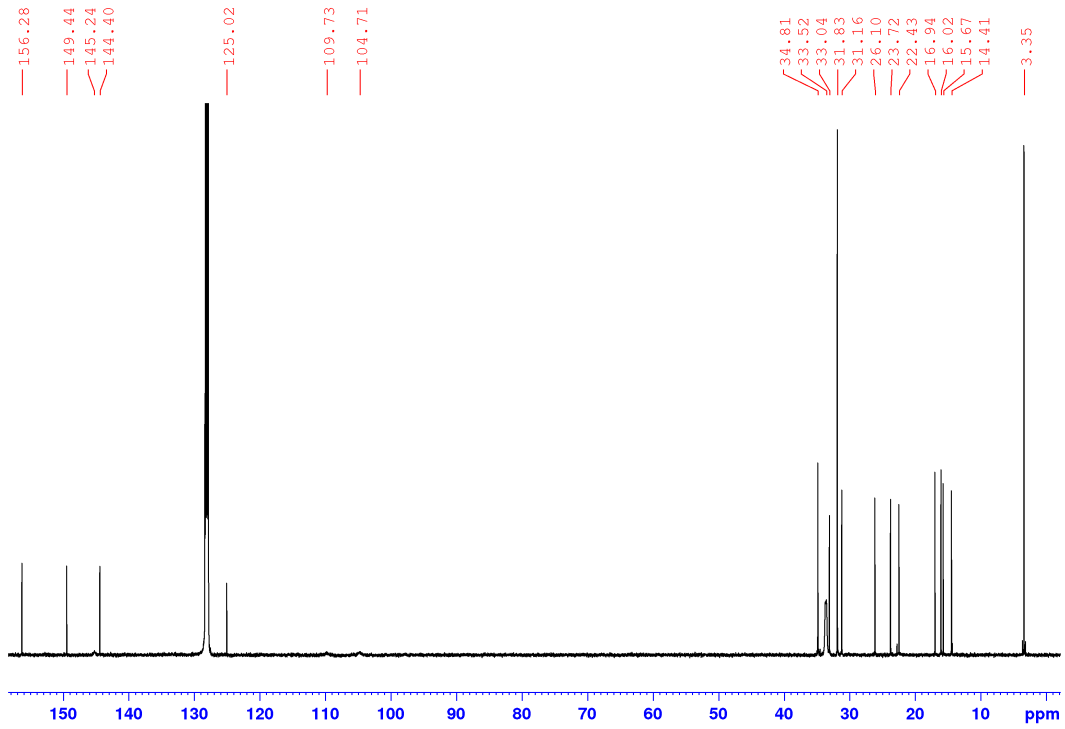


Figure S12. $^{13}C\{^{1}H\}$ NMR spectrum of **3** in d_6-benzene.

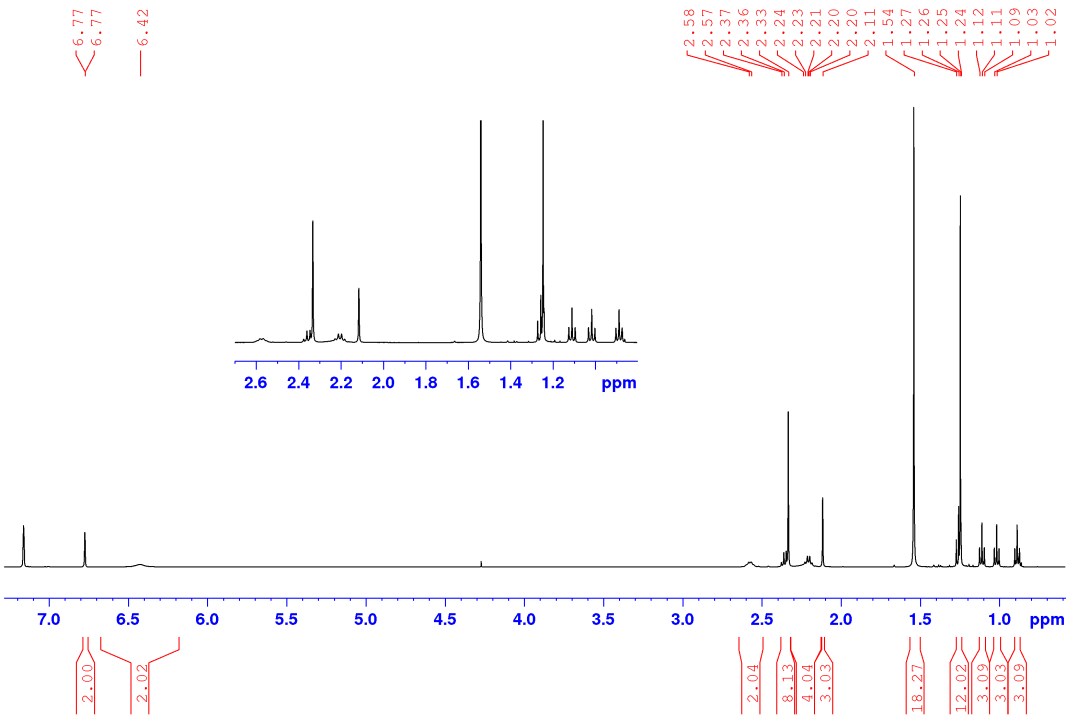


Figure S13. ^{1}H NMR spectrum of **4** in d_6-benzene.

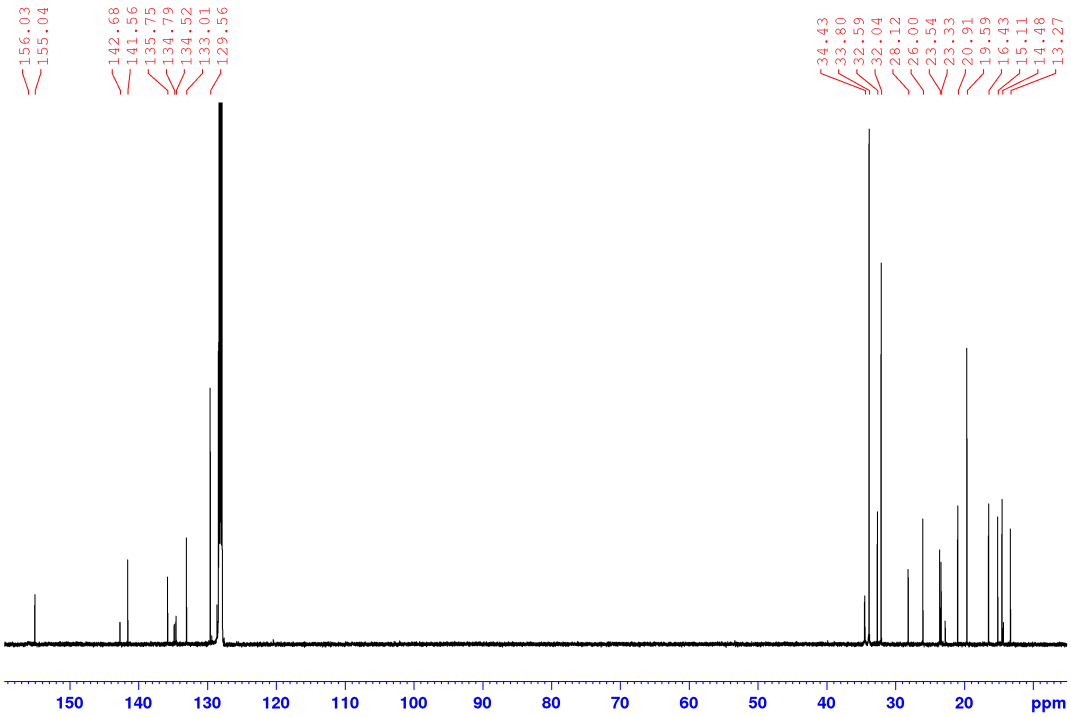


Figure S14. $^{13}C\{^{1}H\}$ NMR spectrum of **4** in d_6-benzene.

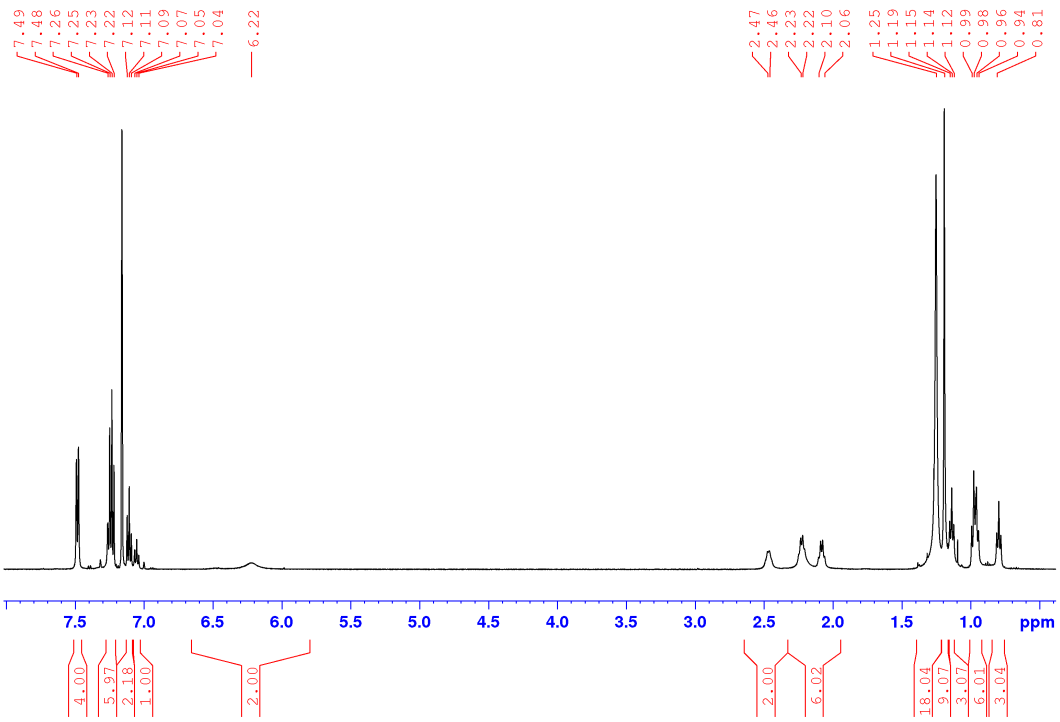


Figure S15. ^{1}H NMR spectrum of **5** in d_6-benzene.

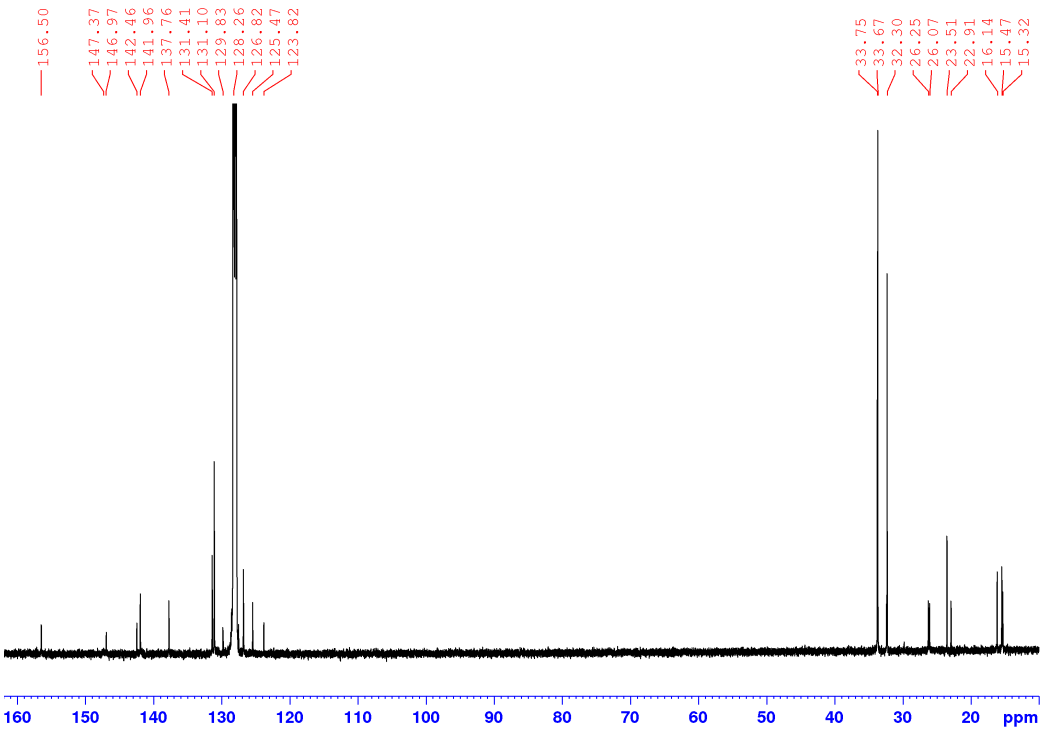


Figure S16. $^{13}C\{^{1}H\}$ NMR spectrum of **5** in d_6-benzene.

Crystallographic Details

The crystal data of **1**, **2**, **3**, **4**, and **5** were collected on a Bruker X8-APEX II diffractometer with a CCD area detector and multi-layer mirror monochromated $Mo_{K\alpha}$ radiation. The structure was solved using the intrinsic phasing method,[6] refined with the *SHELXL* program[7] and expanded using Fourier techniques. All non-hydrogen atoms were refined anisotropically. Hydrogen atoms were included in structure factor calculations. All hydrogen atoms were assigned to idealized geometric positions.

The crystallographic data have been deposited with the Cambridge Crystallographic Data Center as supplementary publication numbers CCDC-1987119 (**1**), CCDC-1987122 (**2**), CCDC-1987118 (**2-DMAP**), CCDC-1987121 (**3**), CCDC-1987117 (**4**), and CCDC-1987120 (**5**). These data can be obtained free of charge *via* www.ccdc.cam.ac.uk/data_request/cif

Crystal data for **1:** $C_{32}H_{58}Al_2$, M_r = 496.74, colorless block, 0.42×0.294×0.188 mm^3, monoclinic space group $P2_1/n$, a = 8.755(4) Å, b = 15.965(5) Å, c = 11.067(5) Å, β = 96.64(2)°, V = 1536.6(11) Å^3, Z = 2, ρ_{calcd} = 1.074 g·cm^{-3}, μ = 0.112 mm^{-1}, $F(000)$ = 552, T = 100(2) K, R_1 = 0.0612, wR^2 = 0.1288, 3028 independent reflections [2θ≤52.042°] and 161 parameters.

Crystal data for **2:** $C_{29}H_{49}Al$, $M_r = 424.66$, colorless block, 0.18×0.13×0.10 mm^3, monoclinic space group $P2_1/n$, $a = 9.335(4)$ Å, $b = 16.672(9)$ Å, $c = 17.185(7)$ Å, $\beta = 93.88(3)°$, $V = 2668(2)$ Å^3, $Z = 4$, $\rho_{calcd} = 1.057$ g·cm^{-3}, $\mu = 0.089$ mm^{-1}, $F(000) = 944$, $T = 100(2)$ K, $R_1 = 0.1040$, $wR^2 = 0.1767$, 5262 independent reflections [2θ≤52.044°] and 284 parameters.

Crystal data for **2-DMAP:** $C_{36}H_{59}AlN_2$, $M_r = 546.83$, colorless block, 0.544×0.35×0.317 mm^3, monoclinic space group $P2_1/n$, $a = 12.957(6)$ Å, $b = 16.692(7)$ Å, $c = 15.618(6)$ Å, $\beta = 96.13(2)°$, $V = 3358(2)$ Å^3, $Z = 4$, $\rho_{calcd} = 1.081$ g·cm^{-3}, $\mu = 0.086$ mm^{-1}, $F(000) = 1208$, $T = 100(2)$ K, $R_1 = 0.0505$, $wR^2 = 0.0956$, 6611 independent reflections [2θ≤52.042°] and 367 parameters.

Crystal data for **3:** $C_{32}H_{58}AlNSi$, $M_r = 511.86$, colorless block, 0.555×0.441×0.42 mm^3, triclinic space group $P\bar{1}$, $a = 9.601(2)$ Å, $b = 12.750(3)$ Å, $c = 13.314(2)$ Å, $\alpha = 97.397(6)°$, $\beta = 93.793(15)°$, $\gamma = 94.404(7)°$, $V = 1606.7(6)$ Å^3, $Z = 2$, $\rho_{calcd} = 1.058$ g·cm^{-3}, $\mu = 0.120$ mm^{-1}, $F(000) = 568$, $T = 100(2)$ K, $R_1 = 0.0360$, $wR^2 = 0.0889$, 6282 independent reflections [2θ≤52.044°] and 332 parameters.

Crystal data for **4:** $C_{38}H_{60}AlN_3$, $M_r = 585.87$, orange block, 0.472×0.36×0.292 mm^3, monoclinic space group $P2_1/n$, $a = 10.2360(15)$ Å, $b = 32.920(5)$ Å, $c = 10.7797(14)$ Å, $\beta = 105.178(5)°$, $V = 3505.8(8)$ Å^3, $Z = 4$, $\rho_{calcd} = 1.110$ g·cm^{-3}, $\mu = 0.087$ mm^{-1}, $F(000) = 1288$, $T = 100(2)$ K, $R_1 = 0.0465$, $wR^2 = 0.1083$, 6894 independent reflections [2θ≤52.04°] and 395 parameters.

Crystal data for **5:** One of the phenyl groups and two of the *tert*-butyl groups are disordered. For this reason, the atomic displacement parameters of atoms C1 > C6 of the residues 4 and 14, as well as the atoms C1 > C4 of the residues 5 and 15, 6 and 16 were restrained with the RIGU keyword (enhanced rigid bond restraint; *SHELXL* input). Standard values of 0.004 for both parameters s1 and s2 were used. The displacement parameters of atoms C1 > C6 of the residues 4 and 14, as well as the atoms C1 > C4 of the residues 5 and 15, 6 and 16 were restrained to the same value with the similarity restraint keyword SIMU. The distances between all atoms of the residues 4 and 14 were restrained during refinement to the same value. The Uii displacement parameters of atoms C1 > C6 of the residues 4 and 14, as well as the atoms C1 > C4 of the residues 5 and 15, 6 and 16 were restrained with the ISOR keyword to approximate isotropic behavior.
$C_{47}H_{62}AlN_3$, $M_r = 695.97$, yellow block, 0.229×0.175×0.118 mm^3, monoclinic space group $P2_1/c$, $a = 19.5714(5)$ Å, $b = 14.2192(3)$ Å, $c = 14.8360(4)$ Å, $\beta = 96.3970(10)°$, $V = 4103.00(18)$ Å^3, $Z = 4$, $\rho_{calcd} = 1.127$ g·cm^{-3}, $\mu = 0.084$ mm^{-1}, $F(000) = 1512$, $T = 105(2)$ K, $R_1 = 0.1059$, $wR^2 = 0.2266$, 8083 independent reflections [2θ≤52.038°] and 601 parameters.

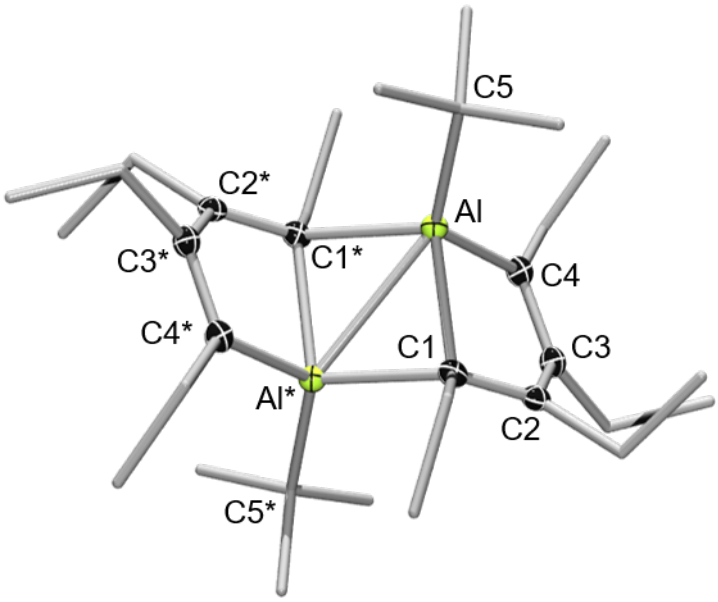


Figure S17. Solid-state structure of **1**. Ellipsoids are set at 50% probability. Some ellipsoids and all hydrogen atoms have been removed for clarity. Selected bond lengths (Å) and angles (º): Al−C4 1.990(2), C4−C3 1.360(3), C3−C2 1.494(2), C2−C1 1.373(2), C1−Al 2.154(2), Al*−C1 2.117(2), Al−Al* 2.638(1), C1*−Al 2.117(2), Al1−C5 2.003(2), C1−Al−C4 89.53(7), C3−C2−C1 121.6(2), C2−C1−Al 96.3(1), C4−C3−C2 117.1(2), Al−C4−C3 106.2(1).

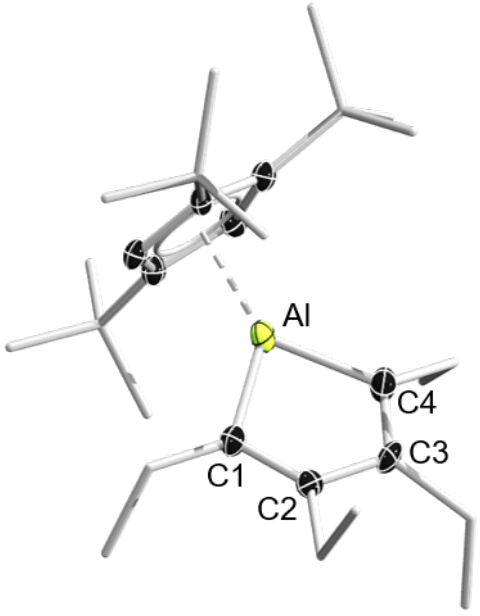


Figure S18. Solid-state structure of **2**. Ellipsoids shown at the 50% probability level. Some ellipsoids and all hydrogen atoms have been removed for clarity. Selected bond lengths (Å) and angles (º): Al−C4 1.976(3), C4−C3 1.357(3), C3−C2 1.518(4), C2−C1 1.345(4), C1−Al 1.966(3), Cp(Centroid)−Al 1.933, C4−Al−C1 91.6(1), Al−C1−C2 104.8(2), C1−C2−C3 119.0(2), C2−C3−C4 118.8(2), C3−C4−Al 104.6(2).

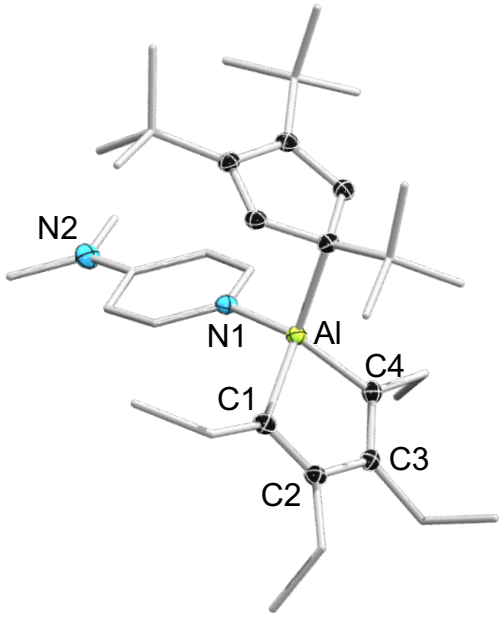


Figure S19: Solid-state structure of **2-DMAP**. Ellipsoids shown at the 50% probability level. Some ellipsoids and all hydrogen atoms have been removed for clarity. Selected bond lengths (Å) and angles (º): C2−C3 1.518(2), C4−C3 1.359(2), C4−Al1 1.990(2), C2−C1 1.353(2), C1−Al 1.970(2), C5−C9 1.461(2), C8−C9 1.372(2), C7−C8 1.485(2), C6−C7 1.373(2), C5−C6 1.458(2), Al−C5 2.081(1), Al−N1 1.967(1), C1−Al−C4 91.47(5), C4−Al−C5 118.55(5), C1−Al−N1 105.51(5).

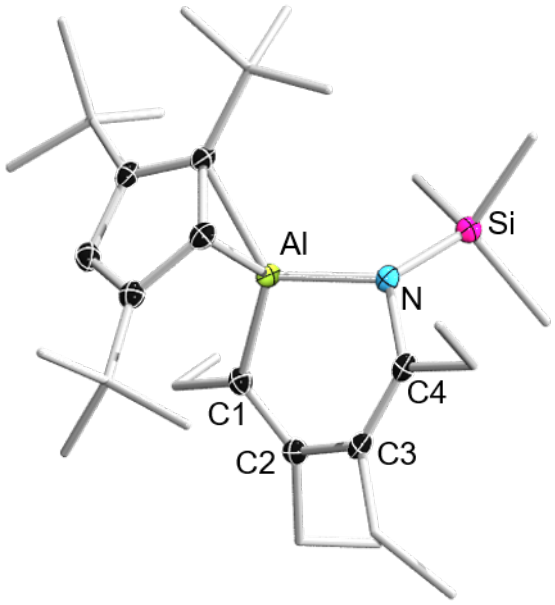


Figure S20: Solid-state structure of **3**. Ellipsoids shown at the 50% probability level. Some ellipsoids and all hydrogen atoms have been removed for clarity. Selected bond lengths (Å) and angles (º): Al−N1 1.8280(11), N1−C4 1.4356(15), C4−C3 1.3592(17), C3−C2 1.5005(16), C2−C1 1.3581(17), C1−Al 1.9395(12), N1−Si 1.7325(11), C1−Al−N1 102.75(5), Al−N1−C4 102.34(7), N1−C4−C3 123.46(10), C4−C3−C2 124.25(10), C3−C2−C1 122.33(10), C2−C1−Al 108.84(9).

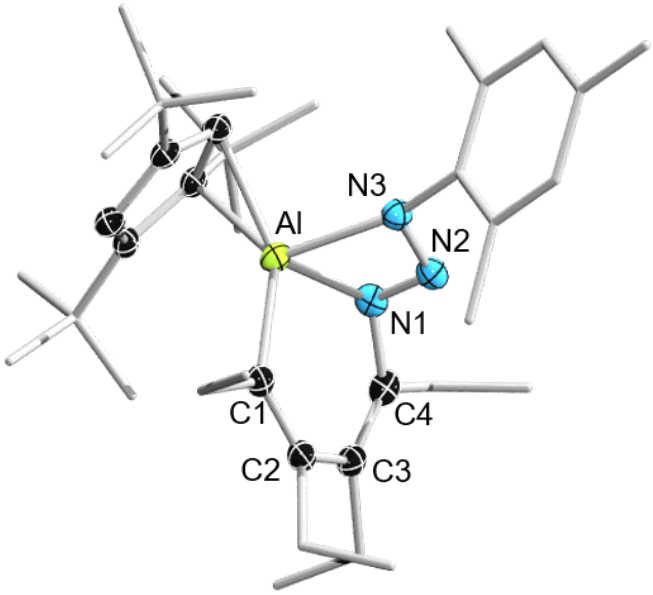


Figure S21: Solid-state structure of **4**. Ellipsoids shown at the 50% probability level. Some ellipsoids and all hydrogen atoms have been removed for clarity. Selected bond lengths (Å) and angles (º): Al−N1 1.9210(12), N1−C4 1.4268(17), C4−C3 1.341(2), C3−C2 1.5124(19), C2−C1 1.3676(19), C1−Al 1.9947(14), N1−N2 1.3198(16), N2−N3 1.3079(16), Al−N3 2.0800(12), C1−Al−N1 91.26(5), Al−N1−C4 128.66(9), N1−C4−C3 117.52(12), C4−C3−C2 124.69(12), C3−C2−C1 126.51(12), C2−C1−Al 121.12(10).

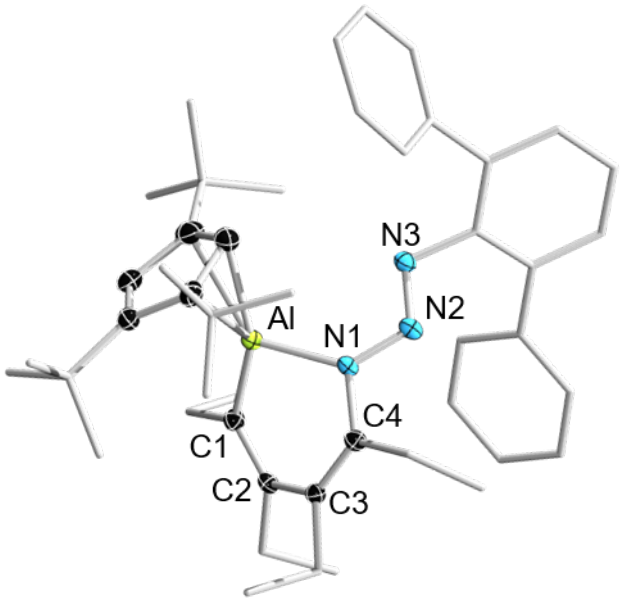


Figure S22: Solid-state structure of **5**. Ellipsoids shown at the 50% probability level. Some ellipsoids and all hydrogen atoms have been removed for clarity. Selected bond lengths (Å) and angles (º): Al−N1 1.884(3), N1−C4 1.427(5), C4−C3 1.356(5), C3−C2 1.499(5), C2−C1 1.354(5), C1−Al 1.940(4), N1−N2 1.342(4), N2−N3 1.277(4), C1−Al−N1 97.48(15), Al−N1−C4 114.1(2), N1−C4−C3 120.9(3), C4−C3−C2 124.6(3), C3−C2−C1 124.5(3), C2−C1−Al 114.9(3).

UV-vis Spectroscopy

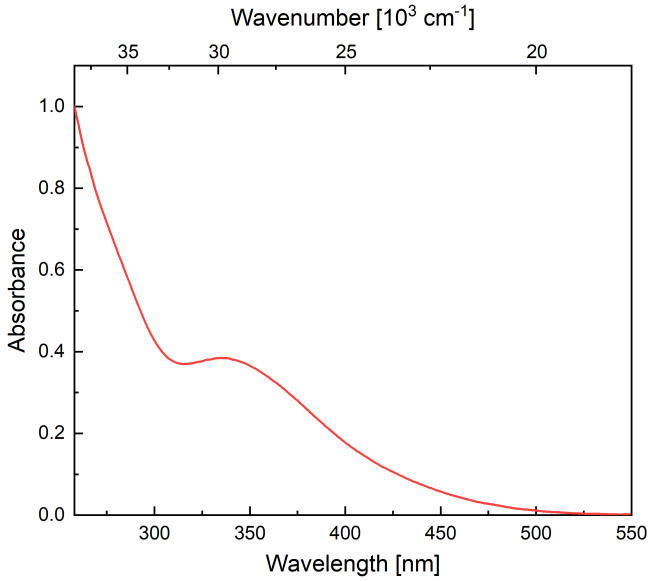


Figure S23: UV-vis absorption spectrum of **4** in pentane (λ_{max} = 335 nm).

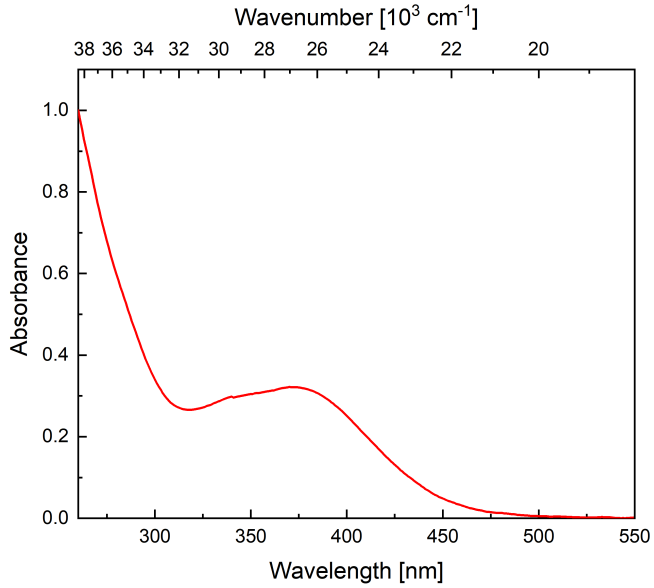


Figure S24: UV-vis absorption spectrum of **5** in pentane (λ_{max} = 370 nm).

IR Spectroscopy

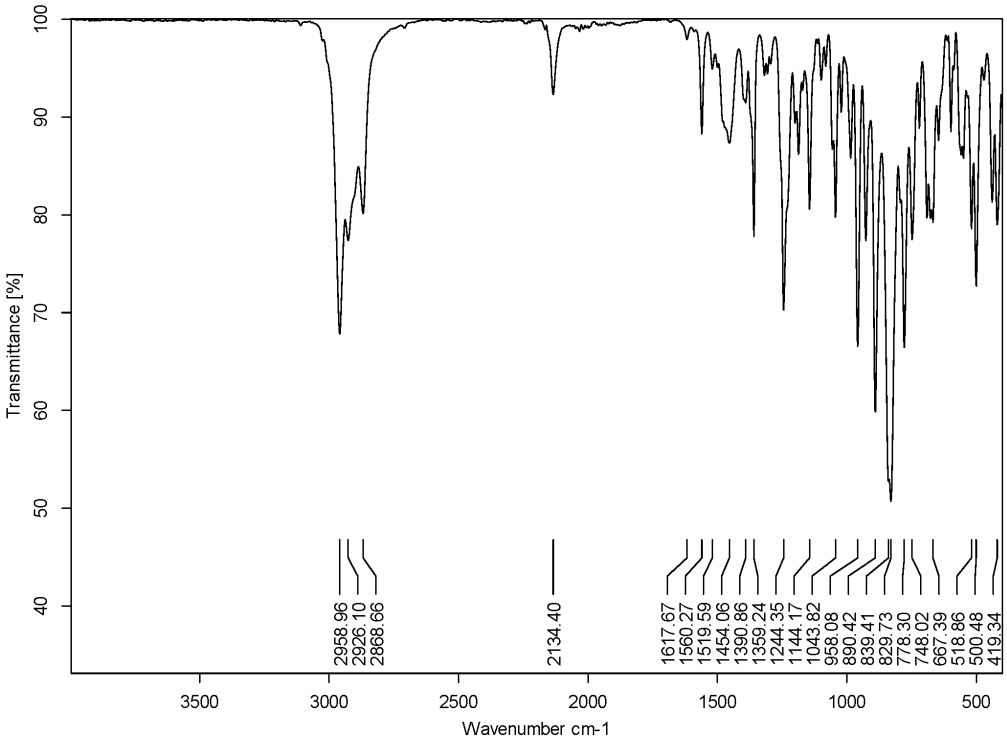


Figure S25: IR spectrum of **3**.

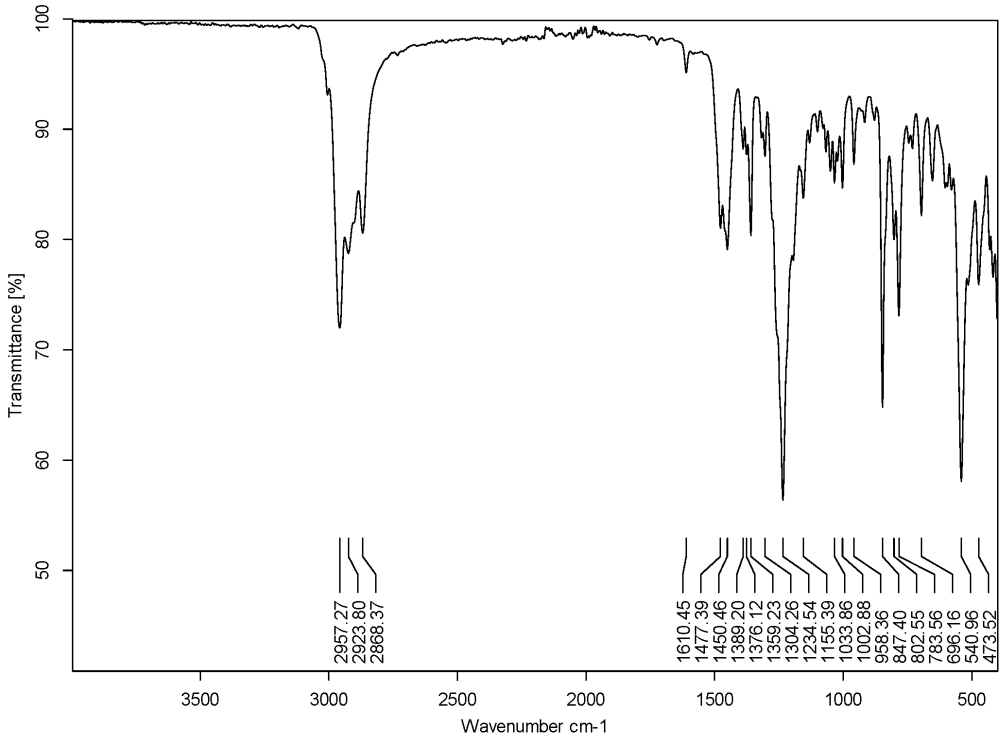


Figure S26: IR spectrum of **4**.

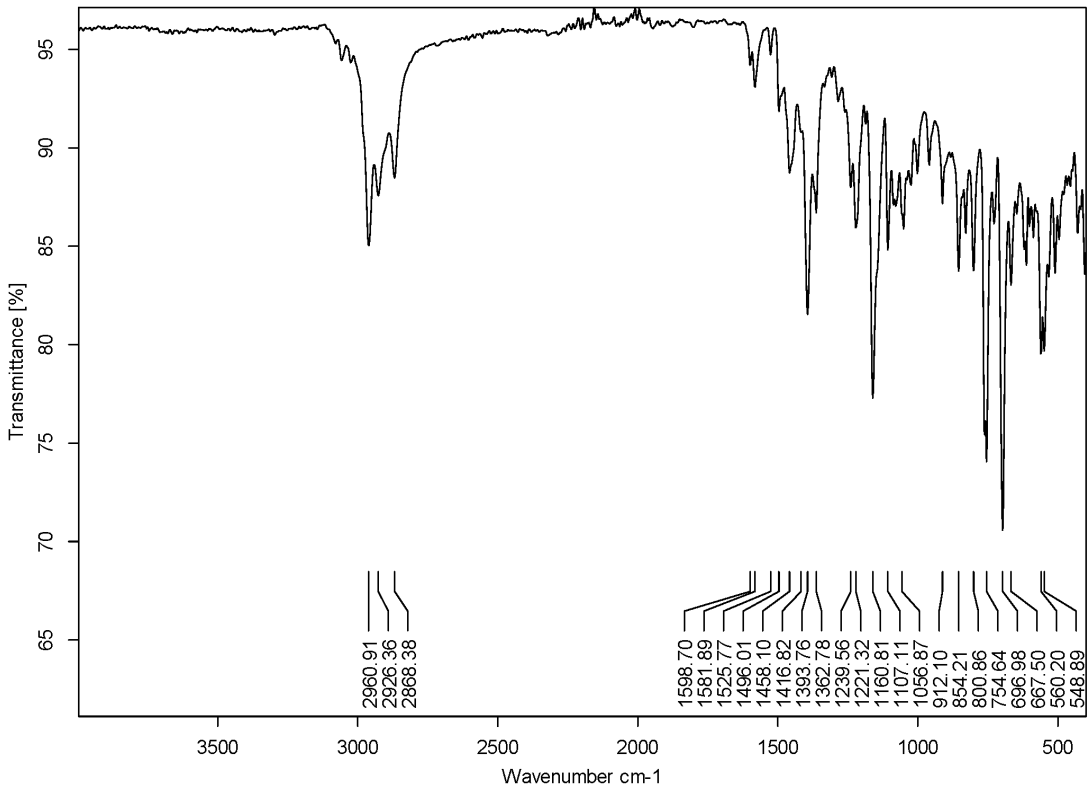
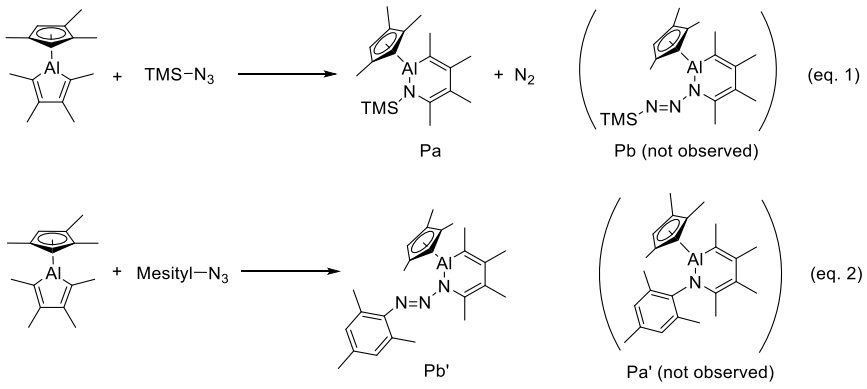


Figure S27: IR spectrum of **5**.

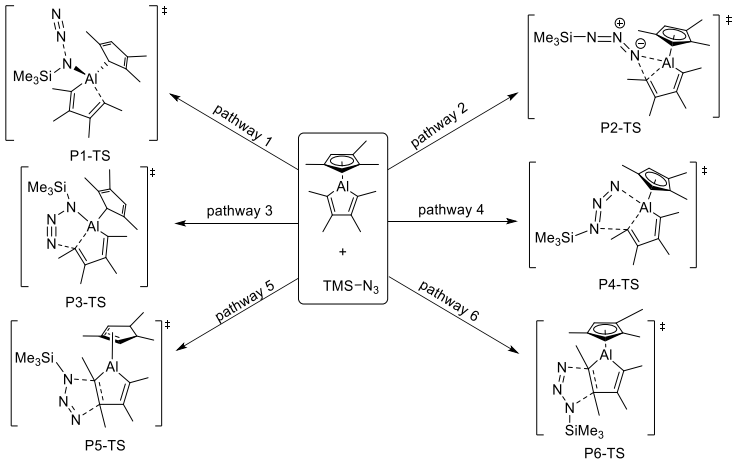
Computational Details

All molecular geometries were fully optimized at the DFT level using the B3LYP functional.[8] The Al and Si atoms are described by the polarization triple-ζ basis set Def2TZVP.[9] For other atoms including H, C, N and O, the 6-31G* basis set was used. Vibrational frequency calculations were performed at the same level of theory to verify the nature of the stationary points as local minima (which have no imaginary frequency) or transition states (which have only one imaginary frequency). Intrinsic reaction coordinate (IRC) calculations were also carried out to make sure that the transition states could connect two relevant minima.[10] To take into account the effects of solvent, single-point energy calculations were carried out using the SMD solvation model and toluene as the solvent. All of the DFT calculations were performed with the Gaussian 09 software package.[11]



Scheme S1: The two model reactions (eq. 1 and 2) considered for the mechanistic studies.

1. Mechanistic studies related to the reaction in equation 1



Scheme S2. Overview of the pathways considered for the reaction of the alumole with trimethylsilyl azide (eq. 1 in Scheme S1). Our calculations indicate that pathway 3 is kinetically the most favorable, while pathways 2 and 6 are the next favorable ones, with noticeably higher reaction barriers.

1.1 Calculated energy profiles

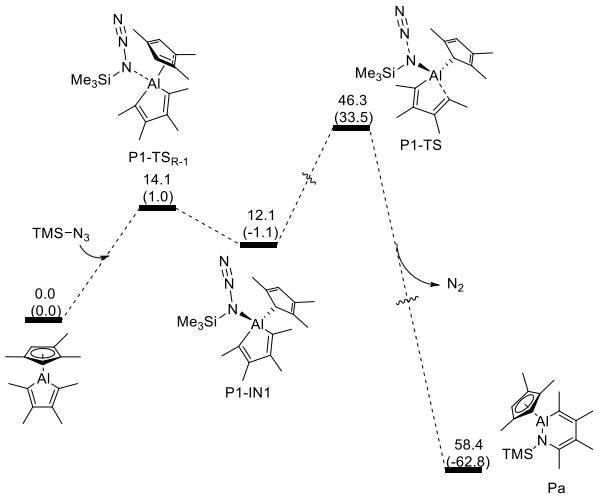


Figure S28. Energy profile calculated for pathway 1. The relative free energy and electronic energies (in parentheses) are given in kcal/mol.

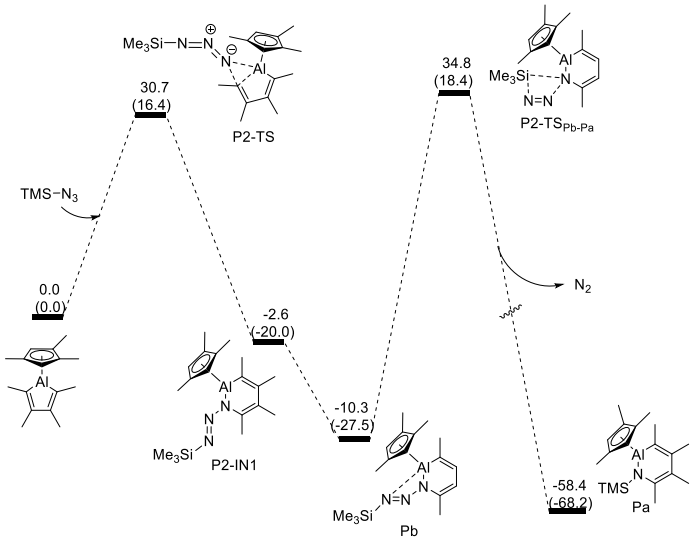


Figure S29. Energy profile calculated for pathway 2. The relative free energy and electronic energies (in parentheses) are given in kcal/mol.

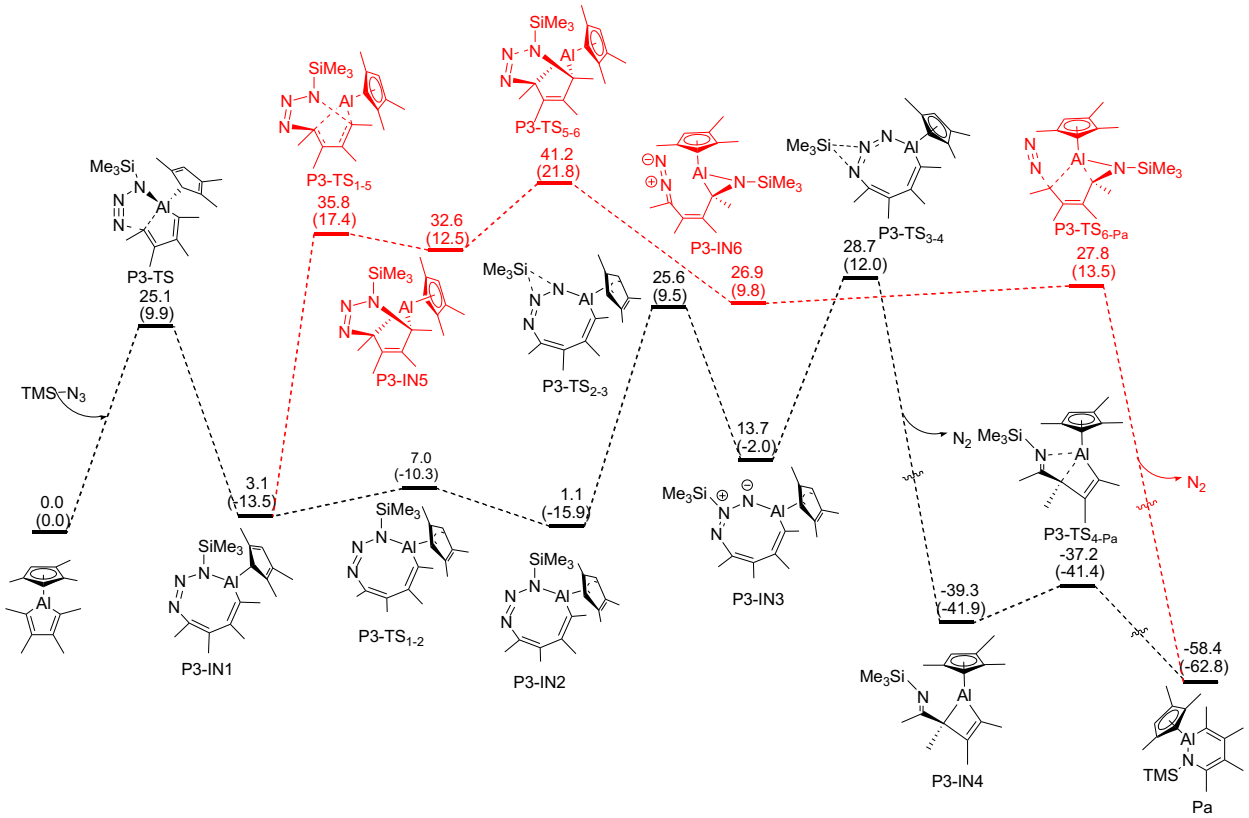


Figure S30. Energy profiles calculated for pathway 3. The relative free energy and electronic energies (in parentheses) are given in kcal/mol.

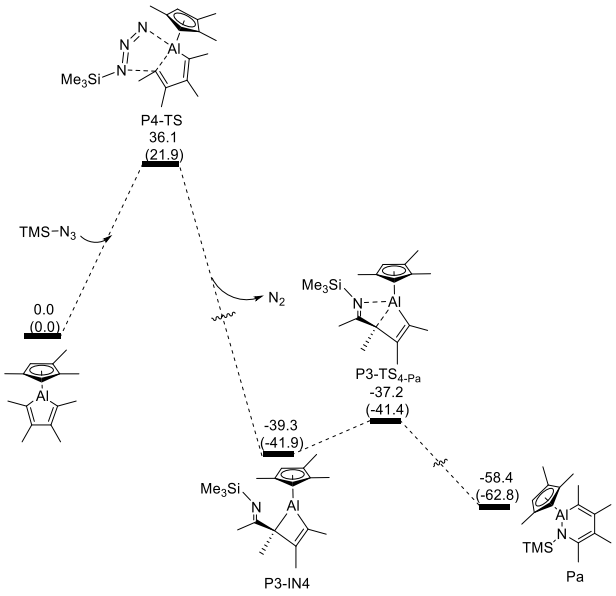


Figure S31. Energy profile calculated for pathway 4. The relative free energy and electronic energies (in parentheses) are given in kcal/mol.

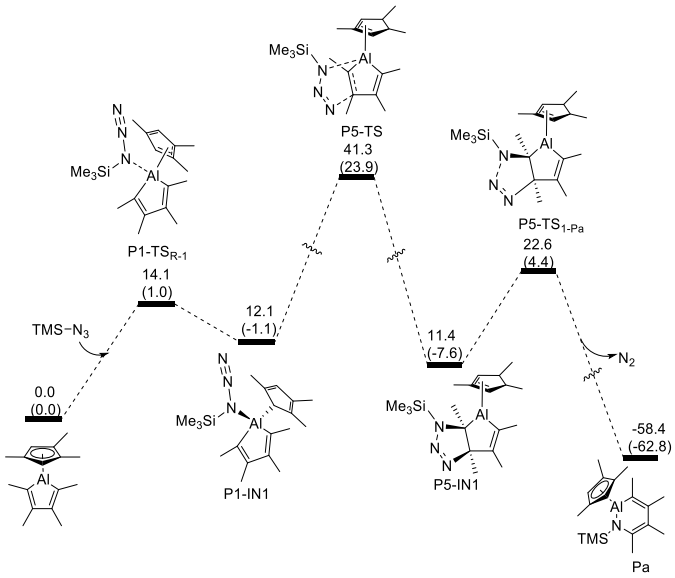


Figure S32. Energy profile calculated for pathway 5. The relative free energy and electronic energies (in parentheses) are given in kcal/mol.

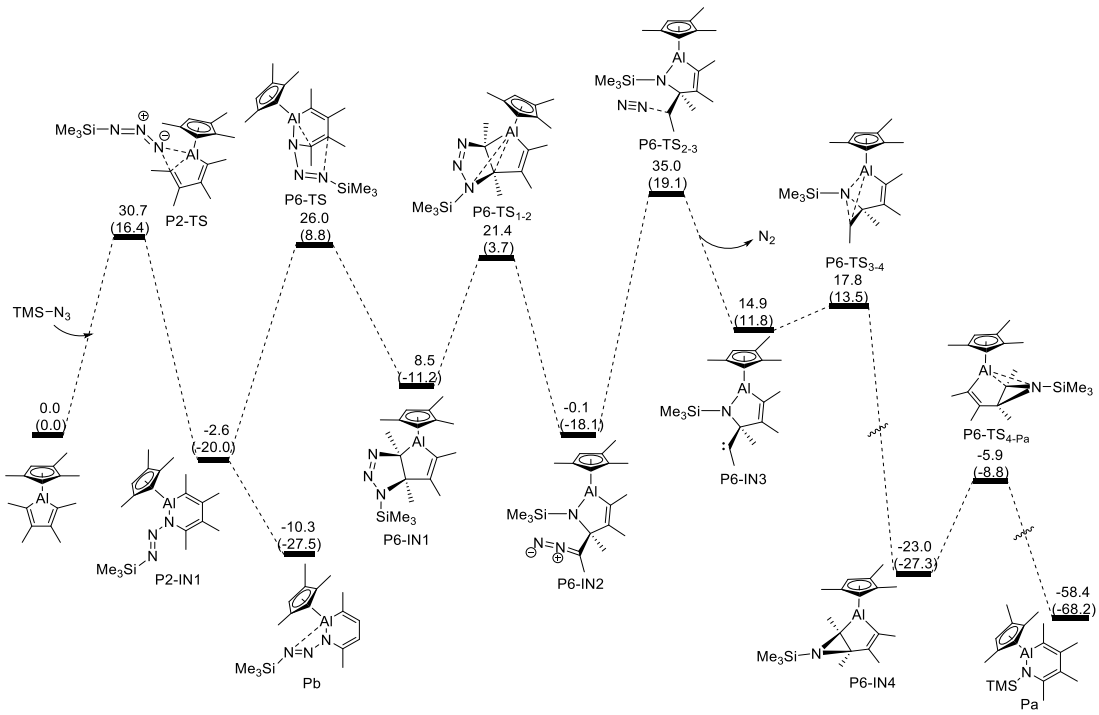


Figure S33. Energy profile calculated for pathway 6. The relative free energy and electronic energies (in parentheses) are given in kcal/mol.

2. Mechanistic studies related to the reaction in equation 2

Only pathways 2, 3 and 6 were calculated (cf. Scheme S2), marked as pathways 2', 3' and 6', respectively. Pathway 2' becomes the most favored mechanism.

2.1 Calculated energy profiles

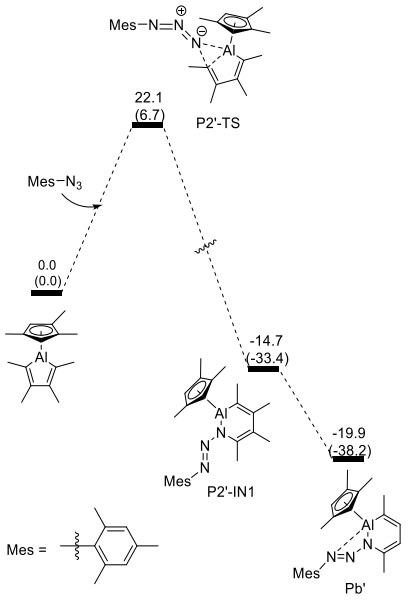


Figure S34. Energy profile calculated for pathway 2' for the reaction between mesityl azide and the alumole. The relative free energy and electronic energies (in parentheses) are given in kcal/mol.

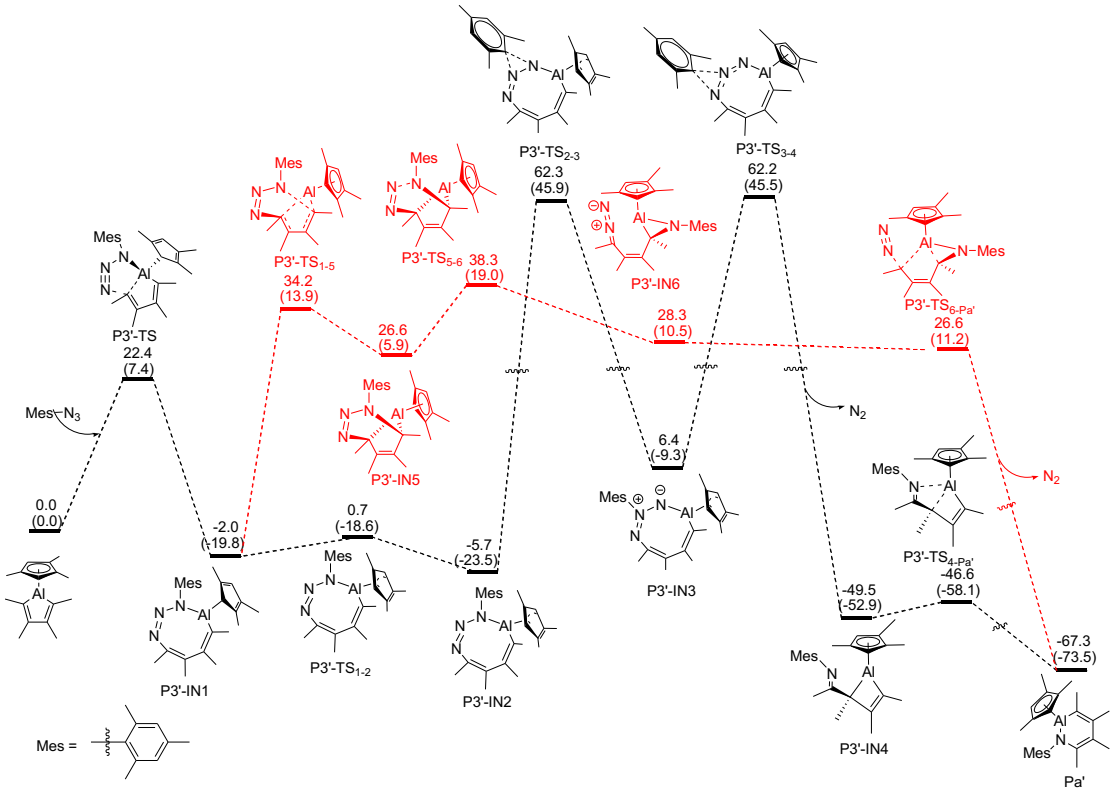


Figure S35. Energy profile calculated for pathway 3' for the reaction between mesityl azide and the aluminole. The relative free energy and electronic energies (in parentheses) are given in kcal/mol.

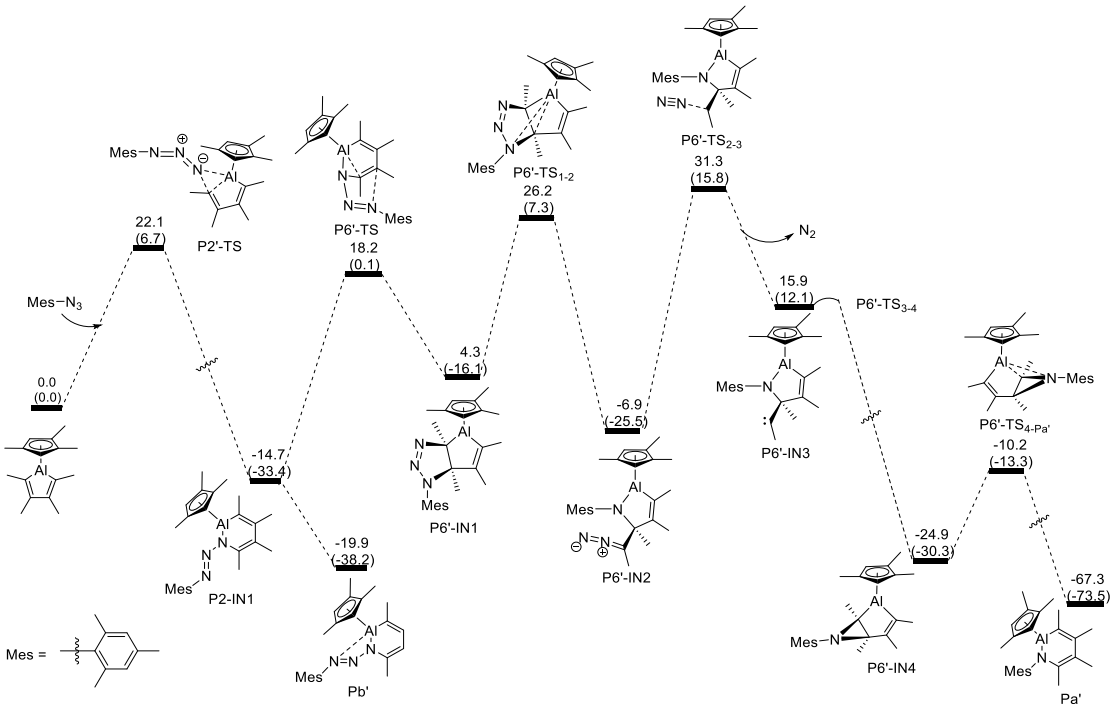
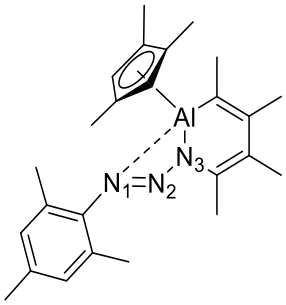


Figure S36. Energy profile calculated for pathway 6' for the reaction between mesityl azide and the aluminole. The relative free energy and electronic energies (in parentheses) are given in kcal/mol. Note:

Attempts to locate the transition state P6'-TS_{3-4} were unsuccessful as it is presumably very close in energy to P6'-IN3.

2.2 Calculated IR data



N1-N2: 1343 cm^{-1}, 1347 cm^{-1}

N2-N3: 1292 cm^{-1}, 1310 cm^{-1}

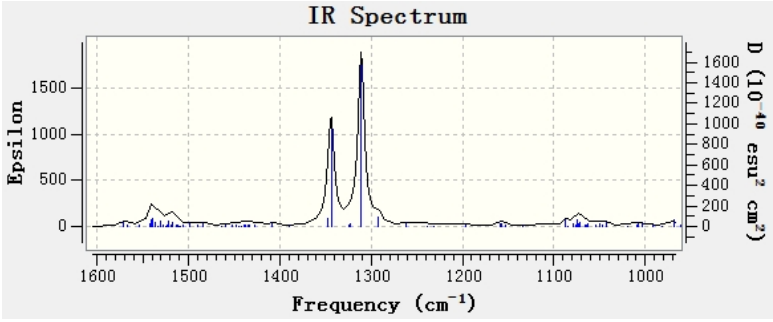
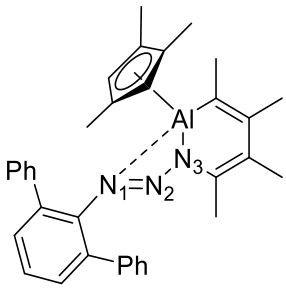


Figure S37. Calculated IR spectrum of **4**.



N1-N2: 1357 cm^{-1}

N2-N3: 1318 cm^{-1}, 1332 cm^{-1}, 1336 cm^{-1}, 1339 cm^{-1}

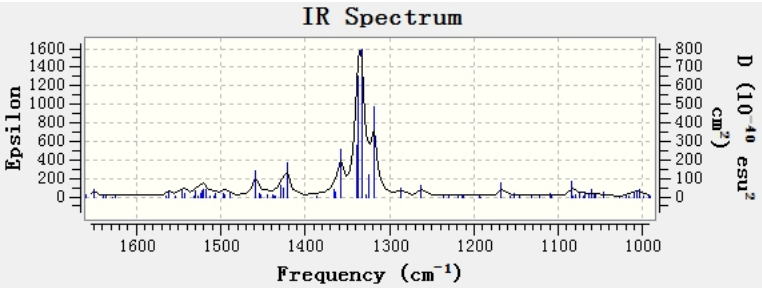


Figure S38. Calculated IR spectrum of **5**.

3. Cartesian coordinates of all investigated species and relative zero point corrected energies

40

Alumole E = -865.9878099

Al	-0.17382900	-0.02125400	0.14139200
C	-2.10177200	1.05251000	0.75775100
H	-2.05351300	2.02919900	1.22524300
C	-2.16382400	0.81590500	-0.64094000
C	-2.15409700	-0.60900300	-0.83574100
C	1.16272300	1.40829700	0.13138300
C	2.36025600	-0.76709900	-0.09053400
C	2.34676600	0.75894400	0.00315600
C	1.17928500	-1.43282800	-0.03948000
C	3.68330100	1.47063700	-0.06053700
H	4.36634200	1.13091500	0.72908300
H	3.56821000	2.55194900	0.04510700
C	-2.09893800	-1.21294900	0.45071100
H	-2.03823500	-2.27871500	0.63770600
C	-2.03140700	-0.19629000	1.44708900
C	3.71961700	-1.42210500	-0.23456300
H	4.24981200	-1.06051000	-1.12527000
H	3.64648700	-2.50849600	-0.31628700
C	1.04137200	2.91161200	0.22737900
H	0.00406900	3.22508800	0.39580000
H	1.37673500	3.41932300	-0.68970500
C	1.00775200	-2.92710600	-0.11415600
H	1.94247600	-3.49137000	-0.22235900
H	0.36389300	-3.21201300	-0.95977600
C	-2.02296200	-0.39923400	2.94008900
H	-3.04724600	-0.45857400	3.33094500
H	-1.51266600	-1.32747800	3.21836000

H	-1.52337400	0.42667400	3.45756800
C	-2.28934000	1.86477700	-1.71348400
H	-1.75403700	1.58687000	-2.62811600
H	-3.34087700	2.02136300	-1.98942600
H	-1.89018900	2.82639800	-1.37584200
C	-2.27950600	-1.33545600	-2.14900800
H	-3.33019900	-1.40778600	-2.46053600
H	-1.73792100	-0.82922600	-2.95565300
H	-1.88767000	-2.35517300	-2.07530000
H	0.50406700	-3.31534300	0.78365100
H	4.36789800	-1.20091800	0.62377100
H	4.19665100	1.28597900	-1.01403100
H	1.63371900	3.33448000	1.05229500

16

TMS-N_3 E = -573.523711

N	-0.87668000	0.00000300	-0.84938600
Si	0.66210400	0.00001000	0.01743500
N	-1.99318000	0.00000300	-0.34587200
C	0.76899300	1.53946400	1.07990800
C	1.94514000	0.00048300	-1.33703200
C	0.76943400	-1.53992900	1.07916200
N	-3.07203000	-0.00004600	0.03111600
H	0.69046300	2.45000300	0.47509100
H	-0.03038900	1.56698900	1.83023300
H	1.72461500	1.57732500	1.61794000
H	1.84595200	0.88566600	-1.97526900
H	2.95949500	0.00034000	-0.92001900
H	1.84594300	-0.88428000	-1.97585000
H	0.69122300	-2.45019700	0.47389700
H	1.72504800	-1.57774300	1.61721400
H	-0.02997100	-1.56807600	1.82943900

54

Pa E = -1330.094143

C	-1.86700800	-0.55931000	-1.65720800
H	-1.36430600	-0.53179600	-2.61820200
C	-1.80106700	-1.67587000	-0.71789500
C	-2.75750500	-1.38650200	0.31465400
C	-3.38000100	-0.16184600	0.00264600
H	-4.09623500	0.34890100	0.63733200
C	-2.85192500	0.35464400	-1.19858900
Al	-0.58386000	-0.08599700	0.00222100
C	0.24758700	2.34386600	0.80292200

C	1.13871100	2.17256200	-0.38127600
C	1.63689900	0.97040400	-0.81696300
C	-0.69340400	1.43054600	1.18344400
N	1.21184900	-0.28699900	-0.30258000
Si	2.31665000	-1.46270400	0.35198700
C	1.41323200	-2.40746800	1.71101200
H	2.05190600	-3.20316300	2.11550700
H	0.49511800	-2.89058500	1.35595500
H	1.14528100	-1.74793800	2.54536900
C	3.80996500	-0.62054400	1.13105900
H	4.45107000	-1.36111200	1.62621100
H	3.49752600	0.10887400	1.88747600
H	4.43040100	-0.09037300	0.39982900
C	2.93140400	-2.72227300	-0.91165500
H	3.60897700	-3.44567700	-0.43923900
H	3.47995900	-2.24831700	-1.73381400
H	2.10541600	-3.29042000	-1.35634300
C	1.51769900	3.45905200	-1.10934100
H	2.46656900	3.89089200	-0.75854100
H	1.61234000	3.30596200	-2.18791300
H	0.75071800	4.22712700	-0.96875500
C	2.63563700	0.88691200	-1.95641600
H	2.14256000	0.57561600	-2.88858800
H	3.16058200	1.82545800	-2.14483800
H	3.39220800	0.12523500	-1.74152100
C	0.43506900	3.64210000	1.58240900
H	-0.26156600	4.42697400	1.25407400
H	0.25162500	3.48479000	2.64970800
H	1.44753000	4.04342900	1.47589100
C	-1.56968200	1.66165300	2.39921600
H	-0.98456700	1.69682300	3.33108700
H	-2.12024500	2.61213400	2.34410800
H	-2.31482500	0.86977300	2.51978100
C	-3.09899300	-2.28181400	1.47607200
H	-3.81687100	-3.05809400	1.17689700
H	-2.21992200	-2.79684500	1.87899300
H	-3.55557600	-1.71383200	2.29344300
C	-3.19884900	1.67564100	-1.82769000
H	-4.27907500	1.85526700	-1.78252900
H	-2.70729600	2.51149200	-1.31382700
H	-2.89539700	1.70850400	-2.87958600
C	-1.21420000	-3.02705000	-1.04370400
H	-1.00991000	-3.61877500	-0.14558700
H	-1.91260100	-3.60774300	-1.66234200

H	-0.27866800	-2.93598300	-1.60486100

56

P1-TS(R-1) E = -1439.510713

Al	-0.73267900	0.26664000	0.45054700
C	-1.97615800	-2.03662300	0.30940900
H	-1.48441200	-2.91486400	-0.09635700
C	-3.10629700	-1.41610300	-0.23494700
C	-3.43870900	-0.30625700	0.59358800
C	-0.75414600	1.11922700	-1.30512700
C	0.43599900	2.61401500	0.30596200
C	-0.07679200	2.27979700	-1.09567600
C	0.30988500	1.69127100	1.29801600
C	0.21306900	3.30382000	-2.17746900
H	1.29238000	3.46283100	-2.30584700
H	-0.19131400	3.00559600	-3.14635400
C	-2.52089400	-0.26503100	1.66511800
H	-2.57904500	0.39269700	2.52667400
C	-1.56139000	-1.34825800	1.50399400
C	1.02166700	4.00154200	0.49659900
H	0.27258400	4.78059800	0.30095000
H	1.39017100	4.15518100	1.51279900
C	-1.32030100	0.67350000	-2.62898600
H	-1.12577700	-0.39062400	-2.81136600
H	-2.41460600	0.78163800	-2.64273500
C	0.69092000	1.91189700	2.74093000
H	1.33788700	2.78038700	2.91957600
H	-0.20424000	2.05191700	3.36678400
N	1.41027600	-1.24635300	-0.31537700
N	1.02922900	-1.96324200	-1.24230700
N	0.58983500	-2.61707300	-2.06667500
C	-0.71389400	-1.93303900	2.61241600
H	-0.31170400	-1.15471300	3.27102300
H	-1.30448100	-2.61559200	3.23888100
H	0.13419700	-2.50113000	2.21408800
C	-3.83018500	-1.82344000	-1.48849200
H	-3.88725900	-1.00983900	-2.22232400
H	-3.33166600	-2.66932900	-1.97339300
H	-4.86335600	-2.12935800	-1.27338400
C	-4.55824900	0.66616300	0.34868700
H	-4.58754800	1.44103100	1.12163800
H	-4.46249500	1.16886500	-0.62274200
H	-5.53231200	0.15859600	0.34881000
H	1.20609600	1.03800300	3.16260100

H	1.85581300	4.19476700	-0.18975400
H	-0.21777200	4.28329500	-1.93359600
H	-0.93574000	1.22575400	-3.49532400
Si	3.16582700	-0.95791600	-0.04920700
C	3.60480700	0.69289800	-0.79803300
H	4.66066000	0.93241300	-0.61868900
H	3.43874200	0.70024300	-1.88134300
H	2.99128900	1.48512800	-0.35708900
C	4.09281500	-2.35833000	-0.88043000
H	3.82641700	-3.33441900	-0.45841800
H	3.90339800	-2.39594600	-1.95969500
H	5.17362000	-2.22633700	-0.74584600
C	3.41087300	-0.97405900	1.79900500
H	4.46532500	-0.79569900	2.04430700
H	2.82077500	-0.19074200	2.28508200
H	3.12412100	-1.93711600	2.23596300

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P1-IN1 E = -1439.512569

Al	0.39772200	0.05364900	0.34025200
C	1.59429600	-1.49522700	0.88382700
H	1.27248100	-1.92203500	1.83889500
C	2.86838900	-0.72983600	0.85433500
C	3.50773400	-1.01261600	-0.33687900
C	0.03380300	1.65088600	1.42555700
C	0.26565000	2.34742100	-0.95462300
C	0.00774200	2.66460400	0.51972600
C	0.42414900	1.05168300	-1.34433100
C	-0.27199200	4.11705600	0.85893100
H	-1.18368200	4.48037000	0.36437700
H	-0.40211700	4.27054900	1.93211900
C	2.74285500	-2.01823100	-1.03754300
H	3.01876900	-2.43798500	-2.00157500
C	1.63145600	-2.36447000	-0.31232900
C	0.37211200	3.53605200	-1.89241500
H	1.23803200	4.16343600	-1.64021900
H	0.48982900	3.22914000	-2.93351600
C	-0.22112800	1.79360600	2.90485000
H	-1.07686000	1.17703200	3.22133600
H	0.63433700	1.42659800	3.49023200
C	0.76789000	0.61207600	-2.74634100
H	0.52827600	1.34604700	-3.52688200
H	1.84195200	0.39063000	-2.82770900
N	-1.56461300	-0.92216700	0.47746200

N	-1.64854700	-1.73344800	1.41515800
N	-1.65776600	-2.46787800	2.28137300
C	0.64754200	-3.45058300	-0.64725800
H	0.96050500	-3.98877000	-1.54864800
H	0.56506900	-4.18776700	0.16419200
H	-0.36706000	-3.07199000	-0.83441000
C	3.35014300	0.14845100	1.97881300
H	4.37055700	0.50117200	1.79857000
H	2.72279100	1.03679000	2.12633000
H	3.35755000	-0.39909000	2.93200800
C	4.78596700	-0.42258500	-0.86582200
H	4.60980000	0.20174800	-1.75264700
H	5.28894100	0.20555700	-0.12390500
H	5.49101100	-1.20869100	-1.16749000
H	0.26240700	-0.32469600	-3.01437000
H	-0.50881400	4.18789700	-1.83644800
H	0.54178000	4.77577400	0.53068000
H	-0.42672500	2.81652700	3.24508200
Si	-3.08224500	-0.55424500	-0.48382600
C	-3.37067400	1.27854800	-0.37297100
H	-4.24819700	1.55369800	-0.97212300
H	-3.54834100	1.60262700	0.65776900
H	-2.50505200	1.82617500	-0.75737900
C	-4.45041400	-1.54017200	0.32772800
H	-4.26777800	-2.62062200	0.29792700
H	-4.61086800	-1.25131000	1.37291300
H	-5.39138000	-1.35695400	-0.20601500
C	-2.76296900	-1.12727700	-2.22710900
H	-3.65513300	-0.95914400	-2.84386600
H	-1.93402900	-0.57632400	-2.68143600
H	-2.52584300	-2.19627800	-2.26832500

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P1-TS E = -1439.458683

Al	-0.33928800	-0.05066500	-0.43939600
C	-1.94115100	-1.22133800	-0.80723700
H	-1.76443400	-1.75750500	-1.74875100
C	-3.08191300	-0.25773700	-0.79549700
C	-3.76516400	-0.41291100	0.38719000
C	0.07956400	1.64848700	-1.36692200
C	0.26924100	2.05521700	1.05034900
C	0.39584300	2.52724300	-0.37238900
C	0.11659500	0.72308500	1.33568200
C	0.86995600	3.95427600	-0.57613000

H	1.85960900	4.11923300	-0.12713500
H	0.94826200	4.21002100	-1.63427100
C	-3.17103300	-1.51504300	1.11908800
H	-3.52411600	-1.86963300	2.08443800
C	-2.12949300	-2.05090000	0.41489300
C	0.21273400	3.11556200	2.13310200
H	-0.63354900	3.79543100	1.96999100
H	0.10692200	2.68260300	3.12937600
C	0.19620100	1.94048100	-2.83884900
H	0.94243100	1.27698100	-3.30306100
H	-0.74840700	1.72806300	-3.35747800
C	-0.06340000	0.13604400	2.71016900
H	0.59373300	0.57964000	3.46966300
H	-1.10080900	0.27043700	3.04853300
N	1.27438300	-1.04128100	-0.16869000
N	1.37955900	-2.21911200	-1.36585200
N	0.79184900	-2.98758000	-1.93214700
C	-1.32549700	-3.26306300	0.79145700
H	-1.71068500	-3.70731700	1.71604600
H	-1.36834200	-4.03743100	0.01237700
H	-0.26415400	-3.03124700	0.95294200
C	-3.39621200	0.68757800	-1.92271100
H	-4.41678800	1.07661500	-1.84282600
H	-2.72297600	1.55473200	-1.95577200
H	-3.31458900	0.18480300	-2.89639900
C	-4.94093600	0.37812400	0.89056800
H	-4.66866700	1.01917900	1.74093500
H	-5.36230100	1.02950300	0.11796100
H	-5.74392100	-0.28431800	1.24030500
H	0.11814600	-0.94217800	2.70726000
H	1.11797400	3.73668700	2.12708100
H	0.19170200	4.68189600	-0.11259900
H	0.48336400	2.96876200	-3.09093500
Si	3.00245300	-0.67830200	0.21331000
C	3.65609500	0.77354900	-0.77427200
H	4.70847300	0.96379600	-0.52664300
H	3.60080000	0.57760000	-1.85194400
H	3.08828600	1.68730100	-0.57649200
C	4.01840800	-2.20355100	-0.21436100
H	3.63378400	-3.10533500	0.27646100
H	4.06506300	-2.39897900	-1.29153000
H	5.04929500	-2.05753700	0.13276100
C	3.21115200	-0.37009500	2.04986600
H	4.28298000	-0.39965900	2.28694600

H	2.82574400	0.60549800	2.35630000
H	2.71711100	-1.13700900	2.65512400

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P2-TS E = -1439.48568

Al	-1.44687500	-0.14990200	-0.12086100
C	-2.95048300	-1.33464200	-1.04945800
H	-2.66428600	-1.73171100	-2.01726700
C	-3.66544100	-0.10186400	-0.82452500
C	-3.95121700	-0.02721600	0.56724400
C	-0.17715700	0.70762700	-1.41913400
C	0.30837400	1.68642900	0.82262200
C	0.54302300	1.62586500	-0.66103700
C	-0.67166600	0.90806100	1.36378200
C	1.34948100	2.72844600	-1.31319400
H	2.24071200	2.99160700	-0.73906300
H	1.66624300	2.45002000	-2.32059100
C	-3.42385400	-1.18751500	1.18390500
H	-3.43774400	-1.38881100	2.24956500
C	-2.79798100	-2.00773700	0.21260300
C	1.19918300	2.62644100	1.61110200
H	1.08133500	3.66713600	1.28180000
H	0.98612800	2.59588700	2.68105100
C	-0.04706000	0.60273500	-2.91719000
H	-0.56979600	-0.28177300	-3.29705300
H	-0.49154300	1.47715000	-3.41395700
C	-0.98517800	0.81278300	2.83215100
H	-0.50495400	1.57651000	3.45542600
H	-2.06660200	0.87763500	3.00704900
N	0.31691200	-1.09111300	-0.75659800
N	1.48726600	-1.08214400	-0.41587700
N	2.37739300	-0.19163500	-0.38035800
C	-2.18994800	-3.36850300	0.42464200
H	-1.88475300	-3.50884000	1.46727900
H	-2.90824700	-4.16328600	0.18245600
H	-1.30727200	-3.51746200	-0.20641100
C	-4.11083800	0.86108200	-1.89242400
H	-5.12764900	0.62784000	-2.23773500
H	-4.12176600	1.89597300	-1.53223400
H	-3.45198000	0.82054000	-2.76633200
C	-4.67895300	1.09108900	1.26338800
H	-5.75374400	1.07529600	1.03686800
H	-4.57396100	1.01119700	2.35045000
H	-4.30368500	2.07828100	0.96766600

H	-0.67893200	-0.16681700	3.22973300
H	2.25771300	2.37010700	1.47817900
H	0.74293500	3.64304200	-1.39757000
H	0.99729400	0.53266200	-3.25432700
Si	4.02388500	-0.65029800	0.15267000
C	4.80894100	-1.77867600	-1.13488600
H	5.83557500	-2.04733600	-0.85621300
H	4.23852400	-2.70865600	-1.24226400
H	4.84484100	-1.29496400	-2.11772300
C	3.95931400	-1.51127100	1.82590500
H	3.51038500	-0.86455800	2.58837100
H	3.35870700	-2.42646600	1.77018100
H	4.96272500	-1.79038500	2.17064100
C	4.95734200	0.97587000	0.26059300
H	6.01298900	0.80540700	0.50370900
H	4.91847700	1.51884800	-0.69066900
H	4.54102500	1.62902100	1.03609300

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P2-IN1 E = -1439.539868

Al	1.37970600	-0.39500600	0.01451200
C	2.37467000	-1.78527900	-1.43911000
H	2.66045800	-1.48228000	-2.44045000
C	1.09187500	-2.30491700	-1.07804800
C	1.12237000	-2.56956900	0.32913700
C	2.20605400	1.09959100	0.93713700
C	0.82079700	2.62249700	-0.53838800
C	1.76648100	2.34326300	0.57888500
C	-0.14847200	1.76937900	-0.97800100
C	2.27675700	3.57371500	1.32269400
H	1.58070500	4.41419000	1.25773700
H	2.42772600	3.35326400	2.38336600
C	2.46018000	-2.28385100	0.78146900
H	2.80066300	-2.39084600	1.80526400
C	3.23759500	-1.82014100	-0.29908400
C	0.95566500	3.98539700	-1.20096200
H	1.99179100	4.33856100	-1.18421300
H	0.63830800	3.96515500	-2.24630900
C	3.21735800	0.95232400	2.06223300
H	2.79626100	1.24447900	3.03660700
H	3.56407900	-0.07981100	2.16935400
C	-1.09097400	2.10608700	-2.11840000
H	-1.80816600	2.88678300	-1.84414600
H	-0.52979200	2.45659000	-2.99448800

N	-2.39863900	0.62422000	-0.05519200
N	-1.38094200	-0.13076000	-0.08923600
N	-0.21225400	0.43848800	-0.47582800
C	4.67884700	-1.39146000	-0.26249000
H	5.27016900	-1.95133400	-0.99732600
H	4.80110100	-0.32521200	-0.48764400
H	5.11565000	-1.57353900	0.72412800
C	-0.05260900	-2.56360600	-2.01641500
H	-0.12063900	-3.63399700	-2.25298200
H	-1.00791000	-2.25101300	-1.58490000
H	0.08393900	-2.02467900	-2.95940200
C	0.03260400	-3.21813500	1.14236600
H	-0.95230400	-2.82082500	0.88101800
H	0.01610800	-4.30373100	0.97721800
H	0.18837300	-3.05190000	2.21358300
H	-1.66479000	1.22945900	-2.41968100
H	0.34704300	4.75255200	-0.70156900
H	3.24391800	3.92152600	0.93095600
H	4.11061800	1.57506900	1.91069200
Si	-3.90074200	-0.14643100	0.47440100
C	-5.19008300	1.21299300	0.44084200
H	-6.17265100	0.84577300	0.76201000
H	-4.90804100	2.03800600	1.10544400
H	-5.30241800	1.62777300	-0.56784300
C	-3.71120400	-0.81859000	2.22011100
H	-2.92394400	-1.57994400	2.26827500
H	-3.44385500	-0.02157100	2.92397700
H	-4.64292900	-1.27737700	2.57445800
C	-4.39097500	-1.53292600	-0.69910100
H	-5.33538400	-1.99993500	-0.39198800
H	-4.52265600	-1.16236500	-1.72275100
H	-3.62597900	-2.31798300	-0.72611700

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Pb E = -1439.553816

Al	0.09439400	-0.47669500	0.03501500
C	0.36722900	-2.02460100	1.45776200
H	-0.21611900	-1.82024900	2.35094300
C	1.79099200	-1.92049900	1.35117500
C	2.18281900	-2.54952400	0.14588300
C	0.87545200	2.33342900	0.98645100
C	1.87394100	1.49050300	-1.19596000
C	1.85225400	2.35590800	0.04191600
C	1.22008700	0.30406300	-1.40229500

C	2.99372300	3.35014300	0.19319100
H	2.88005500	4.23211700	-0.45048800
H	3.08565600	3.70531600	1.22133100
C	1.02504500	-3.04628100	-0.48648100
H	1.00684200	-3.56337800	-1.44079200
C	-0.12207600	-2.74189500	0.28766300
C	2.73077500	2.08152300	-2.31585100
H	3.80192400	1.88704800	-2.16384100
H	2.46646200	1.66596400	-3.28871600
C	0.67441900	3.27425200	2.14558000
H	-0.38823200	3.53913800	2.20702900
H	0.93854700	2.79861900	3.10095500
C	1.36834600	-0.41768300	-2.73799800
H	2.41561900	-0.60822400	-3.01139500
H	0.86760200	-1.38957400	-2.72546800
N	-0.04285000	1.25792200	0.91674200
N	-1.29698100	1.47571200	0.62823300
N	-1.80112000	0.34457900	0.17308800
C	-1.48995600	-3.35914800	0.14663500
H	-1.74107800	-3.55021900	-0.90317100
H	-1.54137600	-4.32240700	0.67333800
H	-2.27395100	-2.72170500	0.56975600
C	2.70145300	-1.24823600	2.34275500
H	3.34543000	-1.97979900	2.85024100
H	3.36487900	-0.51499000	1.86709900
H	2.12760800	-0.72469900	3.11464700
C	3.58308300	-2.59859900	-0.39996600
H	4.28787300	-3.02870000	0.32380400
H	3.63043700	-3.20896100	-1.30811600
H	3.95711000	-1.59787500	-0.65577400
H	0.92518700	0.15733500	-3.56511100
H	2.61415300	3.16810300	-2.38642100
H	3.95140200	2.88850100	-0.07118200
H	1.24551800	4.19944100	2.05183600
Si	-3.54194300	0.34450900	-0.24368400
C	-3.71308200	-0.69666500	-1.80015300
H	-4.76541200	-0.78347200	-2.09737000
H	-3.16690500	-0.24724500	-2.63746300
H	-3.32819200	-1.71196200	-1.65452500
C	-4.10879700	2.11073900	-0.54241200
H	-3.96085100	2.73122800	0.34728000
H	-3.55000800	2.57263900	-1.36379600
H	-5.17440800	2.13700700	-0.80111100
C	-4.51845400	-0.42132500	1.17445900

H	-5.59122600	-0.44553800	0.94523500
H	-4.20251800	-1.45059400	1.38029200
H	-4.38880700	0.15693000	2.09677800

56

P2-TS(Pb-Pa) E = -1439.481216

Al	0.76271400	-0.28116700	-0.05604500
C	1.44451500	-1.86014600	1.23468900
H	0.80052300	-2.05654900	2.08310400
C	2.62951800	-1.07102100	1.25401500
C	3.22666500	-1.14951500	-0.04000800
C	-0.94878800	1.48919200	1.02929500
C	0.60921300	2.39574700	-0.76415000
C	-0.23842200	2.51719700	0.45362500
C	1.21881100	1.24002900	-1.16424000
C	-0.33268700	3.90644400	1.07205800
H	-1.20727300	4.47766200	0.72477600
H	-0.39747800	3.85950000	2.16276500
C	2.39536500	-1.94216900	-0.85020600
H	2.56619200	-2.16817100	-1.89747300
C	1.26128100	-2.39124000	-0.09595700
C	0.78763600	3.67684600	-1.57374000
H	1.67969200	4.24051700	-1.26410300
H	0.90872600	3.45566100	-2.63773900
C	-1.83113800	1.77394900	2.24172900
H	-2.55432800	0.97360800	2.39710900
H	-1.23009600	1.84406700	3.15932200
C	2.08647300	1.22031300	-2.40954900
H	2.89398300	1.96592600	-2.37595700
H	2.55814900	0.24636400	-2.56445000
N	-0.93981300	0.15092700	0.58222200
N	-1.56769900	-1.16087100	1.82568100
N	-2.43848100	-1.64985000	1.22752100
C	0.29982800	-3.48310600	-0.49804800
H	0.04453000	-3.42994000	-1.56247200
H	0.74432900	-4.47129300	-0.31983600
H	-0.63071100	-3.44159500	0.07617700
C	3.19054200	-0.34301100	2.44669800
H	4.09451300	-0.84342500	2.81921200
H	3.47089600	0.69001100	2.20892800
H	2.46882200	-0.31436500	3.26927800
C	4.49260200	-0.45505900	-0.45706800
H	5.32834700	-0.72539900	0.20112100
H	4.77405200	-0.72948200	-1.47853600

H	4.39554300	0.63758500	-0.42365500
H	1.50304200	1.43492700	-3.31798200
H	-0.06893000	4.34991000	-1.47228900
H	0.55077500	4.50577600	0.83457000
H	-2.38578600	2.71274000	2.14628900
Si	-2.79434900	-0.73408700	-0.54765700
C	-4.00302700	0.62713400	-0.09843200
H	-4.76863600	0.67261500	-0.88374300
H	-4.51883600	0.43117500	0.84765700
H	-3.52213500	1.60697100	-0.03475200
C	-3.81825100	-2.24920900	-1.06354200
H	-3.18473300	-3.13034500	-1.23122600
H	-4.55060700	-2.52241700	-0.29540100
H	-4.35432800	-2.05655000	-2.00180600
C	-1.88312800	-0.36231600	-2.16555900
H	-2.59172400	-0.42222800	-3.00307700
H	-1.41081100	0.62303400	-2.15917000
H	-1.10020300	-1.10568900	-2.36850600

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P3-TS E = -1439.496401

Al	0.55915400	-0.42048900	0.20275300
C	-0.79693400	-1.73109200	0.95744100
H	-0.12358400	-2.37989000	1.53794900
C	-1.56519100	-2.43245200	-0.11073000
C	-2.88249300	-2.05717300	-0.01942600
C	2.19238400	-0.07900700	1.29996000
C	2.96174100	-0.60069800	-1.01638400
C	3.22711800	-0.42786200	0.45576000
C	1.66451200	-0.68655100	-1.42654200
C	4.63530100	-0.69086500	0.93906000
H	5.35211300	-0.01031900	0.46112100
H	4.73010800	-0.57312800	2.01977400
C	-3.02895100	-1.18375000	1.13507800
H	-3.97328700	-0.75221500	1.45953900
C	-1.82617200	-1.01689400	1.76094300
C	4.17540500	-0.64928400	-1.92581800
H	4.83602700	-1.49063500	-1.68014900
H	3.89742000	-0.75173800	-2.97627500
C	2.38793600	0.04729100	2.79612400
H	1.51290000	0.49485300	3.27892700
H	2.53601300	-0.93522800	3.26977800
C	1.22876600	-0.81114900	-2.86212100
H	2.04295100	-0.86906900	-3.59467700

H	0.59456500	-1.69578500	-3.00812700
N	-0.11226300	1.49495400	0.03841100
N	0.91924600	2.22794600	0.31400400
N	2.00451400	2.20216200	0.72304700
C	-1.56492900	-0.26269000	3.03352200
H	-2.50261400	0.08843300	3.47876000
H	-1.05960600	-0.89137600	3.77986900
H	-0.92524600	0.61806000	2.88098500
C	-0.95826800	-3.45658300	-1.02916800
H	-0.88635000	-4.43972800	-0.53955200
H	-1.54864500	-3.59767600	-1.94144600
H	0.05957700	-3.18387700	-1.33117400
C	-4.03162400	-2.48218100	-0.89231400
H	-3.70361800	-3.11507600	-1.72292700
H	-4.77812300	-3.05206700	-0.32171100
H	-4.55820600	-1.61937500	-1.32326800
H	0.59991900	0.04682200	-3.14534700
H	4.78156700	0.26213700	-1.83428400
H	4.95791700	-1.70854800	0.68094400
H	3.25360800	0.66651300	3.06588200
Si	-1.56369600	2.34874200	-0.61122500
C	-2.33732600	1.17393100	-1.83455200
H	-3.30827200	1.55970100	-2.16978800
H	-1.70698300	1.04497300	-2.72199900
H	-2.50749000	0.18586800	-1.39196000
C	-0.96438100	3.91820700	-1.44007600
H	-0.48133200	4.60002700	-0.73074800
H	-0.24810900	3.70547900	-2.24197700
H	-1.81043300	4.45574700	-1.88626700
C	-2.71714000	2.75109700	0.80376700
H	-3.60494800	3.28374100	0.43980300
H	-3.05335500	1.83758900	1.30444700
H	-2.23073800	3.39055800	1.54988000

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P3-IN1 E = -1439.530714

Al	0.44101400	-0.26364800	-0.06426000
C	-0.50799700	-1.72253000	0.95037000
H	0.28850400	-2.23510000	1.50685700
C	-1.18235600	-2.53899400	-0.10844800
C	-2.53779800	-2.34220000	-0.00393900
C	2.20852400	0.85240100	1.12763400
C	2.94145300	-0.50146000	-0.82918400
C	2.84906100	-0.26488400	0.64951000

C	1.75487900	-0.57203500	-1.48470200
C	3.51169600	-1.28470900	1.55126300
H	4.60214700	-1.15297200	1.52002900
H	3.20817100	-1.19826300	2.59643900
C	-2.79141200	-1.49639800	1.15066200
H	-3.78230400	-1.19412800	1.48019600
C	-1.61861600	-1.16155600	1.76520500
C	4.33351500	-0.67733500	-1.39865300
H	4.85484700	-1.52344700	-0.93197100
H	4.31464900	-0.85574800	-2.47606000
C	2.01241500	1.16906100	2.60073400
H	1.12712500	1.79667200	2.73471300
H	1.89173500	0.27327400	3.21381400
C	1.60081000	-0.76648500	-2.97090900
H	2.54565600	-0.91910000	-3.50635200
H	0.95082900	-1.62183000	-3.19661800
N	-0.12834100	1.53012700	-0.07454900
N	0.92319900	2.40625000	-0.11645200
N	2.04062400	2.05260300	0.33838100
C	-1.45580000	-0.37281800	3.03260200
H	-2.42736600	-0.19874500	3.50780900
H	-0.82353600	-0.90238100	3.75919700
H	-0.99518700	0.60948300	2.86435700
C	-0.45406900	-3.49436600	-1.01262500
H	-0.22037200	-4.43392000	-0.48910700
H	-1.04591200	-3.75897200	-1.89551300
H	0.50128400	-3.08689400	-1.36254300
C	-3.62805100	-2.91820100	-0.86473600
H	-3.22911200	-3.49820100	-1.70270800
H	-4.28258200	-3.58442700	-0.28603900
H	-4.26994600	-2.13156400	-1.28336700
H	1.11281100	0.11113900	-3.41760600
H	4.94455400	0.21609900	-1.21485900
H	3.30353700	-2.30597100	1.21194000
H	2.87383400	1.73360800	2.97764000
Si	-1.65723300	2.26982200	-0.61485100
C	-2.48850800	1.05337800	-1.77811900
H	-3.48762000	1.41116500	-2.05809900
H	-1.91361000	0.92955200	-2.70422400
H	-2.61474900	0.06406400	-1.32276600
C	-1.30579200	3.87820100	-1.50621500
H	-0.84203300	4.61513200	-0.84323900
H	-0.62845500	3.72969600	-2.35406900
H	-2.24101800	4.30578000	-1.89033400

C	-2.76039900	2.58788600	0.86893100
H	-3.70674300	3.05025100	0.56041700
H	-2.99949100	1.65603200	1.39248000
H	-2.27929600	3.26502500	1.58494300

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P3-TS(1-2) E = -1439.525935

Al	-0.35644600	0.27678300	-0.04560200
C	-0.62516000	1.73104600	1.47211300
H	-1.47253300	1.55826500	2.12758400
C	-0.69341400	2.47964600	0.22443500
C	0.63798900	2.73849700	-0.17670800
C	-1.47814400	-1.68246900	1.03989600
C	-2.64266200	-0.81766200	-0.96768300
C	-2.56775600	-1.04808700	0.50829900
C	-1.59885900	-0.14345500	-1.51266900
C	-3.72756500	-0.55746600	1.34736100
H	-4.59541000	-1.21772000	1.21117200
H	-3.50590200	-0.53938200	2.41659100
C	1.50586100	2.23487800	0.83733900
H	2.58884400	2.28471400	0.80406600
C	0.75588700	1.64356100	1.86003600
C	-3.89111700	-1.31597300	-1.66654200
H	-4.79647200	-0.85585900	-1.24871400
H	-3.87855700	-1.10175200	-2.73765500
C	-1.24076400	-1.90906100	2.52237500
H	-0.16777300	-1.97701400	2.72405400
H	-1.65334300	-1.10865600	3.14131000
C	-1.45984100	0.18173200	-2.97855700
H	-2.30100700	-0.14997300	-3.59938700
H	-1.34263800	1.26295000	-3.13595200
N	0.99453100	-1.05014300	-0.04313600
N	0.48893100	-2.32784700	-0.13290300
N	-0.66863100	-2.59450000	0.26575400
C	1.28324300	0.99363900	3.10968700
H	2.26518500	1.40190500	3.37171800
H	0.61378900	1.16635700	3.96078200
H	1.40280300	-0.09165900	3.00111700
C	-1.94562200	3.05023000	-0.38419000
H	-2.17350500	4.03286800	0.05284500
H	-1.84892300	3.18993700	-1.46591500
H	-2.81347900	2.40519500	-0.21371900
C	1.05467800	3.53467500	-1.38540100
H	0.45915600	3.28719900	-2.27167700

H	0.93540600	4.61280800	-1.20960200
H	2.10619000	3.36368300	-1.63673400
H	-0.55218500	-0.28326600	-3.38881700
H	-3.99931400	-2.40148900	-1.54178200
H	-4.04355400	0.44769900	1.04271200
H	-1.69165500	-2.85780700	2.83839300
Si	2.71210100	-1.08094800	-0.53588900
C	3.03554400	0.23463000	-1.83840900
H	4.08154600	0.17863300	-2.16675600
H	2.40735400	0.08007800	-2.72432000
H	2.85952400	1.25027800	-1.47552300
C	3.14120100	-2.74596700	-1.27986600
H	3.02896500	-3.56109900	-0.55892200
H	2.50287800	-2.98064300	-2.13799100
H	4.18401500	-2.73415300	-1.62397800
C	3.81968600	-0.78815300	0.95393300
H	4.87608100	-0.81735400	0.65696900
H	3.63557700	0.17922000	1.43106400
H	3.67040100	-1.56690100	1.71164700

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P3-IN2 E = -1439.534787

Al	-0.16633100	0.07672800	0.03629600
C	-2.07733300	1.18683800	1.55033500
H	-2.80150800	0.57534400	2.07939800
C	-2.37934400	2.09998100	0.53160000
C	-1.16323200	2.68497500	0.09184300
C	-0.14799300	-2.46005400	0.55048600
C	-1.80275100	-1.70559900	-1.13171100
C	-1.45397500	-2.23114100	0.22834800
C	-1.29568400	-0.49099600	-1.45585400
C	-2.61041900	-2.51289000	1.16328200
H	-3.12757000	-3.43253700	0.85639600
H	-2.30188100	-2.64923700	2.20199400
C	-0.10394000	2.11715500	0.84036500
H	0.91130800	2.49534700	0.87553200
C	-0.66663000	1.15120800	1.78666000
C	-2.72299900	-2.57519000	-1.96260900
H	-3.68493400	-2.73472900	-1.45744400
H	-2.93428700	-2.14024000	-2.94196500
C	0.36434800	-2.94394400	1.89270200
H	1.30995400	-2.44784200	2.13484000
H	-0.33803600	-2.75761100	2.70750900
C	-1.52369400	0.20881700	-2.77269400

H	-2.11943700	-0.36751600	-3.49036200
H	-2.03105300	1.17078800	-2.62229900
N	1.61658200	-0.52025500	-0.13922400
N	1.74353600	-1.78030900	-0.69367200
N	0.86956300	-2.64724100	-0.45664900
C	-0.00272900	0.69273400	3.06762400
H	1.04131100	0.39986400	2.91496600
H	-0.01234700	1.49402900	3.81907700
H	-0.52809800	-0.16641800	3.49929800
C	-3.74236300	2.36870200	-0.04395400
H	-3.96148700	3.44386000	-0.07776300
H	-3.84361800	1.99094300	-1.07053700
H	-4.52375600	1.89207400	0.55745400
C	-1.02197900	3.71760000	-0.99197700
H	-1.39417700	3.36357800	-1.96207000
H	-1.59237700	4.62361700	-0.74725000
H	0.02366700	4.01318400	-1.12702200
H	-0.56663300	0.44249000	-3.25929200
H	-2.27802100	-3.56620700	-2.12124200
H	-3.34739200	-1.70275900	1.12652100
H	0.56416700	-4.02129100	1.84728400
Si	3.12906000	0.39983800	-0.33304800
C	2.91161600	1.77939700	-1.59463200
H	3.84802700	2.33766900	-1.72279600
H	2.63671700	1.36980100	-2.57430900
H	2.13761500	2.50136400	-1.31014100
C	4.50665500	-0.73407600	-0.89953000
H	4.66728000	-1.55951300	-0.19749500
H	4.29093400	-1.17556100	-1.87696100
H	5.44510100	-0.16953500	-0.97632100
C	3.61069400	1.13741400	1.33020000
H	4.55749200	1.68525000	1.23819500
H	2.87087400	1.83686100	1.73389100
H	3.76036800	0.34878600	2.07765700

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P3-TS(2-3) E = -1439.494386

Al	0.55566400	-0.27867700	0.18176100
C	2.84018600	-0.22815800	1.32264600
H	3.24638300	0.68347200	1.74908100
C	3.34924600	-0.89919400	0.19450200
C	2.53409200	-2.03352700	-0.04358600
C	-0.80034900	2.23071300	0.78661100
C	0.47504700	1.97609000	-1.34552500

C	0.32529200	2.47541800	0.07024900
C	0.77821500	0.66823700	-1.51576300
C	1.48351000	3.31270500	0.57445400
H	1.57196300	4.23125600	-0.02059900
H	1.38452300	3.61145300	1.62006500
C	1.50916200	-2.05708500	0.94268200
H	0.80813200	-2.86789900	1.11228500
C	1.69838700	-0.92098200	1.83362100
C	0.33650100	3.03699400	-2.41886500
H	1.08057000	3.83500900	-2.29352900
H	0.45355000	2.63371200	-3.42734600
C	-1.06433500	2.64858400	2.21718500
H	-1.43843000	1.79285200	2.79191500
H	-0.17927800	3.03908500	2.72293200
C	1.03243800	0.01835400	-2.85654100
H	0.93375400	0.70013200	-3.70921400
H	2.04319800	-0.40902700	-2.89606000
N	-1.26482900	-0.51385800	0.47322700
N	-2.13636700	0.44327600	0.18831500
N	-2.00659800	1.70985000	0.20460700
C	1.07649900	-0.75921600	3.20014500
H	0.02125000	-1.05249000	3.20340900
H	1.59641400	-1.38326600	3.93958900
H	1.13604300	0.27854000	3.54643100
C	4.50971400	-0.45300200	-0.65162000
H	5.25841200	-1.24835000	-0.76121300
H	4.20064400	-0.16351000	-1.66493900
H	5.01176200	0.41122400	-0.20409200
C	2.71332500	-3.04091500	-1.14594700
H	2.78205500	-2.57286100	-2.13553400
H	3.63783500	-3.61665500	-1.00281700
H	1.88330900	-3.75439100	-1.17117900
H	0.34235200	-0.81965100	-3.02832200
H	-0.65108600	3.51135800	-2.35539800
H	2.42927500	2.77016400	0.45805800
H	-1.84773800	3.41554200	2.24003300
Si	-3.10879200	-1.09375900	-0.22037800
C	-4.43160800	-0.33756700	-1.34409300
H	-5.18722300	-1.08039300	-1.63171900
H	-4.94468400	0.49771200	-0.85239900
H	-3.99386000	0.05428000	-2.27155600
C	-3.92542100	-1.62395700	1.38042900
H	-3.23821500	-2.19436700	2.01396600
H	-4.27217000	-0.75649500	1.95437900

H	-4.80204600	-2.25097700	1.17452100
C	-2.46183800	-2.55672400	-1.22121000
H	-3.28975200	-3.15571100	-1.62305200
H	-1.86929800	-2.21126700	-2.07830700
H	-1.82200700	-3.20853100	-0.61628000

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P3-IN3 E = -1439.511909

Al	0.72304800	-0.37885200	0.15862200
C	3.05496200	-0.06385800	1.27338900
H	3.32886900	0.85922400	1.77485000
C	3.64672500	-0.55901200	0.09845400
C	3.00360200	-1.77735400	-0.23625200
C	-0.95863500	1.79513600	0.96566500
C	0.30821300	1.95539200	-1.17770600
C	0.09537900	2.29910200	0.27574000
C	0.80061100	0.72555500	-1.45818300
C	1.11009200	3.26208500	0.85757200
H	1.04751300	4.23269700	0.34761800
H	0.97450400	3.44752400	1.92521400
C	2.00123900	-2.03067600	0.73698300
H	1.42830100	-2.94643800	0.83992900
C	2.02508400	-0.95158100	1.71711500
C	0.01651600	3.07667800	-2.15512800
H	0.65006900	3.95315500	-1.96290800
H	0.17301200	2.78152200	-3.19542400
C	-1.24632100	2.01172200	2.43754200
H	-1.46899500	1.05059800	2.91660000
H	-0.41847000	2.47570800	2.97777500
C	1.14603200	0.24497300	-2.84899700
H	0.92045100	0.96837900	-3.64166600
H	2.21556100	0.00692300	-2.92220100
N	-1.00005900	-0.94744800	0.42224900
N	-1.99607600	-0.15632500	0.21835700
N	-2.06488600	1.14479300	0.33733800
C	1.41537600	-1.00718000	3.09860700
H	0.42286500	-1.47019800	3.08522300
H	2.04601900	-1.59454500	3.78005500
H	1.31058500	-0.00516500	3.52976800
C	4.72013900	0.12080800	-0.70657600
H	5.55471200	-0.55862400	-0.92365100
H	4.34779800	0.48770800	-1.67289900
H	5.12927900	0.98197900	-0.16743100
C	3.31622400	-2.64732600	-1.42250600

H	3.25709700	-2.10054900	-2.37204300
H	4.33458900	-3.05371500	-1.35473500
H	2.62745300	-3.49639700	-1.48440300
H	0.61148900	-0.68344900	-3.09310200
H	-1.02402500	3.40956600	-2.04920000
H	2.12862400	2.88773400	0.69883900
H	-2.13609100	2.64237100	2.55344800
Si	-3.54624500	-0.99575000	-0.31346400
C	-3.11596800	-1.89548300	-1.89212500
H	-3.98558300	-2.44273800	-2.27661000
H	-2.79145700	-1.19593700	-2.67125900
H	-2.30680900	-2.61154600	-1.72042800
C	-4.87431600	0.28732100	-0.58446300
H	-5.08327500	0.84484200	0.33385000
H	-4.57834700	1.01167100	-1.34980300
H	-5.80563200	-0.19338600	-0.91149800
C	-3.97274900	-2.16172100	1.08220700
H	-4.84965900	-2.76993300	0.82799700
H	-3.13430600	-2.83393900	1.28770700
H	-4.20441000	-1.61410800	2.00316700

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P3-TS(3-4) E = -1439.49013

Al	1.25268500	-0.26931100	-0.29800400
C	3.36127500	-1.06033900	-0.87729700
H	3.75434200	-1.01634700	-1.88708600
C	2.52903100	-2.11139300	-0.36881200
C	2.21666600	-1.78556000	0.98532200
C	-1.08858500	1.17408500	1.29206900
C	0.23401800	2.29729700	-0.52383200
C	-0.06990900	1.98946200	0.92531200
C	1.00634800	1.44313400	-1.23045400
C	0.79308400	2.75469400	1.90953400
H	0.66823100	3.83645600	1.76911400
H	0.57519300	2.53101500	2.95598100
C	2.84087500	-0.52318500	1.27257200
H	2.79625000	-0.01290200	2.22832500
C	3.58478600	-0.09754800	0.13542900
C	-0.34466000	3.61676600	-1.00014200
H	-0.03009600	4.45267800	-0.36086800
H	-0.05809700	3.85782100	-2.02659900
C	-1.54120500	0.88555800	2.70680100
H	-1.44265100	-0.18452200	2.93200200
H	-0.98862000	1.44543000	3.46333800

C	1.45298600	1.67786300	-2.65693600
H	1.24279300	2.68558100	-3.03489300
H	2.53377300	1.51053900	-2.75931200
N	-0.39344600	-1.09316700	-0.48945200
N	-1.51651500	-0.56188600	-0.36920300
N	-1.92152100	0.52332700	0.33526800
C	4.36743000	1.18020600	0.00308600
H	4.87374300	1.43081800	0.94216200
H	5.13425500	1.08816800	-0.77355600
H	3.72684300	2.03071600	-0.26497800
C	2.12455000	-3.36424600	-1.09875400
H	2.68089900	-4.23464700	-0.72615200
H	1.05592900	-3.57196100	-0.98115900
H	2.33044000	-3.27663200	-2.17059300
C	1.42082300	-2.62649300	1.94532500
H	0.50709900	-3.01430500	1.48203200
H	2.00714000	-3.48676900	2.29492000
H	1.12997300	-2.04691500	2.82793100
H	0.96963800	0.96646000	-3.34211900
H	-1.44106700	3.58238100	-0.95552600
H	1.85416200	2.54063300	1.73101000
H	-2.60442700	1.13291400	2.80883500
Si	-3.41361500	-0.67004100	-0.36821200
C	-3.54696500	-2.55164700	-0.50437300
H	-4.58161200	-2.86555700	-0.69294500
H	-2.91466400	-2.93674600	-1.31251900
H	-3.22477800	-3.04459100	0.42235000
C	-3.89586100	0.14139300	-1.98690700
H	-3.85005500	1.23336500	-1.91340800
H	-3.23484300	-0.16912800	-2.80392200
H	-4.92184600	-0.13406800	-2.26259000
C	-4.67603300	-0.22518700	0.96623400
H	-5.65883200	-0.65127400	0.72327200
H	-4.38571200	-0.62409500	1.94617800
H	-4.78924500	0.86002500	1.06843500

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P3-IN4 E = -1330.060218

Al	-1.38332600	0.35294400	0.09457400
C	-1.51019600	-1.64420700	1.04039300
H	-0.62335300	-2.12526700	1.43668000
C	-2.00001300	-1.78874600	-0.29774400
C	-3.17415400	-0.98636200	-0.41050400
C	1.19440900	0.16883600	-1.25766400

C	-0.06930700	2.20832900	-0.40879200
C	-0.07175600	0.97216500	-1.33284900
C	-0.94492200	2.14663900	0.62914700
C	-0.58533300	1.30003100	-2.74667800
H	0.12488600	1.89961300	-3.33754800
H	-0.80405100	0.40029200	-3.33319800
C	-3.41636100	-0.40121400	0.87525600
H	-4.22455800	0.28436700	1.10395200
C	-2.41087400	-0.81548500	1.77993200
C	0.88419300	3.33257300	-0.74035900
H	0.72282900	3.70120800	-1.76217600
H	0.78706800	4.18203800	-0.05752200
C	1.65940300	-0.51567100	-2.54049200
H	2.52829900	-1.14888600	-2.36002300
H	0.86092400	-1.13094600	-2.97093100
C	-1.18128800	3.19285800	1.67977600
H	-0.63498100	4.12909900	1.50320200
H	-2.24760100	3.44582600	1.75318500
N	1.81501500	0.05509000	-0.13860000
C	-2.29333600	-0.44221800	3.23203300
H	-2.81081700	-1.17375900	3.86653900
H	-1.24761500	-0.41061100	3.55598200
H	-2.73697600	0.53883300	3.43127300
C	-1.39617100	-2.65655500	-1.36616400
H	-0.33028300	-2.82643600	-1.18436500
H	-1.88599200	-3.63928000	-1.39366500
H	-1.50126000	-2.21547600	-2.36339100
C	-4.06166900	-0.85588600	-1.62029800
H	-4.76240800	-1.69881400	-1.68670800
H	-4.65815700	0.06150400	-1.57820400
H	-3.48785500	-0.83748200	-2.55323000
H	-0.88521000	2.82619000	2.67233600
H	1.91959500	2.97262800	-0.68772000
H	-1.51485600	1.87880900	-2.69127700
H	1.91963900	0.23065200	-3.30199200
Si	3.21535100	-0.64393200	0.56045400
C	2.63107000	-1.87918400	1.85782500
H	3.47676300	-2.30690000	2.41120600
H	1.96282200	-1.40320100	2.58493700
H	2.08678100	-2.71449800	1.39883600
C	4.16150100	0.74957300	1.39584600
H	4.51529100	1.48500600	0.66269900
H	3.52619500	1.28050900	2.11365900
H	5.04018100	0.37245300	1.93438300

C	4.42793200	-1.54954900	-0.57710500
H	5.30060900	-1.88368900	0.00007700
H	3.98710600	-2.44178000	-1.03860500
H	4.80143500	-0.90642500	-1.38336300

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P3-TS(4-Pa) E = -1330.060048

Al	1.28333800	0.26242400	-0.21514700
C	1.44594500	-1.91610200	-0.53695000
H	0.58693800	-2.48842000	-0.86614700
C	1.80242000	-1.67633900	0.83103500
C	2.99188900	-0.89094800	0.82798400
C	-1.19966300	0.66434500	1.12647800
C	0.15025400	2.29286400	-0.26830900
C	0.11180300	1.39112200	0.98791900
C	0.92716900	1.82580100	-1.28150400
C	0.63710300	2.09920900	2.24514800
H	-0.02444000	2.89900900	2.61306300
H	0.78536400	1.40372500	3.08024700
C	3.36771800	-0.68730700	-0.53783100
H	4.21911000	-0.10252500	-0.86797500
C	2.43753900	-1.33587500	-1.38631900
C	-0.68291700	3.55515400	-0.25801900
H	-0.44632400	4.18350200	0.61046700
H	-0.53890900	4.16006600	-1.15840800
C	-1.90945600	0.73035000	2.47286500
H	-2.84485600	0.17090000	2.46565500
H	-1.26845500	0.32331800	3.26438200
C	1.14318200	2.46620300	-2.62207700
H	0.68884000	3.46162600	-2.71845800
H	2.21404700	2.57312100	-2.84128900
N	-1.64431600	-0.00618400	0.12254000
C	2.47242200	-1.39077300	-2.88877100
H	3.02900800	-2.27138400	-3.23600200
H	1.46458800	-1.45378800	-3.31298000
H	2.95939200	-0.50593600	-3.31205200
C	1.06389800	-2.18429900	2.03780900
H	0.02854100	-2.43701600	1.78901900
H	1.53911700	-3.08968600	2.43898600
H	1.04311800	-1.44498600	2.84655500
C	3.75981500	-0.42025800	2.03436400
H	4.37951500	-1.22792400	2.44653500
H	4.42968900	0.40738600	1.77877200
H	3.09872400	-0.07737900	2.83795200

H	0.72848200	1.84108200	-3.42506800
H	-1.75123300	3.30671000	-0.18910400
H	1.60910100	2.56458900	2.04283600
H	-2.11679500	1.77141600	2.75057700
Si	-3.05145600	-0.84969600	-0.39540600
C	-2.49803500	-2.55108100	-0.98198000
H	-3.34701400	-3.13083800	-1.36564200
H	-1.75923200	-2.47333600	-1.78816300
H	-2.04692400	-3.13297400	-0.16838100
C	-3.76181700	0.11414700	-1.84527300
H	-4.10745500	1.10668700	-1.53123100
H	-3.00979900	0.26047900	-2.62867400
H	-4.61816300	-0.40825200	-2.29039200
C	-4.44581500	-1.10997400	0.85651800
H	-5.27209100	-1.65352500	0.37899700
H	-4.12934000	-1.70218900	1.72378600
H	-4.85606100	-0.16336600	1.22842600

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P3-TS(1-5) E = -1439.482029

Al	-0.74714300	-0.27261400	-0.04932500
C	-2.50411000	-1.57622700	-1.02710300
H	-2.89700700	-1.37788000	-2.01761200
C	-3.03860300	-1.05706300	0.18407100
C	-2.21623300	-1.51503900	1.25061000
C	-0.79911700	1.36678300	-1.25959300
C	0.13057300	2.25689100	0.84590900
C	-0.56555900	2.54137500	-0.29250400
C	0.34364900	0.81946200	1.15083800
C	-0.94802600	3.92117600	-0.76341900
H	-0.42440000	4.17729400	-1.69355100
H	-2.02170300	3.97317900	-0.98317200
C	-1.16232500	-2.29336300	0.67691700
H	-0.39601100	-2.81952100	1.23439100
C	-1.34466400	-2.34290200	-0.74714300
C	0.68512600	3.29958500	1.79286900
H	0.30384000	3.17405500	2.81469500
H	1.77919200	3.22224400	1.85602000
C	-1.88363300	1.59275700	-2.31006600
H	-1.96704700	0.72106700	-2.96828600
H	-2.86225600	1.73997100	-1.83813100
C	1.00583300	0.47970600	2.46193400
H	0.37219800	0.88457000	3.26266300
H	1.06305300	-0.59823900	2.63035500

N	1.24920900	0.02304100	-0.23908100
N	1.49592200	0.84159800	-1.41636000
N	0.51591700	1.40032500	-1.94472400
C	-0.54795300	-3.16555000	-1.72398200
H	0.47846800	-3.32234600	-1.37653100
H	-1.00055700	-4.15718200	-1.85725600
H	-0.49922400	-2.69282100	-2.71095600
C	-4.27242000	-0.20500600	0.31770500
H	-5.11590600	-0.78525600	0.71596600
H	-4.12083500	0.64427400	0.99501600
H	-4.58127900	0.19566000	-0.65300200
C	-2.41952100	-1.24275900	2.71591300
H	-2.58589200	-0.17813900	2.92003100
H	-3.29265200	-1.78636500	3.10051300
H	-1.55070600	-1.56082800	3.30089600
H	2.00763200	0.90695500	2.60670800
H	0.45218300	4.31966500	1.48299300
H	-0.72872000	4.69901400	-0.02924700
H	-1.67734700	2.46104000	-2.94831900
Si	2.85254600	-0.79131800	-0.06011000
C	4.16833700	0.46363000	0.39932700
H	5.16183000	-0.00264100	0.40125600
H	4.18264800	1.28058000	-0.32961300
H	4.00764300	0.89793100	1.39220800
C	3.28141100	-1.58846400	-1.70413100
H	2.50121200	-2.28323600	-2.03598800
H	3.41225600	-0.83690600	-2.48739300
H	4.21448400	-2.15974300	-1.61349600
C	2.80198000	-2.17426200	1.21547000
H	3.70869500	-2.78039800	1.08921200
H	2.78916600	-1.82679200	2.25207300
H	1.94845400	-2.84589500	1.06974900

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P3-IN5 E = -1439.488139

Al	-1.16482100	-0.18769600	-0.10222500
C	-2.96892800	-1.20517300	-1.07743600
H	-3.24805100	-0.97111300	-2.09823700
C	-3.41161200	-0.49624000	0.07319500
C	-2.75130700	-1.07262200	1.21354500
C	-0.70236400	1.35138700	-1.26202500
C	0.39969200	1.68943000	0.90827300
C	-0.25318300	2.27612200	-0.13694400
C	0.60701800	0.18476900	0.77119000

C	-0.53552300	3.75422800	-0.26448500
H	-0.04178800	4.16497900	-1.15528600
H	-1.60760300	3.95172900	-0.38661800
C	-1.92560900	-2.13418700	0.73147300
H	-1.28269900	-2.75232700	1.34710400
C	-2.03372100	-2.20866100	-0.68742400
C	0.93251500	2.40825500	2.12449200
H	0.53380500	1.98022300	3.05317600
H	2.02595300	2.31828600	2.18731600
C	-1.66149700	1.95371600	-2.28476300
H	-1.96333200	1.18946600	-3.00918100
H	-2.57221400	2.34124400	-1.81305700
C	0.93267000	-0.54909100	2.06864600
H	0.15754200	-0.34763200	2.81732300
H	0.95670600	-1.63272500	1.91585700
N	1.66534000	-0.08839300	-0.27860400
N	1.46671600	0.25181000	-1.61529000
N	0.46204600	0.84279300	-2.07342400
C	-1.35439200	-3.20456200	-1.59124700
H	-0.39451200	-3.53188700	-1.17851900
H	-1.97858300	-4.09767700	-1.72345600
H	-1.16523900	-2.78381100	-2.58405300
C	-4.45003900	0.59330800	0.09963400
H	-5.43082800	0.18921700	0.38366100
H	-4.20672000	1.38395200	0.81817500
H	-4.55756200	1.05845600	-0.88477500
C	-3.00360000	-0.73106300	2.65896200
H	-3.13038400	0.34540000	2.81739200
H	-3.91834300	-1.22054600	3.01881700
H	-2.18033800	-1.06871500	3.29615600
H	1.89002000	-0.25747200	2.52297900
H	0.69244500	3.47380300	2.13113400
H	-0.19248700	4.32973900	0.59790800
H	-1.20073100	2.77000200	-2.85829600
Si	3.35190000	-0.61648900	-0.04998800
C	4.31145500	0.59833900	1.02441700
H	5.36788200	0.30171900	1.06923300
H	4.27196100	1.61148200	0.60699800
H	3.94544600	0.64755200	2.05584400
C	4.19264100	-0.72289100	-1.71857500
H	3.66866200	-1.40650200	-2.39352200
H	4.23966800	0.25029900	-2.21544800
H	5.21823700	-1.09251100	-1.58327800
C	3.45467300	-2.32508000	0.74201800

H	4.49053900	-2.68369400	0.67799300
H	3.16950300	-2.34240000	1.79825400
H	2.82706100	-3.05099600	0.21072500

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P3-TS(5-6) E = -1439.477475

Al	-0.77213000	-0.14801200	-0.05694600
C	-2.96913200	-0.73055800	-0.73884200
H	-3.59955200	-0.05476300	-1.30462300
C	-2.96910500	-0.85676700	0.67431600
C	-1.97858200	-1.82388900	1.02051100
C	-0.69043800	1.72122200	-1.02866700
C	0.54092700	2.09316400	1.07067700
C	-0.15065300	2.66866400	0.05359400
C	0.57398900	0.57947000	1.17411000
C	-0.32952000	4.15058500	-0.17749300
H	0.12044600	4.47000300	-1.12842700
H	-1.39256700	4.42031000	-0.22970700
C	-1.37115400	-2.26778600	-0.19266300
H	-0.60246500	-3.02809800	-0.26961400
C	-1.98276800	-1.59027600	-1.29792600
C	1.26464200	2.88952200	2.13512400
H	0.83879900	2.71696800	3.13164800
H	2.31783800	2.58563200	2.19139900
C	-1.86181400	2.25824200	-1.84711700
H	-2.15073100	1.54940500	-2.63031900
H	-2.73060600	2.39921900	-1.19511000
C	1.15119100	0.03304300	2.46834300
H	0.61426800	0.46263000	3.32276100
H	1.02858200	-1.05022500	2.53613000
N	1.15528600	-0.12917900	-0.11580300
N	1.47302200	0.97241600	-1.71416000
N	0.48865400	1.57819800	-1.91173400
C	-1.72347100	-1.84160400	-2.76027900
H	-0.67315600	-2.08747300	-2.95239900
H	-2.32707200	-2.68178100	-3.12903600
H	-1.97695100	-0.96779200	-3.37084300
C	-3.85952000	-0.11882700	1.63711500
H	-4.60403600	-0.78888000	2.08782200
H	-3.29344800	0.33243600	2.46151000
H	-4.40652500	0.68412700	1.13182800
C	-1.68086800	-2.33087200	2.40455400
H	-1.56799600	-1.51583500	3.12850600
H	-2.49189500	-2.97709200	2.76687800

H	-0.75972300	-2.92216400	2.42172400
H	2.22026300	0.25440200	2.61652400
H	1.24575200	3.96554800	1.95546400
H	0.11253100	4.75837000	0.61382600
H	-1.64862300	3.21837500	-2.33158700
Si	2.60348200	-1.12734900	-0.24283600
C	4.16432700	-0.10549700	-0.00571300
H	5.06364200	-0.71690200	-0.15499500
H	4.20154300	0.72436400	-0.71985000
H	4.22206700	0.31920900	1.00373000
C	2.59773000	-1.89966900	-1.95849000
H	1.69418400	-2.50052100	-2.12130800
H	2.64727300	-1.14776200	-2.75159700
H	3.45863200	-2.57013300	-2.07632900
C	2.64338800	-2.56767000	0.97873600
H	3.41481900	-3.28078400	0.65861100
H	2.88697100	-2.26291800	2.00094800
H	1.69292600	-3.11385200	1.00897800

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P3-IN6 E = -1439.494937

Al	-0.82628500	-0.16636200	0.01648400
C	-2.78892100	-0.15831500	-1.08182800
H	-3.00244800	0.52989700	-1.89080200
C	-3.15445700	0.03089700	0.28538000
C	-2.74261800	-1.13217500	0.99829200
C	-0.14524900	1.87529300	-0.91293600
C	1.16144700	1.62869800	1.18030400
C	0.90623400	2.37196000	0.07204500
C	0.55025900	0.27140000	1.34468400
C	1.54994000	3.69717200	-0.28870300
H	1.78642500	3.74432200	-1.36070500
H	0.90271400	4.55978000	-0.07205900
C	-2.13939000	-2.02195400	0.06565800
H	-1.69703000	-2.97999800	0.31153400
C	-2.16661800	-1.43756700	-1.23412300
C	2.03786600	2.15349200	2.29742200
H	1.47549000	2.18935500	3.23828500
H	2.89024400	1.48470500	2.47387400
C	-1.25957200	2.87777600	-1.25277100
H	-1.94900800	2.48559800	-2.00547100
H	-1.82583700	3.07748100	-0.33981100
C	0.65512400	-0.35404500	2.73007200
H	0.18496000	0.27568500	3.49726600

H	0.14493200	-1.32220000	2.74569700
N	0.87332500	-0.70972600	0.19031800
N	0.91530900	0.93959400	-2.96328300
N	0.43706200	1.39865800	-2.04465400
C	-1.74570000	-2.08706500	-2.52560100
H	-0.86410000	-2.72139600	-2.39115500
H	-2.55080200	-2.71891600	-2.92371300
H	-1.50473200	-1.34367800	-3.29335400
C	-3.87272200	1.21612500	0.87149400
H	-4.85712000	0.92591600	1.26159500
H	-3.32072400	1.67017700	1.70484100
H	-4.03838400	1.99262400	0.11800000
C	-2.93509200	-1.38067900	2.46941000
H	-2.62325300	-0.52367400	3.07746400
H	-3.99087100	-1.57678400	2.70026500
H	-2.35891300	-2.24994400	2.80118200
H	1.69197200	-0.53812200	3.05391100
H	2.42625600	3.15704500	2.11391600
H	2.49065100	3.85782900	0.24238300
H	-0.85791100	3.83035500	-1.61933900
Si	2.34643100	-1.52126200	-0.13097400
C	3.80947200	-0.34177500	-0.35117200
H	4.73105600	-0.89381200	-0.57846900
H	3.63954900	0.36882300	-1.16899800
H	3.99914500	0.24462900	0.55648600
C	2.12343700	-2.49486800	-1.73169900
H	1.37195200	-3.28576500	-1.61554800
H	1.80572400	-1.85023800	-2.55972100
H	3.06091800	-2.98047300	-2.03154900
C	2.86135700	-2.75943000	1.20463800
H	3.76203000	-3.30887100	0.89928400
H	3.08737600	-2.27118400	2.16003400
H	2.07275800	-3.49811300	1.39395800

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P3-TS(6-Pa) E = -1439.490627

Al	-0.41212100	-0.25995600	0.31437200
C	-3.51846400	-1.25012200	-0.82329900
H	-4.05889100	-1.38642000	-1.75677900
C	-3.90269500	-0.31281500	0.21259400
C	-3.00615100	-0.42053900	1.25298200
C	-0.42435200	1.32148800	-1.02610800
C	1.22325300	1.93893100	0.71147500
C	0.61194500	2.26068400	-0.50028600

C	1.16440000	0.60770100	1.29326400
C	1.00494900	3.41698700	-1.38443000
H	1.42409600	3.04807200	-2.33946200
H	0.16355500	4.07092700	-1.64950800
C	-1.95869200	-1.39780100	0.85882800
H	-1.58102700	-2.09335500	1.61520100
C	-2.40100100	-1.95003500	-0.44711700
C	1.89668400	3.02973800	1.52151800
H	1.48186400	3.05894800	2.53483800
H	2.97120900	2.83029900	1.63210200
C	-1.75097100	1.93111500	-1.50562900
H	-2.39079200	1.17236100	-1.96387000
H	-2.27554000	2.32497500	-0.63159600
C	1.58910300	0.39192000	2.73686700
H	1.12132700	1.10294900	3.42847500
H	1.30651700	-0.61527800	3.05913700
N	1.34499900	-0.57077000	0.38382300
N	0.85933200	0.54650600	-3.12545900
N	0.17474600	0.69165400	-2.23686700
C	-1.76958500	-3.11106300	-1.16499500
H	-0.68443000	-3.00201200	-1.28769100
H	-1.92806700	-4.05074500	-0.61677800
H	-2.20455500	-3.23615900	-2.16254100
C	-5.09931900	0.59205600	0.10768200
H	-5.25379700	1.18053600	1.01732600
H	-5.00464100	1.29842800	-0.72893100
H	-6.01729000	0.01628300	-0.07026700
C	-3.04265900	0.26273300	2.59274200
H	-3.27833900	-0.44895200	3.39729900
H	-2.07949600	0.72112100	2.85362500
H	-3.79961800	1.05269300	2.62742600
H	2.67963600	0.47455500	2.87847100
H	1.76980500	4.02490800	1.09128400
H	1.78117200	4.03985900	-0.93569500
H	-1.60120000	2.75066800	-2.21887600
Si	2.83224200	-1.33211900	-0.01461600
C	4.13738500	-0.05604900	-0.49558800
H	5.09668800	-0.53460800	-0.73099700
H	3.83190200	0.52392700	-1.37478800
H	4.32203700	0.65529300	0.31944000
C	2.50944800	-2.48964700	-1.46459700
H	1.76644100	-3.25433000	-1.20569000
H	2.14365600	-1.95254300	-2.34752300
H	3.42683200	-3.01607800	-1.75675400

C	3.54342900	-2.36876900	1.39378400
H	4.46523200	-2.87888400	1.08435100
H	3.78628400	-1.75986900	2.27251500
H	2.83181700	-3.13927200	1.71543800

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P4-TS E = -1439.476504

Al	0.84428100	0.60153000	-0.17203900
C	2.56629400	1.08784500	-1.12472700
H	2.34814300	1.53149200	-2.09714800
C	3.20926800	-0.22652900	-1.00449400
C	3.94484100	-0.23385600	0.17545600
C	-0.60304800	-0.44542000	-1.20182800
C	-0.15024500	-1.64732900	0.93449100
C	-0.56719400	-1.63665100	-0.50308300
C	0.63207700	-0.61791900	1.36991400
C	-0.82625900	-2.97698200	-1.15967100
H	-1.67942000	-3.48660900	-0.69052700
H	-1.04043700	-2.88233600	-2.22596000
C	3.84833800	1.06418200	0.77453100
H	4.33009600	1.35217600	1.70518500
C	3.06486400	1.89912600	-0.00556000
C	-0.59932400	-2.83395800	1.76742500
H	-0.16411700	-3.77523300	1.40674300
H	-0.31661200	-2.72698800	2.81642100
C	-0.91313100	-0.36289200	-2.67907400
H	-0.97923000	0.67850800	-3.00895300
H	-0.12211400	-0.83793900	-3.27729600
C	1.15559100	-0.46863100	2.77052900
H	0.93141300	-1.30545700	3.44357300
H	2.24374400	-0.32895100	2.75394200
N	-0.33508800	2.19277500	0.02159600
N	-1.49093500	1.85874300	0.00087900
N	-2.13514500	0.86126100	-0.40297300
C	2.86427200	3.37970700	0.17136300
H	3.21214600	3.70274800	1.15898400
H	3.43441000	3.94781300	-0.57820900
H	1.81490100	3.67899700	0.07222200
C	3.05444500	-1.35258500	-1.99136000
H	3.96364700	-1.96342800	-2.03755100
H	2.22835700	-2.03533500	-1.74344900
H	2.86355700	-0.97088700	-3.00195000
C	4.69017400	-1.39797300	0.76913300
H	5.02796900	-2.10100200	-0.00128600

H	5.57618800	-1.06004500	1.32003400
H	4.07170700	-1.97083900	1.47479200
H	0.75128200	0.44324600	3.23449100
H	-1.69045700	-2.96176400	1.73297700
H	0.03351100	-3.64928900	-1.04190200
H	-1.86083500	-0.84801400	-2.94891400
Si	-3.78685400	0.48007300	0.17920300
C	-4.87725000	1.95955300	-0.17723200
H	-5.90933500	1.76697400	0.14218700
H	-4.52375000	2.84976000	0.35485000
H	-4.89599800	2.19396800	-1.24744400
C	-3.73569400	0.10742700	2.01238100
H	-3.04086500	-0.71020000	2.23372300
H	-3.41017800	0.98368800	2.58517800
H	-4.72722500	-0.18182400	2.38305000
C	-4.32047400	-1.01127600	-0.81063800
H	-5.34768900	-1.29172000	-0.54685800
H	-4.29872800	-0.80823600	-1.88708500
H	-3.68088500	-1.87867200	-0.61800100

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P5-TS E = -1439.473459

Al	-0.39590900	0.28965500	0.27095100
C	-1.74605700	-1.04559800	0.98493600
H	-1.25263300	-1.83865700	1.55100400
C	-2.53831500	-1.41360100	-0.21904500
C	-3.67701400	-0.63877500	-0.23882800
C	-0.66732700	1.77733300	-0.99630000
C	1.45408800	2.24354800	0.23259600
C	0.35920700	2.63970400	-0.79123000
C	1.04779000	1.25777200	1.20737900
C	0.60279400	3.92883900	-1.54573000
H	1.54568000	3.88865300	-2.10649900
H	-0.19636600	4.13675000	-2.25946100
C	-3.69978500	0.17189500	0.96047200
H	-4.49051500	0.87467400	1.20994000
C	-2.60100200	-0.08996400	1.73613600
C	2.41306400	3.34572600	0.67716200
H	1.88861600	4.09257500	1.28538600
H	3.23372000	2.93813800	1.27289900
C	-1.76480300	1.97660400	-2.01122800
H	-1.82431200	1.11576500	-2.69074000
H	-2.74232800	2.02990600	-1.51435800
C	1.88780100	1.00002100	2.41922200

H	2.96887600	0.97393600	2.22127600
H	1.73027900	1.81997300	3.13907600
N	1.46444000	-0.58097900	-0.30927000
N	2.28416000	0.18542900	-1.01350200
N	2.48937900	1.36824800	-0.93275500
C	-2.31874900	0.43356400	3.11741600
H	-1.32609400	0.89470100	3.20501100
H	-3.05829600	1.18842600	3.40567900
H	-2.36014200	-0.37046700	3.86668100
C	-2.11996600	-2.46119200	-1.21418900
H	-1.94819300	-3.43241000	-0.72819100
H	-2.88568100	-2.61589400	-1.98051800
H	-1.19050400	-2.20306100	-1.74081200
C	-4.74813700	-0.58341900	-1.29271700
H	-4.73752200	0.37360300	-1.83218600
H	-4.63879200	-1.37684600	-2.03879800
H	-5.74637400	-0.68506000	-0.84715300
H	1.60518000	0.07374800	2.92938300
H	2.85342600	3.85208000	-0.18411900
H	0.66960700	4.78984900	-0.86821300
H	-1.66029000	2.87480400	-2.63182600
Si	2.12147900	-2.27311500	-0.23644700
C	1.14182200	-3.24090500	1.03995900
H	1.64191800	-4.20277600	1.20983500
H	1.09562300	-2.72458100	2.00541100
H	0.11950500	-3.45741200	0.71697200
C	3.92102400	-2.16703500	0.30296800
H	4.51469000	-1.57401000	-0.40116000
H	4.01571700	-1.70582200	1.29296700
H	4.36977100	-3.16648700	0.35842600
C	1.99702400	-3.06903700	-1.93474200
H	2.42209700	-4.08054800	-1.92677600
H	0.95701500	-3.14700300	-2.27002200
H	2.54583500	-2.48021000	-2.67795600

56

P5-IN1 E = -1439.521993

Al	-0.89173000	0.07972000	0.28577700
C	-1.78280000	-1.80434900	0.61044500
H	-1.06117000	-2.60118700	0.75025900
C	-2.65574400	-1.66464500	-0.51828100
C	-3.64608200	-0.71215500	-0.19006900
C	-1.09104000	1.63269500	-0.84647100
C	1.03297700	2.02181900	0.48106300

C	-0.03895400	2.43838300	-0.56188100
C	0.99300000	0.49354600	0.82737800
C	0.17781400	3.80545700	-1.19368300
H	1.19342300	4.16576100	-1.01995300
H	0.02319000	3.77163000	-2.27730500
C	-3.38815200	-0.25074700	1.11814400
H	-3.96343500	0.50940300	1.63762400
C	-2.25809200	-0.91744400	1.66334500
C	0.98636900	2.97565500	1.68481800
H	0.05134200	2.85838800	2.24460200
H	1.82677100	2.80112300	2.36279100
C	-2.17465000	2.02325500	-1.82165300
H	-2.34861900	1.23239800	-2.56260000
H	-3.13178700	2.17076300	-1.30469900
C	1.50959700	0.15314400	2.23513000
H	2.53006100	0.52314100	2.40691000
H	0.86567400	0.57360500	3.01597200
N	1.98379400	0.01415900	-0.19389900
N	2.77689300	1.07411300	-0.59626500
N	2.35685700	2.18693800	-0.21995800
C	-1.87671900	-0.98466200	3.12286200
H	-0.82235900	-1.24154600	3.26467700
H	-2.05881300	-0.03188100	3.63276000
H	-2.46997000	-1.75053200	3.64068600
C	-2.54817800	-2.42664500	-1.81063100
H	-3.35775500	-3.16407100	-1.89754700
H	-2.61999100	-1.77192500	-2.68768000
H	-1.60164200	-2.97320100	-1.87729300
C	-4.77694500	-0.27129200	-1.07868800
H	-5.28858400	0.60293100	-0.66309700
H	-4.43845700	-0.00826700	-2.08756500
H	-5.52752600	-1.06586600	-1.19060200
H	1.52659600	-0.93284200	2.38646600
H	1.04579900	4.01370200	1.34613800
H	-0.52584000	4.54730600	-0.79230100
H	-1.95817300	2.94565100	-2.37192300
Si	2.80371400	-1.52466900	-0.51758500
C	1.65476500	-2.95098000	-0.10449300
H	2.18037900	-3.89536100	-0.29556000
H	1.34585800	-2.96273600	0.94684600
H	0.75428500	-2.95003100	-0.72825500
C	4.36772200	-1.67967500	0.50942700
H	5.03518700	-0.82978300	0.32806600
H	4.15135700	-1.71013100	1.58366300

H	4.91617900	-2.59567600	0.25490000
C	3.22940100	-1.56806600	-2.33964500
H	3.76329500	-2.49173500	-2.59662900
H	2.32857400	-1.51566200	-2.96204600
H	3.86809100	-0.72060300	-2.60807100

56

P5-PS(1-Pa) E = -1439.505531

Al	-0.51408000	0.16209400	0.23215900
C	-1.83325000	-1.26596000	0.80396600
H	-1.32617000	-2.14702800	1.19920200
C	-2.67594800	-1.38442200	-0.40905700
C	-3.76239800	-0.54419700	-0.25954200
C	-0.77225100	1.86165100	-0.70905400
C	1.53403800	1.98000000	0.28427100
C	0.36608300	2.57401700	-0.55157300
C	1.32296900	0.57680500	0.89726400
C	0.64822800	3.92928800	-1.17747200
H	1.68668900	4.00142100	-1.51822400
H	0.00717200	4.11296200	-2.04238600
C	-3.69189500	0.06287200	1.04913200
H	-4.41839200	0.77260400	1.43612800
C	-2.58820300	-0.39180700	1.73118500
C	2.11908700	3.01437300	1.25005800
H	1.40093900	3.21535300	2.05183000
H	3.05273700	2.66549000	1.69836900
C	-1.96247700	2.33682300	-1.50447600
H	-2.16927700	1.65307500	-2.33884900
H	-2.86476900	2.32815600	-0.88083300
C	2.16051800	0.26265800	2.13079700
H	3.24484600	0.34028200	1.95952400
H	1.90715300	0.93442100	2.95775300
N	1.45598300	-0.33749200	-0.24813800
N	2.59897400	0.58224300	-1.28188100
N	2.58160500	1.68682100	-0.84829600
C	-2.22854700	-0.11882500	3.16671500
H	-1.18241200	0.18846600	3.29496100
H	-2.85833700	0.67521300	3.58221200
H	-2.37201000	-1.01285800	3.79055900
C	-2.37528900	-2.31512500	-1.55275100
H	-2.47612400	-3.36717100	-1.24856500
H	-3.05584800	-2.15610000	-2.39482600
H	-1.35404700	-2.19740600	-1.93826400
C	-4.86228300	-0.26416300	-1.24663600

H	-4.76155000	-0.86057000	-2.15864500
H	-5.84735700	-0.48758900	-0.81582800
H	-4.87951800	0.79204600	-1.54679700
H	1.95591000	-0.75366200	2.48251400
H	2.32535900	3.95576800	0.73848400
H	0.48008700	4.75074600	-0.46759100
H	-1.85751900	3.34570700	-1.91957500
Si	2.19375100	-1.98249300	-0.32818900
C	1.28931000	-3.22787300	0.76489300
H	1.86346400	-4.16325800	0.78091300
H	1.18264100	-2.89624400	1.80352800
H	0.29270200	-3.46642400	0.38002000
C	4.01841500	-1.97809300	0.14909400
H	4.57352700	-1.21405900	-0.40509100
H	4.17598700	-1.80463200	1.21879200
H	4.46356600	-2.95154100	-0.09437800
C	2.02098300	-2.49414200	-2.12787800
H	2.44763200	-3.49164600	-2.28988100
H	0.97106200	-2.52749300	-2.44058000
H	2.54389800	-1.79062500	-2.78331700

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P6-TS E = -1439.496764

Al	1.53738500	0.05333200	-0.06754300
C	3.55449300	-0.25650500	-0.99410700
H	3.67589200	-0.11605700	-2.06240300
C	3.11037400	-1.47296700	-0.36872700
C	3.11417400	-1.23896500	1.04614900
C	0.59916600	1.58558400	0.78740900
C	-0.77345600	1.13244900	-1.20253100
C	-0.52466300	1.87728900	0.07764600
C	0.00578500	-0.01012700	-1.50258100
C	-1.54116600	2.93928700	0.45399400
H	-2.56445100	2.56453900	0.34421500
H	-1.42408300	3.27029700	1.48768000
C	3.60544200	0.08232700	1.26097700
H	3.68394500	0.56258500	2.22982600
C	3.87900000	0.69750200	0.01826900
C	-1.51131800	1.85809400	-2.30214400
H	-0.84173500	2.58367300	-2.78762300
H	-1.87176600	1.17011100	-3.06977000
C	0.96604700	2.22961200	2.09845700
H	1.99170000	2.62152200	2.06819400
H	0.31257900	3.05336600	2.40785700

C	-0.04409800	-0.65065800	-2.87649500
H	-1.04259600	-1.04834500	-3.11792900
H	0.23330300	0.05959500	-3.66452800
N	-2.16065500	-0.32038800	-0.16353500
N	-1.26340900	-1.16287600	0.14902900
N	-0.06667500	-1.06188100	-0.40469800
C	4.41322500	2.08589600	-0.20631000
H	4.06429300	2.50371000	-1.15708200
H	4.10630900	2.77125500	0.59133700
H	5.51126400	2.08879900	-0.23379900
C	2.80196200	-2.77463900	-1.05722300
H	3.57525900	-3.52355500	-0.83938500
H	1.83666900	-3.18465600	-0.74281300
H	2.77026400	-2.64399100	-2.14373900
C	2.75390700	-2.24552700	2.10629100
H	1.83841000	-2.79259000	1.85475000
H	3.55263800	-2.98826100	2.23710000
H	2.59718500	-1.75889000	3.07471500
H	0.65506700	-1.49106000	-2.92831600
H	-2.36460600	2.42048100	-1.91769100
H	-1.45505600	3.82946700	-0.18439400
H	0.95805300	1.48577700	2.90923200
Si	-3.79998000	-0.65134500	0.48118500
C	-4.93696600	0.60443000	-0.33717500
H	-5.98070400	0.42406800	-0.05223800
H	-4.69139100	1.63233200	-0.04669900
H	-4.87624100	0.54222700	-1.42985300
C	-3.79818700	-0.43200600	2.35111600
H	-3.10796100	-1.14188100	2.82065500
H	-3.48070300	0.57825400	2.63339400
H	-4.79618200	-0.60113600	2.77433300
C	-4.32660000	-2.39947100	0.02141900
H	-5.32572000	-2.63372500	0.40957500
H	-4.35065800	-2.53359600	-1.06626100
H	-3.62283200	-3.13242300	0.43094400

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P6-IN1 E = -1439.528453

Al	-1.67413600	0.22083900	0.13358800
C	-3.63323100	-0.54705800	1.00726600
H	-3.73600400	-0.77057100	2.06335900
C	-3.23399700	-1.47849900	0.00368700
C	-3.21983400	-0.77765800	-1.24585500
C	-0.63499700	1.80016800	-0.37707300

C	1.08702200	0.38914200	0.85662900
C	0.64131700	1.64266900	0.04795100
C	-0.05767900	-0.67848100	0.94050400
C	1.69435900	2.69900100	-0.22793700
H	2.70391700	2.37963600	0.03585000
H	1.70323000	2.97981000	-1.28837600
C	-3.68480200	0.55324700	-0.99584800
H	-3.77317100	1.33087900	-1.74559000
C	-3.92763000	0.71573200	0.39072300
C	1.63785900	0.82600900	2.22285700
H	0.83760200	1.27494900	2.82149700
H	2.04685800	-0.02439500	2.77632800
C	-1.05085600	3.04025600	-1.13735100
H	-2.12043800	3.04204900	-1.37293400
H	-0.84246500	3.96227200	-0.57440400
C	-0.19774600	-1.44541200	2.26119100
H	0.73907700	-1.93488700	2.56381000
H	-0.51469900	-0.79016800	3.08074600
N	2.08897800	-0.38944600	0.05763000
N	1.45939500	-1.45633200	-0.55176700
N	0.29876000	-1.65692400	-0.11781500
C	-4.46201900	1.94401500	1.07811200
H	-4.11900700	2.00804400	2.11657200
H	-4.15166800	2.86082900	0.56583100
H	-5.55984800	1.93521200	1.09877600
C	-2.90586600	-2.93388000	0.19958000
H	-3.59404100	-3.56560400	-0.37715800
H	-1.88448900	-3.16864700	-0.12036100
H	-3.00558200	-3.21797500	1.25206700
C	-2.89487200	-1.37516200	-2.59001400
H	-2.00659900	-2.01394100	-2.54430100
H	-3.72628300	-1.99112900	-2.95845000
H	-2.70914300	-0.59411500	-3.33445000
H	-0.95008800	-2.23286000	2.15822000
H	2.42772700	1.57516600	2.12536300
H	1.48614400	3.61975400	0.33543600
H	-0.51322300	3.13435800	-2.09326700
Si	3.83190700	-0.33832800	-0.35459800
C	4.81065200	0.66356000	0.90825600
H	5.87492500	0.57434900	0.65416700
H	4.57420000	1.73211200	0.92036600
H	4.68544500	0.27613800	1.92492000
C	4.07811400	0.37922800	-2.07879300
H	3.48916900	-0.18253300	-2.81260900

H	3.77303700	1.42952900	-2.13817800
H	5.13181100	0.31939800	-2.37968000
C	4.47135000	-2.10684600	-0.31685500
H	5.53593500	-2.13820400	-0.58111600
H	4.35901000	-2.54838900	0.68004500
H	3.92294500	-2.73665400	-1.02326000

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P6-TS(1-2) E = -1439.50723

Al	0.71954700	-0.01497400	0.03940600
C	3.24138800	-0.85966900	0.92272000
H	3.74761600	-0.65664000	1.86067000
C	3.31929000	-0.04631300	-0.22739300
C	2.44290400	-0.59140600	-1.21683000
C	0.40541900	0.94953500	1.73482300
C	-1.33148700	1.28136300	-0.00596900
C	-0.76287900	1.55769400	1.45083400
C	-0.21684300	1.83805600	-0.98933400
C	-1.55719200	2.47737700	2.34735900
H	-2.57348000	2.10272000	2.52666800
H	-1.07392000	2.59064300	3.32088900
C	1.81269300	-1.75909600	-0.61319400
H	1.20374300	-2.47691200	-1.15073500
C	2.32669400	-1.91145500	0.70987300
C	-2.70589600	1.91063600	-0.26633000
H	-2.67530000	2.99648500	-0.13267200
H	-3.02684800	1.70110600	-1.29066100
C	1.16806100	1.05125900	3.02538500
H	1.32034800	0.05852400	3.47029000
H	2.17419800	1.45655300	2.85281400
C	0.22329300	3.28023400	-0.95054100
H	-0.59849200	3.99290900	-1.11759100
H	0.66018000	3.50034300	0.02755500
N	-1.23796700	-0.15141000	-0.32272700
N	-1.01559700	0.25620100	-2.47352900
N	-0.50309100	1.28098700	-2.22382700
C	1.97940700	-3.00556400	1.68339100
H	0.96829800	-3.39377000	1.51855700
H	2.66935500	-3.85503400	1.58680200
H	2.03810500	-2.65725100	2.72073100
C	4.20229200	1.15864900	-0.40650000
H	5.08461600	0.92165900	-1.01753900
H	3.68065900	1.98270700	-0.90735300
H	4.56360400	1.53106500	0.55789600

C	2.42409400	-0.23945400	-2.68329300
H	2.37060200	0.84248800	-2.84941300
H	3.33502900	-0.60193800	-3.17928500
H	1.56814900	-0.69212600	-3.19210500
H	0.98828800	3.47435100	-1.70949800
H	-3.46772000	1.51464600	0.41285400
H	-1.66512900	3.48174600	1.91530600
H	0.68685500	1.68020300	3.78529900
Si	-2.47228600	-1.39435600	-0.11181500
C	-4.01634400	-1.12193900	-1.16718900
H	-4.66079300	-2.00883300	-1.11276200
H	-4.61392600	-0.26529500	-0.83897500
H	-3.75243200	-0.96607800	-2.21909600
C	-2.99305800	-1.51967700	1.70238800
H	-2.13387600	-1.72531600	2.35112800
H	-3.45871000	-0.59351100	2.06016200
H	-3.72232800	-2.32757600	1.84418700
C	-1.70109400	-3.02779300	-0.65036700
H	-2.45159900	-3.82749100	-0.62602900
H	-1.31866200	-2.96558000	-1.67575200
H	-0.87641500	-3.33421600	0.00238400

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P6-IN2 E = -1439.542449

Al	-0.90729300	0.06488300	-0.16215800
C	-3.68066900	0.31566000	-0.65868400
H	-4.23123000	1.07546300	-1.20341700
C	-3.46392200	0.32086700	0.73666900
C	-2.62635100	-0.77958400	1.06536300
C	-0.60996800	1.94936600	-0.52308000
C	1.66586600	0.83776900	-0.51781100
C	0.72919000	2.08229000	-0.64985100
C	2.69175500	1.12038200	0.61598000
C	1.43703500	3.39244400	-0.94012100
H	1.75767100	3.45781500	-1.98859500
H	0.79314800	4.25280700	-0.74745600
C	-2.33227300	-1.46971700	-0.18986800
H	-1.90349600	-2.46223600	-0.27053400
C	-3.00382300	-0.76792800	-1.24899400
C	2.42410800	0.68571600	-1.86084700
H	3.01517900	1.57204100	-2.10967600
H	3.10345400	-0.17039600	-1.84587400
C	-1.60644200	3.07375000	-0.65459200
H	-2.28496800	2.89019400	-1.49800700

H	-2.24482100	3.14053200	0.23499200
C	4.14227800	1.50475100	0.44167800
H	4.70731500	0.73561200	-0.09982400
H	4.26531000	2.44624100	-0.11006400
N	0.88263100	-0.38960300	-0.21442800
N	1.77730300	0.87295500	2.86913000
N	2.23560800	1.01474700	1.82095700
C	-3.02469700	-1.16817900	-2.70004500
H	-2.10008800	-1.67573800	-2.99716200
H	-3.85268900	-1.86055600	-2.90459700
H	-3.15655800	-0.30093800	-3.35605400
C	-4.03765700	1.30754600	1.71713100
H	-4.81427700	0.84403000	2.34077000
H	-3.27733300	1.70515800	2.40004700
H	-4.49674700	2.15588400	1.19952500
C	-2.35867700	-1.29679100	2.45749400
H	-2.21893100	-0.47980000	3.17371500
H	-3.20393800	-1.90150600	2.81545600
H	-1.46781100	-1.92830000	2.49953700
H	4.61921100	1.63379400	1.41838700
H	1.69134000	0.52718000	-2.65789200
H	2.33144200	3.51188700	-0.32077800
H	-1.15636100	4.06074200	-0.81020800
Si	1.60468300	-1.99683100	-0.15329300
C	3.43719600	-2.03482400	0.32133100
H	3.76156100	-3.08345300	0.35028300
H	4.09650200	-1.51701500	-0.38200400
H	3.60750400	-1.61146100	1.31687600
C	1.41993800	-2.89548700	-1.81225800
H	0.36741400	-2.95631100	-2.11723000
H	1.96061300	-2.38233700	-2.61621100
H	1.80467100	-3.92201600	-1.75761000
C	0.75983500	-3.05489800	1.16860900
H	1.30392000	-4.00288400	1.26903700
H	0.78776100	-2.55707700	2.14486000
H	-0.28064400	-3.31068600	0.94564100

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P6-TS(2-3) E = -1439.48314

Al	0.86415100	0.07311800	-0.44359200
C	3.42062600	0.13417500	-1.03888800
H	3.86359400	-0.30851700	-1.92550100
C	3.54848300	-0.36774200	0.27111900
C	2.77993000	0.45447400	1.13147400

C	0.55579200	-1.80539000	-0.77468000
C	-1.70776900	-0.70161100	-0.69700700
C	-0.78671100	-1.95991900	-0.84340100
C	-2.75319600	-0.82117200	0.40070600
C	-1.45650300	-3.30070500	-1.06422200
H	-2.24510600	-3.26556900	-1.82261200
H	-0.73328600	-4.05311100	-1.38499300
C	2.19247600	1.49147400	0.33807700
H	1.69755500	2.37104700	0.73104500
C	2.59008500	1.28837600	-1.04712000
C	-2.45765900	-0.52623800	-2.06288100
H	-3.03767400	-1.40921400	-2.34430900
H	-3.13512900	0.32930000	-2.03129200
C	1.53613800	-2.94302800	-0.94248600
H	2.50163600	-2.58291000	-1.30866400
H	1.73401000	-3.44402000	0.01635500
C	-3.93969700	-1.70446500	0.20562800
H	-4.66672500	-1.03113300	-0.27945000
H	-3.86628200	-2.59696800	-0.43033400
N	-0.89335900	0.52789100	-0.45460500
N	-1.29821200	-1.50116400	2.93600800
N	-1.75829500	-1.71881200	1.94515000
C	2.44398600	2.26717100	-2.18757200
H	1.47868400	2.78136000	-2.17724400
H	3.22504500	3.03806400	-2.13997300
H	2.54298800	1.76056900	-3.15393300
C	4.34755700	-1.56966800	0.69477200
H	5.15772600	-1.28648700	1.37992300
H	3.73602700	-2.31632700	1.21662200
H	4.80606300	-2.06390200	-0.16776800
C	2.65067300	0.31051200	2.62394700
H	2.49973800	-0.73186800	2.92847500
H	3.55839600	0.66411600	3.13230800
H	1.81033600	0.89542900	3.01206900
H	-4.39048000	-1.97686000	1.16627100
H	-1.70690800	-0.33745300	-2.83527700
H	-1.91469700	-3.67437700	-0.13949900
H	1.19362300	-3.71785500	-1.63993000
Si	-1.64915300	1.96435200	0.20160000
C	-3.45445300	2.26192900	-0.27774400
H	-3.77816400	3.18988500	0.21328700
H	-3.58062600	2.41486700	-1.35616200
H	-4.13762500	1.47192800	0.04527300
C	-0.78061000	3.49104100	-0.50728000

H	0.26430400	3.61378600	-0.20600800
H	-0.81063900	3.48658500	-1.60402400
H	-1.31112100	4.39243200	-0.17283800
C	-1.52279100	2.07879800	2.07930200
H	-1.90882300	3.03967100	2.44452100
H	-2.09721400	1.27906100	2.55741500
H	-0.48413600	1.99352600	2.42419700

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P6-IN3 E = -1329.973573

Al	-0.72477100	0.05571900	-0.26439200
C	-3.18091300	0.02504300	-1.03401100
H	-3.59627100	0.65235800	-1.81611000
C	-3.35805400	0.22532800	0.35143900
C	-2.60405200	-0.76043500	1.03695500
C	2.27561000	1.18212200	1.07308800
C	0.86517200	2.18619800	-0.29820300
C	1.82206200	0.92621100	-0.31428700
C	-0.47422300	1.97489600	-0.26362100
C	2.75683200	1.02943700	-1.54494400
H	3.31262000	1.97048600	-1.58053900
H	3.48446600	0.21537500	-1.54575500
C	-1.97767200	-1.59361100	0.04808800
H	-1.46061800	-2.52414200	0.24743500
C	-2.33427200	-1.09288000	-1.26273800
C	1.44647300	3.58181200	-0.42927800
H	1.04089200	4.08135600	-1.31899800
H	1.16761200	4.20172200	0.43272300
C	3.51554300	1.98564700	1.28223900
H	4.19480000	1.27992800	1.79124900
H	4.06334600	2.41418000	0.42625200
C	-1.43625900	3.13155600	-0.36348400
H	-2.46199200	2.80281400	-0.54185400
H	-1.43822500	3.72378500	0.56433000
N	1.04567100	-0.34267300	-0.38301400
C	-2.06473300	-1.76029600	-2.58822800
H	-1.07068200	-2.21692900	-2.62752000
H	-2.79829100	-2.55459100	-2.78117900
H	-2.13449700	-1.04240900	-3.41267000
C	-4.18696100	1.29829600	1.00337400
H	-3.59321000	1.94521800	1.66160600
H	-4.66384700	1.93839500	0.25407000
H	-4.98555100	0.86351700	1.61887800
C	-2.55292000	-0.96030500	2.52820900

H	-1.69470600	-1.57031200	2.82533500
H	-2.48608800	-0.00869400	3.06769300
H	-3.45795800	-1.47118500	2.88502200
H	-1.16661600	3.82725500	-1.17091000
H	2.53217000	3.60432900	-0.51149800
H	2.16042600	0.94990200	-2.45924900
H	3.34240500	2.76654200	2.03527000
Si	1.80215100	-1.81937700	0.17056700
C	3.69034300	-1.77420000	0.14522400
H	4.05791100	-2.68405800	0.63757600
H	4.10103400	-1.77202400	-0.87045300
H	4.12203500	-0.92526800	0.68559900
C	1.31332300	-3.23950500	-0.97346400
H	0.23515900	-3.43289400	-0.99641700
H	1.63267500	-3.04109300	-2.00395900
H	1.79811800	-4.17042900	-0.65118400
C	1.31511800	-2.28726000	1.93217400
H	1.86121600	-3.17715100	2.27230600
H	1.54551600	-1.45959000	2.61195400
H	0.24585400	-2.50909400	2.03005400

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P6-TS(3-4) E = -1329.970632

Al	-0.76273400	0.06181500	-0.23375500
C	-3.26533400	-0.19388600	-0.81493900
H	-3.81886000	0.38809500	-1.54413400
C	-3.23377000	0.05968500	0.57236600
C	-2.33371000	-0.86566500	1.16971500
C	1.99314100	1.28635100	1.23172200
C	0.62227500	2.28393000	-0.44050800
C	1.67607600	1.16182300	-0.24008000
C	-0.68604800	1.96453700	-0.52907000
C	2.76577000	1.33556200	-1.32380900
H	3.20353100	2.33869100	-1.29854900
H	3.58149600	0.62229000	-1.20552300
C	-1.83052100	-1.71151200	0.11413500
H	-1.22990600	-2.60072000	0.25658800
C	-2.40445500	-1.27426600	-1.13164900
C	1.14719700	3.70494100	-0.52489700
H	0.40945500	4.41890500	-0.14701100
H	2.06745500	3.84880500	0.05109500
C	3.37147100	1.71749000	1.59408000
H	3.70533900	1.26789800	2.53796900
H	4.17925500	1.67402600	0.84518300

C	-1.75105800	3.00686300	-0.77520100
H	-2.69188900	2.55777100	-1.10570400
H	-1.97587500	3.57476100	0.14031100
N	1.05943800	-0.19927600	-0.31512100
C	-2.26297900	-1.93878300	-2.47693000
H	-1.25609100	-2.33525600	-2.64146800
H	-2.96341900	-2.77933300	-2.57245800
H	-2.48193900	-1.23696900	-3.28882700
C	-3.99962900	1.13078400	1.29970200
H	-4.70687100	0.69657600	2.01857900
H	-3.34113600	1.80255200	1.86415000
H	-4.57612000	1.74446200	0.60059400
C	-2.08410400	-1.03330600	2.64618100
H	-2.87728800	-1.63609700	3.10978100
H	-1.13256800	-1.53484700	2.84344200
H	-2.06186800	-0.06949000	3.16616800
H	-1.45276300	3.73879000	-1.53724000
H	1.37571100	3.98965600	-1.56152000
H	2.32239700	1.18370000	-2.31385800
H	3.21433400	2.78483000	1.84754600
Si	1.92077200	-1.69203900	-0.00616200
C	3.80574300	-1.58876400	-0.06804200
H	4.19609700	-2.56032100	0.26299900
H	4.19466100	-1.41552900	-1.07706800
H	4.23319000	-0.83091300	0.59654300
C	1.44499300	-2.96203200	-1.31695600
H	0.38408200	-3.23319100	-1.29962600
H	1.67370100	-2.58791400	-2.32231400
H	2.01528900	-3.88873100	-1.17092000
C	1.53190600	-2.41063000	1.69665800
H	2.18778000	-3.26285000	1.91741000
H	1.68939800	-1.65135900	2.47173400
H	0.50029700	-2.76713800	1.79220100

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P6-IN4 E = -1330.038112

Al	-0.74055400	0.13596400	0.23768100
C	-3.28422300	-0.51213200	-1.11523700
H	-3.81466300	-0.05947400	-1.94699300
C	-3.51140400	-0.20354000	0.25545500
C	-2.59011600	-0.93565400	1.02981900
C	0.75120000	0.45103600	1.45839400
C	0.56389900	2.32031200	-0.36911900
C	1.44643900	1.41576200	0.52002700

C	-0.65208600	1.84108400	-0.71265800
C	2.80633400	1.98327700	0.89756100
H	2.68293400	2.92401500	1.44574000
H	3.36908300	1.30186400	1.53609300
C	-1.72929800	-1.66801600	0.09605900
H	-1.11864600	-2.51947300	0.38207300
C	-2.22682400	-1.41197400	-1.23685700
C	1.14626500	3.65283500	-0.78881900
H	2.07862600	3.53448000	-1.35745100
H	0.45228300	4.21504200	-1.41726400
C	1.29872900	0.03778500	2.80184500
H	0.87906400	0.69183100	3.57690700
H	0.99004700	-0.98501400	3.05214000
C	-1.65132800	2.54086600	-1.59364200
H	-2.59247100	2.71744000	-1.05540500
H	-1.31170000	3.50890400	-1.98264700
N	1.38353800	-0.03330000	0.14327500
C	-1.69846900	-2.00811300	-2.51306900
H	-0.61482500	-1.87504600	-2.62422300
H	-1.89320600	-3.08834300	-2.56153600
H	-2.17658200	-1.54872000	-3.38467000
C	-4.58070900	0.71948500	0.77483800
H	-4.28378200	1.20580400	1.71066600
H	-4.81398300	1.50753500	0.05028500
H	-5.51604100	0.17836700	0.97624400
C	-2.60051800	-1.12217700	2.52513700
H	-2.93615200	-0.22101200	3.05065000
H	-3.27817400	-1.93807900	2.81450400
H	-1.60674900	-1.37545500	2.91060400
H	-1.91678100	1.91510400	-2.45594200
H	1.38647000	4.28592200	0.07609100
H	3.41998700	2.19722500	0.01495200
H	2.39201700	0.08080800	2.88994900
Si	2.61517700	-1.17480800	-0.37652500
C	4.20972400	-1.20634000	0.62766700
H	4.85165900	-2.01553000	0.25450300
H	4.78280500	-0.27655100	0.54898300
H	4.02841600	-1.40191300	1.69083200
C	3.02040400	-0.73115100	-2.15396500
H	2.11992800	-0.73308900	-2.77860900
H	3.46734600	0.26770700	-2.22513400
H	3.73380000	-1.44283000	-2.58804300
C	1.85708700	-2.89011500	-0.27849100
H	2.58425100	-3.64419400	-0.60530300

H	1.56252900	-3.14630900	0.74660000
H	0.97183300	-2.98751200	-0.91569900

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P6-TS(4-Pa) E = -1330.007723

Al	0.53764500	-0.10026600	-0.21628400
C	3.43693600	-0.91179100	1.02140500
H	3.92534200	-0.86885600	1.99134900
C	3.78499200	-0.08537600	-0.10441300
C	2.94701600	-0.41117500	-1.16057200
C	-0.91293400	0.62258000	-1.29607500
C	-0.59267200	2.19743700	0.68510300
C	-1.39016500	1.71465000	-0.44688100
C	0.54914500	1.49223000	0.99911800
C	-2.67725500	2.42225500	-0.76668300
H	-2.42844100	3.33794000	-1.32649900
H	-3.32466300	1.82187800	-1.40787800
C	1.98284700	-1.42068800	-0.67584100
H	1.58229600	-2.18183900	-1.34728900
C	2.39563400	-1.75619500	0.69462300
C	-1.11077800	3.39966400	1.45534500
H	-2.00555800	3.15015900	2.04223700
H	-0.36456300	3.77608800	2.15703700
C	-1.40225600	0.47438500	-2.71797700
H	-1.01889500	1.29173200	-3.34351800
H	-1.02348300	-0.46292900	-3.14089300
C	1.45363100	1.84255000	2.13664300
H	2.50063200	1.69711800	1.84775400
H	1.33560000	2.85607200	2.53823100
N	-1.29679500	-0.49705700	-0.28486100
C	1.82760700	-2.86647500	1.53484600
H	0.73246800	-2.90650300	1.49542900
H	2.18865200	-3.84741200	1.19347800
H	2.12217100	-2.75833400	2.58467200
C	4.89140900	0.93470900	-0.09157500
H	4.93001800	1.51057600	-1.02157500
H	4.77948900	1.65134800	0.73321100
H	5.87271000	0.45791100	0.03785100
C	3.00658200	0.07958600	-2.58189000
H	3.54833000	1.02748200	-2.66662300
H	3.51773600	-0.64499600	-3.23277700
H	2.00609400	0.23611000	-3.00268700
H	1.28570900	1.13817600	2.96616400
H	-1.38254800	4.23126500	0.79405000

H	-3.23216300	2.73603900	0.12095200
H	-2.49694400	0.45354300	-2.83172100
Si	-2.78220500	-1.21537300	0.22188800
C	-4.06399800	-1.35998300	-1.15651600
H	-4.92518300	-1.94661400	-0.81046100
H	-4.45111700	-0.38662800	-1.48118900
H	-3.65382400	-1.86427000	-2.03899300
C	-3.59981400	-0.31694200	1.66963100
H	-2.89874500	-0.19749800	2.50476300
H	-3.95480400	0.68314400	1.39225300
H	-4.46815600	-0.87464500	2.04450700
C	-2.34259300	-2.94760800	0.81452000
H	-3.23632400	-3.47966600	1.16509400
H	-1.88963700	-3.54548000	0.01527800
H	-1.63314200	-2.91570600	1.65019300

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Mes-N_3 E = -513.7765387

N	1.85927000	0.66779500	-0.34864400
N	2.78336400	0.05215600	0.19165400
N	3.74200300	-0.39816700	0.62132000
C	0.49845500	0.26667200	-0.16593900
C	0.08193700	-1.07771700	-0.15718400
C	-0.43070000	1.32291000	-0.07711700
C	-1.28638600	-1.33668500	-0.00841000
C	-1.78215800	1.00643400	0.06082300
C	-2.23427100	-0.31818000	0.10622900
H	-1.61678500	-2.37336200	0.00355500
H	-2.50175100	1.81917300	0.13849100
C	1.04943600	-2.22432100	-0.34150300
H	1.71401300	-2.05625600	-1.19746800
H	1.68824600	-2.38766900	0.53520300
H	0.50334400	-3.15447900	-0.52324100
C	0.03213100	2.75888200	-0.11968300
H	0.71071700	2.98674600	0.71088700
H	0.58434300	2.97426800	-1.04169700
H	-0.82022800	3.44251700	-0.06163200
C	-3.70586200	-0.62843700	0.25413300
H	-4.27899900	-0.27727700	-0.61358100
H	-3.87927400	-1.70472100	0.35245600
H	-4.13156800	-0.13877800	1.13862900

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P2'-TS E = -1379.753196

Al	-2.10302900	0.10622900	0.18750300
C	-3.51261300	0.40630300	1.75229200
H	-3.23525500	-0.00578900	2.71606000
C	-4.29667600	-0.26394900	0.74936500
C	-4.50494800	0.65926200	-0.31323700
C	-1.08107700	-1.59644500	0.43742700
C	-0.53220000	-0.75141700	-1.83561500
C	-0.45006900	-1.80546500	-0.77139300
C	-1.35786200	0.31413000	-1.62586000
C	0.19771500	-3.12749600	-1.12362400
H	1.17280400	-2.98981500	-1.60043200
H	0.33613900	-3.75880100	-0.24348100
C	-3.86287300	1.87314400	0.03504900
H	-3.79903800	2.75089500	-0.59846200
C	-3.23952700	1.74118500	1.30123800
C	0.32842500	-0.95990000	-3.06718000
H	0.10057900	-1.90942500	-3.56822500
H	0.19644400	-0.16293800	-3.80135500
C	-1.03238800	-2.57132500	1.58453800
H	-1.45060600	-2.13235400	2.49691900
H	-1.62361000	-3.47293800	1.36652500
C	-1.52044000	1.47240200	-2.57236300
H	-1.09448500	1.31193900	-3.57004900
H	-2.58041800	1.72526100	-2.70390500
N	-0.35425800	0.24078400	1.20871600
N	0.83590000	0.30179900	1.02565400
N	1.71771200	-0.46675400	0.55042000
C	-2.52409900	2.81443100	2.07705200
H	-2.15277300	3.60377400	1.41442400
H	-3.19645800	3.28648400	2.80574600
H	-1.66935600	2.41109100	2.63071300
C	-4.86268800	-1.65429900	0.85967600
H	-5.89426200	-1.63229300	1.23721500
H	-4.88350700	-2.16647200	-0.10890100
H	-4.27543300	-2.27050900	1.54846100
C	-5.27424200	0.39443800	-1.57906400
H	-6.35781100	0.40052300	-1.39812200
H	-5.06575300	1.15900100	-2.33460800
H	-5.02818800	-0.57973000	-2.01800700
H	-1.04866800	2.37942400	-2.16452500
H	1.39380100	-0.98880000	-2.80301900
H	-0.42598800	-3.68341500	-1.83857000
H	-0.01100100	-2.90084400	1.82148000
C	3.04233600	0.02225700	0.40811600

C	4.06781600	-0.91249600	0.66527400
C	3.35277200	1.31839700	-0.06217100
C	5.39568800	-0.52449700	0.47726900
C	4.69882100	1.65548800	-0.23180900
C	5.73722300	0.75827600	0.03738200
H	6.18486500	-1.24538000	0.68214200
H	4.94079100	2.65164300	-0.59819000
C	3.73449700	-2.30376300	1.14912000
H	3.20858800	-2.27809900	2.11098900
H	3.07465500	-2.82666700	0.44772800
H	4.64442000	-2.89917700	1.27496000
C	2.27982100	2.32354400	-0.41020000
H	1.48182500	1.86940400	-1.00923900
H	1.80623600	2.74786100	0.48340100
H	2.70615000	3.15195600	-0.98526200
C	7.18207300	1.16842500	-0.12818300
H	7.82526200	0.30269800	-0.31941200
H	7.30756200	1.87265000	-0.95821800
H	7.56348600	1.66328100	0.77556700

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P2'-IN1 E = -1379.814155

Al	-1.96713700	-0.53213300	0.03855700
C	-2.85633200	-1.83472300	1.63114500
H	-3.26650500	-1.43795300	2.55339000
C	-1.48607600	-2.19547900	1.43392200
C	-1.35922900	-2.66164500	0.08657800
C	-2.91969400	0.68634500	-1.13570700
C	-1.87491000	2.58032300	0.18112200
C	-2.68164800	2.01797900	-0.93881800
C	-0.83535900	1.94567800	0.79642200
C	-3.29446800	3.04944900	-1.88100700
H	-2.71996800	3.97936700	-1.90443900
H	-3.34005000	2.66546500	-2.90413200
C	-2.68029900	-2.64852200	-0.48935600
H	-2.91448100	-2.95274900	-1.50332900
C	-3.60557100	-2.16178700	0.45760500
C	-2.25265200	3.98330700	0.63260900
H	-3.32344700	4.17055100	0.50299000
H	-2.02100900	4.15159400	1.68700500
C	-3.81223300	0.24016700	-2.28217100
H	-3.37088500	0.47032600	-3.26403800
H	-3.99107500	-0.83909900	-2.26618600
C	-0.04724600	2.56057300	1.93719600

H	0.60060700	3.37723800	1.60029500
H	-0.72137100	2.96190800	2.70417700
N	1.62814500	0.99417400	0.23926300
N	0.70270900	0.12957000	0.25759200
N	-0.54859000	0.58772500	0.48231400
C	-5.08498300	-1.97017600	0.26525700
H	-5.65050700	-2.51905300	1.02820100
H	-5.38007400	-0.91620900	0.33362100
H	-5.40293600	-2.33989700	-0.71433700
C	-0.39739900	-2.13816300	2.46798000
H	-0.21682900	-3.13616800	2.88958600
H	0.54389900	-1.77651100	2.04430200
H	-0.67412700	-1.47624400	3.29491000
C	-0.12263100	-3.24675500	-0.54389700
H	0.77024600	-2.66863500	-0.28991400
H	0.03415600	-4.27974500	-0.20566300
H	-0.21072800	-3.27087600	-1.63535200
H	0.59065400	1.81535000	2.41242600
H	-1.72049000	4.75990700	0.06515300
H	-4.32377400	3.31070000	-1.59471900
H	-4.79786600	0.72715300	-2.26360100
C	2.90781700	0.44889600	-0.07519600
C	3.94922700	0.65074700	0.85420700
C	3.17095400	-0.15683000	-1.32107500
C	5.23150800	0.19484800	0.54294800
C	4.47562400	-0.58784600	-1.59027900
C	5.51766800	-0.43745800	-0.67217000
H	6.03041500	0.34429500	1.26743600
H	4.68233200	-1.04517400	-2.55662000
C	3.67599700	1.34104300	2.16915800
H	3.16805800	2.29934600	2.01427300
H	3.02272700	0.74074200	2.81572500
H	4.60697700	1.52466100	2.71542800
C	2.10401100	-0.29429800	-2.38509500
H	1.42765400	-1.13367200	-2.18834300
H	1.48287000	0.60587600	-2.44570500
H	2.56303500	-0.46065600	-3.36555900
C	6.90885900	-0.94375300	-0.97726700
H	7.67765300	-0.28552500	-0.55660700
H	7.07476900	-1.94410500	-0.55387400
H	7.08139700	-1.01628300	-2.05660200

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Pb' E = -1379.823328

Al	0.74291300	0.41499800	-0.05704000
C	0.84771400	1.63753000	-1.75475700
H	0.26914300	1.21911000	-2.57309300
C	2.27685300	1.67337000	-1.68025500
C	2.63457600	2.55086100	-0.63092000
C	1.59682800	-2.45385300	-0.47670600
C	2.70210700	-1.12794400	1.39676100
C	2.64130700	-2.23578200	0.37061200
C	1.95545700	0.02251400	1.43512800
C	3.81255700	-3.20264800	0.34216700
H	3.88666300	-3.81341800	1.25048300
H	3.75620800	-3.88325700	-0.50875200
C	1.44896800	3.06123600	-0.06440500
H	1.40295100	3.74557800	0.77709800
C	0.31841000	2.52353200	-0.72698000
C	3.69838500	-1.42453300	2.51592000
H	4.72987900	-1.47531400	2.14576200
H	3.67560200	-0.66712700	3.29817200
C	1.34985400	-3.65496100	-1.35610600
H	0.27564800	-3.86972500	-1.37191100
H	1.65527300	-3.46768600	-2.39544300
C	2.10323800	0.99314000	2.60331500
H	3.11475800	1.41595100	2.68443900
H	1.42243000	1.84371300	2.50358400
N	0.65325300	-1.41700100	-0.57944000
N	-0.62513600	-1.62902000	-0.36866400
N	-1.13702100	-0.46150100	-0.06928400
C	-1.09603700	3.04207900	-0.65328500
H	-1.31170200	3.47269300	0.33117700
H	-1.25829800	3.83518900	-1.39650700
H	-1.83956600	2.26158900	-0.84473000
C	3.22629600	0.90708900	-2.56066900
H	3.82949300	1.58833000	-3.17637700
H	3.92938000	0.29442300	-1.98226700
H	2.68668300	0.24034800	-3.24144200
C	4.03452100	2.81795700	-0.15232800
H	4.69769600	3.10797000	-0.97769400
H	4.05073200	3.62877200	0.58382500
H	4.48127100	1.93310800	0.32181800
H	1.87837400	0.51741200	3.56848800
H	3.48908200	-2.39200300	2.99073000
H	4.76195800	-2.66049800	0.25080500
H	1.86395900	-4.55149600	-1.00511400
C	-2.54647300	-0.37202000	0.06456500

C	-3.42112300	-0.84165500	-0.93891000
C	-3.05231300	0.25745000	1.22331200
C	-4.79763900	-0.68014100	-0.74476700
C	-4.43378000	0.39642200	1.36357400
C	-5.32849400	-0.07008600	0.39409300
H	-5.47464500	-1.03370200	-1.52006300
H	-4.82161600	0.87613000	2.26027300
C	-2.12384900	0.74929100	2.30867100
H	-1.45498000	-0.04516300	2.65826100
H	-1.48627000	1.57218400	1.96109100
H	-2.69407300	1.11678600	3.16748300
C	-2.92304600	-1.47599700	-2.21834100
H	-2.08574100	-0.91483400	-2.64868000
H	-2.56900100	-2.49978100	-2.05834100
H	-3.72560100	-1.50873600	-2.96204100
C	-6.82115400	0.06829400	0.58360600
H	-7.21428100	-0.71616300	1.24439100
H	-7.08135300	1.03130600	1.03748500
H	-7.35457400	-0.01087100	-0.36945600

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P3'-TS E =-1379.754228

Al	-1.21950700	0.16502900	0.34562100
C	-0.59668200	1.65404100	1.58044400
H	-1.30536400	1.55912000	2.41512400
C	-0.65615900	2.93863600	0.82573100
C	0.63014900	3.37677400	0.61910800
C	-2.43729200	-1.24732500	1.03049700
C	-3.42623300	-0.40387100	-1.09165300
C	-3.49818500	-1.25728100	0.15377900
C	-2.36327500	0.43304200	-1.25040900
C	-4.77379600	-2.03765500	0.38025800
H	-5.00781100	-2.68414400	-0.47451100
H	-4.72361300	-2.66496700	1.27196000
C	1.53934700	2.46645700	1.29642000
H	2.62079200	2.57660300	1.30846200
C	0.83842000	1.47708700	1.92469900
C	-4.54756900	-0.55898000	-2.10143200
H	-5.53428300	-0.37829600	-1.65626600
H	-4.43390600	0.12879900	-2.94177000
C	-2.42259600	-2.00728100	2.33490400
H	-1.40073100	-2.28146000	2.62649600
H	-2.81097600	-1.38413500	3.15547600
C	-2.19279300	1.32039400	-2.46218800

H	-3.13491700	1.75337300	-2.82490300
H	-1.51270300	2.15445300	-2.25859600
N	0.29950600	-1.12522700	-0.27869100
N	-0.28328000	-2.24490900	-0.56090900
N	-1.24192100	-2.88172500	-0.48218200
C	1.38044300	0.43181000	2.85600600
H	2.47400800	0.38859200	2.81011800
H	1.10151300	0.64311600	3.89903300
H	0.99976300	-0.57281000	2.63195500
C	-1.94302500	3.62243300	0.45725200
H	-2.44385800	4.03044100	1.34813000
H	-1.78170100	4.45850400	-0.23152100
H	-2.65655000	2.93763700	-0.01795400
C	1.08912300	4.59693000	-0.13156300
H	0.25322200	5.15237100	-0.56843200
H	1.63454600	5.28831900	0.52563500
H	1.77497000	4.33730000	-0.94996500
H	-1.76036100	0.76505800	-3.30928700
H	-4.57416000	-1.57620300	-2.51614000
H	-5.63062600	-1.36060800	0.50083100
H	-3.01251000	-2.93271700	2.32913500
C	1.73313400	-1.10016600	-0.46409300
C	2.54807200	-2.02793000	0.21537900
C	2.28448100	-0.11667300	-1.30311000
C	3.93155600	-1.94545900	0.03309500
C	3.67530300	-0.07422600	-1.44197100
C	4.51783400	-0.97329100	-0.78296500
H	4.56720700	-2.66034100	0.55154200
H	4.10859600	0.68041500	-2.09472300
C	1.97440300	-3.10121700	1.11183200
H	1.51369300	-3.91616200	0.53864600
H	2.76229200	-3.54356100	1.72840500
H	1.20512700	-2.70528500	1.78365600
C	1.41622200	0.85885700	-2.05626800
H	0.60830400	0.35041100	-2.59177100
H	0.95538800	1.59210500	-1.38247700
H	2.01053800	1.41529100	-2.78760700
C	6.01896100	-0.88491900	-0.92904800
H	6.46113100	-0.28707800	-0.12083400
H	6.48547100	-1.87534300	-0.89130900
H	6.30189700	-0.41227100	-1.87538000

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P3'-IN1 E= -1379.795872

Al	-1.01602800	0.18145900	0.40457000
C	-1.26523300	-1.13998800	1.98836200
H	-2.31897800	-1.18443100	2.25450900
C	-0.34058400	-0.12156600	2.52125600
C	0.96386300	-0.64620200	2.37628500
C	-2.21477400	-0.64231300	-1.67211800
C	-3.30723900	1.24586900	-0.49766800
C	-3.25861700	-0.19097600	-0.91178900
C	-2.24000600	1.70834200	0.20172700
C	-4.41517600	-1.06654300	-0.47523200
H	-5.30195700	-0.86042300	-1.09043900
H	-4.20578500	-2.13430500	-0.56387200
C	0.86512300	-1.94826000	1.82283700
H	1.71502400	-2.56940900	1.55910000
C	-0.47388600	-2.27796500	1.60860900
C	-4.55631300	2.00923700	-0.88721900
H	-5.46352500	1.50952400	-0.52395100
H	-4.55949000	3.02901900	-0.49606900
C	-2.03030900	-2.07231000	-2.14178800
H	-0.97176700	-2.34397800	-2.11528100
H	-2.58337700	-2.79375700	-1.53916200
C	-2.10014800	3.14322100	0.65484100
H	-3.04909000	3.69234800	0.68497200
H	-1.65067600	3.21390900	1.65198300
N	0.28200300	0.10578700	-0.95963600
N	-0.19035800	0.47096600	-2.19336400
N	-1.39435700	0.23753200	-2.47333000
C	-1.01154000	-3.58950100	1.10553300
H	-0.40516300	-4.00587400	0.29269900
H	-1.02416800	-4.33745200	1.91031200
H	-2.04015700	-3.49172800	0.74332400
C	-0.75469900	1.01811100	3.42166700
H	-0.80333700	0.68484300	4.46840500
H	-0.05030200	1.85704500	3.38329400
H	-1.74593300	1.40368300	3.16134700
C	2.24332700	0.01909000	2.80168000
H	2.17662700	1.11078600	2.75031100
H	2.49386900	-0.24099500	3.84018200
H	3.08321600	-0.29121500	2.17242800
H	-1.43329300	3.69590500	-0.02168500
H	-4.64310100	2.06963000	-1.98036400
H	-4.69317300	-0.85837500	0.56475500
H	-2.36565800	-2.16021200	-3.18214600
C	1.71546000	0.24342400	-0.88680900

C	2.52807200	-0.85175700	-1.24063800
C	2.30131900	1.46469000	-0.50334600
C	3.91748900	-0.71812700	-1.15723200
C	3.69661700	1.55633800	-0.44189400
C	4.52482800	0.47700900	-0.75891100
H	4.54197600	-1.56886600	-1.42416400
H	4.14583500	2.50255300	-0.14597900
C	1.92446200	-2.14556700	-1.72988500
H	1.41020900	-2.00306100	-2.68819900
H	2.69843500	-2.90601900	-1.87551300
H	1.18691100	-2.53396800	-1.02042000
C	1.45695800	2.67486500	-0.18526600
H	0.75570900	2.89408500	-0.99694400
H	0.86056600	2.53579400	0.72591400
H	2.08684900	3.55638500	-0.02954300
C	6.03003800	0.60769700	-0.71557400
H	6.50594400	-0.33060300	-0.40945300
H	6.43572600	0.86865800	-1.70245300
H	6.34519000	1.39064300	-0.01757700

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P3'-TS(1-2) E= -1379.793748

Al	-0.91850000	0.36819500	0.16365600
C	-1.54745200	0.86424600	2.14426500
H	-2.59951700	0.72483700	2.36810400
C	-0.97491900	2.07364800	1.58761900
C	0.43805900	1.92230800	1.63250800
C	-2.04248200	-1.90394900	-0.46247200
C	-3.15920500	0.10868500	-1.35510400
C	-3.11897800	-1.06373500	-0.43018500
C	-2.11709600	0.97388500	-1.28479900
C	-4.31706300	-1.27223900	0.47264400
H	-5.14863000	-1.72001600	-0.08923600
H	-4.10982400	-1.93275300	1.31734300
C	0.72435600	0.68030000	2.27048500
H	1.71900500	0.27366300	2.41051100
C	-0.47276600	0.03671000	2.61431300
C	-4.37087600	0.20142100	-2.26022700
H	-5.30679800	0.14166700	-1.68997900
H	-4.39106900	1.12967000	-2.83595700
C	-1.85623500	-3.12449400	0.41739800
H	-0.80763100	-3.22574200	0.71126900
H	-2.46523600	-3.09433300	1.32297000
C	-1.98266700	2.17522500	-2.19364300

H	-2.93929700	2.53610000	-2.59228900
H	-1.50439500	3.02124700	-1.68680800
N	0.41992000	-0.75687300	-0.56523600
N	0.01455500	-1.56658100	-1.59531500
N	-1.16590700	-1.99744100	-1.60672500
C	-0.62785800	-1.22962200	3.40967500
H	0.25285800	-1.87446000	3.32983400
H	-0.76237900	-0.99683500	4.47504400
H	-1.50200900	-1.81026300	3.09801100
C	-1.75770000	3.30633700	1.22559500
H	-1.99992500	3.88464800	2.12793700
H	-1.19811400	3.96886300	0.55773300
H	-2.70227100	3.05490200	0.73174400
C	1.46467700	2.94042500	1.21291500
H	1.07742700	3.62981200	0.45523600
H	1.78018500	3.55006200	2.07067200
H	2.35957500	2.46104000	0.80400300
H	-1.34873800	1.93599900	-3.05902200
H	-4.38079800	-0.63376700	-2.97367700
H	-4.67922000	-0.31662300	0.86983700
H	-2.12399000	-4.02616800	-0.14676200
C	1.84862400	-0.56073500	-0.59668200
C	2.68486400	-1.46634000	0.08626300
C	2.41383400	0.49644400	-1.33629900
C	4.06746800	-1.25511100	0.07612400
C	3.80316400	0.66828600	-1.32299100
C	4.64912100	-0.18543000	-0.61046900
H	4.70723100	-1.95557200	0.60988500
H	4.23399500	1.48433800	-1.90024200
C	2.11783000	-2.67621000	0.78815800
H	1.66355500	-3.37043300	0.07074400
H	2.90167400	-3.21689600	1.32808300
H	1.33587400	-2.39914000	1.50152400
C	1.55618100	1.41003100	-2.17740200
H	0.94032000	0.83636100	-2.87786400
H	0.87099100	2.01393400	-1.57071800
H	2.17792500	2.10248100	-2.75356500
C	6.14289400	0.04157100	-0.58044000
H	6.69098400	-0.90403200	-0.50556000
H	6.48718500	0.56178700	-1.48080900
H	6.43693500	0.65541800	0.28192000

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P3'-IN2 E= -1379.801018

Al	0.73865000	0.06393000	-0.06956900
C	2.16332200	1.30655900	-1.93744100
H	3.02704400	0.83029000	-2.39103700
C	2.19303000	2.47511000	-1.16886700
C	0.86245300	2.76559900	-0.75792900
C	1.41582800	-2.44640100	-0.00790500
C	2.79776500	-0.89641100	1.36000600
C	2.60262800	-1.79897600	0.17950600
C	2.00064000	0.19785900	1.42097500
C	3.79632200	-1.95671700	-0.73930000
H	4.56358100	-2.57790300	-0.25695200
H	3.55084400	-2.43292300	-1.69058100
C	0.01115900	1.76196000	-1.27305800
H	-1.07383200	1.78459400	-1.26940900
C	0.82107300	0.80882900	-2.03338400
C	3.91173900	-1.28369000	2.31022200
H	4.88115900	-1.32593000	1.79641800
H	4.01100700	-0.58653800	3.14502800
C	1.09860600	-3.35270600	-1.18291900
H	0.03987800	-3.27832700	-1.44342200
H	1.68695100	-3.11397400	-2.07120000
C	2.08004400	1.24168400	2.50804200
H	2.91300000	1.09518300	3.20534900
H	2.18616300	2.24560400	2.07809200
N	-0.79686200	-0.95844000	0.35329700
N	-0.61572600	-2.06392300	1.14334200
N	0.47468300	-2.68518800	1.06006300
C	0.29337100	-0.07567700	-3.14197200
H	-0.67566800	-0.51474900	-2.88516700
H	0.15367400	0.50358500	-4.06476000
H	0.98338700	-0.89563800	-3.37034600
C	3.41983800	3.25657000	-0.78761600
H	3.30271600	4.32547300	-1.00907100
H	3.64890600	3.17654800	0.28369600
H	4.29826100	2.90077000	-1.33643000
C	0.43585800	3.94146700	0.07678000
H	0.91118300	3.95403100	1.06634000
H	0.70720500	4.88615600	-0.41328800
H	-0.64843700	3.94896000	0.22800200
H	1.15889900	1.26112800	3.10524700
H	3.72797000	-2.28286500	2.72625100
H	4.25698500	-0.98439700	-0.94908600
H	1.29390000	-4.39685000	-0.90947700
C	-2.16794600	-0.51658000	0.34299100

C	-3.09607500	-1.15829300	-0.50526200
C	-2.59020700	0.54092400	1.17307900
C	-4.41230900	-0.68993700	-0.54833100
C	-3.91736800	0.97938100	1.09302000
C	-4.84449400	0.38470300	0.23499200
H	-5.12076300	-1.18362200	-1.21114400
H	-4.23577100	1.79975100	1.73344000
C	-2.70301800	-2.35194000	-1.34303100
H	-1.87582200	-2.12063300	-2.02333500
H	-2.37427200	-3.18647200	-0.71308100
H	-3.54898800	-2.69698500	-1.94561100
C	-1.65514700	1.17855400	2.17264000
H	-1.16788600	0.42135500	2.79583900
H	-0.86057300	1.76115900	1.69000800
H	-2.20183000	1.86176600	2.83035700
C	-6.27928500	0.85674000	0.18239400
H	-6.66398500	0.85874800	-0.84392000
H	-6.93621000	0.20256800	0.77124800
H	-6.38276500	1.87024600	0.58370900

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P3'-TS(2-3) E=-1379.689193

Al	-1.15392500	-0.55913100	-0.08226800
C	-2.27038700	-1.32485600	-1.87532500
H	-2.58208100	-0.66291000	-2.67577700
C	-3.11440800	-1.82136000	-0.83223700
C	-2.33788100	-2.68189800	-0.02529000
C	-0.60852400	2.60987900	-0.63196600
C	-2.04136800	1.74042100	1.23601300
C	-1.83656000	2.30664100	-0.14815400
C	-1.96220700	0.40623000	1.42938300
C	-3.12932000	2.62730200	-0.87525500
H	-3.68289000	3.42271700	-0.35755900
H	-2.98405500	2.94481900	-1.90973800
C	-1.01035600	-2.71238100	-0.56816700
H	-0.18863500	-3.31417500	-0.19585000
C	-0.97647300	-1.92488000	-1.76134900
C	-2.39127300	2.79580100	2.26937700
H	-3.29279000	3.35392400	1.98266500
H	-2.56312700	2.38132200	3.26521300
C	-0.32822500	3.32167300	-1.93804500
H	0.18984800	2.66252300	-2.64413800
H	-1.22928100	3.70260300	-2.42204300
C	-2.24399500	-0.26916800	2.75565600

H	-2.50941000	0.42624100	3.55975400
H	-3.07067800	-0.98546100	2.66370300
N	0.58293500	0.09512200	-0.00769200
N	1.02438800	1.28185400	0.36748300
N	0.60790400	2.46083800	0.11858300
C	0.16080800	-1.82477000	-2.73856400
H	1.12999000	-1.76461300	-2.23347000
H	0.17826200	-2.70692600	-3.39225400
H	0.05798900	-0.94372100	-3.38017000
C	-4.55276300	-1.43932900	-0.61231200
H	-5.21417500	-2.31129400	-0.69205000
H	-4.71682200	-0.99347200	0.37646300
H	-4.88149300	-0.71067400	-1.36048800
C	-2.80775200	-3.46912700	1.16707800
H	-3.68755800	-3.01697900	1.63566500
H	-3.08629100	-4.49014600	0.87236800
H	-2.02822300	-3.55587600	1.93162100
H	-1.37705300	-0.84838500	3.10257700
H	-1.57743400	3.52827400	2.34253600
H	-3.78498000	1.74808600	-0.88188600
H	0.34173400	4.16651600	-1.74265400
C	2.29758600	0.26682300	0.23431500
C	3.11271600	0.38527900	-0.91642100
C	2.81643600	-0.26344800	1.44840300
C	4.42617100	-0.09725600	-0.83044000
C	4.12631100	-0.72523300	1.45154200
C	4.96200600	-0.66676700	0.32368400
H	5.05138500	-0.01074400	-1.71813100
H	4.51457900	-1.14141500	2.38052800
C	1.95068900	-0.32293900	2.67340400
H	1.49294400	0.65422700	2.88015000
H	1.12012800	-1.03199200	2.54916600
H	2.53015400	-0.62722500	3.55054300
C	2.63731500	1.07509000	-2.17066400
H	1.68996400	0.66796100	-2.53867000
H	2.48489300	2.14918400	-1.99952300
H	3.37859900	0.96817300	-2.96895900
C	6.37560200	-1.19763900	0.36862700
H	6.40316500	-2.29275700	0.45998500
H	6.92680300	-0.93393800	-0.54070400
H	6.93608400	-0.79438300	1.22224900

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P3'-IN3 E=-1379.777337

Al	-1.30107000	-0.45022400	0.05249300
C	-3.69590300	-0.98306200	-0.79043600
H	-4.17234000	-0.40076800	-1.57296600
C	-4.10996700	-1.03744700	0.55219900
C	-3.22377300	-1.89693900	1.24928100
C	-0.08293300	1.43929300	-1.78196700
C	-1.23590500	2.25838100	0.28533000
C	-1.17129000	2.00436300	-1.20097700
C	-1.49368300	1.19937800	1.08841900
C	-2.39164600	2.47789100	-1.96556300
H	-2.49832500	3.56683900	-1.87348800
H	-2.36131600	2.24359300	-3.03149000
C	-2.25066100	-2.37047300	0.32943100
H	-1.51731600	-3.14709200	0.52037500
C	-2.54151900	-1.80555800	-0.98282900
C	-1.09911000	3.71154700	0.69454300
H	-1.90108500	4.32719700	0.26534900
H	-1.12489300	3.84817700	1.77810600
C	0.06461900	1.10597400	-3.25295700
H	0.38086200	0.06178000	-3.36851800
H	-0.85362200	1.24570900	-3.82644100
C	-1.69343300	1.29313100	2.58401600
H	-1.56642900	2.30376800	2.98973800
H	-2.70205600	0.95729400	2.85906000
N	0.47712200	-0.80350800	-0.20407100
N	1.31969600	0.11673100	-0.48222600
N	1.16349600	1.24957600	-1.11448000
C	-2.01069200	-2.32380200	-2.29894300
H	-0.94552900	-2.57145100	-2.23698800
H	-2.54514200	-3.23385500	-2.60386600
H	-2.13564300	-1.58548200	-3.09888700
C	-5.24518700	-0.26090100	1.16072500
H	-5.90787100	-0.90847400	1.74939400
H	-4.89424800	0.53319100	1.83411300
H	-5.85473000	0.21585900	0.38558200
C	-3.29060000	-2.24386000	2.71121700
H	-3.26977500	-1.35634400	3.35588700
H	-4.21924800	-2.78229800	2.94424100
H	-2.45467800	-2.88746400	3.00428400
H	-0.99818300	0.63428600	3.12231800
H	-0.15206500	4.12280000	0.32224100
H	-3.30123400	2.03543200	-1.54174700
H	0.85109100	1.72960400	-3.69408900
C	2.71308600	-0.10454000	-0.05838100

C	3.21304900	0.61305900	1.03438000
C	3.47720000	-1.04530300	-0.76122200
C	4.53028100	0.34987300	1.42766400
C	4.78938300	-1.26194900	-0.32979200
C	5.33311500	-0.58257500	0.76510200
H	4.93698600	0.89620100	2.27624800
H	5.40117200	-1.98339600	-0.86757600
C	2.38940000	1.64825900	1.76081300
H	2.22750400	2.53100100	1.13289700
H	1.39939100	1.26413000	2.02743600
H	2.89443700	1.96330000	2.67900100
C	2.92074500	-1.79997700	-1.94346300
H	2.10376600	-2.46151000	-1.63664200
H	2.51633100	-1.11452200	-2.69810800
H	3.70050800	-2.40308100	-2.41798500
C	6.74167100	-0.86687700	1.23379200
H	7.18616800	0.00773300	1.72081300
H	6.76075900	-1.68916700	1.96183600
H	7.39098100	-1.15698700	0.40061100

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P3'-TS(3-4) E=-1379.690435

Al	1.76737700	-0.38502800	-0.30739100
C	3.92916600	-1.36729300	-0.88407300
H	4.48623100	-1.11741700	-1.78042000
C	2.84520400	-2.29815200	-0.83641600
C	2.35511200	-2.30850000	0.51020800
C	-0.45437100	1.54876400	1.19920600
C	1.45466500	2.33611900	-0.26096800
C	0.83135400	1.97427100	1.06825000
C	2.09279400	1.41086700	-1.00751200
C	1.60666200	2.43795400	2.29119300
H	1.42587900	3.50171700	2.50651000
H	1.34204900	1.87791200	3.19342400
C	3.10821500	-1.32116600	1.23739400
H	2.98697600	-1.10463200	2.29327000
C	4.10584600	-0.77262600	0.38055900
C	1.31183600	3.81637800	-0.57329900
H	1.77246500	4.43817800	0.20646800
H	1.76320400	4.09375100	-1.52866500
C	-1.20718300	1.61020000	2.51682700
H	-0.77206200	0.94181700	3.26905100
H	-1.17436400	2.62446200	2.93207700
C	2.80231200	1.70529100	-2.30964400

H	2.87771100	2.77220200	-2.55016000
H	3.82335300	1.30194100	-2.29644200
N	-0.01654800	-0.70434600	-0.67167600
N	-0.97221000	0.09401300	-0.71817400
N	-1.24621500	1.19914200	0.08104600
C	5.07787200	0.32082100	0.72910800
H	5.32796800	0.30319800	1.79571800
H	6.01098900	0.20692300	0.16632100
H	4.67504500	1.31602900	0.49874500
C	2.40148700	-3.21364400	-1.94767800
H	2.80627300	-4.22561100	-1.81234200
H	1.31038600	-3.29703300	-1.99546700
H	2.74998000	-2.84796400	-2.91916700
C	1.37206200	-3.28571000	1.09126700
H	0.55055800	-3.49903700	0.40068000
H	1.86999500	-4.23853200	1.31844800
H	0.93966900	-2.91181900	2.02467000
H	2.29418500	1.21664900	-3.15352600
H	0.24933700	4.09035000	-0.60847400
H	2.68357200	2.32468800	2.12651200
H	-2.25363300	1.33225700	2.38043700
C	-2.57841900	0.08217500	-0.22617000
C	-3.51801500	0.64063600	-1.13658600
C	-2.95682000	-0.90726200	0.70588300
C	-4.83585000	0.21516000	-1.05793200
C	-4.30806100	-1.29645600	0.71463000
C	-5.26782900	-0.75245100	-0.13283800
H	-5.55503600	0.64686500	-1.75249100
H	-4.60277000	-2.06786500	1.42433000
C	-3.07114000	1.65406700	-2.15002200
H	-2.70525100	2.56747200	-1.66568800
H	-2.23116100	1.26427500	-2.74140600
H	-3.88743900	1.91677400	-2.83007100
C	-1.98308500	-1.59921200	1.62399200
H	-1.07880000	-1.89998700	1.08259200
H	-1.65981800	-0.96927000	2.45949700
H	-2.44202500	-2.49580100	2.05307900
C	-6.71507100	-1.18022000	-0.07313400
H	-6.85165800	-2.02547900	0.60983700
H	-7.36673800	-0.36743700	0.27582900
H	-7.08861600	-1.48595800	-1.05893800

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P3'-IN4 E=-1270.331818

Al	2.12603400	0.15585100	0.08944800
C	3.83274100	-0.68762000	1.29138800
H	4.37661600	-0.09898000	2.02215000
C	4.22602000	-0.88238000	-0.07319500
C	3.26757200	-1.73015100	-0.67901800
C	-0.68432500	0.84530200	0.88543300
C	0.99484000	2.09275700	-0.58038000
C	0.69320300	1.42703100	0.77943800
C	1.95402400	1.46327900	-1.31056200
C	1.08355800	2.32504400	1.97366700
H	0.40550800	3.18356200	2.10046300
H	1.08733000	1.77960300	2.92368500
C	2.28748400	-2.05693600	0.31725200
H	1.43478000	-2.70939100	0.16787700
C	2.66313500	-1.45809800	1.55635600
C	0.24360200	3.34828200	-0.95331800
H	0.32717200	4.10760900	-0.16470100
H	0.60501400	3.79107100	-1.88622500
C	-1.20863100	0.52641100	2.27840500
H	-0.45034100	0.01976000	2.88393600
H	-1.46959000	1.45082600	2.80936500
C	2.47227500	1.86427500	-2.66217000
H	2.04459200	2.80254900	-3.03955000
H	3.56408900	1.98452500	-2.65146600
N	-1.36450000	0.61490800	-0.18647700
C	1.99345900	-1.64984000	2.88774200
H	0.93728700	-1.91223700	2.77178700
H	2.47322200	-2.46524600	3.44519300
H	2.05525400	-0.75024400	3.50951800
C	5.43172800	-0.27307700	-0.73394200
H	6.24348700	-1.00682900	-0.82627500
H	5.20821800	0.09139900	-1.74283500
H	5.81746200	0.57050000	-0.15234100
C	3.25575200	-2.19501500	-2.10930700
H	3.53299500	-1.39310300	-2.80282200
H	3.96555900	-3.01869800	-2.26289300
H	2.26437800	-2.55810000	-2.39876300
H	2.25628600	1.08826300	-3.40941500
H	-0.82098500	3.11911500	-1.07345600
H	2.09116600	2.73485400	1.83471600
H	-2.10179300	-0.10032100	2.22830300
C	-2.65281300	0.04434400	-0.19002900
C	-3.80190100	0.85156500	-0.02767400
C	-2.80430900	-1.32810400	-0.49038300

C	-5.06611100	0.26560000	-0.14444000
C	-4.08836900	-1.86909400	-0.59432900
C	-5.23879200	-1.09263400	-0.42621700
H	-5.94430000	0.89602200	-0.01246800
H	-4.19008100	-2.93023800	-0.81792900
C	-3.67340300	2.33026400	0.25104200
H	-3.19707200	2.53361500	1.21868700
H	-3.06025000	2.82638000	-0.51088700
H	-4.65701800	2.81105600	0.26120900
C	-1.58663900	-2.19566200	-0.69409800
H	-0.90028700	-1.74199200	-1.41972000
H	-1.01862200	-2.32726600	0.23725500
H	-1.86788100	-3.19102500	-1.05386800
C	-6.61795500	-1.69252300	-0.58030200
H	-7.36017000	-1.15084900	0.01685200
H	-6.95914200	-1.66225100	-1.62456600
H	-6.63668100	-2.74249700	-0.26644300

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P3'-TS(4-Pa') E =-1270.330265

Al	2.04271200	0.06717000	0.05727500
C	3.74134700	-1.20869200	0.82477600
H	4.33796600	-0.91819600	1.68261900
C	4.07971600	-0.95554600	-0.54365700
C	3.04931600	-1.49919600	-1.34809200
C	-0.64406800	0.64148700	1.22327400
C	1.10929300	2.19560800	0.22336200
C	0.79059000	1.10430500	1.27139300
C	1.95124200	1.80184000	-0.76887600
C	1.30188400	1.48194000	2.67468800
H	0.74971300	2.31640200	3.13431800
H	1.24861600	0.64153400	3.37649500
C	2.07830100	-2.08635200	-0.46925100
H	1.18597900	-2.61228400	-0.78725900
C	2.52882000	-1.95443100	0.87974600
C	0.49323000	3.56288300	0.41274200
H	0.80797300	4.00499100	1.36748900
H	0.76665500	4.26155200	-0.38372100
C	-1.36916700	0.40078200	2.53753300
H	-0.85722100	-0.36759600	3.12962700
H	-1.37625300	1.31072500	3.14890900
C	2.44265300	2.63042100	-1.92080000
H	2.08586200	3.66897000	-1.90524400
H	3.54043500	2.66405500	-1.94676800

N	-1.20004400	0.45582900	0.07298900
C	1.87672600	-2.51917300	2.11075000
H	0.79258900	-2.60818500	1.98936600
H	2.26514500	-3.52312500	2.32757600
H	2.07043300	-1.89673400	2.99088900
C	5.29987000	-0.22130700	-1.02713700
H	6.04821100	-0.91853300	-1.42680400
H	5.06135300	0.49048500	-1.82560400
H	5.77364900	0.33713400	-0.21328700
C	2.96507300	-1.45795300	-2.84913200
H	3.22014300	-0.46924600	-3.24785100
H	3.65595300	-2.18015200	-3.30394600
H	1.95624200	-1.70521100	-3.19462000
H	2.12674600	2.19363500	-2.87810200
H	-0.60036000	3.49166900	0.43934000
H	2.35320600	1.79076000	2.62735500
H	-2.39995900	0.08277400	2.37008300
C	-2.53284400	0.03180600	-0.10797400
C	-3.49055700	0.97380900	-0.55354700
C	-2.90185200	-1.32734000	0.00517600
C	-4.78982000	0.54833900	-0.83564900
C	-4.21559400	-1.70671700	-0.29415300
C	-5.18244700	-0.78853900	-0.70768800
H	-5.51589100	1.28602100	-1.17462100
H	-4.48507500	-2.75811700	-0.20499600
C	-3.10681400	2.42282600	-0.72506100
H	-2.93474900	2.91667500	0.24089800
H	-2.17591400	2.51629900	-1.29555100
H	-3.89491500	2.97915900	-1.24315000
C	-1.89473300	-2.37353400	0.41726000
H	-0.97733700	-2.29173200	-0.17654500
H	-1.60147200	-2.27780400	1.47138300
H	-2.30133700	-3.38107500	0.28205500
C	-6.60267700	-1.21721500	-0.99778800
H	-7.27478200	-0.98691200	-0.15944900
H	-7.00546000	-0.70625600	-1.88032700
H	-6.66603400	-2.29599900	-1.17741700

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Pa' E = -1270.36593845

C	-0.22873300	-2.12863700	-0.85656500
H	0.77298100	-1.98979800	-1.24602800
C	-0.53776100	-2.39786600	0.54760800
C	-1.90841300	-2.79960300	0.58539700

C	-2.41672200	-2.76282400	-0.72593400
H	-3.44987100	-2.95332100	-0.99783800
C	-1.40908100	-2.35336500	-1.62428500
Al	-1.02147500	-0.34054200	-0.05873300
C	-2.51172600	2.02322600	0.23441500
C	-1.30614200	2.80306300	-0.07080600
C	-0.01796300	2.31303100	-0.13379600
C	-2.63381500	0.64718700	0.23577700
N	0.29942500	0.95164900	-0.05944200
C	-1.50165100	4.29205400	-0.34259100
H	-1.45533900	4.91715300	0.56338600
H	-0.75127900	4.68186000	-1.03466700
H	-2.47166400	4.48555800	-0.80858200
C	1.13962900	3.28653900	-0.30113200
H	1.25892700	3.60159900	-1.34763300
H	0.98648800	4.19285400	0.29027100
H	2.08756900	2.84597600	0.00917300
C	-3.74424500	2.85714600	0.58884800
H	-4.33503500	3.11360200	-0.30267100
H	-4.41015300	2.31691600	1.26425200
H	-3.47846200	3.79675700	1.07951900
C	-3.99106400	0.02872000	0.54128500
H	-4.31123700	0.20854400	1.57933700
H	-4.78532700	0.43162300	-0.10322500
H	-3.98608700	-1.05167800	0.39729900
C	-2.66338200	-3.21006800	1.81987900
H	-2.26152500	-4.14082800	2.24324600
H	-2.61201300	-2.45124800	2.61042500
H	-3.72095700	-3.38103800	1.59504800
C	-1.54492900	-2.21240700	-3.11660600
H	-1.47186600	-3.19094200	-3.61032700
H	-2.51048200	-1.77847000	-3.40024600
H	-0.75659000	-1.57928100	-3.53749900
C	0.47691300	-2.66369200	1.63489200
H	0.09303000	-2.40470700	2.62826700
H	0.73977900	-3.73085800	1.65902800
H	1.40278000	-2.10445700	1.47664300
C	1.68010100	0.55547300	0.00806500
C	2.30499200	0.41936200	1.26842600
C	2.40438300	0.27178100	-1.16859200
C	3.62725900	-0.03273600	1.32773700
C	3.72312000	-0.18870800	-1.05944100
C	4.35391000	-0.35316700	0.17562700
H	4.10151300	-0.13672100	2.30219000

H	4.27398200	-0.41601900	-1.97032000
C	1.80170300	0.49703100	-2.53593100
H	1.63988400	1.56462700	-2.72948000
H	2.46259000	0.11377800	-3.31989300
H	0.82580600	0.01285300	-2.64334700
C	1.56886600	0.77925000	2.53811900
H	1.23219100	1.82234800	2.52655100
H	0.66983300	0.16782100	2.67722900
H	2.21137500	0.63853900	3.41293800
C	5.78448500	-0.83238900	0.26817500
H	6.46704300	-0.00958400	0.51923400
H	5.90313600	-1.59605900	1.04576800
H	6.12377300	-1.26230900	-0.67984000

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P3'-TS(1-5) E=-1379.742291

Al	-1.18777800	-0.32385300	0.08696000
C	-3.71069500	-1.59819700	-0.76160100
H	-4.39525900	-1.41287900	-1.58271800
C	-3.85115900	-1.05352300	0.55023200
C	-2.75082600	-1.46912500	1.31896100
C	-1.51642200	1.23080700	-1.16044600
C	-0.37757900	2.22791400	0.79800300
C	-1.25486000	2.43144600	-0.22291000
C	0.08888300	0.81607400	1.00733400
C	-1.87459300	3.75400200	-0.59604100
H	-1.56267200	4.06429000	-1.60181800
H	-2.96953700	3.68615500	-0.61486800
C	-1.86614700	-2.23274200	0.43047800
H	-1.12507400	-2.93654000	0.79377100
C	-2.53462400	-2.33423800	-0.85443300
C	0.07827400	3.29739100	1.76853500
H	-0.27164300	3.08463900	2.78771300
H	1.17219100	3.35283300	1.82278400
C	-2.76002600	1.36213000	-2.03872900
H	-2.85643700	0.49105400	-2.69326200
H	-3.66934500	1.41652200	-1.43089000
C	0.97117000	0.53980700	2.20331600
H	0.40135700	0.79386800	3.10612500
H	1.23911500	-0.51816700	2.28188800
N	0.85193500	0.17501700	-0.42310100
N	0.76879800	0.89645600	-1.69759800
N	-0.33938000	1.30873600	-2.06114400
C	-2.04645800	-3.10281200	-2.05191600

H	-1.01938700	-2.84044600	-2.33349500
H	-2.05795200	-4.18469700	-1.86211100
H	-2.68383600	-2.91342200	-2.92172600
C	-5.01021100	-0.21861900	1.02288500
H	-5.83234100	-0.84894300	1.38954800
H	-4.72687800	0.44979400	1.84317400
H	-5.41596700	0.39915600	0.21401500
C	-2.57145300	-1.33590100	2.80903000
H	-3.00291300	-0.40557000	3.19507800
H	-3.06239700	-2.16498400	3.33805600
H	-1.51401000	-1.35233400	3.09567800
H	1.90454500	1.11741200	2.23004500
H	-0.28477500	4.29179900	1.50307000
H	-1.61069700	4.55594800	0.09612500
H	-2.71762300	2.25087400	-2.68012500
C	2.24932800	-0.18938700	-0.25988200
C	2.60948900	-1.54153600	-0.09781300
C	3.25782000	0.80421500	-0.29150000
C	3.95989900	-1.87562900	0.06347000
C	4.59056700	0.41746300	-0.12174100
C	4.96944500	-0.91408500	0.06425700
H	4.22388300	-2.92452100	0.18312100
H	5.35811900	1.18915000	-0.14303400
C	1.59601300	-2.65864200	-0.09999200
H	1.06236200	-2.72582800	0.85630400
H	0.84532700	-2.52640600	-0.88375600
H	2.08959800	-3.62226800	-0.26110400
C	2.97502400	2.26905800	-0.53873600
H	2.94602900	2.47961300	-1.61356600
H	2.01432300	2.58975100	-0.13434600
H	3.76138800	2.88828400	-0.09314900
C	6.41737200	-1.29295800	0.27045500
H	6.58767800	-2.35341200	0.05706000
H	7.08131900	-0.70708500	-0.37522600
H	6.73375800	-1.11249300	1.30674000

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P3'-IN5 E=-1379.752673

Al	-1.64269200	-0.34423100	-0.08010500
C	-3.49368400	-1.60067100	-0.59351800
H	-3.95558200	-1.52070600	-1.57060500
C	-3.78379600	-0.75919100	0.51835200
C	-2.90947500	-1.14881400	1.59050600
C	-1.51444500	1.00307900	-1.53833800

C	-0.58608900	1.87066100	0.57940200
C	-1.34085400	2.13480700	-0.53411600
C	0.07015600	0.49936100	0.58867100
C	-2.05268300	3.44260100	-0.79655900
H	-1.74598400	3.85236200	-1.76741400
H	-3.14140200	3.31645300	-0.84515500
C	-2.09461500	-2.21617200	1.10533500
H	-1.32037700	-2.71690300	1.67541200
C	-2.44094100	-2.49438300	-0.25098400
C	-0.42848400	2.79463200	1.76444100
H	-0.73765600	2.30368100	2.69603500
H	0.61823700	3.09225600	1.90805200
C	-2.60849400	1.20929000	-2.58397400
H	-2.71175300	0.30547600	-3.19369100
H	-3.58464400	1.41854000	-2.13117100
C	0.66587100	0.05061500	1.92033400
H	-0.09454100	0.08376300	2.70751800
H	1.02711000	-0.98127900	1.86522400
N	1.11469300	0.40944900	-0.50402900
N	0.83210500	0.37862100	-1.84694500
N	-0.29629800	0.63295900	-2.33184700
C	-1.87714400	-3.58829600	-1.11953000
H	-0.84056600	-3.82143300	-0.85657000
H	-2.46052500	-4.51092300	-1.00334500
H	-1.90118300	-3.31630000	-2.17984900
C	-4.87950000	0.27092000	0.59369900
H	-5.75788900	-0.13231000	1.11502400
H	-4.56786200	1.17155800	1.13437600
H	-5.20240300	0.57661100	-0.40618900
C	-2.94863100	-0.62625400	3.00216300
H	-3.01429500	0.46684500	3.04323800
H	-3.82262600	-1.02206700	3.53625500
H	-2.05868200	-0.93025600	3.56112900
H	1.50919400	0.66829500	2.25645600
H	-1.02066600	3.70783800	1.67340000
H	-1.84250100	4.20086400	-0.03947200
H	-2.37120600	2.03072800	-3.27449800
C	2.48607000	0.06325600	-0.24863200
C	2.91206200	-1.27385600	-0.40933100
C	3.40921700	1.05933800	0.11504100
C	4.24937100	-1.59284200	-0.17140100
C	4.74155200	0.69182500	0.35280700
C	5.18180000	-0.62480000	0.22311200
H	4.57446200	-2.62394300	-0.29980500

H	5.45531100	1.46569700	0.63002100
C	1.94383500	-2.34588500	-0.84780200
H	1.12180100	-2.46280000	-0.12942900
H	1.49420300	-2.09489100	-1.81459700
H	2.44723600	-3.31370600	-0.93904500
C	3.00960100	2.51048900	0.23365100
H	2.15158500	2.74123400	-0.40260500
H	2.73535100	2.77071200	1.26493300
H	3.84211100	3.16382200	-0.04903000
C	6.61931400	-1.00309700	0.49690100
H	6.71124300	-1.58104700	1.42620500
H	7.03163000	-1.62331600	-0.30794900
H	7.25428600	-0.11675500	0.59687400

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P3'-TS(5-6) E=-1379.736032

Al	-1.08435100	-0.22193100	-0.49851800
C	-3.31209800	-1.18080600	-0.63469200
H	-3.94830300	-0.58001300	-1.27610000
C	-3.52511700	-1.43524700	0.71423100
C	-2.51441600	-2.35638900	1.16228300
C	-1.41005400	1.67570300	-1.32174600
C	-0.64796600	2.07251500	1.00505200
C	-1.27693800	2.58629000	-0.08740100
C	-0.15813500	0.63585900	0.96637900
C	-1.81141700	3.99380900	-0.22353900
H	-1.39224200	4.49078200	-1.10946200
H	-2.90280800	4.00629400	-0.34629500
C	-1.69107600	-2.65143400	0.08635700
H	-0.86007700	-3.34831100	0.10534300
C	-2.11412400	-1.89545700	-1.09078700
C	-0.52399600	2.82187800	2.31326800
H	-1.07264800	2.29614800	3.10521800
H	0.51753300	2.88215200	2.64719100
C	-2.61777700	1.96408800	-2.21142300
H	-2.64482700	1.28492300	-3.07112400
H	-3.53619000	1.80656400	-1.63709700
C	0.35025800	0.02141600	2.25798200
H	-0.44604400	0.04172000	3.01163800
H	0.61862900	-1.02881300	2.10871500
N	0.76062800	0.26880800	-0.29399100
N	0.92478600	1.62248500	-1.83495700
N	-0.16335000	1.94580700	-2.08893200
C	-1.95580800	-2.39165700	-2.51944900

H	-0.93919800	-2.74388100	-2.72087600
H	-2.63976900	-3.22789400	-2.71690000
H	-2.18375500	-1.60578200	-3.24961000
C	-4.59046600	-0.82982300	1.58393100
H	-5.18264800	-1.60377100	2.08985800
H	-4.16478000	-0.19288800	2.37126600
H	-5.27977300	-0.21413200	0.99676900
C	-2.36595400	-2.86011800	2.57008100
H	-2.14182800	-2.04932800	3.27661800
H	-3.28664600	-3.34262900	2.92437100
H	-1.55696100	-3.59423900	2.64391300
H	1.22543300	0.52032800	2.69441100
H	-0.91874600	3.83811000	2.26836300
H	-1.57680400	4.62164200	0.63773100
H	-2.63916000	2.98998200	-2.59752100
C	2.12023700	-0.08942300	-0.13533900
C	2.58860700	-1.30471700	-0.70188300
C	3.06587000	0.77968600	0.46871700
C	3.92645800	-1.67152600	-0.54773800
C	4.39513500	0.36297800	0.60109000
C	4.84962600	-0.86720800	0.12650800
H	4.25931200	-2.61380500	-0.97972300
H	5.10389600	1.04278300	1.07173000
C	1.68262600	-2.20276700	-1.50653600
H	0.86285200	-2.60782700	-0.90652400
H	1.23098200	-1.66661000	-2.35045900
H	2.24464000	-3.04876500	-1.91497500
C	2.71996600	2.17888000	0.91984200
H	1.90326900	2.60921400	0.33486900
H	2.42099300	2.21383600	1.97450400
H	3.59315100	2.83195100	0.81659100
C	6.28170500	-1.30701100	0.31861500
H	6.39256400	-1.93618200	1.21270100
H	6.64007900	-1.89467800	-0.53427300
H	6.95111600	-0.44859600	0.44221200

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P3'-IN6 E=-1379.748559

Al	-1.15243600	-0.43095300	-0.11747200
C	-3.36015300	-0.98474600	-0.73107800
H	-3.92745400	-0.36857800	-1.41765300
C	-3.52040700	-1.00572200	0.66998600
C	-2.60743100	-1.96408200	1.19840200
C	-1.12333000	1.41319400	-1.46556800

C	-0.55301800	2.14595300	0.84322700
C	-0.89574600	2.50804000	-0.42704300
C	-0.24221700	0.72517800	1.18858600
C	-1.11947400	3.92410100	-0.91939700
H	-0.61518000	4.09217600	-1.88135300
H	-2.18096500	4.16560200	-1.07732500
C	-1.89611500	-2.52930300	0.11190800
H	-1.16601800	-3.32451000	0.18379200
C	-2.33963300	-1.92139600	-1.11688000
C	-0.63778300	3.13792600	1.98591400
H	-1.43117000	2.82970000	2.67925700
H	0.28670400	3.17705600	2.57112000
C	-2.27323000	1.65570100	-2.45964000
H	-2.41249100	0.79959000	-3.12687900
H	-3.19290900	1.79145600	-1.88568200
C	0.04192300	0.39212400	2.64753400
H	-0.75932700	0.73055200	3.31581000
H	0.13656800	-0.69119500	2.76953000
N	0.59912300	-0.11153900	0.21236000
N	0.96256500	0.89400800	-2.75504000
N	0.03058200	1.15708100	-2.17628100
C	-2.06364400	-2.42306700	-2.51268400
H	-1.05911600	-2.84957000	-2.60099900
H	-2.77765500	-3.20997100	-2.79051100
H	-2.15534200	-1.62769100	-3.26108500
C	-4.44941800	-0.13939600	1.47414300
H	-5.14754400	-0.74642200	2.06498800
H	-3.90861800	0.50433400	2.18012500
H	-5.04548600	0.50937800	0.82396400
C	-2.44632300	-2.32460800	2.64915500
H	-2.33393400	-1.44026800	3.28636400
H	-3.32234600	-2.87750000	3.01481600
H	-1.56841400	-2.95965700	2.80464100
H	0.98025300	0.83171800	3.01945800
H	-0.87823600	4.15186700	1.66120300
H	-0.71877400	4.66814700	-0.22783300
H	-2.12309000	2.55079300	-3.07510600
C	1.98739000	-0.26997100	0.19840000
C	2.94014800	0.74148400	0.51993300
C	2.50574400	-1.52794400	-0.24168700
C	4.30928400	0.44892400	0.46515400
C	3.87961400	-1.75377500	-0.30294200
C	4.81661600	-0.78606900	0.06737300
H	5.00861200	1.24248900	0.72593600

H	4.22765500	-2.72846100	-0.64339100
C	1.58179300	-2.64844700	-0.64022100
H	0.95500300	-2.96638800	0.20069400
H	0.90204400	-2.35859000	-1.45276200
H	2.15249400	-3.51790000	-0.98334900
C	2.56420000	2.16177800	0.87186600
H	2.08249300	2.24349100	1.85190800
H	3.46183400	2.78833200	0.90406100
H	1.87755700	2.59934700	0.14075800
C	6.30051200	-1.06769700	0.03952900
H	6.59607000	-1.59717400	-0.87487900
H	6.88272900	-0.14082200	0.09029100
H	6.61402200	-1.69486300	0.88615600

63

P3'-TS(6-Pa') E=-1379.748165

Al	-0.85358300	-0.27616900	0.16067700
C	-3.84416600	-1.82582300	-0.86145300
H	-4.48485700	-1.95926300	-1.72969300
C	-4.24620900	-1.13705400	0.34960800
C	-3.19711900	-1.17452700	1.23978300
C	-1.35290600	1.29074100	-1.11615500
C	-0.12000900	2.29420300	0.77215300
C	-0.80232900	2.49060300	-0.42571700
C	0.36521100	0.98803700	1.19836200
C	-1.03276300	3.84028100	-1.07486400
H	-0.79615800	3.80149800	-2.14897400
H	-2.07174400	4.19240400	-0.99887900
C	-2.04042600	-1.83175400	0.56536400
H	-1.44714900	-2.53972600	1.15265200
C	-2.56223900	-2.29092200	-0.74809200
C	-0.00146400	3.43975100	1.75977900
H	-0.53905000	3.19336900	2.68338000
H	1.04131500	3.62253800	2.04648700
C	-2.74777200	1.42661600	-1.74072300
H	-3.02575500	0.52729900	-2.29604600
H	-3.46498700	1.54318400	-0.92391800
C	0.94408300	0.81366000	2.59250200
H	0.30756400	1.25152900	3.36964900
H	1.05658600	-0.25118800	2.82215400
N	0.90615300	0.02108200	0.17033100
N	0.39173500	1.03640300	-3.05692700
N	-0.43367400	1.00279900	-2.29250600
C	-1.82266800	-3.14404900	-1.74191700

H	-0.88781400	-2.68857800	-2.09654200
H	-1.54853500	-4.11705900	-1.31128700
H	-2.44489400	-3.33717700	-2.62249200
C	-5.60768400	-0.52802400	0.54134000
H	-5.71483000	-0.05380600	1.52167900
H	-5.82110300	0.23532900	-0.21955300
H	-6.39793300	-1.28592500	0.45475800
C	-3.17138100	-0.71335500	2.67162100
H	-3.14540200	-1.56672300	3.36483700
H	-2.28929000	-0.09920200	2.89555400
H	-4.05501000	-0.11839000	2.92334100
H	1.94421300	1.26259900	2.69872200
H	-0.42684900	4.37121100	1.38245000
H	-0.39107500	4.61714300	-0.65232200
H	-2.83399100	2.29753900	-2.40140400
C	2.26376900	-0.32912700	0.11080800
C	2.64476300	-1.69688200	0.15681100
C	3.28270100	0.64651300	-0.05152400
C	3.99338200	-2.04784700	0.05997100
C	4.62019500	0.24496800	-0.12197300
C	5.00794300	-1.09520200	-0.06502000
H	4.25913200	-3.10346900	0.09754100
H	5.38345600	1.01138700	-0.25098500
C	2.95591400	2.11185800	-0.20485000
H	2.14094400	2.26754600	-0.91937800
H	2.63658600	2.57108600	0.73872900
H	3.83252300	2.66570700	-0.55714400
C	1.61602300	-2.78778000	0.32480100
H	1.00868900	-2.63342300	1.22559200
H	0.91897900	-2.84134400	-0.52108400
H	2.09957800	-3.76659000	0.41027500
C	6.46330200	-1.49861000	-0.12032400
H	7.07007300	-0.74022300	-0.62776900
H	6.88644000	-1.63132600	0.88540900
H	6.59851900	-2.44739300	-0.65256600

63

P6'-TS E = -1379.763603

Al	2.19894600	0.01744500	0.06134000
C	4.27803400	0.81181300	-0.07347400
H	4.50907100	1.79838700	0.31241300
C	3.77531100	0.53989000	-1.38823100
C	3.61166800	-0.88041700	-1.48762600
C	1.16422100	-1.06652600	1.35628000

C	-0.05198000	1.06288400	1.30988200
C	0.08772400	-0.35262600	1.79070200
C	0.84456100	1.51857800	0.28732200
C	-0.98484100	-0.85306300	2.74019300
H	-1.98839000	-0.65774600	2.34398500
H	-0.90808400	-1.92775000	2.91536600
C	4.05460600	-1.44913300	-0.25856700
H	4.01715000	-2.50527300	-0.01723400
C	4.46312700	-0.41920900	0.62248600
C	-0.69347000	2.05009600	2.25318200
H	-0.00278200	2.25175400	3.08494600
H	-0.91380600	2.99905800	1.76233000
C	1.42185000	-2.50480800	1.72365100
H	2.44655800	-2.63598400	2.09628000
H	0.74452300	-2.91755100	2.48003000
C	0.91894800	2.99568900	-0.05754900
H	-0.04519200	3.40399500	-0.39796600
H	1.25019700	3.59058500	0.80217900
N	-1.43193700	0.57389400	-0.22431000
N	-0.60100400	0.29537100	-1.15348600
N	0.63654800	0.67399600	-0.97909000
C	5.01128800	-0.58117600	2.01458800
H	4.84349400	0.31681000	2.61916700
H	4.55133000	-1.42639800	2.53844600
H	6.09437600	-0.76200700	1.99370500
C	3.54917600	1.53948900	-2.48964500
H	4.28196000	1.40340500	-3.29628700
H	2.54864800	1.44674600	-2.92516600
H	3.65857000	2.56342700	-2.11760000
C	3.13402800	-1.62861300	-2.70335500
H	2.22418800	-1.18448900	-3.12305000
H	3.89524100	-1.62515400	-3.49502000
H	2.91609500	-2.67424600	-2.46187900
H	1.63881600	3.15980100	-0.86482900
H	-1.61491600	1.65931500	2.69018300
H	-0.92267800	-0.35992700	3.71964800
H	1.34706500	-3.14824500	0.83428100
C	-2.77759600	0.13574100	-0.37184300
C	-3.80924600	1.08937100	-0.23564000
C	-3.08701600	-1.22610100	-0.59323500
C	-5.13690200	0.66172700	-0.31106900
C	-4.43313300	-1.59976800	-0.65910100
C	-5.47497000	-0.67965500	-0.51394000
H	-5.92917600	1.40264700	-0.21999800

H	-4.67143500	-2.64807600	-0.82965200
C	-2.01343700	-2.27325200	-0.77171400
H	-1.55609300	-2.20904200	-1.76572700
H	-1.20497200	-2.15088800	-0.04429000
H	-2.43462300	-3.27731000	-0.65593900
C	-3.50131500	2.55768500	-0.05594800
H	-3.12726800	2.77810800	0.95050500
H	-2.73564500	2.89526400	-0.76228500
H	-4.40115500	3.16120900	-0.21231400
C	-6.91953100	-1.12122500	-0.55545200
H	-7.04226700	-2.03710600	-1.14351900
H	-7.30487700	-1.32786400	0.45252600
H	-7.56209500	-0.34940600	-0.99383100

63

P6'-IN1 E = -1379.789826

Al	2.24645400	0.13942600	-0.23811900
C	4.34325200	-0.69094500	-0.33260900
H	4.62284200	-1.48993400	-1.01038000
C	3.88776200	-0.87033100	1.00459300
C	3.61290600	0.42942600	1.53793100
C	1.03148500	1.48975200	-0.94858200
C	-0.39147800	-0.60669400	-1.02333000
C	-0.15797500	0.91461000	-1.24920800
C	0.85966000	-1.30698900	-0.38353400
C	-1.29399700	1.71107500	-1.86885600
H	-2.25098100	1.18724400	-1.84803400
H	-1.43298300	2.66827800	-1.35278400
C	3.98017300	1.38836800	0.53969900
H	3.87632100	2.46211100	0.64350600
C	4.41708300	0.71106800	-0.62585100
C	-0.85750800	-1.23316500	-2.34765600
H	-0.09615600	-1.06981600	-3.11883300
H	-1.02448700	-2.30750600	-2.25173400
C	1.26199300	2.96414200	-1.20334300
H	2.27944800	3.27728800	-0.94475900
H	1.09981300	3.23372300	-2.25742500
C	1.28787700	-2.65284200	-0.98284800
H	0.48775300	-3.40553400	-0.94708400
H	1.60683800	-2.55032500	-2.02674000
N	-1.37078200	-0.84809600	0.09939500
N	-0.72189000	-1.23538000	1.24299800
N	0.48181300	-1.52516300	1.03320100
C	4.93226100	1.33129700	-1.89749100

H	4.77746500	0.67207300	-2.75853300
H	4.43913200	2.28483700	-2.11319900
H	6.01026200	1.52731500	-1.82720100
C	3.73338500	-2.17425800	1.73903600
H	4.35651800	-2.18319100	2.64268700
H	2.69512500	-2.34923000	2.04153700
H	4.05227400	-3.01374200	1.11290300
C	3.14524800	0.73022800	2.93814700
H	2.33796900	0.05878600	3.24900100
H	3.96624000	0.61572900	3.65854600
H	2.77801400	1.75850900	3.01917700
H	2.13274600	-3.06003800	-0.41929700
H	-1.78537400	-0.77724300	-2.70354600
H	-1.06909700	1.95191500	-2.91808800
H	0.57677000	3.59431100	-0.61606200
C	-2.70807500	-0.35830400	0.26017500
C	-3.78853400	-1.07632600	-0.29226300
C	-2.95100700	0.80359300	1.03241300
C	-5.08471100	-0.56241800	-0.14809000
C	-4.26250100	1.26485700	1.15856200
C	-5.34443100	0.61234200	0.55654900
H	-5.91537600	-1.11825800	-0.57939800
H	-4.44477700	2.16077700	1.74921600
C	-1.83967100	1.52544300	1.75804300
H	-1.48225000	0.92913900	2.60539200
H	-0.97482300	1.70389500	1.11287600
H	-2.19242000	2.48823600	2.14145300
C	-3.61327100	-2.41352200	-0.97645500
H	-3.52537400	-2.31810800	-2.06538700
H	-2.71855300	-2.92733000	-0.61678800
H	-4.48103900	-3.05184200	-0.77855300
C	-6.74658000	1.16255900	0.67641600
H	-7.49802400	0.39171300	0.47576700
H	-6.93509300	1.56691100	1.67747200
H	-6.91669700	1.97944900	-0.03801300

63

P6'-TS(1-2) E = -1379.755347

Al	1.23248300	-0.15301500	-0.09648500
C	2.19048500	-2.52236000	0.03204200
H	1.92422100	-3.26201500	0.78016700
C	3.38299200	-1.75631100	0.02975600
C	3.33347000	-0.87828600	-1.07704900
C	1.33455300	0.46365300	1.76631400

C	-0.16660300	1.77669900	0.29057200
C	0.44993100	1.47810100	1.72725600
C	1.10457500	2.04160700	-0.60253000
C	-0.00871000	2.33940600	2.87964300
H	-1.10097100	2.33005800	2.98802200
H	0.41952500	1.99298800	3.82375400
C	2.09451400	-1.11544300	-1.76761300
H	1.81454900	-0.70211800	-2.72905700
C	1.38363800	-2.16476400	-1.07784300
C	-1.16749200	2.93483200	0.28353500
H	-0.74727600	3.81321800	0.78115900
H	-1.41756400	3.21954800	-0.73968400
C	2.05469000	-0.03136100	2.98880900
H	1.88709700	-1.10728100	3.13456000
H	3.14096400	0.08976700	2.88273700
C	2.05223600	3.17205400	-0.28913100
H	1.56395100	4.15794000	-0.28931100
H	2.49375900	3.02048000	0.69956200
N	-0.64088700	0.50979500	-0.32233200
N	-0.08148200	1.14153500	-2.36137300
N	0.73691700	1.86008100	-1.92138100
C	0.14546900	-2.86173300	-1.57787300
H	-0.55101000	-2.16443700	-2.05465200
H	0.40968000	-3.62418900	-2.32307400
H	-0.39005700	-3.36797000	-0.76836200
C	4.50181500	-1.86219600	1.02973600
H	5.33420300	-2.46183300	0.63574900
H	4.91521200	-0.88155100	1.29385300
H	4.16589200	-2.34095500	1.95524400
C	4.39596300	0.09571500	-1.50697100
H	4.90932800	0.54932600	-0.65129500
H	5.16383700	-0.39848600	-2.11822400
H	3.97248100	0.90525700	-2.11108300
H	2.86788600	3.20634600	-1.01840200
H	-2.09484600	2.66390800	0.79856900
H	0.28522000	3.39079300	2.75538600
H	1.76296700	0.47430800	3.91837300
C	-1.97778800	0.00381300	-0.14392500
C	-2.21887400	-1.04141900	0.80263600
C	-3.08952000	0.45946300	-0.90911700
C	-3.50041500	-1.57574300	0.95188900
C	-4.35485500	-0.11624500	-0.70654800
C	-4.59567500	-1.12981800	0.21123600
H	-3.64476100	-2.37022900	1.68171300

H	-5.18141400	0.25145600	-1.31198200
C	-3.06807000	1.54736100	-1.96464200
H	-3.40325600	2.50615500	-1.54858000
H	-2.09015800	1.69723600	-2.41187300
H	-3.76745800	1.29234900	-2.76847500
C	-1.15924900	-1.61279100	1.71848400
H	-0.26400500	-1.94389600	1.18556500
H	-0.82974900	-0.88482400	2.46342600
H	-1.55739400	-2.48301000	2.25008100
C	-5.96969000	-1.72713800	0.40137000
H	-5.95891700	-2.81461600	0.25574000
H	-6.34974600	-1.54431900	1.41487800
H	-6.69064400	-1.30267800	-0.30480000

63

P6'-IN2 E = -1379.807663

Al	-1.34688100	-0.48088700	-0.14077500
C	-3.17931300	-2.08897600	-0.10848700
H	-4.18969400	-1.85130600	-0.42090300
C	-2.67563000	-1.92162800	1.20450500
C	-1.27930200	-2.24727700	1.17993000
C	-2.38317400	1.10114500	-0.57322100
C	0.02115200	1.83162400	-0.68641300
C	-1.50274200	2.09636700	-0.81436100
C	0.60549500	2.80506400	0.36892400
C	-1.88493900	3.50092300	-1.24503800
H	-1.96168700	3.57631400	-2.33861500
H	-2.85315800	3.79956800	-0.83379300
C	-0.95343200	-2.60374100	-0.17486500
H	0.02249100	-2.92968300	-0.51456300
C	-2.13342200	-2.49589700	-0.97568100
C	0.68404800	2.16932000	-2.04553600
H	0.57180600	3.22899500	-2.29373700
H	1.75279800	1.93701800	-2.03124300
C	-3.88027000	1.25244800	-0.69167100
H	-4.25270500	0.77820900	-1.61161300
H	-4.39768800	0.75242200	0.13656600
C	1.97136300	3.44877100	0.29423600
H	2.76848800	2.69838000	0.21452000
H	2.06287900	4.11971500	-0.56939400
N	0.23106300	0.40273300	-0.32597200
N	-0.75006200	3.14075200	2.37592200
N	-0.09581000	3.00177700	1.43647800
C	-2.25571100	-2.82707700	-2.43991600

H	-1.31383600	-2.66046600	-2.97330300
H	-2.52643200	-3.88198900	-2.57949400
H	-3.02998000	-2.22454100	-2.92714800
C	-3.47086400	-1.52028700	2.41814900
H	-3.72355400	-2.39482800	3.03269100
H	-2.92263000	-0.82241200	3.06103800
H	-4.41124000	-1.03792900	2.13229100
C	-0.36964800	-2.39744000	2.37056700
H	-0.58371600	-1.65888500	3.14997700
H	-0.49207400	-3.39134400	2.82219200
H	0.68054900	-2.28930000	2.08507400
H	2.16209300	4.04421700	1.19277700
H	0.21247900	1.58101200	-2.83645400
H	-1.14558300	4.23927700	-0.91950800
H	-4.22320500	2.29392200	-0.70991400
C	1.55502600	-0.12073500	-0.21244800
C	2.16934600	-0.78311400	-1.31132800
C	2.26025000	-0.08525600	1.02224200
C	3.45297800	-1.32487900	-1.17312200
C	3.54531900	-0.63642100	1.10545200
C	4.17290500	-1.24788800	0.01936000
H	3.89833400	-1.83055800	-2.02903400
H	4.06373400	-0.59806900	2.06268500
C	1.67699200	0.49917700	2.29059300
H	2.05553800	1.51001400	2.48382000
H	0.58885500	0.56380400	2.25275300
H	1.95761400	-0.11407500	3.15475900
C	1.48891300	-0.95576100	-2.65341300
H	1.83428500	-0.21071100	-3.38141800
H	1.71723700	-1.94204700	-3.07388700
H	0.40498900	-0.85081300	-2.57942100
C	5.57255100	-1.80652800	0.13039600
H	5.71494000	-2.66793300	-0.53165600
H	6.32618300	-1.05715100	-0.14805000
H	5.79767600	-2.12572100	1.15398500

63

P6'-TS(2-3) E = -1379.742802

Al	-1.22295700	-0.59637800	-0.12701600
C	-2.82211500	-2.50602900	-0.23821600
H	-3.84037900	-2.44400500	-0.60516000
C	-2.42915500	-2.30588800	1.10331400
C	-0.99796200	-2.37789200	1.15554500
C	-2.48786500	0.81904500	-0.45773000

C	-0.20609900	1.87560400	-0.76404200
C	-1.76270600	1.91948200	-0.76136500
C	0.32333600	3.13308800	-0.13663100
C	-2.41418500	3.22895900	-1.16021500
H	-2.86531300	3.15788800	-2.16060000
H	-3.22800600	3.48283300	-0.47003200
C	-0.54081100	-2.63326900	-0.18814200
H	0.49295500	-2.78370700	-0.47582900
C	-1.67572000	-2.69649300	-1.05287200
C	0.23825500	2.18173200	-2.25567900
H	-0.03938500	3.18891800	-2.57791100
H	1.31883900	2.06476900	-2.36467900
C	-3.99920200	0.84765000	-0.47724300
H	-4.39347800	1.10268400	-1.47223600
H	-4.43493400	-0.11613600	-0.19621300
C	1.77840100	3.31861200	0.13444000
H	2.41949100	2.45582100	0.34643700
H	2.14842800	3.77060400	-0.80133100
N	0.21703100	0.50055800	-0.35215000
N	-1.25910400	3.74815000	2.37595100
N	-0.55704100	3.17060000	1.73317400
C	-1.66593200	-3.00254700	-2.52751300
H	-0.71930700	-2.71393600	-2.99551800
H	-1.79977800	-4.07853300	-2.70092500
H	-2.47489200	-2.48488500	-3.05454900
C	-3.34664300	-2.09317200	2.27711800
H	-3.43075900	-3.00449900	2.88460100
H	-2.99443000	-1.29630300	2.94239300
H	-4.35457300	-1.82505300	1.94506100
C	-0.15167100	-2.45486600	2.40004400
H	-0.49132000	-1.76367400	3.17877300
H	-0.19246500	-3.46688800	2.82573800
H	0.89648800	-2.22964200	2.18414500
H	1.93150200	4.09380000	0.89447400
H	-0.26669500	1.46002600	-2.90186200
H	-1.69660600	4.05112600	-1.14943600
H	-4.40400800	1.59965300	0.21614700
C	1.57513500	0.08598900	-0.20681700
C	2.29541300	-0.49948700	-1.28263600
C	2.19877100	0.10614700	1.07464500
C	3.60267600	-0.96417600	-1.07898400
C	3.50162600	-0.37734900	1.22782300
C	4.23682000	-0.90022300	0.16016800
H	4.13223100	-1.40696000	-1.92158200

H	3.95455200	-0.34817400	2.21793600
C	1.50248600	0.65246200	2.30086700
H	1.67835500	1.72832200	2.41738700
H	0.42040900	0.51700900	2.25039800
H	1.87762700	0.16363600	3.20634200
C	1.70230100	-0.69570200	-2.66145800
H	2.01024900	0.09209500	-3.36042700
H	2.03879400	-1.64765900	-3.08821500
H	0.61117200	-0.69200000	-2.63513100
C	5.65768700	-1.37920400	0.34653500
H	5.94076600	-2.10493800	-0.42355400
H	6.37205500	-0.54670300	0.28690200
H	5.79760400	-1.85257100	1.32510900

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P6'-IN4 E = -1270.297257

Al	-1.41298100	-0.00969100	0.19022300
C	-3.30153600	-1.05584500	-1.67400300
H	-3.80869400	-0.58868900	-2.51186300
C	-3.81319800	-1.11825900	-0.35163500
C	-2.83370500	-1.72256200	0.47245400
C	-0.23647800	0.49054300	1.69019900
C	-0.72789400	2.52495700	0.13446500
C	0.27414800	1.72823800	0.98772000
C	-1.71371900	1.81420700	-0.45885900
C	1.40005700	2.50668900	1.65203800
H	0.99941900	3.13022700	2.46005200
H	2.14868000	1.83952800	2.08364000
C	-1.67496900	-1.99330600	-0.37522500
H	-0.84714500	-2.63975400	-0.10129500
C	-2.00879700	-1.59119700	-1.71546900
C	-0.52416200	4.02205700	0.04471200
H	0.41822700	4.28460700	-0.45522200
H	-1.33090300	4.50530700	-0.51093000
C	0.15927100	0.17494300	3.11197400
H	-0.41923700	0.84099200	3.76623800
H	-0.10397300	-0.84807000	3.39585100
C	-2.77841000	2.38349300	-1.35707500
H	-3.78082500	2.18844100	-0.95233800
H	-2.69847500	3.46504000	-1.52328000
N	0.63449100	0.37306500	0.42465000
C	-1.12521500	-1.73448200	-2.92470500
H	-0.08244000	-1.47706900	-2.70508300

H	-1.12838000	-2.76752100	-3.29908900
H	-1.46470600	-1.08961800	-3.74230100
C	-5.17534900	-0.64955800	0.08474800
H	-5.16206800	-0.22952500	1.09704300
H	-5.56487100	0.12122500	-0.58905000
H	-5.90234500	-1.47388600	0.08954800
C	-3.00926000	-2.20681000	1.88887400
H	-3.67480200	-1.55555000	2.46646900
H	-3.44401800	-3.21614400	1.90880000
H	-2.05362700	-2.25514000	2.42267000
H	-2.75769800	1.89889800	-2.34210000
H	-0.48898200	4.48676700	1.03907800
H	1.91713800	3.16960700	0.95269500
H	1.21971100	0.32805500	3.34718800
C	1.96569500	-0.07960300	0.14294900
C	2.65650000	0.58046300	-0.90695900
C	2.54538300	-1.22091600	0.73916000
C	3.94336300	0.16266100	-1.24754300
C	3.83942500	-1.59867900	0.35250600
C	4.57253800	-0.91300200	-0.61376000
H	4.46110500	0.68461900	-2.05042800
H	4.27674100	-2.47782300	0.82281300
C	2.01237900	1.68927000	-1.70561800
H	0.96749600	1.46241500	-1.93836900
H	2.01246200	2.64611700	-1.17122100
H	2.55387700	1.84315700	-2.64441500
C	1.84125600	-2.10647200	1.74459600
H	2.03735400	-1.79815900	2.77789900
H	0.75842500	-2.11760900	1.60705500
H	2.19912200	-3.13648700	1.64322300
C	5.98002400	-1.32388200	-0.97760200
H	6.72514500	-0.70305600	-0.46158800
H	6.17744000	-2.36526300	-0.70175800
H	6.16408900	-1.21880900	-2.05302000

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P6'-TS(4-Pa') E = -1270.269754

Al	-1.06907500	0.08019200	0.15697700
C	-2.82917900	-2.17261900	-1.35616800
H	-3.12898200	-2.34870300	-2.38583300
C	-3.73743600	-1.86099300	-0.28348500
C	-3.00056500	-1.69255800	0.87790500
C	0.08874300	1.33869800	1.22516100
C	-1.34201900	2.73382000	-0.29603600

C	-0.09166700	2.52873800	0.35580100
C	-2.12506300	1.59561400	-0.50146000
C	1.10778800	3.39269200	0.04257100
H	1.08564100	4.28180000	0.69389200
H	2.03934200	2.86418900	0.26173500
C	-1.57649400	-1.83569500	0.53672200
H	-0.87055800	-2.26449100	1.25071100
C	-1.53226800	-2.22742500	-0.88606300
C	-1.68027100	4.07982200	-0.91410000
H	-1.60931900	4.05893700	-2.00997300
H	-2.71050200	4.36307500	-0.67054700
C	0.24832700	1.53426400	2.71612900
H	-0.54181700	2.21995100	3.04795300
H	0.14359800	0.61014200	3.28991200
C	-3.46131600	1.68745600	-1.18153300
H	-4.09286800	0.83285500	-0.92667400
H	-4.01312100	2.61006500	-0.95474500
N	0.80538700	0.48742800	0.29314800
C	-0.31541500	-2.72463300	-1.61909900
H	0.59609400	-2.18044900	-1.34674600
H	-0.12714000	-3.78379700	-1.38999600
H	-0.44387600	-2.64699800	-2.70478300
C	-5.23091900	-1.76545900	-0.44651400
H	-5.50830400	-1.14176800	-1.30619200
H	-5.67879100	-2.75423400	-0.61792100
H	-5.71573400	-1.34112900	0.43889800
C	-3.50899500	-1.43881300	2.27089300
H	-4.52207700	-1.02226600	2.27029000
H	-3.54245700	-2.36547400	2.86268100
H	-2.86761400	-0.73750900	2.81923300
H	-3.33142800	1.65688000	-2.27566500
H	-1.02734800	4.87839900	-0.55195700
H	1.14616900	3.75560200	-0.99113200
H	1.20956300	1.99685500	2.99482100
C	2.11690900	-0.00523600	0.15433800
C	2.65152100	0.04624200	-1.16754400
C	2.89782200	-0.60099900	1.17982100
C	3.94191000	-0.42181900	-1.41365000
C	4.18668600	-1.05386700	0.87588100
C	4.74142400	-0.96259100	-0.40177600
H	4.33464300	-0.36172000	-2.42715100
H	4.77023200	-1.51580800	1.67069700
C	1.83549600	0.60204600	-2.30985000
H	0.92954300	0.00851500	-2.48655700

H	1.49773100	1.62342700	-2.11152900
H	2.42000100	0.60427600	-3.23566000
C	2.38019000	-0.84323800	2.57767100
H	2.46768000	0.04135000	3.21752500
H	1.32640300	-1.13831100	2.57141100
H	2.95064600	-1.64633100	3.05542000
C	6.15058200	-1.42846500	-0.68173100
H	6.86450100	-0.59424200	-0.63894000
H	6.47935200	-2.17397700	0.05035400
H	6.23631100	-1.87349600	-1.67956500

References

1 L. Liu, W.-X. Zhang, Q. Luo, H. Li, and Z. Xi, *Organometallics* 2010, **29**, 278-281.

2 A. Hofmann, T. Tröster, T. Kupfer, and H. Braunschweig, *Chem. Sci.* 2019, **10**, 3421-3428.

3 H. Lehmkuhl, O. Olbrysch, and H. Nehl, *Justus Liebigs Ann. Chem.* 1973, **4**, 708-714.

4 F. Sebest, L. Casarrubios, H. S. Rzepa, A. J. P. White, and S. Díez-González, *Green Chem.* 2018, **20**, 4023-4035.

5 Adopted from ref. 4.

6 G. Sheldrick, *Acta Cryst.* 2015, **A71**, 3-8.

7 G. Sheldrick, *Acta Cryst.* 2008, **A64**, 112-122.

8 a) A. D. Becke, *J. Chem. Phys.* 1993, **98**, 5648-5652; b) B. Miehlich, A. Savin, H. Stoll, and H. Preuss, *Chem. Phys. Lett.* 1989, **157**, 200-206; c) C. Lee, W. Yang, and R. G. Parr, *Phys. Rev. B: Condens. Matter Mater. Phys.* 1988, **37**, 785-789; d) P. J. Stephens, F. J. Devlin, and C. F. Chabalowski, *J. Phys. Chem.* **1994**, *98*, 11623-11627.

9 a) F. Weigend and R. Ahlrichs, *Phys. Chem. Chem. Phys.* 2005, **7**, 3297– 3305; b) F. Weigend, *Phys. Chem. Chem. Phys.* 2006, **8**, 1057– 1065.

10 a) K. Fukui, *J. Phys. Chem.* 1970, **74**, 4161-4163; b) K. Fukui, *Acc. Chem. Res.* 1981, **14**, 363-368.

11 M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A., Jr. Montgomery, J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, M. J. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, *Gaussian 09, Revision D.01*; Gaussian, Inc., Wallingford, CT, 2009.