Electronic Supplementary Information for

Catalyst-Dependent Intrinsic Ring Walking Behavior on π-Face of Conjugated Polymers

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1. Materials.

2-Bromo-3-hexyl-5-iodothiophene (**1**) and [1,3-bis(2,6-diisopropylphenyl)imidazol-2-ylidene]triphenylphosphine nickel(II) dichloride ($NiCl_2(PPh_3)IPr$) were purchased from Tokyo Chemical Industry Co., Ltd. $NiCl_2$(dppp), PEPPSI-IPr, 2,5-dibromothiophene and isopropylmagnesium chloride (2.0 M solution in THF) were purchased from Sigma-Aldrich Co. Commercially available dehydrated tetrahydrofuran (THF, stabilizer-free, Kanto Chemical Co., Inc.) was used as a dry solvent. 2-Thienylmagnesium chloride (0.475 M solution in THF) was prepared from 2-chlorothiophene and magnesium turning in the presence of 1,2-dibromoethane, and titrated with hydrochloric acid (1.0 M), sodium hydroxide (0.5 M) by using methyl red as a pH indicator.

2. General.

^{1}H NMR spectra were obtained on a JEOL ECA-600 spectrometer. The internal standard of ^{1}H NMR spectra in $CDCl_3$ was tetramethylsilane (0.00 ppm). Conversion of 2,5-dibromothiophene and ratio of 2-(5-bromothienyl)-2-thiophene to alpha-terthiophene were determined by analytical GC performed on a Shimadzu GC-2010 gas chromatograph equipped with a Restek dimethylpolylsiloxane fluid Rtx-1 column (15 m) and flame ionization detector (FID). The M_n and M_w/M_n values of poly(3-hexylthiophen-2,5-diyl) (P3HT) were measured on a Tosoh HLC-8020 gel permeation chromatography (GPC) unit (eluent, THF; calibration, polystyrene standards) with two TSK-gel columns (2 × Multipore H_{XL}-M). MALDI-TOF mass spectra were recorded on a Shimadzu/Kratos AXIMA-CFR plus in the reflectron ion mode by use of a laser (λ = 337 nm). Dithranol (1,8-dihydroxy-9[10*H*]-anthracenone) was used as the matrix for the MALDI-TOF mass measurements.

3. Computational Details.

Density functional theory (DFT) calculations were performed using Gaussian 09 program package.[S1] Geometry optimizations and vibrational analyses of all local equilibrium and transition state structures were performed using the Becke's three-parameter hybrid functional,[S2] LYP correlation functional[S3-S4] (B3LYP) together with effective core potentials (ECPs) with the LANL2DZ basis sets for Ni, Pd and Br, and 6-31G(d) basis sets for the other atoms. The energy diagram of the reaction pathway was obtained by the global reaction route mapping method (GRRM)[S5-S12] based on Gaussian 09. Second-order perturbation analysis of **TS4** was calculated with the natural bond orbital (NBO) 5.9 program package[S13-S15] at the same level as used for geometry optimization. The calculated geometries of starting material (**SM**), intermediates (**CP1**–**CP7**) and transition states (**TS1**–**TS5)** are shown in Figures S13–S27. All stationary points were optimized without any symmetry assumptions and were characterized by normal coordinate analysis at the same level of theory (number of imaginary frequencies, NIMAG, 0 for minima and 1 for transition states). The intrinsic reaction coordinate (IRC) method[S16-S18] was used to track minimum energy paths from transition structures to the corresponding local minima. The values of electronic energies (ΔE) were evaluated by single-point energy calculations using B3LYP functional together with ECPs with SDD basis sets for Ni, Pd, Br and 6-311++G(d,p) basis sets for the other atoms. The values of electronic energies (ΔE) were shown in kcal/mol unless otherwise noted. Cartesian coordinates and energies of the computed structures are listed in Appendix (pages S50–S94).

4. Synthesis.

4-1. General procedure for the model reaction (Table 1).

All glass apparatuses were dried prior to use. Addition of reagents into a reaction flask and withdrawal of a small aliquot of the reaction mixture for analysis were carried out via a syringe from a three-way stopcock under a stream of nitrogen. A round-bottomed flask equipped with a three-way stopcock was heated under reduced pressure, and then cooled to room temperature under an argon atmosphere. Ni or Pd catalyst (0.0095 mmol) was placed in the flask, and the atmosphere in the flask was replaced with argon. A solution of 2,5-dibromothiophene (91.9mg, 0.38 mmol) and naphthalene (used as an internal standard for GC analysis, 24.4 mg, 0.19 mmol) in dry THF (3.1 mL) was added via a syringe, and the reaction mixture was stirred at 0 ^{o}C. To the mixture was added 2-chloromagnesiothiophene (0.475 M solution in THF, 0.8 mL, 0.38 mmol) via a syringe, and stirring was continued at room temperature. The reaction was allowed to proceed for 2 h, followed by quenching in 5 M hydrochloric acid. The organic layer was extracted with diethyl ether and subjected to GC to determine the product composition and distribution.

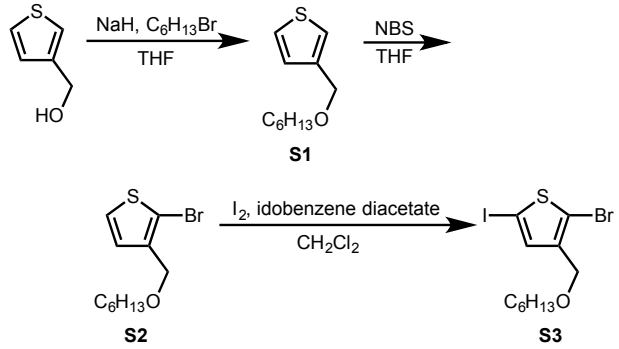
4-2. General procedure for the polymerization (Table 2).

All glass apparatuses were dried prior to use. Addition of reagents into a reaction flask and withdrawal of a small aliquot of the reaction mixture for analysis were carried out via a syringe from a three-way stopcock under a stream of nitrogen. A round-bottomed flask equipped with a three-way stopcock was heated under reduced pressure, and then cooled to room temperature under an argon atmosphere. A solution of **1** (149.2 mg, 0.4 mmol) in dry THF (2.7 mL) was added via a syringe, and the reaction mixture was stirred at 0 ^{o}C. Isopropylmagnesium chloride (2.0 M solution in THF, 0.2 mL, 0.4 mmol) was added via a syringe, and stirring was continued at room temperature for 90 min. A suspension of $NiCl_2$(dppp) or a solution of $NiCl_2(PPh_3)$IPr or PEPPSI-IPr (0.0114 mmol, 2.85 mol%) in dry THF (2.4 mL) was added via a syringe, and

stirring was continued at room temperature. After 90 min, 5 M hydrochloric acid was added. The mixture was extracted with chloroform, and the organic layer was washed with water, dried over anhydrous $MgSO_4$, and concentrated under reduced pressure. The residue was dissolved in $CHCl_3$, and the solution was added to methanol. Insoluble material was collected by filtration, washed with methanol, and dried in a desiccator to give P3HT as a dark purple solid. ^{1}H NMR (600 MHz, $CDCl_3$) δ 6.98 (s, 1 H), 2.80 (t, J = 7.7 Hz, 2 H), 1.71 (m, 2 H), 1.48-1.38 (m, 2 H), 1.37-1.30 (m, 4 H), 0.91 (t, J = 7.2 Hz, 3 H).

4-3. Synthesis of monomers.

Synthesis of **S3**



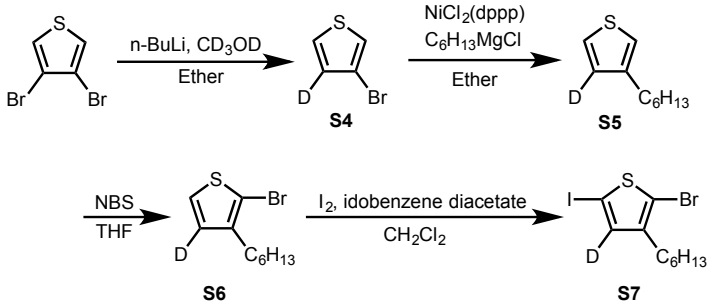
To a flask 50% sodium hydrade (2.237 g, 59.95 mmol) was added and washed with dry hexane, to which dry THF (85 mL) was added. To the mixture 3-thiophenemethanol (5.00 g, 43.8 mmol) was added dropwise over 30 min, and the mixture was stiired at room temperature for 30 min. To the mixture 1-bromohexane (7.8 mL, 55 mmol) was added, and the mixture was refluxed for 12 h. The reaction mixture was cooled to room temperature, quenched with water, and extracted with ether. The collected organic layer was washed with brine, and dried over $MgSO_4$. After filtration, the solvent was removed under reduced pressure, and resultant residue was purified by distillation (55 ˚C/ 20 mmHg) to afford **S1** (4.15g, 48%) as a colorless liquid. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.29 (dd, J = 5.0 and 2.9 Hz, 1H), 7.20 (d, J =2.8 Hz, 1 H), 7.07 (d, J = 4.8Hz, 1

H), 4.50 (s, 1H), 3.45 (t, J = 6.7 Hz, 2 H), 1.60 (quint, J = 6.9 Hz, 2 H), 1.36-1.26 (m, 6 H), 0.88 (t, J = 6.8Hz, 3 H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 139.9, 127.3, 125.8, 122.5, 70.4, 68.1, 31.7, 29.7, 25.8, 22.6, 14.0.

To a mixture of **S1** (3.968 g, 19.99 mmol) and dry THF (40 mL) was added NBS (3.596 g, 20.20 mmol), and the mixture was stirred at room temperature for 1.5 h. Additional dry THF (15 mL) was added to the mixture, which was stirred at room temperature for 4 h, quenched with 10wt% sodium thiosulfate aqueous solution, and extracted with hexane. The collected organic layer was washed with 10w% sodium thiosulfate aqueous solution and water, and dried over $MgSO_4$. After filtration, the solvent was removed under reduced pressure, and the residure was purified with distillation (82 ˚C, 0.3 mmHg) to afford **S2** (3.051 g, 56%) as a colorless viscous liquid. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.24 (d, J = 5.5 Hz, 1 H), 6.99 (d, J = 5.5 Hz, 1 H), 4.44 (s, 1 H), 3.45 (t, J = 6.5 Hz, 2 H), 1.59 (quint, J = 7.0 Hz, 2 H), 1.37-1.24 (m, 6 H), 0.88 (t, J = 6.9 Hz, 3 H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 138.6, 128.2, 125.8, 110.8, 70.5, 66.7, 31.6, 29.4, 25.8, 22.6, 14.0.

To a mixture of **S2** (2.778 g, 10.02 mmol) and dry CH_2Cl_2 (26 mL) was added iodine (1.663 g, 6.55 mmol) and iodobenzene diacetate (1.937 g, 6.01 mmol) at 0 ˚C. The mixture was stirred at 0 ˚C for 8 h, quenched with 10w% sodium thiosulfate aqueous solution and extracted with CH_2Cl_2. The collected organic layer was washed with brine, and dried over $MgSO_4$. After filtration, the solvent was removed under reduced pressure, and the residure was purified with column chromatograpy (SiO_2; hexane/CH_2Cl_2 = 19/1) to afford **S3** (3.929 g, 97%) as a colorless liquid. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.16 (s, 1 H), 4.38 (s, 1 H), 3.43 (t, J = 6.5 Hz, 2 H), 1.59 (quint, J = 7.1 Hz, 2 H), 1.37-1.25 (m, 6 H), 0.89 (t, J = 6.9 Hz, 3 H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 140.8, 137.8, 113.4, 71.9, 70.7, 66.3, 31.6, 29.6, 25.8, 22.6, 14.1.

Synthesis of **S7**



All glass apparatuses were dried prior to use. A round-bottomed flask equipped with a three-way stopcock was heated under reduced pressure, and then cooled to room temperature under an argon atmosphere. To the flask a mixture of 3,4-dibromothiophene (9.081 g, 37.54 mmol) and dry ether (75 mL) was added and stirred at –78 ˚C. To the mixture 1.63 M n-buthyl lithium in hexane (25.5 mL, 41.57 mmol) was added at –78 ˚C, and stirred for 25 min. To the mixture CD_3CD (5.0 mL, 191 mmol) was added dropwise, and stirred at –78 ˚C for 5 min and at room temperature for 1 h, quenched with water, and extracted with ether. The collected organic layer was washed with water, dried over $MgSO_4$, and filtered. The solvent was removed under reduced pressure to afford **S4** (8.46 g) as a pale red viscous liquid. This compound was used for next reaction without further purification.

All glass apparatuses were dried prior to use. A round-bottomed flask equipped with a three-way stopcock was heated under reduced pressure, and then cooled to room temperature under an argon atmosphere. To the flask $NiCl_2$(dppp) (207.9 mg, 0.384 mmol) was added, and the flask was replaced with Ar gas, to which a mixture of **S4** (8.455 g, 37.5 mmol) and dry ether (5.0 mL) was added with nitrogen gas flowing. To the mixture 1.62 M n-hexyl magnesium bromide in ether (24 mL, 39 mmol) was added. The mixture was stirred at room temperature overnight, quenched with 1 M HCl solution at 0 ˚C, and extracted with ether. The collected organic layer was washed with saturated $NaHCO_{3aq}$ and brine, and dired over $MgSO_4$, and filtered. The

solvent was removed under reduce pressure, and the residue was purified by column chromatography (SiO_2; hexane) and distillation (98-99 ˚C, 10 mmHg) to afford **S5** (3.872 g, 61%) as a colorless liquid. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.23 (d, *J* = 2.7 Hz, 1 H), 6.91 (d, *J* = 2.7 Hz, 1 H), 2.62 (t, *J* = 7.7 Hz, 2 H), 1.61 (quint, *J* = 7.5 Hz, 2 H), 1.36-1.26 (m, 6 H), 0.90-0.87 (m, 3 H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 143.2, 128.9, 128.2, 128.0, 124.9, 119.7, 31.9, 31.7, 30.5, 30.3, 29.71, 29.67, 29.4, 29.0, 22.7, 22.6, 14.11, 14.8.

To a mixture of **S5** (3.389 g, 20.00 mmol) and dry THF (33 mL) was added NBS (3.596 g, 20.20 mmol), and the mixture was stirred at room temperature for 1.5 h. Additional dry THF (30 mL) was added to the mixture. The mixture was stirred at room temperature for 2.5 h, quenched with 10wt% sodium thiosulfate aqueous solution, and extracted with ether. The collected organic layer was washed with 10wt% sodium thiosulfate aqueous solution and 10wt% KOH_{aq}, and dried over $MgSO_4$. After filtration, the solvent was removed under reduced pressure, and purified with distillation (67 ˚C, 0.3 mmHg) to afford **S6** (3.766 g, 76%) as a colorless viscous liquid. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.17 (s, 1 H), 2.56 (t, *J* = 7.7 Hz, 2 H), 1.57 (quint, *J* = 7.6 Hz, 2 H), 1.35-1.26 (m, 6 H), 0.89 (t, *J* = 7.6 Hz, 3 H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 141.9, 128.2, 128.0, 127.8, 125.0, 108.8, 31.6, 29.7, 29.4, 28.9, 22.6, 14.1.

To a mixture of **S6** (991.9 mg, 4.00 mmol) and dry CH_2Cl_2 (20 mL) was added iodine (577.2 mg, 4.55 mmol) and iodobenzene diacetate (777.7 mg, 2.41 mmol) at 0 ˚C. The mixture was stirred at room temperature overnight, quenched with saturated $NaHCO_{3aq}$, and extracted with ether. The collected organic layer was washed with saturated $NaHCO_{3aq}$, dried over $MgSO_4$ and filtered. The solvent was removed under reduced pressure, and the residure was purified with column chromatograpy (SiO_2; hexane) and distillation (120 ˚C, 0.25 mmHg) to afford **S7** (873.4 mg, 58%) as a colorless liquid. ^{1}H NMR (600 MHz, $CDCl_3$) δ 2.52 (t, *J* = 7.7 Hz, 2 H), 1.55 (quint, *J* = 7.1 Hz, 2 H), 1.34-1.26 (m, 6 H), 0.88 (t, *J* = 6.9 Hz, 3 H); ^{13}C NMR (150 MHz, $CDCl_3$) δ

144.2, 143.0, 138.0, 137.9, 137.7, 137.5, 111.7, 110.2, 70.9, 31.6, 29.60, 29.58, 29.53, 29.4, 29.2, 29.1, 28.80, 28.77, 22.5, 14.1.

4-4. General procedure for the copolymerization (Fig. 3a).

All glass apparatuses were dried prior to use. Addition of reagents into a reaction flask and withdrawal of a small aliquot of the reaction mixture for analysis were carried out via a syringe from a three-way stopcock under a stream of nitrogen. A round-bottomed flask equipped with a three-way stopcock was heated under reduced pressure, and then cooled to room temperature under an argon atmosphere. A solution of **1** (223.88 mg, 0.600 mmol) and naphthalene (24.94 mg, 0.195 mmol) as an internal standard in dry THF (3.6 mL) was added via a syringe, and the reaction mixture was stirred at 0 °C. Isopropylmagnesium chloride (2.0 M solution in THF, 0.3 mL, 0.6 mmol) was added via a syringe, and stirring was continued at room temperature for 90 min. A suspension of $NiCl_2$(dppp) or a solution of $NiCl_2(PPh_3)$IPr or PEPPSI-IPr (0.03 mmol) in dry THF (3.6 mL) was added via a syringe, and stirring was continued at room temperature for 1 h. To another flask a monomer (**S3**, **S7** or 1,4-dibromo-2,5-dihexyloxybenezene[S19]) (0.4 mmol) and dry THF (2.7 mL) was added, to which 2 M isopropyl magnesium chloride in THF (0.2 mL, 0.4 mmol) at 0 ˚C, and the mixture was stirred at room temperature for 1 h. The prepared chloromagnesio monomer (**2**, **1-d**, **3**[S19]) solution was added to the flask containing prepolymer via cannula, and stirred at room temperature. After 5 min, 5 M hydrochloric acid was added. The mixture was extracted with chloroform, and concentrated under reduced pressure. The residue was dissolved in $CHCl_3$, and the solution was added to methanol. Insoluble material was collected by filtration, washed with methanol, and dried in a desiccator to give a desired copolymer.

5. Supporting Figures and Tables.

5-1. Energy decomposition analysis (EDA) in each step (unit = kcal/mol).

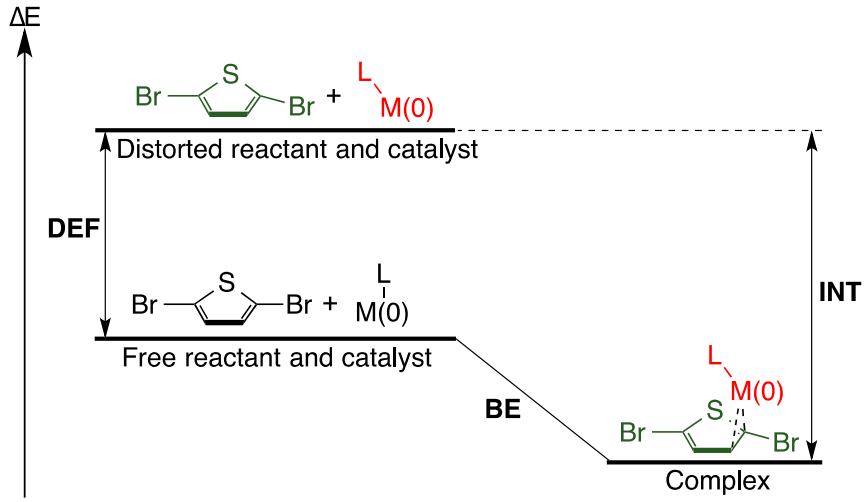


Fig. S1 A representative model of EDA (formation of **CP1**). BE, DEF and INT indicate binding energy, deformation energy and interaction energy, respectively. The DEF of thiophene units and the catalyst were designated by DEF_{Th} and DEF_{cat} respectively. The total DEF was designated by DEF_{total} (DEF_{Th} + DEF_{cat}).

Table S1. EDA of **CP1** and **TS1** in OA step.

CP1

	Ni(0)dppp	Ni(0)NHC	Pd(0)dppp	Pd(0)NHC
DEF_{Th}	18.6	15.2	17.6	10.8
DEF_{cat}	11.2	4.3	9.6	2.2
DEF_{total}	29.9	19.4	27.2	13.0
INT	–60.6	–56.6	–42.8	–36.9
BE	–30.8	–37.2	–15.6	–23.9

TS1

	Ni(0)dppp	Ni(0)NHC	Pd(0)dppp	Pd(0)NHC
DEF_{Th}	27.0	17.3	24.7	18.0
DEF_{cat}	12.2	4.1	9.6	2.3
DEF_{total}	39.2	21.4	34.3	20.3
INT	–61.8	–55.0	–39.1	–40.0
BE	–22.5	–33.6	–4.7	–19.7

Table S2. EDA of **TS2** in RE step.

	Ni(0)dppp	Ni(0)NHC	Pd(0)dppp	Pd(0)NHC
DEF_{Th}	54.9	55.8	61.0	72.1
DEF_{cat}	15.6	6.2	12.2	4.4
DEF_{total}	70.5	62.0	73.2	76.5
INT	–63.6	–69.9	–50.0	–64.2
BE	–6.9	–7.9	–23.2	–12.3

Table S3. EDA of **CP4**, **TS3** and **CP6** in unidirectional pathway.

CP4

	Ni(0)dppp	Ni(0)NHC	Pd(0)dppp	Pd(0)NHC
DEF_{Th}	13.6	8.9	10.2	6.0
DEF_{cat}	10.4	3.4	7.1	1.6
DEF_{total}	23.9	12.3	17.3	7.6
INT	–47.5	–42.4	–27.8	–27.0
BE	–23.5	–30.2	–10.5	–19.5

TS3

	Ni(0)dppp	Ni(0)NHC	Pd(0)dppp	Pd(0)NHC
DEF_{Th}	6.3	5.2	0.4	1.6
DEF_{cat}	8.0	3.3	1.4	0.8
DEF_{total}	14.2	8.5	1.7	2.4
INT	–26.3	–28.8	–5.5	–16.2
BE	–12.1	–20.3	–3.7	–13.8

CP6

	Ni(0)dppp	Ni(0)NHC	Pd(0)dppp	Pd(0)NHC
DEF_{Th}	17.1	13.8	15.5	9.8
DEF_{cat}	11.2	4.2	8.6	2.1
DEF_{total}	28.2	18.0	24.1	11.9
INT	–57.7	–54.1	–38.4	–35.1
BE	–29.5	–36.1	–14.2	–23.2

Table S4. EDA of **TS4**, **CP5**, **TS5** and **CP7** in bidirectional pathway.

TS4

	Ni(0)dppp	Ni(0)NHC	Pd(0)dppp	Pd(0)NHC
DEF_{Th}	3.3	4.6	0.6	1.4
DEF_{cat}	7.9	4.0	1.5	1.2
DEF_{total}	11.1	8.6	2.1	2.6
INT	–22.5	–34.4	–4.9	–17.9
BE	–11.4	–25.9	–2.7	–15.3

CP5

	Ni(0)dppp	Ni(0)NHC	Pd(0)dppp	Pd(0)NHC
DEF_{Th}	12.9	8.3	9.3	5.6
DEF_{cat}	9.6	3.1	6.8	1.4
DEF_{total}	22.6	11.3	16.1	7.0
INT	–44.4	–40.1	–25.3	–25.5
BE	–21.8	–28.8	–9.2	–18.5

TS5

	Ni(0)dppp	Ni(0)NHC	Pd(0)dppp	Pd(0)NHC
DEF_{Th}	5.1	4.3	0.2	1.5
DEF_{cat}	7.3	2.8	1.3	0.7
DEF_{total}	12.4	7.1	1.5	2.3
INT	–24.1	–27.6	–5.2	–16.3
BE	–11.7	–20.5	–3.6	–14.1

CP7

	Ni(0)dppp	Ni(0)NHC	Pd(0)dppp	Pd(0)NHC
DEF_{Th}	11.7	8.4	8.5	4.8
DEF_{cat}	9.9	3.4	6.8	1.6
DEF_{total}	21.6	11.8	15.3	6.4
INT	–46.8	–42.4	–28.0	–28.4
BE	–25.2	–30.6	–12.7	–22.0

5-2. Differential EDA (unit = kcal/mol)

Table S5. Differential EDA between **TS1** and **CP1** in OA step (**TS1**–**CP1**).

	Ni(0)dppp	Ni(0)NHC	Pd(0)dppp	Pd(0)NHC
ΔDEF_{Th}	8.4	2.1	7.1	7.2
ΔDEF_{cat}	1.0	–0.1	0.04	0.1
ΔDEF_{total}	9.4	1.2	7.2	7.3
ΔINT	–1.1	1.6	3.7	–3.2
ΔBE	8.3	3.6	10.9	4.2

Table S6. Differential EDA between **TS3**, **CP4** and **CP6** in unidirectional pathway.

TS3–CP4

	Ni(0)dppp	Ni(0)NHC	Pd(0)dppp	Pd(0)NHC
ΔDEF_{Th}	–7.3	–3.7	–9.9	–4.3
ΔDEF_{cat}	–2.4	–0.1	–5.7	–0.8
ΔDEF_{total}	–9.7	–3.8	–15.6	–5.2
ΔINT	21.1	13.6	22.3	10.9
ΔBE	11.5	9.9	6.8	5.7

TS3–CP6

	Ni(0)dppp	Ni(0)NHC	Pd(0)dppp	Pd(0)NHC
ΔDEF_{Th}	–10.8	–8.6	–15.2	–8.2
ΔDEF_{cat}	–3.2	–0.9	–7.3	–1.3
ΔDEF_{total}	–14.0	–9.5	–22.4	–9.4
ΔINT	31.4	25.3	32.9	18.9
ΔBE	17.4	15.7	10.5	9.4

Table S7. Differential EDA between **CP4**, **CP5**, **CP7**, **TS4** and **TS5** in bidirectional pathway.

TS4–CP4

	Ni(0)dppp	Ni(0)NHC	Pd(0)dppp	Pd(0)NHC
ΔDEF_{Th}	–10.3	–4.3	–9.6	–4.6
ΔDEF_{cat}	–2.5	0.62	–5.6	–0.4
ΔDEF_{total}	–12.8	–3.7	–15.2	–5.0
ΔINT	24.9	8.0	22.9	9.2
ΔBE	12.1	4.3	7.7	4.2

TS4–CP5

	Ni(0)dppp	Ni(0)NHC	Pd(0)dppp	Pd(0)NHC
ΔDEF_{Th}	–9.7	–3.7	–8.7	–4.2
ΔDEF_{cat}	–1.7	0.9	–5.3	–0.2
ΔDEF_{total}	–11.4	–2.8	–14.0	–4.4
ΔINT	21.9	5.7	20.4	7.6
ΔBE	10.4	2.9	6.5	3.2

TS5–CP5

	Ni(0)dppp	Ni(0)NHC	Pd(0)dppp	Pd(0)NHC
ΔDEF_{Th}	–7.9	–4.0	–9.1	–4.1
ΔDEF_{cat}	–2.3	–0.2	–5.5	–0.7
ΔDEF_{total}	–10.2	–4.2	–14.6	–4.8
ΔINT	20.3	12.5	20.1	9.2
ΔBE	10.1	8.2	5.6	4.4

TS5–CP7

	Ni(0)dppp	Ni(0)NHC	Pd(0)dppp	Pd(0)NHC
ΔDEF_{Th}	–6.6	–4.1	–8.3	–3.4
ΔDEF_{cat}	–2.6	–0.6	–5.5	–0.8
ΔDEF_{total}	–9.2	–4.6	–13.8	–4.2
ΔINT	22.7	14.8	22.8	12.0
ΔBE	13.5	10.1	9.1	7.9

5-3. Comparison among important bond lengths in OA and RE (unit = Å).

Table S8. Comparison among bond lengths of C-Br bond of **CP1** and **TS1**.

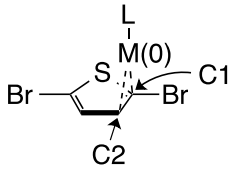
	Ni(0)dppp	Ni(0)NHC	Pd(0)dppp	Pd(0)NHC
CP1	2.033	2.041	2.022	2.004
TS1	2.303	2.184	2.277	2.197
Δ(**TS1**–**CP1**)	0.270	0.143	0.255	0.193

Table S9. Comparison among bond lengths of C-C bond of **CP3** and **TS2**.

	Ni(0)dppp	Ni(0)NHC	Pd(0)dppp	Pd(0)NHC
CP3	2.631	2.625	2.716	2.729
TS2	1.878	1.915	1.924	2.061
Δ(**CP3-TS2**)	0.753	0.710	0.792	0.668

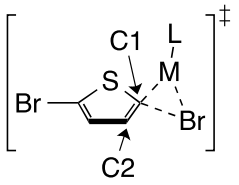
5-4. Important bond lengths of CPs and TSs (unit = Å).

Table S10. Important bond lengths of **CP1.**



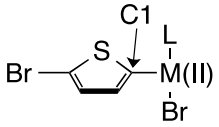
Catalyst	C1-M(0)	C2-M(0)	C1-Br	M(0)-Br
Ni(0)dppp	1.912	2.020	2.033	3.311
Ni(0)NHC	1.862	2.029	2.041	3.264
Pd(0)dppp	2.130	2.197	2.022	3.519
Pd(0)NHC	2.080	2.273	2.004	3.348

Table S11. Important bond lengths of **TS1.**



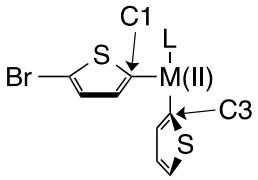
Catalyst	C1-M	C2-M	C1-Br	M-Br
Ni(0)dppp	1.842	2.319	2.303	2.838
Ni(0)NHC	1.808	2.280	2.184	2.876
Pd(0)dppp	2.055	2.659	2.277	2.956
Pd(0)NHC	2.009	2.825	2.197	2.897

Table S12. Important bond lengths of **CP2.**



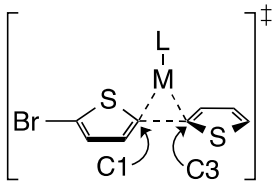
Catalyst	C1-M(II)	M(II)-Br
Ni(0)dppp	1.914	2.429
Ni(0)NHC	1.853	2.338
Pd(0)dppp	2.045	2.583
Pd(0)NHC	1.985	2.518

Table S13. Important bond lengths of **CP3.**



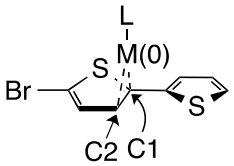
Catalyst	C1-M(II)	C3-M(II)	C1-C3
Ni(0)dppp	1.913	1.918	2.631
Ni(0)NHC	1.857	1.851	2.625
Pd(0)dppp	2.059	2.046	2.716
Pd(0)NHC	1.986	2.002	2.729

Table S14. Important bond lengths of **TS2.**



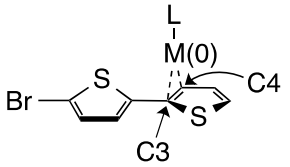
Catalyst	C1-M	C3-M	C1-C3
Ni(0)dppp	1.906	1.910	1.878
Ni(0)NHC	1.857	1.848	1.915
Pd(0)dppp	2.084	2.082	1.924
Pd(0)NHC	2.030	2.011	2.061

Table S15. Important bond lengths of **CP4.**



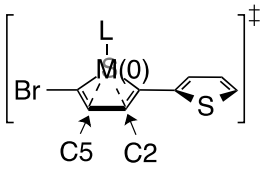
Catalyst	C1-M(0)	C2-M(0)
Ni(0)dppp	2.023	1.999
Ni(0)NHC	1.952	1.999
Pd(0)dppp	2.270	2.213
Pd(0)NHC	2.199	2.252

Table S16. Important bond lengths of **CP5.**



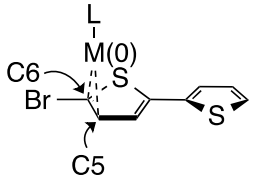
Catalyst	C3-M(0)	C4-M(0)
Ni(0)dppp	2.039	2.005
Ni(0)NHC	1.960	2.007
Pd(0)dppp	2.294	2.228
Pd(0)NHC	2.213	2.263

Table S17. Important bond lengths of **TS3.**



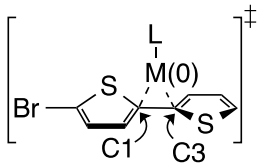
Catalyst	C2-M(0)	C5-M(0)
Ni(0)dppp	2.116	2.169
Ni(0)NHC	2.018	2.114
Pd(0)dppp	2.723	2.594
Pd(0)NHC	2.367	2.329

Table S18. Important bond lengths of **CP6.**



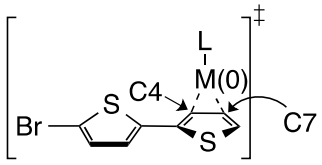
Catalyst	C6-M(0)	C5-M(0)
Ni(0)dppp	1.914	2.035
Ni(0)NHC	1.860	2.054
Pd(0)dppp	2.141	2.216
Pd(0)NHC	2.081	2.309

Table S19. Important bond lengths of **TS4.**



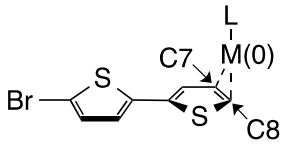
Catalyst	C1-M(0)	C3-M(0)	C1-C3
Ni(0)dppp	2.155	2.093	1.457
Ni(0)NHC	2.154	1.972	1.442
Pd(0)dppp	2.665	2.724	1.460
Pd(0)NHC	2.339	2.318	1.453

Table S20. Important bond lengths of **TS5.**



Catalyst	C4-M(0)	C7-M(0)
Ni(0)dppp	2.132	2.173
Ni(0)NHC	2.028	2.124
Pd(0)dppp	2.673	2.669
Pd(0)NHC	2.311	2.410

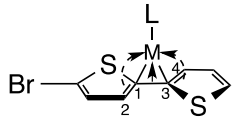
Table S21. Important bond lengths of **CP7.**



Catalyst	C7-M(0)	C8-M(0)
Ni(0)dppp	2.028	1.984
Ni(0)NHC	2.019	1.939
Pd(0)dppp	2.263	2.207
Pd(0)NHC	2.280	2.181

Important NBOs in TS4.

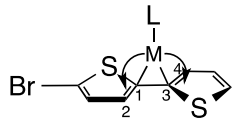
Table 22. Donation. (unit: kcal/mol)



Catalyst	$\pi_{C1\text{-}C2}\rightarrow d$	$\pi_{C3\text{-}C4}\rightarrow d$	$\sigma_{C1\text{-}C3}\rightarrow d$
Ni(0)dppp	9.0	8.1	16.8
Ni(0)NHC	11.8	41.6	12.5
Pd(0)dppp	6.0	N.D.	N.D.
Pd(0)NHC	13.5	16.0	11.5

(N.D. indicates not determined (the value was less than 5.0 kcal/mol))

Table 23. Backdonation. (unit: kcal/mol)



Catalyst	$d\rightarrow\pi^*_{C1\text{-}C2}$	$d\rightarrow\pi^*_{C3\text{-}C4}$
Ni(0)dppp	10.4	16.4
Ni(0)NHC	13.1	37.7
Pd(0)dppp	N.D.	N.D.
Pd(0)NHC	7.5	5.8

(N.D. indicates not determined (the value was less than 5.0 kcal/mol))

5-5. GPC profiles.

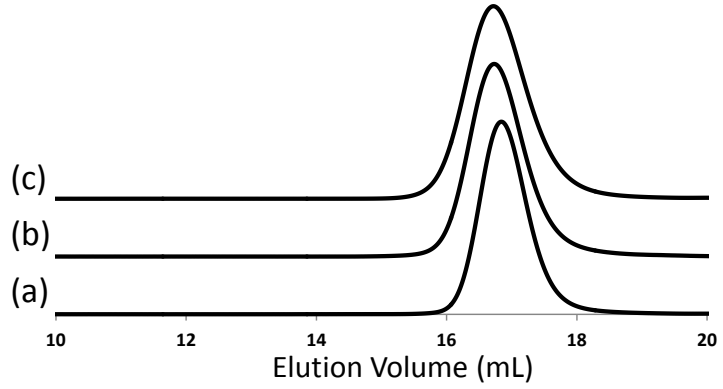


Fig. S2 GPC profiles of the P3HT obtained by treatment of **1** with 1.0 equiv. of ^{i}PrMgCl, followed by polymerization with 2.85 mol% of catalysts in THF at rt for 90 min, (a) $NiCl_2$(dppp) (M_n = 7270, M_w/M_n = 1.12), (b) $NiCl_2(PPh_3)$IPr (M_n = 7540, M_w/M_n = 1.18), (c) PEPPSI-IPr (M_n = 7630, M_w/M_n = 1.19).

5-6. MALDI-TOF mass spectra.

Not only Br/H end set but also Br/Br end set should be observed in MALDI-TOF mass spectra, if the π-arene complex were as stable as the complex of C–Pd(II)L–Br. In this case, however, the energy difference between these states is still high, and the catalyst should favor the oxidative addition state at either of end groups even if a π-arene complex formed. Therefore, Br/H end sets are observed in MALDI-TOF mass spectra.

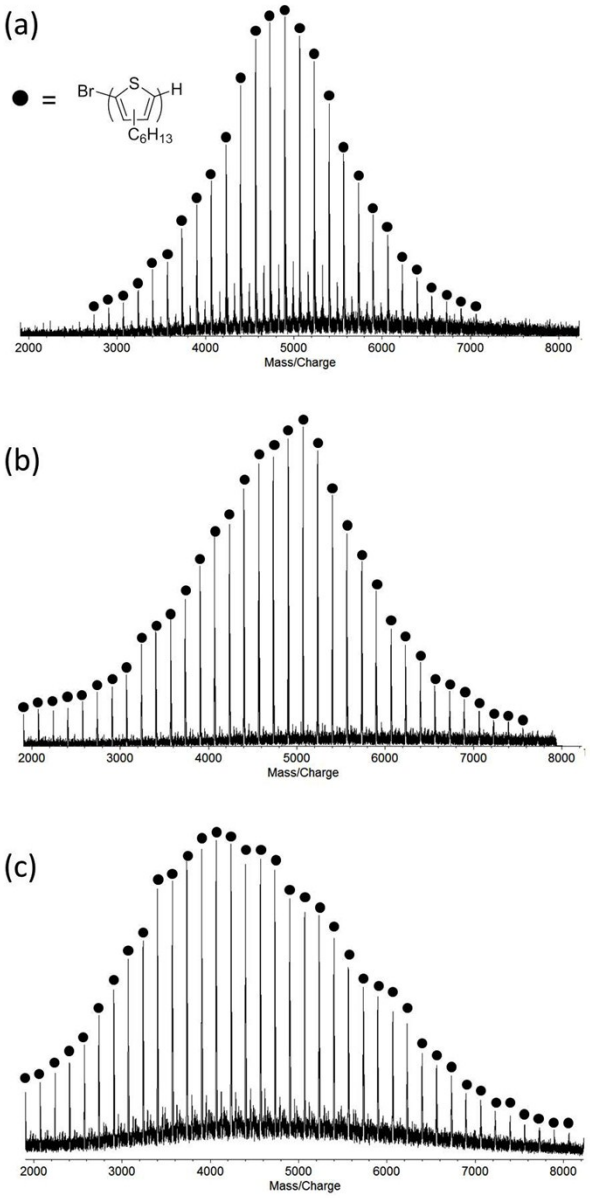


Fig. S3 MALDI-TOF-MS spectra of the P3HT obtained by treatment of **1** with 1.0 equiv. of ^{i}PrMgCl, followed by polymerization with 2.85 mol% of catalysts in THF at rt for 90 min, (a) $NiCl_2$(dppp) (M_n = 7270, M_w/M_n = 1.12), (b) $NiCl_2(PPh_3)$IPr (M_n = 7540, M_w/M_n = 1.18), (c) PEPPSI-IPr (M_n = 7630, M_w/M_n = 1.19).

5-7. ^{1}H NMR spectra in $CDCl_3$ of the polythiophenes obtained by polymerizations with $NiCl_2$(dppp), $NiCl_2(PPh_3)$IPr, and PEPPSI-IPr.

According to a literature,[S20] these ratio of the structure **A**, **B**, and **C** (Table 2 in the maniscript) were calculated using the integral ratio of signals **a**, **c**, and **d** (**A**:**B**:**C** = **a**:c:(d-c)) on the polythiophene obtained by the use of $NiCl_2$(dppp), $NiCl_2(PPh_3)$IPr, and PEPPSI-IPr, respectively (Figure S4-S6).

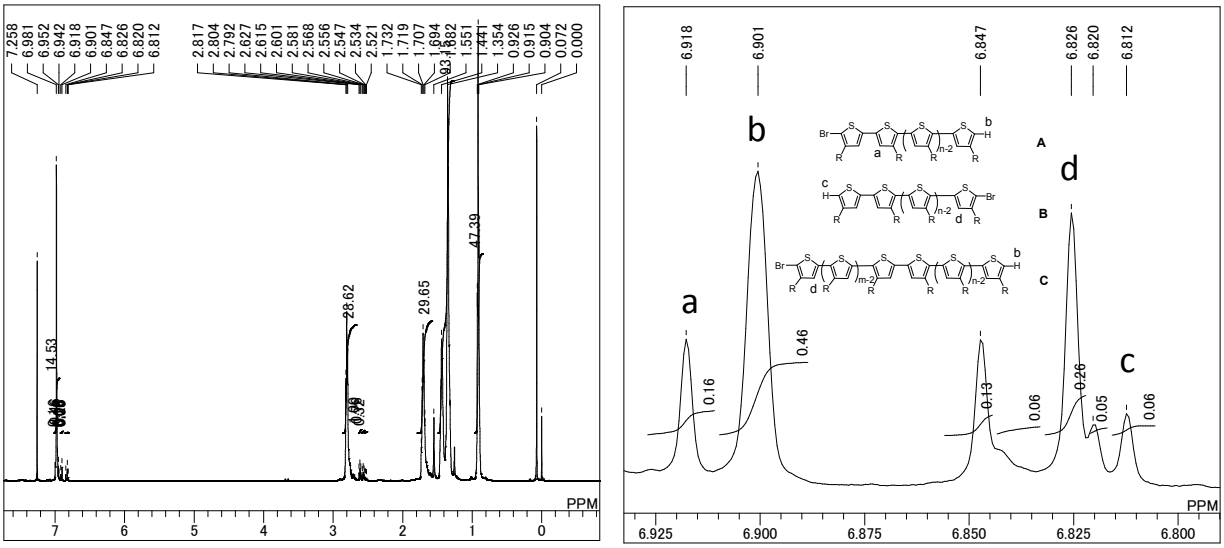


Fig. S4 ^{1}H NMR spectrum of P3HT (M_n = 7270, M_w/M_n = 1.12), which was purified by reprecipitation from MeOH, obtained by the polymerization with 2.85 mol% of $NiCl_2$(dppp).

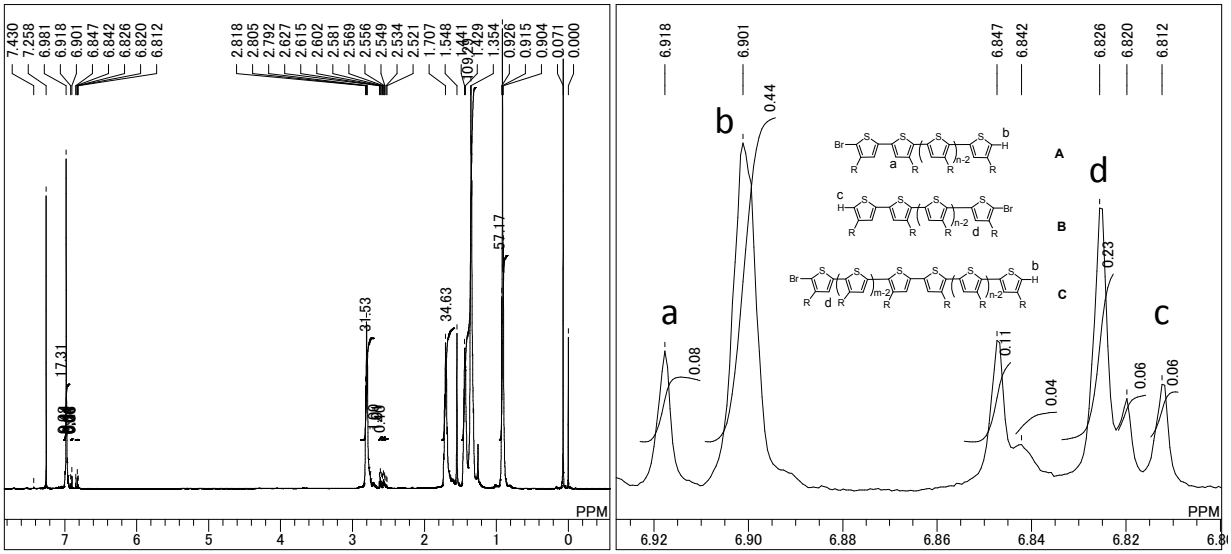


Fig. S5 ^{1}H NMR spectrum of P3HT (M_n = 7540, M_w/M_n = 1.18), which was purified by reprecipitation from MeOH, obtained by the polymerization with 2.85 mol% of $NiCl_2(PPh_3)IPr$.

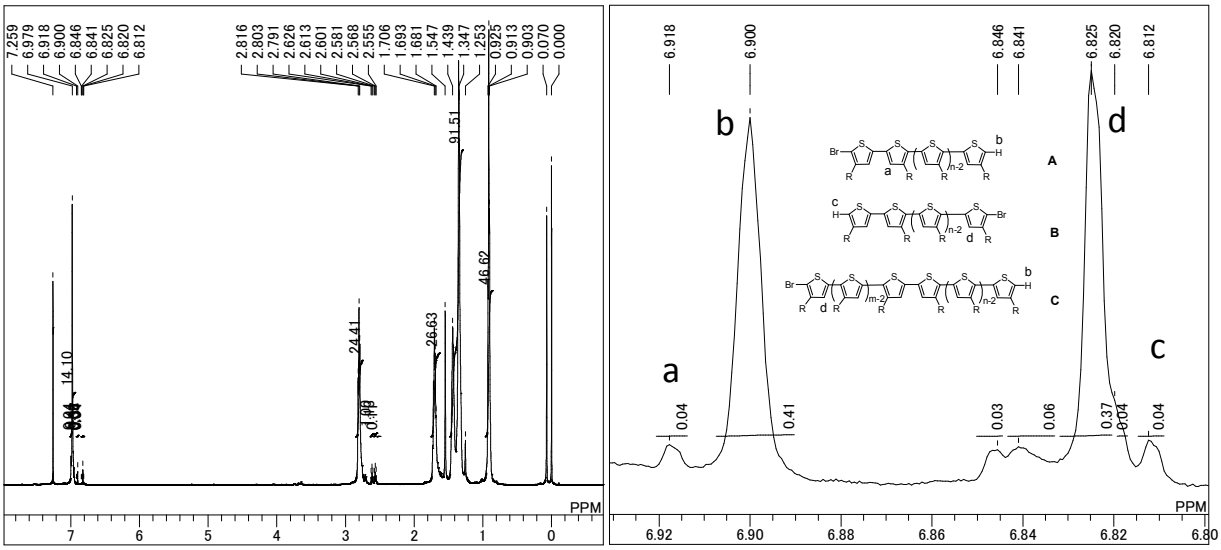


Fig. S6 ^{1}H NMR spectrum of P3HT (7630, M_w/M_n = 1.19), which was purified by reprecipitation from MeOH, obtained by the polymerization with 2.85 mol% of PEPPSI-IPr.

5-8. GPC profiles and ^{1}H NMR spectra in $CDCl_3$ of block copolymers, and estimation of block copolymerization nature.

The block copolymerization nature discussed in the manuscript (Fig. 3) was estimated from ^{1}H NMR spectra in $CDCl_3$ (Figure S8, S10, and S12). The integral ratio of signal 1-5 decreased in the case of copolymerization between **1** and **1-d** or **3** (Figure S10, and 12), indicating that these copolymers have high triblock nature due to the catalysts bidirectionally walking. On the other hand, the integral ratio of the signal 3 dramatically decreased, and signals 1, 2, 4, and 5 almost unchanged even after consumption of **2** (Figure S8), which suggest that the catalyst moved unidirectionally to afford block copolymer with high diblock nature.

On the other hand, if the block copolymerization completely proceeded, the signals derived from the end group of prepolymer should disappear. In fact, these signals almost disappeared in the case of phenylene monomer **3**. In the case of block copolymerization with **2** and **1-d**, however, signals of the end group of the prepolymer were observed, presumably because living polymerization nature of the homopolymerization of **2** is not so high, and because the deuterium ratio of the monomer **1d** is not 100%.

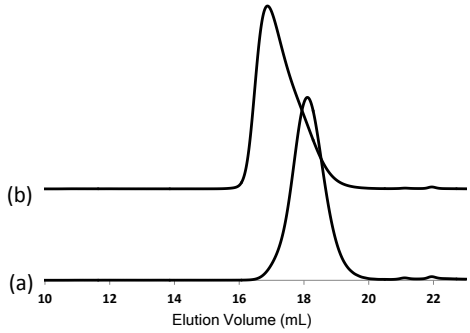


Fig. S7 GPC profile of products obtained by the polymerization of **1** with 5.0 mol% of PEPPSI-IPr in THF ($[\mathbf{1}]_0$ = 0.08 M) at room temperature for (a) 1 h (M_n = 4740, M_w/M_n = 1.18) and (b) followed by addition of **2** ($[\mathbf{2}]_0/[\text{catalyst}]_0$ = 20) and stirring for 5 min (M_n = 8740, M_w/M_n = 1.29).

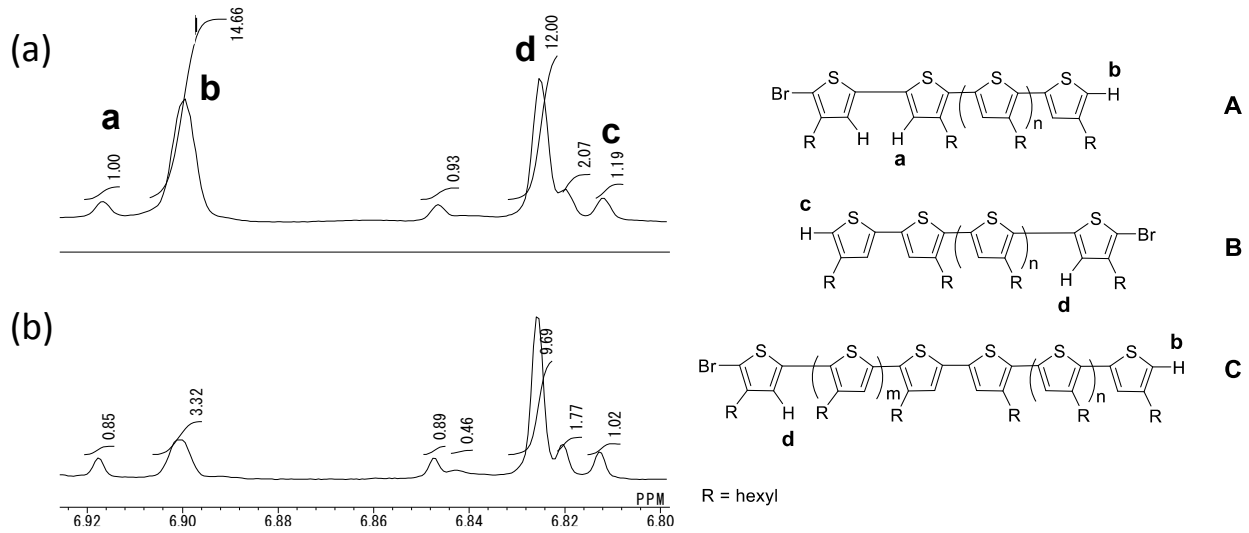


Fig. S8 ^{1}H NMR spectra of products obtained by polymerization of **1** with 5.0 mol% of PEPPSI-IPr in THF ($[\mathbf{1}]_0$ = 0.08 M) at room temperature for (a) 1 h (M_n = 4740, M_w/M_n = 1.18) and (b) followed by addition of **2** ($[\mathbf{2}]_0/[\text{catalyst}]_0$ = 20) and stirring for 5 min (M_n = 8740, M_w/M_n = 1.29).

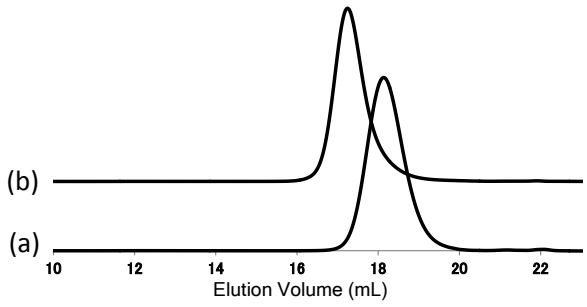


Fig. S9 GPC profile of products obtained by the polymerization of **1** with 5.0 mol% of PEPPSI-IPr in THF ($[\mathbf{1}]_0$ = 0.08 M) at room temperature for (a) 1 h (M_n = 4480, M_w/M_n = 1.14) and (b) followed by addition of **1-d** ($[\mathbf{1\text{-}d}]_0/[\text{catalyst}]_0$ = 20) and stirring for 90 min (M_n = 8590, M_w/M_n = 1.12).

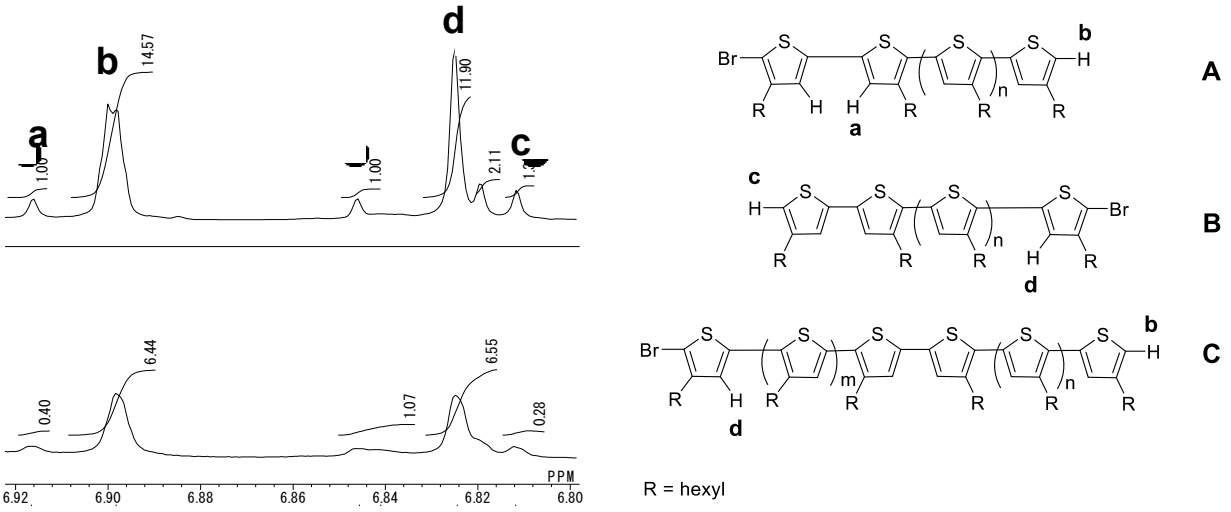


Fig. S10 ^{1}H NMR spectra of products obtained by polymerization of **1** with 5.0 mol% of PEPPSI-IPr in THF ($[\mathbf{1}]_0$ = 0.08 M) at room temperature for (a) 1 h (M_n = 4480, M_w/M_n = 1.14) and (b) followed by addition of **1-d** ($[\mathbf{1\text{-}d}]_0/[\text{catalyst}]_0$ = 20) and stirring for 90 min (M_n = 8590, M_w/M_n = 1.12).

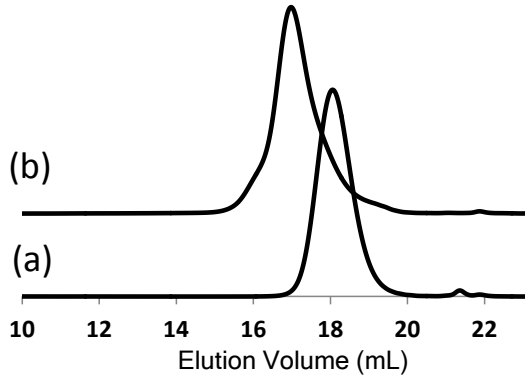


Fig. S11 GPC profile of products obtained by the polymerization of **1** with 5.0 mol% of PEPPSI-IPr in THF ($[\mathbf{1}]_0$ = 0.08 M) at room temperature for (a) 1 h (M_n = 4810, M_w/M_n = 1.15) and (b) followed by addition of **3** ($[\mathbf{3}]_0/[\text{catalyst}]_0$ = 20) and stirring for 3 h (M_n = 9220, M_w/M_n = 1.37).

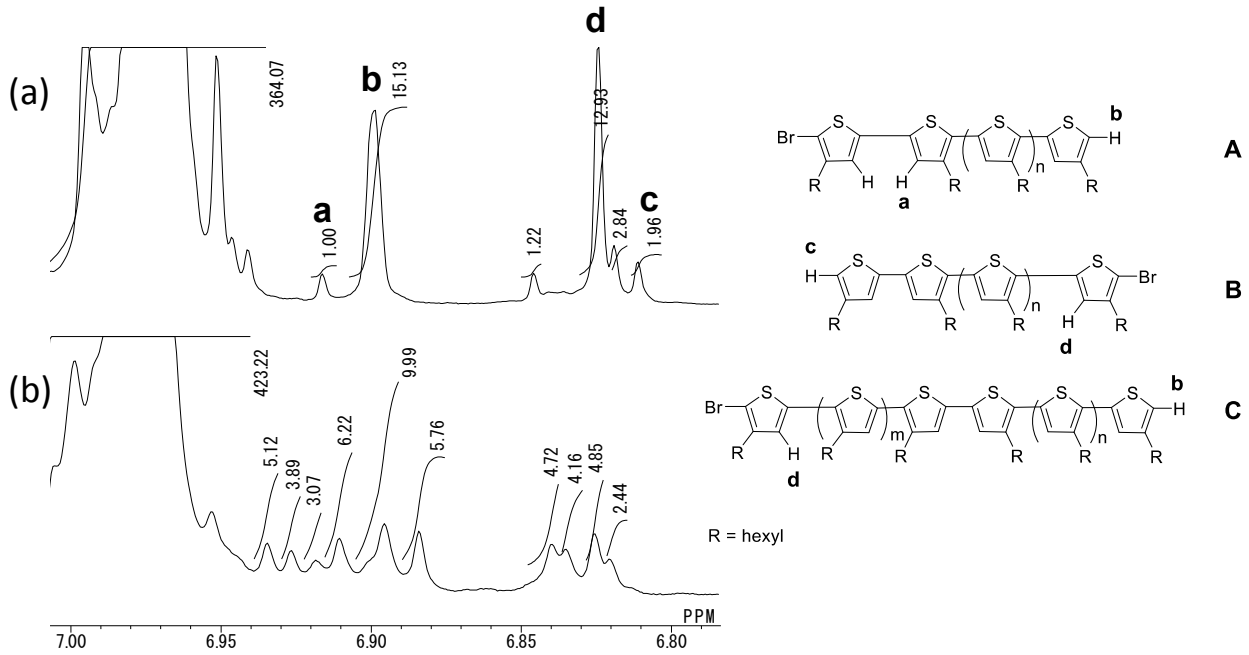


Fig. S12 ^{1}H NMR spectra of products obtained by polymerization of **1** with 5.0 mol% of PEPPSI-IPr in THF in THF ($[\mathbf{1}]_0$ = 0.08 M) at room temperature for (a) 1 h (M_n = 4810, M_w/M_n = 1.15) and (b) followed by addition of **3** ($[\mathbf{3}]_0/[\text{catalyst}]_0$ = 20) and stirring for 3 h (M_n = 9220, M_w/M_n = 1.37).

6. Supporting References

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7. Appendix.

7-1. Optimized geometries.

The geometries were given by tube type model (atom color: yellow = sulfer, silver = carbon, red = bromide, white = hydrogen, light yellow = magnesium, dark yellow = phosphine, light green = chloride, blue = nitrogen, light blue = nickel, dark blue = palladium).

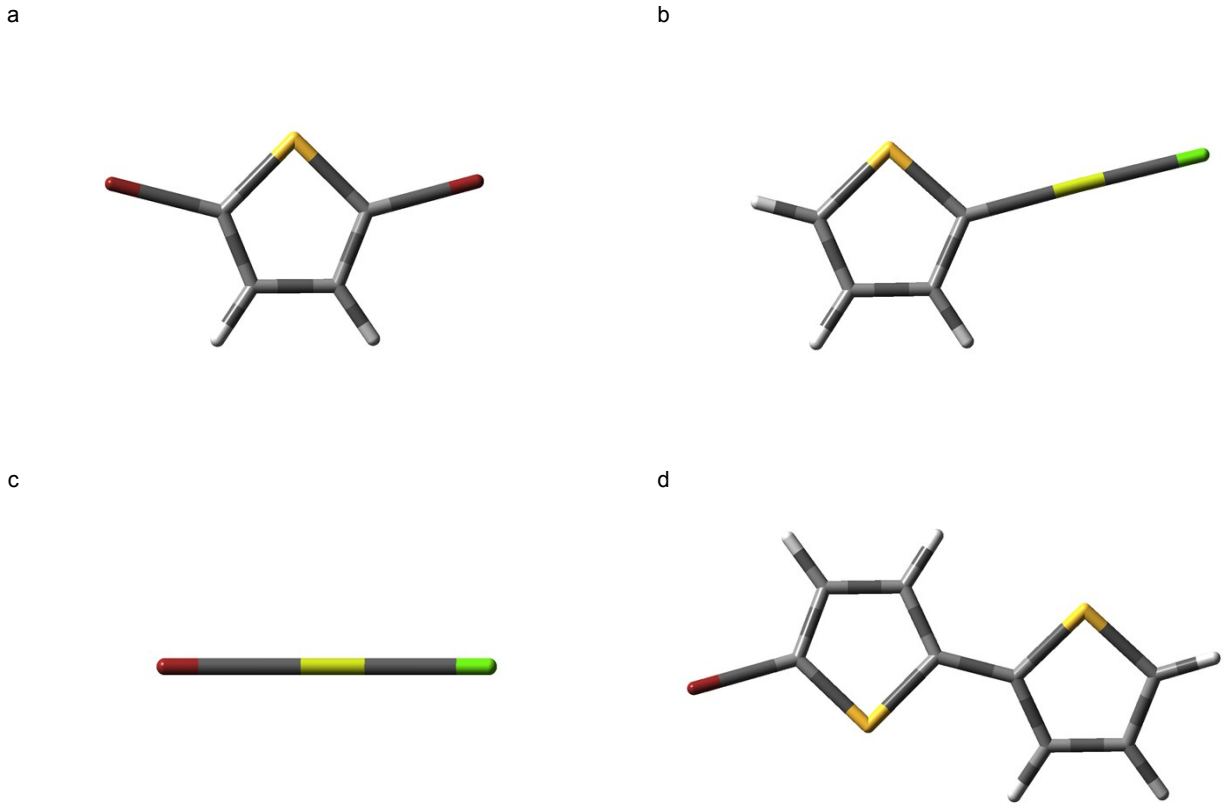

Fig. S13 Optimized geometries of (a) 2,5-dibromothiophene, (b) 2-chloromagnesio thiophene, (c) MgBrCl and (d) 2-bromobithiophene.

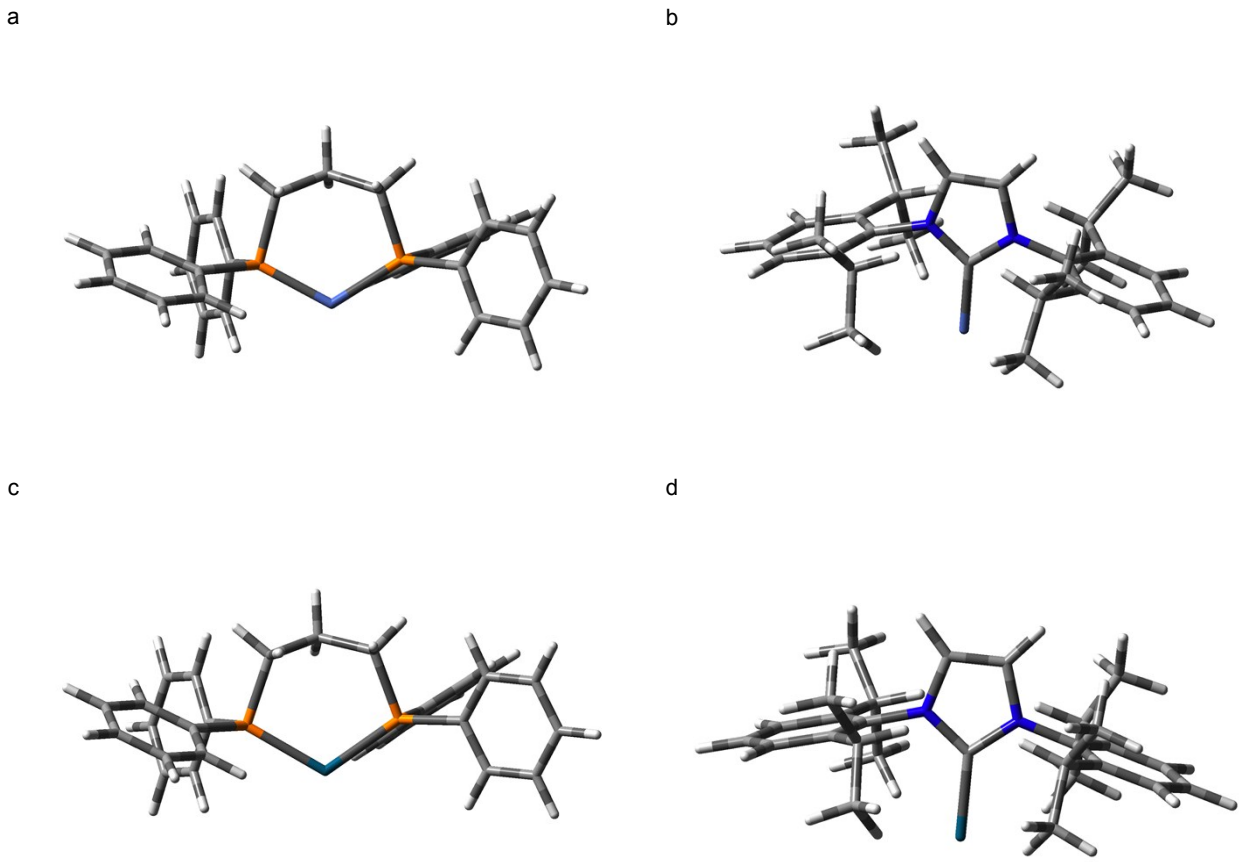

Fig. S14 Optimized geometries of (a) Ni(0)dppp, (b) Ni(0)NHC, (c) Pd(0)dppp and (d) Pd(0)NHC.

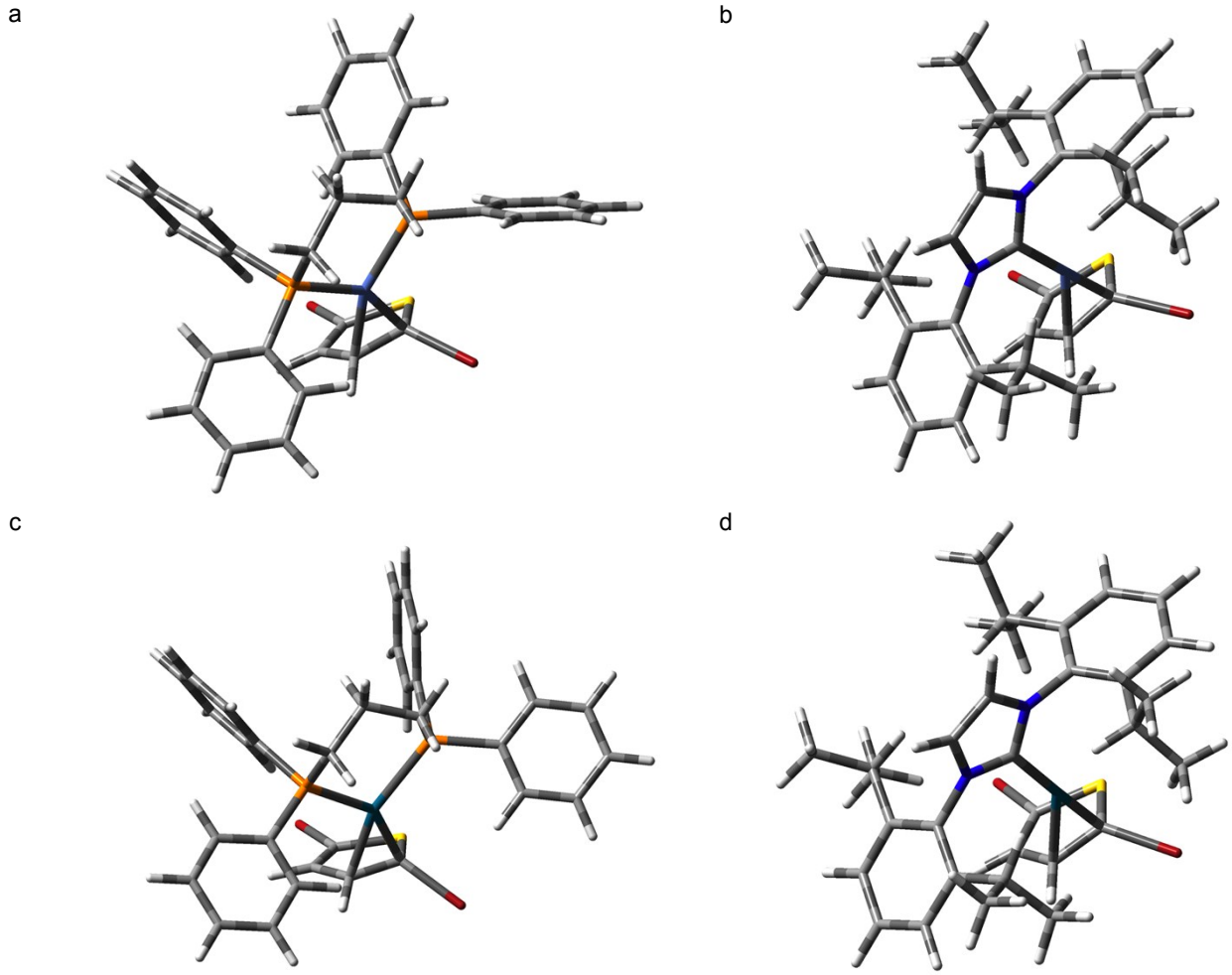

Fig. S15 Optimized geometries of **CP1s** with (a) Ni(0)dppp, (b) Ni(0)NHC, (c) Pd(0)dppp and (d) Pd(0)NHC.

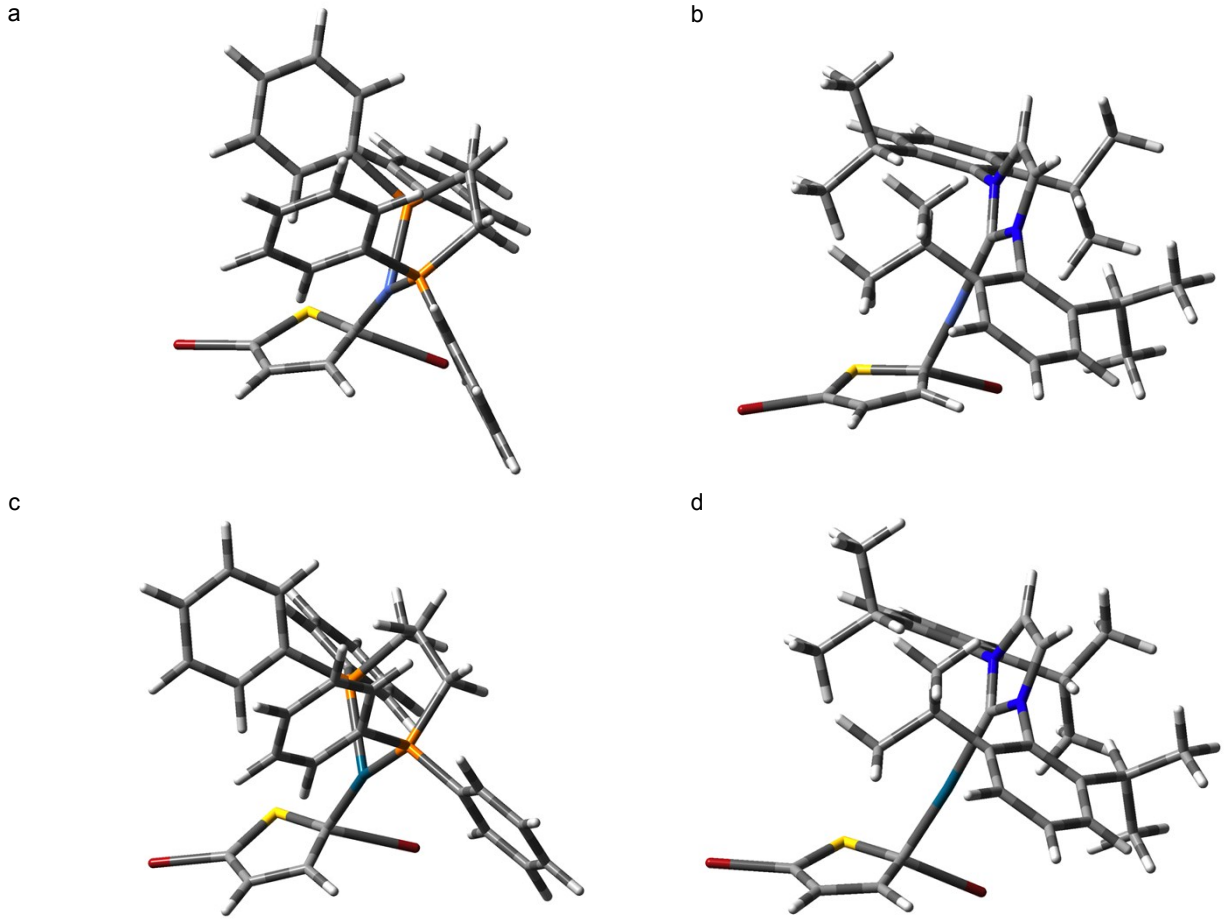

Fig. S16 Optimized geometries of **TS1s** with (a) Ni(0)dppp, (b) Ni(0)NHC, (c) Pd(0)dppp and (d) Pd(0)NHC.

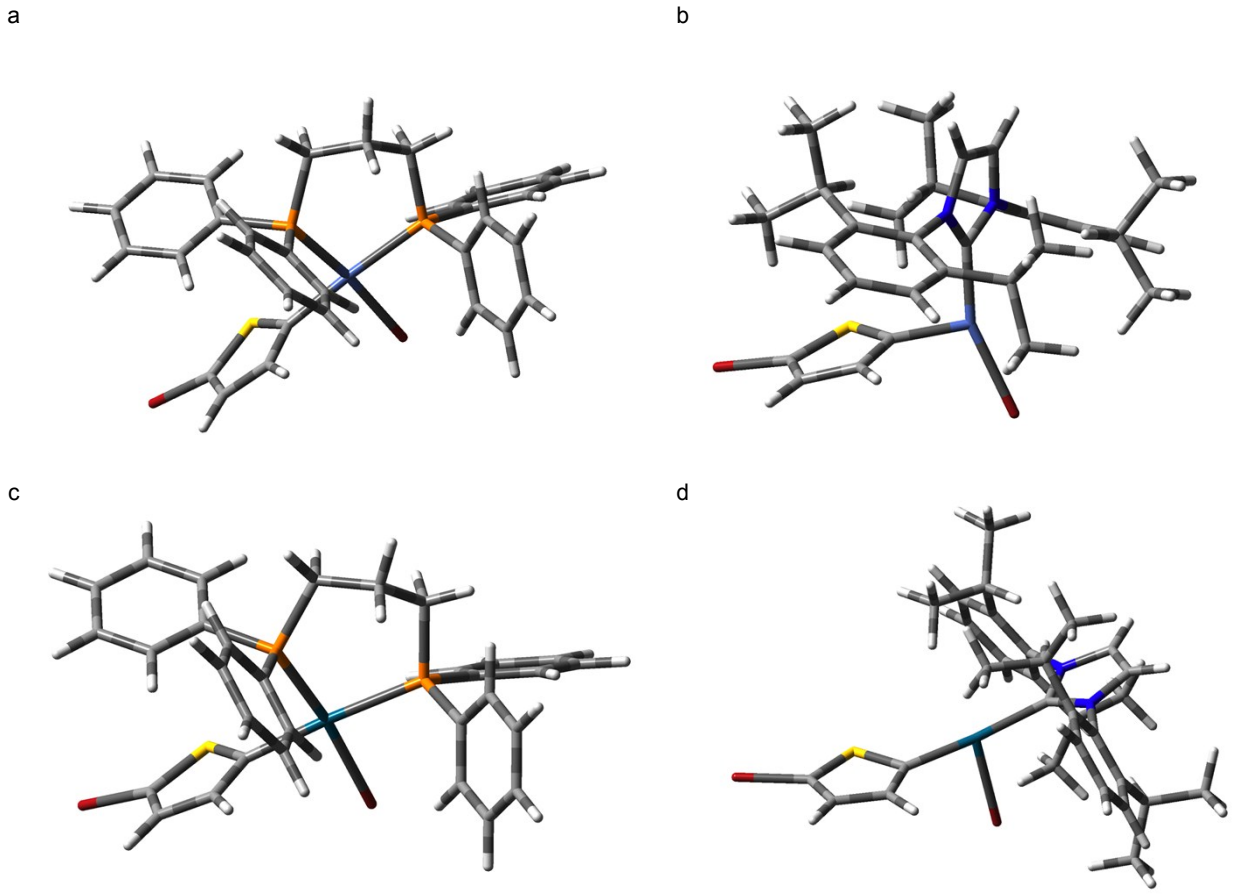

Fig. S17 Optimized geometries of **CP2s** with (a) Ni(0)dppp, (b) Ni(0)NHC, (c) Pd(0)dppp and (d) Pd(0)NHC.

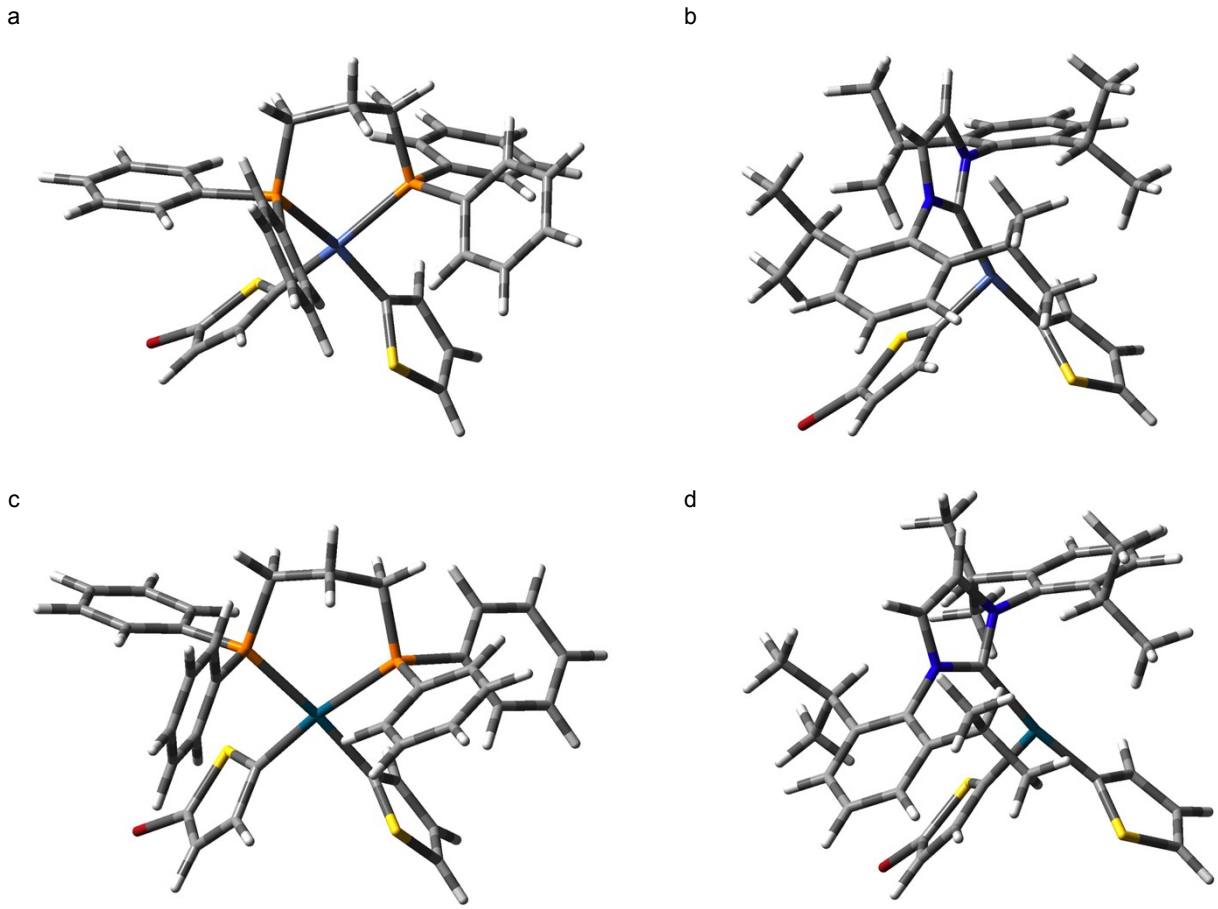

Fig. S18 Optimized geometries of **CP3s** with (a) Ni(0)dppp, (b) Ni(0)NHC, (c) Pd(0)dppp and (d) Pd(0)NHC.

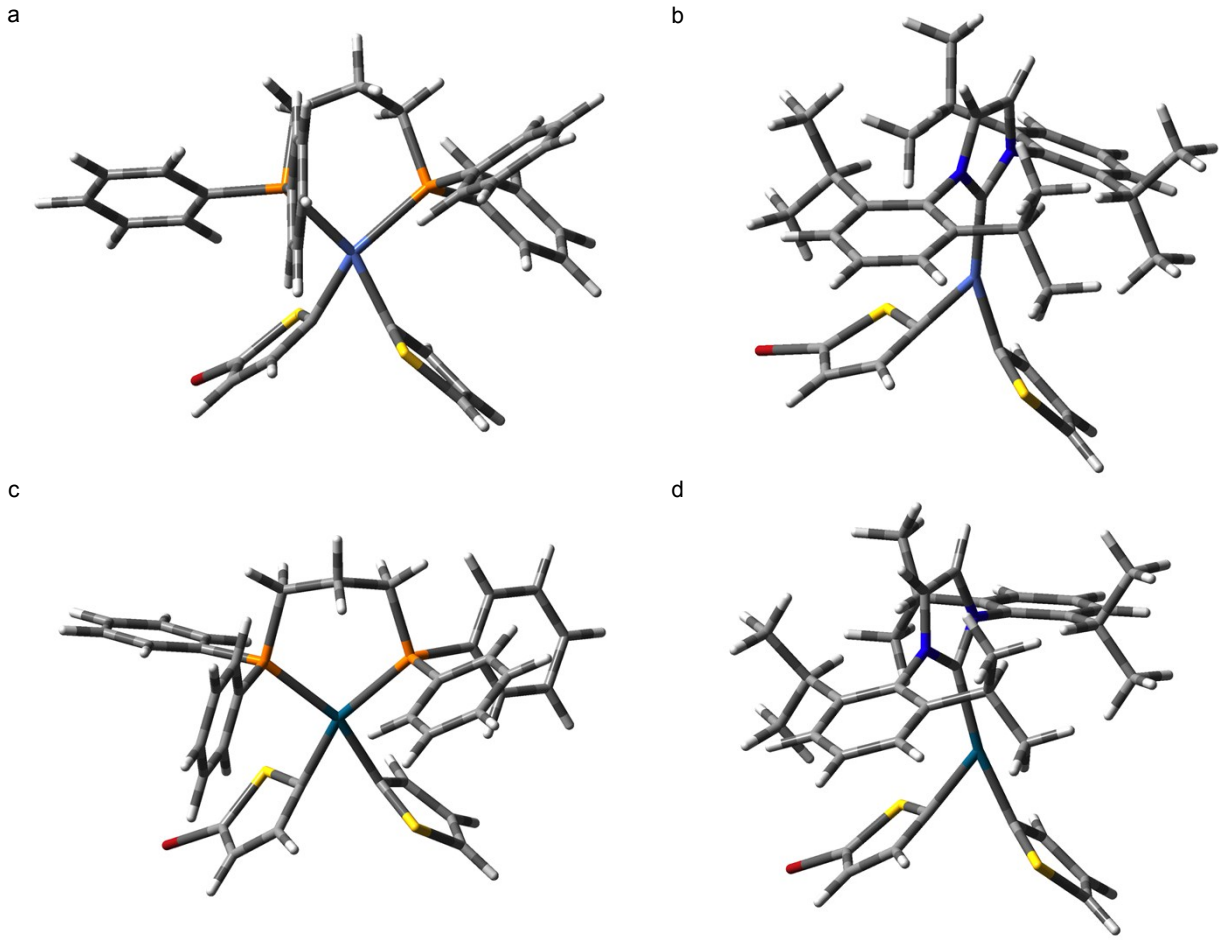

Fig. S19 Optimized geometries of **TS2s** with (a) Ni(0)dppp, (b) Ni(0)NHC, (c) Pd(0)dppp and (d) Pd(0)NHC.

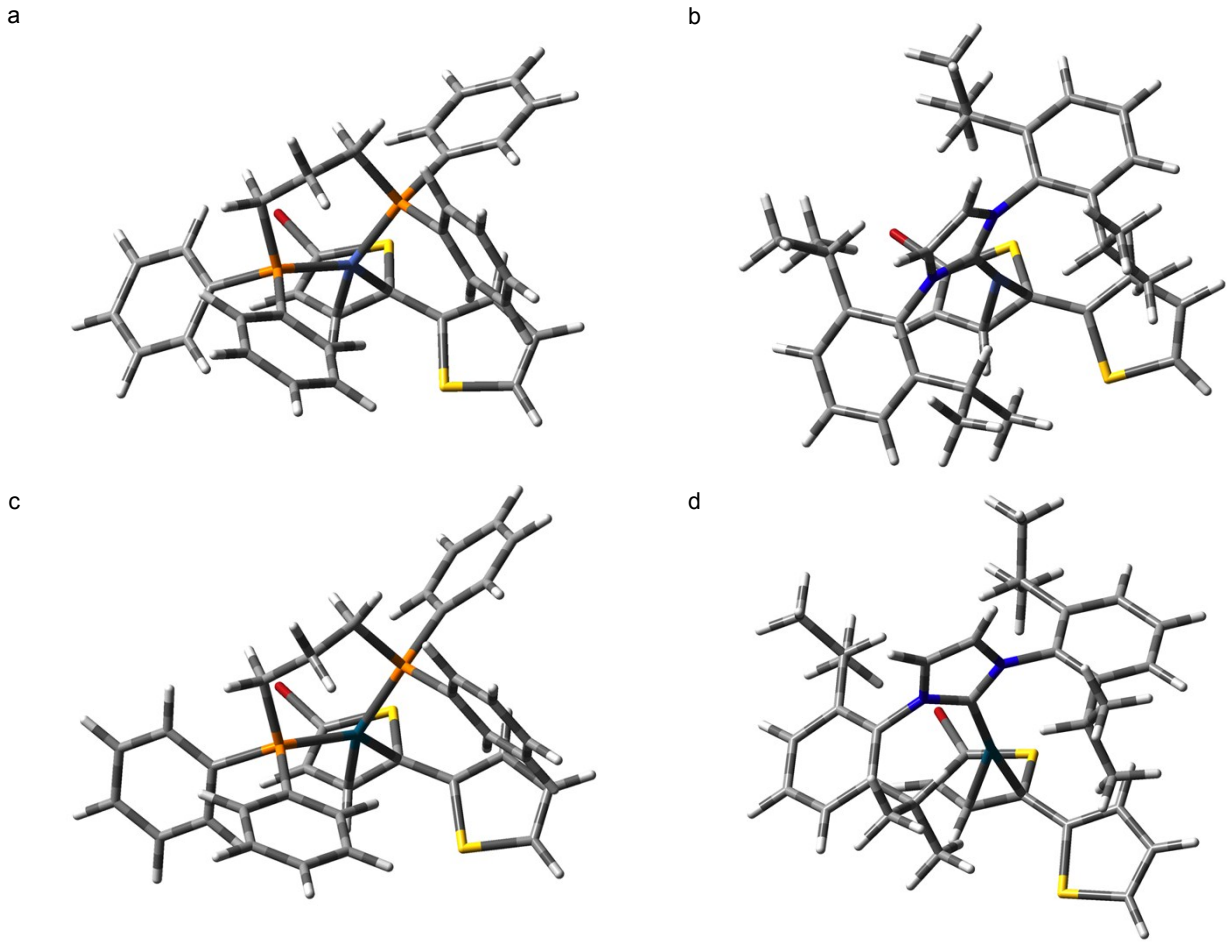

Fig. S20 Optimized geometries of **CP4s** with (a) Ni(0)dppp, (b) Ni(0)NHC, (c) Pd(0)dppp and (d) Pd(0)NHC.

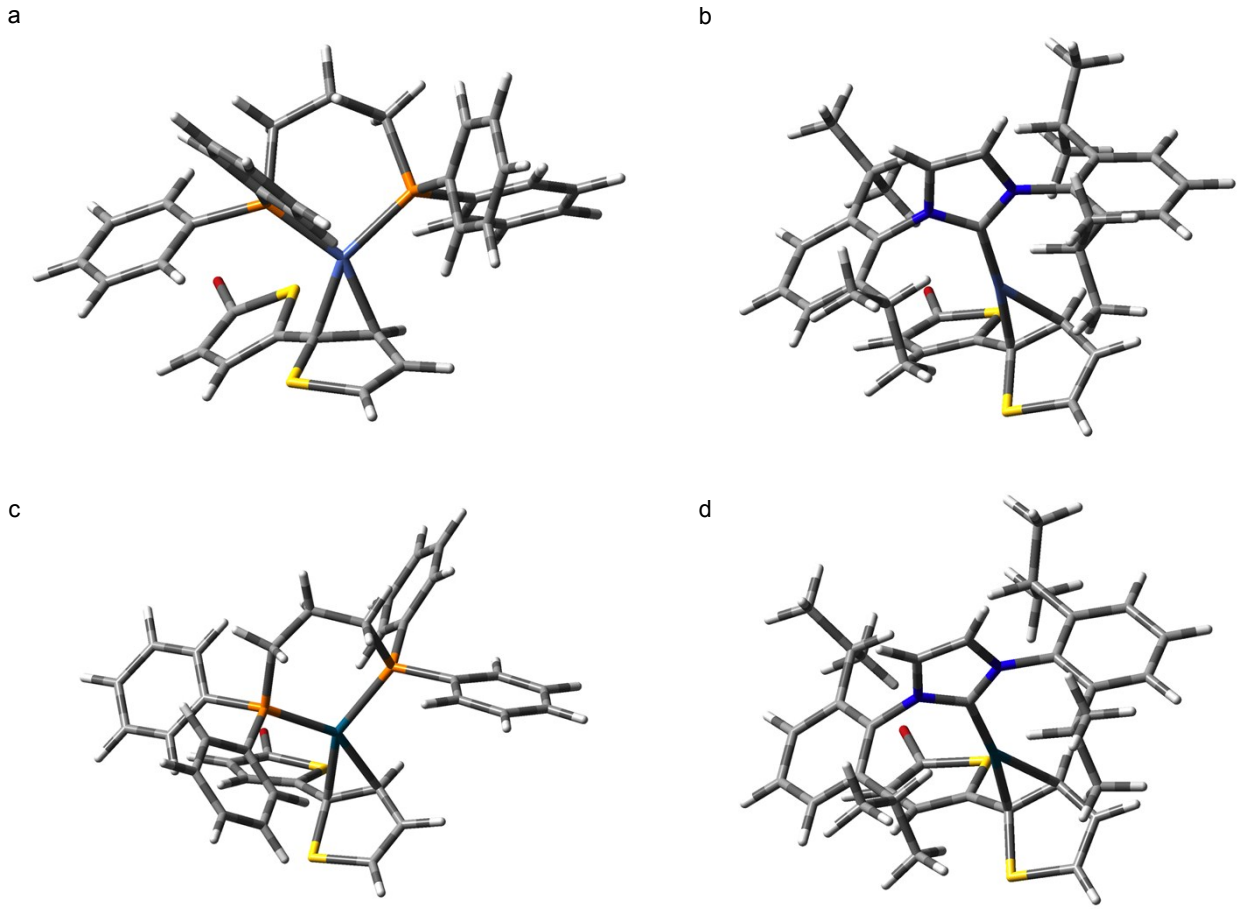

Fig. S21 Optimized geometries of **CP5s** with (a) Ni(0)dppp, (b) Ni(0)NHC, (c) Pd(0)dppp and (d) Pd(0)NHC.

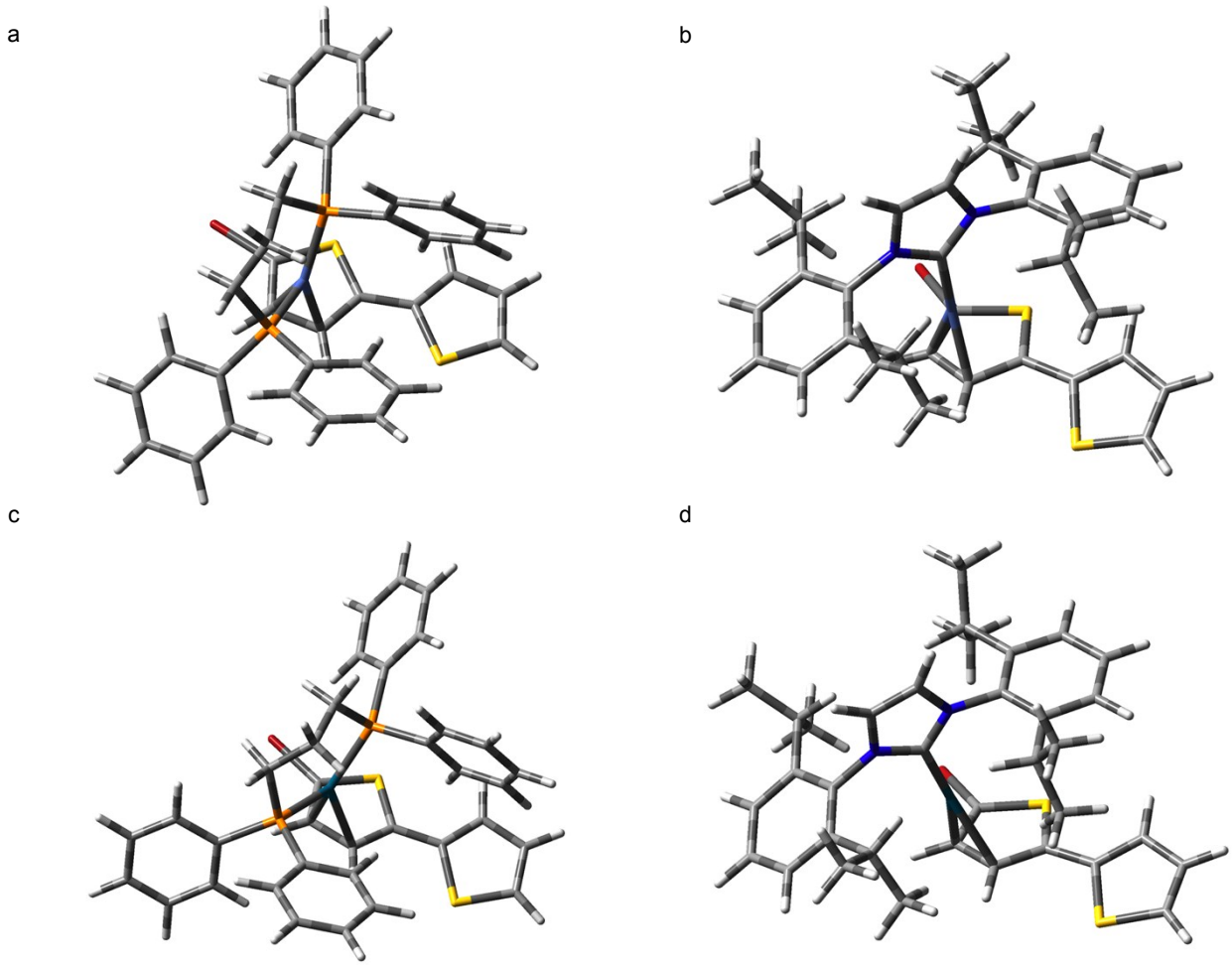

Fig. S22 Optimized geometries of **TS3s** with (a) Ni(0)dppp, (b) Ni(0)NHC, (c) Pd(0)dppp and (d) Pd(0)NHC.

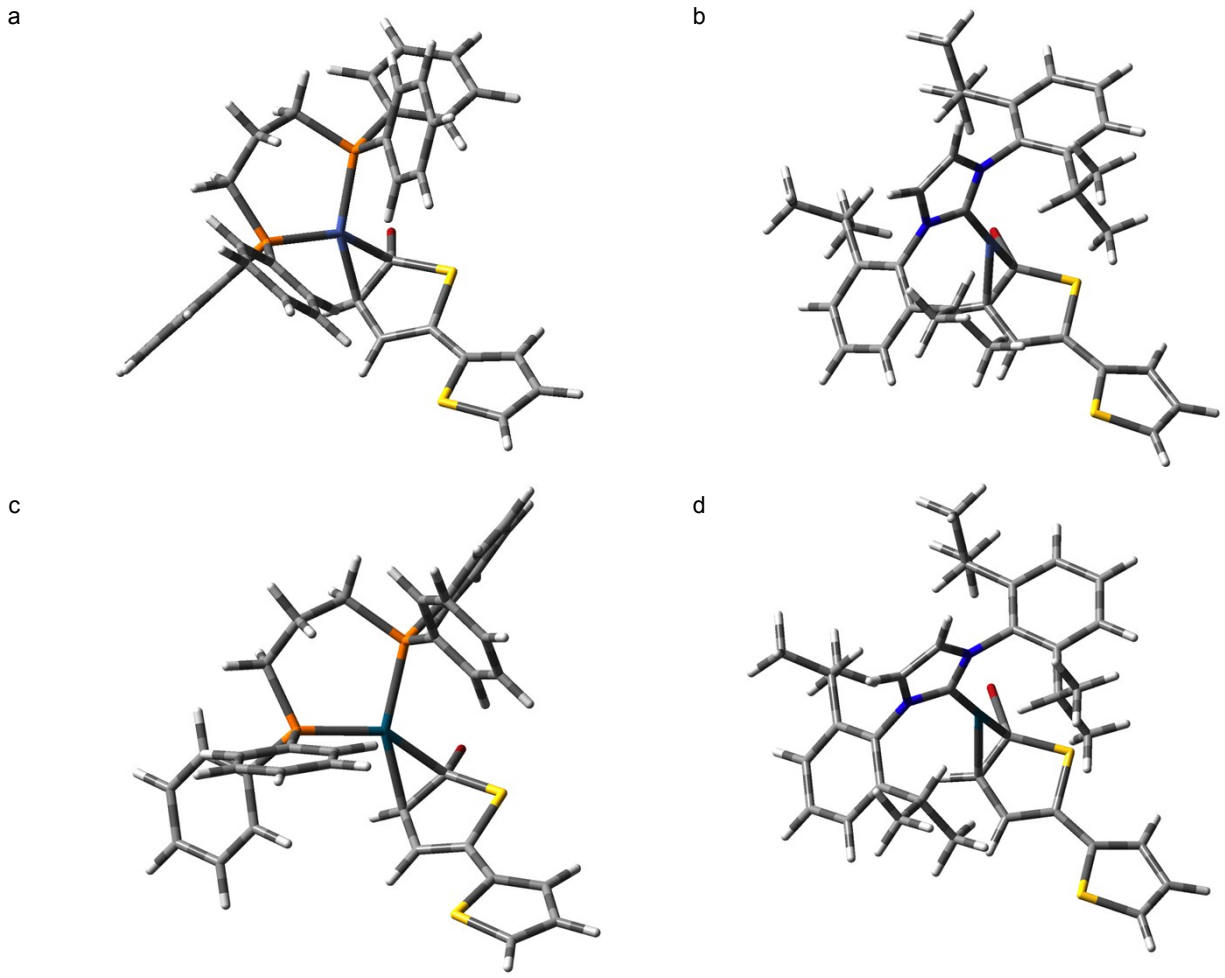

Fig. S23 Optimized geometries of **CP6s** with (a) Ni(0)dppp, (b) Ni(0)NHC, (c) Pd(0)dppp and (d) Pd(0)NHC.

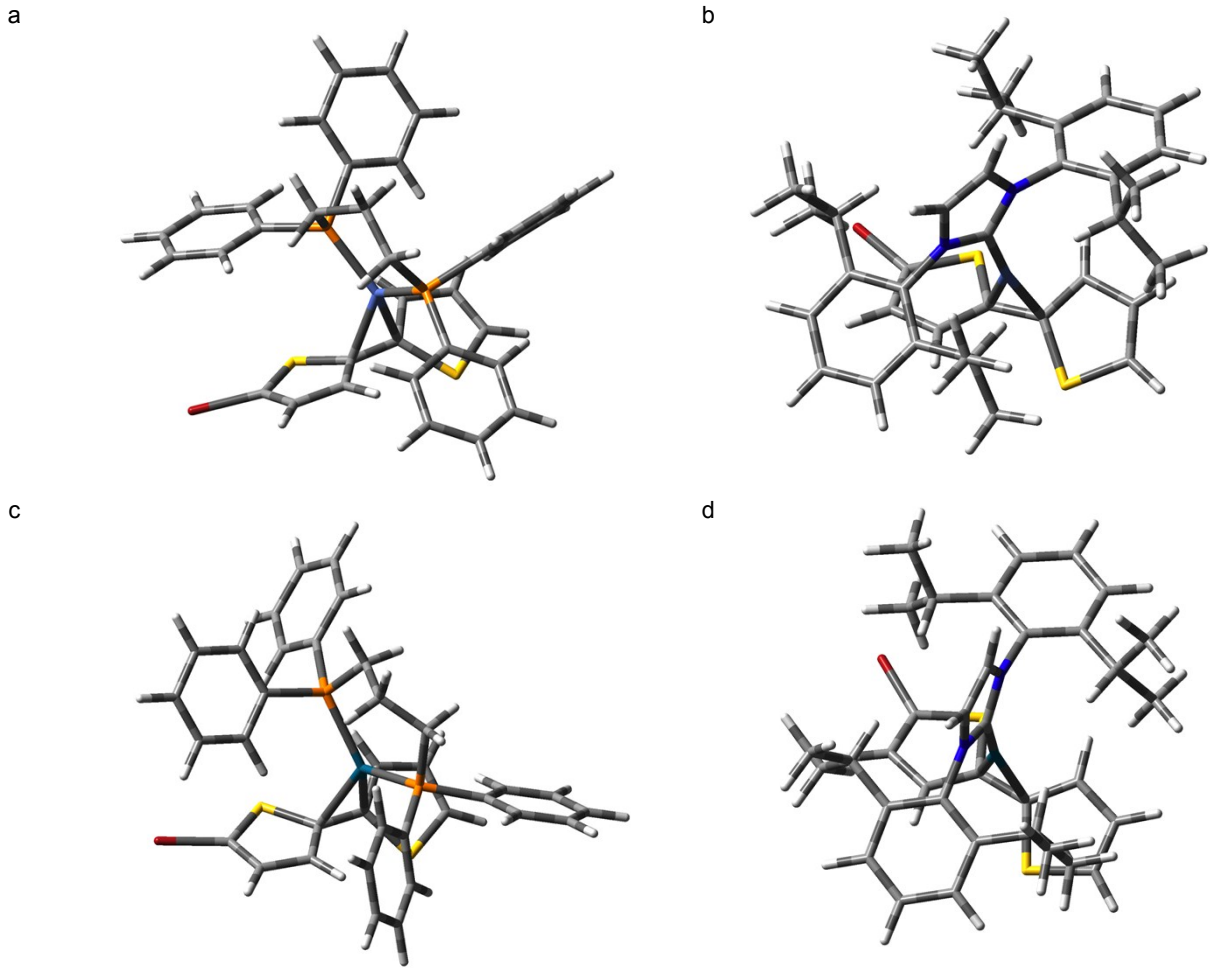

Fig. S24 Optimized geometries of **TS4s** with (a) Ni(0)dppp, (b) Ni(0)NHC, (c) Pd(0)dppp and (d) Pd(0)NHC.

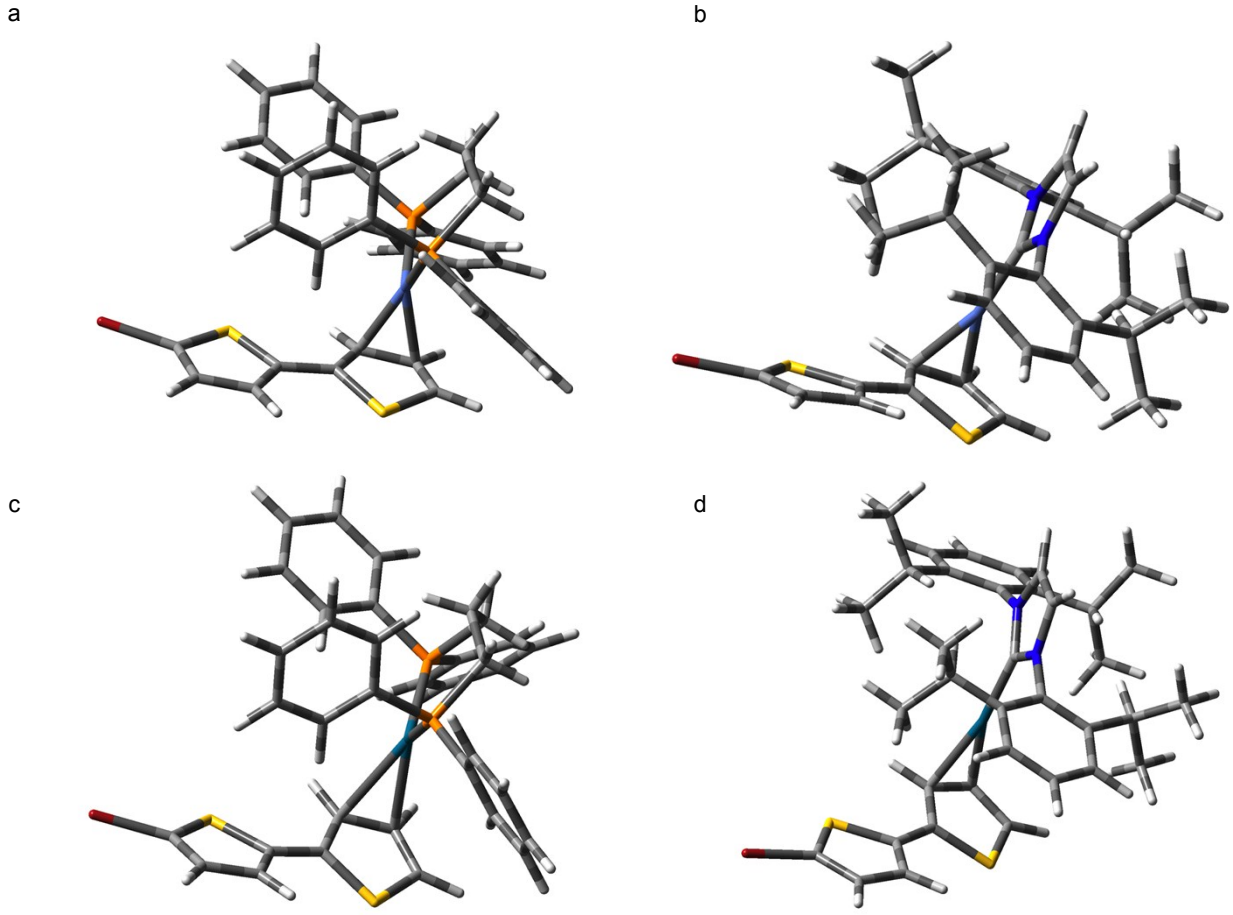

Fig. S25 Optimized geometries of **TS5s** with (a) Ni(0)dppp, (b) Ni(0)NHC, (c) Pd(0)dppp and (d) Pd(0)NHC.

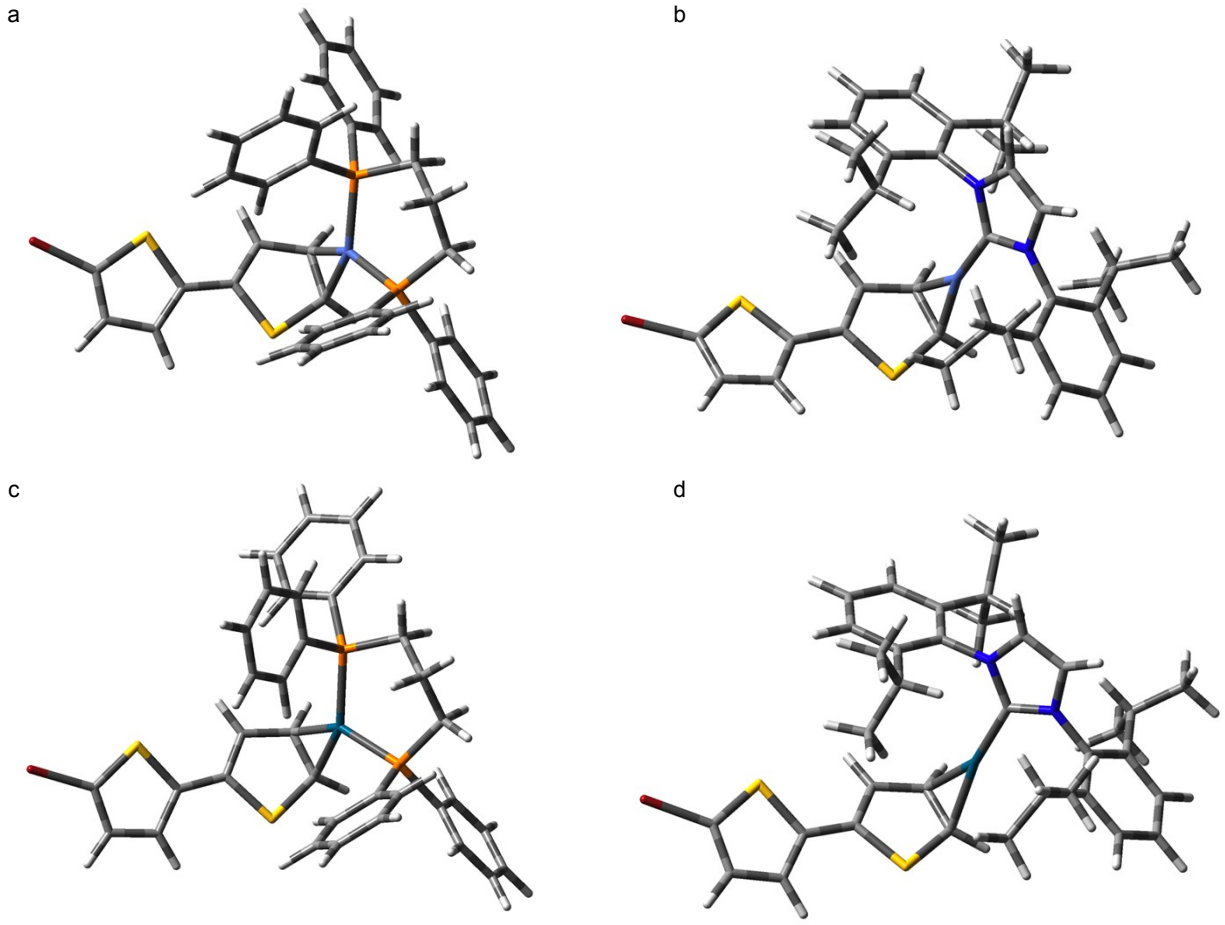

Fig. S26 Optimized geometries of **CP7s** with (a) Ni(0)dppp, (b) Ni(0)NHC, (c) Pd(0)dppp and (d) Pd(0)NHC.

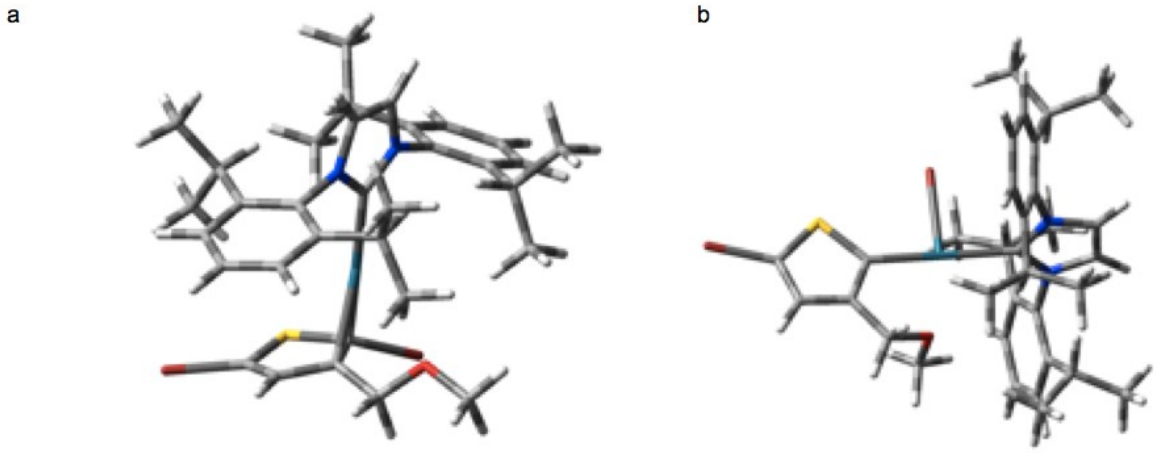

Fig. S27 Optimized geometries of (a) **CP8** and (b) **CP9** with Pd(0)NHC.

7-2. Cartesian Coordinates (in Å) and Energies

SM

Dibromothiophene

Energy (RB3LYP) = -578.100651074622 A.U.
Free Energy = -578.087551752611 A.U.

C	0.71604200	1.57153400	0.00003900
S	0.00001500	-0.92503200	0.00015800
C	-0.71606200	1.57151600	0.00008300
H	1.32221900	2.46931500	-0.00002700
C	-1.22960200	0.30795100	0.00015400
H	-1.32226100	2.46928300	0.00001500
Br	-3.10220300	-0.18131500	-0.00006900
C	1.22960800	0.30797900	0.00006100
Br	3.10220000	-0.18131300	-0.00006100

2-magneciochlorothiophene

Energy (RB3LYP) = -1212.764690363633 A.U.
Free Energy = -1212.741298320730 A.U.

C	0.55966600	0.21982300	-0.00001700
C	1.35795100	1.35095400	-0.00000800
C	2.76299100	1.09693900	0.00000800
C	3.05620300	-0.23983600	0.00001500
S	1.60573800	-1.18676700	-0.00000400
H	0.95470700	2.36065500	-0.00001400
H	3.51911400	1.87541700	0.00001200
H	4.02962100	-0.71269300	0.00002100
Mg	-1.48683300	0.08654000	-0.00000400
Cl	-3.69259600	-0.00828600	0.00000600

Br-Th-Th

Energy (RB3LYP) = -1117.357193399719 A.U.
Free Energy = -1117.291270001274 A.U.

C	-0.73634800	0.27303200	0.10697500
C	-0.18951500	1.51762700	0.29913700
C	1.22875200	1.53251700	0.26592300
S	0.51587400	-0.92360700	-0.13750700
H	-0.79595100	2.40226100	0.48244400
H	1.84265800	2.41706500	0.40657200
C	-2.12816200	-0.11644700	0.07662800
C	-2.68248000	-1.35690200	0.27750800
S	-3.36890500	1.06289900	-0.26134400
C	-4.09658800	-1.36227400	0.17209400
H	-2.08725000	-2.23556500	0.51800800
C	-4.60992600	-0.12878600	-0.10583600
H	-4.71019400	-2.24861000	0.30748300
C	1.73818800	0.28810100	0.04801700
Br	3.59726100	-0.18860000	-0.05555400
H	-5.64842400	0.15596600	-0.23117300

BrMgCl

Energy (RB3LYP) = -673.597620404358 A.U.
Free Energy = -673.622017823457 A.U.

Cl	0.00000000	0.00000000	-2.90701500
Mg	0.00000000	0.00000000	-0.71269200
Br	0.00000000	0.00000000	1.65633000

CPs and TSs with Ni(0)dppp

Ni(0)dppp

Energy (RB3LYP) = -1896.527249213089 A.U.

Free Energy = -1896.137431604210 A.U.

Ni	0.01495000	-0.63595700	-1.01217300
P	-1.81087300	-0.37294600	0.01115800
P	1.82666100	-0.29405200	0.02722900
C	1.32826900	-0.45542400	1.83988000
H	2.12702000	-0.03675600	2.46579300
H	1.26865400	-1.52868200	2.06204700
C	-1.30037600	-0.51334900	1.81761200
H	-1.18285400	-1.58954500	1.99638900
H	-2.12925300	-0.19207900	2.46195800
C	-0.00474700	0.22656200	2.21970900
H	-0.01371000	0.31524200	3.31510300
H	-0.01889700	1.25596200	1.83930300
C	-2.56333400	1.31736000	-0.11804200
C	-2.77361800	1.82338300	-1.41314100
C	-2.90929400	2.12842600	0.97431700
C	-3.33163000	3.08584100	-1.61096000
H	-2.48895600	1.21797000	-2.27063900
C	-3.45664900	3.39960600	0.77826400
H	-2.75271100	1.77895300	1.99023100
C	-3.67351300	3.88018400	-0.51335400
H	-3.49075300	3.45350300	-2.62142800
H	-3.71356900	4.01287500	1.63837900
H	-4.09971100	4.86842600	-0.66459600
C	-3.30237100	-1.48291700	0.02456200
C	-4.54414100	-1.11564600	0.56597000
C	-3.15811700	-2.76939300	-0.51702500
C	-5.61091900	-2.01589500	0.57129100
H	-4.68426200	-0.11858600	0.97480900
C	-4.22142600	-3.67411200	-0.50410500
H	-2.20413600	-3.05393900	-0.95568300
C	-5.45117000	-3.29789100	0.03947000
H	-6.56864500	-1.71567600	0.98933300
H	-4.09202900	-4.66737500	-0.92652000
H	-6.28341600	-3.99705200	0.04300200
C	2.52927000	1.42601000	0.00752200
C	1.71776900	2.46460800	-0.47720600
C	3.81480200	1.74055700	0.47599800
C	2.17296800	3.78475600	-0.48009400
H	0.72604500	2.22965200	-0.85572000
C	4.27319600	3.05890200	0.46498200
H	4.46712500	0.95215200	0.84091200
C	3.45270400	4.08479200	-0.01018000
H	1.52952000	4.57598600	-0.85636800
H	5.27368700	3.28470300	0.82577400
H	3.81189500	5.11068900	-0.01923600
C	3.34810400	-1.35499700	-0.05723900
C	4.06395300	-1.82131300	1.05731600
C	3.78673900	-1.73671200	-1.33650300
C	5.18659400	-2.63796100	0.89580600
H	3.75188300	-1.55303600	2.06209000
C	4.91463400	-2.54010800	-1.50044000
H	3.22781700	-1.40376500	-2.20836000
C	5.61733700	-2.99601200	-0.38222000
H	5.72476700	-2.99239400	1.77147100
H	5.23847500	-2.81976100	-2.49969400
H	6.49042600	-3.63122000	-0.50644100

CP1

Energy (RB3LYP) = -2474.678360319427 A.U.

Free Energy = -2474.253168841656 A.U.

Ni	-0.03786000	-0.03859600	-0.64537800
P	1.42328100	-1.54006300	0.16665700
P	-1.92788800	-1.22845400	-0.44961200
C	-1.64735500	-3.07186700	-0.59374900
H	-2.58801400	-3.60589000	-0.41477200
H	-1.40247500	-3.24287900	-1.65005200
C	0.90739100	-3.31016300	-0.15648200
H	0.99197400	-3.48935500	-1.23565100
H	1.61650800	-3.98454500	0.33817500
C	-0.52792700	-3.64388400	0.29797800
H	-0.62760500	-4.73740200	0.29204500
H	-0.67388100	-3.33639400	1.34131400
C	1.55277100	-1.52594500	2.01154700
C	0.74787600	-0.64753200	2.74984400
C	2.43057600	-2.38130600	2.69917500
C	0.80922600	-0.62921000	4.14591000
H	0.07556100	0.02683300	2.22826600
C	2.49123500	-2.36416500	4.09167600
H	3.08129200	-3.05165800	2.14348100
C	1.67848800	-1.48808700	4.81796400
H	0.17892200	0.05847600	4.70300900
H	3.17592700	-3.02956700	4.61117400
H	1.72926600	-1.47328900	5.90353100
C	3.19788600	-1.52616700	-0.33868100
C	3.74141500	-2.44023600	-1.25285700
C	4.02342700	-0.50391900	0.16146300
C	5.07732000	-2.34092600	-1.64994100
H	3.13204200	-3.23768800	-1.66622900
C	5.35596700	-0.40749000	-0.23412100
H	3.62197700	0.21906100	0.86636000
C	5.88818600	-1.32651600	-1.14205300
H	5.48117100	-3.06009500	-2.35788000
H	5.97829800	0.38925600	0.16438800
H	6.92659200	-1.24942600	-1.45278400
C	-2.86153000	-1.01577700	1.12891600
C	-2.86534200	0.26701300	1.70477500
C	-3.55111200	-2.04709500	1.78583100
C	-3.55149700	0.51382900	2.89429400

H	-2.32227900	1.07333000	1.21921200
C	-4.22970000	-1.80176300	2.98194100
H	-3.56635900	-3.05085600	1.37248500
C	-4.23403900	-0.52123400	3.53716600
H	-3.54492100	1.51303700	3.32136500
H	-4.75498500	-2.61346900	3.47840800
H	-4.76266700	-0.33222200	4.46759800
C	-3.20012200	-0.99106200	-1.77061300
C	-4.58220500	-1.04523400	-1.53935600
C	-2.74030100	-0.76454100	-3.07895400
C	-5.48290500	-0.88200100	-2.59440900
H	-4.95929700	-1.20879300	-0.53427800
C	-3.64094800	-0.61399800	-4.13378600
H	-1.67134300	-0.69731700	-3.26835800
C	-5.01569900	-0.66993900	-3.89262800
H	-6.55159000	-0.92074200	-2.39965400
H	-3.26889600	-0.44143400	-5.14019000
H	-5.71873400	-0.54246700	-4.71141400
C	-0.02110500	3.32978700	0.24637200
C	-1.00431500	2.79421800	-0.50993700
C	-0.52366900	1.76201400	-1.42235200
C	0.88648000	1.52116900	-1.25216100
S	1.58437100	2.66814300	-0.04600600
H	-2.03816400	3.12016200	-0.46670000
H	-1.01815300	1.61795800	-2.37938100
Br	-0.26190000	4.66566100	1.64681300
Br	2.03642200	1.21541600	-2.90050100

CP2

Energy (RB3LYP) = -2474.718558580249 A.U.

Free Energy = -2474.289656515730 A.U.

Ni	-0.29005100	-0.43232000	-0.07045900
P	0.42788900	1.36401400	1.06029400
P	-2.52390800	-0.23150000	0.59610000
C	-2.83294700	0.74358700	2.15714300
H	-3.91296700	0.87965400	2.28162200
H	-2.52147000	0.08097800	2.97483300
C	-0.58744700	1.94165400	2.52463400
H	-0.42667300	1.23590000	3.34723900
H	-0.16380400	2.90066400	2.84365600
C	-2.09427600	2.08681200	2.26873100
H	-2.52286700	2.64202600	3.11352200
H	-2.27130200	2.70536200	1.38031000
C	0.38331100	2.85860200	-0.01220600
C	-0.27024200	2.79420700	-1.25137800
C	0.92016500	4.08615800	0.41159000
C	-0.38502300	3.93264500	-2.05247600
H	-0.68949300	1.85109200	-1.59013300
C	0.80900500	5.22056900	-0.39175100
H	1.44009900	4.15457200	1.36317000
C	0.15542000	5.14566400	-1.62492000
H	-0.89531900	3.86634000	-3.00912000
H	1.23383500	6.16259300	-0.05573400
H	0.07015400	6.03081200	-2.24941400
C	2.10934300	1.31539000	1.80789300
C	2.30026400	0.69832300	3.05477600
C	3.22633800	1.82256400	1.12717800
C	3.57395500	0.61067800	3.61672200
H	1.46284900	0.26485800	3.59356700
C	4.49879500	1.73313800	1.69185800
H	3.10785700	2.27114300	0.14758300
C	4.67656500	1.13117300	2.93816600
H	3.70277700	0.12817800	4.58166900
H	5.35349000	2.12569700	1.14832100
H	5.66951300	1.05801200	3.37288600
C	-3.52698900	0.63951000	-0.68926300
C	-3.35913300	0.26360700	-2.03464000
C	-4.43817100	1.66483600	-0.38596400
C	-4.09107700	0.89329800	-3.04179300
H	-2.65936700	-0.52816400	-2.28574300
C	-5.16396300	2.29666800	-1.39857600
H	-4.59493100	1.98464800	0.63876100
C	-4.99324600	1.91231800	-2.72872300
H	-3.95227000	0.58390200	-4.07417500
H	-5.86287800	3.08880200	-1.14321400
H	-5.55940600	2.40353700	-3.51561200
C	-3.46481400	-1.75749500	1.01376900
C	-4.86180200	-1.81115100	0.90629700
C	-2.77273200	-2.86044300	1.53472800
C	-5.55597800	-2.94879500	1.32159300
H	-5.40960000	-0.97142300	0.48812000
C	-3.47070500	-3.99174700	1.95812900
H	-1.68835500	-2.84538800	1.57753400
C	-4.86220100	-4.03830800	1.85145300
H	-6.63802600	-2.98404600	1.22643300
H	-2.92393000	-4.84334700	2.35340000
H	-5.40349900	-4.92470500	2.17130800
C	3.86736400	-1.22293400	-1.17852800
C	3.46530400	-0.24054000	-2.03381700
C	2.11095200	0.15768300	-1.77741200
C	1.49599700	-0.52333000	-0.75157900
S	2.60692000	-1.69196100	-0.07412900
H	4.09292400	0.18120300	-2.81085600
H	1.61591000	0.92665000	-2.36161600
Br	5.61670500	-2.07845400	-1.14552700
Br	-0.84454500	-2.36631700	-1.43119000

CP3

Energy (RB3LYP) = -3013.888025309811 A.U.

Free Energy = -3013.410125246395 A.U.

Ni	0.20653200	-0.21184300	0.10088800
P	-0.40409400	1.81068800	-0.86223500

P	2.29087700	-0.25628200	-0.92525000
C	2.44357000	0.72964000	-2.51195100
H	3.48281200	0.67605200	-2.85219300
H	1.84760700	0.20414500	-3.26819200
C	0.46480800	2.37435000	-2.41976100
H	0.02065700	1.79443500	-3.23893200
H	0.20193500	3.42014900	-2.61307600
C	1.99054500	2.19578500	-2.42298000
H	2.38903800	2.72687300	-3.29745400
H	2.43646500	2.68465100	-1.54705500
C	0.00847700	3.13661500	0.35433300
C	0.24034000	2.76665200	1.68932800
C	0.11698500	4.49385900	0.00592200
C	0.56569000	3.72560700	2.65054400
H	0.16620400	1.72116100	1.97514800
C	0.44540400	5.45186900	0.96601600
H	-0.06181100	4.81574200	-1.01578100
C	0.66984200	5.06970100	2.29061500
H	0.73894500	3.41856900	3.67820500
H	0.52506300	6.49685900	0.67848300
H	0.92567400	5.81693500	3.03693200
C	-2.15355300	2.10173400	-1.36408900
C	-2.74095000	1.17064900	-2.23603200
C	-2.90763400	3.20505400	-0.94294000
C	-4.04650000	1.35007700	-2.69100300
H	-2.18811300	0.28626200	-2.54108500
C	-4.21740100	3.37960600	-1.39560200
H	-2.48194600	3.92717800	-0.25410800
C	-4.78819800	2.45673200	-2.27222600
H	-4.48921400	0.61578100	-3.35816000
H	-4.79203500	4.23738200	-1.05606300
H	-5.80901400	2.59177100	-2.61912800
C	3.74913500	0.32659100	0.03974400
C	3.59131700	0.62133500	1.40167200
C	5.01370700	0.50755400	-0.54903800
C	4.66888500	1.09223500	2.15582400
H	2.63096500	0.45965700	1.87746700
C	6.08807600	0.97778700	0.20499100
H	5.17204100	0.26824000	-1.59671700
C	5.91637000	1.27455000	1.55989300
H	4.52886300	1.31104700	3.21075200
H	7.05902400	1.11094200	-0.26469700
H	6.75424800	1.64163300	2.14662600
C	2.74785700	-1.92458200	-1.56662400
C	3.87880700	-2.63082100	-1.13721700
C	1.88858700	-2.52625400	-2.50175900
C	4.15456400	-3.90195000	-1.64683700
H	4.54327200	-2.19652600	-0.39802800
C	2.16602300	-3.79441400	-3.01086400
H	0.98535900	-2.01279500	-2.82337800
C	3.30322100	-4.48550400	-2.58531800
H	5.03473200	-4.43774000	-1.30157400
H	1.48962900	-4.24532100	-3.73190700
H	3.51837000	-5.47560300	-2.97776400
C	-3.92161500	-1.40782900	0.81087300
C	-3.77359800	-0.32932000	1.62972200
C	-2.44084600	0.19898200	1.57162300
C	-1.58479500	-0.46506100	0.72287900
S	-2.44066000	-1.80971800	-0.01215000
H	-4.56839600	0.07794300	2.24460200
H	-2.14412000	1.06376000	2.15760300
Br	-5.55075100	-2.44467600	0.54569500
C	0.70253700	-1.63473400	1.28826300
C	1.05994800	-2.95220600	1.10867800
S	0.72001300	-1.28778500	3.01279700
C	1.37493600	-3.66038700	2.31539600
H	1.09393100	-3.42620700	0.13401300
C	1.25737700	-2.88878500	3.43615600
H	1.67844100	-4.70312800	2.33655800
H	1.44187800	-3.16133300	4.46726100

CP4

Energy (RB3LYP) = -3013.923239401618 A.U.

Free Energy = -3013.444334914759 A.U.

Ni	-0.20140900	-0.01919800	0.12711300
P	1.55094500	-0.33327900	-1.22992200
P	-0.95244200	1.91285800	-0.68864700
C	-0.69739600	2.07191700	-2.53930200
H	-1.02777500	3.06522500	-2.86503100
H	-1.35899400	1.34424400	-3.02480300
C	1.23601000	0.36784100	-2.93939900
H	0.47836600	-0.28947000	-3.38524100
H	2.13708100	0.24425800	-3.55200500
C	0.75362500	1.83080700	-2.99629300
H	0.82748100	2.16094600	-4.04137300
H	1.43395000	2.47917400	-2.42990500
C	3.11151000	0.49656900	-0.68525700
C	3.46036200	0.39125100	0.67247000
C	3.95904800	1.22027100	-1.53910200
C	4.62598300	0.98461700	1.15823400
H	2.82242700	-0.16840100	1.34912600
C	5.11887800	1.82576800	-1.04927700
H	3.72631000	1.31763900	-2.59474300
C	5.45621600	1.70871600	0.29988300
H	4.87922000	0.88150400	2.20992500
H	5.75922300	2.38625400	-1.72555500
H	6.36000200	2.17842700	0.67909500
C	2.11105600	-2.03324000	-1.70170800
C	1.11988900	-2.98074800	-2.00867500
C	3.45869000	-2.41608700	-1.78021400
C	1.46859000	-4.27328300	-2.40256500
H	0.07102000	-2.71289400	-1.91949600
C	3.80532900	-3.71311000	-2.16491100
H	4.24100300	-1.70274800	-1.54050900

C	2.81295800	-4.64316200	-2.48040800
H	0.68860100	-4.99344700	-2.63494000
H	4.85380400	-3.99524200	-2.21911000
H	3.08526500	-5.65202500	-2.77918100
C	-0.13685200	3.44995700	-0.06526900
C	0.84325600	3.33204900	0.93084800
C	-0.44108700	4.72783500	-0.56600800
C	1.50757900	4.46235000	1.41446700
H	1.08837300	2.34903200	1.32294500
C	0.22130100	5.85606600	-0.08372700
H	-1.20976400	4.84590600	-1.32536900
C	1.19866100	5.72448200	0.90751300
H	2.26695000	4.35203900	2.18372900
H	-0.02538600	6.83805700	-0.47909300
H	1.71472800	6.60460600	1.28212500
C	-2.75743400	2.28618900	-0.53339800
C	-3.25049100	3.17654600	0.43414500
C	-3.68289300	1.56897400	-1.31196000
C	-4.62473600	3.35873200	0.60337500
H	-2.55999400	3.73709000	1.05663800
C	-5.05559200	1.75643200	-1.14684200
H	-3.33780800	0.84641000	-2.04644700
C	-5.53230200	2.65368400	-0.18850800
H	-4.98417000	4.05564900	1.35615500
H	-5.75213400	1.19439600	-1.76330600
H	-6.60133100	2.79693300	-0.05699700
C	-0.42708000	-1.49657100	1.49218600
C	-1.46996100	-0.50300900	1.59251300
C	-2.74955300	-0.99023600	1.09734600
C	-2.69772400	-2.27400800	0.68247700
S	-1.13145600	-3.04740100	0.85654000
H	-1.45161200	0.27178700	2.35834500
H	-3.64248200	-0.37836800	1.05302600
C	0.72326000	-1.61884900	2.39200700
C	1.75363800	-2.53454300	2.36772900
S	0.94145600	-0.51406600	3.74591400
C	2.71524800	-2.34620600	3.40512800
H	1.82895400	-3.30878000	1.61162800
C	2.42606400	-1.28700900	4.22003200
H	3.59093600	-2.97450200	3.53106300
Br	-4.15327100	-3.25352000	-0.17225800
H	2.97982600	-0.91911400	5.07328000

CP5

Energy (RB3LYP) = -3013.921189211170 A.U.

Free Energy = -3013.441716737629 A.U.

C	4.31203300	1.12917200	0.25079100
C	4.62671000	0.17207800	1.16667500
C	3.47919900	-0.26525100	1.89856400
C	2.30707300	0.35609200	1.53767000
S	2.61253400	1.51222400	0.23819800
H	5.63031500	-0.20266200	1.32875900
H	3.52663900	-1.01124600	2.68354400
Br	5.53599000	2.04097700	-0.95088300
C	0.94492700	0.17600900	2.04263400
C	-0.02395200	1.23374000	2.21000200
S	0.67876900	-1.10197900	3.29509500
C	-0.95198700	0.93371300	3.29110100
H	0.20987400	2.26763800	1.96216200
C	-0.71697800	-0.24026000	3.92593300
H	-1.75280300	1.61022800	3.57678900
H	-1.28626000	-0.68019700	4.73562800
Ni	-0.41797100	0.17693000	0.55339000
P	-0.04410000	-1.57278400	-0.78220100
P	-1.98479500	1.23127500	-0.61185000
C	-0.24733400	-1.12483100	-2.59019900
C	-1.24279800	-2.97312300	-0.61584700
C	1.57809300	-2.45854700	-0.76509200
C	-1.76377100	0.99328000	-2.45620700
C	-3.72861900	0.70793400	-0.28701100
C	-2.06790000	3.08087900	-0.53927200
H	0.56233400	-0.43277700	-2.85186900
H	-0.11198200	-2.02365000	-3.20350100
C	-1.60105700	-0.46638800	-2.92521500
C	-2.27120900	-2.87854300	0.33171600
C	-1.16680600	-4.12414400	-1.41870100
C	2.63562700	-2.09986200	-1.61534400
C	1.80438400	-3.45682400	0.19898500
H	-2.58972000	1.47385500	-2.99430100
H	-0.86406200	1.56699700	-2.71358100
C	-4.07185600	0.40862000	1.04324300
C	-4.71719400	0.58404300	-1.27584300
C	-3.26559400	3.81113100	-0.54663000
C	-0.85126700	3.78188600	-0.48288100
H	-1.70674800	-0.47361900	-4.01838300
H	-2.42328700	-1.08390500	-2.54178300
C	-3.20964000	-3.90492400	0.47015200
H	-2.33296000	-1.99611400	0.96136900
C	-2.10277600	-5.14829500	-1.28189600
H	-0.36339000	-4.22811800	-2.14340200
C	3.87673500	-2.73285700	-1.51800200
H	2.50485600	-1.32052500	-2.35949300
C	3.04390000	-4.08877200	0.29426600
H	1.00487800	-3.74679000	0.87448400
C	-5.36782800	0.01281300	1.37572700
H	-3.31350300	0.48029700	1.81851200
C	-6.01181600	0.17641300	-0.94474500
H	-4.48835200	0.80540200	-2.31375900
C	-3.24538400	5.20724200	-0.50442700
H	-4.21845900	3.29193200	-0.58188200
C	-0.83170400	5.17656700	-0.45383600
H	0.08564300	3.23104100	-0.45589400
C	-3.12797600	-5.03930900	-0.33710900
H	-4.00238800	-3.81389300	1.20783400

H	-2.03136800	-6.03339700	-1.90886500
C	4.08450800	-3.73142400	-0.56626000
H	4.68063000	-2.44114900	-2.18868600
H	3.19536800	-4.86293900	1.04219700
C	-6.34140200	-0.10695000	0.38144100
H	-5.61485000	-0.20911800	2.41074000
H	-6.76233000	0.08248300	-1.72535200
C	-2.03056500	5.89332000	-0.46152600
H	-4.18244300	5.75834400	-0.50629400
H	0.11912200	5.70150100	-0.41379800
H	-3.85638800	-5.83898500	-0.23053300
H	5.04996800	-4.22497100	-0.49276000
H	-7.34926500	-0.42244100	0.63776800
H	-2.01758100	6.97951600	-0.42871400

CP6

Energy (RB3LYP) = -3013.932680227658 A.U.
Free Energy = -3013.453952330182 A.U.

Ni	-0.17071900	-0.49684500	-0.58644900
P	-1.84916500	-1.03464700	0.80365500
P	1.37935500	-1.94783800	0.13522800
C	0.64588000	-3.51514700	0.84486500
H	1.44267700	-4.14601100	1.25628000
H	0.24690100	-4.06221200	-0.01917400
C	-1.82080500	-2.83424700	1.31962800
H	-2.06914800	-3.43649400	0.43669400
H	-2.61231600	-3.00570600	2.05888900
C	-0.46899700	-3.31041900	1.88891200
H	-0.64262600	-4.27701600	2.38026200
H	-0.13233400	-2.62922400	2.68071100
C	-1.75207900	-0.18324100	2.44324200
C	-0.67788700	0.67756000	2.70720900
C	-2.72122200	-0.38360200	3.44102900
C	-0.56618400	1.31725100	3.94475300
H	0.06899400	0.85052500	1.93848500
C	-2.60963800	0.25338600	4.67590100
H	-3.57525500	-1.02726200	3.24627100
C	-1.52960900	1.10447600	4.93041000
H	0.27276400	1.98165200	4.13271900
H	-3.36707400	0.09094600	5.43841700
H	-1.44531800	1.60294200	5.89258400
C	-3.61640900	-0.76699700	0.34369700
C	-4.46972800	-1.80512100	-0.05739700
C	-4.10636500	0.55059900	0.32562200
C	-5.78111100	-1.53491100	-0.45674700
H	-4.12364500	-2.83387700	-0.06440200
C	-5.41513900	0.81810000	-0.07031700
H	-3.46029300	1.37146400	0.62476400
C	-6.25810400	-0.22461800	-0.46327600
H	-6.42803500	-2.35323500	-0.76232100
H	-5.77559400	1.84329100	-0.07657400
H	-7.27782700	-0.01550200	-0.77519500
C	2.51730900	-1.32301400	1.44798000
C	2.89875000	0.02826900	1.37390400
C	3.00948700	-2.10099500	2.50779900
C	3.75859800	0.58142300	2.32320000
H	2.51408700	0.64957300	0.56965600
C	3.86278400	-1.54447200	3.46366700
H	2.73314700	-3.14696100	2.59919400
C	4.24122100	-0.20401200	3.37236200
H	4.04184800	1.62756600	2.24431900
H	4.23101000	-2.16095500	4.27959700
H	4.90504800	0.22670800	4.11723100
C	2.50537300	-2.66995100	-1.14225700
C	3.85010100	-2.98883000	-0.90443800
C	1.96302700	-2.92560800	-2.41307400
C	4.63202300	-3.55559000	-1.91362400
H	4.29225400	-2.78978000	0.06718000
C	2.74174900	-3.50307900	-3.41636000
H	0.92786400	-2.66176600	-2.61785200
C	4.08018700	-3.81710000	-3.16889300
H	5.67452400	-3.79235000	-1.71688800
H	2.30642600	-3.69599700	-4.39328000
H	4.69111400	-4.25717500	-3.95251700
C	0.83129100	2.80526700	-1.26591400
C	1.48867600	1.71220300	-1.75549700
C	0.64596600	0.58662500	-2.10330100
C	-0.73749400	0.85454300	-1.81765100
S	-0.93032100	2.53573800	-1.21007000
H	2.56344700	1.70563700	-1.91768300
H	0.95088700	-0.10780200	-2.88091800
C	1.38545600	4.05811100	-0.79412100
C	0.75621200	5.27156100	-0.61316400
S	3.08405700	4.19319200	-0.35498300
C	1.62287100	6.30214300	-0.14668000
H	-0.29592600	5.42149200	-0.83015800
C	2.91023200	5.87781400	0.03331700
H	1.29914200	7.32085200	0.03854300
Br	-2.15015700	0.24555100	-3.15113200
H	3.76770600	6.44816100	0.36420800

CP7

Energy (RB3LYP) = -3013.926605224619 A.U.
Free Energy = -3013.448679807625 A.U.

Ni	1.28606000	0.29237800	-0.85342700
P	2.96580300	-0.69117500	0.20857700
P	1.16464800	2.20886500	0.27136100
C	2.81772800	2.75860000	0.96110400
H	2.68424800	3.65002400	1.58520300
H	3.40670500	3.08339500	0.09352300
C	4.19750000	0.55189700	0.87848400
H	4.68913900	0.98306500	-0.00322600

H	4.98456300	0.03042600	1.43594000
C	3.59232300	1.67809900	1.74036700
H	4.42004100	2.17723500	2.26233800
H	2.95618700	1.25251000	2.52719700
C	2.51225000	-1.70706400	1.68428800
C	1.29861100	-2.41365300	1.62617300
C	3.29157000	-1.80604400	2.84846800
C	0.88341700	-3.20546800	2.69767300
H	0.67917400	-2.34298200	0.73595300
C	2.87014100	-2.59102100	3.92405800
H	4.23485300	-1.27405800	2.92756200
C	1.66622700	-3.29382000	3.85048100
H	-0.05661000	-3.74689700	2.63262200
H	3.48422800	-2.65245100	4.81890500
H	1.33915900	-3.90394100	4.68831300
C	4.11069200	-1.78327800	-0.75438500
C	4.43075500	-1.38764100	-2.06429400
C	4.67280000	-2.96652100	-0.25374200
C	5.30600300	-2.14208500	-2.84562800
H	3.98159700	-0.48559800	-2.47420700
C	5.53882800	-3.72920500	-1.04113600
H	4.43149500	-3.29882700	0.75127200
C	5.86098400	-3.31823100	-2.33546500
H	5.54504300	-1.81870000	-3.85550200
H	5.96177400	-4.64685600	-0.64021100
H	6.53458600	-3.91368400	-2.94598800
C	0.05506700	2.15955100	1.74706800
C	-1.03464000	1.27356100	1.70114400
C	0.23498700	2.94223400	2.89937500
C	-1.92623000	1.18094200	2.77096300
H	-1.18266600	0.65442600	0.82056100
C	-0.65109200	2.84252100	3.97390600
H	1.06504500	3.63943900	2.96717700
C	-1.73437500	1.96350300	3.91099300
H	-2.76591700	0.49399100	2.71191100
H	-0.49488400	3.45330800	4.85941600
H	-2.42368700	1.88784000	4.74778000
C	0.66733300	3.75115000	-0.62658500
C	-0.24127000	4.69537100	-0.12752000
C	1.23383700	3.96829400	-1.89477900
C	-0.56646200	5.83126800	-0.87371000
H	-0.70151400	4.54519900	0.84405500
C	0.91995500	5.10888900	-2.63311800
H	1.91943300	3.23176100	-2.30870400
C	0.01521000	6.04414000	-2.12403000
H	-1.27656100	6.55071800	-0.47392500
H	1.37201000	5.26197300	-3.60973600
H	-0.23913800	6.92858700	-2.70197400
C	-1.77007100	-1.02590500	-1.77434000
C	-1.36517600	0.24153700	-2.09032500
C	0.03027700	0.37082400	-2.44412900
C	0.72862400	-0.87910100	-2.35422300
S	-0.43033300	-2.18870000	-1.92952100
H	-2.04579500	1.08896600	-2.09114300
H	0.36754500	1.19228800	-3.07246000
C	-3.07429200	-1.47495400	-1.33629900
C	-3.57665100	-2.75761800	-1.27731700
S	-4.28610800	-0.32462800	-0.76824400
C	-4.91933500	-2.83970900	-0.80345500
H	-3.00154600	-3.62437500	-1.58459100
C	-5.42637800	-1.61091300	-0.49835100
H	-5.47618500	-3.76366000	-0.70370800
Br	-7.20927500	-1.22194600	0.15893000
H	1.53404600	-1.18460200	-3.01604800

TS1

Energy (RB3LYP) = –2474.667287331640 A.U.

Free Energy = –2474.242280460076 A.U.

Ni	0.31288000	-0.46831500	-0.37341500
P	-0.64929300	1.39360300	-1.22708300
P	2.46109300	0.23458500	-0.31938500
C	2.85196400	1.43873600	-1.69116100
H	3.88692700	1.78757100	-1.59257500
H	2.82030300	0.84173500	-2.61169200
C	0.49613400	2.32508100	-2.38229400
H	0.59370600	1.71013400	-3.28532100
H	0.00959400	3.25687500	-2.69276500
C	1.89367400	2.64026200	-1.81332500
H	2.36421100	3.36682500	-2.48922300
H	1.79758400	3.15108800	-0.84677600
C	-1.02159900	2.65235000	0.07298500
C	-1.03076800	2.24355700	1.41501400
C	-1.29286700	3.99933500	-0.22353400
C	-1.30203100	3.15654200	2.43682200
H	-0.82674400	1.20368400	1.65398100
C	-1.55770100	4.91260700	0.79690600
H	-1.31220200	4.33946000	-1.25531900
C	-1.56204100	4.49229300	2.12986500
H	-1.30799100	2.82175100	3.47045200
H	-1.76423800	5.95118500	0.55178700
H	-1.76989600	5.20453000	2.92400500
C	-2.19379100	1.31723900	-2.23464700
C	-2.15867400	0.65825600	-3.47610100
C	-3.41879600	1.82907100	-1.77899700
C	-3.31039800	0.54488600	-4.25338000
H	-1.23570700	0.20895600	-3.83012800
C	-4.57298400	1.70494600	-2.55569200
H	-3.47635200	2.32754600	-0.81714900
C	-4.52169000	1.06933200	-3.79638100
H	-3.26294500	0.03360000	-5.21107500
H	-5.51282900	2.10683900	-2.18620300
H	-5.42050800	0.97381700	-4.39962900
C	2.96613800	1.09811800	1.23042900
C	2.43671400	0.61028900	2.43737600

C	3.83873800	2.19660300	1.27516100
C	2.78585700	1.19204600	3.65596800
H	1.74260900	-0.22615200	2.41351300
C	4.17908200	2.78629000	2.49500900
H	4.25969400	2.60417400	0.36094800
C	3.65701700	2.28336900	3.68746000
H	2.37043500	0.79845400	4.57983000
H	4.85294000	3.63886400	2.51105300
H	3.92322400	2.74265400	4.63562900
C	3.77023000	-1.04265900	-0.58002500
C	5.09848300	-0.87115900	-0.16014900
C	3.41345300	-2.22157800	-1.25407400
C	6.05216500	-1.85701500	-0.41648000
H	5.38788100	0.02615800	0.37948100
C	4.37235000	-3.20264000	-1.51575400
H	2.38388500	-2.37319200	-1.56978500
C	5.69169800	-3.02277400	-1.09695500
H	7.07660100	-1.71593900	-0.08163500
H	4.08302000	-4.10988700	-2.03922600
H	6.43589500	-3.78999900	-1.29366900
C	-2.27071700	-2.09494500	2.09762400
C	-0.96709100	-2.46339600	2.20062800
C	-0.25120800	-2.27943900	0.96136700
C	-1.04175400	-1.66679900	-0.02652700
S	-2.70472500	-1.44286500	0.52450600
H	-0.53931200	-2.91773200	3.08733600
H	0.67290000	-2.80120700	0.74454300
Br	-3.61374800	-2.22484000	3.49942900
Br	-0.58831600	-2.51684000	-2.11864800

TS2

Energy (RB3LYP) = –3013.872841600292 A.U.

Free Energy = -3013.395035631298 A.U.

Ni	0.07849700	-0.18839200	0.14444600
P	-0.28484400	1.89597300	-0.77762400
P	2.01518700	-0.63751500	-1.01317500
C	2.00825300	0.12031400	-2.72446700
H	2.93128800	-0.16657700	-3.24187400
H	1.17312600	-0.32133300	-3.28207800
C	0.43679800	2.18102300	-2.48077100
H	-0.26129600	1.68331200	-3.16665000
H	0.38171900	3.24977400	-2.72171200
C	1.86299700	1.65436700	-2.72861600
H	2.17463900	2.01357300	-3.71854800
H	2.56752600	2.09820300	-2.01477600
C	0.57106500	3.13081600	0.30008200
C	0.33856800	3.04224500	1.68472200
C	1.43797200	4.12969700	-0.16852900
C	0.94762500	3.93012700	2.57075000
H	-0.32450600	2.27150500	2.06778500
C	2.05559100	5.01397900	0.72050700
H	1.64172800	4.22988800	-1.22983900
C	1.81171300	4.91786900	2.09063500
H	0.75172300	3.84587200	3.63624300
H	2.72677000	5.77849600	0.33788200
H	2.29184600	5.60658600	2.78056900
C	-1.95499600	2.65187000	-1.01985700
C	-3.05019000	1.80578900	-1.24716000
C	-2.15579800	4.04192700	-1.02748900
C	-4.31833200	2.33873100	-1.48978700
H	-2.91583800	0.72941200	-1.22351300
C	-3.42395500	4.57195500	-1.26573100
H	-1.32315200	4.71330900	-0.83723900
C	-4.50748800	3.72108300	-1.49936400
H	-5.15718600	1.66895800	-1.65785100
H	-3.56648000	5.64963000	-1.26590500
H	-5.49568700	4.13554300	-1.68113700
C	3.63878000	-0.04618500	-0.35926000
C	3.65529800	0.84107600	0.72616000
C	4.85913400	-0.43401700	-0.93906300
C	4.86582700	1.33881000	1.21700300
H	2.72114800	1.13600100	1.19278700
C	6.06571700	0.06154200	-0.44776300
H	4.86599400	-1.13680200	-1.76809600
C	6.07054300	0.95111000	0.63138500
H	4.86165800	2.02533700	2.05918000
H	7.00280400	-0.24786100	-0.90340300
H	7.01233900	1.33480500	1.01502400
C	2.34623800	-2.41807900	-1.35619300
C	2.86457500	-3.21883500	-0.32267800
C	2.01945600	-3.02926200	-2.57738100
C	3.07107700	-4.58428200	-0.51655000
H	3.11244500	-2.77334800	0.63558800
C	2.22210800	-4.39819100	-2.76690800
H	1.60789600	-2.44591800	-3.39484700
C	2.75136400	-5.17922600	-1.73900900
H	3.47846000	-5.18458400	0.29263900
H	1.96788600	-4.85072600	-3.72184200
H	2.91032100	-6.24386900	-1.88780800
C	-3.95412500	-1.44759400	0.59558500
C	-3.81122600	-0.61882800	1.67095500
C	-2.45463100	-0.23551700	1.88181700
C	-1.54778600	-0.75008100	0.96433200
S	-2.43126200	-1.78081400	-0.19091300
H	-4.63743200	-0.29866600	2.29591700
H	-2.14429000	0.37267100	2.72490300
Br	-5.61531200	-2.22386600	-0.05605400
C	0.08172300	-1.46547400	1.56505700
C	0.19267600	-2.84365100	1.68856400
S	0.77262100	-0.71347200	3.02092800
C	0.82413800	-3.28050800	2.88920600
H	-0.20902800	-3.52599400	0.94807500
C	1.19581800	-2.25615800	3.71671300
H	0.98597700	-4.32700900	3.13010900

H	1.68955300	-2.30882300	4.67816500

TS3

Energy (RB3LYP) = -3013.907788216182 A.U.
Free Energy = -3013.427909077884 A.U.

Ni	-0.14052300	-0.49667600	0.04186800
P	1.17746300	0.47264100	-1.44281300
P	-2.12524100	-0.20107500	-0.87380900
C	-2.02871700	-0.30238500	-2.74491100
H	-3.02024100	-0.10576000	-3.17005300
H	-1.76707000	-1.33447000	-3.00742800
C	0.48152900	0.28066600	-3.17425000
H	0.62778900	-0.77828300	-3.42374600
H	1.10661500	0.84386400	-3.87799300
C	-0.99988800	0.66053000	-3.36825900
H	-1.19089500	0.68773400	-4.44986000
H	-1.18186700	1.68090500	-3.00805800
C	1.31898400	2.30611500	-1.22268900
C	1.54626500	2.77878100	0.08100600
C	1.21564000	3.24282700	-2.26315500
C	1.67629900	4.14416800	0.33624700
H	1.61973100	2.07142500	0.90166100
C	1.33309800	4.61164400	-2.00647000
H	1.04444800	2.91643800	-3.28425200
C	1.56534300	5.06588400	-0.70753600
H	1.85527400	4.48211700	1.35349500
H	1.24434800	5.32140500	-2.82508200
H	1.65725300	6.13079300	-0.51023200
C	2.93220200	-0.03268500	-1.77883900
C	3.25303000	-1.39371700	-1.66044900
C	3.93687900	0.86546300	-2.17095300
C	4.54041000	-1.85055700	-1.94608000
H	2.49287300	-2.09639800	-1.33282100
C	5.22778500	0.40928900	-2.44539700
H	3.71551700	1.92471600	-2.25942900
C	5.53226700	-0.94919400	-2.33742300
H	4.76913800	-2.90861100	-1.84874800
H	5.99625100	1.11792200	-2.74432500
H	6.53818700	-1.30169800	-2.55033100
C	-3.00180900	1.41727100	-0.65673700
C	-2.38965200	2.41018100	0.12105300
C	-4.23674800	1.70283900	-1.26538700
C	-2.99289800	3.66015900	0.28669300
H	-1.43286700	2.20252900	0.59151500
C	-4.84016200	2.94888300	-1.09963200
H	-4.73802000	0.94328600	-1.85998300
C	-4.21746500	3.93126900	-0.32318100
H	-2.50107800	4.41843000	0.88987700
H	-5.79615400	3.15439500	-1.57461700
H	-4.68830900	4.90261400	-0.19553100
C	-3.44950000	-1.43903000	-0.49416700
C	-4.46653400	-1.16931900	0.43802300
C	-3.36639700	-2.74000300	-1.02435100
C	-5.38086500	-2.15768500	0.80827300
H	-4.55409900	-0.17689600	0.86990000
C	-4.28428000	-3.72536000	-0.65849500
H	-2.57687300	-2.99449200	-1.72663700
C	-5.29756500	-3.43799800	0.25882000
H	-6.16208000	-1.92258900	1.52676200
H	-4.20451300	-4.71994600	-1.08979700
H	-6.01073100	-4.20589300	0.54580400
C	0.81939500	-0.45672400	2.40940600
C	-0.44732800	-0.96535900	2.08243800
C	-0.38317100	-2.20349900	1.35801200
C	0.92751000	-2.57661200	1.12594000
S	2.10920500	-1.64200700	2.04322800
H	-1.37481700	-0.53818900	2.44758400
H	-1.24492500	-2.79475700	1.07459800
C	1.13514000	0.72669500	3.17728200
C	2.37235600	1.20918700	3.55920300
S	-0.13325500	1.78928300	3.77913200
C	2.30705000	2.40966300	4.32455700
H	3.30204000	0.71881400	3.29071400
C	1.02776000	2.84895500	4.52464600
H	3.18175200	2.92267100	4.71009800
Br	1.45553700	-4.29111600	0.36086800
H	0.68985200	3.72197100	5.06638400

TS4

Energy (RB3LYP) = –3013.907241709024 A.U.
Free Energy = -3013.426547463246 A.U.

C	3.32726300	-2.09862100	0.29992400
C	2.28546300	-2.73000600	-0.31350700
C	1.02943400	-2.39038700	0.27668800
C	1.13385300	-1.46803000	1.31875800
S	2.84373700	-1.06900900	1.61191400
H	2.40173200	-3.42044800	-1.14026800
H	0.09876600	-2.87672000	0.01264500
Br	5.20138100	-2.26889700	-0.18170200
C	0.06463800	-0.99743100	2.18945000
C	-0.02748400	0.27938900	2.76236500
S	-1.15509000	-2.07474800	2.90931600
C	-1.10568500	0.39319800	3.69555400
H	0.72318700	1.04542300	2.61422900
C	-1.79564100	-0.77365500	3.86983600
H	-1.34186000	1.30959900	4.22652000
H	-2.65104400	-0.95062400	4.50919500
Ni	-0.20299600	-0.11044700	0.31239700
P	-1.98961200	-0.64136200	-0.90042700
P	0.59140200	1.69099600	-0.69942300
C	-1.77240900	-0.06383200	-2.67539100
C	-3.61305800	0.13280100	-0.43642800

C	-2.49804600	-2.40807000	-1.18988900
C	0.18296900	1.65530100	-2.53311800
C	-0.12574500	3.34711900	-0.25435100
C	2.40783500	2.06859300	-0.73112000
H	-1.03035000	-0.72739200	-3.13495300
H	-2.70505100	-0.21706000	-3.23020700
C	-1.30700700	1.39697500	-2.83534400
C	-3.75851200	0.62940700	0.86735200
C	-4.70576200	0.22947200	-1.31426500
C	-1.72464900	-3.24082100	-2.01940200
C	-3.58140000	-2.98434500	-0.50544800
H	0.49452800	2.60245700	-2.98934300
H	0.78585400	0.86443400	-2.99533700
C	-1.13900700	3.41253000	0.71128400
C	0.28302200	4.53796300	-0.88004500
C	2.97637700	2.93103900	0.22238900
C	3.27093800	1.40099300	-1.61577100
H	-1.48365000	1.68305400	-3.88100000
H	-1.93767500	2.06562900	-2.23500300
C	-4.95884300	1.21234500	1.28261200
H	-2.92699400	0.54723200	1.56142300
C	-5.90129700	0.82078800	-0.90513300
H	-4.63543900	-0.16913500	-2.32239100
C	-2.03756000	-4.59179700	-2.17825500
H	-0.86594000	-2.83737400	-2.54992400
C	-3.89031300	-4.33718200	-0.65872800
H	-4.19428200	-2.37124600	0.14772300
C	-1.73468000	4.63297200	1.04307400
H	-1.45985700	2.49700600	1.19823000
C	-0.30750000	5.75681600	-0.54861300
H	1.07904900	4.51576900	-1.61973700
C	4.35588100	3.13272100	0.27630100
H	2.33579300	3.46047500	0.92198600
C	4.65077600	1.60508200	-1.56445800
H	2.87360300	0.70601800	-2.34988200
C	-6.03037800	1.31565000	0.39536700
H	-5.05324400	1.58673400	2.29888300
H	-6.73439000	0.89072400	-1.59997900
C	-3.12369100	-5.14658800	-1.49849900
H	-1.43041500	-5.21061200	-2.83436500
H	-4.73661000	-4.75736200	-0.12101900
C	-1.32036200	5.80667100	0.41408600
H	-2.52273400	4.66319600	1.79118000
H	0.02233200	6.66864500	-1.04014000
C	5.19959100	2.47315500	-0.61949800
H	4.77079200	3.80917600	1.01943600
H	5.29690500	1.07788600	-2.26128700
H	-6.96272400	1.77478500	0.71375800
H	-3.36698500	-6.19868500	-1.61966800
H	-1.78109600	6.75701700	0.67112400
H	6.27409800	2.62964900	-0.57795500

TS5

Energy (RB3LYP) = -3013.907253938963 A.U.

Free Energy = -3013.430103025902 A.U.

Ni	-1.16322500	0.02101100	-0.71215400
P	-1.60709100	1.68628900	0.65427700
P	-1.86257600	-1.72438300	0.42384700
C	-3.34120900	-1.29393600	1.49765200
H	-3.61090600	-2.16446700	2.10756200
H	-4.19064500	-1.09267200	0.83389700
C	-3.11081300	1.29793200	1.70791300
H	-3.96686000	1.36329000	1.02385400
H	-3.25546400	2.09677600	2.44527300
C	-3.10984800	-0.07403500	2.41100500
H	-3.91925500	-0.06256300	3.15374600
H	-2.18277900	-0.20684900	2.98325600
C	-0.27442400	2.02123300	1.89642900
C	1.05368200	1.97425000	1.43970500
C	-0.50402300	2.31054400	3.25100500
C	2.11937200	2.21949800	2.30640400
H	1.25189500	1.73769500	0.39829900
C	0.56298500	2.54393800	4.12254000
H	-1.51626700	2.35791500	3.64073700
C	1.87656300	2.50124100	3.65267800
H	3.13735500	2.17915000	1.92818000
H	0.36478800	2.76009100	5.16931400
H	2.70524700	2.68269100	4.33209800
C	-2.08907100	3.39222300	0.09090500
C	-2.93274200	3.49622300	-1.02679600
C	-1.67484700	4.57078000	0.72894400
C	-3.36970500	4.74030400	-1.48164500
H	-3.23643100	2.59191800	-1.54862600
C	-2.10010500	5.81805200	0.26475700
H	-1.01585700	4.51951200	1.59001600
C	-2.95138000	5.90706400	-0.83743600
H	-4.02685200	4.79999100	-2.34573500
H	-1.76482000	6.72132300	0.76838900
H	-3.28129600	6.87831100	-1.19671500
C	-0.74828100	-2.50897000	1.68066800
C	0.52261800	-1.95425700	1.88677200
C	-1.13649500	-3.61358400	2.45913100
C	1.38713000	-2.48672900	2.84754200
H	0.83109300	-1.09826600	1.29355000
C	-0.27458600	-4.14674900	3.41674000
H	-2.11127300	-4.06993000	2.30625700
C	0.98990600	-3.58262100	3.61325700
H	2.36804400	-2.04268700	2.99332800
H	-0.58737900	-5.00291300	4.00916600
H	1.66110400	-3.99932100	4.35978500
C	-2.48817400	-3.18425500	-0.52971200
C	-1.66748800	-4.29941500	-0.77581100
C	-3.74159700	-3.13433000	-1.16711200
C	-2.09336300	-5.33475400	-1.60992300

H	-0.69279800	-4.36715700	-0.30156000
C	-4.16928200	-4.17231400	-1.99627200
H	-4.39561200	-2.27888000	-1.01982800
C	-3.34732200	-5.27880000	-2.22079600
H	-1.44245800	-6.18895500	-1.77862200
H	-5.14732000	-4.11494200	-2.46752100
H	-3.67938700	-6.08619300	-2.86771100
C	0.85778300	0.41712100	-2.26827500
C	0.05464200	-0.73454100	-2.28992900
C	-1.25443500	-0.48381400	-2.82325800
C	-1.43598500	0.84547300	-3.15755000
S	0.05477500	1.77380900	-3.10704500
H	0.43089200	-1.72737500	-2.06925000
H	-2.00594200	-1.25202600	-2.96564600
C	2.24142200	0.53126600	-1.87477600
C	3.07597800	1.63168100	-1.93270000
S	3.11493700	-0.85343900	-1.21283400
C	4.39992500	1.38748300	-1.46315900
H	2.74849300	2.59689200	-2.30377700
C	4.56316800	0.09961400	-1.04452000
H	5.18563700	2.13316100	-1.44100000
Br	6.17784500	-0.69227000	-0.31973500
H	-2.31962300	1.28623700	-3.59975800

CPs and TSs with Ni(0)NHC

Ni(0)NHC

Energy (RB3LYP) = -1329.315385641056A.U.

Free Energy = -1328.807160728671 A.U.

Ni	-0.00001400	-0.00001000	-1.89737200
C	0.67722700	0.00001200	2.06758100
C	-0.67719500	0.00001200	2.06759100
H	1.38855000	0.00001600	2.87877400
H	-1.38850600	0.00001700	2.87879500
N	1.08278600	0.00000500	0.73411900
N	-1.08277500	0.00000500	0.73413600
C	-0.00000100	0.00000000	-0.12536300
C	-2.46222100	0.00000200	0.31918800
C	-3.11852100	1.23466300	0.13922200
C	-3.11851900	-1.23466200	0.13923600
C	-4.46417800	1.20589800	-0.24701700
C	-4.46417700	-1.20590300	-0.24700300
C	-5.13279500	-0.00000400	-0.43995100
H	-4.99389800	2.14162500	-0.40243600
H	-4.99389600	-2.14163200	-0.40241200
H	-6.17726900	-0.00000600	-0.74093800
C	2.46222600	0.00000200	0.31915000
C	3.11852300	1.23466300	0.13917400
C	3.11852100	-1.23466200	0.13918700
C	4.46417400	1.20589800	-0.24708500
C	4.46417300	-1.20590300	-0.24707300
C	5.13278800	-0.00000400	-0.44003000
H	4.99389200	2.14162500	-0.40251200
H	4.99389000	-2.14163200	-0.40249000
H	6.17725700	-0.00000600	-0.74103300
C	-2.40857200	2.57267500	0.31913600
C	-3.13109300	3.48091800	1.33200500
C	-2.22037300	3.27943500	-1.03745200
H	-1.40938300	2.37303200	0.71703200
H	-3.24605500	2.98590400	2.30321500
H	-2.56032800	4.40422900	1.48674700
H	-4.13035700	3.76712100	0.98363100
H	-1.64362000	2.64396300	-1.71883600
H	-3.18494800	3.50531800	-1.50816100
H	-1.68021200	4.22501400	-0.90521000
C	-2.40856900	-2.57267100	0.31916500
C	-2.22036900	-3.27944600	-1.03741500
C	-3.13109000	-3.48090400	1.33204400
H	-1.40938100	-2.37302200	0.71705900
H	-1.64361700	-2.64398100	-1.71880600
H	-1.68020700	-4.22502300	-0.90516200
H	-3.18494300	-3.50533500	-1.50812200
H	-3.24605300	-2.98588000	2.30324800
H	-4.13035300	-3.76711100	0.98367200
H	-2.56032400	-4.40421300	1.48679600
C	2.40857700	2.57267500	0.31910000
C	2.22035700	3.27943500	-1.03748500
C	3.13111400	3.48091700	1.33195800
H	1.40939500	2.37303100	0.71701100
H	1.64359300	2.64396400	-1.71886100
H	1.68019700	4.22501400	-0.90523400
H	3.18492400	3.50531900	-1.50820900
H	3.24609100	2.98590400	2.30316600
H	4.13037200	3.76712000	0.98356800
H	2.56035100	4.40422900	1.48670900
C	2.40857400	-2.57267100	0.31912800
C	3.13111000	-3.48090400	1.33199500
C	2.22035300	-3.27944600	-1.03745000
H	1.40939200	-2.37302200	0.71703600
H	3.24608800	-2.98588000	2.30319800
H	2.56034600	-4.40421300	1.48675600
H	4.13036800	-3.76711100	0.98360800
H	1.64359000	-2.64398100	-1.71883200
H	3.18492000	-3.50533600	-1.50817200
H	1.68019200	-4.22502200	-0.90518900

CP1

Energy (RB3LYP) = -1907.480039673722 A.U.

Free Energy = -1906.940249014491 A.U.

Ni	0.10993400	-0.29098900	-0.62756800
C	3.46972000	-0.95561600	-0.57978400
C	3.02070800	0.25813000	-0.98523300
C	1.76389400	0.17985000	-1.70504800
C	1.27686100	-1.16485800	-1.78544200
S	2.42433900	-2.30091500	-0.99460400
H	3.55522600	1.18496300	-0.81071500
H	1.48942800	0.94824900	-2.42239800
Br	0.36759400	-1.88382300	-3.46494300
Br	5.06297700	-1.27586700	0.49174300
C	-2.32258700	2.15765700	1.73270300
C	-2.85478800	0.94434500	2.02197400
H	-2.58414400	3.14899600	2.06809800
H	-3.67565600	0.65960300	2.66131900
N	-1.27504000	1.93147200	0.84438800
N	-2.11833000	0.00763900	1.30388700
C	-1.12789600	0.59794800	0.56111900
C	-2.36444500	-1.41462800	1.33983700
C	-3.29049100	-1.96521900	0.43027800
C	-1.68036500	-2.19590600	2.29362100
C	-3.51597400	-3.34589400	0.49404700
C	-1.94301300	-3.57126800	2.30986600
C	-2.84943400	-4.14262200	1.42088900
H	-4.22117500	-3.80214700	-0.19461700
H	-1.42761200	-4.20258700	3.02794000
H	-3.03675100	-5.21269400	1.45027300
C	-0.44411900	2.97820200	0.29992200
C	-0.79336000	3.54411500	-0.94242600

C	0.67668900	3.40496900	1.04033900
C	0.03684700	4.55179200	-1.44974000
C	1.46684900	4.42158400	0.48927100
C	1.15620200	4.98643700	-0.74497600
H	-0.19960900	5.00327500	-2.40907500
H	2.33793300	4.77363100	1.03458100
H	1.78562200	5.77107600	-1.15655500
C	-4.04758100	-1.11959400	-0.58939200
C	-5.55822400	-1.09750300	-0.28101200
C	-3.78082700	-1.58748300	-2.03278700
H	-3.68418800	-0.09044400	-0.51341900
H	-5.75656800	-0.72105800	0.72923800
H	-6.08390200	-0.45112400	-0.99370600
H	-5.99618800	-2.09988800	-0.35423400
H	-2.71101200	-1.57074200	-2.26427800
H	-4.14705800	-2.60677600	-2.20229100
H	-4.29539300	-0.92914800	-2.74297500
C	-0.68606800	-1.60265800	3.28709300
C	0.73086200	-2.16913000	3.07393000
C	-1.15606000	-1.80376500	4.74139300
H	-0.63111700	-0.52457300	3.10966700
H	1.07813200	-1.98454800	2.05223700
H	1.43650500	-1.69594900	3.76712300
H	0.76348300	-3.25046900	3.25194800
H	-2.14824100	-1.36797100	4.90653200
H	-1.21139500	-2.86666100	5.00390300
H	-0.45518900	-1.32673300	5.43650600
C	-2.02345200	3.10641300	-1.73225800
C	-1.63133700	2.42350800	-3.05665000
C	-2.98806500	4.28402400	-1.97459500
H	-2.56260400	2.36430600	-1.13609900
H	-1.01744100	1.53645700	-2.87016300
H	-2.52854800	2.10696800	-3.60186100
H	-1.06733300	3.10240200	-3.70744300
H	-3.28946700	4.75580400	-1.03229600
H	-2.53390700	5.05787700	-2.60423800
H	-3.89310100	3.93315200	-2.48413100
C	1.03475900	2.81955500	2.40344800
C	0.85204200	3.86740800	3.52017900
C	2.45676300	2.22847600	2.42570600
H	0.34424900	1.99693600	2.61093900
H	-0.17201200	4.25786900	3.54114100
H	1.06640900	3.42362600	4.49953800
H	1.52923900	4.71885300	3.38395800
H	2.57291700	1.45183600	1.66358600
H	3.21912700	2.99657700	2.24962000
H	2.66269800	1.77916800	3.40437000

CP2

Energy (RB3LYP) = -1907.526205082677 A.U.

Free Energy = -1906.983525661697 A.U.

Ni	-0.55967700	-0.10792700	-1.18961100
C	3.61372600	-1.10036700	-0.95211900
C	3.57161000	0.14309600	-1.51104300
C	2.23337700	0.65783900	-1.57498100
C	1.28728200	-0.19994400	-1.07608300
S	2.03333100	-1.67127400	-0.49291900
H	4.44615000	0.67380600	-1.86977600
H	1.99706300	1.62674700	-2.00002400
Br	-1.06835100	-0.62200100	-3.41245600
Br	5.19941100	-2.18543400	-0.65469600
C	-1.21766700	1.58934300	2.51559200
C	-2.01423600	0.49337000	2.56937500
H	-1.08207200	2.40540600	3.20662800
H	-2.71543300	0.15625500	3.31582500
N	-0.52017200	1.52728900	1.31463100
N	-1.79175500	-0.21804800	1.39770300
C	-0.87642400	0.41697300	0.60536800
C	-2.51346100	-1.42600500	1.04566500
C	-3.73989700	-1.29736700	0.36118600
C	-1.98531500	-2.67229300	1.44491200
C	-4.43856900	-2.47576800	0.06958200
C	-2.73018100	-3.81357700	1.12623000
C	-3.94115400	-3.71903700	0.44504200
H	-5.38394700	-2.41581500	-0.46044100
H	-2.35578200	-4.79100400	1.41163600
H	-4.49858900	-4.62037700	0.20532700
C	0.40901100	2.55942800	0.90183400
C	-0.01563400	3.52021000	-0.03789400
C	1.68318300	2.59251100	1.50645300
C	0.90139000	4.51861200	-0.39296500
C	2.54915400	3.62312900	1.12337600
C	2.16928000	4.57123400	0.17745900
H	0.60981800	5.27212100	-1.11847000
H	3.53853700	3.67803500	1.56660600
H	2.86162500	5.35769000	-0.11077400
C	-4.34224400	0.05240700	-0.02188100
C	-5.52728900	0.39951100	0.90354300
C	-4.76309500	0.11383400	-1.50250300
H	-3.57875500	0.82330900	0.12635100
H	-5.22693300	0.41560300	1.95765200
H	-5.93325000	1.38602200	0.65105900
H	-6.33583700	-0.33340600	0.79899700
H	-3.92748900	-0.12846200	-2.16659800
H	-5.58417000	-0.57845800	-1.72086800
H	-5.11468900	1.12330200	-1.74610700
C	-0.68392600	-2.79565800	2.23348400
C	0.17036300	-4.00090600	1.80115000
C	-0.96862700	-2.85999700	3.74978500
H	-0.08788100	-1.89668700	2.04397600

H	0.33241700	-4.01283900	0.71933100
H	1.15014500	-3.95238700	2.28856200
H	-0.28912800	-4.95341900	2.08960200
H	-1.50880100	-1.97469200	4.10279400
H	-1.57400800	-3.74076600	3.99505500
H	-0.02994300	-2.92776100	4.31201100
C	-1.42329600	3.55697500	-0.62772000
C	-1.41659900	3.53221000	-2.16788700
C	-2.20135900	4.77841400	-0.09525000
H	-1.96009800	2.66335800	-0.29581300
H	-0.92156300	2.63493000	-2.55259500
H	-2.44510200	3.53348800	-2.54670900
H	-0.91032100	4.41015300	-2.58553800
H	-2.24689000	4.77984600	0.99996300
H	-1.73261600	5.71791200	-0.41032700
H	-3.22818300	4.77225700	-0.47912500
C	2.12636000	1.58488500	2.56503700
C	2.09050300	2.21747900	3.97270900
C	3.52027700	0.99680500	2.27946900
H	1.41994000	0.74881200	2.55553500
H	1.09489700	2.59606500	4.23053900
H	2.37743100	1.47925300	4.73067000
H	2.79056900	3.05851800	4.04109200
H	3.57627000	0.56994600	1.27510400
H	4.30837800	1.75302100	2.37435000
H	3.74306300	0.20400700	3.00272400

CP3

Energy (RB3LYP) = -2446.696001181410 A.U.

Free Energy = -2446.103835579917 A.U.

Ni	-0.45577100	-0.51479000	-0.84088300
C	3.76056300	-1.30431200	-0.29652400
C	3.70122300	-0.19480800	-1.08690400
C	2.34720500	0.19015900	-1.36918400
C	1.39750900	-0.61218400	-0.78224500
S	2.17567500	-1.90493300	0.10916200
H	4.57454500	0.33395900	-1.45204700
H	2.10282300	1.04499500	-1.99058100
C	-1.52331800	2.65646100	1.76342600
C	-2.35751600	1.66492500	2.16367200
H	-1.43147300	3.68238200	2.08271600
H	-3.14130200	1.64675200	2.90436300
N	-0.70813200	2.12041500	0.77215600
N	-2.02995500	0.54737000	1.40588800
C	-1.01028900	0.80945600	0.52926200
C	-2.69948000	-0.72905600	1.52656100
C	-3.80610300	-0.99608100	0.69346100
C	-2.24010400	-1.64185100	2.49965600
C	-4.45491100	-2.22649600	0.85861400
C	-2.92905600	-2.85472300	2.61990300
C	-4.02338700	-3.14642900	1.80952600
H	-5.30998300	-2.46505600	0.23346300
H	-2.60364700	-3.58073600	3.35857800
H	-4.54213800	-4.09485900	1.92061600
C	0.31369600	2.89396900	0.10168600
C	0.02330000	3.45774600	-1.15624200
C	1.54508200	3.09125500	0.75970700
C	1.02732000	4.22053900	-1.76739100
C	2.50449200	3.87540600	0.10852900
C	2.25433900	4.42882900	-1.14431500
H	0.83930400	4.66422400	-2.74084400
H	3.46428700	4.04679100	0.58625300
H	3.01708900	5.02764000	-1.63495000
C	-4.33088000	0.00551400	-0.33210700
C	-5.65276400	0.63834400	0.14925000
C	-4.49406500	-0.61869100	-1.73137800
H	-3.59817200	0.81340400	-0.42435600
H	-5.53071400	1.13746000	1.11740000
H	-6.00667600	1.38226600	-0.57411600
H	-6.43614100	-0.12049500	0.26145900
H	-3.56462400	-1.08654300	-2.07218800
H	-5.28103200	-1.38162700	-1.74680700
H	-4.77561000	0.15541500	-2.45473900
C	-1.06871500	-1.33326700	3.42823500
C	-0.04212100	-2.47900700	3.48898500
C	-1.57504600	-0.97629100	4.84161000
H	-0.54478500	-0.45761300	3.03311500
H	0.33491100	-2.72981700	2.49311300
H	0.81306500	-2.17909100	4.10509500
H	-0.46488900	-3.38631100	3.93572700
H	-2.26099900	-0.12163300	4.82209100
H	-2.10845500	-1.82071100	5.29417200
H	-0.73362200	-0.72014600	5.49594400
C	-1.32756600	3.30053400	-1.84855600
C	-1.19564200	2.59845300	-3.21318600
C	-2.04037000	4.66085500	-1.98920100
H	-1.96147600	2.66732800	-1.22074600
H	-0.74300100	1.60725000	-3.10756900
H	-2.18369900	2.47169300	-3.67134600
H	-0.57973000	3.18013500	-3.90894600
H	-2.17055600	5.14777800	-1.01591000
H	-1.47529200	5.34618600	-2.63152100
H	-3.03166200	4.52615300	-2.43775700
C	1.84404600	2.51394100	2.14093400
C	1.79566200	3.61792300	3.21807800
C	3.18785300	1.76426300	2.19074200
H	1.06347100	1.78453300	2.37841000
H	0.82399200	4.12482200	3.24101900
H	1.97802100	3.19131600	4.21145500
H	2.56230100	4.38005900	3.03447100
H	3.24168200	0.99071900	1.42033400
H	4.03795500	2.44274700	2.05216700
H	3.31031200	1.28638100	3.16968000
C	-0.48458100	-1.79666100	-2.17606800

C	-1.07947900	-3.04525400	-2.08529600
S	-0.06753200	-1.49020900	-3.85030700
C	-1.24503300	-3.71312500	-3.33792700
H	-1.39215300	-3.47983700	-1.13984800
C	-0.74516400	-2.99343000	-4.39175800
H	-1.70842000	-4.68923600	-3.44661700
H	-0.73904500	-3.26280500	-5.44032100
Br	5.37409300	-2.16586900	0.37185600

CP4

Energy (RB3LYP) = -2446.724739909582 A.U.

Free Energy = -2446.131183911042 A.U.

Ni	-0.00861000	-0.37104900	-0.44683600
C	0.31462100	-2.02511700	-1.43122600
C	1.26567500	-1.03116500	-1.83818000
C	2.58851400	-1.27255200	-1.29685700
C	2.64895300	-2.38612700	-0.52631900
S	1.13377300	-3.24711100	-0.37012700
H	1.14266000	-0.43252100	-2.73878800
H	3.43720500	-0.62618600	-1.48797200
Br	4.20578600	-2.99104600	0.47698000
C	-1.56706000	2.56509100	2.03680400
C	-0.63541700	3.30831400	1.39179300
H	-2.27948600	2.82444900	2.80415900
H	-0.36908400	4.34996400	1.47980200
N	-1.47295600	1.27510500	1.52135800
N	0.00669500	2.45512600	0.49758800
C	-0.49728800	1.17757000	0.55713600
C	1.07464200	2.87196900	-0.37714300
C	2.39651400	2.85361000	0.11175100
C	0.75539500	3.30328300	-1.68030500
C	3.41492700	3.26265700	-0.75846000
C	1.81352900	3.69394800	-2.51066700
C	3.13031400	3.67212400	-2.05856400
H	4.44455100	3.25937500	-0.41198200
H	1.60151100	4.02288000	-3.52412200
H	3.93623400	3.98138400	-2.71904000
C	-2.30847500	0.17959700	1.94831000
C	-1.86306500	-0.64368400	3.00259600
C	-3.55280800	-0.01039600	1.31225100
C	-2.70504200	-1.68650000	3.40938400
C	-4.35605700	-1.06515300	1.76292900
C	-3.93829200	-1.89708400	2.79859000
H	-2.38944100	-2.34048300	4.21726200
H	-5.32123900	-1.23675200	1.29516200
H	-4.57697800	-2.71084900	3.13219200
C	2.73993600	2.43281000	1.53775500
C	3.25624000	3.63236800	2.35803800
C	3.74261900	1.26475400	1.57265400
H	1.82188600	2.07984100	2.01629800
H	2.52611600	4.44979000	2.37783300
H	3.45578800	3.33015900	3.39294200
H	4.18888400	4.03012500	1.94061400
H	3.35627900	0.39842100	1.02764300
H	4.70748600	1.54300400	1.13228200
H	3.93005200	0.95947300	2.60890200
C	-0.67806500	3.36149200	-2.20002200
C	-0.91190000	2.33741400	-3.32687200
C	-1.06052700	4.78544900	-2.64912700
H	-1.34679800	3.09112600	-1.37760100
H	-0.72426100	1.32030600	-2.96836700
H	-1.94920300	2.38833000	-3.67928100
H	-0.25703100	2.52814900	-4.18570000
H	-0.91829000	5.51223700	-1.84108700
H	-0.46061500	5.11693000	-3.50463400
H	-2.11349000	4.81645100	-2.95299200
C	-0.52906300	-0.42667600	3.71022700
C	0.38262100	-1.66384800	3.60635500
C	-0.74125900	-0.01118700	5.17987300
H	-0.01058800	0.39581400	3.20932700
H	0.56474300	-1.93134900	2.56055300
H	1.35014300	-1.46022300	4.08040300
H	-0.05565200	-2.53413600	4.10921400
H	-1.35238400	0.89565400	5.25635600
H	-1.24393400	-0.80046600	5.75132400
H	0.22285300	0.18706500	5.66288500
C	-4.04660300	0.89692900	0.18927500
C	-5.20926400	1.78791700	0.67187700
C	-4.44298400	0.10278900	-1.06908700
H	-3.22281200	1.55718100	-0.09675500
H	-4.91631100	2.39969300	1.53293700
H	-5.53286800	2.46302700	-0.12929800
H	-6.07456600	1.18458400	0.97150500
H	-3.61806900	-0.52547800	-1.41830100
H	-5.30793200	-0.54577100	-0.88585000
H	-4.71623400	0.79256700	-1.87654600
C	-0.91083200	-2.42586200	-2.12063700
C	-2.00229100	-3.10153800	-1.61466500
S	-1.14932400	-2.10096900	-3.83207500
C	-3.02369800	-3.34202100	-2.58005900
H	-2.07201600	-3.39888100	-0.57358300
C	-2.71732800	-2.84719500	-3.81824300
H	-3.95400500	-3.85313700	-2.35536800
H	-3.31498000	-2.87197000	-4.71958800

CP5

Energy (RB3LYP) = -2446.722798783168 A.U.

Free Energy = -2446.129783765468 A.U.

Ni	-0.29007000	-0.22044400	-0.77092000
C	4.62353700	-0.73248800	-0.57200600
C	4.37076500	0.55144600	-0.95837100
C	3.07656600	0.68632200	-1.54358500

C	2.35649000	-0.48844900	-1.59860700
S	3.30923600	-1.81305600	-0.92938500
H	5.06761900	1.36999600	-0.82318400
H	2.67884800	1.63067200	-1.89951400
Br	6.22499800	-1.38008700	0.31450800
C	-3.13037500	0.61648400	2.14669000
C	-2.43824300	1.78126300	2.15772100
H	-3.98281200	0.28888500	2.72092600
H	-2.56294900	2.67912600	2.74258200
N	-2.52704000	-0.19767200	1.19080000
N	-1.42730200	1.65200800	1.20892200
C	-1.45784100	0.42405400	0.58869700
C	-0.45653500	2.68115900	0.92934900
C	-0.74008800	3.62891500	-0.07526300
C	0.73107900	2.71544900	1.68861300
C	0.21556800	4.62424400	-0.31537600
C	1.65148400	3.73251000	1.40638700
C	1.40009100	4.67702100	0.41475100
H	0.02735900	5.36825900	-1.08426400
H	2.57786100	3.78313900	1.97153600
H	2.12788300	5.45858500	0.21238700
C	-2.97859700	-1.53178500	0.88224900
C	-3.98831200	-1.69902600	-0.08692700
C	-2.41280200	-2.61772500	1.58004200
C	-4.41479900	-3.00469300	-0.36039300
C	-2.86951900	-3.90257500	1.26007900
C	-3.85852400	-4.09739800	0.29962900
H	-5.19316400	-3.16669800	-1.10072700
H	-2.44624900	-4.76132500	1.77349700
H	-4.20095200	-5.10291000	0.06917000
C	-2.03535500	3.61161700	-0.88105000
C	-2.89084000	4.86024400	-0.58754900
C	-1.76672300	3.46109100	-2.39033100
H	-2.61477400	2.73759800	-0.57016500
H	-3.12124900	4.94636000	0.48065000
H	-3.83868400	4.81099600	-1.13656800
H	-2.37703100	5.77969200	-0.89217400
H	-1.19604400	2.55003100	-2.59803000
H	-1.20478300	4.31424600	-2.78883400
H	-2.71502900	3.40450600	-2.93844000
C	1.03523600	1.70154200	2.78718600
C	2.29886000	0.88097500	2.46678900
C	1.14516400	2.38290700	4.16559300
H	0.19998800	0.99720700	2.83778700
H	2.19857700	0.36742000	1.50578600
H	2.46781300	0.12708000	3.24501300
H	3.19202700	1.51474100	2.41952400
H	0.23106000	2.93420600	4.41495400
H	1.98092300	3.09167800	4.19922400
H	1.31416500	1.63354300	4.94787600
C	-4.63364800	-0.52132200	-0.81133500
C	-4.53981800	-0.65766800	-2.34240100
C	-6.09618300	-0.33120600	-0.36037500
H	-4.08477300	0.38434300	-0.53807600
H	-3.49869300	-0.76336000	-2.66258800
H	-4.96000500	0.23298900	-2.82499100
H	-5.10145200	-1.52528100	-2.70906800
H	-6.16590300	-0.17995000	0.72300500
H	-6.70819900	-1.20508700	-0.61384400
H	-6.53901800	0.54211300	-0.85392200
C	-1.34054600	-2.43854900	2.65071400
C	-1.77689800	-3.04101700	4.00043400
C	0.01281700	-3.01436200	2.19180500
H	-1.19545700	-1.36564500	2.80716000
H	-2.72873500	-2.61656700	4.33992200
H	-1.02071700	-2.83703000	4.76756200
H	-1.89970500	-4.12864900	3.94031200
H	0.35363900	-2.51226900	1.28086700
H	-0.05628500	-4.09011300	1.98975800
H	0.77355900	-2.86736300	2.96785900
C	1.02015300	-0.72231500	-2.13953100
C	0.14995900	-1.83190700	-1.88397900
S	0.57805100	0.03519200	-3.71795600
C	-0.81171600	-2.02477700	-2.94893300
H	0.41328000	-2.64795800	-1.21406500
C	-0.71062800	-1.12396100	-3.96181900
H	-1.55218400	-2.81818100	-2.93179500
H	-1.34758500	-1.03417700	-4.83309900

CP6

Energy (RB3LYP) = -2446.734565144036A.U.

Free Energy = -2446.141653568827 A.U.

Ni	0.10644600	-0.21125000	-0.69683000
C	-3.33631700	-0.35180400	-1.06247600
C	-2.63966900	0.79232500	-1.35754300
C	-1.33427500	0.58048200	-1.92813800
C	-1.02587500	-0.81045500	-2.04545100
S	-2.39562800	-1.80277500	-1.46020300
H	-3.06032400	1.78316500	-1.21314200
H	-0.84978200	1.34616700	-2.52658900
Br	-0.01980700	-1.55869700	-3.66074800
C	2.90330900	0.26661700	2.34971500
C	2.71794200	1.57300400	2.03671200
H	3.54479800	-0.20885000	3.07503400
H	3.16442300	2.47129300	2.43350900
N	2.05999200	-0.46343800	1.51838100
N	1.76687800	1.60789900	1.02106100
C	1.34041500	0.34963400	0.67929100
C	1.28326900	2.82626300	0.41792200
C	1.90648100	3.29783300	-0.75460500
C	0.21574500	3.50776000	1.03614200
C	1.41066900	4.47980100	-1.31950300
C	-0.23571500	4.68762400	0.43163000
C	0.35006400	5.16810500	-0.73652300

H	1.86385200	4.86610200	-2.22806100
H	-1.05897000	5.23513200	0.88185800
H	-0.01836700	6.08370500	-1.19170400
C	1.94896300	-1.90264900	1.54612300
C	2.82951200	-2.66638000	0.75298700
C	0.97551800	-2.48973000	2.38011900
C	2.70757500	-4.06030500	0.81092100
C	0.89585500	-3.88762500	2.39499800
C	1.75070600	-4.66668000	1.62006400
H	3.36950600	-4.67778700	0.21067000
H	0.15159000	-4.37116000	3.02122200
H	1.67060500	-5.75018100	1.64641000
C	3.08210000	2.57982200	-1.41052000
C	4.32955400	3.48306400	-1.47526200
C	2.70873400	2.04119800	-2.80489700
H	3.33963400	1.71570000	-0.79103100
H	4.61482500	3.84487500	-0.48068700
H	5.17815300	2.92761000	-1.89150200
H	4.16316200	4.35887800	-2.11319100
H	1.87328400	1.33671300	-2.74002000
H	2.42347300	2.85177500	-3.48614900
H	3.56179900	1.51564500	-3.25044100
C	-0.44284200	3.01490700	2.32142800
C	-1.93960900	2.71303700	2.11848800
C	-0.22799100	4.01257300	3.47717700
H	0.03628300	2.07481700	2.60969300
H	-2.08591300	1.96428800	1.33387500
H	-2.37700000	2.32536600	3.04614500
H	-2.49974600	3.61356000	1.83977000
H	0.83770500	4.19887500	3.65380100
H	-0.70373500	4.97796700	3.26822400
H	-0.66279100	3.62118900	4.40443800
C	3.89844000	-2.03470500	-0.13381300
C	3.74593800	-2.45584800	-1.60774400
C	5.31295700	-2.35195800	0.39202800
H	3.77185300	-0.94861200	-0.09610800
H	2.75343900	-2.20147200	-1.99314300
H	4.49392700	-1.94307300	-2.22427400
H	3.89387000	-3.53416300	-1.73884800
H	5.44337100	-2.01090100	1.42565600
H	5.51489200	-3.42938100	0.36954500
H	6.07070300	-1.85727100	-0.22704600
C	0.02753600	-1.66766600	3.24781100
C	0.22938300	-1.97102300	4.74560300
C	-1.44095300	-1.87141300	2.82830300
H	0.26046500	-0.60962200	3.09651300
H	1.26522500	-1.79060000	5.05566300
H	-0.42346700	-1.33365500	5.35354500
H	-0.01211300	-3.01385000	4.98218100
H	-1.58742600	-1.61152800	1.77510200
H	-1.75890200	-2.91147000	2.96753000
H	-2.09964800	-1.23752300	3.43389900
C	-4.64709900	-0.48278000	-0.45968900
C	-5.50230400	-1.56526300	-0.47416200
S	-5.37191000	0.84229100	0.44052800
C	-6.72876000	-1.33366500	0.21152300
H	-5.26246700	-2.49216400	-0.98403800
C	-6.81058300	-0.07846600	0.74959400
H	-7.52106700	-2.07029300	0.29137800
H	-7.62589000	0.36286000	1.30694500

CP7

Energy (RB3LYP) = -2446.725997535359 A.U.

Free Energy = -2446.134309075778 A.U.

Ni	0.95199500	-0.21609800	-1.06990500
C	-2.23009000	-0.95480300	-1.66173400
C	-1.65827300	0.21757500	-2.09168200
C	-0.32093400	0.08523500	-2.60785800
C	0.16214600	-1.25066800	-2.50752600
S	-1.12053100	-2.31905400	-1.86806800
H	-2.17480000	1.17210000	-2.04604000
H	0.10945700	0.83383800	-3.26853800
C	3.69990700	0.46033000	1.97023600
C	3.03249100	1.63815200	2.02945300
H	4.53762100	0.08616100	2.53775500
H	3.16780700	2.50311000	2.65984500
N	3.09464000	-0.28964200	0.96474200
N	2.03406900	1.58009700	1.05962700
C	2.05035900	0.38627800	0.37813600
C	1.09382700	2.64611900	0.81565800
C	1.42848300	3.64599900	-0.11959300
C	-0.11821900	2.65775700	1.53459000
C	0.49400700	4.66512100	-0.34148200
C	-1.01632300	3.70037500	1.27369200
C	-0.71787000	4.69261900	0.34383200
H	0.71838100	5.44635700	-1.06230600
H	-1.96349400	3.73220200	1.80459200
H	-1.43024100	5.49151900	0.15507900
C	3.51831100	-1.61592400	0.58850400
C	4.47730100	-1.75728900	-0.43539300
C	2.97222800	-2.72183800	1.27085200
C	4.87206200	-3.05612500	-0.77892500
C	3.40730100	-3.99769400	0.89065200
C	4.34418300	-4.16643600	-0.12502400
H	5.60282500	-3.19924300	-1.56989000
H	3.00285400	-4.87022500	1.39585200
H	4.66536900	-5.16580100	-0.40683000
C	2.74430800	3.64056400	-0.89188900
C	3.53548800	4.94715500	-0.68989100
C	2.50807600	3.35335400	-2.38742000
H	3.36120400	2.82506200	-0.50301700
H	3.72338000	5.14135800	0.37230300
H	4.50367800	4.88636100	-1.20076400
H	3.00221500	5.81374500	-1.09756000

H	2.01282200	2.38525300	-2.51566800
H	1.88147700	4.12586800	-2.84926400
H	3.46237300	3.32753900	-2.92764900
C	-0.47758900	1.58526700	2.55817100
C	-1.67230800	0.73694200	2.08193100
C	-0.73972500	2.19173000	3.95048100
H	0.37789500	0.91035100	2.65496900
H	-1.45489500	0.26518800	1.11862600
H	-1.89293800	-0.05237500	2.81063500
H	-2.57680200	1.34564700	1.96558200
H	0.12021600	2.77240800	4.30401600
H	-1.61155200	2.85619200	3.94618500
H	-0.93549000	1.39617000	4.67900500
C	5.07088000	-0.56224900	-1.17513300
C	4.57628900	-0.51392300	-2.63413900
C	6.60981300	-0.54622400	-1.10326000
H	4.71434500	0.34894500	-0.68586500
H	3.48307100	-0.44561100	-2.66355500
H	4.99116900	0.36089900	-3.14967000
H	4.88222600	-1.40848900	-3.19002300
H	6.96260500	-0.56090400	-0.06566400
H	7.05139500	-1.40756900	-1.61765800
H	7.00118700	0.35882000	-1.58255500
C	1.94530600	-2.57372600	2.38928600
C	2.50593700	-3.07568900	3.73475200
C	0.61969700	-3.27655100	2.03943200
H	1.72244900	-1.50918400	2.50515900
H	3.42659500	-2.54713500	4.00801000
H	1.77361100	-2.91832200	4.53542000
H	2.73551900	-4.14723600	3.69996500
H	0.20430400	-2.88692600	1.10441200
H	0.75371300	-4.35916500	1.92770100
H	-0.11561400	-3.11375200	2.83666600
C	-3.53396500	-1.15933800	-1.06843400
C	-4.05283200	-2.29345600	-0.47931100
S	-4.73380600	0.13348100	-1.05176300
C	-5.39029600	-2.14841300	-0.00713800
H	-3.48530400	-3.21210300	-0.37831600
C	-5.87903200	-0.89752100	-0.24470700
H	-5.95247500	-2.93268300	0.48523300
H	0.88573700	-1.72246300	-3.16766700
Br	-7.63705600	-0.22958300	0.22716600

TS1

Energy (RB3LYP) = -1907.476141663962 A.U.

Free Energy = -1906.936865315967 A.U.

Ni	0.20898800	-0.09911000	-0.60173700
C	3.95951700	0.01241800	-0.61082000
C	3.31906100	1.20572100	-0.75093200
C	2.02135000	1.06097500	-1.35443700
C	1.69666300	-0.28727300	-1.61266400
S	3.02966500	-1.36638200	-1.15500500
H	3.75756300	2.15771500	-0.47401600
H	1.47941300	1.89720100	-1.78091000
Br	0.51573600	-0.86275200	-3.35710300
Br	5.71974300	-0.25053400	0.16957000
C	-2.97842700	1.11605800	1.80785300
C	-3.08157500	-0.22846100	1.94975000
H	-3.56126000	1.92343800	2.22267400
H	-3.77138100	-0.83486100	2.51542600
N	-1.89832300	1.34464200	0.96016300
N	-2.06332800	-0.78765500	1.18389800
C	-1.30968300	0.17260800	0.55812700
C	-1.82160100	-2.20710900	1.07876100
C	-2.51760900	-2.94298400	0.09753700
C	-0.91534900	-2.80699100	1.97696600
C	-2.27543100	-4.32060000	0.03085900
C	-0.70733600	-4.18691800	1.85980800
C	-1.37820800	-4.93758600	0.89845300
H	-2.79476400	-4.91696700	-0.71344300
H	-0.00992300	-4.67872800	2.53186200
H	-1.20189700	-6.00745100	0.82532000
C	-1.44679100	2.66012900	0.57544500
C	-1.95960500	3.23697700	-0.60361600
C	-0.52366500	3.32694900	1.40648200
C	-1.50727000	4.51763400	-0.94682400
C	-0.10870100	4.60642500	1.01689700
C	-0.59114000	5.19677700	-0.14828300
H	-1.88042800	4.98849000	-1.85183200
H	0.60333300	5.14614900	1.63486200
H	-0.25436200	6.19007200	-0.43321400
C	-3.52575800	-2.30077900	-0.85099300
C	-4.96576600	-2.71093900	-0.47984000
C	-3.22420600	-2.61818200	-2.32760300
H	-3.45366200	-1.21499500	-0.73624100
H	-5.20897800	-2.43802400	0.55361000
H	-5.68737900	-2.21564500	-1.14024000
H	-5.10776300	-3.79359700	-0.57989400
H	-2.20997900	-2.31024600	-2.60032200
H	-3.32627100	-3.68803600	-2.54389300
H	-3.92954300	-2.08453000	-2.97566500
C	-0.17609500	-2.01923000	3.05437000
C	1.34857800	-2.05526300	2.83608600
C	-0.55030100	-2.51129100	4.46657300
H	-0.48611000	-0.97262900	2.98282200
H	1.61279400	-1.65785600	1.85074300
H	1.85522400	-1.45005400	3.59736300
H	1.74209100	-3.07619700	2.90574900
H	-1.63125500	-2.45231200	4.63846500
H	-0.24412000	-3.55179000	4.62562100
H	-0.05116100	-1.89903200	5.22685100
C	-2.97967800	2.53169400	-1.49221700
C	-2.43326600	2.29892900	-2.91368000
C	-4.31552000	3.30091300	-1.52618100

H	-3.18208700	1.54688400	-1.06117700
H	-1.51836000	1.69847100	-2.89127200
H	-3.17360300	1.76382900	-3.52008600
H	-2.21059500	3.24514600	-3.42101100
H	-4.72725500	3.43455700	-0.51911900
H	-4.19594400	4.29555400	-1.97152500
H	-5.05355500	2.75504200	-2.12554600
C	0.01940200	2.71414500	2.69409300
C	-0.42741100	3.52185500	3.92901700
C	1.55187500	2.56214700	2.65263400
H	-0.39859200	1.70833900	2.79387100
H	-1.51955700	3.59538500	3.98654400
H	-0.07034800	3.04233900	4.84803400
H	-0.02628500	4.54197300	3.90839800
H	1.86184300	1.94983600	1.80005600
H	2.05261500	3.53464700	2.57546100
H	1.90872700	2.07871700	3.56989600

TS2

Energy (RB3LYP) = -2446.687270723211 A.U.

Free Energy = -2446.094811317539 A.U.

Ni	0.05878500	-0.13237300	0.82222700
C	-4.16984100	-0.14093600	0.53950300
C	-3.90312800	0.99756600	1.24481100
C	-2.53606500	1.07174200	1.64854100
C	-1.74718700	0.00842000	1.23294800
S	-2.75795100	-1.14008700	0.33361600
H	-4.64894300	1.74834900	1.48006500
H	-2.14921600	1.87738200	2.26256900
C	2.57377900	1.26820600	-2.24248500
C	2.83962400	-0.06028400	-2.31906700
H	2.96365600	2.10608100	-2.79875500
H	3.50974800	-0.61730300	-2.95469300
N	1.62849600	1.42645100	-1.23658800
N	2.04351200	-0.67913100	-1.36321800
C	1.28041100	0.22707900	-0.67323300
C	2.03263900	-2.10776200	-1.14469100
C	2.84060800	-2.64620000	-0.12257400
C	1.24262700	-2.91146600	-1.99241000
C	2.83395000	-4.03740000	0.03868300
C	1.27775700	-4.29607200	-1.78645300
C	2.06229300	-4.85540200	-0.78158600
H	3.44462500	-4.48480300	0.81731100
H	0.68134300	-4.94404800	-2.42190600
H	2.07343000	-5.93269400	-0.63849200
C	1.10092100	2.71316500	-0.84301100
C	1.81383200	3.47090300	0.10732800
C	-0.08064200	3.17711900	-1.45621900
C	1.30250100	4.73070900	0.44370900
C	-0.54373000	4.44483600	-1.08350900
C	0.13684300	5.21424200	-0.14341400
H	1.82662700	5.34026900	1.17420200
H	-1.45067100	4.83393600	-1.53608600
H	-0.24231700	6.19507000	0.13126600
C	3.73106600	-1.78551600	0.76889500
C	5.21855800	-1.98949400	0.41532300
C	3.47632600	-2.03854700	2.26676700
H	3.48944000	-0.73598900	0.57811800
H	5.41704000	-1.75683200	-0.63738300
H	5.85092600	-1.33965700	1.03183500
H	5.53057900	-3.02575700	0.59189300
H	2.42327100	-1.88427600	2.52158700
H	3.75310700	-3.05823400	2.55973200
H	4.07925300	-1.34912200	2.86944700
C	0.39410700	-2.33309200	-3.12184300
C	-1.07022200	-2.80532200	-3.05736600
C	1.01539900	-2.65796300	-4.49612700
H	0.38267400	-1.24425900	-3.01454200
H	-1.52732200	-2.55042300	-2.09662700
H	-1.65406000	-2.32103600	-3.84888800
H	-1.15764500	-3.88838500	-3.20180400
H	2.04069600	-2.27861700	-4.57612600
H	1.04770600	-3.74012400	-4.66989000
H	0.42326700	-2.20634100	-5.30076300
C	3.11085800	2.98444200	0.74775300
C	3.02023600	2.95044100	2.28490300
C	4.31004600	3.83496800	0.28173500
H	3.29063200	1.95763000	0.41556300
H	2.19843800	2.30925500	2.61864200
H	3.95228000	2.55675400	2.70782400
H	2.86439900	3.95093000	2.70503000
H	4.40979800	3.82491100	-0.80984300
H	4.20390000	4.88005100	0.59570200
H	5.24237900	3.44982400	0.71134100
C	-0.82329100	2.37273400	-2.51902900
C	-0.53786900	2.93859700	-3.92582700
C	-2.33722700	2.29440900	-2.25281500
H	-0.44412600	1.34708600	-2.49079600
H	0.53483400	2.93755500	-4.15189200
H	-1.04580100	2.33877500	-4.69033500
H	-0.89629800	3.97113900	-4.01568200
H	-2.54400000	1.90298300	-1.25264600
H	-2.82090500	3.27415600	-2.34540600
H	-2.80933200	1.62865900	-2.98437700
C	-0.48990900	-0.69287000	2.49516200
C	-0.67965700	-1.97313800	2.99532400
S	0.08106000	0.35593600	3.80380100
C	-0.33988700	-2.11814800	4.37218300
H	-1.08093400	-2.77965900	2.39162700
C	0.08090900	-0.95052800	4.95164600
H	-0.41808200	-3.05638500	4.91271300
H	0.39414200	-0.78463000	5.97436400
Br	-5.89366100	-0.66363500	-0.19650400

TS3

Energy (RB3LYP) = -2446.709505803522 A.U.

Free Energy = -2446.115614890211 A.U.

Ni	-0.18541900	0.18555800	-0.80168600
C	1.75028200	0.69398000	-2.03525000
C	0.52789900	0.39608400	-2.67767300
C	-0.46134400	1.42006200	-2.49591400
C	0.02028000	2.46274400	-1.71627900
S	1.74453800	2.36058300	-1.40851700
H	0.39040600	-0.47017300	-3.31648700
H	-1.45070500	1.41111500	-2.93691500
Br	-0.90658900	4.14697800	-1.40947400
C	-0.85317700	-1.35950200	2.99521800
C	-1.96165900	-1.78004000	2.34155200
H	-0.53038500	-1.50587300	4.01394100
H	-2.80735800	-2.36162500	2.67393300
N	-0.09044500	-0.64017300	2.07530500
N	-1.85718300	-1.30719100	1.03605400
C	-0.69366000	-0.59010000	0.83456500
C	-2.84245600	-1.55416000	0.01526400
C	-3.93767900	-0.67396200	-0.10018000
C	-2.69308600	-2.68390000	-0.81583900
C	-4.88304700	-0.93899900	-1.09899400
C	-3.66468100	-2.89875300	-1.80139800
C	-4.74773800	-2.03555800	-1.94632700
H	-5.73634300	-0.27629500	-1.21374300
H	-3.57253700	-3.75656700	-2.46180400
H	-5.49158900	-2.22194400	-2.71669600
C	1.21816100	-0.12009900	2.38477600
C	1.35061900	1.23498100	2.75626100
C	2.31486200	-1.00483500	2.35030700
C	2.63038600	1.69023200	3.09443500
C	3.57254700	-0.49632000	2.70128400
C	3.73120200	0.83598100	3.06900400
H	2.76991300	2.72695500	3.38272200
H	4.43635200	-1.15494300	2.68572200
H	4.71475600	1.21193600	3.33938700
C	-4.12200500	0.53000500	0.81793600
C	-5.39852600	0.39374300	1.67136800
C	-4.11702300	1.85136100	0.02735400
H	-3.27133100	0.56472700	1.50425700
H	-5.38672100	-0.52708600	2.26592000
H	-5.48849400	1.24169000	2.36062300
H	-6.30014500	0.37515600	1.04764300
H	-3.18148900	1.96652200	-0.52809900
H	-4.94930400	1.90108800	-0.68502000
H	-4.21285500	2.70359900	0.71061600
C	-1.53022300	-3.66111100	-0.67278700
C	-0.60422100	-3.61827100	-1.90313400
C	-2.02409200	-5.09393100	-0.39278900
H	-0.93177500	-3.34934800	0.18785600
H	-0.19700400	-2.61067600	-2.03683500
H	0.23555700	-4.31154600	-1.77401600
H	-1.13704400	-3.90260000	-2.81872700
H	-2.66039500	-5.13084800	0.49889800
H	-2.60361900	-5.49575800	-1.23220000
H	-1.17143900	-5.76367700	-0.22979500
C	0.14284400	2.16509200	2.83668500
C	0.46717400	3.61949900	2.45700900
C	-0.49600400	2.10951100	4.24107900
H	-0.59633600	1.80398400	2.11488200
H	0.97218800	3.67578800	1.48788800
H	-0.46005600	4.19883300	2.38773600
H	1.10106000	4.11091400	3.20507700
H	-0.81556600	1.09512600	4.50213900
H	0.21448300	2.44667900	5.00592500
H	-1.37647300	2.76184800	4.28731000
C	2.17199600	-2.47769700	1.97574800
C	2.41006800	-3.38515900	3.19989900
C	3.09350700	-2.87485900	0.80816800
H	1.14443500	-2.64228100	1.63988900
H	1.72071900	-3.14713400	4.01813300
H	2.26524200	-4.43821100	2.93031800
H	3.43138100	-3.27574300	3.58392300
H	2.91235600	-2.24703300	-0.06868700
H	4.15297400	-2.78303300	1.07425200
H	2.91416400	-3.92015000	0.52856700
C	3.00133600	-0.03231300	-2.09280000
C	4.14513800	0.15006300	-1.34090200
S	3.25565800	-1.31113600	-3.27391000
C	5.20859700	-0.72657800	-1.70045400
H	4.20549800	0.87099500	-0.53285900
C	4.87998800	-1.57983400	-2.71755900
H	6.17683400	-0.72715900	-1.21113800
H	5.48566000	-2.35085200	-3.17418600

TS4

Energy (RB3LYP) = -2446.719049105191 A.U.

Free Energy = -2446.123221742965 A.U.

Ni	0.14337800	-0.21233200	0.87798900
C	-3.81458200	-1.07968900	0.82936700
C	-3.55745500	0.22299000	1.13985900
C	-2.30080400	0.38663300	1.79605200
C	-1.60406400	-0.81218900	1.98514700
S	-2.54926900	-2.16915400	1.32799600
H	-4.22659100	1.04143500	0.90327700
H	-1.94773500	1.33665400	2.17957100
Br	-5.36167600	-1.74960000	-0.13628800
C	2.37197900	0.75064700	-2.47530000
C	1.68511700	1.90794500	-2.32428700
H	3.11568200	0.45452000	-3.19822000
H	1.70136500	2.82402500	-2.89338400

N	1.95423500	-0.09961800	-1.45424900
N	0.85450600	1.73829700	-1.21957100
C	1.00147600	0.49031500	-0.64966000
C	-0.07991000	2.74106900	-0.77317600
C	0.27156100	3.56963800	0.31391200
C	-1.29949200	2.87990700	-1.46690500
C	-0.65059200	4.54822400	0.70504100
C	-2.18182900	3.87912600	-1.03581700
C	-1.86539900	4.70248600	0.04050600
H	-0.41239000	5.20418200	1.53649200
H	-3.12866800	4.01236300	-1.55138500
H	-2.56419200	5.47127100	0.36018600
C	2.51911800	-1.40881800	-1.24064100
C	3.78182700	-1.50196400	-0.62151600
C	1.80950500	-2.54410900	-1.68819200
C	4.32899300	-2.78066500	-0.44970600
C	2.40112400	-3.79665500	-1.48548100
C	3.64685100	-3.91698500	-0.87236700
H	5.30212000	-2.88483900	0.02200300
H	1.88363900	-4.69158000	-1.81560800
H	4.08712700	-4.90030800	-0.72840700
C	1.62919400	3.46622800	1.00447800
C	2.61117000	4.49844500	0.41061800
C	1.54683700	3.60989700	2.53369600
H	2.02933200	2.46853800	0.80367100
H	2.73492100	4.36116300	-0.66948500
H	3.59827900	4.40325700	0.87888200
H	2.25468800	5.52196600	0.57936500
H	0.85583100	2.87825000	2.96428300
H	1.22743700	4.61268100	2.84119500
H	2.53575100	3.43665600	2.97387900
C	-1.66537600	2.01190800	-2.66821600
C	-3.03006900	1.31955900	-2.49959400
C	-1.62522400	2.83415700	-3.97286800
H	-0.91537500	1.22060500	-2.75479600
H	-3.05713600	0.71577400	-1.58792400
H	-3.22365600	0.65937700	-3.35326500
H	-3.85277100	2.04305100	-2.45351900
H	-0.64115100	3.28915400	-4.13372800
H	-2.36541900	3.64302300	-3.95498000
H	-1.84802300	2.19504200	-4.83548400
C	4.56928500	-0.27563300	-0.16561800
C	4.95114700	-0.34416300	1.32473600
C	5.82031000	-0.06644300	-1.04342600
H	3.93052400	0.60329700	-0.28923000
H	4.06198600	-0.44782800	1.95369500
H	5.47567300	0.57283200	1.61942200
H	5.62069700	-1.18656200	1.53605100
H	5.55748100	0.03592900	-2.10255200
H	6.51431300	-0.91077000	-0.95474800
H	6.35566100	0.84046000	-0.73807600
C	0.47603800	-2.42128000	-2.42199000
C	0.70767000	-2.31877100	-3.94489600
C	-0.50722100	-3.56000400	-2.10374400
H	0.00136800	-1.49325400	-2.09026600
H	1.34246500	-1.46327900	-4.20028100
H	-0.24718200	-2.19933000	-4.47084600
H	1.19368400	-3.22440800	-4.32818700
H	-0.66569000	-3.66259200	-1.02545700
H	-0.16732800	-4.52575800	-2.49634200
H	-1.47844100	-3.34766100	-2.56447300
C	-0.32514200	-0.99606000	2.62582200
C	0.71946100	-1.86167300	2.20511100
S	0.17997400	-0.08005900	4.07188600
C	1.85509600	-1.80269000	3.08770100
H	0.57178900	-2.68253900	1.51064800
C	1.72071500	-0.90629100	4.10284400
H	2.73746600	-2.41897700	2.95155700
H	2.44018900	-0.65841200	4.87255600

TS5

Energy (RB3LYP) = -2446.710218430069 A.U.

Free Energy = -2446.116324765342 A.U.

Ni	-0.66835800	-0.27829300	-1.04416800
C	1.44831700	-0.03110200	-2.05860600
C	0.63820800	-1.15928400	-2.32045000
C	-0.52720900	-0.83452900	-3.08933100
C	-0.60709700	0.51908400	-3.38591100
S	0.85200000	1.38381800	-2.95379900
H	0.92765000	-2.17011100	-2.05229100
H	-1.27002900	-1.55789000	-3.40624600
C	-2.50554000	1.21373200	2.36072700
C	-3.15538000	0.03580100	2.20785600
H	-2.60219600	1.98699600	3.10655400
H	-3.93792600	-0.42656900	2.78914000
N	-1.58318400	1.30384700	1.31813500
N	-2.62116000	-0.56961600	1.07301900
C	-1.62966700	0.19837100	0.49110500
C	-3.05700600	-1.84309000	0.56224300
C	-4.14257900	-1.87980600	-0.33710900
C	-2.39783800	-3.01257500	0.99405300
C	-4.54414100	-3.13049700	-0.82261300
C	-2.83838900	-4.23676300	0.47538400
C	-3.89772300	-4.29845000	-0.42617300
H	-5.37437700	-3.18960600	-1.52108000
H	-2.34462600	-5.15418300	0.78339800
H	-4.22410900	-5.25921500	-0.81594400
C	-0.65666300	2.39887500	1.18360000
C	-0.98335000	3.47228400	0.32801700
C	0.52605200	2.37806100	1.95001900
C	-0.08365200	4.54224500	0.25737500
C	1.39068100	3.47546200	1.84215700
C	1.09162300	4.54679500	1.00585600
H	-0.30458400	5.38499500	-0.39013600

H	2.30836900	3.48933800	2.42338600
H	1.77417200	5.39014900	0.93776400
C	-4.87248600	-0.61986800	-0.79267000
C	-6.37053100	-0.66854200	-0.43474900
C	-4.66453800	-0.36681400	-2.29834700
H	-4.43832200	0.23227700	-0.26225500
H	-6.51987000	-0.81875400	0.64059900
H	-6.85971600	0.27113000	-0.71749300
H	-6.88719900	-1.48101400	-0.95904300
H	-3.59773200	-0.26364300	-2.52177500
H	-5.06828100	-1.18702500	-2.90425500
H	-5.17286500	0.55598600	-2.60403300
C	-1.23613700	-2.98121900	1.98230900
C	0.08533900	-3.38703800	1.30166100
C	-1.51687000	-3.84873200	3.22444900
H	-1.11493800	-1.95017900	2.32669000
H	0.30784700	-2.70873800	0.47102000
H	0.91539500	-3.33762300	2.01659100
H	0.03801000	-4.41116200	0.91164400
H	-2.44499000	-3.54627600	3.72298100
H	-1.60700600	-4.91085000	2.96831200
H	-0.69678100	-3.75278600	3.94571300
C	-2.29101400	3.50146500	-0.45851800
C	-2.13339300	4.08418500	-1.87350100
C	-3.38008600	4.26632300	0.32295400
H	-2.62494100	2.46652300	-0.57719300
H	-1.33267600	3.57711200	-2.42100000
H	-3.06755500	3.95743000	-2.43326300
H	-1.90993400	5.15753300	-1.85863400
H	-3.56406800	3.81484500	1.30385900
H	-3.08593700	5.31081200	0.48354900
H	-4.32617000	4.26349900	-0.23206400
C	0.86884100	1.23088100	2.89628200
C	0.74519500	1.67406000	4.36844300
C	2.26125700	0.63753700	2.61525300
H	0.14240500	0.43044600	2.73038500
H	-0.26132200	2.04434400	4.59468700
H	0.95611900	0.83385200	5.04078000
H	1.45496500	2.47657400	4.60266000
H	2.34885200	0.31277000	1.57450700
H	3.06145100	1.36086100	2.81171300
H	2.43739700	-0.22906700	3.26361300
C	2.75719900	0.01297400	-1.44557400
C	3.47946600	1.10828300	-1.01530400
S	3.69392700	-1.46302100	-1.20601100
C	4.76352600	0.78801400	-0.48653700
H	3.08403300	2.11770400	-1.04769200
C	5.00778500	-0.55423400	-0.51697900
H	5.46032400	1.51808200	-0.09261600
H	-1.38299500	1.02081700	-3.94800800
Br	6.59373100	-1.45974000	0.13505300

CPs and TSs with Pd(0)dppp

Pd(0)dppp

Energy (RB3LYP) = -1854.006154752044 A.U.

Free Energy = -1853.617597560421 A.U.

P	-1.92852200	-0.30706800	0.04020700
P	1.94870500	-0.24418100	0.05018300
C	1.34075400	-0.38911400	1.82769300
H	2.11542700	0.01054000	2.49473000
H	1.24452400	-1.45988600	2.04763900
C	-1.29739700	-0.44163300	1.80650300
H	-1.14645500	-1.51576700	1.96953200
H	-2.09441900	-0.14444900	2.50042700
C	0.00470700	0.32710000	2.14261900
H	-0.00493500	0.50612800	3.22640900
H	-0.00530200	1.32216300	1.68046600
C	-2.73686000	1.35817200	-0.02520500
C	-3.11714400	1.83386500	-1.29260900
C	-2.97065600	2.17852200	1.08942200
C	-3.73201000	3.07624900	-1.43890000
H	-2.91951300	1.22290700	-2.17028300
C	-3.57385800	3.43110700	0.94256300
H	-2.68200500	1.85217100	2.08365500
C	-3.96034500	3.88146000	-0.31963300
H	-4.02327700	3.42107300	-2.42767500
H	-3.74090600	4.05305100	1.81840900
H	-4.42957100	4.85518600	-0.43272200
C	-3.38039800	-1.45956400	0.14145300
C	-3.23793100	-2.74089500	-0.41234700
C	-4.59352800	-1.12385000	0.76311100
C	-4.27545100	-3.67189500	-0.33314200
H	-2.30805700	-3.00076900	-0.91352900
C	-5.63454100	-2.05082200	0.83411200
H	-4.73146400	-0.13130600	1.18338700
C	-5.47676200	-3.32760700	0.28924800
H	-4.14851900	-4.66083400	-0.76612100
H	-6.57057900	-1.77539800	1.31369500
H	-6.28921700	-4.04757800	0.34387600
C	2.65234200	1.47305100	0.06297900
C	1.93498400	2.49137000	-0.58320600
C	3.85368700	1.80172900	0.71160200
C	2.39824600	3.80911800	-0.56992900
H	1.01207100	2.23915400	-1.10053600
C	4.32097500	3.11640700	0.71783100
H	4.43502200	1.02622500	1.20312300
C	3.59272900	4.12387500	0.07953200
H	1.82875100	4.58610300	-1.07337800
H	5.25608100	3.35428500	1.21882300
H	3.95900600	5.14727700	0.08408000
C	3.47254400	-1.30098500	0.06614100
C	4.03966900	-1.61821200	-1.18016100
C	4.07337000	-1.82345100	1.22281400
C	5.18235000	-2.41176300	-1.26832300
H	3.57070200	-1.24398200	-2.08742600
C	5.21071400	-2.63118700	1.13483300
H	3.66035700	-1.60735100	2.20320400
C	5.77075900	-2.92378700	-0.10886300
H	5.60688400	-2.64066400	-2.24239300
H	5.65848900	-3.02972900	2.04182600
H	6.65500600	-3.55207700	-0.17585500
Pd	0.01355300	-0.57481100	-1.15608800

CP1

Energy (RB3LYP) = -2432.131175428226 A.U.

Free Energy = -2431.707195061825 A.U.

Pd	0.03835400	0.09104600	-0.66466800
P	1.68704300	-1.51357000	0.07604500
P	-1.80339700	-1.44463000	-0.62230700
C	-1.29937400	-3.21386300	-0.95676300
H	-2.17839200	-3.86623000	-0.89238400
H	-0.98059300	-3.23694400	-2.00666900
C	1.25077600	-3.27411100	-0.39450400
H	1.41027400	-3.32907600	-1.47915800
H	1.98875800	-3.95291200	0.04996900
C	-0.17406800	-3.75581800	-0.05236200
H	-0.17753700	-4.85006100	-0.14733600
H	-0.40435600	-3.54836800	1.00026800
C	1.80140700	-1.55619300	1.91912300
C	1.74843300	-0.32460000	2.59461800
C	1.93375200	-2.73136300	2.67640300
C	1.84034400	-0.27018200	3.98560900
H	1.62960500	0.59431700	2.02663000
C	2.01553000	-2.67646200	4.06992600
H	1.97509400	-3.70044200	2.18839000
C	1.97173400	-1.44622000	4.72729800
H	1.80096500	0.69209500	4.48886800
H	2.11368900	-3.59690000	4.63974900
H	2.03536200	-1.40466300	5.81140400
C	3.45194800	-1.48438800	-0.47826800
C	3.72980500	-0.98905000	-1.76137800
C	4.51042800	-1.96960400	0.30593900
C	5.03475700	-0.99548600	-2.25724600
H	2.92629400	-0.57652400	-2.36420800
C	5.81563700	-1.96671500	-0.18815500
H	4.31951500	-2.34119700	1.30835500
C	6.08018100	-1.48367200	-1.47172800
H	5.23408700	-0.60413500	-3.25125000
H	6.62685300	-2.33938300	0.43212300
H	7.09781700	-1.47945900	-1.85338600
C	-2.72859500	-1.53562500	0.97168000
C	-2.70772500	-0.39794000	1.79574000
C	-3.43612000	-2.66833000	1.40795600
C	-3.38770800	-0.38721500	3.01457000

H	-2.14786400	0.47824500	1.48002300
C	-4.11009400	-2.65984400	2.63065400
H	-3.46854400	-3.56612100	0.79743200
C	-4.08917900	-1.51854500	3.43504600
H	-3.35990700	0.50254900	3.63753700
H	-4.65027800	-3.54577400	2.95428700
H	-4.61290500	-1.51394300	4.38725200
C	-3.10270000	-1.21169800	-1.91825200
C	-4.47001300	-1.44420600	-1.70926500
C	-2.67659900	-0.78121300	-3.18646300
C	-5.38656100	-1.25966300	-2.74708300
H	-4.82543900	-1.76087600	-0.73358900
C	-3.59124100	-0.61030400	-4.22580900
H	-1.62280200	-0.56863400	-3.35316400
C	-4.95041500	-0.84759700	-4.00730000
H	-6.44381600	-1.43757600	-2.56784200
H	-3.24398100	-0.27999000	-5.20125600
H	-5.66584800	-0.70415100	-4.81261300
C	-0.55224300	3.39934100	0.69993800
C	-1.39125100	2.82890300	-0.19363500
C	-0.69016900	2.08520200	-1.23013500
C	0.73011000	2.07483200	-1.01487700
S	1.15542300	3.10205400	0.40106900
H	-2.47057700	2.92500100	-0.15454000
H	-1.11704600	1.99160800	-2.22407000
Br	1.96130900	2.31356200	-2.60091800
Br	-1.08470600	4.37219100	2.30214800

CP2

Energy (RB3LYP) = -2432.173754466570 A.U.

Free Energy = -2431.746852892057 A.U.

Pd	-0.28779900	-0.40723700	-0.06903300
P	0.45513300	1.50391800	1.03190900
P	-2.61598100	-0.15713800	0.59932500
C	-2.88348700	0.91793800	2.09882900
H	-3.95838400	1.09171400	2.22279100
H	-2.58174200	0.29937100	2.95345000
C	-0.61473900	2.10877800	2.43919200
H	-0.48352500	1.42282700	3.28329900
H	-0.20466100	3.07646800	2.75034000
C	-2.11362000	2.25069300	2.12393900
H	-2.55446200	2.87819600	2.90937200
H	-2.25482000	2.80153000	1.18580700
C	0.47155600	2.96832500	-0.08066300
C	-0.11740800	2.87680000	-1.35010400
C	1.00250700	4.20031800	0.33874400
C	-0.17501400	3.99490900	-2.18561100
H	-0.52833400	1.92705000	-1.68164000
C	0.94715700	5.31381400	-0.49855500
H	1.47480800	4.28810700	1.31340000
C	0.35749800	5.21271200	-1.76190000
H	-0.63376400	3.90911700	-3.16651300
H	1.36601200	6.25967800	-0.16594700
H	0.31643500	6.08158600	-2.41313300
C	2.11585900	1.43965200	1.81702100
C	2.26925200	0.85661100	3.08526300
C	3.25706300	1.89091500	1.13647500
C	3.53142200	0.75066000	3.66922600
H	1.41111400	0.46403700	3.62267400
C	4.51798700	1.78130300	1.72297200
H	3.16616400	2.31201800	0.14168300
C	4.65888700	1.21593600	2.99095700
H	3.63208600	0.29667500	4.65116400
H	5.39208100	2.12943400	1.18013000
H	5.64275400	1.12732100	3.44303500
C	-3.62366500	0.63387200	-0.72867800
C	-3.48764500	0.13987100	-2.03905500
C	-4.50542500	1.70201500	-0.49700700
C	-4.22567300	0.69748800	-3.08310200
H	-2.80584800	-0.68355600	-2.23488100
C	-5.23628000	2.26194500	-1.54783200
H	-4.63407900	2.11128500	0.49972600
C	-5.09948900	1.76039300	-2.84234000
H	-4.11293500	0.29931500	-4.08780000
H	-5.91231600	3.08966100	-1.35018500
H	-5.66944700	2.19578500	-3.65880900
C	-3.55846600	-1.65321400	1.10746200
C	-4.96134700	-1.67374000	1.08589600
C	-2.86151000	-2.76765100	1.59579800
C	-5.65536300	-2.78871800	1.55679800
H	-5.51373200	-0.82595600	0.69005300
C	-3.55983800	-3.87789700	2.07311000
H	-1.77664000	-2.77777700	1.57217500
C	-4.95551300	-3.89030500	2.05440200
H	-6.74177500	-2.79843000	1.52975300
H	-3.01024200	-4.73939200	2.44198400
H	-5.49721400	-4.75991000	2.41690200
C	3.99697800	-1.29310200	-1.12805500
C	3.61116800	-0.34033000	-2.02365000
C	2.25403100	0.07098100	-1.80370700
C	1.62789000	-0.57518000	-0.76468800
S	2.71930500	-1.71977500	-0.02587800
H	4.25177600	0.05140600	-2.80570600
H	1.76789500	0.82123600	-2.41876000
Br	-0.86476200	-2.51451500	-1.44674500
Br	5.74152600	-2.15451200	-1.04097300

CP3

Energy (RB3LYP) = -2971.343093019863 A.U.

Free Energy = -2970.865601207367 A.U.

Pd	-0.21816400	-0.29783700	0.06484200
P	0.56769000	1.90299900	0.79204400

P	-2.49402400	0.12878800	0.80505800
C	-2.68512700	1.41706000	2.14506100
H	-3.75727300	1.56542600	2.31792800
H	-2.26183200	1.00930700	3.07055600
C	-0.48736600	2.77997200	2.06067600
H	-0.25230300	2.29072300	3.01415000
H	-0.12230700	3.80902100	2.15757400
C	-2.01060700	2.76626100	1.83805700
H	-2.44805700	3.51460800	2.51174100
H	-2.26275900	3.09499400	0.82250100
C	0.65275900	3.07209500	-0.63123200
C	1.32866500	2.64509400	-1.78898700
C	0.07096300	4.34963100	-0.62318200
C	1.42489400	3.48085400	-2.90159600
H	1.78105400	1.65816100	-1.81374300
C	0.16010600	5.17927300	-1.74367300
H	-0.45645400	4.71398500	0.25192000
C	0.83791200	4.74839400	-2.88428300
H	1.95660500	3.13713500	-3.78473000
H	-0.30002900	6.16354600	-1.72020700
H	0.90838700	5.39570300	-3.75429300
C	2.20546400	2.05432500	1.62413200
C	2.50042700	1.15720500	2.66291600
C	3.13579500	3.05185100	1.30166900
C	3.69320600	1.26656000	3.37645400
H	1.80260100	0.35919100	2.90490500
C	4.33537100	3.15174100	2.00986200
H	2.92986000	3.74948000	0.49616900
C	4.61470900	2.26365400	3.04925100
H	3.91039300	0.56162200	4.17410600
H	5.05156500	3.92529100	1.74586400
H	5.55005300	2.34169800	3.59669500
C	-3.56530300	0.82767100	-0.52200900
C	-2.97205300	1.31880300	-1.69379000
C	-4.95829200	0.92766400	-0.36889900
C	-3.75453600	1.90608600	-2.69119500
H	-1.89732000	1.23084600	-1.82721800
C	-5.73796000	1.51091800	-1.36663300
H	-5.43636700	0.53487500	0.52444200
C	-5.13658900	2.00250100	-2.52906100
H	-3.28180900	2.27906900	-3.59545900
H	-6.81519700	1.57830700	-1.23960400
H	-5.74653800	2.45364200	-3.30719000
C	-3.47147100	-1.28594100	1.46640300
C	-3.96118700	-2.25394800	0.57247500
C	-3.69667200	-1.46347000	2.84060500
C	-4.67183300	-3.35685800	1.04320900
H	-3.78395800	-2.15038200	-0.49292600
C	-4.40474800	-2.57281500	3.30881000
H	-3.32683300	-0.74318500	3.56265400
C	-4.89676900	-3.52051600	2.41172300
H	-5.03970400	-4.09470600	0.33586300
H	-4.57131700	-2.69068600	4.37627000
H	-5.44762400	-4.38335300	2.77638200
C	3.92615200	-1.86968700	-0.86912700
C	3.42578200	-1.47794600	-2.07480900
C	2.10806000	-0.92617100	-1.94519400
C	1.62088800	-0.87807500	-0.65778600
S	2.80883900	-1.56312800	0.42975100
H	3.95843400	-1.58143500	-3.01348500
H	1.52552000	-0.61166500	-2.80588100
Br	5.67565900	-2.66374400	-0.54393300
C	-0.80314800	-2.10198600	-0.70194100
C	-0.74960300	-3.36246600	-0.16050400
S	-1.48539900	-2.19429100	-2.31316200
C	-1.26117200	-4.39372900	-1.01693600
H	-0.34471100	-3.56352000	0.82617700
C	-1.70020700	-3.92319800	-2.22186200
H	-1.29059400	-5.44327500	-0.73902000
H	-2.12311500	-4.47587900	-3.05076200

CP4

Energy (RB3LYP) = -2971.378146147386 A.U.

Free Energy = -2970.901488340466 A.U.

Pd	-0.19031000	-0.06970200	0.13559000
P	1.72993400	0.10735800	-1.28093200
P	-1.33453700	1.87140500	-0.64996900
C	-0.95091800	2.20029400	-2.45225600
H	-1.45987100	3.12114800	-2.76330100
H	-1.38171300	1.37698700	-3.03576200
C	1.32728200	0.98497100	-2.88547400
H	0.73577700	0.26341200	-3.46343000
H	2.25182500	1.13797400	-3.45597700
C	0.55509200	2.31667800	-2.77195700
H	0.63934500	2.82191000	-3.74337600
H	1.04136000	2.98343600	-2.04894700
C	3.12020200	1.08937900	-0.55943700
C	3.48644900	0.79594800	0.76651900
C	3.81218000	2.10679000	-1.23497500
C	4.52339900	1.48907200	1.39034700
H	2.95816800	0.01766200	1.31016900
C	4.84275600	2.80969500	-0.60451100
H	3.55574500	2.36323200	-2.25817100
C	5.20269200	2.50145400	0.70776700
H	4.79296100	1.23976100	2.41309300
H	5.36349100	3.59757200	-1.14277700
H	6.00483800	3.04829800	1.19643000
C	2.57661800	-1.39412400	-1.95620100
C	1.80804800	-2.55772100	-2.11890300
C	3.92818300	-1.41524500	-2.33492000
C	2.37385700	-3.71205500	-2.66429200
H	0.76859600	-2.56250600	-1.80195700
C	4.49427800	-2.57261800	-2.87176800
H	4.54319200	-0.52952600	-2.20340500

C	3.71821200	-3.72190800	-3.04078100
H	1.76578000	-4.60498100	-2.78293700
H	5.54320400	-2.57669500	-3.15749100
H	4.16176700	-4.62238000	-3.45764400
C	-0.87104900	3.48930000	0.12072600
C	0.24523500	3.53863600	0.96865100
C	-1.58224700	4.67413200	-0.13387900
C	0.64859600	4.74709400	1.54314800
H	0.79543000	2.62490200	1.17757600
C	-1.18214800	5.87880300	0.44337700
H	-2.45995800	4.65254800	-0.77469400
C	-0.06424100	5.91754600	1.28218600
H	1.51689100	4.76872300	2.19620700
H	-1.74365700	6.78746400	0.24158200
H	0.24515500	6.85705000	1.73276000
C	-3.18089300	1.93394900	-0.60160000
C	-3.80257800	1.98416400	0.66015500
C	-3.99513800	1.84989700	-1.74101200
C	-5.19067300	1.96503500	0.77638300
H	-3.19153800	2.04478700	1.55760300
C	-5.38829000	1.82112200	-1.62347000
H	-3.55428100	1.80649200	-2.73165700
C	-5.99050600	1.88044400	-0.36775600
H	-5.64984600	2.01304500	1.76041500
H	-6.00014800	1.75444300	-2.51939100
H	-7.07312100	1.85819600	-0.27789700
C	-0.20939800	-1.84957500	1.54410300
C	-1.40745400	-1.07894900	1.68392900
C	-2.56900600	-1.73744300	1.11757900
C	-2.27980200	-2.95609700	0.60722800
S	-0.60115800	-3.43190800	0.77011600
H	-1.52203500	-0.33460300	2.46806000
H	-3.55378400	-1.28649600	1.09060800
C	0.96354700	-1.80648800	2.42084100
C	2.14275100	-2.51377600	2.32330400
S	0.99983400	-0.77688600	3.84616100
C	3.07240900	-2.22454400	3.36593300
H	2.34541800	-3.20484800	1.51188900
C	2.60709200	-1.29688500	4.25658100
H	4.05073700	-2.68744700	3.44171800
Br	-3.51003800	-4.10835700	-0.36680400
H	3.09888000	-0.89337000	5.13139500

CP5

Energy (RB3LYP) = -2971.373285096131 A.U.

Free Energy = -2970.897708143739 A.U.

Pd	-0.64120700	0.41033500	-0.64064000
P	0.26930600	1.82772000	1.05431400
P	-2.73708100	-0.03410200	0.40445100
C	-3.28547400	1.41856000	1.45076000
H	-4.22789600	1.16271100	1.95105500
H	-3.49443800	2.25399900	0.77072300
C	-1.08243200	2.72893200	1.98659800
H	-1.46038800	3.48130600	1.28253300
H	-0.63688000	3.29243200	2.81582000
C	-2.25425800	1.86971400	2.50740600
H	-2.79556400	2.47630100	3.24576100
H	-1.87774800	0.99937700	3.05907300
C	1.21521800	0.94173400	2.37335200
C	2.15872700	-0.01173600	1.95050600
C	1.04230000	1.14480400	3.75152500
C	2.91549300	-0.72889600	2.87689900
H	2.30110200	-0.19009100	0.88839800
C	1.79239300	0.41768900	4.68009300
H	0.32145300	1.86984400	4.11647200
C	2.73144800	-0.51839600	4.24592200
H	3.64158400	-1.45754000	2.52667000
H	1.64048800	0.58595100	5.74325800
H	3.31380300	-1.08319100	4.96914500
C	1.36672900	3.26220400	0.64298100
C	1.25622900	3.82176900	-0.63959800
C	2.27474900	3.82619100	1.55307700
C	2.02406900	4.93169900	-0.99882400
H	0.57904500	3.37423900	-1.36224300
C	3.04726300	4.93036400	1.18982100
H	2.38702700	3.39716300	2.54479200
C	2.92133500	5.48760700	-0.08517400
H	1.92811500	5.35281400	-1.99624700
H	3.74952800	5.35487700	1.90291700
H	3.52537800	6.34636100	-0.36644200
C	-2.78782500	-1.41023100	1.64203200
C	-1.58181300	-2.00302800	2.04387900
C	-3.98954900	-1.86496400	2.21092500
C	-1.57461100	-3.02264200	2.99968400
H	-0.64865900	-1.66258700	1.60278700
C	-3.98230400	-2.88517000	3.16149200
H	-4.93557400	-1.42936500	1.89975700
C	-2.77370300	-3.46511900	3.55873900
H	-0.63151300	-3.47044200	3.30109200
H	-4.91943800	-3.23051300	3.59073000
H	-2.76995200	-4.26173100	4.29819500
C	-4.23353200	-0.38657400	-0.62250300
C	-4.26158100	-1.59209300	-1.34856100
C	-5.29948600	0.51126400	-0.78498200
C	-5.32563500	-1.89481100	-2.19519200
H	-3.44388000	-2.30111400	-1.24324900
C	-6.36294300	0.21152900	-1.64227500
H	-5.31470600	1.45214700	-0.24441100
C	-6.38177300	-0.99068000	-2.34759200
H	-5.33063200	-2.83592300	-2.73906100
H	-7.17865500	0.92157700	-1.75250100
H	-7.20943400	-1.22312400	-3.01219300
C	0.68244600	0.05140500	-2.47962200
C	-0.56479400	-0.63173700	-2.60861600

C	-1.43462300	-0.00835500	-3.58529400
C	-0.89268000	1.07732300	-4.19092600
S	0.73840700	1.41554000	-3.64804200
H	-0.68061600	-1.67832100	-2.33826000
H	-2.43506000	-0.37312200	-3.79272900
C	1.95359400	-0.51817500	-2.03291700
C	3.18454200	0.08925100	-1.91196000
S	2.07441900	-2.22146900	-1.58974000
C	4.22242300	-0.77630500	-1.45165900
H	3.34217800	1.14069900	-2.12655000
C	3.76754300	-2.04230200	-1.22840700
H	5.24775900	-0.46553300	-1.29039800
Br	4.79875800	-3.54996900	-0.57068800
H	-1.36098800	1.73992800	-4.90786400

CP6

Energy (RB3LYP) = -2971.385224941946 A.U.
Free Energy = -2970.908747210777 A.U.

Pd	-0.21907600	-0.32167800	-0.69457300
P	-2.10940400	-0.93904900	0.67178300
P	1.16626300	-2.16917000	-0.04688400
C	0.18421500	-3.69334900	0.40766700
H	0.87560900	-4.47839900	0.73791900
H	-0.30784200	-4.05490400	-0.50396700
C	-2.18336100	-2.77736100	1.02549000
H	-2.51664400	-3.23480700	0.08500000
H	-2.98521500	-2.96805400	1.74924400
C	-0.87996800	-3.45296500	1.49879400
H	-1.15391100	-4.43532000	1.90595500
H	-0.44066300	-2.89721800	2.33656000
C	-1.99767900	-0.16086000	2.34466200
C	-1.62025500	1.19301900	2.39666900
C	-2.25034800	-0.83282700	3.55121100
C	-1.51267800	1.85644700	3.61925100
H	-1.40367600	1.72621300	1.47449700
C	-2.13254700	-0.16987500	4.77562300
H	-2.54072500	-1.87891200	3.54990100
C	-1.76606700	1.17602600	4.81273600
H	-1.22288800	2.90364200	3.63762600
H	-2.32815200	-0.70820300	5.69946900
H	-1.67493000	1.69056800	5.76567300
C	-3.87227000	-0.66368200	0.18106200
C	-4.18840200	-0.69865400	-1.18556100
C	-4.90448100	-0.46718600	1.11215900
C	-5.51047400	-0.55776700	-1.61138500
H	-3.39531700	-0.81355800	-1.91833200
C	-6.22419600	-0.31742500	0.68371600
H	-4.67877600	-0.42139700	2.17353700
C	-6.53062700	-0.36626300	-0.67817000
H	-5.73849000	-0.58254400	-2.67362600
H	-7.01308800	-0.15986700	1.41488100
H	-7.55867800	-0.24653000	-1.00999000
C	2.21360900	-1.94061500	1.45929500
C	1.99507200	-0.81887800	2.27213900
C	3.20485300	-2.86548900	1.82872600
C	2.74510200	-0.62907000	3.43603300
H	1.23751500	-0.09348800	1.98842200
C	3.95478000	-2.67367800	2.98830800
H	3.40064600	-3.73081200	1.20061200
C	3.72468900	-1.55497800	3.79504200
H	2.56392100	0.24509800	4.05530600
H	4.72144500	-3.39421600	3.26150100
H	4.31212400	-1.40555300	4.69722700
C	2.38330700	-2.80650700	-1.28182700
C	3.44207400	-1.95886300	-1.65586400
C	2.27390400	-4.05497400	-1.91223200
C	4.36824200	-2.35339000	-2.61855800
H	3.54141900	-0.98466200	-1.18392100
C	3.19828900	-4.44620600	-2.88571200
H	1.47026700	-4.73623100	-1.65227700
C	4.24776600	-3.60000500	-3.24026600
H	5.18274300	-1.68612100	-2.88798300
H	3.09499300	-5.41728300	-3.36300300
H	4.96572000	-3.90559600	-3.99644900
C	1.32099600	3.00081900	-0.88585600
C	1.85249200	1.89201600	-1.48217200
C	0.89008800	0.99925900	-2.08656200
C	-0.45369600	1.44810300	-1.87612700
S	-0.45179000	3.03141800	-1.03642000
H	2.92296600	1.71390700	-1.52892800
H	1.15912700	0.35977100	-2.92136600
C	2.00122800	4.04981100	-0.15361100
C	1.57661700	5.33499100	0.11207800
S	3.59265300	3.78598900	0.54421300
C	2.52032900	6.10694000	0.84843000
H	0.62323100	5.71880700	-0.23526400
C	3.66115500	5.41258600	1.14602100
H	2.35869400	7.14067200	1.13489700
Br	-1.78366400	1.30475600	-3.39052500
H	4.53704700	5.75561400	1.68019000

CP7

Energy (RB3LYP) = -2971.383534383272 A.U.
Free Energy = -2970.907618705002 A.U.

Pd	1.15698100	0.16880000	-0.91197100
P	2.91375700	-0.95533100	0.23664700
P	1.36149400	2.30008600	0.14988000
C	3.10513300	2.60776300	0.76193100
H	3.11883700	3.53760500	1.34399100
H	3.74071200	2.76655300	-0.11883300
C	4.21927300	0.24224300	0.84271600
H	4.75025000	0.57302000	-0.05899900

H	4.96139700	-0.29555600	1.44532100
C	3.69644600	1.46885900	1.62056600
H	4.54680000	1.89025900	2.17296600
H	2.97264600	1.15890100	2.38516300
C	2.40471400	-1.87817800	1.75475500
C	1.18883600	-2.58245800	1.69196500
C	3.13301100	-1.90502900	2.95486700
C	0.72575600	-3.30559500	2.79154500
H	0.60164000	-2.55622000	0.77733300
C	2.66281800	-2.62030100	4.05911500
H	4.07291400	-1.36848500	3.04173800
C	1.46059300	-3.32460000	3.97936200
H	-0.21431000	-3.84639800	2.72180300
H	3.23832600	-2.62573700	4.98126900
H	1.09605000	-3.88047300	4.83915400
C	3.98715700	-2.16047000	-0.67243000
C	4.21772600	-1.92132000	-2.03742700
C	4.58651500	-3.27897700	-0.07397500
C	5.04255900	-2.76612500	-2.78101800
H	3.73896000	-1.06998500	-2.51651900
C	5.40129900	-4.13178600	-0.82178800
H	4.41222000	-3.49106500	0.97671800
C	5.63459600	-3.87626500	-2.17438100
H	5.21302300	-2.56438000	-3.83543400
H	5.85387800	-4.99778700	-0.34536300
H	6.26827600	-4.54207300	-2.75426900
C	0.39396100	2.53001200	1.71205100
C	-0.20149300	1.40776900	2.30690500
C	0.25291800	3.78170500	2.33378800
C	-0.91373100	1.53087900	3.50276800
H	-0.10744000	0.43766700	1.82579800
C	-0.46214400	3.90493900	3.52476200
H	0.69139700	4.66590300	1.87830100
C	-1.04556000	2.77876500	4.11259600
H	-1.36948900	0.65194500	3.95062300
H	-0.56822400	4.88041100	3.99267400
H	-1.60541000	2.87699800	5.03901600
C	0.97808700	3.85390700	-0.77968500
C	-0.30049500	3.95819400	-1.35673900
C	1.88678000	4.90406400	-0.98085500
C	-0.66492100	5.08283300	-2.09354600
H	-1.01196500	3.14661700	-1.22549200
C	1.52600300	6.02664500	-1.73285800
H	2.88363800	4.86069700	-0.55413300
C	0.25053200	6.12179900	-2.28749900
H	-1.66103400	5.14652800	-2.52380600
H	2.24594500	6.82784000	-1.87962700
H	-0.02906800	6.99542500	-2.87014100
C	-2.15771800	-1.15045900	-1.76885400
C	-1.71165300	0.07011500	-2.19984900
C	-0.33193300	0.09798900	-2.61405500
C	0.30377400	-1.16388600	-2.45006200
S	-0.87422600	-2.37110600	-1.86960500
H	-2.35642100	0.94285600	-2.24875900
H	0.04804000	0.86622300	-3.28087500
C	-3.46184400	-1.50468300	-1.24906500
C	-4.04977400	-2.74764500	-1.14951700
S	-4.54772300	-0.26774200	-0.61910200
C	-5.36352600	-2.72942200	-0.59603700
H	-3.55946100	-3.65473200	-1.48639000
C	-5.76113100	-1.46416200	-0.27491200
H	-5.97974200	-3.60929200	-0.45564500
Br	-7.47120400	-0.94389900	0.47703800
H	1.10572900	-1.54408600	-3.07270900

TS1

Energy (RB3LYP) = -2432.115962805660 A.U.

Free Energy = -2431.692945534719 A.U.

Pd	-0.38283300	-0.63437500	0.11397500
P	0.49484200	1.17778300	1.48216300
P	-2.66908800	0.10509600	0.19108000
C	-3.07831700	0.95883000	1.80154200
H	-4.12385100	1.28956400	1.78409700
H	-3.02291500	0.17228700	2.56488400
C	-0.76946300	1.75609100	2.73807300
H	-0.86150300	0.93249000	3.45726800
H	-0.35214900	2.60120500	3.29871400
C	-2.16138700	2.13604300	2.19188300
H	-2.67526200	2.69750400	2.98371100
H	-2.06048600	2.83404700	1.35121900
C	0.87768500	2.70033800	0.50863300
C	1.34767100	2.53419800	-0.80495800
C	0.72250600	4.00554800	1.00484900
C	1.66657400	3.63984700	-1.59420500
H	1.46118000	1.53163800	-1.20732200
C	1.03112300	5.11215900	0.21087500
H	0.36280600	4.17108500	2.01610300
C	1.50616500	4.93164100	-1.08930300
H	2.03465700	3.49000100	-2.60550100
H	0.90084000	6.11460100	0.61038100
H	1.74684500	5.79334000	-1.70620700
C	1.96591100	0.94568800	2.57628400
C	2.09537300	-0.28872300	3.23561900
C	2.94428200	1.93062700	2.78250200
C	3.16621000	-0.52173600	4.09956100
H	1.37021000	-1.07793100	3.05561000
C	4.01901300	1.69047300	3.64056500
H	2.87428200	2.88440400	2.26914200
C	4.13066700	0.46706900	4.30392400
H	3.25294500	-1.48269000	4.59938200
H	4.77175300	2.46089500	3.78706800
H	4.97032200	0.28165300	4.96854300
C	-3.18224000	1.30748700	-1.11185900
C	-2.58137500	1.18069400	-2.37532000

C	-4.12450800	2.33028100	-0.91713500
C	-2.92758700	2.03754300	-3.42020600
H	-1.83118300	0.40922100	-2.53104200
C	-4.46356300	3.19503000	-1.96023200
H	-4.60077900	2.46446300	0.04963300
C	-3.86909200	3.04820600	-3.21445900
H	-2.45394100	1.92211300	-4.39138200
H	-5.19200400	3.98364600	-1.79055600
H	-4.13308600	3.72213300	-4.02502500
C	-3.96889100	-1.20900900	0.15362300
C	-5.30673600	-0.95546600	-0.18720100
C	-3.59242000	-2.51326900	0.51190200
C	-6.24928400	-1.98410000	-0.16151800
H	-5.61326000	0.04217000	-0.48845100
C	-4.53957700	-3.53885800	0.54515100
H	-2.55434500	-2.72655800	0.75676600
C	-5.86846100	-3.27645400	0.20803400
H	-7.28095500	-1.77664100	-0.43385500
H	-4.23395900	-4.54339400	0.82503200
H	-6.60395100	-4.07641300	0.22553400
C	2.97920700	-1.39676100	-2.24051700
C	1.80221900	-1.82965700	-2.77060000
C	0.81952700	-2.08984100	-1.75804500
C	1.24835100	-1.73555500	-0.47679000
S	2.94125800	-1.22503800	-0.49649600
H	1.64711500	-2.01071400	-3.82799800
H	-0.09493600	-2.64032300	-1.94128600
Br	0.59379900	-3.24472800	1.09766300
Br	4.59540100	-0.96485300	-3.23012100

TS2

Energy (RB3LYP) = -2971.322959624901 A.U.

Free Energy = -2970.845879558413 A.U.

Pd	-0.25730400	-0.29994600	0.07433500
P	0.60396400	1.89515900	0.79319300
P	-2.56373100	0.22156900	0.77190700
C	-2.73262000	1.57356800	2.05367500
H	-3.79832000	1.79416100	2.18796500
H	-2.36024000	1.17665600	3.00657500
C	-0.46556000	2.84447400	1.99924600
H	-0.28568400	2.37094800	2.97265200
H	-0.07434800	3.86523700	2.08731100
C	-1.97986700	2.87484500	1.71422900
H	-2.41215800	3.67383100	2.33109100
H	-2.17683000	3.16392800	0.67436700
C	0.80453300	3.03823000	-0.64165100
C	1.54502800	2.56627100	-1.74158900
C	0.24854700	4.32506100	-0.70974100
C	1.73326800	3.36675900	-2.86764200
H	1.97209700	1.56761800	-1.71375000
C	0.42886400	5.12070000	-1.84457200
H	-0.32891100	4.72277900	0.11832800
C	1.17308400	4.64575400	-2.92438100
H	2.31426600	2.98801800	-3.70435200
H	-0.01217500	6.11348500	-1.87943900
H	1.31485400	5.26638700	-3.80509900
C	2.22274200	2.01194200	1.67417000
C	2.53890000	1.00878300	2.60390200
C	3.11984100	3.07534100	1.49176600
C	3.71769800	1.07582000	3.34762600
H	1.86675000	0.16507000	2.73478800
C	4.30360600	3.13517200	2.22901000
H	2.89783000	3.85613300	0.77058900
C	4.60347500	2.13836200	3.15974400
H	3.95060200	0.28943200	4.06039500
H	4.99218700	3.96188000	2.07465400
H	5.52732200	2.18521800	3.73005500
C	-3.62036200	0.89060000	-0.58921800
C	-3.00145200	1.38567100	-1.74661100
C	-5.02008900	0.94919500	-0.48929600
C	-3.76385300	1.94060600	-2.77757500
H	-1.92021200	1.32660500	-1.84086700
C	-5.78065600	1.49819400	-1.52118400
H	-5.51754900	0.55227600	0.39167400
C	-5.15340600	1.99701800	-2.66652300
H	-3.27013000	2.31936500	-3.66840500
H	-6.86354100	1.53325600	-1.43391200
H	-5.74808300	2.42170400	-3.47103700
C	-3.59187200	-1.13906200	1.47229100
C	-3.74637100	-2.30406100	0.69962100
C	-4.18728700	-1.09169900	2.74315700
C	-4.48878400	-3.38116700	1.18070500
H	-3.28321800	-2.37255200	-0.27926300
C	-4.92483400	-2.17635100	3.22509400
H	-4.08749900	-0.21156700	3.36970400
C	-5.07990200	-3.32221500	2.44506000
H	-4.59441300	-4.27154600	0.56707900
H	-5.37920000	-2.12030500	4.21098000
H	-5.65337700	-4.16533700	2.82106700
C	3.81010600	-1.89350100	-0.83491600
C	3.35188000	-1.44260900	-2.03880300
C	1.96127800	-1.12548100	-1.99829500
C	1.34873900	-1.32615000	-0.76748300
S	2.55919500	-1.92109800	0.37845700
H	3.96968800	-1.36157800	-2.92603700
H	1.40645900	-0.82128300	-2.87946200
Br	5.61937300	-2.48144600	-0.43170600
C	-0.36981600	-2.19123200	-0.78846700
C	-0.46663600	-3.42181600	-0.15660600
S	-1.22117900	-2.28101300	-2.33708300
C	-1.18601400	-4.40882200	-0.89392000
H	0.01558900	-3.62850800	0.79252200
C	-1.64907900	-3.95627100	-2.09901200
H	-1.33245900	-5.42569700	-0.54253300

H	-2.20186300	-4.49619900	-2.85669900

TS3

Energy (RB3LYP) = -2971.370871158452 A.U.

Free Energy = -2970.895715739267 A.U.

Pd	-0.35301600	-0.32944100	-0.12539300
P	0.91442600	0.70833100	-1.77652500
P	-2.58198100	0.22888900	-0.49963200
C	-2.70105000	0.62929900	-2.33139900
H	-3.70005200	1.03349800	-2.54018300
H	-2.61190400	-0.31692500	-2.87970400
C	-0.25383600	1.02744800	-3.21065000
H	-0.38452900	0.05036200	-3.69274700
H	0.24205300	1.66288200	-3.95566700
C	-1.63571800	1.62193300	-2.85359600
H	-2.04016800	2.06368400	-3.77426500
H	-1.52362800	2.45782200	-2.15150000
C	1.54325800	2.39384800	-1.33124900
C	2.20400800	2.51845300	-0.09636700
C	1.39030900	3.54391800	-2.12160100
C	2.71477700	3.74568500	0.32513200
H	2.30876100	1.64494700	0.54203500
C	1.89032300	4.77753900	-1.69468900
H	0.87680300	3.49153100	-3.07683400
C	2.55699600	4.88142400	-0.47338800
H	3.22464700	3.81326300	1.28270500
H	1.75674500	5.65704900	-2.31965100
H	2.94470100	5.84158100	-0.14292700
C	2.34132500	-0.02905800	-2.71118400
C	2.50376000	-1.42192800	-2.65908500
C	3.24147100	0.72672700	-3.47899200
C	3.52909900	-2.04792300	-3.37104900
H	1.82463400	-2.01330300	-2.04947100
C	4.27298700	0.10246700	-4.18221700
H	3.14549700	1.80831500	-3.51983500
C	4.41706000	-1.28635600	-4.13288700
H	3.63898800	-3.12815500	-3.32062900
H	4.96586900	0.70131400	-4.76832200
H	5.22171300	-1.77064300	-4.68022400
C	-3.19017000	1.82169100	0.23384100
C	-2.26015600	2.67917500	0.84122700
C	-4.53653900	2.21876000	0.17744800
C	-2.66284300	3.90709500	1.37266200
H	-1.21721400	2.37539700	0.89331000
C	-4.94018600	3.44126000	0.71483300
H	-5.27512600	1.56479100	-0.27851800
C	-4.00361600	4.28924300	1.31252500
H	-1.92836300	4.55991200	1.83720800
H	-5.98670400	3.73224200	0.66817700
H	-4.31993600	5.24096500	1.73176800
C	-4.04571300	-0.87975100	-0.23956300
C	-4.35919500	-1.23886000	1.08510900
C	-4.80307000	-1.44921400	-1.27501500
C	-5.40058400	-2.12035300	1.36532100
H	-3.78182200	-0.81545200	1.90448400
C	-5.84041600	-2.34466300	-0.99532100
H	-4.59459100	-1.19973100	-2.31036400
C	-6.14501800	-2.68137200	0.32269000
H	-5.62920700	-2.37511600	2.39711000
H	-6.41228700	-2.77469800	-1.81388100
H	-6.95183000	-3.37662900	0.53842400
C	1.71408000	-0.99576000	2.50344800
C	0.34155700	-1.10870600	2.38964500
C	-0.08857600	-2.23515900	1.61519400
C	0.98298200	-2.94982900	1.14048600
S	2.51648500	-2.32069900	1.66761500
H	-0.34896900	-0.41572800	2.85715000
H	-1.12194600	-2.52708200	1.47746200
C	2.49318300	0.01506300	3.19155900
C	3.81314500	0.36933100	3.00244000
S	1.78074600	0.99242100	4.46409100
C	4.24806500	1.41988300	3.86094000
H	4.44533000	-0.09642400	2.25380700
C	3.26184000	1.86513600	4.69848600
H	5.25240100	1.82914600	3.84869400
Br	0.90291300	-4.57881800	0.09815900
H	3.31331400	2.64955100	5.44153900

TS4

Energy (RB3LYP) = -2971.368774987662 A.U.

Free Energy = -2970.892862621616 A.U.

Pd	-0.42346800	0.31404000	0.21656000
P	1.00298300	1.59081000	-1.11962300
P	-2.43588600	0.04292800	-0.90734700
C	-2.40870800	1.15017000	-2.43074800
H	-3.14271200	0.77463600	-3.15549500
H	-2.79091600	2.11867100	-2.08515600
C	-0.08420500	2.36239400	-2.44059300
H	-0.66842200	3.15885500	-1.96325400
H	0.55248700	2.83601600	-3.19855900
C	-1.04745500	1.36659200	-3.12979500
H	-1.26457300	1.76535500	-4.12996100
H	-0.53756000	0.40949200	-3.29668500
C	2.23854400	0.70156400	-2.18185400
C	2.25891600	-0.70030100	-2.16023300
C	3.13867700	1.37738200	-3.02242300
C	3.15082300	-1.41281200	-2.96663000
H	1.57598100	-1.22719100	-1.49826100
C	4.03173600	0.66734400	-3.82444800
H	3.15131100	2.46433200	-3.04037300
C	4.03786900	-0.73047100	-3.79963000
H	3.15709900	-2.49917300	-2.93498800

H	4.72605700	1.20374500	-4.46650500
H	4.73657100	-1.28287800	-4.42271900
C	2.00357100	3.03766900	-0.53156700
C	1.75829300	4.37302200	-0.88723500
C	3.03228600	2.77508400	0.39329600
C	2.51806700	5.41158900	-0.33893600
H	0.97545800	4.61849800	-1.59765100
C	3.79732600	3.80838100	0.93015900
H	3.23459000	1.74814600	0.69003400
C	3.54010300	5.13447400	0.56784400
H	2.30981600	6.43870700	-0.62846500
H	4.59246000	3.58016300	1.63547600
H	4.13063400	5.94235200	0.99167000
C	-2.81793400	-1.63073400	-1.60239600
C	-3.31032300	-2.61904700	-0.72915500
C	-2.54975200	-1.99629700	-2.93040400
C	-3.53977500	-3.91993300	-1.17229300
H	-3.52877900	-2.36012600	0.30450300
C	-2.76946000	-3.30451900	-3.37289500
H	-2.16479900	-1.26480100	-3.63403800
C	-3.26657800	-4.26996600	-2.49846900
H	-3.93249500	-4.66267000	-0.48230300
H	-2.55379100	-3.56395700	-4.40641400
H	-3.43971800	-5.28568500	-2.84379600
C	-4.08574100	0.54204500	-0.21752400
C	-5.30326900	0.24396000	-0.85186400
C	-4.10858400	1.28995300	0.96883900
C	-6.51192300	0.68669600	-0.31360700
H	-5.30816300	-0.34597200	-1.76460500
C	-5.31845800	1.73937300	1.50421900
H	-3.17183600	1.51147000	1.47449300
C	-6.52179400	1.43798500	0.86497000
H	-7.44676400	0.44570000	-0.81365800
H	-5.31940500	2.31805800	2.42453500
H	-7.46418200	1.78170100	1.28376600
C	2.53129400	-2.50656100	1.56263300
C	1.32585000	-3.02137000	1.18177400
C	0.23896200	-2.19175900	1.59063200
C	0.63246200	-1.04149100	2.25338700
S	2.38879800	-1.01180200	2.43385600
H	1.21022000	-3.94656600	0.63052800
H	-0.80047000	-2.43582900	1.40502200
Br	4.27586700	-3.26532700	1.18942800
C	-0.19701700	-0.03437300	2.90843400
C	0.02949000	1.32508900	3.03812800
S	-1.63132300	-0.50115400	3.81279500
C	-0.95990300	1.98670900	3.82226800
H	0.87258500	1.82600400	2.57583100
C	-1.92165200	1.13640900	4.29872900
H	-0.95547900	3.05382300	4.01577000
H	-2.78752600	1.37547400	4.90196900

TS5

Energy (RB3LYP) = -2971.370790507723 A.U.

Free Energy = -2970.896222148246 A.U.

Pd	-1.02890100	0.35232600	-0.65369600
P	-0.53361100	2.18680000	0.68087900
P	-2.92891200	-0.67070000	0.21917900
C	-3.83297900	0.67267100	1.17250600
H	-4.66009500	0.21496800	1.73047800
H	-4.27572500	1.35565200	0.43654900
C	-2.13573300	2.64763300	1.54486400
H	-2.73408200	3.15867900	0.77997900
H	-1.93410600	3.40100200	2.31722100
C	-2.95095500	1.48222100	2.15182800
H	-3.62736600	1.92071400	2.89788900
H	-2.29392900	0.80558900	2.71272000
C	0.64020000	1.85144400	2.07554000
C	1.85707300	1.22838800	1.74597600
C	0.39268300	2.15339700	3.42392000
C	2.80399800	0.93700200	2.72717800
H	2.05685400	0.96366800	0.71063100
C	1.33556400	1.84990700	4.41041200
H	-0.53918600	2.62474500	3.72090100
C	2.54444900	1.24522300	4.06521300
H	3.73837400	0.45806900	2.44630700
H	1.12156600	2.08733900	5.44954400
H	3.27626600	1.00899300	4.83326600
C	-0.00892300	3.87795400	0.11210700
C	-0.15428500	4.18517100	-1.24892000
C	0.49749300	4.86309600	0.97487500
C	0.18001700	5.45104600	-1.73515700
H	-0.52313300	3.41824100	-1.92627500
C	0.84108300	6.12524900	0.48827600
H	0.63623900	4.64142200	2.02963000
C	0.67961300	6.42346700	-0.86721300
H	0.05955300	5.67368300	-2.79244800
H	1.23669300	6.87638200	1.16757900
H	0.94873000	7.40658000	-1.24485500
C	-2.68079300	-1.92803900	1.56156900
C	-1.39387700	-2.09219900	2.09645400
C	-3.73177100	-2.69962000	2.08457100
C	-1.16278500	-2.99877100	3.13423000
H	-0.57455900	-1.50276900	1.69144600
C	-3.49981100	-3.61069800	3.11529900
H	-4.73405700	-2.59648900	1.67722400
C	-2.21469000	-3.76122100	3.64373100
H	-0.15995600	-3.11145600	3.53797300
H	-4.32231200	-4.20488500	3.50580400
H	-2.03535300	-4.47258000	4.44582700
C	-4.29634700	-1.44584800	-0.76595400
C	-3.98078300	-2.59575800	-1.51439700
C	-5.59292500	-0.92008600	-0.87862100
C	-4.92937100	-3.20691200	-2.33105500

H	-2.97964600	-3.01702400	-1.44928200
C	-6.54210900	-1.52494700	-1.70906500
H	-5.87841700	-0.03568200	-0.31822200
C	-6.21648600	-2.66970100	-2.43498900
H	-4.66413100	-4.09970900	-2.89171400
H	-7.53974900	-1.09890500	-1.78174700
H	-6.95545400	-3.13927500	-3.07868600
C	1.70063200	-0.39197500	-2.45576000
C	0.49290200	-1.05862700	-2.33790600
C	-0.54806100	-0.49128100	-3.13961300
C	-0.12539000	0.60745000	-3.84830600
S	1.55878000	0.93838600	-3.59153000
H	0.36284000	-1.94384000	-1.72495100
H	-1.54679200	-0.90525200	-3.21231100
C	2.96398200	-0.67675700	-1.80469000
C	4.04451200	0.15540100	-1.60259700
S	3.29361500	-2.27549300	-1.14641200
C	5.13316900	-0.46102700	-0.91872900
H	4.05309200	1.19305300	-1.91883700
C	4.86368900	-1.76245200	-0.60664400
H	6.05962700	0.04101800	-0.66778700
Br	6.02620200	-2.99030400	0.33860800
H	-0.69782900	1.21909900	-4.53250300

CPs and TSs with Pd(0)NHC

Pd(0)NHC

Energy (RB3LYP) = -1286.796900951381 A.U.

Free Energy = -1286.290512363789 A.U.

C	-0.67688300	0.00655100	2.21915300
C	0.67729900	0.00477900	2.21891000
H	-1.38887300	0.00999400	3.02960700
H	1.38958100	0.00633400	3.02911000
N	-1.07857400	0.00288600	0.88437000
N	1.07848400	0.00003100	0.88399000
C	-0.00020100	-0.00142800	0.02836600
C	2.46089200	-0.00033800	0.47423600
C	3.11615800	-1.23510700	0.29549300
C	3.11728300	1.23429800	0.29921600
C	4.46599000	-1.20612500	-0.07615400
C	4.46725200	1.20533400	-0.07199800
C	5.13760000	-0.00041500	-0.25864700
H	4.99636900	-2.14206800	-0.22809400
H	4.99859800	2.14129200	-0.22050600
H	6.18539700	-0.00046500	-0.54786200
C	-2.46116600	0.00390800	0.47512500
C	-3.11924000	-1.23029700	0.30301400
C	-3.11468900	1.23909400	0.29311800
C	-4.46893600	-1.20036800	-0.06906900
C	-4.46438000	1.21104100	-0.07911200
C	-5.13751400	0.00582400	-0.25914300
H	-5.00142000	-2.13596300	-0.21568300
H	-4.99335100	2.14734700	-0.23365400
H	-6.18511900	0.00660400	-0.54905100
C	2.40723200	-2.57430400	0.46922700
C	3.09299000	-3.45415900	1.53205200
C	2.28416300	-3.31185200	-0.87824000
H	1.39000600	-2.37520000	0.81813300
H	3.15471900	-2.94041400	2.49842000
H	2.52895500	-4.38324200	1.67678700
H	4.11196600	-3.72995000	1.23613900
H	1.73717300	-2.69558200	-1.60036400
H	3.26966800	-3.54590900	-1.29887400
H	1.74187200	-4.25647000	-0.74804400
C	2.40990400	2.57371000	0.47800500
C	2.29955900	3.32369800	-0.86366600
C	3.08946600	3.44232600	1.55405100
H	1.38934400	2.37428100	0.81683200
H	1.75802500	2.71550900	-1.59650600
H	1.75761300	4.26790500	-0.72925700
H	3.28878700	3.56042800	-1.27388100
H	3.14070000	2.92037100	2.51663100
H	4.11214500	3.71612700	1.26923800
H	2.52787700	4.37245500	1.70164100
C	-2.41365700	-2.57021200	0.48483800
C	-2.30022400	-3.32075800	-0.85625700
C	-3.09697200	-3.43791600	1.55922300
H	-1.39390900	-2.37148000	0.82653300
H	-1.75645600	-2.71286600	-1.58771700
H	-1.75913100	-4.26523100	-0.72023600
H	-3.28857800	-3.55697500	-1.26889400
H	-3.15131900	-2.91537600	2.52131100
H	-4.11872400	-3.71190900	1.27123900
H	-2.53598000	-4.36802400	1.70918900
C	-2.40408700	2.57788100	0.46345800
C	-3.09016800	3.46245900	1.52216600
C	-2.27804000	3.31049500	-0.88643100
H	-1.38766700	2.37868200	0.81464600
H	-3.15414300	2.95223800	2.49025800
H	-2.52499300	4.39122100	1.66451900
H	-4.10829500	3.73871700	1.22375500
H	-1.73126100	2.69080000	-1.60573800
H	-3.26267000	3.54459400	-1.30907400
H	-1.73440800	4.25470500	-0.75888500
Pd	0.00000700	-0.00981800	-1.93969100

CP1

Energy (RB3LYP) = -1864.935856787257 A.U.

Free Energy = -1864.398111939889 A.U.

Pd	0.25547500	-0.25065900	-0.60068500
C	3.84009400	-0.23245600	-0.34089500
C	3.21371900	0.84150600	-0.89061100
C	2.09777800	0.46398600	-1.72346200
C	1.87243500	-0.93628000	-1.71572400
S	3.11629500	-1.77285400	-0.74004300
H	3.52352100	1.86766600	-0.73212500
H	1.70561200	1.11912700	-2.49295600
Br	1.22304200	-1.92825700	-3.33166700
Br	5.30971800	-0.16136600	0.92765200
C	-3.01442100	1.67626400	1.49787200
C	-3.27242900	0.38431600	1.81651100
H	-3.52765500	2.58997200	1.75358000
H	-4.05710900	-0.06185100	2.40713800
N	-1.86844200	1.66901900	0.70621300
N	-2.27724800	-0.37892500	1.21203000
C	-1.39040500	0.39906800	0.51473400
C	-2.19716900	-1.81675800	1.31605900
C	-2.88528800	-2.60375700	0.37053300
C	-1.45034600	-2.37891300	2.37113700
C	-2.80574700	-3.99525400	0.50665000
C	-1.40363700	-3.77582500	2.45737000
C	-2.07284400	-4.57770000	1.53694200
H	-3.32257400	-4.63011000	-0.20734400
H	-0.83197500	-4.24049900	3.25566700
H	-2.02195400	-5.65997300	1.62206400
C	-1.26412100	2.86552200	0.17156500
C	-1.65621700	3.31155300	-1.10613300

C	-0.32015300	3.55513600	0.95833800
C	-1.06172400	4.48242300	-1.59337300
C	0.23956600	4.72224600	0.42352900
C	-0.12351500	5.18225300	-0.83942400
H	-1.33880700	4.84993600	-2.57743700
H	0.97132500	5.27617400	1.00488400
H	0.32434600	6.08958700	-1.23634900
C	-3.70190300	-1.99992300	-0.76782900
C	-5.20173600	-2.32118000	-0.61145300
C	-3.17650200	-2.44798400	-2.14512500
H	-3.59436400	-0.91227400	-0.72258100
H	-5.59067300	-1.96377700	0.34909100
H	-5.77994000	-1.84309200	-1.41102100
H	-5.38854500	-3.40020600	-0.66499500
H	-2.12082500	-2.18553200	-2.26837200
H	-3.27531900	-3.53116400	-2.28299600
H	-3.74734900	-1.95915800	-2.94378900
C	-0.70611400	-1.53201600	3.39866700
C	0.81374300	-1.77754400	3.33601100
C	-1.25254000	-1.76284700	4.82146800
H	-0.87062000	-0.47879100	3.15352000
H	1.20235000	-1.56531400	2.33459600
H	1.33231700	-1.12752500	4.05096700
H	1.06508800	-2.81505900	3.58626300
H	-2.32671700	-1.55157100	4.87788400
H	-1.09928100	-2.79763400	5.14948100
H	-0.73956300	-1.10897500	5.53658700
C	-2.68399800	2.57351300	-1.95838300
C	-2.04925400	2.01734900	-3.24767900
C	-3.90293900	3.46298600	-2.27269900
H	-3.04678400	1.71569700	-1.38488900
H	-1.23001600	1.33033100	-3.01045300
H	-2.79680700	1.46887300	-3.83333100
H	-1.65400300	2.82108700	-3.88049300
H	-4.37524100	3.83417900	-1.35584000
H	-3.62431900	4.33270000	-2.87914000
H	-4.65282600	2.89430000	-2.83507000
C	0.09984100	3.08124000	2.34643100
C	-0.30389000	4.09817500	3.43247200
C	1.60711400	2.76851300	2.40814600
H	-0.42864800	2.14789200	2.56032500
H	-1.38284500	4.29127100	3.42002100
H	-0.03803200	3.71992400	4.42661500
H	0.20716700	5.05830800	3.29452800
H	1.87947400	2.00966600	1.66793900
H	2.21327600	3.66316300	2.22161500
H	1.87457900	2.38913300	3.40157600

CP2

Energy (RB3LYP) = -1864.953568775482 A.U.

Free Energy = -1864.414845163126 A.U.

Pd	-0.42500300	-0.30277100	-0.09501500
C	-4.78542000	-1.06613900	-0.34558500
C	-4.20211300	-2.30258900	-0.39283400
C	-2.77715100	-2.21143200	-0.44192600
C	-2.29098200	-0.92259200	-0.36862200
S	-3.61997600	0.22319500	-0.35160800
H	-4.75993500	-3.23198100	-0.39698900
H	-2.13216400	-3.07865800	-0.54062400
Br	-0.15119000	-0.32951700	-2.59767400
Br	-6.69136000	-0.70496200	-0.22956600
C	3.74022800	0.33237500	1.00086800
C	3.30726600	1.61700400	1.02332000
H	4.70274400	-0.09900800	1.22473400
H	3.81447000	2.53646200	1.26886300
N	2.65459600	-0.44853300	0.61556100
N	1.96661600	1.59072500	0.65261800
C	1.54313800	0.31650400	0.40322400
C	1.13063000	2.76936500	0.58422100
C	1.18796900	3.57638100	-0.57069000
C	0.31164600	3.07890100	1.68930400
C	0.38276500	4.72189300	-0.59370700
C	-0.48375300	4.22810900	1.60292600
C	-0.44897400	5.04306100	0.47530400
H	0.40145900	5.36652500	-1.46685500
H	-1.13660900	4.48840000	2.43085300
H	-1.07238600	5.93190300	0.42918900
C	2.71324000	-1.88989700	0.50117800
C	3.26252000	-2.45550000	-0.66889500
C	2.25504500	-2.67241500	1.58049400
C	3.33848000	-3.85216700	-0.73254000
C	2.34569900	-4.06450400	1.45495000
C	2.88207400	-4.65040700	0.31277200
H	3.75534700	-4.32139200	-1.61803500
H	1.99504300	-4.69583000	2.26634500
H	2.94587300	-5.73257800	0.23646800
C	2.10171900	3.26220200	-1.75202200
C	3.33664900	4.18783000	-1.74691500
C	1.36786400	3.33826200	-3.10340800
H	2.45438700	2.23229200	-1.64168200
H	3.90650000	4.10363000	-0.81416500
H	4.00718600	3.93476100	-2.57649600
H	3.04200000	5.23790700	-1.86133900
H	0.50095800	2.67184300	-3.11751900
H	1.03297200	4.35686500	-3.33199100
H	2.04471100	3.02914200	-3.90827000
C	0.25712600	2.21347600	2.94489100
C	-1.08492700	1.46296000	3.04204100
C	0.52818200	3.02859300	4.22430900
H	1.04782100	1.46020000	2.87413400

H	-1.26021500	0.84130100	2.15253500
H	-1.10167900	0.80821200	3.92123500
H	-1.92887200	2.15800700	3.11916500
H	1.48801300	3.55391900	4.16669500
H	-0.25200300	3.77633500	4.40546800
H	0.55526900	2.36450300	5.09604400
C	3.79631000	-1.60982700	-1.82228000
C	3.31671300	-2.10918000	-3.19735400
C	5.33772800	-1.53968300	-1.77923700
H	3.40862200	-0.59361100	-1.70264300
H	2.22539000	-2.16178600	-3.23698600
H	3.65056100	-1.41528600	-3.97739000
H	3.72716500	-3.09583200	-3.44254700
H	5.70368600	-1.12841800	-0.83150500
H	5.77917200	-2.53623900	-1.90027700
H	5.71387000	-0.90466100	-2.58990600
C	1.68747600	-2.07139100	2.86299200
C	2.54019900	-2.45071800	4.09003600
C	0.21280000	-2.46880900	3.06834100
H	1.71978500	-0.98161600	2.77356000
H	3.58283600	-2.13804100	3.96351000
H	2.14658500	-1.96622600	4.99133200
H	2.53559600	-3.53249200	4.26605000
H	-0.40316900	-2.17377900	2.21010400
H	0.10236700	-3.55182100	3.19729300
H	-0.19373800	-1.98319100	3.96331700

CP3

Energy (RB3LYP) = -2404.139237981727 A.U.

Free Energy = -2403.548542383114 A.U.

Pd	-0.47821900	-0.76680500	-0.71058800
C	3.87749500	-1.13137900	0.08167600
C	3.77960900	-0.25440500	-0.95729400
C	2.41562800	-0.03241600	-1.34761900
C	1.50395000	-0.72493100	-0.59225600
S	2.31806800	-1.70802600	0.60503100
H	4.63182500	0.22046800	-1.42993500
H	2.13963600	0.62700100	-2.16231300
C	-1.60129900	3.02439500	1.22685800
C	-2.47587900	2.14919200	1.78085600
H	-1.49591900	4.09198200	1.33657200
H	-3.28945300	2.29399900	2.47409000
N	-0.76063200	2.28462100	0.39950200
N	-2.14777600	0.89622000	1.27599300
C	-1.08745000	0.95740800	0.41268200
C	-2.86560200	-0.31684100	1.59632000
C	-3.94239300	-0.70294300	0.77122600
C	-2.47824700	-1.05240700	2.73567300
C	-4.62984200	-1.87463600	1.11317600
C	-3.20656800	-2.21048600	3.03264600
C	-4.26823300	-2.62130400	2.23045100
H	-5.46034400	-2.20365900	0.49545600
H	-2.93566300	-2.80056500	3.90306200
H	-4.81606700	-3.52650200	2.47808900
C	0.30420400	2.89266000	-0.36783800
C	0.07817100	3.19198500	-1.72585700
C	1.51050700	3.20752300	0.29072200
C	1.12107700	3.80493100	-2.43285000
C	2.51137200	3.83323200	-0.46193300
C	2.32459400	4.12348800	-1.81058400
H	0.98251300	4.04304600	-3.48356200
H	3.45328500	4.08845800	0.01393600
H	3.11832300	4.60280400	-2.37747800
C	-4.38646200	0.10455600	-0.44552700
C	-5.81248300	0.65983900	-0.25624800
C	-4.27973300	-0.71506600	-1.74635600
H	-3.71697500	0.96397100	-0.54838000
H	-5.88498700	1.27738200	0.64625900
H	-6.09724100	1.27834700	-1.11536400
H	-6.54914600	-0.14704100	-0.16810800
H	-3.26056400	-1.08483800	-1.91045000
H	-4.94657900	-1.58477300	-1.73148100
H	-4.55799100	-0.09649200	-2.60765500
C	-1.33353400	-0.61787400	3.64591900
C	-0.29973200	-1.73917300	3.85920900
C	-1.87244700	-0.09919800	4.99510600
H	-0.80948400	0.21032600	3.15977900
H	0.10403900	-2.09252300	2.90554000
H	0.53653300	-1.36728900	4.46205900
H	-0.73051400	-2.59750500	4.38771900
H	-2.56794400	0.73679900	4.85699000
H	-2.40496000	-0.88812300	5.53945100
H	-1.04745200	0.24709900	5.62851500
C	-1.24262200	2.90634500	-2.43458500
C	-1.06175200	1.91756600	-3.60182200
C	-1.91522400	4.21088200	-2.90755900
H	-1.92020400	2.43527800	-1.71655800
H	-0.63790800	0.97015000	-3.25183900
H	-2.02882300	1.70419800	-4.07250300
H	-0.39836600	2.32255900	-4.37500900
H	-2.07826700	4.90299200	-2.07343600
H	-1.30602000	4.72978100	-3.65664900
H	-2.88789700	3.99295300	-3.36414200
C	1.74130700	2.92058800	1.77218700
C	1.67158400	4.22090700	2.60020700
C	3.06731300	2.18231000	2.03077700
H	0.93756200	2.26362000	2.11883400
H	0.70978500	4.73235200	2.47804900
H	1.80575900	4.00321700	3.66636000
H	2.45959800	4.92137700	2.29910700
H	3.13873100	1.26942200	1.43402200
H	3.93534100	2.80977400	1.79669700
H	3.14024900	1.90900200	3.08986700
C	-0.25137100	-2.43755000	-1.78930500

C	-0.41063700	-3.75180200	-1.39598100
S	-0.04696000	-2.38193200	-3.52996200
C	-0.41898500	-4.69081500	-2.47444500
H	-0.51405800	-4.04487700	-0.35559300
C	-0.23435700	-4.10111200	-3.69657200
H	-0.55291500	-5.76020000	-2.34151800
H	-0.20543000	-4.57297200	-4.67038900
Br	5.51529900	-1.70958200	0.96037300

CP4

Energy (RB3LYP) = -2404.184875762993 A.U.

Free Energy = -2403.593611438597 A.U.

Pd	0.25333000	-0.28622300	-0.41701600
C	1.72791700	-1.68763600	-1.25176600
C	2.05411200	-0.40730700	-1.76375100
C	3.22062700	0.17242300	-1.14551100
C	3.77883700	-0.64915600	-0.21851300
S	2.93626400	-2.16144800	-0.00853900
H	1.66297400	-0.03477900	-2.70546600
H	3.60149800	1.15622400	-1.39130800
Br	5.27733200	-0.20636900	0.93769100
C	-3.03790900	1.43933500	1.76257400
C	-2.66609000	2.53084400	1.05133600
H	-3.82518400	1.29323100	2.48539400
H	-3.06232900	3.53383200	1.02523700
N	-2.17037000	0.41268000	1.39668600
N	-1.58043200	2.14445700	0.26823100
C	-1.25105400	0.82699400	0.46557900
C	-0.89394700	3.03942300	-0.63119000
C	0.16648400	3.82057800	-0.13024900
C	-1.32509200	3.11845300	-1.97035500
C	0.80512700	4.69341400	-1.02009700
C	-0.64886500	4.00535000	-2.81745900
C	0.40591100	4.78521400	-2.35075300
H	1.62781100	5.30755400	-0.66456700
H	-0.95380800	4.08502300	-3.85717100
H	0.91629000	5.46805400	-3.02509400
C	-2.24890300	-0.92283500	1.93707500
C	-1.50141700	-1.23386800	3.09064800
C	-3.09353800	-1.85896100	1.30673600
C	-1.61919800	-2.52993000	3.60836900
C	-3.17656700	-3.13861400	1.86946800
C	-2.44762800	-3.47380600	3.00749600
H	-1.05321800	-2.80172200	4.49487900
H	-3.82036800	-3.88208100	1.40798600
H	-2.52597400	-4.47318100	3.42777000
C	0.62962400	3.74733000	1.32146800
C	0.41861000	5.09118300	2.04673900
C	2.09354100	3.27949400	1.42640600
H	0.01836200	2.99963900	1.83467200
H	-0.63054200	5.40678500	2.00949100
H	0.71035100	5.00567000	3.10018600
H	1.02190000	5.88965600	1.59883600
H	2.22359900	2.30012400	0.95544400
H	2.77927500	3.98685200	0.94460200
H	2.39001600	3.19567200	2.47881400
C	-2.47833800	2.28176800	-2.51553000
C	-1.98975500	1.28020600	-3.57962300
C	-3.61545900	3.16847100	-3.05972800
H	-2.89048600	1.69478800	-1.68977900
H	-1.23406400	0.60918600	-3.15766800
H	-2.82672700	0.67027000	-3.94076600
H	-1.55308100	1.79387800	-4.44469000
H	-3.98503700	3.86073100	-2.29439400
H	-3.28835100	3.76597500	-3.91871800
H	-4.45618000	2.54716800	-3.39037800
C	-0.59225100	-0.22255400	3.78166600
C	0.87442700	-0.69375900	3.79243600
C	-1.08879100	0.09563900	5.20602700
H	-0.62436300	0.70815100	3.20827500
H	1.23420100	-0.87129700	2.77372400
H	1.51309500	0.06906800	4.25369900
H	0.99743800	-1.62044000	4.36574000
H	-2.11852100	0.47158100	5.19729600
H	-1.06422500	-0.79234000	5.84872400
H	-0.45246400	0.85882500	5.66951100
C	-3.91162300	-1.52176600	0.06397300
C	-5.42077400	-1.50396600	0.37949900
C	-3.59857100	-2.47419100	-1.10520800
H	-3.63168200	-0.51591300	-0.26142500
H	-5.65593700	-0.78821700	1.17575900
H	-5.99477700	-1.22132500	-0.51102400
H	-5.77271200	-2.49032900	0.70458400
H	-2.53012400	-2.46896800	-1.34176100
H	-3.89205300	-3.50610100	-0.87809200
H	-4.15084200	-2.16457400	-2.00064700
C	0.95851700	-2.74793900	-1.90798700
C	0.31468000	-3.82501900	-1.33838700
S	0.81108900	-2.81109400	-3.65613200
C	-0.30881600	-4.68257300	-2.29088800
H	0.26830400	-3.97584700	-0.26528700
C	-0.14125400	-4.25930800	-3.58141900
H	-0.86938800	-5.57165500	-2.02248200
H	-0.51997800	-4.70687200	-4.49052200

CP5

Energy (RB3LYP) = -2404.183502001091 A.U.

Free Energy = -2403.592823227298 A.U.

Pd	-0.28958200	-0.47315100	-0.66592000
C	4.78434700	-0.79154900	-0.22919400
C	4.42050200	0.44202100	-0.68671900
C	3.15326600	0.41383600	-1.34082100

C	2.56692400	-0.83097200	-1.37182800
S	3.61163600	-2.01821600	-0.59823600
H	5.01822200	1.33547900	-0.55282900
H	2.67028800	1.29583200	-1.74642700
C	-2.52689900	2.28095200	1.76854200
C	-3.34920600	1.20861600	1.86467600
H	-2.59550300	3.27215000	2.18865800
H	-4.28319700	1.07087200	2.38658700
N	-1.45774200	1.89067500	0.96511600
N	-2.76285300	0.18922600	1.11705000
C	-1.58082500	0.58920800	0.54558300
C	-3.34445400	-1.12330700	0.97565300
C	-4.23998900	-1.35770400	-0.08654900
C	-3.01569800	-2.11565200	1.92059400
C	-4.80711400	-2.63429700	-0.18674300
C	-3.60890700	-3.37542100	1.77089300
C	-4.49583700	-3.63518800	0.72957400
H	-5.50021100	-2.84654300	-0.99605600
H	-3.37077200	-4.16345900	2.47981900
H	-4.94644700	-4.61962200	0.63280600
C	-0.35662500	2.76055100	0.63009100
C	-0.45187400	3.56194500	-0.52546500
C	0.76323600	2.79570600	1.48510900
C	0.62271700	4.41245800	-0.81478600
C	1.80846200	3.66506000	1.14864200
C	1.74237200	4.46569100	0.01147000
H	0.57975600	5.04203000	-1.69915700
H	2.68616000	3.71296100	1.78702200
H	2.56421400	5.13480800	-0.23040500
C	-4.60030900	-0.28710600	-1.11155500
C	-6.10106600	0.06074900	-1.06074900
C	-4.16860700	-0.69939600	-2.53195000
H	-4.04526000	0.62125400	-0.86138900
H	-6.40155100	0.39434100	-0.06072900
H	-6.33011000	0.86500200	-1.76998000
H	-6.72428200	-0.80190000	-1.32463500
H	-3.09294000	-0.89996900	-2.56699900
H	-4.69815600	-1.59901800	-2.86853700
H	-4.39392700	0.10420400	-3.24371100
C	-2.04191900	-1.86880300	3.06856800
C	-0.75782700	-2.70337300	2.89661600
C	-2.69729000	-2.12313000	4.43985300
H	-1.74515000	-0.81643500	3.04050800
H	-0.26742200	-2.46003000	1.94808000
H	-0.05463700	-2.49341300	3.71169800
H	-0.97376200	-3.77861100	2.90925000
H	-3.59521200	-1.50911700	4.57504400
H	-2.99018600	-3.17246700	4.56203000
H	-1.99527300	-1.88065800	5.24634900
C	-1.66681400	3.53701000	-1.44765600
C	-1.28668500	3.10102600	-2.87545500
C	-2.39437400	4.89617300	-1.45261700
H	-2.36823800	2.79155200	-1.06257500
H	-0.81714500	2.11189600	-2.86839500
H	-2.18247400	3.05145700	-3.50637100
H	-0.59117200	3.80841900	-3.34286500
H	-2.70367700	5.18899800	-0.44256500
H	-1.75464200	5.69369300	-1.84873600
H	-3.29134400	4.84633600	-2.08129900
C	0.86938200	1.93445200	2.73960300
C	0.93163300	2.80113200	4.01293000
C	2.06577300	0.96714900	2.66165000
H	-0.03349500	1.32091600	2.80557100
H	0.05974100	3.46084700	4.09259400
H	0.95876900	2.16489600	4.90548800
H	1.82844500	3.43171800	4.02770500
H	1.99156200	0.32785200	1.77643900
H	3.01969600	1.50533200	2.61394400
H	2.09110000	0.32533100	3.55059100
C	1.30523400	-1.24435200	-1.99340700
C	0.49286000	-2.35241500	-1.65493700
S	0.99402000	-0.77799700	-3.69302000
C	-0.36464100	-2.76597700	-2.73625500
H	0.68563300	-2.98115900	-0.79117300
C	-0.20872700	-2.02637300	-3.86949100
H	-1.07027900	-3.58495300	-2.64751000
H	-0.77136800	-2.10071100	-4.79144700
Br	6.39550200	-1.22792500	0.76050400

CP6

Energy (RB3LYP) = -2404.191235478396 A.U.

Free Energy = -2403.599784421540 A.U.

Pd	0.01262800	-0.14520400	-0.71785400
C	-3.60680500	0.15529000	-0.97934100
C	-2.81347200	1.23463900	-1.28902200
C	-1.60474700	0.90793700	-1.98478800
C	-1.45028800	-0.48933200	-2.15737800
S	-2.86662000	-1.35817400	-1.51466400
H	-3.09693500	2.25610100	-1.05568000
H	-1.03770300	1.63852400	-2.54946000
Br	-0.59661200	-1.27552400	-3.79588000
C	3.06998900	-0.27641400	2.33339800
C	3.15404300	1.04036800	2.02313400
H	3.61992800	-0.87969000	3.03857700
H	3.79227300	1.82296500	2.40246800
N	2.06527000	-0.80918500	1.53038800
N	2.19887000	1.27804900	1.03779100
C	1.50606200	0.13999400	0.71413800
C	1.97026200	2.57614000	0.45051600
C	2.67252600	2.92569000	-0.71985900
C	1.06980700	3.45529200	1.08456800
C	2.44104800	4.19794000	-1.25792300
C	0.87858600	4.71584600	0.50516800
C	1.55401300	5.08545600	-0.65483600

H	2.96349600	4.49582400	-2.16264100
H	0.18890600	5.41559000	0.96888500
H	1.38978500	6.06820100	-1.08917000
C	1.66595100	-2.19604500	1.56644600
C	2.33720700	-3.11667300	0.73679200
C	0.63376800	-2.58072500	2.44578100
C	1.94306600	-4.45866100	0.80756000
C	0.27910300	-3.93503800	2.47358700
C	0.92490000	-4.86619700	1.66489700
H	2.43881700	-5.19262400	0.17860900
H	-0.51718700	-4.26262100	3.13589100
H	0.63260400	-5.91235400	1.70167000
C	3.65615900	1.98213200	-1.40475300
C	5.07813400	2.57622300	-1.43836600
C	3.17654100	1.59730800	-2.81754200
H	3.70266000	1.05883800	-0.82022500
H	5.43541500	2.81849500	-0.43076600
H	5.77853500	1.86019100	-1.88425700
H	5.11870000	3.49471500	-2.03559000
H	2.19349500	1.11655800	-2.77652300
H	3.10402600	2.47489900	-3.47118400
H	3.88145100	0.89550500	-3.27934400
C	0.31290400	3.08423900	2.35626300
C	-1.21090800	3.08667600	2.12925500
C	0.70402500	4.00150200	3.53182600
H	0.59240600	2.06345300	2.63184400
H	-1.48562000	2.39248800	1.32890700
H	-1.73112200	2.77797400	3.04387800
H	-1.57713700	4.08470400	1.85994800
H	1.78302600	3.97070800	3.72265900
H	0.43075700	5.04520300	3.33666300
H	0.18815800	3.68868300	4.44734500
C	3.45762600	-2.70632400	-0.21382900
C	3.09998700	-3.01813900	-1.67973200
C	4.79748100	-3.35675500	0.18430200
H	3.58609600	-1.62258600	-0.13919000
H	2.17053100	-2.51932400	-1.97301500
H	3.89966900	-2.67170900	-2.34549700
H	2.97438100	-4.09478200	-1.84465400
H	5.07693800	-3.10234900	1.21330700
H	4.75024300	-4.44980400	0.11321400
H	5.59988000	-3.01466300	-0.48002600
C	-0.09823500	-1.58810000	3.34333800
C	0.08759500	-1.92993700	4.83477800
C	-1.59065900	-1.49158100	2.97215400
H	0.33701200	-0.59807000	3.17973000
H	1.14823700	-1.96271900	5.10988000
H	-0.40287600	-1.17567000	5.46141900
H	-0.35106700	-2.90327800	5.08394300
H	-1.71314000	-1.20140400	1.92360000
H	-2.10560200	-2.44775100	3.12365000
H	-2.08942600	-0.74146700	3.59766100
C	-4.85751700	0.13395500	-0.24990600
C	-5.84137600	-0.83351900	-0.24509800
S	-5.31228400	1.45964700	0.81042600
C	-6.95283000	-0.51205400	0.58423400
H	-5.77539400	-1.73785700	-0.84065800
C	-6.81850900	0.69750000	1.21033000
H	-7.82134500	-1.15139900	0.70035200
H	-7.51146300	1.18778600	1.88085200

CP7

Energy (RB3LYP) = -2404.189158462626 A.U.

Free Energy = -2403.598030229379 A.U.

Pd	0.91485500	-0.48847800	-0.98000400
C	-2.49189400	-1.41947000	-1.64767400
C	-1.89640100	-0.37413100	-2.31199000
C	-0.54543700	-0.63038600	-2.72195200
C	-0.08897300	-1.89628600	-2.30994500
S	-1.37737300	-2.77535400	-1.47365600
H	-2.41348800	0.55372700	-2.53445100
H	-0.04223400	-0.02973700	-3.47221700
C	3.78901900	1.03841500	1.84583900
C	2.89506600	2.05543200	1.89499700
H	4.72281200	0.88387200	2.36343400
H	2.88843700	2.97193900	2.46397700
N	3.28644900	0.11231400	0.93465300
N	1.86759000	1.72482100	1.01423600
C	2.08810500	0.51705100	0.40088700
C	0.71470200	2.56370100	0.79206300
C	0.77873700	3.55236500	-0.20981500
C	-0.42401000	2.37864000	1.60089900
C	-0.34830600	4.36287300	-0.39392000
C	-1.52354000	3.21560900	1.37271400
C	-1.48943000	4.19766300	0.38655500
H	-0.33208900	5.13120600	-1.16193700
H	-2.41983500	3.09228100	1.97385900
H	-2.35446100	4.83588600	0.22597000
C	3.95779400	-1.12138100	0.60450400
C	4.87056400	-1.13074400	-0.46926700
C	3.69411200	-2.26634100	1.38267100
C	5.51986800	-2.33740300	-0.75782300
C	4.37255000	-3.44589300	1.05108300
C	5.27532200	-3.48471000	-0.00788500
H	6.22473300	-2.37826700	-1.58353100
H	4.18757600	-4.34655700	1.62974100
H	5.79009300	-4.41114400	-0.24905700
C	2.00687200	3.75058900	-1.09271100
C	2.57870600	5.17594000	-0.96729200
C	1.69745000	3.39696700	-2.56035000
H	2.78270300	3.05775700	-0.75444200
H	2.82843800	5.41710500	0.07238600
H	3.49131000	5.27346900	-1.56721000
H	1.86786100	5.93124500	-1.32228400

H	1.34940700	2.36151100	-2.63801600
H	0.92401400	4.05363200	-2.97672600
H	2.59770100	3.50691800	-3.17736500
C	-0.49956500	1.30704100	2.68371100
C	-1.53920100	0.22759100	2.32496500
C	-0.77789800	1.91614200	4.07166700
H	0.47369100	0.81044600	2.73661200
H	-1.29576100	-0.23899500	1.36469900
H	-1.55628100	-0.55412900	3.09425100
H	-2.54879700	0.64942700	2.25399800
H	-0.02265100	2.66374200	4.34088600
H	-1.75874300	2.40403500	4.11163000
H	-0.76839900	1.13218400	4.83810900
C	5.15437700	0.10393900	-1.31870500
C	4.65565000	-0.09135100	-2.76371100
C	6.64566000	0.49061600	-1.28620400
H	4.59153800	0.94154000	-0.89690600
H	3.58133600	-0.30604200	-2.77067100
H	4.83145700	0.81666900	-3.35347400
H	5.17712800	-0.91901300	-3.25963700
H	6.99349700	0.65932100	-0.26051300
H	7.27725000	-0.28909600	-1.72780800
H	6.81129500	1.41206000	-1.85689600
C	2.70872100	-2.26234600	2.54722400
C	3.40581600	-2.60281000	3.87909000
C	1.51987200	-3.20558600	2.28033800
H	2.30024200	-1.25222800	2.64198800
H	4.22917200	-1.91030700	4.08921700
H	2.69135300	-2.54270000	4.70857700
H	3.81920000	-3.61822000	3.87074000
H	0.99525500	-2.91941500	1.36279700
H	1.84718100	-4.24729300	2.17844100
H	0.80606400	-3.16039400	3.11173700
C	-3.82301100	-1.48587500	-1.07963900
C	-4.56559300	-2.59365000	-0.73109100
S	-4.72854400	-0.01437500	-0.73629700
C	-5.85546500	-2.28967700	-0.20661500
H	-4.20348000	-3.60721400	-0.86627400
C	-6.07951900	-0.94406600	-0.16193200
H	-6.57761400	-3.03282100	0.10906000
H	0.70068300	-2.48103400	-2.76901700
Br	-7.69253800	-0.05944200	0.44941200

TS1

Energy (RB3LYP) = -1864.930843925680 A.U.

Free Energy = -1864.393159271368 A.U.

Pd	-0.23853900	-0.28717400	-0.51402900
C	-4.15437900	-1.18767100	-0.26353000
C	-3.46138000	-2.36832900	-0.22170400
C	-2.20524400	-2.28074800	-0.88400600
C	-1.92102300	-0.99516200	-1.35267100
S	-3.29784900	0.09306200	-1.06884200
H	-3.83775700	-3.26710500	0.25307100
H	-1.55712800	-3.12765400	-1.07363600
Br	-0.91612700	-0.75430000	-3.29145200
Br	-5.88339100	-0.85688200	0.55403300
C	3.44428600	0.50867900	1.63262400
C	2.94571500	1.76809400	1.58506700
H	4.35313500	0.11707500	2.06183800
H	3.32969800	2.70196300	1.96458900
N	2.52397400	-0.30735900	0.97898100
N	1.73383800	1.68967500	0.90348500
C	1.44914300	0.40622800	0.51660200
C	0.88831100	2.83062600	0.64411700
C	1.09235200	3.57071400	-0.53803100
C	-0.09374000	3.17595000	1.59453900
C	0.27335200	4.68643800	-0.75196400
C	-0.88397200	4.30111700	1.32909200
C	-0.70501400	5.04988700	0.16923000
H	0.40379300	5.27678200	-1.65439100
H	-1.65176400	4.59198300	2.04036600
H	-1.33061500	5.91865200	-0.01786700
C	2.69491400	-1.73135100	0.81788200
C	3.38815200	-2.20702400	-0.31337500
C	2.18472100	-2.59189200	1.81089100
C	3.56139500	-3.59180200	-0.43129100
C	2.38649700	-3.96732400	1.64168500
C	3.06677300	-4.46494400	0.53356300
H	4.09024200	-3.99014700	-1.29241500
H	2.00433300	-4.65708200	2.38893900
H	3.21219500	-5.53622100	0.42176900
C	2.16339200	3.21058600	-1.56311300
C	3.25618200	4.29644500	-1.63006400
C	1.55821900	2.94341700	-2.95450900
H	2.64423900	2.28274200	-1.24001100
H	3.72223100	4.45764300	-0.65104500
H	4.04222200	4.00421200	-2.33639900
H	2.84673600	5.25662400	-1.96553900
H	0.81323800	2.14233500	-2.91455100
H	1.07525600	3.83805200	-3.36485700
H	2.34558300	2.64211300	-3.65574600
C	-0.31373800	2.38286900	2.87899500
C	-1.74170100	1.80922800	2.95455900
C	0.01304700	3.23097400	4.12430600
H	0.37363800	1.53200700	2.87416600
H	-1.95789300	1.17963800	2.08523100
H	-1.85713200	1.19909500	3.85841900
H	-2.49566600	2.60421100	2.99273500
H	1.04318100	3.60457300	4.09576000
H	-0.65306600	4.09792500	4.20593000
H	-0.10621000	2.63280200	5.03544200
C	3.95616900	-1.27917700	-1.38295500
C	3.38652500	-1.59596500	-2.77888300
C	5.49775600	-1.31681200	-1.38908700

H	3.65485300	-0.25635100	-1.13901300
H	2.29403500	-1.52845500	-2.78474400
H	3.77640700	-0.88248900	-3.51466300
H	3.66842100	-2.60146100	-3.11307600
H	5.91012400	-1.04540900	-0.41033000
H	5.87272800	-2.31548500	-1.64258200
H	5.89389500	-0.61362100	-2.13118000
C	1.44301200	-2.08170600	3.04257300
C	2.22665400	-2.38750200	4.33457400
C	0.00902000	-2.64026300	3.11526600
H	1.35859300	-0.99433400	2.96097300
H	3.23265500	-1.95330500	4.30509700
H	1.70375000	-1.97412900	5.20512200
H	2.33490200	-3.46700200	4.49282100
H	-0.55598500	-2.38469600	2.21279800
H	0.00502200	-3.73140800	3.22371200
H	-0.51743800	-2.21939500	3.98022700

TS2

Energy (RB3LYP) = -2404.130431088510 A.U.

Free Energy = -2403.539877770159 A.U.

Pd	0.12211400	-0.21156700	0.94369900
C	-4.23171500	-0.30024000	0.15518300
C	-4.03925700	0.87673000	0.81697000
C	-2.71361900	0.98585400	1.34479400
C	-1.90045500	-0.09377000	1.06751000
S	-2.79906800	-1.29313300	0.14294700
H	-4.80559900	1.63389700	0.93721900
H	-2.38618300	1.83084400	1.93937900
C	2.65863200	1.47813000	-2.20150200
C	3.03503900	0.17811300	-2.29096400
H	2.99195700	2.35503700	-2.73383200
H	3.76508400	-0.31164600	-2.91592100
N	1.67522600	1.54027600	-1.22047400
N	2.26828600	-0.52004100	-1.36460100
C	1.41391500	0.30780400	-0.68558900
C	2.37575000	-1.94671400	-1.16077800
C	3.22230400	-2.42592100	-0.14092300
C	1.65399400	-2.80529300	-2.01504900
C	3.32371700	-3.81414800	0.01491100
C	1.79762600	-4.18385000	-1.81620100
C	2.62012700	-4.68565600	-0.81118700
H	3.96488000	-4.21598500	0.79413100
H	1.25546100	-4.87311000	-2.45683700
H	2.71414000	-5.75947700	-0.67275700
C	1.02185600	2.77115200	-0.83678900
C	1.57726500	3.53494100	0.20857700
C	-0.12327200	3.17734900	-1.55104700
C	0.94257400	4.73999900	0.53520900
C	-0.71288600	4.39357800	-1.18536400
C	-0.18941700	5.16724400	-0.15292400
H	1.34303500	5.35146700	1.33877200
H	-1.59633800	4.73673600	-1.71540800
H	-0.66528900	6.10669400	0.11580500
C	4.03313900	-1.50432900	0.76533400
C	5.54575300	-1.67001800	0.51553000
C	3.68873000	-1.71435800	2.25236400
H	3.77437500	-0.47041700	0.51871000
H	5.80244500	-1.47647600	-0.53236400
H	6.11425000	-0.97042800	1.13960000
H	5.88332400	-2.68421000	0.75922300
H	2.61870800	-1.56878800	2.43596800
H	3.95457700	-2.72277600	2.59048900
H	4.24290200	-1.00003100	2.87273100
C	0.76380700	-2.28968800	-3.14235400
C	-0.66426500	-2.86058400	-3.06661400
C	1.39965600	-2.57553800	-4.51848900
H	0.67850700	-1.20397100	-3.03814500
H	-1.13200500	-2.62954700	-2.10500200
H	-1.28452800	-2.42363100	-3.85790900
H	-0.67746900	-3.94832300	-3.20198300
H	2.39633700	-2.12715800	-4.60364100
H	1.50484900	-3.65331200	-4.69068400
H	0.77451200	-2.16722600	-5.32127300
C	2.83028100	3.11054400	0.96865000
C	2.55446500	2.93898500	2.47455100
C	3.99164500	4.09485400	0.72388000
H	3.14542100	2.13474800	0.58735300
H	1.76093100	2.20505200	2.64940500
H	3.45957500	2.59246200	2.98772100
H	2.25121000	3.88401700	2.94026100
H	4.22006600	4.18792500	-0.34413600
H	3.75508900	5.09640600	1.10176700
H	4.89780000	3.75099500	1.23650100
C	-0.70634600	2.36311200	-2.70219500
C	-0.40570800	3.03643300	-4.05721600
C	-2.21547700	2.10918300	-2.53420000
H	-0.21798600	1.38422700	-2.70421500
H	0.67155200	3.16573200	-4.21433200
H	-0.79797700	2.42945000	-4.88177400
H	-0.87195900	4.02706100	-4.11873600
H	-2.43341400	1.63629800	-1.57243500
H	-2.79470200	3.03811300	-2.59711500
H	-2.57369200	1.44711100	-3.33102000
C	-0.77520400	-0.79162600	2.64747100
C	-1.02646200	-2.07686500	3.08989700
S	-0.57458600	0.27709800	4.03324700
C	-1.02486300	-2.20966700	4.51092400
H	-1.23464500	-2.89827300	2.41327000
C	-0.80187700	-1.02586800	5.16156800
H	-1.19409000	-3.15044200	5.02532400
H	-0.74533900	-0.84653500	6.22749000
Br	-5.86542500	-0.87956400	-0.72682800

TS3

Energy (RB3LYP) = -2404.176355799019 A.U.

Free Energy = -2403.585333290901 A.U.

Pd	-0.03683200	0.38354900	-0.53931200
C	2.84429800	1.07117000	-1.40097700
C	1.61968500	1.10516600	-2.06860700
C	0.79218700	2.22330100	-1.70207700
C	1.40540300	3.00178400	-0.73715200
S	2.99138700	2.44306900	-0.31634100
H	1.38323200	0.42926500	-2.88328900
H	-0.12014400	2.51186400	-2.21050300
Br	0.72220200	4.65279000	0.00241500
C	-2.08611500	-2.31472800	2.09026500
C	-3.09051400	-2.04450700	1.22237900
H	-2.04950600	-2.94855000	2.96248800
H	-4.11072900	-2.39296900	1.18216300
N	-0.98017700	-1.58480100	1.65981600
N	-2.57492900	-1.15584300	0.28158900
C	-1.25644700	-0.85003400	0.53007200
C	-3.34753300	-0.62876400	-0.81554900
C	-4.08075500	0.55887700	-0.62096100
C	-3.36345800	-1.33405400	-2.03560500
C	-4.83500800	1.04020600	-1.69838300
C	-4.13364300	-0.80780100	-3.08015700
C	-4.86200200	0.36752200	-2.91700600
H	-5.40665400	1.95656500	-1.58043500
H	-4.16070300	-1.32569400	-4.03488800
H	-5.45322600	0.75912000	-3.74081200
C	0.29605000	-1.62006200	2.33019300
C	0.54899700	-0.69143400	3.35932100
C	1.23258100	-2.60338700	1.95344000
C	1.78629700	-0.76594200	4.01114000
C	2.45452100	-2.63179300	2.63685800
C	2.73146300	-1.72427800	3.65566400
H	2.01201700	-0.06066100	4.80615000
H	3.19948900	-3.37394100	2.36385900
H	3.68601400	-1.76422900	4.17426000
C	-4.06925000	1.32570500	0.69748900
C	-5.48174200	1.43477100	1.30421000
C	-3.42115800	2.71341700	0.53059800
H	-3.45152500	0.76835000	1.40727300
H	-5.93084600	0.44615600	1.45456800
H	-5.43968700	1.94007500	2.27639300
H	-6.15597700	2.01198600	0.66054600
H	-2.39534800	2.61662400	0.16024400
H	-3.98480000	3.33917800	-0.17203100
H	-3.39032400	3.23722500	1.49368100
C	-2.57084400	-2.61924800	-2.25226300
C	-1.44412300	-2.40973400	-3.28233000
C	-3.48401800	-3.79494700	-2.65006900
H	-2.09189400	-2.88478200	-1.30561700
H	-0.76730000	-1.61571100	-2.94831000
H	-0.86192300	-3.33136000	-3.40394600
H	-1.84465800	-2.13343900	-4.26529400
H	-4.26789000	-3.96363000	-1.90267600
H	-3.97571700	-3.61983600	-3.61419200
H	-2.89764900	-4.71695700	-2.74130900
C	-0.45982400	0.37594400	3.77036900
C	0.08054300	1.79158400	3.49192100
C	-0.88681500	0.21715300	5.24270600
H	-1.35512100	0.24936700	3.15519100
H	0.32716100	1.90778000	2.43164400
H	-0.67244600	2.54460100	3.75434100
H	0.98179300	2.00167100	4.08046400
H	-1.30532400	-0.77790500	5.43360800
H	-0.04189200	0.35943000	5.92682600
H	-1.64979200	0.96150100	5.49990600
C	0.96531300	-3.60904900	0.83821800
C	1.04336000	-5.06117700	1.34825800
C	1.91223600	-3.38106300	-0.35558800
H	-0.05314500	-3.44666700	0.47396100
H	0.34701300	-5.23320300	2.17724400
H	0.79136300	-5.76073300	0.54234900
H	2.05008200	-5.31358000	1.70154800
H	1.80256500	-2.36372900	-0.74469600
H	2.96158700	-3.52614000	-0.07262400
H	1.68226900	-4.08707900	-1.16318200
C	3.93301700	0.13034500	-1.54311000
C	4.97903800	-0.12553900	-0.67952000
S	4.07767500	-0.87207700	-2.97915000
C	5.88192700	-1.11678300	-1.15785100
H	5.07902500	0.36537200	0.28265600
C	5.52512400	-1.61872700	-2.37971000
H	6.75587500	-1.44894800	-0.60791800
H	6.01994200	-2.38202400	-2.96492000

TS4

Energy (RB3LYP) = -2404.178530147158 A.U.

Free Energy = -2403.583870033867 A.U.

Pd	0.02472400	-0.37524000	-0.64488100
C	-3.91166400	-1.54210700	-0.20657600
C	-3.03514300	-2.45708900	0.30004500
C	-1.81750200	-2.50256600	-0.43916000
C	-1.77222400	-1.60065300	-1.50446900
S	-3.29661800	-0.69724400	-1.59720400
H	-3.24121800	-3.07168800	1.16793500
H	-1.02157200	-3.20984500	-0.23821900
Br	-5.65924100	-1.10248300	0.51220300
C	2.10461100	2.37889200	1.90451900
C	2.82206500	1.26049600	2.16459800
H	2.19246900	3.38587300	2.28133000
H	3.66730300	1.09042300	2.81294200

N	1.12446400	2.01848900	0.98179100
N	2.26277500	0.24085100	1.39656800
C	1.19831200	0.68562900	0.64552400
C	2.76177900	-1.11109900	1.39771700
C	3.75169600	-1.46983800	0.46097100
C	2.26838500	-2.01671300	2.35862000
C	4.23238000	-2.78473900	0.49572000
C	2.78628400	-3.31785800	2.35089900
C	3.75500500	-3.70224400	1.42757700
H	4.99271400	-3.09230800	-0.21680600
H	2.42624600	-4.03884000	3.07960400
H	4.14228400	-4.71782400	1.43765500
C	0.15911900	2.94966700	0.45402600
C	0.49394600	3.69695000	-0.69333400
C	-1.07102200	3.10506800	1.12354600
C	-0.45538500	4.60644400	-1.17569400
C	-1.98470700	4.02663400	0.59696400
C	-1.68468100	4.76852100	-0.54213800
H	-0.22707900	5.19633400	-2.05913100
H	-2.94421800	4.16391000	1.08753600
H	-2.40855200	5.47819800	-0.93433900
C	4.31708300	-0.48331600	-0.55589100
C	5.81788400	-0.22887800	-0.31090300
C	4.05678500	-0.94160200	-2.00275100
H	3.79801900	0.47030100	-0.42580000
H	6.00153400	0.13755700	0.70575600
H	6.19758300	0.52057800	-1.01559900
H	6.40894300	-1.14237200	-0.44682100
H	2.98437200	-1.05627000	-2.18794900
H	4.54775100	-1.89844900	-2.21813800
H	4.45015800	-0.20041900	-2.70936700
C	1.22735500	-1.62079900	3.40138200
C	-0.02609100	-2.51256200	3.33355800
C	1.83480600	-1.62213000	4.81870900
H	0.90237600	-0.59970400	3.18333400
H	-0.48251500	-2.45979100	2.34031900
H	-0.76756900	-2.17761400	4.06890400
H	0.20676100	-3.56143000	3.55283800
H	2.69852000	-0.95047400	4.88463700
H	2.17076200	-2.62469400	5.10934200
H	1.09164200	-1.29221900	5.55443600
C	1.84120000	3.56351500	-1.39699200
C	1.68170100	3.14053800	-2.86905100
C	2.66220300	4.86312300	-1.27671700
H	2.40603400	2.77101800	-0.89823300
H	1.15535400	2.18365700	-2.93922100
H	2.66663700	3.02498700	-3.33771300
H	1.12462400	3.88642600	-3.44858300
H	2.81697900	5.14323600	-0.22835700
H	2.16087100	5.70201300	-1.77399600
H	3.64662500	4.73859000	-1.74353200
C	-1.42305200	2.32722300	2.38748000
C	-1.60161200	3.27189100	3.59280800
C	-2.66505900	1.44062400	2.18328800
H	-0.58777600	1.65949000	2.61637000
H	-0.70335400	3.87606700	3.76563200
H	-1.80268900	2.69420000	4.50286500
H	-2.44202400	3.96023200	3.44420500
H	-2.50585300	0.73228500	1.36466800
H	-3.55594200	2.03607800	1.95145200
H	-2.87666300	0.86940100	3.09531200
C	-0.75538700	-1.46713400	-2.53435600
C	-0.49552700	-0.36872300	-3.36038200
S	0.24095300	-2.84240500	-3.03350400
C	0.49245700	-0.63533300	-4.35213800
H	-1.04530700	0.56230900	-3.28807500
C	0.98208700	-1.91116700	-4.29953000
H	0.82935300	0.10292300	-5.07178400
H	1.75402700	-2.35715900	-4.91238200

TS5

Energy (RB3LYP) = -2404.176915436665 A.U.

Free Energy = -2403.585274079994 A.U.

Pd	-0.60657100	-0.21548900	-0.96253300
C	2.03845300	0.05620000	-2.30773400
C	1.07119900	-0.95367900	-2.37012500
C	-0.01125500	-0.63624400	-3.25928800
C	0.13400700	0.60563000	-3.84725600
S	1.60931800	1.37742600	-3.37493200
H	1.21856900	-1.93121200	-1.92165900
H	-0.80806300	-1.32465200	-3.51574700
C	-2.75486500	1.16204200	2.47934000
C	-3.48405000	0.05732900	2.19173700
H	-2.85085900	1.89397800	3.26603700
H	-4.34744900	-0.37235500	2.67528100
N	-1.74888600	1.23710000	1.51808700
N	-2.90696700	-0.51698400	1.06114700
C	-1.81871800	0.19958700	0.61683400
C	-3.40890900	-1.71675400	0.43957700
C	-4.39717500	-1.60167000	-0.55861300
C	-2.91374100	-2.96404800	0.86986300
C	-4.87961000	-2.78323100	-1.13507000
C	-3.43056900	-4.11384900	0.25968100
C	-4.40243600	-4.02802000	-0.73346000
H	-5.63830500	-2.72604400	-1.91076000
H	-3.06393700	-5.08955400	0.56626200
H	-4.78991600	-4.93306100	-1.19423400
C	-0.75810300	2.28435000	1.49621100
C	-1.02694200	3.45949300	0.76646000
C	0.42922400	2.11023800	2.23505300
C	-0.06196700	4.47406000	0.78994700
C	1.36065000	3.15602100	2.22335000
C	1.12048900	4.32716600	1.51005700
H	-0.24014600	5.39094500	0.23484800

H	2.28746400	3.04868900	2.77995700
H	1.85610500	5.12750400	1.51575700
C	-4.93670600	-0.25476500	-1.02937200
C	-6.45807900	-0.14201400	-0.81144000
C	-4.55881400	0.01390900	-2.49886400
H	-4.46242700	0.52740300	-0.43003600
H	-6.72451700	-0.30062000	0.23990600
H	-6.81157200	0.85364000	-1.10475500
H	-7.00929800	-0.87775900	-1.40882400
H	-3.47070100	-0.00389000	-2.62192500
H	-4.99658500	-0.73511200	-3.16994800
H	-4.92611900	0.99891600	-2.81227500
C	-1.84310000	-3.09555100	1.94827200
C	-0.53485800	-3.66422400	1.36579800
C	-2.33629400	-3.93285000	3.14425100
H	-1.61626400	-2.09355300	2.32321300
H	-0.16507700	-3.01911900	0.56132600
H	0.23589600	-3.72176800	2.14398200
H	-0.67975900	-4.67365000	0.96202000
H	-3.25024300	-3.51131600	3.57849700
H	-2.55237000	-4.96782300	2.85417500
H	-1.57032500	-3.96281300	3.92819300
C	-2.31009400	3.65441700	-0.03463700
C	-2.01352000	3.81214200	-1.53820000
C	-3.13799600	4.83877100	0.50136200
H	-2.91812800	2.75244800	0.07696200
H	-1.47204900	2.93854200	-1.91562600
H	-2.94999300	3.90919400	-2.10133300
H	-1.41002100	4.70558700	-1.73895900
H	-3.38380500	4.70776500	1.56155000
H	-2.59825800	5.78777500	0.40004700
H	-4.07785200	4.93051100	-0.05609000
C	0.72832600	0.83973900	3.02429100
C	0.89770000	1.13191300	4.52806700
C	1.95536000	0.10308500	2.45401200
H	-0.12672300	0.16638800	2.91701500
H	0.01002200	1.62288400	4.94371900
H	1.05986900	0.19891400	5.08077900
H	1.75852500	1.78343000	4.71931900
H	1.79915100	-0.14714000	1.39972800
H	2.86407500	0.71187300	2.52944100
H	2.13065100	-0.82744100	3.00758200
C	3.29157200	0.06868000	-1.58715000
C	4.10141100	1.13894900	-1.26734700
S	4.01232500	-1.43240000	-1.01063400
C	5.28658700	0.78198300	-0.56231400
H	3.84110000	2.16346500	-1.51041300
C	5.36552400	-0.56421400	-0.35029400
H	6.03225900	1.49072000	-0.22304300
H	-0.53296700	1.09271500	-4.54537000
Br	6.77373600	-1.50802000	0.58823800

CP8

Energy (RB3LYP) = -2020.79638598 A.U.

Free Energy = -2403.593611438597 A.U.

Pd	0.04645800	-0.53775500	-0.16134700
C	3.48002100	-1.51038200	0.06523000
C	3.08956200	-0.91467600	-1.09206400
C	1.77923100	-1.32897700	-1.54041000
C	1.16481700	-2.20140700	-0.59474600
S	2.27400100	-2.55527100	0.76984700
H	3.70429200	-0.21099600	-1.64223400
Br	0.00494100	-3.74642100	-1.14164000
Br	5.12693000	-1.14119700	1.02961000
C	-1.93079500	3.19750900	0.89995000
C	-2.89363800	2.30748200	1.24280600
H	-1.89814000	4.27368800	0.96648500
H	-3.87461800	2.44619700	1.66956000
N	-0.86615700	2.45624500	0.39274400
N	-2.39213500	1.04558300	0.93653300
C	-1.12985800	1.11112500	0.40506600
C	-3.12125400	-0.18017100	1.15990700
C	-3.94325000	-0.67710800	0.12852800
C	-2.99951800	-0.82317400	2.40841600
C	-4.64925400	-1.86040600	0.37767300
C	-3.72923100	-2.00244500	2.60286300
C	-4.54472800	-2.51867200	1.59975000
H	-5.28666800	-2.27291100	-0.39920600
H	-3.65361000	-2.52450900	3.55250600
H	-5.09972500	-3.43733800	1.77064300
C	0.35980700	3.05341400	-0.07938400
C	0.42648200	3.49579100	-1.41551600
C	1.43361200	3.19748400	0.82124200
C	1.62463200	4.08051400	-1.84443300
C	2.60961900	3.78435800	0.33751200
C	2.70816500	4.21954600	-0.98120600
H	1.70834500	4.43145100	-2.86920100
H	3.45873400	3.90162600	1.00480400
H	3.63013100	4.67327600	-1.33561500
C	-4.08728400	0.02023700	-1.22049400
C	-5.54062000	0.47192800	-1.46632000
C	-3.57339900	-0.86530900	-2.37210900
H	-3.46473100	0.91947600	-1.20633800
H	-5.89721700	1.13037800	-0.66568700
H	-5.61389000	1.01890000	-2.41380800
H	-6.22483000	-0.38281900	-1.52329100
H	-2.51881500	-1.12161600	-2.23002200
H	-4.14712700	-1.79660400	-2.44978900
H	-3.67443800	-0.33268800	-3.32624600
C	-2.11750200	-0.28557200	3.53120600
C	-0.99593500	-1.27807500	3.89330300
C	-2.95218200	0.09074200	4.77141800
H	-1.63352800	0.62841300	3.17492200
H	-0.37428200	-1.50073100	3.01972600
H	-0.35160100	-0.85386400	4.67277400
H	-1.40074700	-2.22334500	4.27370800
H	-3.72631200	0.82677600	4.52529100
H	-3.45115600	-0.78529500	5.20211700
H	-2.30845600	0.52128300	5.54755900
C	-0.74932200	3.38319600	-2.38149700
C	-0.39355500	2.55400400	-3.62962900
C	-1.27986700	4.77801100	-2.77056700
H	-1.55971900	2.85594600	-1.86997100
H	-0.10331700	1.53560800	-3.35352700
H	-1.26224600	2.49262000	-4.29702100
H	0.42556600	3.01068400	-4.19833800
H	-1.57368400	5.35702400	-1.88728600
H	-0.52259300	5.35854200	-3.31076000
H	-2.15656200	4.68513200	-3.42257200
C	1.35337700	2.75270100	2.27808900
C	1.54217200	3.94202700	3.24056700
C	2.35589300	1.62329700	2.57923900
H	0.35246500	2.34833700	2.45404300
H	0.80767300	4.73321800	3.05016900
H	1.42447600	3.61177500	4.27942600
H	2.54060500	4.38467200	3.14528400
H	2.17545900	0.76180100	1.92881300
H	3.39134100	1.95139800	2.43121100
H	2.25581800	1.29477800	3.62087400
C	1.45984800	-1.27827500	-3.01495200
H	2.11086700	-0.53113300	-3.49803500
H	1.70507000	-2.26026600	-3.45821400
O	0.10027800	-0.97850400	-3.27100100
C	-0.25050900	-1.19832200	-4.62346300
H	-1.30777600	-0.94240300	-4.72224500
H	0.33747100	-0.56452200	-5.30689100
H	-0.10646900	-2.25140600	-4.91090800

CP9

Energy (RB3LYP) = -2020.83174504 A.U.

Free Energy = -2403.593611438597 A.U.

Pd	-0.47801100	-0.16316400	0.01023100
C	-4.96258000	-0.44702100	0.33216400
C	-4.37939600	-0.94190700	1.46364200
C	-2.95231200	-0.86795000	1.37242900
C	-2.47983200	-0.33192400	0.18915700
S	-3.80546400	0.10154300	-0.84829000
H	-4.93275900	-1.33320000	2.31050900
Br	-0.73475300	1.07895600	-2.16890100
Br	-6.87750300	-0.34288300	-0.00656100
C	3.88906100	-0.09181300	-0.32689100
C	3.66262800	1.19764900	0.01376800
H	4.80016300	-0.62217200	-0.55365600
H	4.33858500	2.02563100	0.14907900
N	2.64831600	-0.72377700	-0.33282100

N	2.28867600	1.33367800	0.19477100
C	1.64029800	0.14551400	-0.01752700
C	1.69626000	2.58430100	0.63029000
C	1.64071200	3.66663500	-0.27374200
C	1.27592000	2.69846000	1.97490600
C	1.12485000	4.87878300	0.20419600
C	0.76072100	3.93208200	2.38894200
C	0.68228400	5.01223900	1.51467900
H	1.06343400	5.72888700	-0.46746400
H	0.42255400	4.05328900	3.41251900
H	0.27855000	5.96075900	1.85861300
C	2.51991600	-2.15333400	-0.50758700
C	2.12204400	-2.66621500	-1.76017900
C	2.86219300	-2.98330600	0.58253300
C	2.03929600	-4.05961900	-1.88434400
C	2.76896800	-4.36868400	0.39485800
C	2.35499300	-4.90297700	-0.82192300
H	1.73093200	-4.48972100	-2.83157300
H	3.02318500	-5.03522400	1.21418600
H	2.28553000	-5.98046800	-0.94617200
C	2.14994000	3.59065900	-1.71230300
C	3.53751900	4.25692900	-1.84156300
C	1.17704600	4.22708300	-2.72324100
H	2.24542700	2.53502200	-1.98281000
H	4.28486700	3.80536400	-1.18019200
H	3.90571000	4.17167600	-2.87077800
H	3.48145000	5.32349500	-1.59281700
H	0.17231500	3.81203800	-2.61745400
H	1.12326400	5.31628700	-2.60882300
H	1.52441400	4.02539200	-3.74315100
C	1.44025600	1.56544200	2.98704300
C	0.32342200	1.52514000	4.04461300
C	2.82146600	1.65126400	3.67225200
H	1.39510700	0.61572400	2.44684600
H	-0.66815300	1.55929200	3.58072700
H	0.40049600	0.60091800	4.62874700
H	0.39228200	2.35902800	4.75280900
H	3.63829600	1.60349200	2.94399100
H	2.92180700	2.59168900	4.22751000
H	2.95167500	0.82445000	4.38128500
C	1.86194900	-1.76758200	-2.96527100
C	0.66086500	-2.21966500	-3.81286400
C	3.13556400	-1.66488600	-3.83225600
H	1.62333000	-0.76568100	-2.60105500
H	-0.24206300	-2.31636300	-3.20249600
H	0.45647000	-1.46945100	-4.58340600
H	0.84499600	-3.17390600	-4.32147800
H	3.98521700	-1.27499600	-3.25971100
H	3.42265100	-2.64547400	-4.23164300
H	2.96299600	-0.99133000	-4.67959300
C	3.34534400	-2.44086900	1.92759700
C	4.80895000	-2.84915100	2.19271500
C	2.43457000	-2.86963700	3.09442200
H	3.31620100	-1.34866600	1.88961000
H	5.47265000	-2.51292600	1.38801300
H	5.16356600	-2.40804600	3.13154600
H	4.91315500	-3.93728900	2.27479400
H	1.41557400	-2.49674900	2.95397500
H	2.39302200	-3.96016400	3.19957800
H	2.81906800	-2.46288400	4.03751700
C	-1.95299700	-1.30196400	2.40446200
H	-1.67225400	-0.49937000	3.09320000
H	-2.29036100	-2.16029400	3.00098100
O	-0.70655600	-1.66013600	1.73551400
C	-0.77816000	-2.99284700	1.18760100
H	0.13083700	-3.15607300	0.61313700
H	-0.83092600	-3.71344400	2.01336700
H	-1.65537700	-3.09342600	0.54173100
