ELECTRONIC SUPPLEMENTARY INFORMATION

Skeletal Diversity in Pt- and Au-Catalyzed Annulations of Allenedienes: Dissecting Unconventional Mechanistic Pathways

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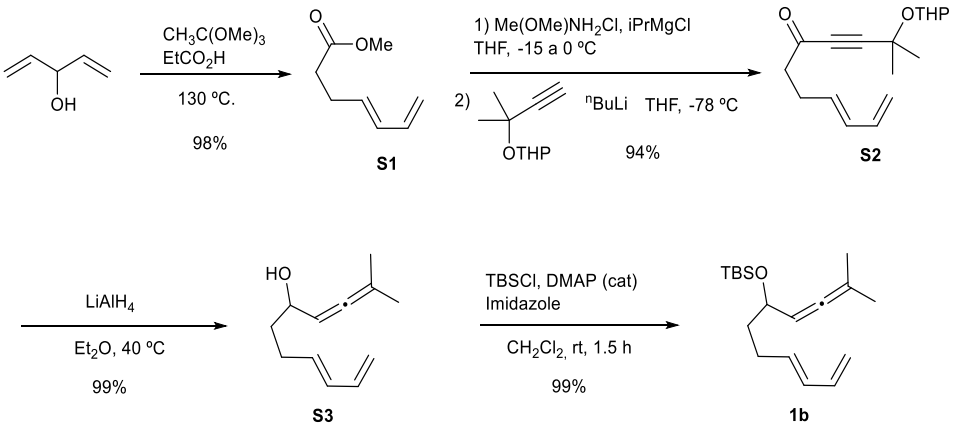
General Contents

1. General Procedures

All the reactions were conducted in dry solvents under argon atmosphere unless otherwise stated. Dry solvents were freshly distilled under argon from an appropriate drying agent before use. Gold complexes and $PtCl_2$ were purchased from Aldrich or Strem Chemicals. All reagents used were bought from Aldrich, Alfa Aesar, TCI or Acros and used without further purification. The abbreviation "rt" refers to reactions carried out approximately at 23 °C. Reaction mixtures were stirred using Teflon-coated magnetic stirring bars. Reaction temperatures were maintained using Thermowatch-controlled silicone oil baths. The reactions were monitored by Thin-layer chromatography (TLC). TLC was performed on silica gel plates and components were visualized by observation under UV light, and/or by treating the plates with *p*-anisaldehyde or cerium nitrate solutions, followed by heating. Flash chromatography was carried out on silica gel (40-63 μm) unless otherwise stated. Dryings were performed with anhydrous Na_2SO_4. Concentration refers to the removal of volatile solvents via distillation using a Büchi rotary evaporator followed by residual solvent removal under high vacuum. NMR spectra were recorded in $CDCl_3$, at 300 MHz (Varian), 400 MHz (Varian) or 500 MHz (Bruker and Varian). Chemical shifts were reported in parts per million (δ) using the residual solvent signals ($CDCl_3$: δ_H 7.26, δ_C 77.16, C_6D_6: δ_H 7.16, δ_C 128.06; CD_2Cl_2: δ_H 5.32, δ_C 54.00) as the internal standards for the ^1H and ^{13}C NMR spectra and coupling constants (*J*) in Hz. Carbon types and structure assignments were determined from DEPT-NMR and two-dimensional experiments (HSQC and HMBC, COSY 1D-nOe and NOESY). NMR spectra were analyzed using MestreNova© NMR data processing software (www.mestrelab.com). The following abbreviations are used to indicate signal multiplicity: s, singlet; d, doublet; t, triplet; q, quartet; p, pentet; dd, double doublet; td, triple doublet; ddd, doublet of doublet of doublets; m, multiplet; br, broad. Mass spectra (ESI-MS) were acquired using IT-MS Bruker AmaZon SL at CIQUS and also using chemical ionization (CI) electron impact (EI), electrospray ionization (ESI) or atmospheric-pressure chemical ionization (APCI) at the CACTUS facility of the University of Santiago de Compostela. Melting points were determined on a Büchi M-560 and were uncorrected.

X-Ray diffraction experiments were carried out at the CACTUS facilities at the University of Santiago. CCDC-1964184-1964188 contains the crystallographic data of this manuscript, which can be obtained via www.ccdc.cam.ac.uk/data_request/cif.

2. Synthesis of allenedienes 1a and 1b (exemplified for the synthesis of **1b**)



Propionic acid (231 µL, 3.09 mmol, 10 mol%) was added to 1,4-pentadien-3-ol (3.0 mL, 2.60 g, 30.9 mmol) in trimethyl orthoacetate (26.7 mL, 210 mmol) at rt. The mixture was stirred at 130 °C for 1 h. Then, the mixture was cooled to 100 °C and the reflux condenser was removed to boil off liberated alcohol for 30 min, and then reattached as the reaction was brought back to 130 °C reflux for 2.5 h. The excess of trimethyl orthoacetate was distilled out at 140 °C and the crude product was purified by flash chromatography (SiO_2, 10% Et_2O/pentane) to give **methyl (*E*)-hepta-4,6-dienoate** (**S1**) as a colorless oil (4.25 g, 98% yield).[1] **^{1}H NMR** (300 MHz, $CDCl_3$) δ 6.19 (dt, *J* = 16.9, 10.2 Hz, 1H), 5.99 (dd, *J* = 14.4, 10.3 Hz, 1H), 5.66 – 5.49 (m, 1H), 5.01 (d, *J* = 16.8 Hz, 1H), 4.89 (d, *J* = 10.0 Hz, 1H), 3.57 (s, 3H), 2.35 – 2.28 (m, 4H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 173.03 (CO), 136.75 (CH), 132.42 (CH), 131.89 (CH), 115.51 (CH_2), 51.31 (CH_3), 33.42 (CH_2), 27.63 (CH_2).

MeNHOMe·HCl (5.89 g, 59.9 mmol) and ^{i}PrMgCl (2.0 M in THF, 62.9 mL, 125.84 mmol) were successively added to a solution of **S1** (4.20 g, 30.0 mmol) in THF (227 mL) at −15 °C. The resulting mixture was warmed to 0 °C and stirred for 3 h before NH_4Cl (sat.) (50 mL) was added. The layers were separated and the aqueous layer was extracted with EtOAc (3× 50 mL). The combined organic layers were washed with brine (50 mL), dried over Na_2SO_4 and concentrated in vacuo to give a crude product that was purified by flash chromatography (SiO_2, 20 - 60% EtOAc/hexanes) to provide the corresponding Weinreb amide [**(*E*)-N-methoxy-N-methylhepta-4,6-dienamide**] as a colorless oil (4.29 g, 99% yield). **^{1}H NMR** (300 MHz, $CDCl_3$) δ 6.29 (dt, *J* = 16.8, 10.0 Hz, 1H), 6.09 (dd, *J* = 15.1, 10.4 Hz, 1H), 5.81 – 5.65 (m, 1H), 5.10 (ddd, *J* = 16.9, 1.2, 0.6 Hz, 1H), 4.97 (ddd, *J* = 10.0, 1.2, 0.6 Hz, 1H), 3.66 (s, 3H), 3.16 (s, 3H), 2.52 (t, *J* = 7.6 Hz, 2H), 2.47 – 2.33 (m, 2H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 173.37 (CO), 136.79 (CH), 133.33 (CH), 131.46 (CH), 115.12 (CH_2), 60.99 (CH_3), 31.97 (CH_3), 31.23 (CH_2), 27.21 (CH_2). **LRMS** (*m/z*, ESI): 170.12 $[M+H]^+$, 138.09. **HRMS-ESI** calculated for $C_9H_{16}NO_2$ $[M+H]^+$: 170.1176, found 170.1181.

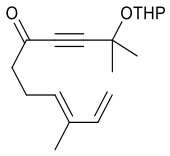
^{n}BuLi (12.13 ml, 2.5M in hexanes, 30.3 mmol) was slowly added (0.2 mL/min) to a solution of 2-((2-methylbut-3-yn-2-yl)oxy)tetrahydro-2H-pyran (5.27 g, 31.3 mmol) in THF (175 mL) at −78 °C. The reaction was stirred 30 min at −78 °C and a solution of the previously obtained amide (3.42 g, 20.2 mmol) in THF (25 mL) was added. The solution was warmed to −15 °C. After 1 h, consumption of starting material was observed by TLC, NH_4Cl (sat.) was added and the resulting mixture was diluted with EtOAc and water. The aqueous layer was separated and extracted with EtOAc (3× 100 mL). The combined organic layers were washed with brine, dried, filtered and concentrated in vacuo. Purification of the crude material by flash chromatography (SiO_2, 1 - 20% EtOAc/hexanes) affords the diene-ynone **S2 [(*E*)-2-methyl-2-((tetrahydro-2H-pyran-2-yl)oxy)undeca-8,10-dien-3-yn-5-one]** as a colorless oil (5.25 g, 94% yield). **^{1}H NMR** (300 MHz, $CDCl_3$) δ 6.29 (dt, *J* = 16.8, 10.2 Hz, 1H), 6.09 (dd, *J* = 15.2, 10.5 Hz, 1H), 5.67 (dt, *J* = 14.5, 6.8 Hz, 1H), 5.12 (d, *J* = 16.9 Hz, 1H), 5.05 – 4.96 (m, 2H),

4.02 – 3.87 (m, 1H), 3.58 – 3.43 (m, 1H), 2.67 (t, *J* = 7.3 Hz, 2H), 2.45 (q, *J* = 7.1 Hz, 2H), 1.93 – 1.77 (m, 1H), 1.77 – 1.65 (m, 1H), 1.62 – 1.53 (m, 4H), 1.54 (s, 6H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 186.42 (CO), 136.65 (CH), 132.11 (CH), 132.00 (CH), 115.77 (CH_2), 96.03 (CH), 94.29 (C), 82.59 (C), 70.41 (C), 63.02 (CH_2), 44.71 (CH_2), 31.67 (CH_2), 29.48 (CH_3), 29.22 (CH_3), 26.68 (CH_2), 25.22 (CH_2), 20.02 (CH_2). **LRMS** (*m/z*, ESI): 299.16 $[M+Na]^+$, 277.18 $[M+H]^+$, 247.13, 175.11. **HRMS-ESI** calculated for $C_{17}H_{24}NaO_3$ $[M+Na]^+$: 299.1618, found 299.1620.

A solution of diene-ynone **S2** (4.0 g, 14.5 mmol) in Et_2O (25 mL) was added to a suspension of $LiAlH_4$ (1.37 g, 36.2 mmol) in Et_2O (125 mL) at rt. The mixture was warmed to 40 °C and, after 2 h, the reaction was cooled in an ice bath and cold water was slowly added, stirred for 1 h, filtered over silica and concentrated in vacuo. Purification of the crude residue by flash chromatography (SiO_2, 10 - 30% EtOAc/hexanes) afforded the allenediene **S3 [(E)-2-methylundeca-2,3,8,10-tetraen-5-ol]** as a colorless oil (2.58 g, 99% yield). **^{1}H NMR** (300 MHz, $CDCl_3$) δ 6.25 (dt, *J* = 16.9, 10.2 Hz, 1H), 6.08 – 5.95 (m, 1H), 5.66 (dt, *J* = 14.6, 7.0 Hz, 1H), 5.07 – 4.96 (m, 2H), 4.90 (dd, *J* = 10.1, 1.7 Hz, 1H), 4.04 (q, *J* = 6.3 Hz, 1H), 2.46 (s, 1H), 2.22 – 2.07 (m, 2H), 1.66 (dd, *J* = 3.0, 1.5 Hz, 6H), 1.62 – 1.50 (m, 2H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 200.02 (C), 137.13 (CH), 134.53 (CH), 131.24 (CH), 114.80 (CH_2), 97.96 (C), 93.43 (CH), 69.61 (CH), 36.70 (CH_2), 28.48 (CH_2), 20.56 (CH_3), 20.48 (CH_3). **LRMS** (*m/z*, APCI): 179.14 $[M+H]^+$, 161.13, 133.10. **HRMS-APCI** calculated for $C_{12}H_{19}O$ $[M+H]^+$: 179.1430, found 179.1429.

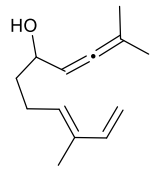
A solution of allenediene **S3** (2.50 g, 14.0 mmol) in CH_2Cl_2 (12 mL) was added to a solution of imidazole (3.82 g, 56.1 mmol), DMAP (343 mg, 2.80 mmol) and TBSCl (4.23 g, 28.0 mmol) in CH_2Cl_2 (70 mL). The resulting reaction mixture was stirred for 1.5 h at rt, water (20 mL) was then added and the resulting mixture was extracted with CH_2Cl_2 (3x 20 mL). The combined extracts were washed with brine (30 mL), dried, filtered and concentrated in vacuo. The residue was purified by column chromatography (SiO_2, 5% Et_2O/hexanes with 0.5% Et_3N) to give allenediene **1b [(*E*)-*tert*-butyldimethyl((2-methylundeca-2,3,8,10-tetraen-5-yl)oxy)silane**] as a colorless oil (4.10 g, 99% yield). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 6.31 (dt, *J* = 17.0, 10.3 Hz, 1H), 6.06 (dd, *J* = 15.2, 10.4 Hz, 1H), 5.77 – 5.66 (m, 1H), 5.08 (d, *J* = 17.0 Hz, 1H), 4.95 (d, *J* = 10.4 Hz, 1H), 4.94 – 4.90 (m, 1H), 4.12 – 4.04 (m, 1H), 2.24 – 2.05 (m, 2H), 1.69 (dd, *J* = 6.3, 2.9 Hz, 6H), 1.67 – 1.52 (m, 2H), 0.90 (s, 9H), 0.07 (s, 3H), 0.06 (s, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 200.61 (C), 137.41 (CH), 134.94 (CH), 131.31 (CH), 114.73 (CH_2), 96.07 (C), 93.85 (CH), 71.94 (CH), 38.36 (CH_2), 28.73 (CH_2), 26.04 (CH_3), 20.83 (CH_3), 20.29 (CH_3), 18.31 (C), -4.03 (CH_3), -4.73 (CH_3). **LRMS** (*m/z*, ESI): 293.23 $[M+H]^+$, 279.21, 270.04, 265.19. **HRMS-ESI** calculated for $C_{18}H_{33}OSi$ $[M+H]^+$: 293.2295, found 293.2296.

(*E*)-2,9-Dimethyl-2-((tetrahydro-2H-pyran-2-yl)oxy)undeca-8,10-dien-3-yn-5-one



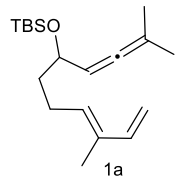
Prepared using the above-mentioned procedure for the synthesis of **S2**, using (*E*)-N-Methoxy-N,5-dimethylhepta-4,6-dienamide.[2] Colorless oil (98% yield). **^{1}H NMR** (300 MHz, $CDCl_3$) δ 6.28 (dd, *J* = 17.4, 10.7 Hz, 1H), 5.38 (t, *J* = 7.3 Hz, 1H), 5.06 (d, *J* = 17.4 Hz, 1H), 4.96 (q, *J* = 3.0 Hz, 1H), 4.91 (d, *J* = 10.7 Hz, 1H), 4.01 – 3.74 (m, 1H), 3.53 – 3.27 (m, 1H), 2.66 – 2.54 (m, 2H), 2.45 (q, *J* = 7.3 Hz, 2H), 1.86 – 1.73 (m, 1H), 1.71 (s, 3H), 1.71 – 1.57 (m, 1H), 1.53 (s, 3H), 1.52 – 1.44 (m, 7H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 186.75 (CO), 141.03 (CH), 135.34 (C), 129.91 (CH), 111.42 (CH_2), 96.14 (CH), 94.35 (C), 82.69 (C), 70.51 (C), 63.13 (CH_2), 45.12 (CH_2), 31.75 (CH_2), 29.59 (CH_3), 29.29 (CH_3), 25.30 (CH_2), 22.74 (CH_2), 20.11 (CH_2), 11.67 (CH_3). **LRMS** (*m/z*, ESI): 313.18 $[M+Na]^+$, 291.19 $[M+H]^+$, 273.18, 253.16. **HRMS-ESI** calculated for $C_{18}H_{26}NaO_3$ $[M+Na]^+$: 313.1774, found 313.1773.

(*E*)-2,9-dimethylundeca-2,3,8,10-tetraen-5-ol



Colorless oil (86% yield). **^{1}H NMR** (300 MHz, $CDCl_3$) δ 6.36 (dd, *J* = 17.4, 10.7 Hz, 1H), 5.55 – 5.44 (m, 1H), 5.12 – 5.04 (m, 2H), 4.92 (d, *J* = 10.7 Hz, 1H), 4.09 (q, *J* = 6.2 Hz, 1H), 2.32 – 2.17 (m, 2H), 1.81 (s, 1H), 1.75 (s, 3H), 1.72 (dd, *J* = 2.9, 2.1 Hz, 6H), 1.66 – 1.57 (m, 2H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 199.95 (C), 141.59 (CH), 134.48 (C), 132.57 (CH), 110.71 (CH_2), 98.83 (C), 93.75 (CH), 69.77 (CH), 37.20 (CH_2), 24.34 (CH_2), 20.74 (CH_3), 11.75 (CH_3). **LRMS** (*m/z*, APCI): 193.16 $[M+H]^+$, 175.15, 160.12. **HRMS-APCI** calculated for $C_{13}H_{21}O$ $[M+H]^+$: 193.1587, found 193.1587.

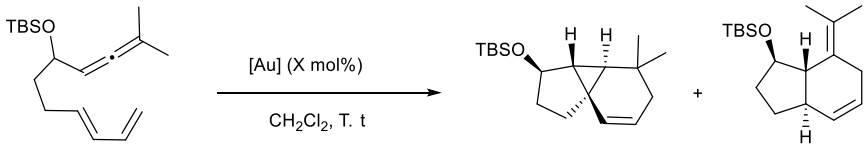
(E)-*tert*-Butyl((2,9-dimethylundeca-2,3,8,10-tetraen-5-yl)oxy)dimethylsilane (1a)



Colorless oil (99% yield). **^{1}H NMR** (300 MHz, $CDCl_3$) δ 6.38 (dd, *J* = 17.1, 11.0 Hz, 1H), 5.57 – 5.46 (m, 1H), 5.09 (d, *J* = 17.1 Hz, 1H), 5.00 – 4.87 (m, 2H), 4.12 (dt, *J* = 7.2, 6.3 Hz, 1H), 2.33 – 2.05 (m, 2H), 1.75 (s, 3H), 1.71 (dd, *J* = 4.9, 2.9 Hz, 6H), 1.65 – 1.56 (m, 2H), 0.92 (s, 9H), 0.09 (s, 6H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 200.58 (C), 141.73 (CH), 134.19 (C), 133.06 (CH), 110.47 (CH_2), 96.26 (C), 93.83 (CH), 72.10 (CH), 38.59 (CH_2), 26.04 (CH_3), 24.50 (CH_2), 20.88 (CH_3), 20.35 (CH_3), 18.37 (C), 11.77 (CH_3), -4.06 (CH_3), -4.73 (CH_3). **LRMS** (*m/z*, ESI): 307.24 $[M+H]^+$, 295.19, 281.22, 267.21. **HRMS-ESI** calculated for $C_{19}H_{35}OSi$ $[M+H]^+$: 307.2452, found 307.2445.

3. Optimization studies

Table S1. Reactivity of the substrate **1b** with gold complexes.[a]



1b **4b** **3b**

Entry	[Au] (X mol%)	T (°C)	t (h)	Conv. (%)	Ratio[b] **4b** : **3b**	% yield (product)[c]
1	AuCl (10)	-15	0.5	>99	-	Complex mixture
2	$AuCl_3$ (10)	rt	12	51	-	Complex mixture
3	IPrAuCl/$AgSbF_6$ (**Au1**)(10)	rt	2	>99	5 : 1	70 (**4b**)
4	IPrAu-NTf_2 (**Au1´**)(10)	rt	2	>99	5.2 : 1	75 (**4b**)
5	IPrAu-NTf_2 (**Au1´**)(5)	rt	2.5	>99	5 : 1	72 (**4b**)
6	IMesAu-NTf_2 (**Au8**)(10)	-15	0.5	>99	-	Complex mixture
7	IPr^{Me}AuCl/$AgNTf_2$ (**Au6**)(10)	rt	2	>99	1 : 0	96 (**4b**)
8	Ph_3PAu-NTf_2 (10)	rt	1	>99	0 : 1	22 (**3b**)[d]
9	JohnPhosAu-NTf_2 (**Au2´**)(10)	rt	12	>99	-	Complex mixture
10	MorDalPhosAu-NTf_2 (**Au9**)(5)	40	12	26	5.5 : 1	11 (**4b**)[d]
11	RuPhosAu-NTf_2 (**Au5**)(5)	40	12	60	16 : 1	32 (**4b**)[d]
12[e]	XPhosAu-NTf_2 (**Au4**)(5)	80	12	80	1.1 : 1	18 (**4b**)[d]
13	**Au3**/$AgSbF_6$ (10)	-15	1.5	>99	1 : 7	66 (**3b**)
14	**Au10**/$AgNTf_2$ (10)	rt	2.5	>99	0 : 1	66 (**3b**)
15	$(C_6F_5)_3$PAuCl/$AgNTf_2$ (**Au7**)(5)	-15	1	>99	1 : 12	70 (**3b**)
16	$AuBr_3$ (10)	rt	12	37	-	Complex mixture
17	$PicAuCl_2$	rt	12	0	-	-
18[f]	$PicAuCl_2$	110	8	60	1 : 0	17 (**4b**)

[a] *Conditions*: Allenediene **1b** (1.0 eq.), was treated with [Au] (X mol%) in CH_2Cl_2 (0.05 M) at the indicated temperature (°C) and time (h), unless otherwise noted. Conversions calculated from the ^{1}H-NMR of the crude mixture. [b] Ratio of products determined by ^{1}H-NMR spectroscopy in the crude reaction mixtures. [c] Isolated yield. [d] Yield by ^{1}H-NMR with internal standard. [e] Carried out at 80 °C in 1,2-DCE. [f] Carried out in toluene

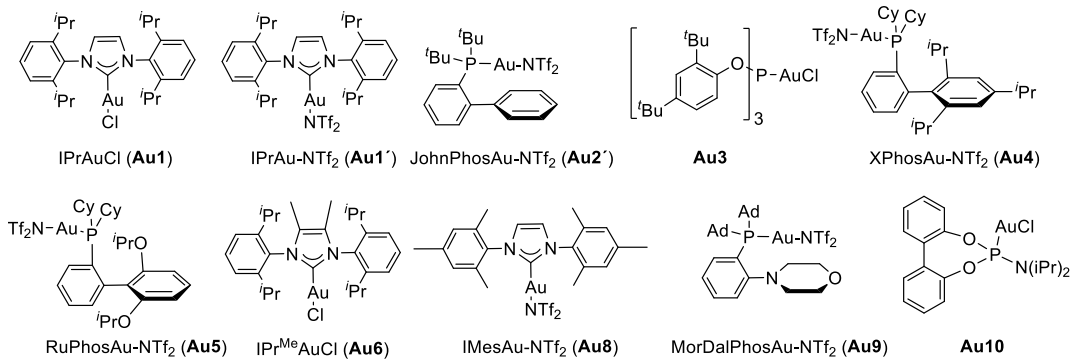
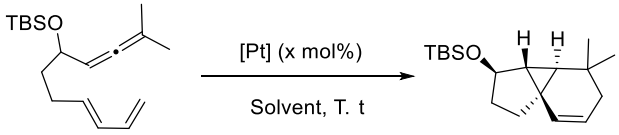


Table S2. Reactivity of allenediene **1b** with platinum complexes; influence of the solvent.[a]

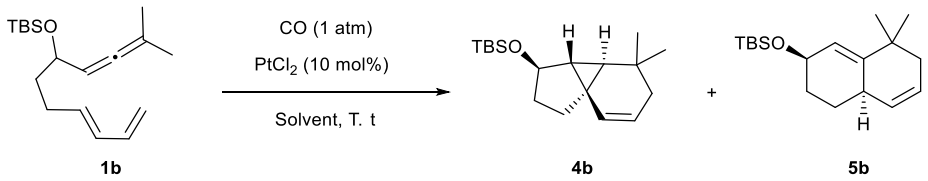


1b **4b**

Entry	[Pt] (x mol%)	Solvent	T (°C)	t (h)	Conv. (%)	**4b**, %yield[b]
1[c]	$PtCl_2$ (10%)	Toluene	110	0.5	>99	43
2[c]	$PtCl_2$ (10%)	Toluene	50	1	>99	60
3	$PtCl_2$ (10%)	Toluene	70	2	>99	81
4	$PtCl_2$ (10%)	Toluene	50	2	>99	71
5	$PtCl_2$ (10%)	Toluene	30	8	>99	79
6	$PtCl_2$ (10%)	$CHCl_3$	30	10	>99	60
7	$PtCl_2$ (10%)	$PhCF_3$	30	72	>99	90
8	$PtCl_2$ (10%)	Et_2O	30	8	>99	58
9	$PtCl_2$ (10%)	THF	30	8	>99	51
10	$PtCl_2$ (10%)	^{t}BuOMe	30	12	>99	89
11	$PtCl_2$ (10%)	Dioxane	30	2.5	>99	99
12[d]	$PtCl_2$ (10%)	Dioxane	30	4	>99	99
13	$PtCl_2$ (1%)	Dioxane	30	24	>99	92
14	$PtCl_2$ (10%)	Cyclohexane [e]	50	2	>99	88
15[e]	$PtCl_4$ (10%)	Toluene	110	3	>99	37
16	$PtBr_2$ (10%)	Toluene	110	8	>99	40
16	$(CH_3CN)_2PtCl_2$ (10%)	Toluene	110	2	50	29
17	$(COD)PtCl_2$ (10%)	Toluene	110	5	0	-
18	$[PtCl_2(ethene)]_2$ (5%)	Toluene	110	1	>99	53
19	$[PtCl_2(ethene)]_2$ (5%)/ ($p$$CF_3$-$C_6H_4$)$_3$P (10%)	Toluene	110	1	>99	50
20	$PtCl_2$ (10%)/ (C_6F_5)$_3$P (10%)	Toluene	110	1	>99	62

[a] *Conditions*: Allenediene **1b** (1.0 eq.), was treated with [Pt] (x mol%) in the indicated solvent (0.05 M), temperature (°C) and time (h), unless otherwise noted. Conversions calculated from the ^{1}H-NMR of the crude mixture. [b] Isolated yield. [c] Toluene (0.1M). [d] Carried out with 1.0 g of **1b.** [e] with 1 ppm of water

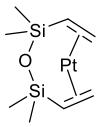
Table S3. Reactivity of allenediene **1b** with $PtCl_2$ [with and without CO (1 atm)][a]



1b **4b** **5b**

Entry	Solvent	T (°C)	t (h)	Conv. (%)	Ratio **4b** : **5b**[b]	%yield (product)[c]
1	Toluene	110	0.25	>99	-	Complex mixture
2	Toluene	50	1	>99	1 : 8	59 (**5b**)
3	$PhCF_3$	50	5	14	-	Traces (**5b**)
4	Dioxane	50	3	>99	1 : 8	68 (**5b**)
5	^{t}BuOMe	50	5	>99	1 : 12	63 (**5b**)
6	Cyclohexane	50	5	>99	1 : 8	79 (**5b**)
7[d]	**Cyclohexane**	**50**	**2**	**>99**	**1 : 9**	**85** (**5b**)
8 [d,e]	Cyclohexane	50	3	>99	1 : 9	81 (**5b**)
9[d,f]	Cyclohexane	50	2	>99	1 : 0	88 (**4b**)
10[d,g]	Cyclohexane	50	12	0	-	-
11[d,f,g]	Cyclohexane	50	12	0	-	-

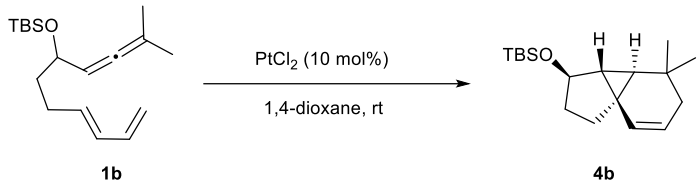
[a] *Conditions*: Allenediene **1b** (1.0 eq.), was treated with $PtCl_2$ (10 mol%) and CO (1 atm) at the indicated solvent (0.05 M), temperature (°C) and time (h), unless otherwise noted. [b] Ratio of products determined by ^{1}H-NMR spectroscopy of the crude reaction mixtures.[c] Isolated yield. [d] Cyclohexane wet (1 ppm H_2O). [e] Carried out with 0.5 g of **1b**. [f] Carried out without CO. [g] Carried out with the Pt(0) complex [**Pt-1**].



[Pt-1]

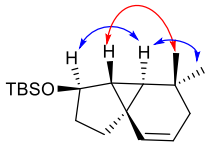
4. General procedure for the annulation reactions and characterization data of products

4.1. Annulations catalyzed by $PtCl_2$ and related neutral Pt and Au salts (exemplified for the cycloaddition of allenediene **1b** with $PtCl_2$)



1b **4b**

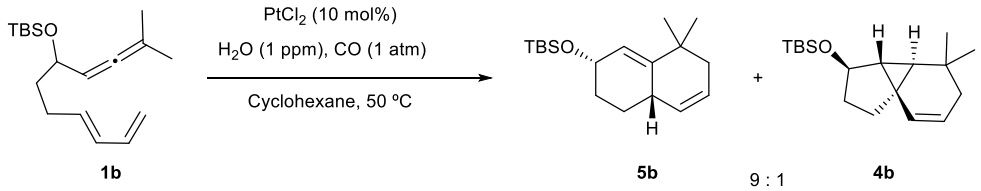
A solution of allenediene **1b** (100 mg, 0.342 mmol) in 1,4-dioxane (1 mL) was added to a suspension of $PtCl_2$ (9.1 mg, 34.2 µmol) in dioxane (6 mL) at rt. The mixture was stirred at that temperature for 1 h (the progress of the reaction was easily monitored by TLC) and filtered through a short pad of Florisil® eluting with Et_2O. The filtrate was concentrated in vacuo and purified by flash chromatography (SiO_2, 0.1 - 5% Et_2O/hexanes) to afford the cycloadduct **4b** (99.8 mg, 99% yield) as a colorless oil. ***t*-Butyl (((3*R**,3a*R**,3b*S**,7a*R**)-4,4-dimethyl-2,3,3a,3b,4,5-hexahydro-1H-cyclopenta[1,3]cyclopropa[1,2]benzen-3-yl)oxy)dime thylsilane (4b):** **^{1}H NMR** (500 MHz, $CDCl_3$) δ 5.98 (dd, *J* = 9.8, 1.9 Hz, 1H), 5.36 (ddd, *J* = 9.4, 5.9, 3.1 Hz, 1H), 4.18 (d, *J* = 4.8 Hz, 1H), 2.03 (td, *J* = 11.8, 8.4 Hz, 1H), 1.74 – 1.65 (m, 1H), 1.65 – 1.61 (m, 2H), 1.55 (dd, *J* = 14.2, 8.5 Hz, 1H), 1.49 – 1.40 (m, 2H), 1.05 (s, 3H), 0.88 (s, 9H), 0.87 (s, 3H), 0.55 (dd, *J* = 4.1, 1.8 Hz, 1H), 0.05 (s, 3H), 0.05 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 130.87 (CH), 121.16 (CH), 75.22 (CH), 36.78 (CH_2), 36.70 (CH), 34.71 (CH), 32.94 (CH_2), 30.59 (C), 30.39 (CH_3), 30.04 (CH_2), 28.63 (C), 28.01 (CH_3), 26.14 (CH_3), 18.40 (C), -4.31 (CH_3), -4.37 (CH_3). **LRMS** (m/z, ESI): 293.23 $[M+H]^+$, 315.21 $[M+Na]^+$. **HRMS-ESI** calculated for $C_{18}H_{32}NaOSi$ $[M+Na]^+$: 315.2115 found 315.2106. The relative stereochemistry of **4b** was determined by NMR.



4b

Figure S1. Significant nOe's observed for **4b**

4.2. Annulations catalyzed by $PtCl_2$ / CO (1 atm), (exemplified for the annulation of allenediene **1b**)



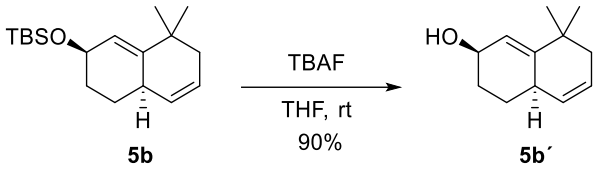
1b **5b** 9 : 1 **4b**

A solution of allenediene **1b** (100.0 mg, 0.342 mmol) in cyclohexane (1.0 mL) was added to a suspension of $PtCl_2$ (9.1 mg, 34.0 µmol) and H_2O (6.8 µL, 1 ppm). Carbon monoxide was bubbled for 5-10 min and the mixture was heated at 50 °C under a CO atmosphere (filled balloon) for 2 h. The mixture was allowed to cool down to rt and filtered through a short pad of Florisil® eluting with Et_2O. The filtrate was concentrated and purified by flash chromatography (SiO_2 15-40 µm, 0.1-5% Et_2O/hexanes) to afford **5b** (84.9 mg, 85% yield, colorless oil) and **4b** (9.1 mg, 9% yield, colorless oil).

***t*-Butyl(((2*S**,4a*S**)-8,8-dimethyl-2,3,4,4a,7,8-hexahydronaphthalen-2-yl)oxy)dimethylsilane (5b).** Colorless oil. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 5.61 – 5.53 (m, 1H), 5.48 (dt, *J* = 9.8, 2.6 Hz, 1H), 5.47 – 5.41 (m, 1H), 4.23 –

4.13 (m, 1H), 2.67 – 2.55 (m, 1H), 2.08 – 1.99 (m, 1H), 1.86 (dd, *J* = 17.3, 5.2 Hz, 1H), 1.78 – 1.72 (m, 1H), 1.70 – 1.64 (m, 1H), 1.60 – 1.54 (m, 1H), 1.53 – 1.45 (m, 1H), 1.10 (s, 3H), 1.04 (s, 3H), 0.88 (s, 9H), 0.06 (s, 3H), 0.06 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 147.58 (C), 130.29 (CH), 124.50 (CH), 119.35 (CH), 65.50 (CH), 41.68 (CH_2), 35.45 (CH), 34.86 (C), 31.97 (CH_2), 27.71 (CH_3), 27.58 (CH_3), 26.17 (CH_3), 25.12 (CH_2), 18.49 (C), -4.06 (CH_3), -4.21 (CH_3). **LRMS** (*m/z*, APCI): 293.23 $[M+H]^+$, 241.19, 161.13, 133.10, 119.08. **HRMS-APCI** calculated for $C_{18}H_{33}OSi$ $[M+H]^+$: 293.2295, found 293.2293. The structure of compound **5b** was confirmed X-ray analysis of its unprotected analog **5b´**.

(2*R,4a*R**)-8,8-Dimethyl-2,3,4,4a,7,8-hexahydronaphthalen-2-ol** (**5b'**)



A TBAF solution (1.08 mL, 1.0 M in THF, 1.08 mmol) was added to a solution of **5b** (45.0 mg, 0.18 mmol) in THF (8.9 mL) at rt. After stirring the mixture at rt for 6 h, NH_4Cl (sat.) (10 mL) was added. The layers were separated, and the aqueous layer was extracted with EtOAc (3× 10 mL). The combined organic layers were washed with brine (20 mL), dried over Na_2SO_4 and concentrated in vacuo. The crude product was purified by flash chromatography (SiO_2, 5 to 20% EtOAc/hexanes) to give the alcohol **5b´** as colorless crystals (29.1 mg, 90% yield). **m.p.:** 73-75 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 5.61 – 5.59 (m, 1H), 5.57 (dq, *J* = 7.6, 2.5 Hz, 1H), 5.52 – 5.42 (m, 1H), 4.16 (t, *J* = 4.6 Hz, 1H), 2.70 – 2.59 (m, 1H), 2.04 – 1.96 (m, 1H), 1.90 (dt, *J* = 5.2, 1.3 Hz, 1H), 1.87 – 1.83 (m, 1H), 1.79 – 1.70 (m, 1H), 1.64 (tdd, *J* = 13.8, 4.3, 3.1 Hz, 1H), 1.58 (br s, 1H), 1.45 – 1.31 (m, 1H), 1.10 (s, 3H), 1.04 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 150.01 (C), 129.88 (CH), 124.55 (CH), 118.30 (CH), 64.68 (CH), 41.68 (CH_2), 35.46 (CH), 35.00 (C), 31.05 (CH_2), 27.67 (CH_3), 27.45 (CH_3), 24.84 (CH_2). **LRMS** (*m/z*, ESI): 161.13 $[M-H_2O+H]^+$, 147.12, 131.09. **HRMS-ESI** calculated for $C_{12}H_{17}$ $[M-H_2O+H]^+$: 161.1325, found 161.1325. Further confirmation of the structure of **5b´** was obtained by X-ray crystallography (from hexane/EtOAc (2:1) mixture).

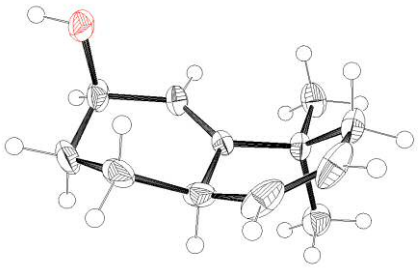
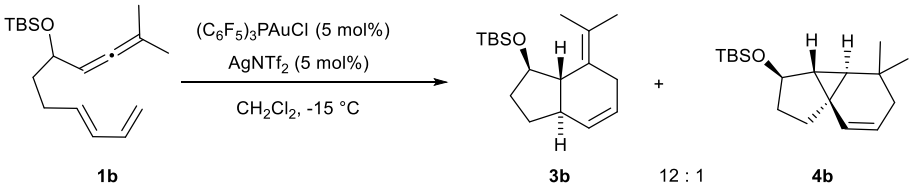


Figure S2. X-ray crystallographic analysis of **5b'** (CCDC 1964187)

4.3. Annulations catalyzed by $(C_6F_5)_3PAuCl$ / $AgNTf_2$ and related cationic gold(I) complexes (exemplified for the cycloaddition of allenediene **1b**)



A solution of allenediene **1b** (100.0 mg, 0.342 mmol) in CH_2Cl_2 (0.5 mL) was added to a suspension of $(C_6F_5)_3PAuCl$ (13.1 mg, 17.1 µmol) and $AgNTf_2$ (6.63 mg, 17.1 µmol) in CH_2Cl_2 (6 ml) at –15 °C. The mixture was stirred at that temperature for 1 h (the progress of the reaction was easily monitored by TLC) and filtered through a short pad of Florisil® eluting with Et_2O. The filtrate was concentrated and purified by flash chromatography (SiO_2 15-40 µm, 0.1-5% Et_2O/hexanes) to afford **3b** as a yellow oil (69.9 mg, 70% yield) and **4b** (5.8 mg, 6% yield, colorless oil). ***t*-Butyldimethyl(((1*R**,3a*R**,7a*S**)-7-(propan-2-ylidene)-2,3,3a,6,7,7a-hexahydro-1H-inden-1-yl)oxy)silane** (**3b**)**: ^{1}H NMR** (400 MHz, $CDCl_3$) δ 5.71 (dd, *J* = 9.5, 1.8 Hz, 1H), 5.59 (ddt, *J* = 9.5, 4.0, 2.6 Hz, 1H), 4.60 (td, *J* = 8.8, 6.3 Hz, 1H), 3.08 – 2.91 (m, 1H), 2.64 (d, *J* = 19.6 Hz, 1H), 2.24 – 2.12 (m, 2H), 2.12 – 2.00 (m, 1H), 1.87 (s, 3H), 1.84 – 1.73 (m, 1H), 1.68 (s, 3H), 1.66 – 1.57 (m, 1H), 1.48 – 1.34 (m, 1H), 0.88 (s, 9H), 0.07 (s, 3H), 0.06 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 130.86 (CH), 127.80 (C), 127.29 (CH), 122.05 (C), 74.95 (CH), 57.32 (CH), 42.48 (CH), 33.71 (CH_2), 33.52 (CH_2), 27.29 (CH_2), 26.19 (CH_3), 22.54 (CH_3), 21.60 (CH_3), 18.18 (C), -3.00 (CH_3), -4.04 (CH_3). **LRMS** (*m/z*, APCI): 293.23 $[M+H]^+$, 251.15, 190.16, 175.11, 161.14. **HRMS-APCI** calculated for $C_{18}H_{33}OSi$ $[M+H]^+$: 293.2295, found 293.2294. The relative stereochemistry of the **3b** was determined by nOe experiments (Figure S3A). Further confirmation was obtained by X-ray crystallographic analysis of the deprotected analog **3b'** (Figure S3B).

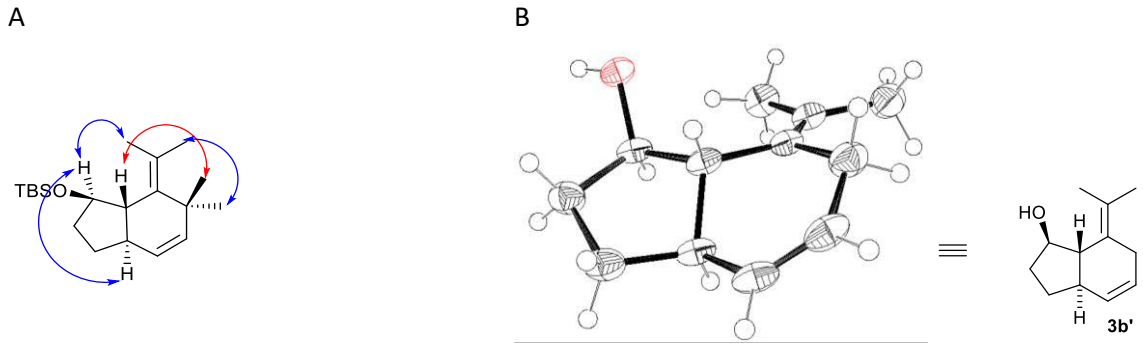
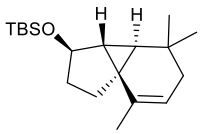


Figure S3. Significant nOe's observed for **3b** (A) and X-ray analysis of **3b'** (CCDC 1964184) (B)

4.4. Characterization data of products obtained from allenediene 1a

***t*-Butyldimethyl(((3*R**,3a*R**,3b*S**,7a*R**)-4,4,7-trimethyl-2,3,3a,3b,4,5-hexahydro-1H-cyclopenta[1,3]cyclopropa[1,2]benzen-3-yl)oxy)silane** (**4a**)



4a

Colorless oil at rt, crystalline solid at -20 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 5.10 (ddd, *J* = 5.2, 3.4, 1.6 Hz, 1H), 4.17 (d, *J* = 4.7 Hz, 1H), 2.22 (td, *J* = 11.7, 8.4 Hz, 1H), 1.85 (s, 3H), 1.62 – 1.55 (m, 3H), 1.52 (dd, *J* = 13.8, 8.3 Hz, 1H), 1.47 – 1.41 (m, 1H), 1.42 – 1.36 (m, 1H), 1.02 (s, 3H), 0.87 (s, 9H), 0.86 (s, 3H), 0.53 (dd, *J* = 4.2, 1.6 Hz, 1H), 0.04 (s, 6H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 136.07 (C), 115.81 (CH), 74.75 (CH), 36.64 (CH_2), 36.62 (CH), 34.94 (CH), 32.43 (CH_2), 31.92 (C), 30.42 (CH_3), 28.73 (CH_3), 28.04 (C), 27.19 (CH_2), 26.11 (CH_3), 21.31 (CH_3), 18.29 (C), -4.28 (CH_3), -4.39 (CH_3). **LRMS** (*m/z*, ESI): 307.24 $[M+H]^+$, 297.07, 281.04, 175.15. **HRMS-ESI** calculated for $C_{19}H_{35}OSi$ $[M+H]^{+\cdot}$ 307.2452 found 307.2452. The relative stereochemistry of the tricyclic product **4a** was determined by NMR (1D, 2D and nOe experiments). Further confirmation of its structure was obtained by X-ray crystallography.

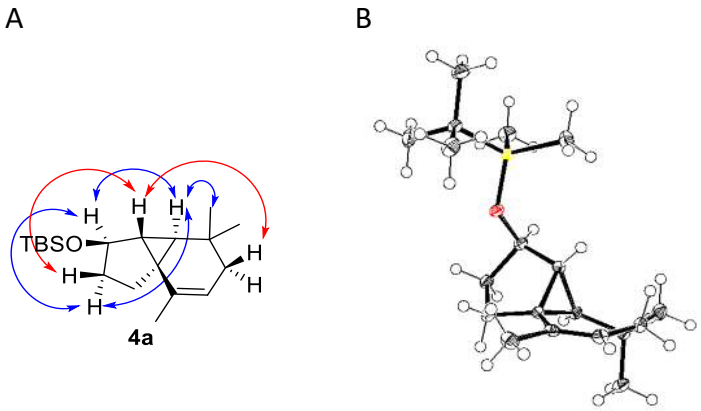
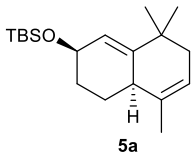
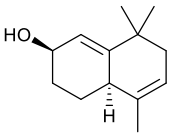


Figure S4. Significant nOe's observed (A) and X-ray crystallographic analysis (B) for **4a** (CCDC 1964188)

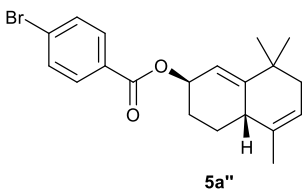
***t*-Butyldimethyl(((2*R**,4a*R**)-5,8,8-trimethyl-2,3,4,4a,7,8-hexahydronaphthalen-2-yl)oxy) silane (5a)**



Colorless oil. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 5.45 (ddd, *J* = 4.7, 2.3, 1.3 Hz, 1H), 5.37 – 5.30 (m, 1H), 4.25 – 4.12 (m, 1H), 2.56 – 2.42 (m, 1H), 1.99 (ddd, *J* = 16.8, 5.4, 2.7 Hz, 1H), 1.92 – 1.85 (m, 1H), 1.83 – 1.80 (m, 1H), 1.80 – 1.76 (m, 1H), 1.70 (s, 3H), 1.60 – 1.51 (m, 1H), 1.49 – 1.39 (m, 1H), 1.09 (s, 3H), 1.00 (s, 3H), 0.89 (s, 9H), 0.07 (s, 3H), 0.06 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 148.16 (C), 135.16 (C), 120.54 (CH), 119.16 (CH), 65.05 (CH), 41.35 (CH_2), 39.11 (CH), 34.75 (C), 32.12 (CH_2), 27.88 (CH_3), 27.31 (CH_3), 26.18 (CH_3), 22.64 (CH_2), 21.15 (CH_3), 18.49 (C), -4.01 (CH_3), -4.20. (CH_3). **LRMS** (*m/z*, APCI): 307.24 $[M+H]^+$, 195.17, 175.15, 133.10. **HRMS-APCI** calculated for $C_{19}H_{35}OSi$ $[M+H]^+$: 307.2452 found 307.2451. The relative stereochemistry of the **5a** was determined by nOe experiments (Figure S5A) and further confirmed by X-ray analysis of its *p*-bromobenzoic ester analog **5a''**, obtained through the following two-steps sequence.



The TBS group of **5a** was removed following the above-mentioned procedure for **5b**. Thus, **5a'** was obtained as a white solid in 95% yield. **m.p.:** 71-73 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 5.60 (d, *J* = 5.0 Hz, 1H), 5.33 (d, *J* = 6.0 Hz, 1H), 4.20 – 4.07 (m, 1H), 2.52 (d, *J* = 10.8 Hz, 1H), 1.99 – 1.86 (m, 3H), 1.81 (dd, *J* = 16.9, 6.0 Hz, 1H), 1.69 (s, 3H), 1.65 – 1.57 (m, 1H), 1.56 (s, 1H), 1.31 (q, *J* = 11.9 Hz, 1H), 1.08 (s, 3H), 0.99 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 150.47 (C), 134.91 (C), 120.63 (CH), 118.27 (CH), 64.29 (CH), 41.38 (CH_2), 39.06 (CH), 34.91 (C), 31.16 (CH_2), 27.82 (CH_3), 27.14 (CH_3), 22.48 (CH_2), 21.01 (CH_3). **LRMS** (*m/z*, ESI): 175.15 $[M-H_2O+H]^+$, 161.13, 145.10, 133.10. **HRMS-ESI** calculated for $C_{13}H_{19}$ $[M-H_2O+H]^+$: 175.1481, found 175.1483.



4-bromobenzoyl chloride (109.6 mg, 0.50 mmol) and Et_3N (69.0 µL, 0.50 mmol) were added to a solution of the alcohol **5a'** (80.0 mg, 0.416 mmol) in CH_2Cl_2 (8 mL). The mixture was cooled in an ice-water bath and DMAP (5.10 mg, 0.042 mmol) was added. After 10 min, the ice bath was removed and stirring was continued at rt for additional 4 h. Then, water (20 mL) and CH_2Cl_2 (20 mL) were added and the aqueous phase was extracted with CH_2Cl_2 (3× 40 mL). The combined organic layers were washed with brine, dried over Na_2SO_4, filtered and concentrated in vacuo. Purification of the crude residue by flash chromatography (SiO_2, 5% EtOAc/hexanes) afforded **5a''** (113.5 mg, 73% yield) as a white solid. **m.p.:** 104-105 °C. **^{1}H-NMR** (500 MHz, $CDCl_3$) δ 7.89 (d, *J* = 8.5 Hz, 2H), 7.55 (d, *J* = 8.5 Hz, 2H), 5.68 – 5.63 (m, 1H), 5.48 (t, *J* = 5.1 Hz, 1H), 5.42 – 5.35 (m, 1H), 2.61 (d, *J* = 11.6 Hz, 1H), 2.12 – 2.04 (m, 2H), 2.00 (dq, *J* = 17.1, 2.9 Hz, 1H), 1.85 (dd, *J* = 17.0, 5.9 Hz, 1H), 1.80 – 1.75 (m, 1H), 1.74 (s, 3H), 1.50 – 1.37 (m, 1H), 1.10 (s, 3H), 1.04 (s, 3H).**^{13}C-NMR** (126 MHz, $CDCl_3$) δ 165.66 (CO), 153.03 (C), 134.64 (C), 131.66 (CH), 131.33 (CH), 130.04 (C), 127.83 (C), 120.9 (CH), 114.31 (CH), 68.67 (CH), 41.27 (CH_2), 38.96 (CH), 35.19 (C), 28.53 (CH_2),

27.78 (CH_3), 27.22 (CH_3), 23.39 (CH_2), 21.04 (CH_3). **LRMS** (*m/z*, ESI): 398.02 $[M+Na]^+$, 314.97, 238.90. Further confirmation of the structure of **5a''** was obtained by X-ray diffraction analysis (from a ^{i}PrOH/$CHCl_3$ (2:1) mixture).

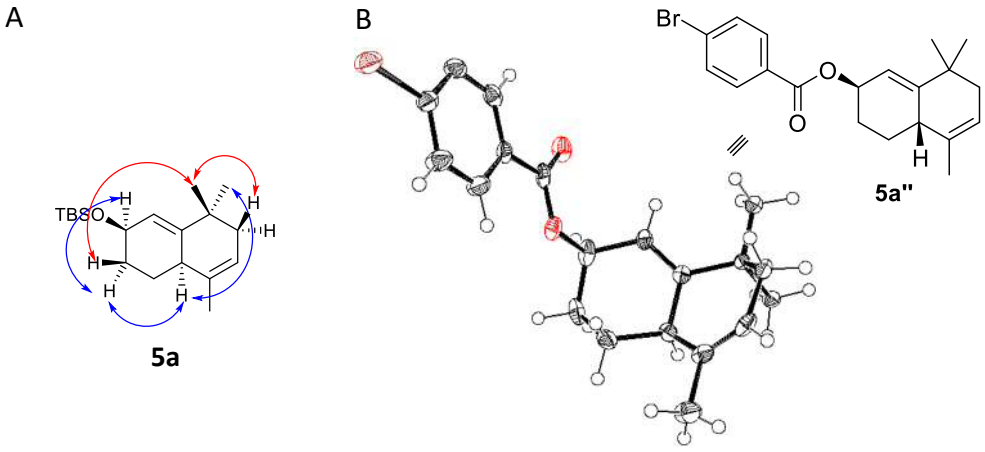
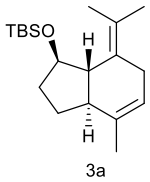


Figure S5. Significant nOe's observed for **5a** (A) and X-ray crystallographic analysis of **5a''** (CCDC 1964185) (B)

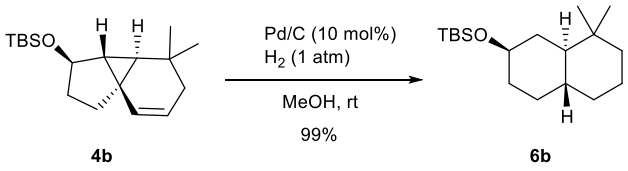
***tert*-Butyldimethyl(((1*R**,3a*S**,7a*S**)-4-methyl-7-(propan-2-ylidene)-2,3,3a,6,7,7a-hexahydro-1H-inden-1-yl)oxy)silane (3a)**



Yellow oil. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 5.39 – 5.21 (m, 1H), 4.60 (ddd, *J* = 9.6, 8.5, 6.1 Hz, 1H), 3.00 – 2.80 (m, 1H), 2.63 (d, *J* = 17.8, 0.9 Hz, 1H), 2.32 – 2.20 (m, 1H), 2.16 – 2.09 (m, 1H), 2.10 – 2.00 (m, 1H), 1.88 (s, 3H), 1.85 – 1.76 (m, 1H), 1.68 (s, 3H), 1.64 (s, 3H), 1.63 – 1.58 (m, 1H), 1.53 – 1.40 (m, 1H), 0.88 (s, 9H), 0.07 (s, 3H), 0.06 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 137.14 (C), 128.01 (C), 121.85 (C), 121.71 (CH), 75.20 (CH), 56.99 (CH), 45.76 (CH), 33.62 (CH_2), 33.53 (CH_2), 26.18, (CH_3) 25.99 (CH_2), 22.54 (CH_3), 21.67 (CH_3), 19.79 (CH_3), 18.18 (C), -3.08 (CH_3), -4.02 (CH_3). **LRMS** (*m/z*, APCI): 307.24 $[M+H]^+$, 187.15, 175.15, 133.10. **HRMS-APCI** calculated for $C_{19}H_{35}OSi$ $[M+H]^+$: 307.2452, found 307.2450.

5. Exploration of the synthetic potential

5.1. Hydrogenation of tricyclic product **4b** with Pd/C



Pd/C (10% wt/wt, 36.4 mg, 34.2 µmol, 10 mol%). was added to a solution of **4b** (100.0 mg, 0.342 mmol) in MeOH (7 mL) at rt. The resulting mixture was stirred under H_2 (1 atm) for 2 h before it was filtered, washed with Et_2O (3 × 20 mL), and concentrated in vacuo to give **6b** as a colorless oil (101.3 mg, 99%). **^{1}H NMR** (300 MHz, $CDCl_3$) δ 3.60 – 3.46 (m, 1H), 1.84 (t, *J* = 12.6 Hz, 2H), 1.69 – 1.52 (m, 2H), 1.50 – 1.31 (m, 3H), 1.29 – 1.12 (m, 2H), 1.12 – 0.93 (m, 3H), 0.89 (s, 12H), 0.84 – 0.74 (m, 2H), 0.76 – 0.65 (m, 1H), 0.06 (s, 6H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 72.79 (CH), 49.79 (CH), 42.22 (CH_2), 39.45 (C), 36.51 (CH_2), 36.46 (CH), 36.24 (CH_2), 34.39 (CH_2), 33.00 (CH_2), 30.47 (CH_3), 26.14 (CH_3), 22.13 (CH_2), 20.21 (CH_3), 18.47 (C), -4.40 (CH_3). Further confirmation of its structure was obtained by X-ray analysis of a 3,5-(NO_2)-benzoate derivative **6b'',** obtained by standard TBS-deprotection (**6b'**) and esterification with the corresponding acid chloride derivative (Figure S6)

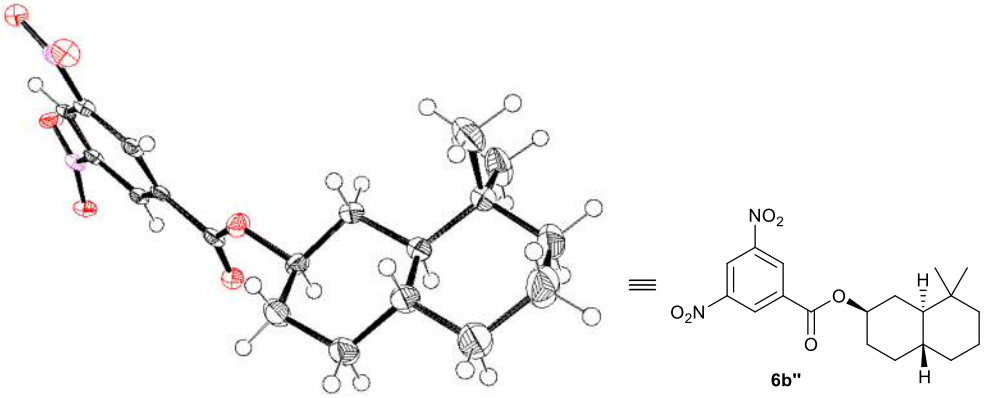
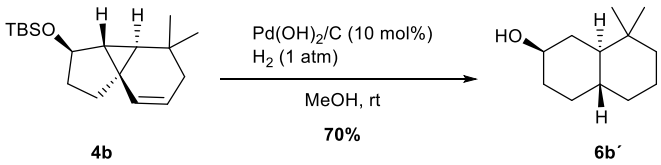


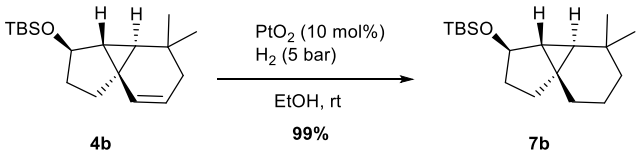
Figure S6. X-ray crystallographic analysis of **6b''** (CCDC 1964186)

5.2. Hydrogenation of tricyclic product **4b** with $Pd(OH)_2/C$



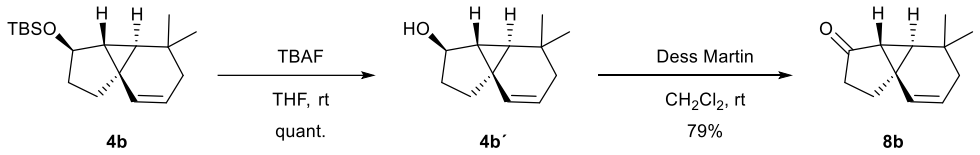
$Pd(OH)_2/C$ (20% wt/wt, 12.0 mg, 17.1 µmol, 10 mol%) was added to a solution of cycloadduct **4b** (50.0 mg, 0.171 mmol) in MeOH (3.5 mL) at rt. The resulting mixture was stirred under H_2 (1 atm) for 1 h before it was filtered, washed through with Et_2O (3 × 20 mL), and concentrated in vacuo. The crude product was purified by flash chromatography (SiO_2, 5 to 40% EtOAc/hexanes) to give the alcohol **6b´** as a colorless oil (21.8 mg, 70%). **^{1}H NMR** (300 MHz, $CDCl_3$) δ 3.55 (ddd, *J* = 15.0, 10.7, 4.2 Hz, 1H), 2.05 – 1.87 (m, 2H), 1.87 – 1.75 (m, 1H), 1.73 – 1.57 (m, 3H), 1.51 – 1.41 (m, 2H), 1.40 – 1.30 (m, 1H), 1.16 (ddd, *J* = 14.5, 6.8, 2.9 Hz, 1H), 1.11 – 0.98 (m, 2H), 0.98 – 0.90 (m, 2H), 0.87 (s, 3H), 0.80 (s, 3H), 0.78 – 0.71 (m, 1H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 71.82 (CH), 49.57 (CH), 42.10 (CH_2), 36.42 (CH), 36.18 (CH_2), 35.82 (CH_2), 34.23 (CH_2), 32.99 (C), 32.75 (CH_2), 30.47 (CH_3), 22.06 (CH_2), 20.18 (CH_3). **LRMS** (*m/z*, APCI): 165.16 [M-H_2O+H]$^+$, 109.10. **HRMS-APCI** calculated for $C_{12}H_{21}$ [M-H_2O+H]$^+$: 165.1638, found 165.1637.

5.3. Hydrogenation of tricyclic product **4b** with PtO_2



A solution of **4b** (36.0 mg, 0.123 mmol, 1.0 eq.) and PtO_2 (2.8 mg, 12.3 µmol, 10 mol%) in EtOH (2.5 mL) was pressurized with H_2 (5 bar) and stirred for 4 h. The mixture was filtered through a pad of SiO_2, eluting with Et_2O). The filtrate was concentrated in vacuo and purified by flash chromatography (SiO_2, 1 to 5% Et_2O/hexanes) to afford the **7b** (35.8 mg, 99% yield) as a colorless oil. **^{1}H NMR** (300 MHz, $CDCl_3$) δ 4.14 (d, *J* = 4.6 Hz, 1H), 1.92 – 1.67 (m, 3H), 1.58 (dd, *J* = 12.1, 7.7 Hz, 1H), 1.39 (tt, *J* = 14.4, 7.3 Hz, 3H), 1.25 – 1.14 (m, 1H), 1.09 – 0.95 (m, 5H), 0.91 (s, 3H), 0.89 (s, 9H), 0.81 (d, *J* = 3.8 Hz, 1H), 0.25 (d, *J* = 3.7 Hz, 1H), 0.06 (s, 3H), 0.05 (s, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 76.74 (CH), 35.94 (CH_2), 33.93 (CH), 32.87 (CH_2), 32.34 (CH_2), 31.37 (CH), 30.96 (CH_3), 30.28 (CH_3), 29.71 (C), 28.41 (C), 26.63 (CH_2), 26.13 (CH_3), 19.01 (CH_2), 18.40 (C), -4.28 (CH_3), -4.39 (CH_3). **LRMS** (*m/z*, APCI): 295.24 [M+H]$^+$, 163.15, 107.08. **HRMS-APCI** calculated for $C_{18}H_{35}OSi$ [M+H]$^+$: 295.2452 found 295.2441.

5.4 Deprotection and oxidation of tricyclic product **4b**



The TBS group of **4b** was removed following the above-described procedure for **5b**. Characterization data of alcohol **4b´**: White solid (21.0 mg, 99% yield). **m.p.:** 84-85 °C. $\mathbf{R_f}$ = 0.13 (30% Et_2O/hexanes). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 5.96 (dd, *J* = 9.8, 3.0 Hz, 1H), 5.38 (ddd, *J* = 9.4, 6.4, 2.6 Hz, 1H), 4.19 (d, *J* = 4.8 Hz, 1H), 2.01 (td, *J* = 12.0, 8.3 Hz, 1H), 1.78 (dd, *J* = 12.4, 8.1 Hz, 1H), 1.68 – 1.59 (m, 3H), 1.55 (d, *J* = 3.2 Hz, 1H), 1.52 – 1.48 (m, 1H), 1.25 (s, 1H), 1.06 (s, 3H), 0.87 (s, 3H), 0.63 (dd, *J* = 3.9, 2.1 Hz, 1H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 130.12 (CH), 121.92 (CH), 74.70 (CH), 36.71 (CH_2), 36.50 (CH), 35.04 (CH), 32.24 (CH_2), 30.23 (CH_3), 30.13 (C), 29.58 (CH_2), 28.48 (CH_3), 28.04 (C). **LRMS** (m/z, ESI): 201.12 $[M+Na]^+$, 161.13, 147.18. **HRMS-ESI** calculated for $C_{12}H_{17}ONa$ $[M+Na]^{+\cdot}$ 201.1255 found 201.1259.

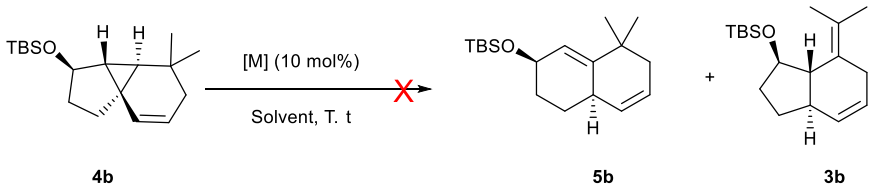
A solution of **4b´** (105.0 mg, 0.589 mmol) in CH_2Cl_2 (2 mL) was added to a solution of Dess-Martin periodinane (274.8 mg, 0.648 mmol) in CH_2Cl_2 (10 mL) at rt. After stirring the mixture for 3 h, the reaction was quenched by addition of aqueous $NaHCO_3$ and $Na_2S_2O_3$ solution. After stirring for another 15 min, the layers were separated, and the aqueous layer was extracted with CH_2Cl_2 (3x 50 mL). The combined organic layers were dried over Na_2SO_4, filtered and concentrated in vacuo. The crude product was purified by flash chromatography (SiO_2, 5 - 20% EtOAc/hexanes) to give the ketone **8b** as a white solid (81.5 mg, 79% yield). **(3a*R**,3b*S**,7a*R**)-4,4-dimethyl-1,2,3a,3b,4,5-hexahydro-3H-cyclopenta[1,3]cyclopropa[1,2]benzen-3-one** (**8b**) **m.p.:** 66-67 °C. **^{1}H NMR** (300 MHz, $CDCl_3$) δ 5.85 (dd, *J* = 9.7, 3.2 Hz, 1H), 5.48 (ddd, *J* = 9.4, 6.8, 2.3 Hz, 1H), 2.27 – 2.02 (m, 4H), 1.96 (dd, *J* = 3.3, 1.2 Hz, 1H), 1.72 (ddd, *J* = 17.0, 6.8, 2.2 Hz, 1H), 1.59 – 1.46 (m, 1H), 1.40 (dd, *J* = 3.3, 2.2 Hz, 1H), 1.07 (s, 3H), 0.96 (s, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 213.14 (CO), 128.02 (CH), 124.30 (CH), 40.08 (CH), 38.66 (CH), 36.21 (CH_2), 34.42 (C), 33.76 (CH_2), 29.73 (CH_3), 28.95 (C), 28.04 (CH_2), 27.80 (CH_3). **LRMS** (m/z, APCI): 177.13 $[M+H]^+$, 131.08. **HRMS-APCI** calculated for $C_{12}H_{17}O$ $[M+H]^{+\cdot}$ 177.1274 found 177.1276.

6. Mechanistic probes

6.1. Complementary data for Scheme 6, equation 1 (main manuscript)

We analyzed if product **5b** could be obtained from **4b** under standard reaction conditions (Table S4). Additionally, we also checked whether **4b** could be obtained from **3b** or **5b,** under standard reaction conditions (Tables S5 and S6).

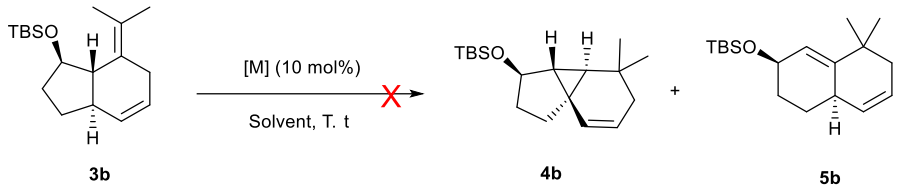
Table S4. Control experiments with **4b**.[a]



Entry	[M]	Solvent	T (°C)	t (h)	Conv. (%)[b]
1	$(C_6F_5)_3PAuCl/AgNTf_2$	CH_2Cl_2	-15	0.5	>99[c]
2	$(C_6F_5)_3PAuCl/AgNTf_2$	CH_2Cl_2	-45	12	<5
3[d]	$PtCl_2$/CO	Cyclohexane	50	2	0
4[d]	$PtCl_2$/CO	Toluene	50	2	>99[c]
5	IPrAu-NTf_2	CH_2Cl_2	rt	12	0
6	IPrAu-NTf_2	CH_2Cl_2	40	4	>99[c]

[a] *Conditions*: **4b** was treated with [M] (10 mol%) in the indicated solvent (0.05M) at the indicated temperature (°C) and time (h), unless otherwise noted. [b] Conversion determined by ^{1}H-NMR of the crude mixtures. [c] Complex mixture of products in which **5b** and **3b** were not observed. [d] Solvent with 1 ppm of water.

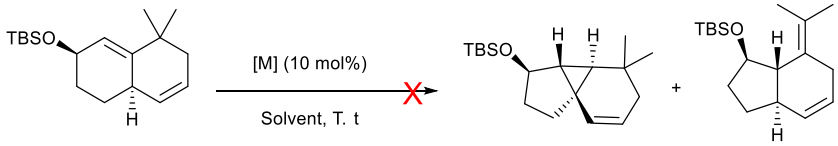
Table S5. Control experiments with the cycloadduct **3b**.[a]



Entry	[M]	Solvent	T (°C)	t (h)	Conv. (%)[b]
1	$PtCl_2$	Dioxane	30	12	0
2	$PtCl_2$	Dioxane	100	2	<5[e]
3[c]	$PtCl_2$/CO	Cyclohexane	50	2	0
4[c]	$PtCl_2$/CO	Cyclohexane	80	2	>99[d]
5	IPrAu-NTf_2	CH_2Cl_2	rt	12	0
6	IPrAu-NTf_2	CH_2Cl_2	40	2	20[e]

[a] *Conditions*: **3b** was treated with [M] (10 mol%) in the indicated solvent (0.05M) at the indicated temperature (°C) and time (h), unless otherwise noted. [b] Conversion determined by ^{1}H-NMR of the crude reaction mixtures. [c] Solvent with 1 ppm of water. [d] Complex mixture of products. [e] **4b** and **5b** were not detected.

Table S6. Control experiments with **5b**[a]



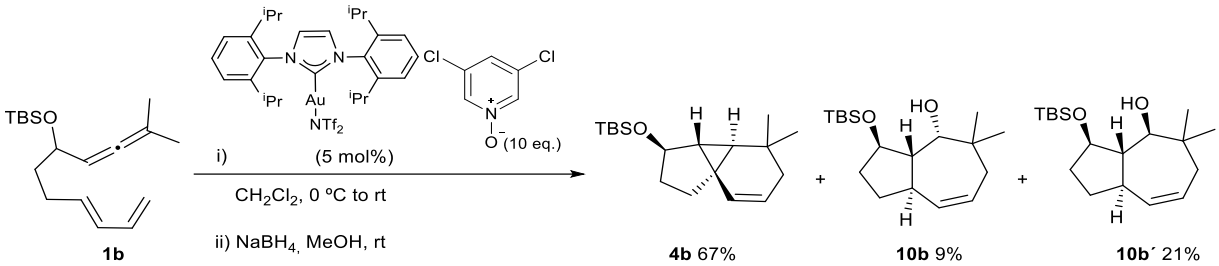
5b **4b** **3b**

Entry	[M]	Solvent	T (°C)	t (h)	Conv. (%)[b]
1	$PtCl_2$	Dioxane	30	12	0
2	$PtCl_2$	Dioxane	100	4	<5[c]
3	$(C_6F_5)_3PAuCl/AgNTf_2$	CH_2Cl_2	rt	12	0
4	$(C_6F_5)_3PAuCl/AgNTf_2$	CH_2Cl_2	40	2	>99[d]
5	IPrAu-NTf_2	CH_2Cl_2	rt	12	0
6	IPrAu-NTf_2	CH_2Cl_2	40	2	<5[c]

[a] *Conditions*: **5b** (1.0 eq) was treated with [M] (10 mol%) in the indicated solvent (0.05M) at the indicated temperature (°C) and time (h), unless otherwise noted. [b]Conversion of **5b** determined by ^{1}H-NMR spectroscopy in the crude mixtures. [c] **4b** and **3b** were not detected [d] A complex mixture of products was obtained.

6.2. Complementary data for Scheme 6, equation 2 (main manuscript)

Reaction of **1b** with IPrAuNTf_2 and 3,5-dichloropyridine N-oxide, followed by reduction with $NaBH_4$.



1b **4b** 67% **10b** 9% **10b´** 21%

A solution of **1b** (250.0 mg, 0.855 mmol) in CH_2Cl_2 (2.0 mL) was added to a suspension of IPrAuNTf_2 (37.0 mg, 42.5 µmol) and 3,5-dichloropyridine *N*-oxide (1.40 g, 8.55 mmol) in CH_2Cl_2 (15 ml) at 0 °C. The mixture was stirred for 12 h at rt, concentrated, redissolved in 10% Et_2O/hexanes and filtered through a Florisil® pad (eluting with 10% Et_2O/hexanes). Then, the solvents were concentrated to provide a crude oil that was used in the next step without further purification. $NaBH_4$ (63.8 mg, 1.69 mmol) was added to a solution of this crude in MeOH (2 mL) at rt. After stirring at rt for 1 h, NH_4Cl (sat.) (5 mL) was added. The volatile materials were concentrated and the aqueous layer was extracted with Et_2O (3× 30 mL). The combined organic layers were washed with brine, dried, filtered and concentrated. Purification by chromatography (SiO_2 15-40 µm, 0 - 20% Et_2O/hexanes) led to **4b** (167.5 mg, 67%) and the epimers **10b´** (55.7 mg, 21%) and **10b** (23.9 mg, 9%).

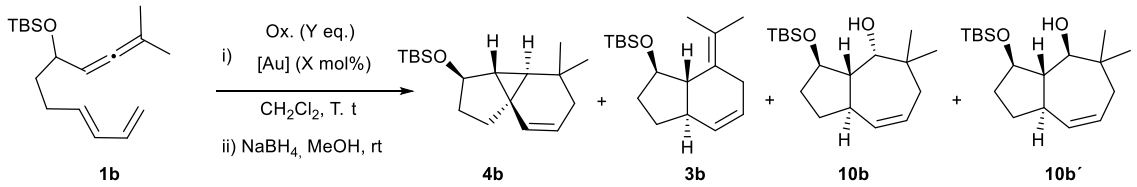
(3*R,3a*S**,4*S**,8a*R**)-3-((*t*-Butyldimethylsilyl)oxy)-5,5-dimethyl-1,2,3,3a,4,5,6,8a-octahydroazulen-4-ol** (**10b**). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 5.64 (dt, *J* = 10.2, 3.0 Hz, 1H), 5.48 (dddd, *J* = 10.5, 8.7, 4.5, 2.8 Hz, 1H), 4.16 – 4.07 (m, 1H), 3.57 (s, 1H), 2.72 – 2.66 (m, 1H), 2.61 – 2.53 (m, 1H), 1.92 – 1.81 (m, 2H), 1.78 (ddd, *J* = 12.1, 8.2, 1.9 Hz, 1H), 1.67 – 1.49 (m, 3H), 1.48 (s, 1H), 1.01 (s, 3H), 0.93 (s, 3H), 0.88 (s, 9H), 0.05 (s, 3H), 0.04 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 137.40 (CH), 128.12 (CH), 77.23 (CH), 74.99 (CH), 52.45 (CH), 36.26 (C), 34.17 (CH_2), 33.80 (CH), 33.72 (CH_2), 29.82 (CH_3), 29.32 (CH_2), 26.03 (CH_3), 24.40 (CH_3), 18.22 (C), -4.26 (CH_3), -4.59 (CH_3). **LRMS** (*m/z*, APCI): 311.24 $[M+H]^+$, 293.24. **HRMS-APCI** calculated for $C_{18}H_{35}O_2Si$ $[M+H]^+$: 311.2401 found 311.2398. The stereochemistry of **10b** was determined by nOe experiments (Figure S7A)

10b´. ^{1}H NMR (500 MHz, $CDCl_3$) δ 5.66 – 5.54 (m, 2H), 4.08 (q, *J* = 8.8, 7.9 Hz, 1H), 3.97 (d, *J* = 1.5 Hz, 1H), 3.34 (dd, *J* = 9.9, 1.4 Hz, 1H), 2.34 – 2.23 (m, 1H), 2.04 – 1.94 (m, 2H), 1.94 – 1.87 (m, 1H), 1.85 – 1.77 (m, 1H), 1.70 – 1.54 (m, 2H), 1.50 (ddd, *J* = 11.5, 9.8, 8.8 Hz, 1H), 1.03 (s, 3H), 0.90 (s, 9H), 0.83 (s, 3H), 0.13 (s, 3H), 0.09 (s, 3H).**^{13}C NMR** (126 MHz, $CDCl_3$) δ 136.09 (CH), 129.62 (CH), 85.92 (CH), 81.12 (CH), 51.31 (CH), 38.76 (CH_2), 37.26 (CH), 36.28 (C), 33.05 (CH_2), 29.55 (CH_3), 28.60 (CH_2), 25.99 (CH_3), 18.73 (CH_3), 17.93 (C), -3.35 (CH_3), -4.78 (CH_3).**LRMS** (*m/z*, APCI): 311.24 $[M+H]^+$, 293.23. **HRMS-APCI** calculated for $C_{18}H_{35}O_2Si$ $[M+H]^+$: 311.2401 found 311.2399. The stereochemistry of the **10b'** was determined by nOe (Figure S7B)

A B

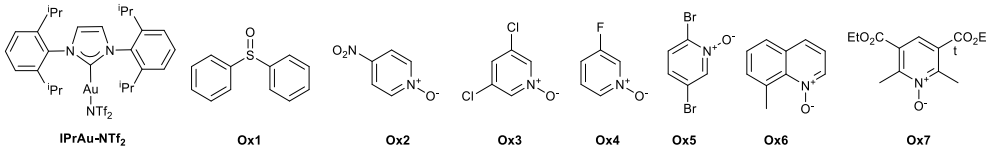
Figure S7. Significant nOe's observed for **10b** (A) and **10b'** (B)

Table S7. Reactivity of the substrate **1b** with other gold complexes and carbene oxidants[a]



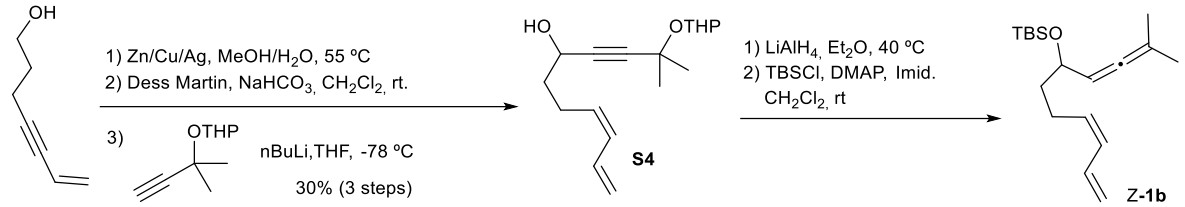
Entry	[M] (X mol%)	Ox. (Y eq.)	Solvent	T (°C)	t (h)	Conv. (%)	**4b** (%)[b]	**3b** (%)[b]	**10b+10b´** (%)[b]
1	IPrAu-NTf_2 (10)	Ox1 (3)	CH_2Cl_2	rt	1	>99	82	-	-
2	IPrAu-NTf_2 (10)	Ox2 (3)	CH_2Cl_2	rt	1	>99	73	-	-
3	IPrAu-NTf_2 (10)	Ox3 (3)	CH_2Cl_2	rt	1	>99	78	-	traces
4	IPrAu-NTf_2 (10)	Ox3 (10)	CH_2Cl_2	rt	1	>99	82	-	7
5	IPrAu-NTf_2 (5)	Ox3 (10)	CH_2Cl_2	0 to rt	24	>99	67[c]	-	30[c]
6	IPrAu-NTf_2 (5)	Ox4 (10)	CH_2Cl_2	0 to rt	24	53	26[c]	-	21[c]
7	IPrAu-NTf_2 (5)	Ox5 (10)	CH_2Cl_2	0 to rt	24	45	21	-	-
8	IPrAu-NTf_2 (5)	Ox6 (10)	CH_2Cl_2	0 to rt	24	<5	-	-	-
9	IPrAu-NTf_2 (5)	Ox7 (10)	CH_2Cl_2	0 to rt	24	<5	-	-	-
10	$(C_6F_5)_3$PAuCl/$AgNTf_2$ (5)	Ox3 (20)	CH_2Cl_2	0 to rt	12	75	-	48[c]	9[c]
11	$PtCl_2$	Ox3 (20)	Dioxane	30	12	<5	-	-	-
12[d]	$PtCl_2$/CO	Ox3 (20)	Cyclohex.	50	2	>99	Complex mixture		

[a] *Conditions*: i) Allenediene **1b** and Ox*n* (Y eq.) were treated with [M] (X mol%) in CH_2Cl_2 (0.05 M) at the indicated temperature (°C) and time (h), unless otherwise noted. ii) the crude was treated with $NaBH_4$ (2 eq.) in MeOH (0.5 M). Conversions calculated from the ^{1}H-NMR of the crude mixture. [b] Yields calculated by ^{1}H-NMR with internal standard. [c] Isolated yield. [d] Cyclohexane with 1 ppm of water.



6.3. Complementary data for scheme 6 equation 3 (main manuscript)

Synthesis of (*Z*)-*tert*-butyldimethyl((2-methylundeca-2,3,8,10-tetraen-5-yl)oxy)silane (*Z*-**1b**)



Following the procedure described by Gilbertson *et al.* (slightly modified).[3] Zinc dust (19.8 g, 303 mmol) was treated with 50 mL of 3% HCl for 1-2 min, and then the liquid was decanted. This was repeated two more times, after which the zinc slurry was rinsed repeatedly with H_2O to remove traces of HCl. A solution of $Cu(OAc)_2{\cdot}H_2O$ (1.69 g, 8.50 mmol) in 50 mL of H_2O was slowly added to the zinc slurry while cooling in an ice bath. The mixture was stirred for 15 min, and a solution of $AgNO_3$ (1.86 g, 11.0 mmol) in 50 mL of H_2O was added likewise. The resulting mixture was filtered, and the active zinc reagent was suspended in a mixture of MeOH (50 mL) and H_2O (60 mL). A solution of hept-6-en-4-yn-1-ol[4] (0.969 g, 8.80 mmol) in MeOH (10 mL) was added, and the mixture was stirred at 55 for 12 h. Then, the Zn/Cu/Ag mixture was filtered off and washed with MeOH (50 mL) and with a mixture of MeOH (80 mL) and HCl (10%, 10 mL). The filtrate was extracted with CH_2Cl_2, dried and evaporated to afford the corresponding hydrogenated product as a yellow oil (0.981 g, E/Z = 1:0, 99% yield) **^{1}H NMR** (300 MHz, $CDCl_3$) δ 6.58 (dt, *J* = 16.8, 10.6 Hz, 1H), 5.96 (t, *J* = 11.0 Hz, 1H), 5.39 (q, *J* = 8.3 Hz, 1H), 5.08 (dd, *J* = 28.5, 13.6 Hz, 2H), 3.54 (t, *J* = 6.4 Hz, 2H), 3.23 (s, 1H), 2.20 (q, *J* = 7.7 Hz, 2H), 1.57 (q, *J* = 7.0 Hz, 2H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 132.07 (CH), 131.83 (CH), 129.74 (CH), 117.17 (CH_2), 61.87 (CH_2), 32.28 (CH_2), 23.99 (CH_2). **LRMS** (*m/z*, APCI): 113.09 $[M+H]^+$, 95.08. **HRMS-APCI** calculated for $C_7H_{13}O$ $[M+H]^+$: 113.0966, found 113.0959.

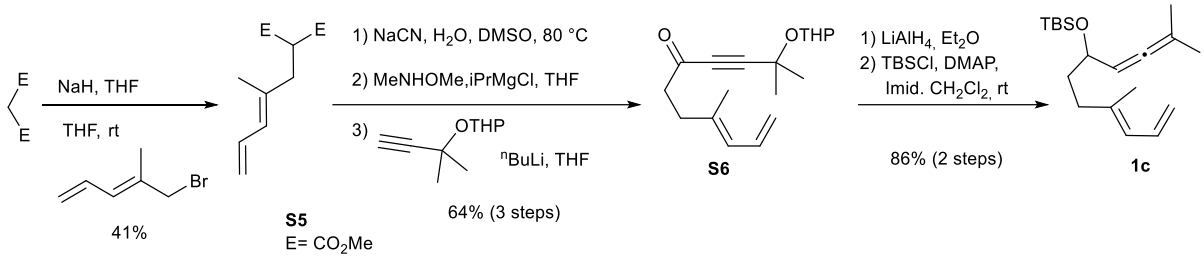
A solution of this diene (0.98 g, 8.74 mmol) in CH_2Cl_2 (2.5 mL) was added to a solution of Dess-Martin periodinane (3.89 g, 9.17 mmol) and $NaHCO_3$ (7.34 g, 87. 4 mmol) in CH_2Cl_2 (70 mL) at rt. After stirring the mixture for 1 h, the reaction was quenched by addition of $NaHCO_3$(aq) and $Na_2S_2O_3$(sat). After stirring for another 15 min, the layers were separated, and the aqueous layer was extracted with CH_2Cl_2 (3x 50 mL). The combined organic layers were dried, filtered and concentrated in vacuo. The crude aldehyde (0.962 g, 99% yield) was used in the next step without further purification.

^{n}BuLi (5.2 ml, 2.5M in hexanes, 13.1 mmol) was slowly added to a solution of 2-((2-methylbut-3-yn-2-yl)oxy)tetrahydro-2H-pyran (2.20 g, 13.10 mmol) in THF (58 mL) at −78 °C. The reaction was stirred 15 min at −78 °C. Then, the solution was warmed to 0 °C and HMPA (1.92 mL, 11.0 mmol) and the crude aldehyde (0.962 g, 8.73 mmol) in THF (5.0 mL) were added. The reaction was stirred at rt. After 1.5 h (consumption of starting material was observed by TLC), NH_4Cl (sat.) was added and the resulting mixture was diluted with EtOAc and water. The aqueous layer was separated and extracted with EtOAc (3× 50 mL). The combined organic layers were washed with brine, dried, filtered and concentrated in vacuo. Purification of the crude material by flash chromatography (SiO_2, 10 - 30% EtOAc/hexanes) afforded the desired propargyl alcohol **S4,** as a pale yellow oil (722.9 mg, 30% global yield). **^{1}H NMR** (300 MHz, $CDCl_3$) δ 6.65 (dt, *J* = 16.9, 10.7 Hz, 1H), 6.01 (t, *J* = 10.9 Hz, 1H), 5.51 – 5.35 (m, 1H), 5.17 (dd, *J* = 16.8, 2.0 Hz, 1H), 5.13 – 5.00 (m, 2H), 4.37 (t, *J* = 6.5 Hz, 1H), 3.99 – 3.86 (m, 1H), 3.55 – 3.42 (m, 1H), 2.83 (s, 1H), 2.34 (qd, *J* = 7.7, 1.5 Hz, 2H), 1.84 – 1.63 (m, 4H), 1.50 (br s, 7H), 1.46 (s, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 132.14 (CH), 131.26 (CH), 130.21 (CH), 117.43 (CH_2), 95.87 (CH), 87.31 (C), 85.11 (C), 70.98 (C), 63.09 (CH_2), 61.64 (C), 37.53 (CH_2), 32.00 (CH_2), 30.59 (CH_3), 30.11 (CH_3), 25.46 (CH_2), 23.62

(CH_2), 20.28 (CH_2). **LRMS** (*m/z*, APCI): 279.19 $[M+H]^+$, 261.18, 177.13. **HRMS-APCI** calculated for $C_{17}H_{27}O_3$ $[M+H]^+$: 279.1955, found 279.1956.

The allenediene Z-**1b** was synthesized from propargyl alcohol **S4** in 68% global yield (two steps),following the same procedure previously described for obtaining **1b**. **(Z)-tert-butyldimethyl((2-methylundeca-2,3,8,10-tetraen-5-yl)oxy)silane** (*Z*-**1b**): Colorless oil (97% yield). **^{1}H NMR** (300 MHz, $CDCl_3$) δ 6.75 – 6.56 (m, 1H), 6.01 (t, *J* = 10.9 Hz, 1H), 5.48 (q, *J* = 8.5 Hz, 1H), 5.19 (d, *J* = 16.9 Hz, 1H), 5.09 (d, *J* = 9.6 Hz, 1H), 5.01 – 4.88 (m, 1H), 4.11 (q, *J* = 7.1, 6.3 Hz, 1H), 2.39 – 2.13 (m, 2H), 1.70 (br s, 6H), 1.67 – 1.53 (m, 2H), 0.91 (s, 9H), 0.08 (s, 6H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 200.57 (C), 132.64 (CH), 132.45 (CH), 129.45 (CH), 116.93 (CH_2), 96.33 (C), 93.77 (CH), 72.01 (CH), 38.77 (CH_2), 26.04 (CH_3), 24.02 (CH_2), 20.88 (CH_3), 20.34 (CH_3), 18.36 (C), -4.06 (CH_3), -4.72 (CH_3). **LRMS** (*m/z*, APCI): 267.21 $[M+H]^+$, 188.15, 173.14. **HRMS-APCI** calculated for $C_{18}H_{33}OSi$ $[M+H]^+$: 293.2295, found 293.2295.

Synthesis of (*E*)-tert-butyl((2,8-dimethylundeca-2,3,8,10-tetraen-5-yl)oxy)dimethylsilane (**1c**)



A solution of dimethyl malonate (12.22 mL, 106.8 mmol) was added to an ice-cooled suspension of NaH (4.89 g, 60% in mineral oil, 122 mmol) in THF (140 mL). After stirring at rt for 1 h, a solution of (*E*)-5-bromo-4-methylpenta-1,3-diene[5] (5.73 g, 35.59 mmol) in THF (40 mL) was added at 0 °C. The reaction mixture was allowed to stir for 3 h at rt, poured into water and extracted with EtOAc. The combined organic layers were dried, filtered and concentrated, and the resulting residue was purified by flash chromatography (SiO_2, 5 - 50% EtOAc/hexanes) to give **S5** as a pale yellow oil (2.37 g, 41% yield). **^{1}H NMR** (300 MHz $CDCl_3$) δ 6.51 (dt, *J* = 16.8, 10.5 Hz, 1H), 5.87 (d, *J* = 10.9 Hz, 1H), 5.13 (d, *J* = 16.8 Hz, 1H), 5.03 (d, *J* = 10.2 Hz, 1H), 3.72 (s, 6H), 3.60 (t, *J* = 7.8 Hz, 1H), 2.66 (d, *J* = 7.9 Hz, 2H), 1.76 (s, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$)) δ 169.25 (CO), 134.15 (C), 132.66 (CH), 127.96 (CH), 116.27 (CH_2), 52.39 (CH_3), 50.25 (CH), 38.58 (CH_2), 16.15 (CH_3). **LRMS** (*m/z*, APCI): 213.11 $[M+H]^+$, 181.08. **HRMS-APCI** calculated for $C_{11}H_{17}O_4$ $[M+H]^+$: 213.1121, found 213.1121.

A solution of **S5** (2.37 g, 11.17 mmol), NaCN (2.74 g, 55.83 mmol, 5.0 eq.), and water (1 mL, 55.8 mmol, 5.0 eq.) in DMSO (112 mL) was stirred for 24 h at 80 °C. When the reaction was complete, water (200 mL) was added, and the resulting mixture was extracted with pentane (3x 100 mL). The combined pentane fractions were washed with water and dried over Na_2SO_4, filtered and concentrated to give the decarboxilated product as a colorless oil (1.30 g, 76% yield), which was used without purification in the next step. **^{1}H NMR** (300 MHz CD_2Cl_2) δ 6.60 (dt, *J* = 16.8, 10.5 Hz, 1H), 5.90 (d, *J* = 10.8 Hz, 1H), 5.10 (s, 1H), 5.03 (dd, *J* = 10.2, 1.5 Hz, 1H), 3.66 (s, 3H), 2.56 – 2.33 (m, 4H), 1.79 (s, 3H). **^{13}C NMR** (75 MHz, CD_2Cl_2) δ 173.74 (CO), 138.01 (C), 133.73 (CH), 126.63 (CH), 115.77 (CH_2), 51.85 (CH_3), 35.24 (CH_2), 33.04 (CH_2), 16.82 (CH_3). **LRMS** (*m/z*, APCI): 177.07 $[M+Na]^+$, 155.11 $[M+H]^+$. **HRMS-APCI** calculated for $C_9H_{15}O_2$ $[M+H]^+$: 155.1067, found 155.1065.

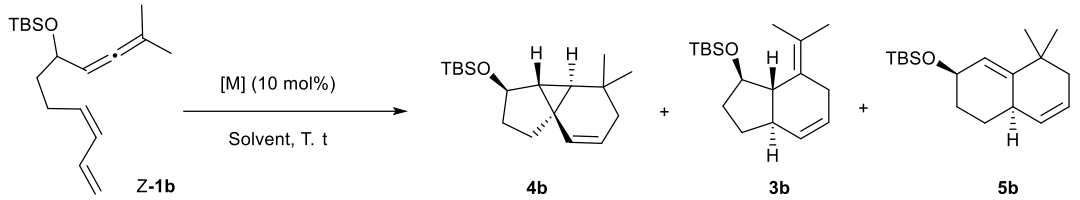
The subsequent Weinreb amide [(*E*)-*N*-methoxy-N,4-dimethylhepta-4,6-dienamide] was synthesized following the procedure described for the synthesis of **1b**. Pale yellow oil (99% yield). **^{1}H NMR** (300 MHz $CDCl_3$) δ 6.45 (dt, *J* = 16.8, 10.5 Hz, 1H), 5.77 (d, *J* = 10.9 Hz, 1H), 4.99 (dd, *J* = 16.8, 2.3 Hz, 1H), 4.93 – 4.83 (m, 1H), 3.57 (s, 3H), 3.06 (s, 3H), 2.43 (q, *J* = 9.4, 8.5 Hz, 2H), 2.27 (dd, *J* = 9.5, 6.2 Hz, 2H), 1.68 (s, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 173.52 (CO), 137.72 (C), 132.78 (CH), 125.47 (CH), 114.83 (CH_2), 60.87 (CH_3), 33.98 (CH_2), 31.84 (CH_3), 30.08

(CH_2), 16.33 (CH_3). **LRMS** (*m/z*, APCI): 206.12 $[M+Na]^+$, 184.13 $[M+H]^+$, 138.09. **HRMS-APCI** calculated for $C_{10}H_{18}NO_2$ $[M+H]^+$: 184.1332, found 184.1350.

The ketone **S6** was synthesized following the procedure described for **S2**. (85% yield). **^{1}H NMR** (300 MHz, $CDCl_3$) δ 6.49 (dt, *J* = 16.9, 10.5 Hz, 1H), 5.81 (d, *J* = 10.9 Hz, 1H), 5.07 (d, *J* = 16.8 Hz, 1H), 4.97 (d, *J* = 9.1 Hz, 2H), 3.96 – 3.83 (m, 1H), 3.52 – 3.39 (m, 1H), 2.71 – 2.55 (m, 2H), 2.37 (t, *J* = 7.8 Hz, 2H), 1.86 – 1.74 (m, 1H), 1.72 (s, 3H), 1.69 – 1.61 (m, 1H), 1.53 (br s, 3H), 1.50 (br s, 7H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 186.88 (CO), 136.72 (C), 132.89 (CH), 126.35 (CH), 115.71 (CH_2), 96.16 (CH), 94.38 (C), 82.65 (C), 70.53 (C), 63.16 (CH_2), 43.77 (CH_2), 33.64 (CH_2), 31.75 (CH_2), 29.59 (CH_3), 29.28 (CH_3), 25.27 (CH_2), 20.12 (CH_2), 16.64 (CH_3). **LRMS** (*m/z*, APCI): 291.19 $[M+H]^+$, 207.14. **HRMS-APCI** calculated for $C_{18}H_{27}O_3$ $[M+H]^+$: 291.1955, found 291.1955.

The allenediene **1c** was synthesized from **S6** following the procedure described for **1b**.: Colorless oil (86% global yield, two steps). **(*E*)-*tert*-butyl((2,8-dimethylundeca-2,3,8,10-tetraen-5-yl)oxy)dimethylsilane** **^{1}H NMR** (300 MHz, $CDCl_3$) δ 6.58 (dt, *J* = 16.7, 10.5 Hz, 1H), 5.88 (d, *J* = 10.9 Hz, 1H), 5.09 (d, *J* = 16.8 Hz, 1H), 5.03 – 4.84 (m, 2H), 4.08 (q, *J* = 6.7 Hz, 1H), 2.24 – 2.00 (m, 2H), 1.77 (s, 3H), 1.70 (t, *J* = 2.9 Hz, 6H), 1.68 – 1.54 (m, 2H), 0.91 (s, 9H), 0.08 (s, 6H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 200.58 (C), 139.60 (C), 133.52 (CH), 125.57 (CH), 114.64 (CH_2), 96.21 (C), 93.79 (CH), 72.22 (CH), 37.11 (CH_2), 35.88 (CH_2), 26.04 (CH_3), 20.89 (CH_3), 20.33 (CH_3), 18.37 (C), 16.86 (CH_3), -4.06 (CH_3), -4.73 (CH_3). **LRMS** (*m/z*, APCI): 307.24 $[M+H]^+$, 249.17, 175.15. **HRMS-APCI** calculated for $C_{19}H_{35}OSi$ $[M+H]^+$: 307.2452, found 307.2445.

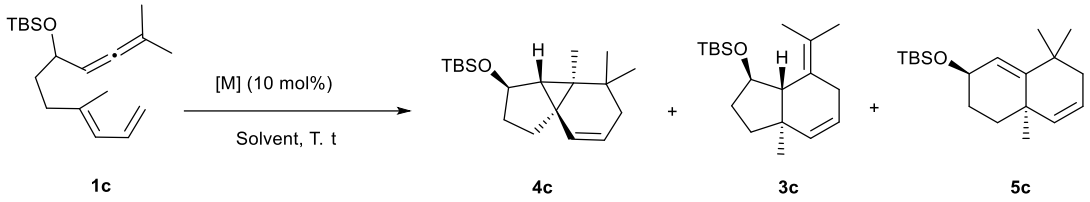
Table S8. Control experiments with *Z*-**1b**[a]



Entry	[M]	Solvent	T (°C)	t (h)	Conv. (%)[b,c]
1	$PtCl_2$	Dioxane	30	12	0
2	$PtCl_2$	Dioxane	100	4	6
3[d]	$PtCl_2$/CO	Cyclohexane	50	12	0
4[d]	$PtCl_2$/CO	Cyclohexane	80	4	0
5	IPrAu-NTf_2	CH_2Cl_2	rt	12	0
6	IPrAu-NTf_2	CH_2Cl_2	40	4	20[d]
7	$(C_6F_5)_3PAuCl/AgNTf_2$	CH_2Cl_2	-15	4	0
8	$(C_6F_5)_3PAuCl/AgNTf_2$	CH_2Cl_2	40	4	14[d]

[a] *Conditions*: Allenediene Z-**1b** was treated with [M] (10 mol%) in the indicated solvent (0.05M) at the indicated temperature (°C) and time (h), unless otherwise noted. [b] Conversion determined by ^{1}H-NMR spectroscopy in the crude reaction mixtures. [c] Isomerization of the *Z*-diene was not detected in the crude NMR. [d] Cyclohexane wet (1 ppm H_2O). [d] **4b**, **3b** and **5b** were not detected in the crude NMR.

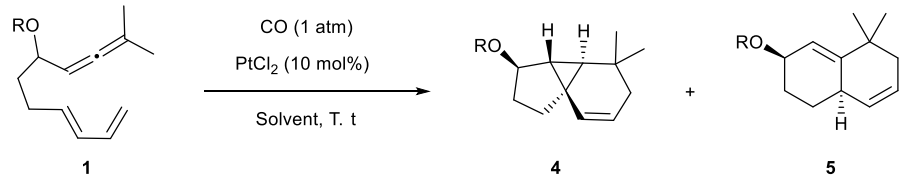
Table S9. Reactivity of the substrate **1c**.[a]



Entry	[M]	Solvent	T (°C)	t (h)	Conv. (%)[b]
1	$PtCl_2$	Dioxane	30	1	0
2	$PtCl_2$	Dioxane	50 to 100	12	>99[c]
3[d]	$PtCl_2$/CO	Cyclohexane	50 to 80	6	<5[e]
5	IPrAu-NTf_2	CH_2Cl_2	rt	1	0
6	IPrAu-NTf_2	$(CH_2)_2Cl_2$	50 to 85	12	>99[c]

[a] *Conditions*: Allenediene **1c** (1.0 eq.), was treated with [M] (10 mol%) in the indicated solvent (0.05M) at the indicated temperature (°C) and time (h), unless otherwise noted. [b] Conversion determined by ^{1}H-NMR spectroscopy in the crude reaction mixtures. [c] A Complex mixture of products was detected in the crude NMR [d] Cyclohexane wet (1 ppm H_2O). [e] Only starting material was observed in the crude NMR.

Table S10. Reactivity of analogs of **1b** with different silyl ethers, using PtCl2/CO (1atm) as catalyst.[a]

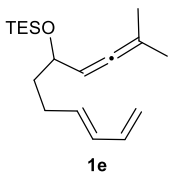


Entry	R (**1**)	T (°C)	t (h)	Conv. (%)	Ratio **4** : **5**[b]	Products (**4** : **5**), yield[c]
1	TBS (**1b**)	50	1.5	>99	1 : 9-	**4b**, 9% **5b**, 80%
2	TES (**1e**)	50	2	>99	1 : 5.2	**4e**, 10% **5e**, 51%
3	TIPS (**1f**)	50	4	99	-1 : 8	**4f**, 10% **5f**, 81%

[a] *Conditions*: Allenediene **1** (1.0 eq.), was treated with $PtCl_2$ (10 mol%) and CO (1 atm) in cyclohexane wet (1 ppm H_2O, 0.05 M), at 50 °C and time (h), unless otherwise noted. [b] Ratio of products determined by ^{1}H-NMR spectroscopy of the crude reaction mixtures.[c] Isolated yield.

Characterization data of allenedienes 1e-1f, and their corresponding annulation products.

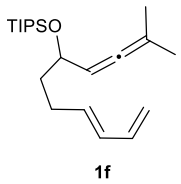
[(E)-Triethyl((2-methylundeca-2,3,8,10-tetraen-5-yl)oxy)silane] (1e)



1e

The allenediene **1e** was synthesized from **S3** following the procedure described for **1b** using TESCl instead of TBSCl: Colorless oil (97% yield). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 6.31 (dt, *J* = 17.0, 10.3 Hz, 1H), 6.06 (dd, *J* = 15.3, 10.4 Hz, 1H), 5.71 (dt, *J* = 14.6, 7.0 Hz, 1H), 5.08 (d, *J* = 17.0 Hz, 1H), 4.97 – 4.91 (m, 2H), 4.07 (d, *J* = 7.3 Hz, 1H), 2.22 – 2.04 (m, 2H), 1.69 (dd, *J* = 5.2, 2.8 Hz, 6H), 1.67 – 1.54 (m, 2H), 0.96 (t, *J* = 7.9 Hz, 9H), 0.61 (qd, *J* = 7.9, 1.5 Hz, 6H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 200.52 (C), 137.42 (CH), 135.06 (CH), 131.23 (CH), 114.77 (CH_2), 96.22 (C), 93.63 (CH), 71.93 (CH), 38.27 (CH_2), 28.77 (CH_2), 20.83 (CH_3), 20.17 (CH_3), 6.99 (CH_3), 5.10 (CH_2). **LRMS** (*m/z*, APCI): 293.23 $[M+H]^+$, 193.16, 161.13. **HRMS-APCI** calculated for $C_{18}H_{33}OSi$ $[M+H]^+$: 293.2295, found 293.2294.

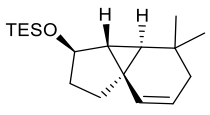
[(*E*)-Triisopropyl ((2-methylundeca-2,3,8,10-tetraen-5-yl)oxy)silane] (1f)



1f

The allenediene **1f** was synthesized from **S3** following the procedure described for **1b** using TIPSCl instead of TBSCl: Colorless oil (92% yield). **^{1}H NMR** (300 MHz, $CDCl_3$) δ 6.31 (dt, *J* = 16.9, 10.2 Hz, 1H), 6.06 (dd, *J* = 15.1, 10.3 Hz, 1H), 5.73 (dt, *J* = 14.6, 6.9 Hz, 1H), 5.08 (d, *J* = 16.6 Hz, 1H), 5.01 – 4.86 (m, 2H), 4.21 (td, *J* = 7.3, 5.2 Hz, 1H), 2.33 – 2.02 (m, 2H), 1.81 – 1.45 (m, 8H), 1.07 (br s, 21H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 200.47 (C), 137.46, (CH) 135.28 (CH), 131.17 (CH), 114.77 (CH_2), 96.11 (C), 93.71 (CH), 72.18 (CH), 38.65 (CH_2), 28.38 (CH_2), 20.95 (CH_3), 20.17 (CH_3), 18.27 (CH_3), 12.58 (CH). **LRMS** (*m/z*, ESI): 335.28 $[M+H]^+$, 327.08, 301.07, 279.09. **HRMS-ESI** calculated for $C_{21}H_{39}OSi$ $[M+H]^+$: 335.2765, found 335.2776.

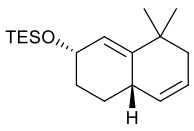
(((3*R,3a*R**,3b*S**,7a*R**)-4,4-dimethyl-2,3,3a,3b,4,5-hexahydro-1H-cyclopenta[1,3]cyclopropa[1,2]benzen-3-yl)oxy)triethylsilane (4e)**



4e

Colorless oil. **^{1}H NMR** (300 MHz, $CDCl_3$) δ 6.08 – 5.88 (m, 1H), 5.36 (ddd, *J* = 9.4, 5.5, 3.5 Hz, 1H), 4.18 (d, *J* = 4.8 Hz, 1H), 2.05 (td, *J* = 11.7, 8.4 Hz, 1H), 1.80 – 1.64 (m, 1H), 1.65 – 1.59 (m, 2H), 1.59 – 1.38 (m, 3H), 1.05 (s, 3H), 1.01 – 0.88 (m, 9H), 0.87 (s, 3H), 0.66 – 0.46 (m, 7H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 130.77 (CH), 121.23 (CH), 74.99 (CH), 36.78 (CH_2), 36.66 (CH), 34.72 (CH), 33.03 (CH_2), 30.67 (C), 30.38 (CH_3), 30.08 (CH_2), 28.57 (CH_3), 28.01 (C), 7.02 (CH_3), 6.96 (CH_3), 6.57 (CH_2), 5.11 (CH_2). **LRMS-IE** (*m/z*, *I*): 292.3 ($[M]^+$, 57), 277.2 (12), 263.2 (19), 217.0 (16), 161.4 (100), 159.4 (98). **HRMS-IE** calculated for $C_{18}H_{32}OSi$ $[M]^{+\cdot}$ 292.2222 found 292.2230.

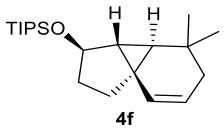
(((2*S,4a*S**)-8,8-dimethyl-2,3,4,4a,7,8-hexahydronaphthalen-2-yl)oxy)triethylsilane (5e)**



5e

Colorless oil. **^{1}H NMR** (300 MHz, $CDCl_3$) δ 5.64 – 5.51 (m, 1H), 5.52 – 5.42 (m, 2H), 4.25 – 4.10 (m, 1H), 2.70 – 2.55 (m, 1H), 2.05 (d, *J* = 17.6 Hz, 1H), 1.86 (dd, *J* = 18.1, 4.9 Hz, 1H), 1.81 – 1.73 (m, 1H), 1.73 – 1.62 (m, 1H), 1.62 – 1.45 (m, 2H), 1.10 (s, 3H), 1.05 (s, 3H), 0.96 (t, *J* = 7.9 Hz, 9H), 0.60 (q, *J* = 7.8 Hz, 6H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 147.83 (C), 130.19 (CH), 124.52 (CH), 119.27 (CH), 65.29 (CH), 41.65 (CH_2), 35.48 (CH), 34.89 (C), 32.01 (CH_2), 27.66 (CH_3), 27.63 (CH_3), 25.17 (CH_2), 7.06 (CH_3), 5.28 (CH_2). **LRMS** (*m/z*, ESI): 293.23 $[M+H]^+$, 265.19, 199.15, 161.13. **HRMS-ESI** calculated for $C_{18}H_{33}OSi$ $[M+H]^+$: 293.2295, found 293.2289.

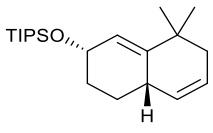
(((3*R,3a*R**,3b*S**,7a*R**)-4,4-dimethyl-2,3,3a,3b,4,5-hexahydro-1H-cyclopenta[1,3]cyclopropa[1,2]benzen-3-yl)oxy)triisopropylsilane (4f)**



4f

Colorless oil. **^{1}H NMR** (300 MHz, $CDCl_3$) δ 5.98 (d, *J* = 9.2 Hz, 1H), 5.36 (ddd, *J* = 9.4, 5.4, 3.7 Hz, 1H), 4.28 (d, *J* = 4.8 Hz, 1H), 2.05 (td, *J* = 11.7, 8.3 Hz, 1H), 1.72 (dd, *J* = 12.0, 8.0 Hz, 1H), 1.67 – 1.57 (m, 3H), 1.54 – 1.38 (m, 4H), 1.06 (br s, 22H), 0.88 (s, 3H), 0.56 (dd, *J* = 4.1, 1.4 Hz, 1H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 130.91 (CH), 121.09 (CH), 75.24 (CH), 36.99 (CH), 36.81 (CH_2), 34.80 (CH), 33.22 (CH_2), 30.57 (C), 30.45 (CH_3), 30.14 (CH_2), 28.61 (CH_3), 28.01 (C), 18.23 (CH_3), 12.42 (CH). **LRMS** (*m/z*, APCI): 335.28 $[M+H]^+$, 321.26, 297.16, 161.14. **HRMS-APCI** calculated for $C_{21}H_{39}OSi$ $[M+H]^+$: 335.2765, found 335.2761.

(((2*S,4a*S**)-8,8-dimethyl-2,3,4,4a,7,8-hexahydronaphthalen-2-yl)oxy)triisopropylsilane (5f)**



5f

Colorless oil. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 5.60 – 5.51 (m, 2H), 5.49 (d, *J* = 9.7 Hz, 1H), 4.33 (dd, *J* = 54.9, 3.5 Hz, 1H), 2.63 (br s, 1H), 2.03 (d, *J* = 17.9 Hz, 1H), 1.92 – 1.80 (m, 2H), 1.75 – 1.62 (m, 1H), 1.63 – 1.49 (m, 2H), 1.10 (s, 3H), 1.06 (s, 18H), 1.05 (s, 3H), 1.05 – 0.97 (m, 8H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 147.40 (C), 130.38 (CH), 124.42 (CH), 119.43 (CH), 65.21 (CH), 41.79 (CH_2), 35.55 (CH), 34.91 (C), 32.12 (CH_2), 27.72 (CH_3), 27.48 (CH_3), 25.13 (CH_2), 18.34 (CH_3), 18.31 (CH_3), 12.71 (CH). **LRMS** (*m/z*, ESI): 335.28 $[M+H]^+$, 313.27, 242.28, 199.15. **HRMS-ESI** calculated for $C_{21}H_{39}OSi$ $[M+H]^+$: 335.2765, found 335.2763.

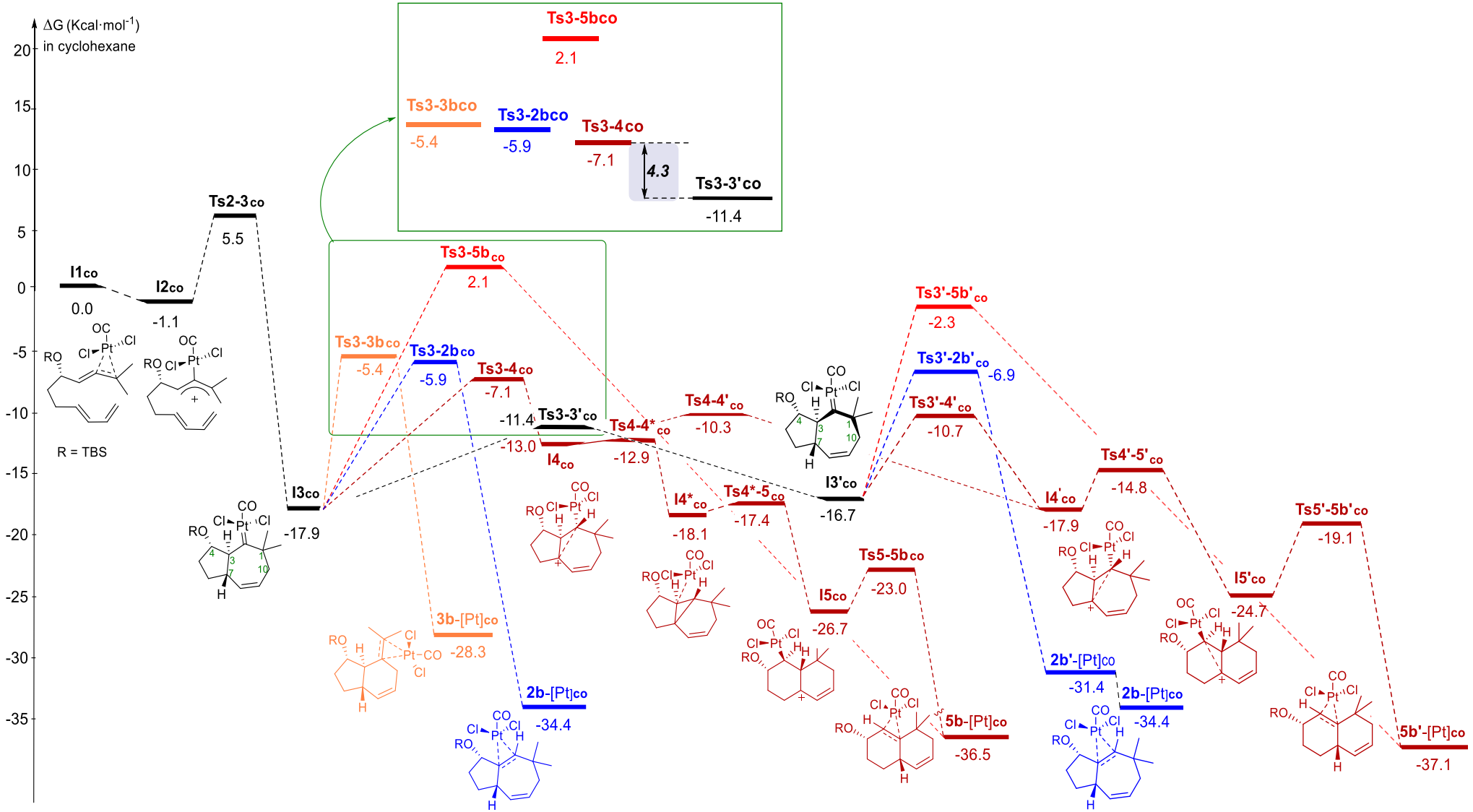
7. Mechanistic Computational Studies

Computational methods

DFT calculations have been carried out with Gaussian 09. [6]The geometries of all complexes were optimized using the B3LYP hybrid functional[7] together with the standard 6-31G(d) basis set for C, H, O, P, Si and Cl and the LANL2DZ basis set for Pt and Au, which includes the relativistic effective core potential (ECP) of Hay and Wadt and employs a split valence (double-zeta) basis set.[8] Using the same level of theory, harmonic vibrational frequencies were calculated in order to characterize the stationary points (Minima – with zero imaginary frequencies- and Transition States – with one imaginary frequency) and determine the zero-point energies (ZPE). The electronic energy values calculated with the smaller basis set have been corrected using the residual energy at the ZPE. The evaluation of Gibbs free energy (G) implies the use of the harmonic-oscillator/rigid rotor approximation, which introduces some uncertainty in the calculation of the vibrational entropy. Connection between all transition states with their corresponding minima were confirmed performing Intrinsic Reaction Coordinate (IRC) studies. Single-point calculations of the optimized systems were carried out using the hybrid functional M06 of Truhlar and Zhao[9] together with the 6-311++g(d,p) basis set for C, H, O, P, Si and Cl and the Stuttgart-Dresden (SDD) ECP for Pt and Au.[10] In this case, a self-consistent reaction field (SCRF) method using the SMD model[11]has been employed in order to obtain the solvation-corrected relative free-energies, using as solvent cyclohexane (ε=2.0165) for the calculations with Pt and dichloromethane (ε=8.93) for the calculations with Au. In order to characterize better some key species, Natural Bond Orbital (NBO) analysis and the determination of the Wiberg bond indices (WBI) have been carried out, calculating the Laplacian of the electron density distribution and the Bond Critical Points (BCP) with the Multiwfn program. [12]

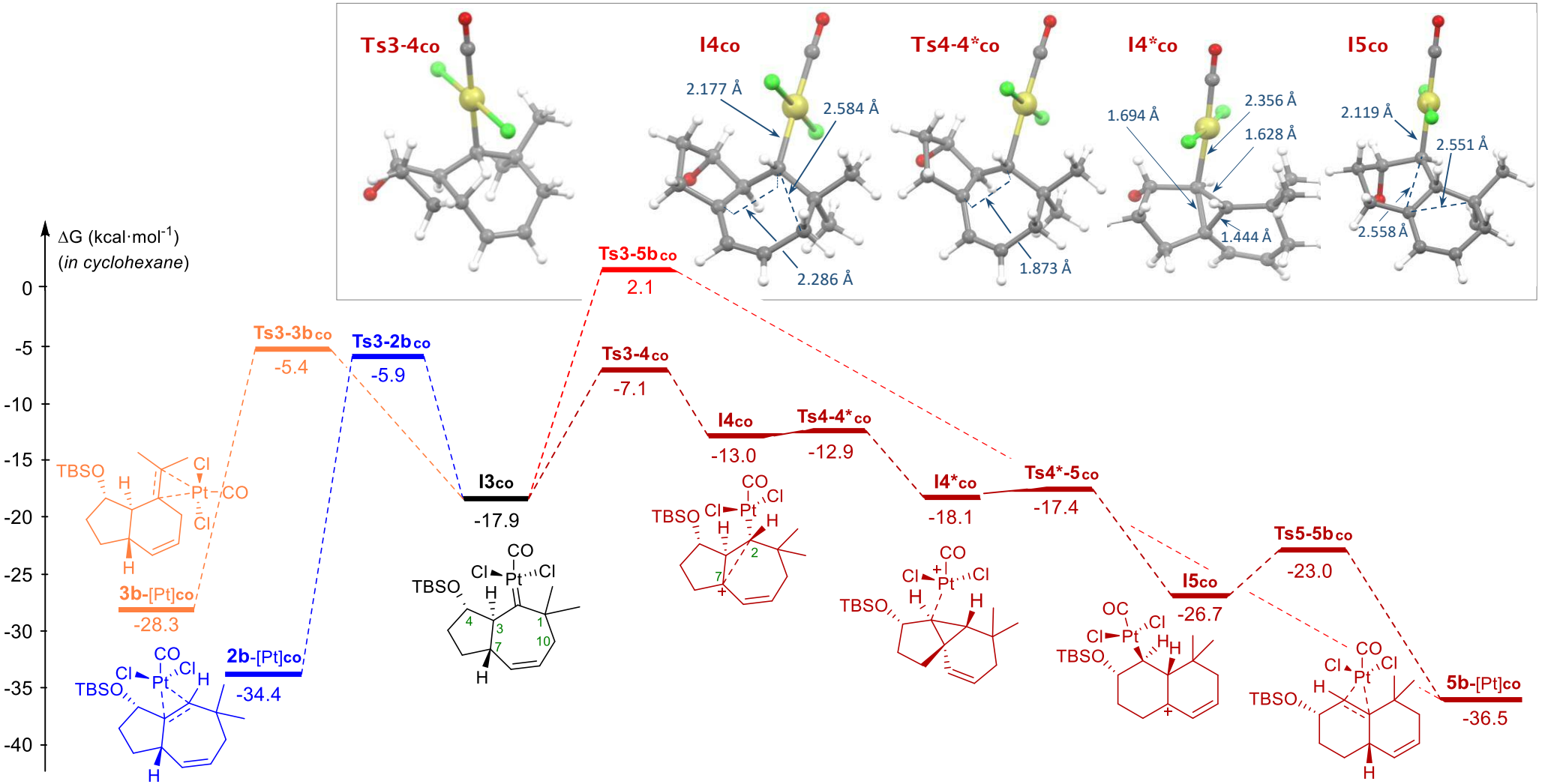
Figure S8. Gibbs energy profile of **1b** using $PtCl_2(CO)$ as catalyst in cyclohexane, involving a *pseudo*-axial conformation of the OTBS group

Fig. S8A) Complete reaction profile



NOTE: As can be deduced from Figure S8, products **5b** and **2b** are respectively obtained as two different conformers from $\mathbf{I3}_{co}$ and $\mathbf{I3'}_{co}$ (**5b**/ **5b'** and **2b**/**2b'**; ($\Delta\Delta G$ = 0.6 and 3.0 kcal·mol^{-1}, respectively) For the sake of simplicity, in the manuscript (Figure 3), we just considered the most stable conformers of each type of product, and were denoted as $\mathbf{5b\text{-}[Pt]}_{co}$, $\mathbf{2b\text{-}[Pt]}_{co}$.

Fig. S8B) Extract of the Gibbs energy profile (kcal mol^{-1}) of the reaction of **1b** with $PtCl_2(CO)$ in cyclohexane corresponding to the different pathways available from **I3$_{co}$** (energy of **I1$_{co}$**, Fig. S8A, is considered as the reference). Optimized structures of selected stationary points (TBS omitted for clarity).



NOTE: As can be deduced from Figure S8, we also found an exergonic pathway towards **5b** from carbene intermediate **I3$_{co}$**. However, the evolution of conformer **I3$_{co}$** to **I3'$_{co}$** is significantly more favored as it involves an activation barrier of only 6.5 kcal·mol^{-1}, 4.3 kcal·mol^{-1} lower than that associated to the formation of **I4$_{co}$** from **Ts3-4$_{co}$** (Fig. S8A).

Also relevant, the energy barriers associated to the formation of the cycloadducts **3b** and **2b** (via **Ts3-3b$_{co}$** and **Ts3-2b$_{co}$**), are very close to that of **Ts3-4$_{co}$**, ($\Delta\Delta G^{‡}$ = 1.7 and 1.2 kcal·mol^{-1}, respectively). Therefore, this path from **I3$_{co}$** towards **5b** would not provide a fully consistent explanation of the experimentally observed selectivity.

Nonetheless, since the pathway from **I3$_{co}$** to **5b** is mechanistically relevant, the key features are discussed below:

1) Similarly to the pathway from **I3'$_{co}$**, the pathway from **I3$_{co}$** starts with the migration of the hydrogen at C7 to the Pt-carbene center (C2) to give the non-classical carbocation cationic intermediate **I4$_{co}$** also stabilized by homohyperconjugation, like its conformer **I4'$_{co}$**. The HOMO-1 molecular orbital of **I4$_{co}$** (NBO analysis) also shows that it is this hyperconjugation, rather than an hypothetical allyl-cation conjugation, the one that accounts for the relative stability of **I4$_{co}$** (Figure S11). Also consistent with the homohyperconjugation, the C2–C7 distance in **I4$_{co}$** (2.286 Å) is significantly shorter than that between C2 and C10 (2.584 Å, Figure S11).

2) The atoms in molecules (AIM) topological analysis of **I4$_{co}$** also confirms this bonding pattern, providing for C2 a sum of Wiberg bond indexes (WBIs) of 3.9, a value which is divided into five different bonds. Thus, this analysis provided WBIs of 0.20 and 0.54 for the critical C2–C7 and C2–Pt bonds, whereas those of C2–C3 and C3–C7 bonds are noticeably higher, of 0.87 and 1.10, respectively (Figure S11).

3) Intermediate **I4$_{co}$** undergoes a skeletal rearrangement to the 6,6-bicyclic system **I5$_{co}$**, but in this case through a stepwise process involving a cyclopropyl-like intermediate **I4*$_{co}$**. This species is formed through an early transition state (**Ts4-4*$_{co}$**) in which the Pt, C2, C3, C7 atoms adopt, together with the p orbital of C7, a W-shape conformation. In the evolution of **I4$_{co}$** to **I4*$_{co}$** the C2–C7 bond is formed with net inversion of configuration at C2, and the Pt center migrates stereospecifically from C2 to C3, like it does in **TS4'-5'$_{co}$**. In the cyclopropyl-platinum intermediate **I4*$_{co}$**,the three different C–C bonds of the cyclopropyl ring are mostly, but not completely formed (see Figure S11 for C–C bond distances and WBI and Laplacian electron density map).

4) Remarkably, we were not able to computationally locate the cyclopropyl adduct (**4b**) resulting from decoordination of the Pt complex from **I4*$_{co}$** (either via associative or dissociative mechanisms). We only found a viable evolution towards **I5$_{co}$** (via **Ts4*-5$_{co}$**).

5) **I5$_{co}$** eventually provides the final cycloadduct through a 1,2-hydride migration from C2 to C7, similarly to that described in the manuscript for **I5'$_{co}$** (Figure 3 and S8). The higher stability of **I5$_{co}$** compared to **I4*$_{co}$** (8.6 kcal·mol^{-1}) seems to be the consequence of the release of the ring strain, since the NBO analysis of **I5$_{co}$** revealed that there is not homohyperconjugation. Indeed, the C7-C3 distance in **I5$_{co}$** (2.558 Å) is basically equal to that of the C7–C1 bond (2.551 Å, Figures S8B and S11). This lack of homo-hyperconjugation in **I5$_{co}$** contrasts with that found for **I5'$_{co}$** and it might be behind the direct formation of biscyclohexyl structure **I5'$_{co}$** from **I4'$_{co}$**, without the intermediacy of cyclopropyl species like **I4*$_{co}$**.

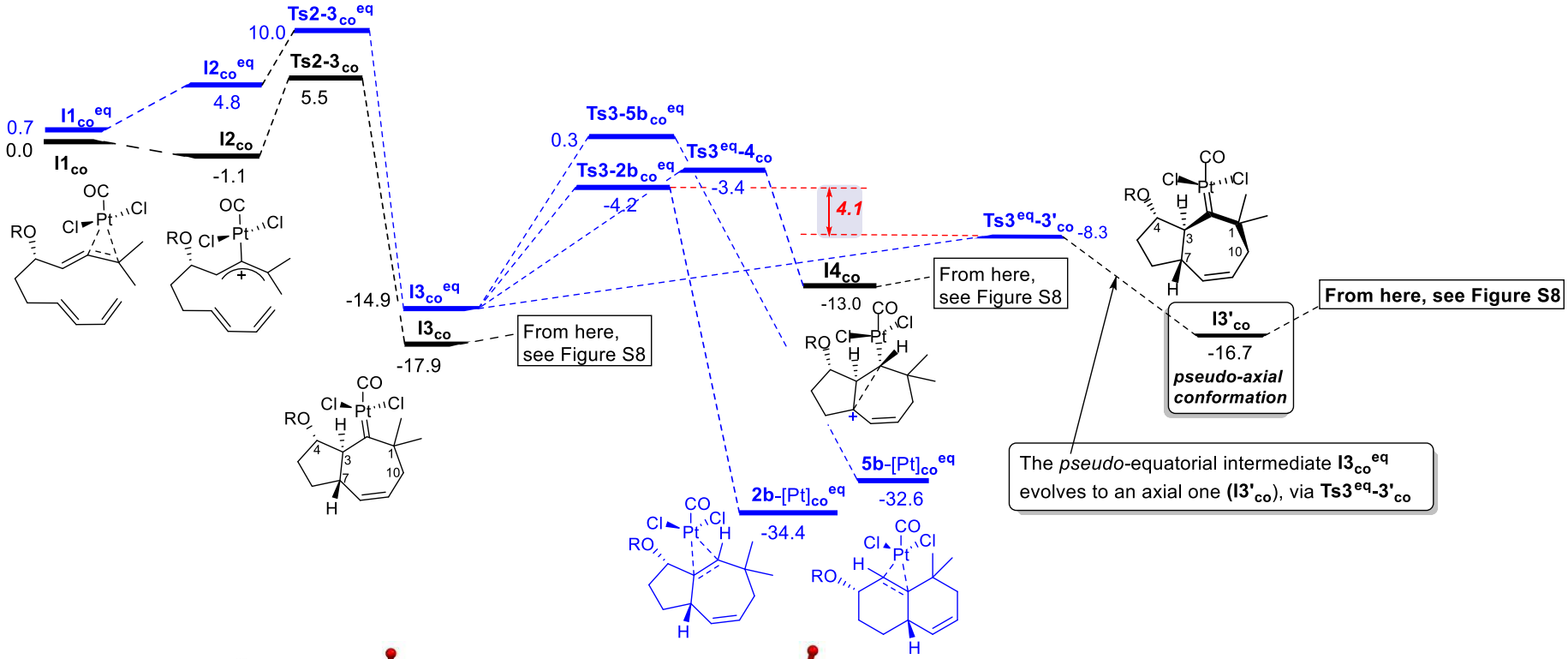
6) The barrier between **I3'$_{co}$** and **I4'$_{co}$** is significantly lower than that for the homologous step from **I3$_{co}$** to **I4$_{co}$** ($\Delta\Delta G^{‡}$ = 4.8 kcal·mol^{-1}, see Figure 8). Moreover, the energy of **I4'$_{co}$**, is also 4.9 kcal·mol^{-1} lower than that of **I4$_{co}$**. These energy differences might be associated to the higher stabilization (due to a better homohyperconjugation) of the carbocation that is generated at C7. Indeed, the energy of the HOMO-1 in **I4'$_{co}$** is 0.1 eV lower than that of **I4$_{co}$**, while all other HOMO and HOMO-*n* orbitals of **I4$_{co}$** and **I4'$_{co}$** have very close energies.

Figure S9. A) Comparison of the profiles of *pseudo*-equatorial (blue pathway) and *pseudo*-axial conformers (black pathway); B) Transition state structures **Ts3^{eq}-4$_{co}$** and **Ts3^{eq}-3'$_{co}$** that connect the *pseudo*-equatorial conformers with the axial ones (via **I4$_{co}$** and **I3'$_{co}$**).

Note: For simplicity, the *pseudo*-axial stationary points are denoted as **In$_{co}$**, and **Ts*n*-*m*$_{co}$**, instead of **In$_{co}^{ax}$** , and **Ts*n*-*m*$_{co}^{ax}$** (*n,m*= numbers)

Comments: a) The lowest energy barrier links the *pseudo*-equatorial intermediate **I3$_{co}^{eq}$** with the axial **I3'$_{co}$** ; b) The *pseudo*-equatorial intermediate **I3$_{co}^{eq}$** evolves to an axial one (**I4$_{co}$**), via **Ts3^{eq}-4$_{co}$**. c) A 1,2-C(10) migration from **I3$_{co}^{eq}$** towards **3b** was not located.

A



B

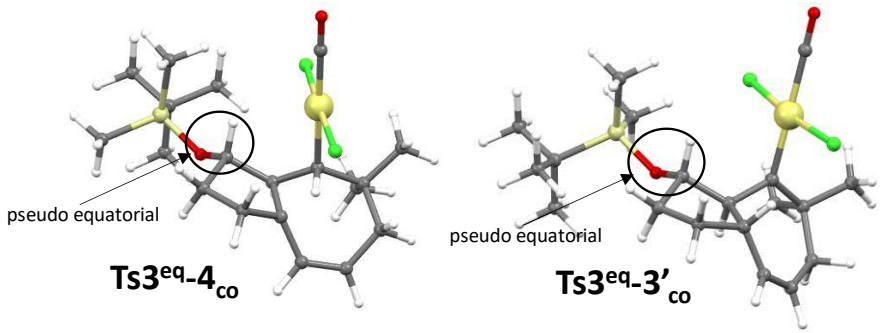


Figure S10. A) Wiberg bond index matrix for **I4'$_{CO}$** and **I5'$_{co}$**; B) Laplacian electron density (**I4'$_{CO}$**, and **I5'$_{co}$**)

A

Wiberg bond index matrix for **I4'$_{co}$**			
	C2	C3	C7
C2	-	0.8951	0.1815
C3	0.8951	-	1.0667
C7	0.1815	1.0667	-
Pt	0.5201	-	-

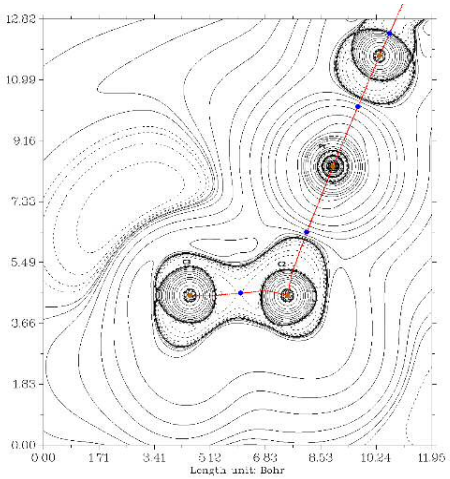
Wiberg bond index matrix for **I5'$_{co}$**			
	C2	**C3**	**C7**
C2	-	0.8607	1.1001
C3	0.8607	-	0.1508
C7	1.1001	0.1508	-
Pt	0.0133	0.5598	-

Wiberg bond index by atom (**I4'co**)			
C2	C3	C7	Pt
3.9080	3.9611	3.8811	3.1575

Wiberg bond index by atom for **I5'$_{co}$**			
C2	**C3**	**C7**	**Pt**
3.9593	3.8999	3.8755	3.1589

B

I4'co



I5'co

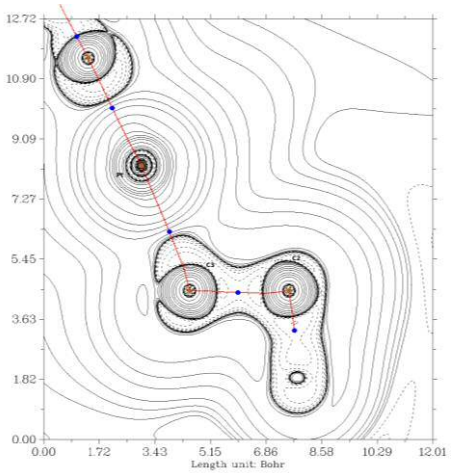
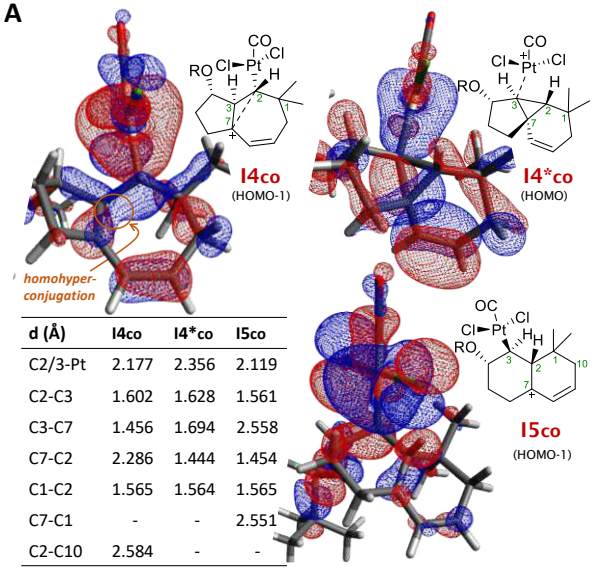


Figure S11. A) Key distances and representation of HOMO s of **I4$_{co}$**, **I4*$_{co}$** and **I5$_{co}$**; B) Wiberg bond index matrix for **I4$_{CO}$** and **I4*$_{co}$**; C) Laplacian electron density (**I4*$_{co}$**)

A



d (Å)	I4co	I4*co	I5co
C2/3-Pt	2.177	2.356	2.119
C2-C3	1.602	1.628	1.561
C3-C7	1.456	1.694	2.558
C7-C2	2.286	1.444	1.454
C1-C2	1.565	1.564	1.565
C7-C1	-	-	2.551
C2-C10	2.584	-	-

B

Wiberg bond index matrix of **I4$_{co}$**			
	C2	C3	C7
C2	-	0.8744	0.1988
C3	0.8744	-	1.0923
C7	0.1988	1.0923	-
Pt	0.5407	0.0103	-

Wiberg bond index matrix of **I4*$_{co}$**			
	C2	C3	C7
C2	-	0.7938	1.0679
C3	0.7938	-	0.6863
C7	1.0679	0.6863	-
Pt	0.0422	0.2822	-

Wiberg bond index by atom **I4co**			
C2	C3	C7	Pt
3.892	3.960	3.842	3.171

Wiberg bond index by atom for **I4*$_{co}$**			
C2	C3	C7	Pt
3.931	3.882	3.975	3.149

C

Laplacian electron density with bond critical points of **I4*$_{co}$**

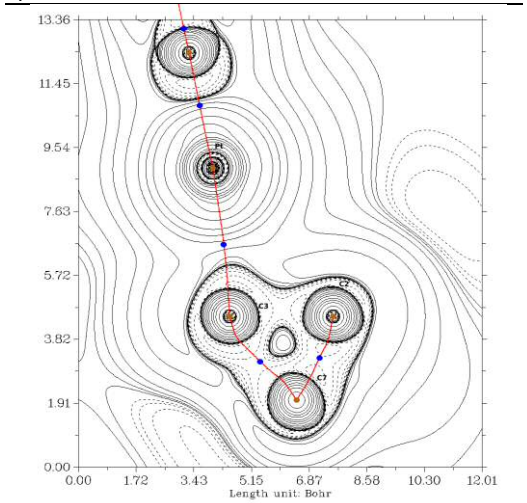
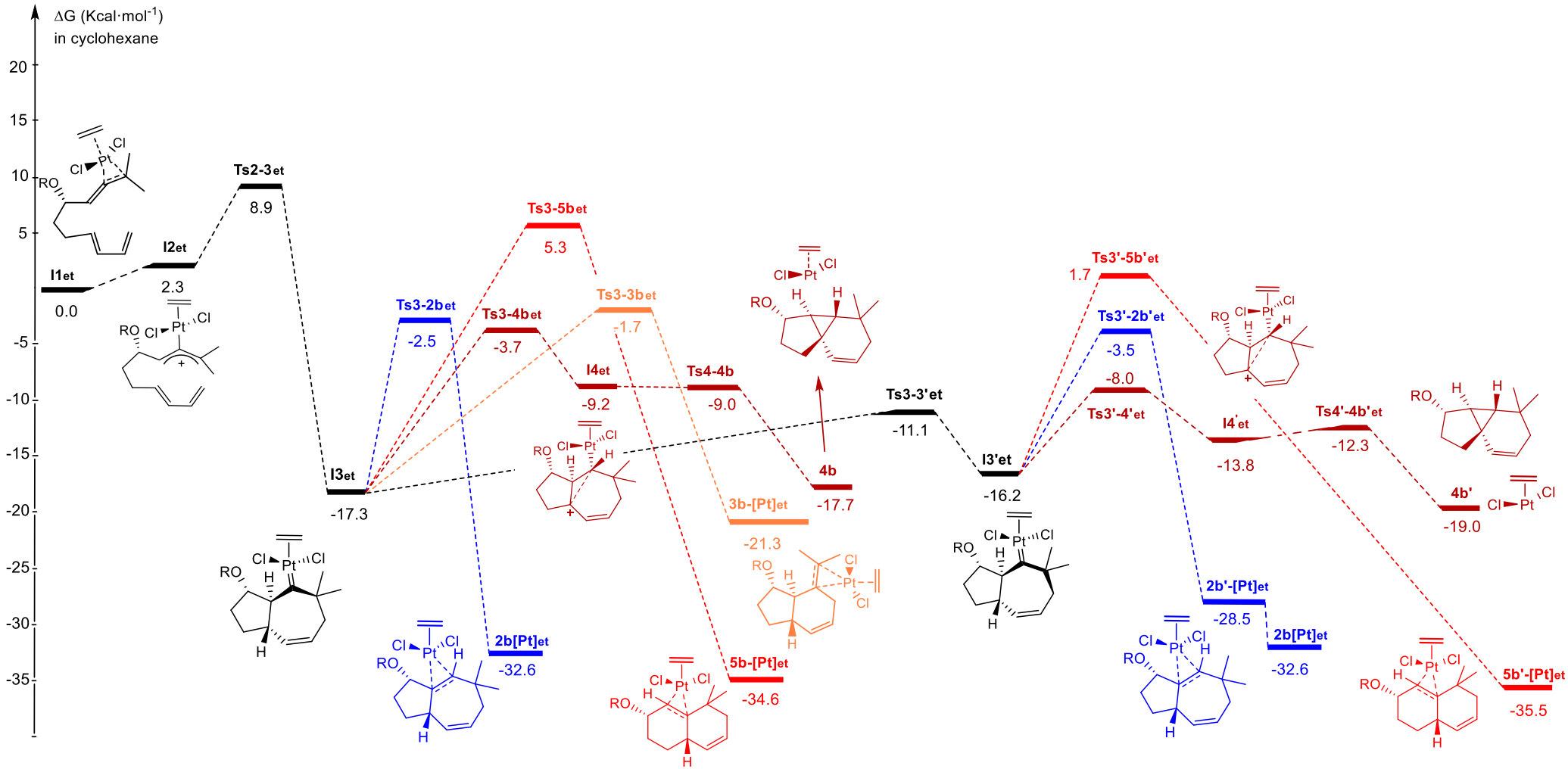
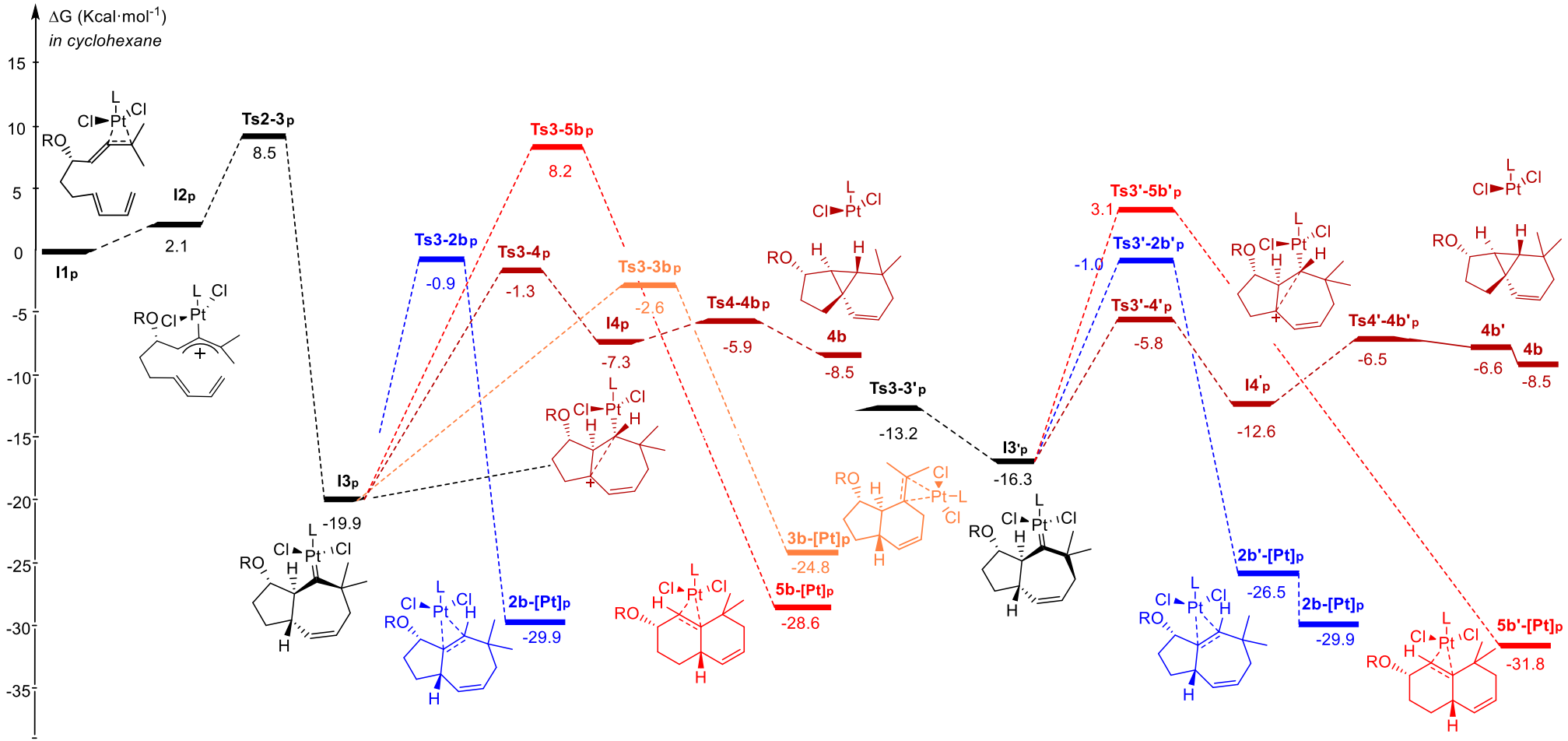


Figure S12. Gibbs energy profile (kcal·mol^{-1}) for the reaction of **1b** catalyzed by $PtCl_2$(ethene) in cyclohexane (SMD model). **NOTE**: Notably, the second preferred pathway also delivers **4b** from **I3$_{et}$**, but with a highest energy barrier of 13.6 kcal·mol^{-1},(via **Ts3-4b$_{et}$**), further supporting the experimental selectivity towards **4b** with this catalyst



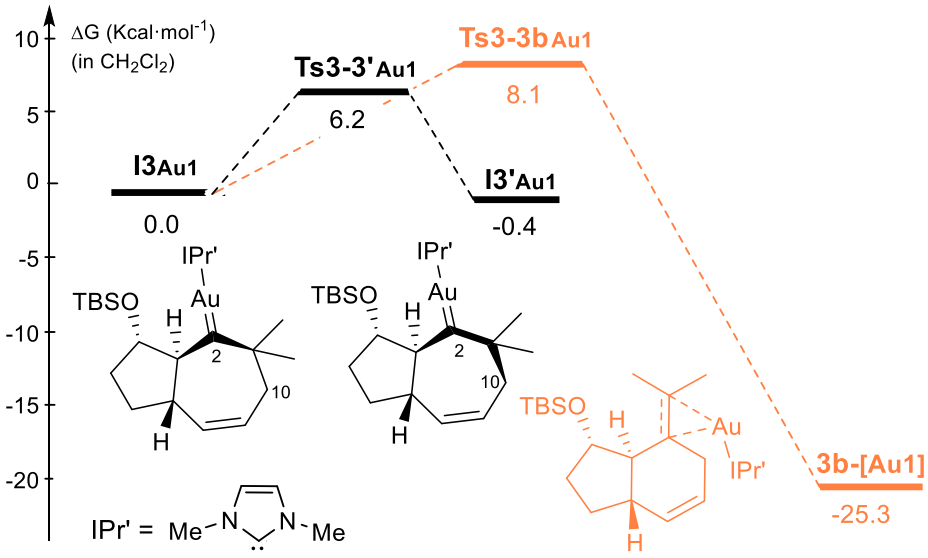
NOTE: As can be deduced from Figure S12, products of type **5b**, **4b** and **2b** are respectively obtained as two different conformers (**5b**/**5b'**, **4b**/**4b'** and **2b**/**2b'**; ΔΔG = 0.9, 1.3 and 3.9 kcal·mol^{-1}, respectively). For the sake of simplicity, in the manuscript (Figure 5), we just considered the most stable conformers, which were denoted as **5b-[Pt]$_{et}$** , **2b-[Pt]$_{et}$** and **4b-[Pt]et** .

Figure S13. Gibbs energy profile (kcal·mol^{-1}) for the reaction of **1b** catalyzed by $PtCl_2P(C_6F_5)_3$ in cyclohexane (SMD model) [L = $P(C_6F_5)_3$, R = TBS].



NOTE: As can be deduced from Figure S13, products of type **5b**, **4b** and **2b** are respectively obtained as two different conformers (**5b**/**5b'**, **4b**/**4b'** and **2b**/**2b'**; ΔΔG = 1.9, 3.2 and 3.4 kcal·mol^{-1}, respectively).

Figure S14 . Key steps of the Gibbs energy profile for the reaction of **1b** catalyzed by [IPr'-Au]$^+$, in CH_2Cl_2.



NOTE: The theoretical analysis with [IPr'Au]$^+$ (Figure S14), a simplistic model of the *N*-heterocyclic carbene gold-complexes **Au1** and **Au6** (Table 1, entries 1 and 5, main manuscript), shows how the energy barrier for the 1,2-alkyl (C10) migration leading to the formal [4 + 2] adduct **3b** increases up to 8.1 kcal·mol^{-1}, so that the conformational change from **I3$_{Au1}$** to **I3'$_{Au1}$** becomes favored by almost 2.0 kcal·mol^{-1} (Figure S14). These relative values are in agreement with the lower proportion of [4+2] adducts with gold complexes bearing σ-donating NHC-ligands (e.g. **Au1** or **Au6**), and the preferential evolution towards cyclopropyl tricyclic product **4b.**

Figure S15 First steps of the energy profile with malonate **1d,** considering both conformers at the connecting tether (denoted as *axial* and *equatorial* in homology to those of **1b**)

NOTE: For simplicity reasons the pseudo-axial stationary points **In$_m^{ax}$** , and **Ts n-m^{ax}** (n,m = any number) are denoted in the manuscript as **In$_m$**, and **TSn$_m$**

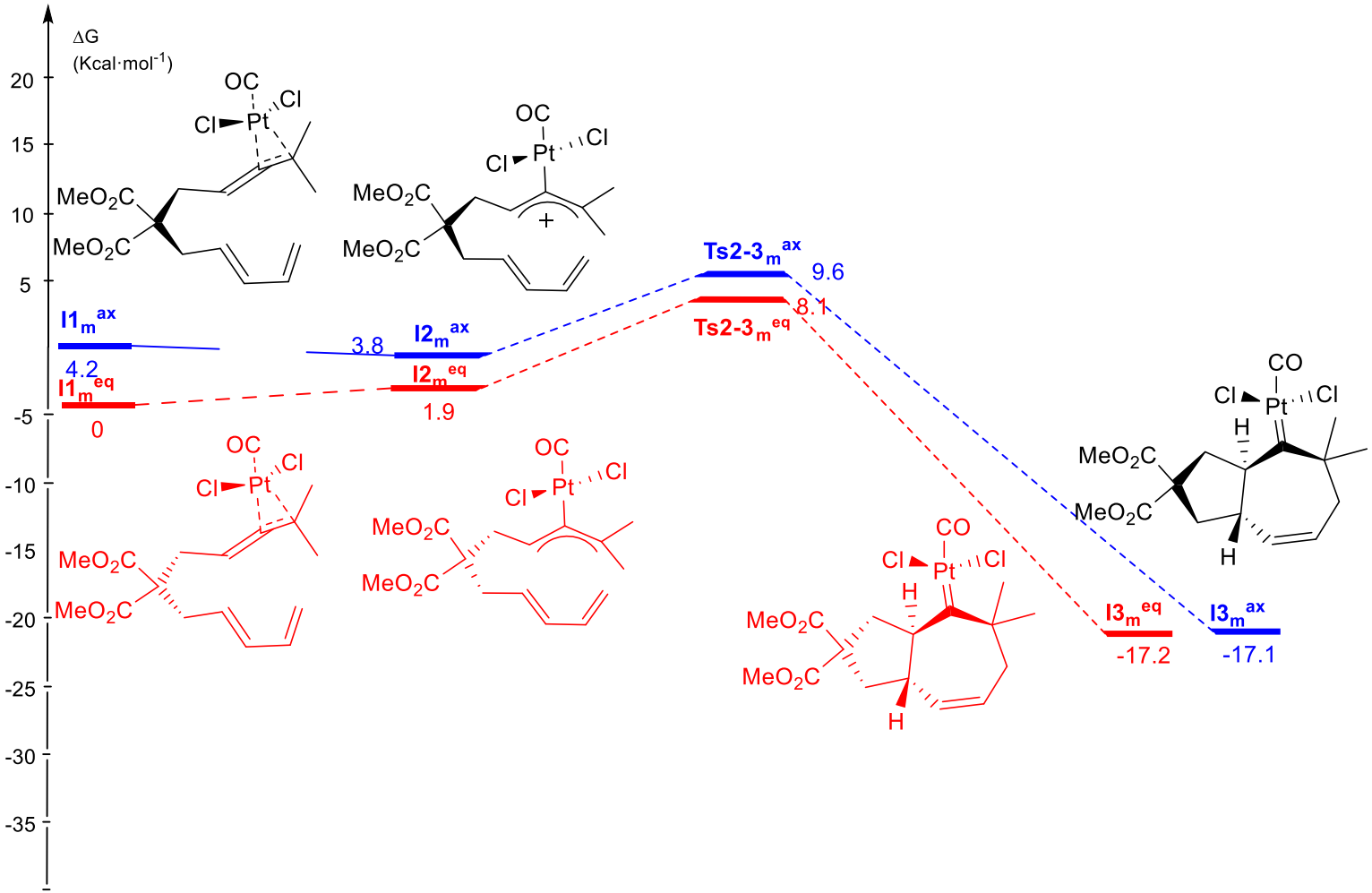
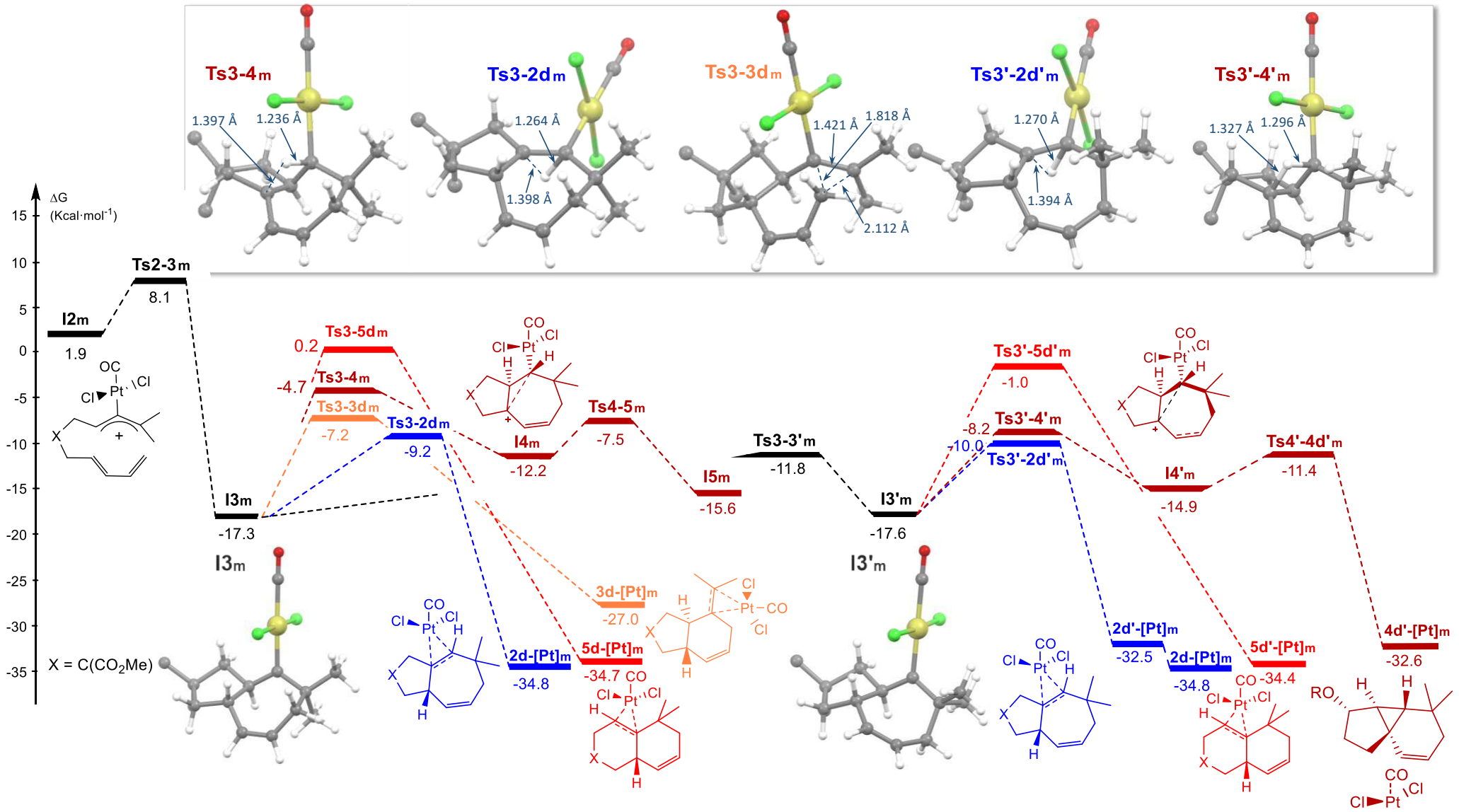


FIGURE S16. Energy profile for the malonate-bearing precursor **1d,** using the more stable *pseudo*-equatorial conformer (energy of **I1$_m^{eq}$**, Fig. S15, considered as reference)



NOTE: As can be deduced from Figure S16, products of type **5d** and **2d** are respectively obtained as two different conformers (**5d**/**5d'** and **2d**/**2d'**; ΔΔG = 0.3 and 2.3 kcal·mol^{-1}, respectively). For simplicity, in the manuscript (Figure 7), we just considered the most stable conformers, which were denoted as **5d-[Pt]$_m$** and **2d-[Pt]$_m$**..

Figure S17. Comparison of key energy barriers towards **2** and **5** on substrates **1b** and **1d** from intermediates **I3$_{co}$** and **I3$_{m}$**

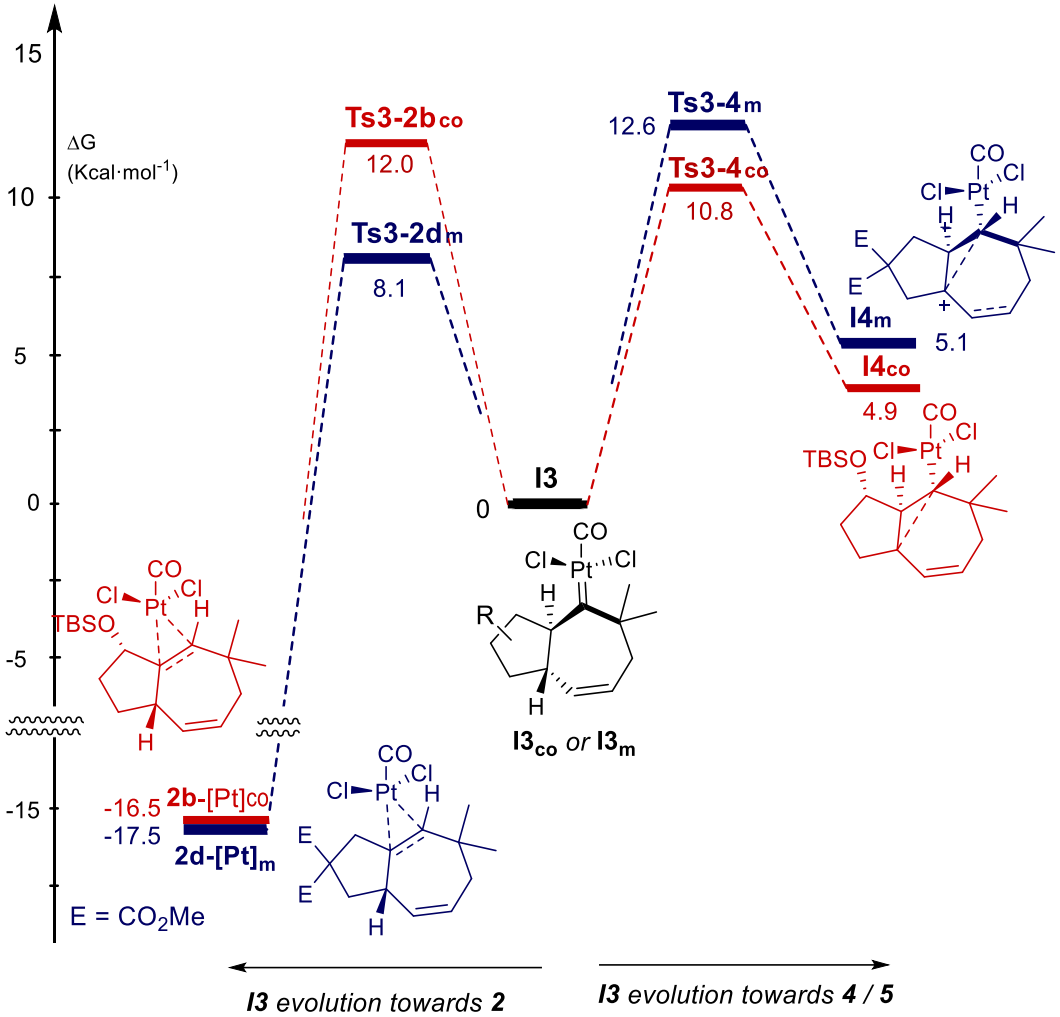
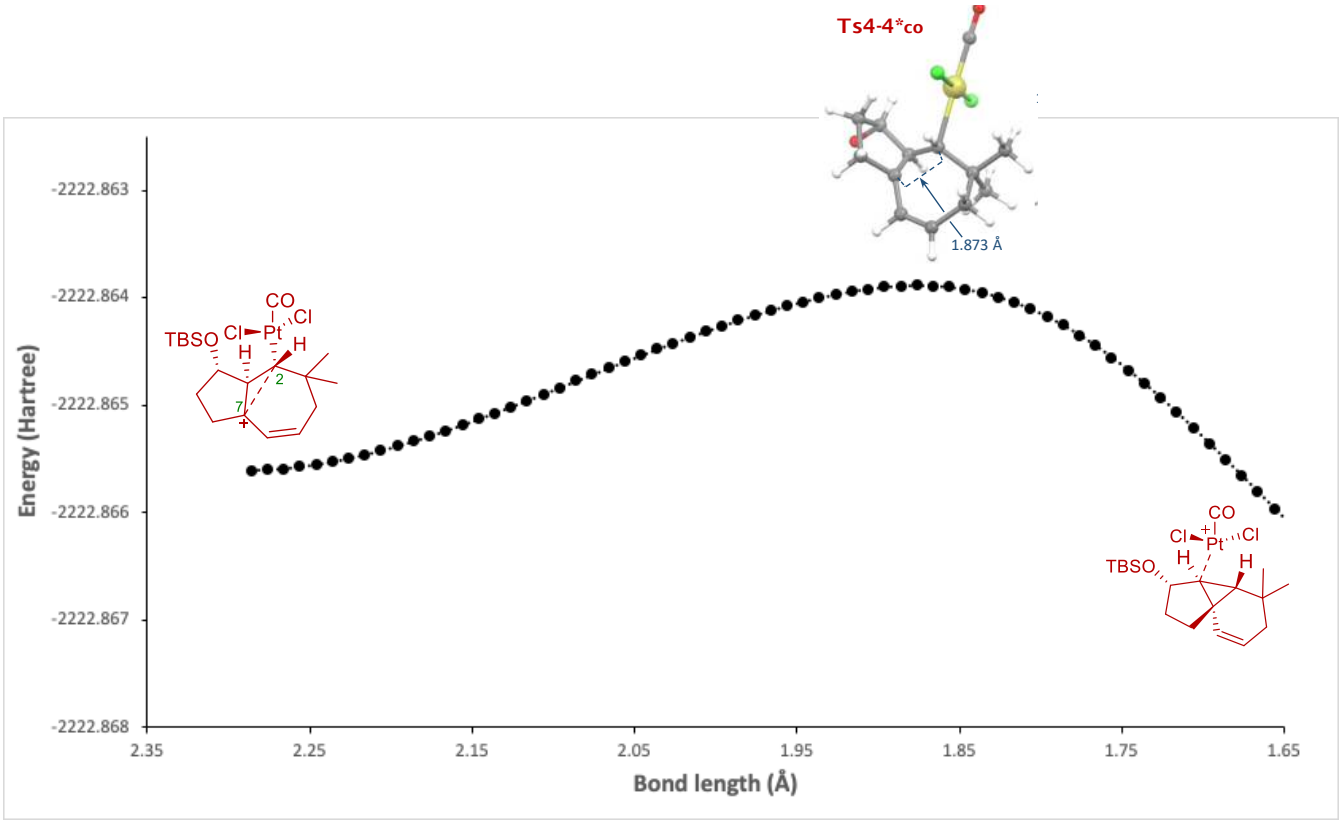
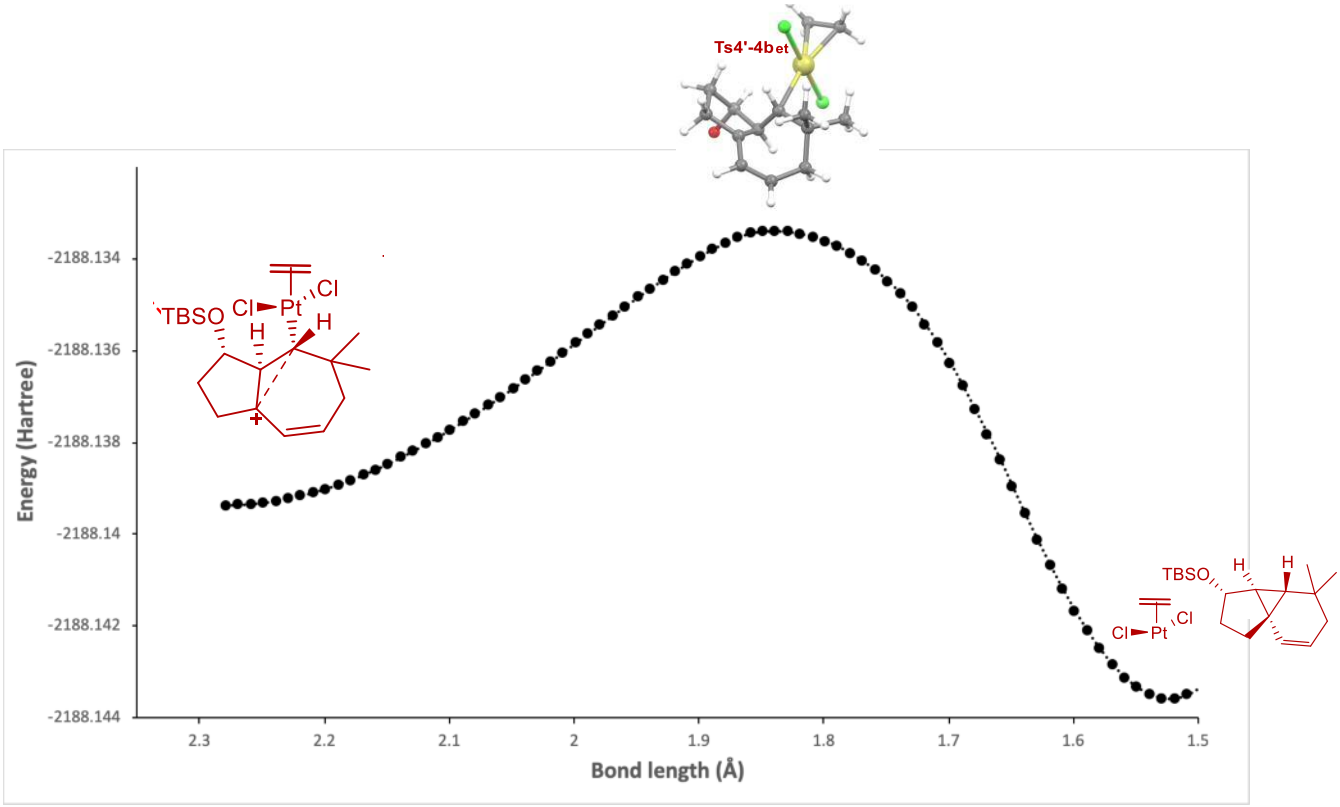


Figure S18. Relaxed Scan analysis of key intermediates **I4$_{co}$** and **I4$_{et}$**

Relaxed scan analysis was carried out to confirm the different evolution of intermediates **I4$_{co}$** an **I4$_{et}$**, respectively affording **I4*$_{co}$** and **4b**





7.1 Cartessian Coordinates

1b-$PtCl_2$(CO)

$I1_{CO}$

Zero-point correction= 0.469851 (Hartree/Particle)
Thermal correction to Energy= 0.505622
Thermal correction to Enthalpy= 0.506566
Thermal correction to Gibbs Free Energy= 0.396911
Sum of electronic and zero-point Energies= -2222.375650
Sum of electronic and thermal Energies= -2222.339880
Sum of electronic and thermal Enthalpies= -2222.338935
Sum of electronic and thermal Free Energies= -2222.448590
HF (M06/6-311++g(d,p) and SDD, SMD(cyclohexane): -2222.65879124

C -2.441158 -2.497374 -1.373810
Si -3.451375 -1.024672 -0.756780
C -4.142854 -1.327923 1.005023
C -4.931656 -0.085970 1.474344
O -2.496639 0.366936 -0.716924
C -1.093814 0.512223 -0.897709
C -0.820852 1.479210 -2.068734
C -1.463351 2.875741 -1.955569
C -0.812746 3.798557 -0.962539
C -1.467707 4.527848 -0.042992
C -0.861366 5.481661 0.895176
C 0.288543 6.149729 0.723088
C -0.498254 0.978032 0.415450
C 0.648795 0.619345 0.958218
Pt 2.044218 -0.809270 -0.070609
Cl 0.982115 -2.682727 0.962165
C 1.599249 0.646015 1.939312
C 1.489324 -0.225674 3.167947
C 2.672892 1.707734 1.984148
C 2.961586 -2.026620 -1.219333
O 3.499555 -2.752830 -1.913401
Cl 3.062615 0.990344 -1.270504
C -4.847156 -0.650478 -1.973232
C -5.084935 -2.552242 1.000418
C -2.985971 -1.589778 1.992963
H 0.670993 6.822178 1.485567
H 0.878156 6.058087 -0.185771
H 0.274073 3.877229 -1.024068
H -1.098211 1.704613 0.962758
H -0.637629 -0.451207 -1.159388
H 3.651319 1.278821 2.224643
H 2.404313 2.391420 2.802977
H 2.741080 2.272220 1.056731
H 0.728404 -0.996640 3.065131
H 1.224292 0.437398 4.004674
H 2.448908 -0.692568 3.413677
H -2.531991 2.773568 -1.735509
H -1.393043 3.339990 -2.951932
H -1.208312 0.992079 -2.973055
H 0.265690 1.568750 -2.192529
H -2.548313 4.401418 0.041760
H -1.429550 5.662594 1.808629
H -3.073973 -3.391385 -1.434313
H -2.049403 -2.312920 -2.382092
H -1.592824 -2.735591 -0.722432
H -5.389774 0.259751 -1.693991
H -4.442134 -0.496269 -2.980567
H -5.573962 -1.469777 -2.029956
H -4.566679 -3.469720 0.695071
H -5.486811 -2.727798 2.008992
H -5.942389 -2.411816 0.330739
H -2.403224 -2.478185 1.722588
H -2.291028 -0.743275 2.037504
H -3.379951 -1.750200 3.007597
H -4.305353 0.813738 1.477457
H -5.800520 0.113906 0.835243
H -5.307045 -0.234482 2.497620

$I2_{CO}$

Zero-point correction= 0.470640 (Hartree/Particle)
Thermal correction to Energy= 0.505736
Thermal correction to Enthalpy= 0.506680
Thermal correction to Gibbs Free Energy= 0.399964
Sum of electronic and zero-point Energies= -2222.378953
Sum of electronic and thermal Energies= -2222.343857
Sum of electronic and thermal Enthalpies= -2222.342913
Sum of electronic and thermal Free Energies= -2222.449629
HF (M06/6-311++g(d,p) and SDD, SMD(cyclohexane): -2222.66365896

C -0.421085 0.772384 0.361875
H -1.063562 1.522960 0.813525
C -1.107136 -0.006378 -0.721690
H -0.806117 -1.057653 -0.592928
C -0.042316 2.759243 -1.635933
C -0.688391 0.398161 -2.156247
C -0.935069 1.886942 -2.463163
H -1.260810 -0.234822 -2.843972
H 0.373211 0.159987 -2.286445
H -0.719503 2.045377 -3.530265
H -1.990140 2.134848 -2.301846
C -0.463755 3.729920 -0.794884
H -1.533755 3.936161 -0.741619
C 0.855694 0.542364 0.857446
C 1.251147 1.216297 2.024691
C 2.661476 1.104554 2.514648
H 2.892011 1.847043 3.284401
H 2.798612 0.104599 2.953398
H 3.371380 1.178132 1.684991
C 0.331938 1.942375 2.964753
H 0.300989 1.378021 3.908988
H 0.745430 2.927304 3.205882
H -0.692900 2.058953 2.615163
Pt 2.111869 -0.819986 -0.052249
Cl 3.291970 0.988519 -1.106024
Cl 0.876028 -2.539258 1.075201
C 3.275390 -2.136854 -0.897208
O 3.954586 -2.910745 -1.392344
H 1.025297 2.564204 -1.733197
C 0.385925 4.537976 0.079192
H -0.111604 5.378391 0.563194
C 1.686356 4.323094 0.354790
H 2.227255 4.991770 1.018909
H 2.252765 3.504136 -0.080957
O -2.512111 0.156423 -0.579246
Si -3.549246 -0.969405 0.151625
C -3.049323 -1.218185 1.956774
H -2.020801 -1.594188 2.025041
H -3.109452 -0.288903 2.535755
H -3.696882 -1.955814 2.446652
C -3.423181 -2.622603 -0.753828
H -4.125928 -3.353777 -0.335403
H -3.640488 -2.525493 -1.823727
H -2.418146 -3.049884 -0.651575
C -5.277013 -0.169270 -0.019931
C -5.281754 1.221662 0.650545
H -4.545525 1.891473 0.192034
H -6.270698 1.692011 0.548112
H -5.061265 1.161220 1.723671
C -5.636743 -0.007112 -1.512608
H -4.906536 0.618305 -2.038551
H -5.683985 -0.973700 -2.028422
H -6.622513 0.468775 -1.618925
C -6.335569 -1.063726 0.662196
H -7.334385 -0.614539 0.564478
H -6.384522 -2.062322 0.210380
H -6.139114 -1.189927 1.734099

TS2-3_{CO}

Zero-point correction= 0.473094 (Hartree/Particle)
Thermal correction to Energy= 0.505988
Thermal correction to Enthalpy= 0.506932
Thermal correction to Gibbs Free Energy= 0.407169
Sum of electronic and zero-point Energies= -2222.372663
Sum of electronic and thermal Energies= -2222.339769
Sum of electronic and thermal Enthalpies= -2222.338824
Sum of electronic and thermal Free Energies= -2222.438587
HF (M06/6-311++g(d,p) and SDD, SMD(cyclohexane): -2222.66028272

C -0.416163 0.941126 0.145513
H -1.094370 1.636900 0.629885
C -1.138235 0.072764 -0.867125
H -0.828823 -0.969157 -0.709953
C 0.171149 2.578493 -1.522113
C -0.791942 0.465382 -2.319001
C -0.818613 1.995527 -2.480213
H -1.497897 -0.025941 -2.996441
H 0.214468 0.097252 -2.549217
H -0.524463 2.252009 -3.508749
H -1.826065 2.391167 -2.310405
C -0.021900 3.680880 -0.716783
H -0.980363 4.197620 -0.758794
C 0.854312 0.727108 0.673630
C 1.279081 1.498189 1.798408
C 2.607712 1.170200 2.440257
H 2.929296 1.952375 3.135423
H 2.484135 0.240815 3.015087

H 3.390504 0.987945 1.700268
C 0.299066 2.148493 2.756528
H -0.049621 1.378103 3.459191
H 0.786774 2.930633 3.345711
H -0.580451 2.577608 2.275515
Pt 2.036500 -0.804886 -0.056971
Cl 3.269503 0.686850 -1.489393
Cl 0.787492 -2.224816 1.418317
C 3.091344 -2.321678 -0.692583
O 3.700253 -3.215590 -1.061048
H 1.171521 2.158396 -1.594558
C 0.891311 4.074449 0.294268
H 0.574014 4.889327 0.943517
C 2.045707 3.394452 0.627097
H 2.658585 3.769097 1.441563
H 2.538999 2.717689 -0.061643
O -2.540759 0.226213 -0.674693
Si -3.520598 -0.821693 0.226809
C -3.054068 -0.731926 2.056053
H -2.010389 -1.038600 2.198226
H -3.172248 0.278361 2.465796
H -3.675614 -1.408225 2.655887
C -3.281507 -2.593155 -0.383424
H -3.982135 -3.276301 0.112594
H -3.440830 -2.679833 -1.464304
H -2.270001 -2.954419 -0.161468
C -5.289648 -0.172047 -0.096251
C -5.392505 1.307057 0.336293
H -4.681192 1.935933 -0.211061
H -6.402944 1.693960 0.138808
H -5.199488 1.434490 1.408779
C -5.627119 -0.276595 -1.599410
H -4.925457 0.301279 -2.211547
H -5.605918 -1.314614 -1.953503
H -6.637521 0.113239 -1.791944
C -6.310065 -1.004854 0.710680
H -7.330184 -0.634864 0.532614
H -6.295531 -2.064173 0.425594
H -6.127785 -0.946063 1.790847

I3$_{CO}$

Zero-point correction= 0.476770 (Hartree/Particle)
Thermal correction to Energy= 0.509119
Thermal correction to Enthalpy= 0.510063
Thermal correction to Gibbs Free Energy= 0.411513
Sum of electronic and zero-point Energies= -2222.402892
Sum of electronic and thermal Energies= -2222.370544
Sum of electronic and thermal Enthalpies= -2222.369599
Sum of electronic and thermal Free Energies= -2222.468150
HF (M06/6-311++g(d,p) and SDD, SMD(cyclohexane): -2222.70185516

C -0.295176 1.194715 -0.164166
H -0.995396 1.724452 0.483390
C -1.123131 0.135027 -0.972251
H -0.779171 -0.880693 -0.759420
C 0.196021 2.289286 -1.287703
C -0.940028 0.513436 -2.452121
C -0.798693 2.037249 -2.431374
H -1.777970 0.151132 -3.053817
H -0.016739 0.060322 -2.834549
H -0.421779 2.453735 -3.372112
H -1.764547 2.506491 -2.207630
C 0.254496 3.656712 -0.691845
H -0.466653 4.392259 -1.045751
C 0.940052 0.821925 0.519557
C 1.456539 1.700560 1.628317
C 2.611830 1.042933 2.413663
H 2.957492 1.726656 3.197906
H 2.279946 0.115149 2.887960
H 3.460812 0.812441 1.763369
C 0.355827 2.129265 2.629274
H -0.121002 1.252049 3.078700
H 0.817770 2.710507 3.434903
H -0.415056 2.751755 2.170614
Pt 1.968171 -0.786974 -0.066645
Cl 3.325652 0.436662 -1.618454
Cl 0.626484 -2.000667 1.528151
C 2.919372 -2.452081 -0.580985
O 3.457492 -3.411849 -0.875963
H 1.188860 1.980790 -1.629962
C 1.093412 3.968539 0.306764
H 1.046855 4.963705 0.744336
C 2.073383 3.000678 0.908293
H 2.646188 3.497283 1.697998
H 2.795621 2.648989 0.162944
O -2.487580 0.297573 -0.618236
Si -3.461543 -0.745445 0.291201
C -3.072046 -0.560102 2.130693
H -2.030445 -0.839353 2.329300
H -3.223475 0.466322 2.484874
H -3.705855 -1.218083 2.737953
C -3.146823 -2.533328 -0.230972
H -3.827716 -3.216090 0.292196
H -3.289088 -2.682040 -1.307703
H -2.125448 -2.840521 0.023160
C -5.240852 -0.169115 -0.113143
C -5.400704 1.327460 0.232831
H -4.690432 1.947420 -0.325711
H -6.414933 1.671731 -0.017731
H -5.247461 1.520431 1.301934
C -5.531102 -0.367152 -1.616581
H -4.834111 0.203671 -2.240647
H -5.461531 -1.421211 -1.912087
H -6.548847 -0.026916 -1.857754
C -6.258809 -0.989271 0.709668
H -7.284584 -0.669853 0.475050
H -6.196656 -2.062837 0.491543
H -6.117437 -0.857617 1.789477

Ts3-2b$_{CO}$

Zero-point correction= 0.472999 (Hartree/Particle)
Thermal correction to Energy= 0.504752
Thermal correction to Enthalpy= 0.505696
Thermal correction to Gibbs Free Energy= 0.409586
Sum of electronic and zero-point Energies= -2222.377745
Sum of electronic and thermal Energies= -2222.345993
Sum of electronic and thermal Enthalpies= -2222.345048
Sum of electronic and thermal Free Energies= -2222.441158
HF (M06/6-311++g(d,p) and SDD, SMD(cyclohexane): -2222.68089572

C 2.121176 1.885107 1.074505
C 1.138968 1.035541 0.207031
C 2.128051 3.417285 0.7761
C -0.157302 3.037423 -0.948457
C 0.140731 1.570247 -0.618729
C -0.891813 0.707017 -1.390213
H -0.463289 -0.245397 -1.710297
H 2.920043 3.853294 1.394425
C 3.559709 1.378095 0.815349
H 3.67644 0.334984 1.12405
H 4.26387 1.984132 1.397922
H 3.829834 1.444766 -0.242694
C 1.783132 1.673994 2.568373
H 0.787032 2.060632 2.81329
H 2.513706 2.213229 3.183695
H 1.810155 0.617256 2.840563
C -1.385651 3.008144 -1.880321
C -1.286891 1.631275 -2.550788
H -2.21316 1.302859 -3.027392
H -0.490684 1.621128 -3.306678
H -2.307614 3.076319 -1.293444
H -1.373137 3.84071 -2.589878
Pt 1.560392 -1.012793 -0.026321
H -0.005038 1.054503 0.699708
Cl 0.508519 -1.585509 2.048486
Cl 2.489852 -0.400236 -2.157986
C -0.230998 3.95841 0.245268
C 0.827966 4.133185 1.036947
H 0.715899 3.326509 -1.559746
H 2.440077 3.573892 -0.266996
H 0.758376 4.792828 1.899192
H -1.177682 4.461486 0.42926
O -1.971886 0.527895 -0.484402
Si -3.159984 -0.694051 -0.524485
C -4.181813 -0.375436 1.057494
C -2.336423 -2.388304 -0.55054
H -3.089078 -3.186133 -0.521199
H -1.749402 -2.533104 -1.466264
H -1.660952 -2.517292 0.301434
C -4.223601 -0.501192 -2.08003
H -3.640971 -0.687755 -2.990349
H -5.046177 -1.22699 -2.07398
H -4.664975 0.498677 -2.16212
C -3.300712 -0.552583 2.3125
H -2.893977 -1.566671 2.392131
H -2.451017 0.138171 2.3174
H -3.893477 -0.361439 3.219027
C -4.749718 1.060725 1.039534
H -3.950097 1.809488 1.006659
H -5.410097 1.233578 0.180441
H -5.341482 1.246059 1.94761
C -5.355413 -1.379659 1.124021
H -5.944969 -1.209269 2.036022
H -6.039558 -1.277689 0.272421
H -5.007237 -2.419534 1.154603
C 2.037213 -2.861931 -0.308515
O 2.32637 -3.95353 -0.480428

2b-[Pt]$_{CO}$

Zero-point correction= 0.477460 (Hartree/Particle)
Thermal correction to Energy= 0.509726
Thermal correction to Enthalpy= 0.510670
Thermal correction to Gibbs Free Energy= 0.411989
Sum of electronic and zero-point Energies= -2222.426699
Sum of electronic and thermal Energies= -2222.394434
Sum of electronic and thermal Enthalpies= -2222.393490
Sum of electronic and thermal Free Energies= -2222.492171
HF (M06/6-311++g(d,p) and SDD, SMD(cyclohexane): -2222.72876700

C 0.688330 2.057275 1.545289
C 0.313511 0.766588 0.806358
C 0.948036 3.273976 0.615891
C -0.043036 1.604160 -1.651265
C -0.084664 0.588935 -0.506020
C -0.940328 -0.602171 -0.974569
H -0.672412 -1.540382 -0.484376
H 1.242085 4.114849 1.255004
C 1.932498 1.827716 2.429969
H 1.817302 0.935333 3.056149
H 2.082829 2.688293 3.092865
H 2.835823 1.705659 1.823688
C -0.520002 2.352496 2.472513
H -1.442694 2.492226 1.900806
H -0.329316 3.267867 3.045658
H -0.677847 1.537462 3.188491
C -0.727961 0.890616 -2.850261
C -0.717816 -0.604502 -2.488109
H -1.483301 -1.186721 -3.009316
H 0.261717 -1.050546 -2.705436
H -1.761931 1.237547 -2.947147
H -0.215791 1.101959 -3.793335
Pt 2.133311 -0.559006 0.018172
H -0.009644 -0.016534 1.491769
Cl 1.154029 -2.343379 1.287411
Cl 3.312834 1.104330 -1.231915
C -0.677802 2.925682 -1.255621
C -0.227122 3.674392 -0.245590
H 1.007748 1.792111 -1.900030
H 1.815671 3.046002 -0.014487
H -0.733485 4.610141 -0.015491
H -1.538101 3.248720 -1.839439
O -2.287784 -0.224574 -0.695777
Si -3.436002 -1.103321 0.182239
C -5.009650 -0.023280 0.066262
C -2.871628 -1.335297 1.970809
H -3.596340 -1.934991 2.535472
H -1.909642 -1.860002 2.016437
H -2.755203 -0.377667 2.491384
C -3.667959 -2.802183 -0.614453
H -2.739506 -3.385283 -0.576802
H -4.435563 -3.384088 -0.089611
H -3.968325 -2.722375 -1.665161
C -4.717346 1.383183 0.633347
H -4.428397 1.345432 1.691105
H -3.911261 1.880639 0.082496
H -5.613422 2.017088 0.563474
C -5.454700 0.112766 -1.405904
H -4.669882 0.561598 -2.025309
H -5.718014 -0.856662 -1.846713
H -6.344450 0.755212 -1.477739
C -6.149590 -0.672468 0.881659
H -7.060384 -0.059826 0.817875
H -6.405493 -1.672428 0.509185
H -5.894858 -0.765476 1.944523
C 3.674432 -1.636416 -0.160553
O 4.605029 -2.288069 -0.260054

TS3-3b$_{CO}$

Zero-point correction= 0.474575 (Hartree/Particle)
Thermal correction to Energy= 0.506683
Thermal correction to Enthalpy= 0.507627
Thermal correction to Gibbs Free Energy= 0.410085
Sum of electronic and zero-point Energies= -2222.378796
Sum of electronic and thermal Energies= -2222.346688
Sum of electronic and thermal Enthalpies= -2222.345744
Sum of electronic and thermal Free Energies= -2222.443286
HF (M06/6-311++g(d,p) and SDD, SMD(cyclohexane): -2222.68022185

C -0.138129 1.499404 -0.101389
H -0.827821 2.068989 0.527297
C -1.082729 0.501610 -0.845370
H -0.663875 -0.505767 -0.891863
C 0.349720 2.511704 -1.179557
C -1.235948 1.104351 -2.267630
C -0.843235 2.586456 -2.141889
H -2.243583 0.943022 -2.659766
H -0.530097 0.602263 -2.942028
H -0.591204 3.048777 -3.102344
H -1.662224 3.165247 -1.693673
C 0.793361 3.754629 -0.469418
H 0.440398 4.729221 -0.802212
C 1.013873 0.947400 0.750344
C 0.879995 0.972126 2.166814
C 1.819179 0.226050 3.064560
H 2.072380 0.809426 3.957089
H 1.285246 -0.676283 3.391733
H 2.719935 -0.107869 2.545857
C -0.237761 1.694843 2.865604
H -1.175354 1.163802 2.657578
H -0.083596 1.734809 3.946513
H -0.361265 2.712089 2.478283
Pt 2.009612 -0.723218 -0.117740
Cl 3.552282 0.620710 -1.368142
Cl 0.492799 -2.133850 1.108027
C 2.808343 -2.295922 -0.922122
O 3.273588 -3.227302 -1.391837
H 1.203652 2.073740 -1.715424
C 1.547205 3.641740 0.635268
H 1.814804 4.516785 1.224126
C 2.115997 2.335612 1.071324
H 2.530543 2.398376 2.080239
H 2.917576 1.973982 0.422028
O -2.329053 0.482166 -0.148895
Si -3.382421 -0.803998 0.131534
C -3.225148 -1.312152 1.945311
H -2.199965 -1.642263 2.147617
H -3.457412 -0.480744 2.622315
H -3.897499 -2.141291 2.197494
C -2.963670 -2.275882 -0.976041
H -3.679508 -3.091938 -0.818124
H -2.983187 -2.021129 -2.042097
H -1.967268 -2.665355 -0.737506
C -5.141770 -0.125311 -0.225024
C -5.412682 1.120533 0.646276
H -4.682363 1.914297 0.451337
H -6.412935 1.526988 0.434905
H -5.377811 0.886355 1.717523
C -5.270752 0.271967 -1.710464
H -4.553993 1.056151 -1.980825
H -5.106763 -0.580836 -2.380869
H -6.278494 0.660741 -1.918918
C -6.196900 -1.205774 0.098995
H -7.209003 -0.825082 -0.102377
H -6.063740 -2.108291 -0.510672
H -6.167804 -1.507029 1.153282

3b-[Pt]$_{CO}$

Zero-point correction= 0.478014 (Hartree/Particle)
Thermal correction to Energy= 0.510362
Thermal correction to Enthalpy= 0.511306
Thermal correction to Gibbs Free Energy= 0.413173
Sum of electronic and zero-point Energies= -2222.416428
Sum of electronic and thermal Energies= -2222.384080
Sum of electronic and thermal Enthalpies= -2222.383136
Sum of electronic and thermal Free Energies= -2222.481269
HF (M06/6-311++g(d,p) and SDD, SMD(cyclohexane): -2222.72014755

C -0.506214 1.125219 0.817180
H -1.101714 1.234101 1.741511
C -1.592880 1.178310 -0.283042
H -1.233024 0.776191 -1.230148
C 0.260422 2.461027 0.690602
C -1.866880 2.710860 -0.454144
C -0.889539 3.462463 0.478813
H -2.908862 2.936430 -0.216497
H -1.698226 2.998615 -1.497671
H -0.549583 4.414746 0.058616
H -1.364242 3.680791 1.443959
C 1.142226 2.698925 1.880484
H 1.523979 3.705901 2.043188
C 0.399190 -0.045013 1.195997
C 0.415403 -1.348684 0.695921
C 0.913724 -2.521180 1.527551
H 0.026541 -3.009068 1.958120
H 1.415205 -3.260369 0.896588
H 1.588137 -2.259167 2.337557
C -0.447739 -1.840224 -0.449228
H -0.711185 -1.077029 -1.170963
H 0.065654 -2.646619 -0.983131
H -1.369741 -2.259166 -0.026256
Pt 2.380554 -0.325450 -0.360509
Cl 3.882435 -1.110000 1.337722
Cl 1.192598 0.479915 -2.283894

C 3.943412 -0.001245 -1.366513
O 4.886936 0.194973 -1.976156
H 0.865368 2.435803 -0.227620
C 1.453695 1.715599 2.729324
H 2.076230 1.917739 3.598849
C 1.035725 0.272789 2.554404
H 0.291560 0.003890 3.325190
H 1.904798 -0.356435 2.743729
O -2.731546 0.441534 0.158882
Si -4.104731 0.009869 -0.715794
C -3.631257 -0.965782 -2.267544
H -2.945560 -0.392156 -2.903587
H -3.143660 -1.918869 -2.036284
H -4.520497 -1.183933 -2.871747
C -5.087625 1.529397 -1.274750
H -6.015807 1.223229 -1.773373
H -5.359658 2.181478 -0.437235
H -4.518666 2.130956 -1.993229
C -5.121664 -1.044565 0.517297
C -4.294365 -2.258148 0.991674
H -3.375005 -1.942622 1.497798
H -4.875580 -2.863337 1.702873
H -4.015617 -2.916655 0.159162
C -5.500726 -0.191509 1.747699
H -4.611642 0.189946 2.262219
H -6.125555 0.667670 1.474750
H -6.072090 -0.793808 2.469173
C -6.412061 -1.552011 -0.163460
H -6.999700 -2.160408 0.539144
H -7.055975 -0.727648 -0.493807
H -6.198657 -2.181256 -1.036544

Ts3-4$_{CO}$

Zero-point correction= 0.473667 (Hartree/Particle)
Thermal correction to Energy= 0.505289
Thermal correction to Enthalpy= 0.506233
Thermal correction to Gibbs Free Energy= 0.409311
Sum of electronic and zero-point Energies= -2222.378765
Sum of electronic and thermal Energies= -2222.347144
Sum of electronic and thermal Enthalpies= -2222.346200
Sum of electronic and thermal Free Energies= -2222.443121
HF (M06/6-311++g(d,p) and SDD, SMD(cyclohexane): -2222.68251754

C 1.628066 2.113595 1.257629
C 1.00577 1.023625 0.28905
C 1.991505 3.409087 0.476156
C -0.032153 1.813543 -1.011925
C -0.50694 0.998099 0.163194
C -1.252587 -0.22827 -0.387183
H -1.048986 -1.116079 0.218751
H 2.366508 4.140734 1.201147
C 2.938487 1.578293 1.876601
H 2.755122 0.695946 2.49521
H 3.377346 2.357041 2.513233
H 3.672967 1.318093 1.108257
C 0.670751 2.456698 2.418839
H -0.204322 3.027879 2.093312
H 1.205151 3.071503 3.151749
H 0.331014 1.549203 2.928561
C -0.379121 1.042262 -2.292141
C -0.745137 -0.381768 -1.835301
H -1.508217 -0.840066 -2.469526
H 0.141887 -1.022627 -1.857078
H -1.257921 1.558854 -2.700144
H 0.414682 1.076414 -3.041954
Pt 2.114421 -0.754716 -0.037395
H -1.052982 1.517796 0.941142
Cl 1.064789 -1.648727 1.924749
Cl 3.142276 0.270877 -1.954487
C -0.026223 3.297977 -0.995925
C 0.872276 4.023802 -0.326087
H 1.259542 1.464031 -0.878552
H 2.836091 3.192636 -0.196319
H 0.818745 5.108709 -0.378116
H -0.809793 3.765144 -1.58875
O -2.638318 0.108157 -0.384656
Si -3.866711 -0.874874 0.231945
C -5.468973 0.105973 -0.123255
C -3.845523 -2.549208 -0.648571
H -4.002757 -2.450979 -1.728814
H -2.884377 -3.056446 -0.498566
H -4.624357 -3.214901 -0.256869
C -3.587199 -1.156019 2.079477
H -2.617341 -1.635403 2.261368
H -3.599765 -0.216625 2.643858
H -4.357603 -1.811445 2.503854
C -5.414781 1.47727 0.585116
H -5.34078 1.373708 1.674633
H -4.560031 2.073013 0.245331
H -6.328111 2.052751 0.374176
C -6.691706 -0.682653 0.395007
H -7.618136 -0.126418 0.191577
H -6.787973 -1.661446 -0.091188
H -6.64543 -0.849663 1.478371
C -5.61981 0.334991 -1.642717
H -4.772342 0.8971 -2.051141
H -5.69297 -0.610038 -2.194567
H -6.534328 0.908086 -1.854369
C 3.130575 -2.373123 -0.260867
O 3.73267 -3.335914 -0.386097

I4$_{CO}$

Zero-point correction= 0.475988 (Hartree/Particle)
Thermal correction to Energy= 0.508144
Thermal correction to Enthalpy= 0.509088
Thermal correction to Gibbs Free Energy= 0.411302
Sum of electronic and zero-point Energies= -2222.389626
Sum of electronic and thermal Energies= -2222.357470
Sum of electronic and thermal Enthalpies= -2222.356526
Sum of electronic and thermal Free Energies= -2222.454311
HF (M06/6-311++g(d,p) and SDD, SMD(cyclohexane): -2222.69383941

C 1.890250 2.043801 1.186785
C 1.277584 1.187662 0.029044
C 2.042576 3.534977 0.792221
C -0.408981 2.440742 -0.870681
C -0.320878 1.251669 -0.036098
C -1.076266 0.159179 -0.835898
H -0.723581 -0.844109 -0.589784
H 2.385085 4.089929 1.676932
C 3.325919 1.530315 1.456642
H 3.305640 0.544004 1.928192
H 3.845811 2.219353 2.135939
H 3.907883 1.454189 0.531760
C 1.102252 1.982559 2.511326
H 0.159011 2.541610 2.464404
H 1.698749 2.437190 3.311578
H 0.884512 0.950399 2.793159
C -0.858645 2.080340 -2.258804
C -0.814928 0.543155 -2.298877
H -1.563757 0.112455 -2.967199
H 0.176778 0.198894 -2.610511
H -1.899679 2.439551 -2.326979
H -0.293108 2.596009 -3.042525
Pt 1.906344 -0.893800 -0.073025
H -0.689546 1.346518 0.982469
Cl 0.642047 -1.493288 1.882375
Cl 3.097630 -0.301809 -2.068732
C -0.135132 3.808600 -0.545353
C 0.896036 4.282619 0.192810
H 1.725233 1.523409 -0.915531
H 2.866654 3.647975 0.063461
H 1.003068 5.367031 0.213977
H -0.725649 4.532120 -1.107136
O -2.468319 0.304521 -0.577374
Si -3.435079 -0.666953 0.418201
C -5.215309 -0.277381 -0.167556
C -2.983533 -2.483222 0.174406
H -3.036281 -2.787716 -0.877335
H -1.968225 -2.684803 0.536000
H -3.662978 -3.130666 0.742302
C -3.178109 -0.194496 2.228937
H -2.144211 -0.400433 2.530551
H -3.382821 0.867139 2.412075
H -3.832083 -0.777688 2.889127
C -5.506807 1.230827 -0.009074
H -5.434970 1.555152 1.036394
H -4.811214 1.839926 -0.597951
H -6.525538 1.462085 -0.353602
C -6.233029 -1.078018 0.674529
H -7.258830 -0.857071 0.345431
H -6.087969 -2.160965 0.575491
H -6.173732 -0.828088 1.740955
C -5.377073 -0.663161 -1.653753
H -4.666479 -0.122663 -2.289529
H -5.223833 -1.736854 -1.817614
H -6.390924 -0.420904 -2.005005
C 2.583093 -2.688151 -0.193065
O 3.006399 -3.748854 -0.255818

Ts4-4*$_{CO}$

Zero-point correction= 0.475445 (Hartree/Particle)
Thermal correction to Energy= 0.507143
Thermal correction to Enthalpy= 0.508087
Thermal correction to Gibbs Free Energy= 0.410965
Sum of electronic and zero-point Energies= -2222.388448
Sum of electronic and thermal Energies= -2222.356751

Sum of electronic and thermal Enthalpies= -2222.355807
Sum of electronic and thermal Free Energies= -2222.452928
HF (M06/6-311++g(d,p) and SDD, SMD(cyclohexane): -2222.69340937

C -0.386422 1.104036 0.03386
H -0.696456 1.185413 1.068605
C -1.094293 0.025854 -0.80997
H -0.798819 -0.989059 -0.531074
C -0.217732 2.263614 -0.793182
C -0.703158 0.377521 -2.256287
C -0.514082 1.906729 -2.243694
H -1.479546 0.052596 -2.952971
H 0.231101 -0.122295 -2.52807
H 0.245101 2.273113 -2.942197
H -1.452269 2.424338 -2.489832
C -0.178337 3.685073 -0.417446
H -1.054233 4.246967 -0.742597
C 1.20091 1.287658 -0.056024
C 1.944556 2.149864 1.022038
C 3.366691 1.57957 1.226661
H 3.946345 2.261524 1.861773
H 3.338608 0.605813 1.726217
H 3.899951 1.462326 0.277344
C 1.229515 2.160165 2.388873
H 1.047964 1.144708 2.749658
H 1.863854 2.671509 3.122471
H 0.27604 2.698244 2.356282
Cl 3.086408 -0.433915 -2.071143
Cl 0.689982 -1.406578 1.968061
H 1.672084 1.355781 -1.039921
C 0.855039 4.312238 0.150035
H 0.790803 5.386666 0.307915
C 2.125279 3.615578 0.542801
H 2.616312 4.178423 1.346306
H 2.826018 3.644568 -0.307308
O -2.492871 0.215682 -0.64417
Si -3.511457 -0.613768 0.425501
C -3.264635 0.028135 2.186181
H -2.257256 -0.211781 2.547547
H -3.398148 1.114475 2.2488
H -3.976117 -0.433979 2.881715
C -3.118454 -2.460315 0.377635
H -3.823205 -3.022995 1.002201
H -3.174805 -2.8688 -0.637949
H -2.113149 -2.658353 0.768321
C -5.26437 -0.222208 -0.230014
C -5.48223 1.306352 -0.2705
H -4.74599 1.800041 -0.914732
H -6.482007 1.539029 -0.665712
H -5.413909 1.758531 0.726994
C -5.43049 -0.787332 -1.65759
H -4.691744 -0.364184 -2.347715
H -5.325484 -1.878965 -1.681012
H -6.429522 -0.547043 -2.049712
C -6.327645 -0.859702 0.691288
H -7.337384 -0.648294 0.310611
H -6.225121 -1.950712 0.747438
H -6.277623 -0.465147 1.713563
Pt 1.893373 -0.904106 -0.044156
C 2.561094 -2.663 -0.058514
O 2.976602 -3.72819 -0.062113

I4*$_{co}$
Zero-point correction= 0.476420 (Hartree/Particle)
Thermal correction to Energy= 0.508850
Thermal correction to Enthalpy= 0.509795
Thermal correction to Gibbs Free Energy= 0.410927
Sum of electronic and zero-point Energies= -2222.395645
Sum of electronic and thermal Energies= -2222.363215
Sum of electronic and thermal Enthalpies= -2222.362271
Sum of electronic and thermal Free Energies= -2222.461139
HF (M06/6-311++g(d,p) and SDD, SMD(cyclohexane): -2222.72876700

C -0.251419 0.898337 0.010965
H -0.054080 0.840410 -1.054227
C 0.930607 0.442788 0.937508
H 0.875077 -0.609816 1.232456
C -0.278338 2.553592 0.367603
C 0.862285 1.351679 2.168810
C 0.633689 2.745199 1.575874
H 1.781723 1.281652 2.756680
H 0.028736 1.037704 2.805213
H 0.178093 3.444142 2.287854
H 1.580952 3.178726 1.241066
C -0.170849 3.521710 -0.743910
H 0.821067 3.802416 -1.089628
C -1.505802 1.806571 0.509669
C -2.723791 2.163734 -0.402709
C -4.015739 1.859997 0.378761
H -4.894867 2.148770 -0.209263
H -4.093082 0.792713 0.610621
H -4.049026 2.411303 1.326286
C -2.768668 1.422893 -1.752524
H -2.887185 0.344537 -1.620187
H -3.627614 1.783810 -2.330912
H -1.869337 1.585913 -2.352989
Cl -2.106084 -0.940174 2.308829
Cl -0.612154 -1.503665 -2.202759
H -1.790509 1.519168 1.517261
C -1.284139 4.094178 -1.220248
H -1.223974 4.866510 -1.984181
C -2.640570 3.689427 -0.693843
H -3.426972 3.959704 -1.407807
H -2.857814 4.258441 0.224044
O 2.135114 0.686954 0.237607
Si 3.236169 -0.404332 -0.446456
C 3.153688 -0.210984 -2.319635
H 2.155396 -0.482942 -2.680575
H 3.357543 0.820524 -2.629644
H 3.878512 -0.861264 -2.824442
C 2.791848 -2.173161 0.045315
H 3.532361 -2.873830 -0.359307
H 2.761019 -2.319253 1.131306
H 1.817106 -2.459447 -0.366636
C 4.960457 0.102172 0.224628
C 5.258852 1.569377 -0.152021
H 4.510626 2.253897 0.264455
H 6.241451 1.873903 0.237510
H 5.279576 1.715949 -1.238814
C 4.996676 -0.037443 1.761059
H 4.243274 0.597583 2.242274
H 4.821975 -1.071011 2.084907
H 5.979551 0.264094 2.151955
C 6.048921 -0.806793 -0.388229
H 7.042356 -0.517319 -0.015868
H 5.900373 -1.861813 -0.126241
H 6.079704 -0.734289 -1.482262
Pt -1.391138 -1.164195 0.033375
C -2.147387 -2.861622 -0.003410
O -2.607803 -3.907915 -0.027473

Ts4*-5$_{co}$
Zero-point correction= 0.476130 (Hartree/Particle)
Thermal correction to Energy= 0.507856
Thermal correction to Enthalpy= 0.508800
Thermal correction to Gibbs Free Energy= 0.411711
Sum of electronic and zero-point Energies= -2222.395932
Sum of electronic and thermal Energies= -2222.364207
Sum of electronic and thermal Enthalpies= -2222.363263
Sum of electronic and thermal Free Energies= -2222.460352
HF (M06/6-311++g(d,p) and SDD, SMD(cyclohexane): -2222.70134387

C -0.265153 0.871113 0.019309
H -0.050553 0.842806 -1.043842
C 0.92694 0.433689 0.940523
H 0.874169 -0.61787 1.239451
C -0.262895 2.573506 0.378694
C 0.867574 1.343331 2.171218
C 0.659919 2.739729 1.578253
H 1.784539 1.262761 2.761638
H 0.02825 1.040657 2.805322
H 0.217626 3.444592 2.293435
H 1.612458 3.159155 1.24115
C -0.134651 3.526317 -0.738768
H 0.86208 3.802324 -1.073653
C -1.485405 1.823921 0.510441
C -2.698153 2.186163 -0.409753
C -3.995679 1.895918 0.367491
H -4.870128 2.186135 -0.22678
H -4.080524 0.830842 0.606212
H -4.029997 2.453823 1.311149
C -2.742324 1.43955 -1.756695
H -2.866269 0.362375 -1.621235
H -3.597672 1.802877 -2.338899
H -1.840444 1.595644 -2.355278
Cl -2.124736 -0.9151 2.303966
Cl -0.608831 -1.51219 -2.197339
H -1.780061 1.541662 1.517067
C -1.24161 4.102181 -1.228503
H -1.169854 4.872001 -1.993985
C -2.603845 3.709171 -0.7097
H -3.383282 3.980498 -1.430703
H -2.822694 4.286593 0.202645
O 2.128706 0.676515 0.234475
Si 3.229733 -0.416841 -0.44649
C 3.151112 -0.22204 -2.319611
H 2.152348 -0.490812 -2.681587
H 3.358601 0.808997 -2.62886
H 3.87456 -0.87432 -2.823785

C 2.782269 -2.184882 0.044262
H 3.521971 -2.886545 -0.360145
H 2.750452 -2.331481 1.130149
H 1.807279 -2.468956 -0.368543
C 4.954254 0.086266 0.22731
C 5.2552 1.553868 -0.145712
H 4.507877 2.238601 0.272122
H 6.238086 1.855992 0.244992
H 5.276597 1.703087 -1.23214
C 4.989596 -0.056865 1.76344
H 4.236466 0.57762 2.245894
H 4.81395 -1.090997 2.084937
H 5.972468 0.243111 2.155586
C 6.042032 -0.822684 -0.386831
H 7.035603 -0.535486 -0.013026
H 5.891821 -1.878119 -0.127507
H 6.073703 -0.747631 -1.480656
Pt -1.400061 -1.165049 0.033504
C -2.172711 -2.861072 -0.000827
O -2.6411 -3.90395 -0.023661

I5$_{CO}$

Zero-point correction= 0.475048 (Hartree/Particle)
Thermal correction to Energy= 0.507197
Thermal correction to Enthalpy= 0.508141
Thermal correction to Gibbs Free Energy= 0.409531
Sum of electronic and zero-point Energies= -2222.408041
Sum of electronic and thermal Energies= -2222.375892
Sum of electronic and thermal Enthalpies= -2222.374947
Sum of electronic and thermal Free Energies= -2222.473558
HF (M06/6-311++g(d,p) and SDD, SMD(cyclohexane): -2222.71390535

C -0.278579 0.149625 -0.111035
H 0.033473 -0.140338 -1.116812
C 0.642474 -0.564068 0.880270
H 0.435196 -1.636768 0.847590
C 0.764806 2.182527 1.037067
C 0.437649 -0.023944 2.294206
C 0.885636 1.446533 2.331367
H 1.023844 -0.597273 3.019584
H -0.618439 -0.111897 2.563941
H 0.287726 2.014632 3.064108
H 1.924834 1.551979 2.667469
C 1.393291 3.465564 0.955670
H 2.079495 3.761633 1.744741
C -0.118661 1.699711 -0.012451
C -0.033547 2.475955 -1.367972
C -1.283460 2.204328 -2.224501
H -1.238614 2.792261 -3.149817
H -1.356578 1.149031 -2.501405
H -2.201651 2.469298 -1.689674
C 1.226947 2.083840 -2.167976
H 1.203782 1.029138 -2.451935
H 1.273811 2.672721 -3.092220
H 2.151417 2.257217 -1.608175
Cl -2.998753 1.351981 1.216919
Cl -1.414113 -2.512857 -1.163132
H -1.093011 2.028922 0.488327
C 1.028896 4.340987 -0.015678
H 1.434864 5.351416 0.000055
C 0.018344 3.990657 -1.053149
H 0.191982 4.572303 -1.966833
H -0.964356 4.325065 -0.672100
O 2.027922 -0.315812 0.544406
Si 3.084795 -1.450533 -0.129661
C 2.676081 -1.757554 -1.947616
H 1.635286 -2.088537 -2.050310
H 2.805257 -0.860179 -2.563616
H 3.314084 -2.544447 -2.368804
C 2.943440 -3.090383 0.802962
H 3.697826 -3.804096 0.448834
H 3.081301 -2.970097 1.883733
H 1.962909 -3.552468 0.638338
C 4.820750 -0.664075 0.088952
C 4.845644 0.750887 -0.526355
H 4.117811 1.411494 -0.041105
H 5.840933 1.204961 -0.408563
H 4.620145 0.735306 -1.599828
C 5.168722 -0.563650 1.589289
H 4.436179 0.043322 2.134893
H 5.205214 -1.550183 2.066380
H 6.155525 -0.097241 1.726571
C 5.881821 -1.537538 -0.615824
H 6.883687 -1.102899 -0.485531
H 5.915642 -2.555061 -0.206661
H 5.698261 -1.616403 -1.694145
Pt -2.251513 -0.612198 0.019724
C -4.035891 -1.398793 0.098790
O -5.077225 -1.870766 0.145506

Ts5-5b$_{CO}$

Zero-point correction= 0.472671 (Hartree/Particle)
Thermal correction to Energy= 0.504345
Thermal correction to Enthalpy= 0.505289
Thermal correction to Gibbs Free Energy= 0.408703
Sum of electronic and zero-point Energies= -2222.406077
Sum of electronic and thermal Energies= -2222.374404
Sum of electronic and thermal Enthalpies= -2222.373459
Sum of electronic and thermal Free Energies= -2222.470046
HF (M06/6-311++g(d,p) and SDD, SMD(cyclohexane): -2222.70727743

C 0.16071 0.126514 0.145414
H -0.162107 -0.193634 1.137202
C -0.789852 -0.460884 -0.907224
H -0.648342 -1.544881 -0.941605
C -0.241977 2.3497 -1.007561
C -0.507924 0.142488 -2.284511
C -0.727921 1.658346 -2.25592
H -1.169899 -0.303365 -3.034025
H 0.524007 -0.084375 -2.57131
H -0.296463 2.146368 -3.138646
H -1.806322 1.876086 -2.278891
C -0.288994 3.81262 -1.000677
H -0.742726 4.295219 -1.861548
C 0.200175 1.626472 0.119281
C 0.428532 2.412082 1.434068
C 1.429873 1.72467 2.380725
H 1.560925 2.344568 3.275889
H 1.083996 0.740786 2.707285
H 2.407181 1.597417 1.905046
C -0.952123 2.506369 2.128942
H -1.358556 1.511671 2.333678
H -0.845636 3.031389 3.085452
H -1.68018 3.050947 1.519132
Cl 2.957821 1.148575 -1.19696
Cl 1.131017 -2.641207 1.128382
H 1.15205 1.90889 -0.720147
C 0.260042 4.520884 -0.001072
H 0.258593 5.60802 -0.037036
C 0.964469 3.834586 1.129566
H 0.910346 4.441173 2.041555
H 2.035723 3.773976 0.873346
O -2.15518 -0.152008 -0.572027
Si -3.266175 -1.22649 0.108014
C -2.85483 -1.549445 1.924105
H -1.855925 -1.992372 2.018801
H -2.871497 -0.629498 2.520689
H -3.568073 -2.250223 2.375511
C -3.227146 -2.871719 -0.825187
H -3.997976 -3.553738 -0.445612
H -3.396999 -2.742886 -1.900425
H -2.262301 -3.376721 -0.696957
C -4.953555 -0.339685 -0.08368
C -4.90877 1.039043 0.610432
H -4.128636 1.679541 0.183231
H -5.870847 1.559439 0.492021
H -4.718058 0.950925 1.687106
C -5.27897 -0.134099 -1.578603
H -4.5102 0.464668 -2.080823
H -5.363303 -1.08735 -2.114385
H -6.238462 0.391501 -1.693588
C -6.069035 -1.191119 0.561622
H -7.042811 -0.691627 0.453249
H -6.157668 -2.178391 0.091397
H -5.900527 -1.345249 1.63448
Pt 2.094155 -0.796515 -0.028346
C 3.786155 -1.729588 -0.182816
O 4.775139 -2.296478 -0.277584

5b-[Pt]$_{CO}$

Zero-point correction= 0.477492 (Hartree/Particle)
Thermal correction to Energy= 0.509652
Thermal correction to Enthalpy= 0.510596
Thermal correction to Gibbs Free Energy= 0.411813
Sum of electronic and zero-point Energies= -2222.431028
Sum of electronic and thermal Energies= -2222.398868
Sum of electronic and thermal Enthalpies= -2222.397923
Sum of electronic and thermal Free Energies= -2222.496706
HF (M06/6-311++g(d,p) and SDD, SMD(cyclohexane): -2222.73180570

C 0.868819 2.273509 1.522269
C 0.483107 1.623886 0.195680
C 1.818560 3.482420 1.302923
C 0.513320 2.463099 -1.062926

C -0.017320 0.322785 0.147639
C -0.961821 -0.140621 -0.972425
H -0.825199 -1.214228 -1.146672
H 1.940127 4.001794 2.260906
C 1.520863 1.319076 2.539480
H 0.885455 0.469335 2.800608
H 1.730701 1.872674 3.461968
H 2.469213 0.923714 2.159546
C -0.484892 2.779767 2.111815
H -0.990987 3.476278 1.438235
H -0.282600 3.303288 3.053545
H -1.158801 1.943374 2.318906
C -0.660276 2.129770 -2.012861
C -0.735659 0.625915 -2.276810
H -1.603478 2.478909 -1.575412
H -0.512418 2.678585 -2.950115
Pt 1.939138 -0.901625 -0.067822
H -0.267929 -0.117989 1.108686
Cl 0.936044 -2.350907 1.557463
Cl 3.055688 0.395769 -1.737464
C 0.689899 3.944661 -0.829969
C 1.319087 4.424849 0.242008
H 1.430053 2.116752 -1.580015
H 2.816276 3.105306 1.031356
H 1.480906 5.493243 0.364511
H 0.327933 4.602768 -1.617237
O -2.292585 0.108576 -0.516628
Si -3.407085 -0.997619 0.110486
C -5.099850 -0.141539 -0.148393
C -3.285888 -2.637901 -0.824085
H -4.057447 -3.335519 -0.475838
H -3.414425 -2.514066 -1.905605
H -2.317288 -3.122912 -0.653329
C -3.058322 -1.309844 1.940973
H -3.075466 -0.382310 2.525401
H -3.801033 -1.989747 2.376514
H -2.073507 -1.773150 2.076177
C -5.348909 0.086094 -1.654508
H -6.315207 0.587159 -1.811936
H -4.571102 0.716322 -2.100381
H -5.377007 -0.858416 -2.211423
C -5.110700 1.224172 0.572418
H -4.973639 1.117898 1.655630
H -4.320444 1.883841 0.196670
H -6.073476 1.732394 0.414933
C -6.230576 -1.024210 0.424194
H -7.205755 -0.538057 0.276425
H -6.279769 -2.003404 -0.068378
H -6.114420 -1.196478 1.501300
C 3.340541 -2.143153 -0.208130
O 4.182061 -2.910450 -0.292824
H 0.197949 0.281694 -2.738713
H -1.555928 0.390308 -2.963041

Ts3-5b$_{CO}$
Zero-point correction= 0.474897 (Hartree/Particle)
Thermal correction to Energy= 0.506723
Thermal correction to Enthalpy= 0.507668
Thermal correction to Gibbs Free Energy= 0.410299
Sum of electronic and zero-point Energies= -2222.369964
Sum of electronic and thermal Energies= -2222.338138
Sum of electronic and thermal Enthalpies= -2222.337193
Sum of electronic and thermal Free Energies= -2222.434562
HF (M06/6-311++g(d,p) and SDD, SMD(cyclohexane): -2222.66883486

C 1.467435 2.05724 1.323819
C 0.844586 1.004427 0.341058
C 2.101647 3.236953 0.504411
C 0.486524 1.831419 -1.330761
C -0.495209 0.668971 0.496529
C -1.283596 -0.299756 -0.337504
H -1.130866 -1.287614 0.123708
H 2.608913 3.909972 1.203554
C 2.600004 1.430863 2.169677
H 2.243221 0.574314 2.748354
H 2.984709 2.182593 2.870445
H 3.435781 1.098761 1.545587
C 0.436266 2.65128 2.309921
H -0.399037 3.145527 1.80156
H 0.928085 3.402631 2.938131
H 0.031532 1.884361 2.980556
C -0.517648 1.114105 -2.224837
C -0.769271 -0.32985 -1.786922
H -1.473558 1.651062 -2.221862
H -0.126686 1.133087 -3.249963
Pt 2.12704 -0.723927 -0.034004
H -1.119249 1.171374 1.237318
Cl 0.952282 -1.84543 1.748607
Cl 3.401638 0.341755 -1.765325
C 0.251372 3.271686 -1.100789
C 1.060529 3.967543 -0.289415
H 1.507932 1.634439 -1.655029
H 2.873511 2.820062 -0.156047
H 0.900015 5.03064 -0.125469
H -0.596934 3.736251 -1.600846
O -2.64758 0.09827 -0.29056
Si -3.951414 -0.922883 0.070767
C -5.477572 0.220462 -0.044033
C -4.013398 -2.335003 -1.185272
H -4.857776 -3.006012 -0.98548
H -4.115348 -1.967736 -2.212771
H -3.101956 -2.943807 -1.138175
C -3.719958 -1.646474 1.800639
H -3.709355 -0.868543 2.572527
H -4.527251 -2.347661 2.0452
H -2.776393 -2.200386 1.88072
C -5.606578 0.786838 -1.474867
H -6.474675 1.458398 -1.542455
H -4.718958 1.36114 -1.763816
H -5.750908 -0.006517 -2.218244
C -5.328093 1.394281 0.947907
H -5.269726 1.048641 1.987272
H -4.429911 1.986228 0.739181
H -6.19515 2.067078 0.877316
C -6.753966 -0.57792 0.302371
H -7.638964 0.070495 0.232049
H -6.913557 -1.418935 -0.383876
H -6.725717 -0.978412 1.323324
C 3.247451 -2.266506 -0.217477
O 3.911158 -3.191165 -0.318501
H 0.155566 -0.913941 -1.840799
H -1.515098 -0.818523 -2.420468

Ts3-3'$_{CO}$
Zero-point correction= 0.476612 (Hartree/Particle)
Thermal correction to Energy= 0.508230
Thermal correction to Enthalpy= 0.509174
Thermal correction to Gibbs Free Energy= 0.411577
Sum of electronic and zero-point Energies= -2222.393131
Sum of electronic and thermal Energies= -2222.361514
Sum of electronic and thermal Enthalpies= -2222.360570
Sum of electronic and thermal Free Energies= -2222.458166
HF (M06/6-311++g(d,p) and SDD, SMD(cyclohexane): -2222.69160379

C -0.281673 1.189158 -0.220812
H -0.960220 1.775373 0.405662
C -1.142087 0.071825 -0.910118
H -0.780415 -0.926703 -0.652448
C 0.175757 2.173773 -1.398391
C -1.033972 0.362083 -2.418749
C -0.871334 1.881985 -2.493237
H -1.904751 -0.021900 -2.957319
H -0.137502 -0.127677 -2.820802
H -0.528209 2.239952 -3.470213
H -1.818970 2.380016 -2.255098
C 0.271493 3.588288 -0.922027
H -0.009385 4.349635 -1.649116
C 0.949440 0.847752 0.492742
C 1.331014 1.701442 1.667377
C 2.760572 1.420469 2.181121
H 2.953781 2.025920 3.074584
H 2.888015 0.368296 2.452752
H 3.505779 1.672089 1.421126
C 0.324383 1.197924 2.770944
H 0.365275 0.111908 2.889575
H 0.626930 1.661523 3.716148
H -0.704909 1.492266 2.550168
Pt 2.055694 -0.714863 -0.052405
Cl 3.456956 0.688950 -1.407439
Cl 0.747672 -2.193633 1.321557
C 3.157272 -2.274816 -0.620354
O 3.784573 -3.164406 -0.953830
H 1.148643 1.842755 -1.780398
C 0.654122 4.000237 0.290221
H 0.649453 5.077389 0.461439
C 1.170838 3.268069 1.509172
H 0.589081 3.623802 2.370722
H 2.176363 3.679317 1.671174
O -2.481500 0.261322 -0.476473
Si -3.534652 -0.887897 0.178462
C -3.109221 -1.202570 1.991202
H -2.087729 -1.589624 2.084173
H -3.178701 -0.289220 2.593592
H -3.783986 -1.945464 2.434361
C -3.388274 -2.510981 -0.780429
H -4.109783 -3.249885 -0.410494
H -3.569492 -2.377156 -1.853161
H -2.389928 -2.948756 -0.660249
C -5.259648 -0.081753 -0.013108
C -5.278134 1.287406 0.701032
H -4.525034 1.967006 0.286663
H -6.261570 1.766363 0.584745

H -5.089670 1.191571 1.777548
C -5.580163 0.130438 -1.507948
H -4.835871 0.773126 -1.991840
H -5.614016 -0.818201 -2.057461
H -6.562413 0.611216 -1.625055
C -6.338614 -0.992932 0.612217
H -7.333239 -0.536627 0.503907
H -6.379957 -1.976530 0.127538
H -6.170442 -1.154446 1.684147

I3'$_{CO}$
Zero-point correction= 0.476853 (Hartree/Particle)
Thermal correction to Energy= 0.509131
Thermal correction to Enthalpy= 0.510075
Thermal correction to Gibbs Free Energy= 0.411521
Sum of electronic and zero-point Energies= -2222.400113
Sum of electronic and thermal Energies= -2222.367835
Sum of electronic and thermal Enthalpies= -2222.366891
Sum of electronic and thermal Free Energies= -2222.465445
HF (M06/6-311++g(d,p) and SDD, SMD(cyclohexane): -2222.69999422

C -0.272318 1.226448 -0.202656
H -0.961057 1.781898 0.441269
C -1.124937 0.176503 -0.989525
H -0.769140 -0.841792 -0.810598
C 0.250251 2.283666 -1.300899
C -0.998846 0.584840 -2.469382
C -0.797266 2.101609 -2.422465
H -1.878313 0.269754 -3.037141
H -0.114129 0.106754 -2.908616
H -0.435200 2.526453 -3.365247
H -1.732266 2.605073 -2.149831
C 0.426061 3.674037 -0.767746
H 0.428780 4.455602 -1.527670
C 0.958746 0.859963 0.490315
C 1.431306 1.771152 1.597614
C 2.950166 2.055476 1.498937
H 3.257895 2.637824 2.374894
H 3.528134 1.128881 1.475551
H 3.189875 2.625142 0.597829
C 1.165490 0.970221 2.916255
H 1.774456 0.066974 2.969045
H 1.425237 1.630020 3.752407
H 0.115363 0.680040 3.018932
Pt 1.977299 -0.771762 -0.046540
Cl 3.339160 0.428465 -1.617312
Cl 0.636987 -2.119481 1.427284
C 2.967299 -2.417378 -0.564746
O 3.535665 -3.358573 -0.859755
H 1.208543 1.930776 -1.705349
C 0.611063 4.028314 0.508421
H 0.728126 5.089573 0.721825
C 0.657408 3.121161 1.719761
H -0.362831 2.927271 2.081140
H 1.140819 3.668534 2.537358
O -2.474548 0.326763 -0.573081
Si -3.442443 -0.782415 0.259876
C -3.049192 -0.718320 2.106894
H -2.005659 -1.005426 2.282869
H -3.204498 0.283224 2.525370
H -3.678057 -1.416030 2.673460
C -3.118009 -2.526605 -0.388966
H -3.799730 -3.249140 0.076303
H -3.252923 -2.594372 -1.474720
H -2.097000 -2.849632 -0.153478
C -5.226445 -0.191362 -0.097375
C -5.395217 1.274395 0.360042
H -4.691821 1.939478 -0.153512
H -6.412939 1.628760 0.139512
H -5.238978 1.388251 1.439943
C -5.520828 -0.276300 -1.610667
H -4.827188 0.342262 -2.191617
H -5.450683 -1.304701 -1.985967
H -6.539969 0.079494 -1.821764
C -6.237185 -1.076930 0.664326
H -7.265190 -0.744322 0.459841
H -6.172423 -2.130173 0.363679
H -6.091085 -1.028831 1.750474

Ts3'-2b'$_{CO}$
Zero-point correction= 0.473001 (Hartree/Particle)
Thermal correction to Energy= 0.504946
Thermal correction to Enthalpy= 0.505890
Thermal correction to Gibbs Free Energy= 0.408802
Sum of electronic and zero-point Energies= -2222.378808
Sum of electronic and thermal Energies= -2222.346863
Sum of electronic and thermal Enthalpies= -2222.345918
Sum of electronic and thermal Free Energies= -2222.443006
HF (M06/6-311++g(d,p) and SDD, SMD(cyclohexane): -2222.68163997

C 0.133979 1.560297 -0.487832
H 0.261617 1.066581 0.839720
C -1.067233 0.741776 -1.029144
H -0.754514 -0.238511 -1.396335
C -0.137411 3.034109 -0.773175
C -1.612961 1.676468 -2.118603
C -1.523561 3.060272 -1.461285
H -2.625112 1.392466 -2.415809
H -0.967348 1.620663 -3.005084
H -1.603422 3.888069 -2.172258
H -2.313956 3.173141 -0.712628
C 0.020904 4.004626 0.370807
H -0.645566 4.863705 0.312483
C 1.269618 1.002894 0.103620
C 2.410387 1.899675 0.664088
C 3.102776 2.653074 -0.498484
H 4.037915 3.090482 -0.130540
H 3.346341 1.964113 -1.313047
H 2.502955 3.474131 -0.897375
C 3.485841 1.026999 1.351827
H 3.958618 0.347244 0.635921
H 4.267939 1.674312 1.766804
H 3.063397 0.428141 2.162731
Pt 1.590141 -1.050761 -0.094033
Cl 2.185653 -0.594734 -2.371888
Cl 0.882165 -1.372675 2.178212
C 1.967169 -2.934049 -0.320125
O 2.199315 -4.043869 -0.458656
H 0.605029 3.271794 -1.554258
C 0.862331 3.930319 1.405497
H 0.801525 4.735988 2.137407
C 1.893664 2.885117 1.748469
H 1.525253 2.296313 2.603667
H 2.774281 3.415311 2.137678
O -1.984627 0.644515 0.045315
Si -2.987690 -0.640403 0.545972
C -2.945149 -0.546074 2.423753
H -1.913772 -0.660195 2.773960
H -3.326539 0.414396 2.789842
H -3.545258 -1.341044 2.881545
C -2.301399 -2.282064 -0.078949
H -2.968167 -3.104466 0.209391
H -2.193649 -2.317564 -1.169349
H -1.320977 -2.476686 0.368377
C -4.774612 -0.354746 -0.104527
C -5.213996 1.102879 0.149631
H -4.582886 1.817908 -0.390522
H -6.250390 1.255524 -0.185538
H -5.173652 1.363538 1.214350
C -4.883023 -0.659408 -1.613936
H -4.220213 -0.025585 -2.215395
H -4.638604 -1.703574 -1.841356
H -5.908748 -0.479083 -1.967099
C -5.734670 -1.303020 0.651826
H -6.757832 -1.194516 0.263748
H -5.455126 -2.357676 0.533264
H -5.768806 -1.084026 1.725171

2b'-[Pt]$_{CO}$
Zero-point correction= 0.477557 (Hartree/Particle)
Thermal correction to Energy= 0.509799
Thermal correction to Enthalpy= 0.510743
Thermal correction to Gibbs Free Energy= 0.412708
Sum of electronic and zero-point Energies= -2222.421606
Sum of electronic and thermal Energies= -2222.389363
Sum of electronic and thermal Enthalpies= -2222.388419
Sum of electronic and thermal Free Energies= -2222.486454
HF (M06/6-311++g(d,p) and SDD, SMD(cyclohexane): -2222.72461672

C -0.074634 0.695650 -0.460578
H 0.000557 -0.016225 1.498354
C -0.898352 -0.477753 -1.019056
H -0.586358 -1.447890 -0.621577
C -0.064197 1.806193 -1.498529
C -0.697324 -0.331013 -2.530304
C -0.764876 1.189108 -2.749932
H -1.451102 -0.888527 -3.093669
H 0.294452 -0.715960 -2.799603
H -0.283065 1.505586 -3.679486
H -1.810491 1.510539 -2.783785
C -0.712700 3.097291 -1.044224
H -1.066913 3.706521 -1.876070
C 0.341373 0.787367 0.849099
C 0.719151 2.066994 1.606736

C 1.975295 2.796092 1.093424
H 2.131187 3.701509 1.692471
H 2.863942 2.166264 1.194987
H 1.897545 3.096277 0.047833
C 0.950061 1.683252 3.083719
H 1.778060 0.971841 3.177437
H 1.195086 2.571019 3.677284
H 0.058658 1.218904 3.522648
Pt 2.128032 -0.552325 -0.000541
Cl 3.174571 0.899226 -1.588996
Cl 1.248963 -2.220125 1.485653
C 3.642252 -1.657752 -0.203608
O 4.559985 -2.326412 -0.310265
H 0.980175 2.017356 -1.764205
C -0.894076 3.587425 0.187722
H -1.404291 4.548731 0.249510
C -0.513590 3.014585 1.534998
H -1.385555 2.496914 1.965136
H -0.315507 3.855292 2.214529
O -2.255131 -0.188204 -0.694943
Si -3.336759 -1.135820 0.195744
C -2.816710 -1.217400 2.010973
H -1.840643 -1.705354 2.121102
H -2.746902 -0.221704 2.464017
H -3.538241 -1.798493 2.598790
C -3.360857 -2.890279 -0.508209
H -4.052528 -3.529255 0.054419
H -3.667698 -2.910511 -1.560149
H -2.369406 -3.354767 -0.440380
C -5.003208 -0.227717 -0.030635
C -4.885622 1.219093 0.498064
H -4.092448 1.774959 -0.014664
H -5.830387 1.759851 0.340727
H -4.673490 1.245590 1.574309
C -5.378088 -0.184498 -1.527827
H -4.613744 0.330683 -2.120037
H -5.507707 -1.189979 -1.946691
H -6.327727 0.352003 -1.668189
C -6.115179 -0.964949 0.747636
H -7.077482 -0.449264 0.617053
H -6.250460 -1.995776 0.396594
H -5.910614 -1.001193 1.824829

Ts3'-4'$_{CO}$

Zero-point correction= 0.473519 (Hartree/Particle)
Thermal correction to Energy= 0.505178
Thermal correction to Enthalpy= 0.506122
Thermal correction to Gibbs Free Energy= 0.409523
Sum of electronic and zero-point Energies= -2222.385045
Sum of electronic and thermal Energies= -2222.353386
Sum of electronic and thermal Enthalpies= -2222.352442
Sum of electronic and thermal Free Energies= -2222.449041
HF (M06/6-311++g(d,p) and SDD, SMD(cyclohexane): -2222.68842128

C -0.515709 0.986593 0.151493
H -1.083797 1.524502 0.904436
C -1.251199 -0.260647 -0.364796
H -1.043333 -1.127712 0.269305
C -0.048737 1.777447 -1.062345
C -0.733875 -0.455205 -1.803944
C -0.404527 0.959943 -2.310540
H -1.479457 -0.959251 -2.424101
H 0.170924 -1.071529 -1.796777
H 0.377705 0.982090 -3.073026
H -1.301367 1.442693 -2.719841
C -0.068493 3.260699 -1.093967
H -0.312403 3.713559 -2.051603
C 0.983014 1.018572 0.302729
C 1.544074 2.140943 1.225243
C 2.958704 2.562784 0.777402
H 3.362068 3.301098 1.480324
H 3.638503 1.707504 0.751231
H 2.954373 3.010093 -0.222084
C 1.613078 1.565492 2.658617
H 2.324174 0.740360 2.727436
H 1.932877 2.360536 3.342982
H 0.640648 1.192154 2.994961
Pt 2.171323 -0.702410 -0.019836
Cl 3.143314 0.316045 -1.969046
Cl 1.119287 -1.749192 1.862656
C 3.286519 -2.259005 -0.234260
O 3.954875 -3.177882 -0.347329
H 1.209470 1.482065 -0.921744
C 0.246700 4.009367 -0.030613
H 0.231085 5.092911 -0.124811
C 0.641461 3.419946 1.294877
H -0.261021 3.202860 1.883353
H 1.189234 4.167589 1.879154
O -2.639785 0.064011 -0.378325
Si -3.867553 -0.929035 0.221694
C -3.595598 -1.228958 2.067874
H -2.626873 -1.710401 2.250142
H -3.611687 -0.295482 2.641913
H -4.367937 -1.888946 2.481508
C -3.839169 -2.594741 -0.674819
H -4.615955 -3.267182 -0.290658
H -3.995523 -2.486418 -1.754215
H -2.876085 -3.099467 -0.528774
C -5.471619 0.050540 -0.128104
C -5.422838 1.415535 0.592845
H -4.569763 2.017157 0.259364
H -6.337866 1.989748 0.385852
H -5.350223 1.302424 1.681588
C -5.619704 0.293504 -1.645685
H -4.772619 0.861281 -2.046923
H -5.689944 -0.646435 -2.206553
H -6.534952 0.866776 -1.853680
C -6.693275 -0.746282 0.380059
H -7.620850 -0.190925 0.179470
H -6.785534 -1.720901 -0.115226
H -6.649075 -0.923000 1.461980

I4'$_{CO}$

Zero-point correction= 0.476464 (Hartree/Particle)
Thermal correction to Energy= 0.508555
Thermal correction to Enthalpy= 0.509499
Thermal correction to Gibbs Free Energy= 0.411855
Sum of electronic and zero-point Energies= -2222.398877
Sum of electronic and thermal Energies= -2222.366787
Sum of electronic and thermal Enthalpies= -2222.365843
Sum of electronic and thermal Free Energies= -2222.463487
HF (M06/6-311++g(d,p) and SDD, SMD(cyclohexane): -2222.70230500

C -0.354651 1.205944 -0.024753
H -0.713737 1.251792 1.002055
C -1.092053 0.111254 -0.839250
H -0.734575 -0.890493 -0.598035
C -0.504198 2.414663 -0.850257
C -0.826955 0.510349 -2.297328
C -0.912020 2.045685 -2.250232
H -1.558236 0.062589 -2.973789
H 0.174867 0.190067 -2.602648
H -0.334795 2.574599 -3.016787
H -1.957635 2.378440 -2.352766
C -0.266117 3.765582 -0.495849
H -0.537919 4.521117 -1.230105
C 1.237360 1.189745 -0.021447
C 1.917638 2.091492 1.049000
C 3.142464 2.775198 0.403347
H 3.691175 3.375950 1.138988
H 3.823185 2.019549 -0.000495
H 2.849883 3.430221 -0.425660
C 2.388926 1.318478 2.304739
H 3.153818 0.582937 2.040738
H 2.828702 2.018387 3.026544
H 1.569903 0.780268 2.786770
Pt 1.955791 -0.873330 -0.054462
Cl 3.292944 -0.245394 -1.938377
Cl 0.534747 -1.520711 1.779571
C 2.697376 -2.638339 -0.112019
O 3.158052 -3.684947 -0.138955
H 1.600835 1.490718 -1.009536
C 0.394689 4.148711 0.633290
H 0.605264 5.210532 0.751109
C 0.950398 3.214804 1.636023
H 0.138168 2.698285 2.163755
H 1.507310 3.774373 2.392698
O -2.488166 0.245543 -0.592032
Si -3.466068 -0.720849 0.395581
C -3.206849 -0.265232 2.211212
H -2.173781 -0.478020 2.510269
H -3.408347 0.795658 2.402689
H -3.863382 -0.851043 2.866486
C -3.041768 -2.541201 0.135830
H -3.723374 -3.184685 0.705595
H -3.109053 -2.836004 -0.917741
H -2.025088 -2.757389 0.484476
C -5.241990 -0.300143 -0.184333
C -5.511785 1.209925 -0.007176
H -4.809887 1.816386 -0.591246
H -6.528455 1.459866 -0.344667
H -5.431493 1.520480 1.041871
C -5.411398 -0.666289 -1.674396
H -4.693822 -0.129101 -2.305064
H -5.274041 -1.740209 -1.850482
H -6.422127 -0.405549 -2.021502
C -6.269495 -1.096106 0.650294
H -7.292759 -0.856155 0.326547
H -6.140455 -2.179744 0.537634
H -6.204185 -0.860288 1.719602

Ts4'-5'$_{CO}$

Zero-point correction= 0.476169 (Hartree/Particle)
Thermal correction to Energy= 0.507822
Thermal correction to Enthalpy= 0.508766
Thermal correction to Gibbs Free Energy= 0.411518
Sum of electronic and zero-point Energies= -2222.391102
Sum of electronic and thermal Energies= -2222.359450
Sum of electronic and thermal Enthalpies= -2222.358505
Sum of electronic and thermal Free Energies= -2222.455753
HF (M06/6-311++g(d,p) and SDD, SMD(cyclohexane): -2222.69675630

C 0.359419 1.098140 -0.059937
H 0.642812 1.144497 -1.105413
C 1.088269 0.053002 0.805208
H 0.790628 -0.974936 0.576247
C 0.208060 2.300523 0.744067
C 0.733733 0.458295 2.247611
C 0.579864 1.991450 2.190651
H 1.516092 0.135261 2.938548
H -0.202567 -0.019144 2.554195
H -0.138291 2.387989 2.916372
H 1.542415 2.483987 2.381081
C 0.291283 3.681925 0.256370
H 0.873390 4.358530 0.879140
C -1.170513 1.388450 0.161235
C -2.054271 2.254392 -0.789495
C -3.020321 3.059823 0.110155
H -3.687643 3.677031 -0.503026
H -3.642804 2.380834 0.703565
H -2.483643 3.720904 0.797108
C -2.910934 1.432183 -1.779507
H -3.607236 0.767509 -1.255361
H -3.514693 2.115868 -2.389663
H -2.296962 0.826421 -2.450423
Pt -1.892330 -0.925601 0.018171
Cl -3.122035 -0.554443 2.038116
Cl -0.655035 -1.341338 -1.990998
C -2.541412 -2.664161 -0.050557
O -2.947596 -3.731974 -0.093503
H -1.608689 1.231527 1.145364
C -0.308387 4.121512 -0.856573
H -0.190802 5.159647 -1.157818
C -1.201388 3.228434 -1.661739
H -0.615408 2.640209 -2.383604
H -1.888588 3.831853 -2.265830
O 2.481285 0.235939 0.601127
Si 3.505706 -0.655519 -0.407822
C 3.284610 -0.117651 -2.205780
H 2.276183 -0.362432 -2.560412
H 3.435294 0.960897 -2.331578
H 3.994980 -0.632002 -2.865036
C 3.103176 -2.495377 -0.257232
H 3.805009 -3.095805 -0.848896
H 3.155703 -2.848199 0.779320
H 2.097208 -2.710153 -0.637420
C 5.253818 -0.236200 0.243652
C 5.500171 1.285590 0.146208
H 4.763439 1.851141 0.727901
H 6.497486 1.535988 0.536763
H 5.457094 1.643595 -0.889838
C 5.382262 -0.667540 1.720862
H 4.636487 -0.170257 2.351151
H 5.258834 -1.750571 1.844570
H 6.377234 -0.406163 2.109994
C 6.321591 -0.976184 -0.591889
H 7.328833 -0.736338 -0.221451
H 6.207149 -2.065957 -0.534678
H 6.289395 -0.690667 -1.650586

I5'$_{CO}$

Zero-point correction= 0.477095 (Hartree/Particle)
Thermal correction to Energy= 0.508926
Thermal correction to Enthalpy= 0.509870
Thermal correction to Gibbs Free Energy= 0.413317
Sum of electronic and zero-point Energies= -2222.409006
Sum of electronic and thermal Energies= -2222.377176
Sum of electronic and thermal Enthalpies= -2222.376231
Sum of electronic and thermal Free Energies= -2222.472784
HF (M06/6-311++g(d,p) and SDD, SMD(cyclohexane): -2222.71434001

C -0.246823 0.498008 0.070342
H 0.185743 0.492947 -0.930485
C 0.816541 -0.053898 1.053251
H 0.635239 -1.121933 1.221902
C 0.531513 2.545190 0.763278
C 0.743116 0.683715 2.392493
C 1.053962 2.178694 2.109746
H 1.470853 0.281098 3.103298
H -0.257463 0.561829 2.815253
H 0.535506 2.803730 2.854093
H 2.123776 2.388942 2.178787
C 1.332848 3.287637 -0.154248
H 2.326410 3.598324 0.155801
C -0.766049 2.003602 0.383548
C -1.465361 2.776026 -0.770444
C -1.990400 4.103723 -0.173750
H -2.483251 4.702259 -0.948764
H -2.727844 3.903116 0.611175
H -1.191248 4.713468 0.263230
C -2.658633 2.018458 -1.372279
H -3.384869 1.752463 -0.597710
H -3.165863 2.655364 -2.108562
H -2.350207 1.098304 -1.877375
Pt -1.877676 -0.904142 0.034707
Cl -2.807376 -0.040067 2.072920
Cl -0.941037 -1.683652 -2.031387
C -3.212888 -2.289612 -0.022236
O -3.986963 -3.131219 -0.057667
H -1.436916 1.920060 1.243479
C 0.878169 3.553319 -1.407583
H 1.524120 4.084817 -2.104838
C -0.446939 3.079289 -1.896800
H -0.262837 2.169524 -2.494828
H -0.867047 3.804551 -2.606498
O 2.142055 0.125946 0.544601
Si 3.079392 -0.944521 -0.371595
C 2.910962 -0.517277 -2.203600
H 1.889050 -0.718482 -2.545339
H 3.135230 0.538566 -2.397704
H 3.588998 -1.119672 -2.820743
C 2.515988 -2.721786 -0.079796
H 3.176712 -3.422757 -0.604978
H 2.518862 -2.998746 0.981119
H 1.503406 -2.874714 -0.471460
C 4.872841 -0.648883 0.237591
C 5.254676 0.836650 0.059445
H 4.582701 1.494144 0.623850
H 6.277618 1.017049 0.421862
H 5.222991 1.145607 -0.992874
C 4.988343 -1.016016 1.732642
H 4.297704 -0.426443 2.347050
H 4.773434 -2.076528 1.911702
H 6.007407 -0.822842 2.098835
C 5.857294 -1.520416 -0.572386
H 6.886993 -1.365046 -0.218593
H 5.638481 -2.590595 -0.471015
H 5.840860 -1.275156 -1.641334

Ts5'-5b'$_{CO}$

Zero-point correction= 0.473110 (Hartree/Particle)
Thermal correction to Energy= 0.504669
Thermal correction to Enthalpy= 0.505613
Thermal correction to Gibbs Free Energy= 0.408725
Sum of electronic and zero-point Energies= -2222.399710
Sum of electronic and thermal Energies= -2222.368151
Sum of electronic and thermal Enthalpies= -2222.367207
Sum of electronic and thermal Free Energies= -2222.464095
HF (M06/6-311++g(d,p) and SDD, SMD(cyclohexane): -2222.70110992

C 0.172251 0.098683 0.109236
H -0.159504 -0.247575 1.085953
C -0.749521 -0.516900 -0.952473
H -0.570312 -1.596172 -0.989272
C -0.414465 2.303931 -1.008396
C -0.497329 0.101417 -2.327451
C -0.791248 1.605863 -2.288076
H -1.140232 -0.370071 -3.077834
H 0.543085 -0.072908 -2.615425
H -0.329450 2.131991 -3.133909
H -1.873548 1.778978 -2.378705
C -0.642218 3.743693 -0.954968
H -0.785550 4.274841 -1.891728
C 0.125184 1.610777 0.100704
C 0.382765 2.425845 1.418128
C 1.812353 3.017072 1.409722
H 1.981210 3.580795 2.334954
H 2.562369 2.224498 1.348134
H 1.974119 3.695900 0.565390
C 0.228800 1.552315 2.676862
H 0.970180 0.749379 2.711072
H 0.375119 2.180395 3.563445
H -0.768535 1.104651 2.746432
Pt 2.142278 -0.717654 -0.031823
Cl 2.829204 1.141612 -1.427136
Cl 1.332057 -2.501026 1.323200

C 3.898707 -1.543447 -0.138489
O 4.927297 -2.040214 -0.198773
H 1.043037 1.914531 -0.708679
C -0.799326 4.347661 0.235833
H -1.078869 5.398480 0.279838
C -0.645389 3.581571 1.515535
H -1.636750 3.194085 1.803800
H -0.343831 4.255109 2.326501
O -2.125775 -0.254710 -0.613817
Si -3.207013 -1.357697 0.064778
C -2.734243 -1.751769 1.851140
H -1.718537 -2.162333 1.902839
H -2.765491 -0.860974 2.490052
H -3.412293 -2.496002 2.287102
C -3.205686 -2.958955 -0.941920
H -3.961421 -3.660103 -0.567135
H -3.416171 -2.775658 -2.001720
H -2.236770 -3.468538 -0.877559
C -4.899296 -0.463730 -0.027689
C -4.824676 0.884028 0.722736
H -4.061983 1.542577 0.290910
H -5.790061 1.408512 0.666560
H -4.590004 0.748109 1.785861
C -5.282942 -0.193221 -1.498351
H -4.531637 0.423667 -2.005192
H -5.394732 -1.121861 -2.071514
H -6.243431 0.340491 -1.552371
C -5.991106 -1.340841 0.623584
H -6.966391 -0.834573 0.578463
H -6.103096 -2.305070 0.112384
H -5.779344 -1.544946 1.680264

5b'-[Pt]$_{CO}$

Zero-point correction= 0.478064 (Hartree/Particle)
Thermal correction to Energy= 0.510098
Thermal correction to Enthalpy= 0.511042
Thermal correction to Gibbs Free Energy= 0.412627
Sum of electronic and zero-point Energies= -2222.433343
Sum of electronic and thermal Energies= -2222.401309
Sum of electronic and thermal Enthalpies= -2222.400365
Sum of electronic and thermal Free Energies= -2222.498779
HF (M06/6-311++g(d,p) and SDD, SMD(cyclohexane): -2222.73368707

C -0.067810 0.301888 0.166193
H -0.280225 -0.140670 1.134243
C -0.966485 -0.237207 -0.950815
H -0.796186 -1.316244 -1.058879
C 0.406280 2.432580 -1.100060
C -0.710090 0.461447 -2.285850
C -0.696431 1.976890 -2.092306
H -1.497383 0.170210 -2.989559
H 0.248188 0.122316 -2.694758
H -0.532806 2.487648 -3.048193
H -1.672501 2.302822 -1.714371
C 0.264450 3.915613 -0.840184
H 0.240291 4.541537 -1.730452
C 0.431412 1.599551 0.167930
C 0.959869 2.278324 1.432516
C 2.462151 2.624995 1.250794
H 2.814209 3.160562 2.139957
H 3.058257 1.714234 1.140281
H 2.640906 3.257471 0.378631
C 0.798812 1.443115 2.712802
H 1.364761 0.508246 2.676086
H 1.169812 2.023653 3.564956
H -0.250114 1.197508 2.913299
Pt 1.978920 -0.827917 -0.039921
Cl 2.948485 0.371255 -1.869378
Cl 1.156781 -2.198681 1.745105
C 3.433747 -2.002237 -0.161142
O 4.311509 -2.728761 -0.233068
H 1.377204 2.254604 -1.594291
C 0.108413 4.447163 0.371446
H -0.047494 5.517945 0.486671
C 0.150726 3.601838 1.612830
H -0.871230 3.366237 1.948138
H 0.613940 4.156940 2.438815
O -2.314398 0.006760 -0.538429
Si -3.451448 -1.157922 -0.080115
C -2.928373 -1.984862 1.535081
H -1.925653 -2.421440 1.452162
H -2.905785 -1.274210 2.369520
H -3.617418 -2.794435 1.805881
C -3.587472 -2.474315 -1.432600
H -4.366450 -3.207512 -1.189935
H -3.832670 -2.036377 -2.406685
H -2.649040 -3.031090 -1.545333
C -5.070572 -0.161961 0.121882
C -4.857200 0.978558 1.141247
H -4.064788 1.663295 0.819088
H -5.780710 1.564587 1.257102
H -4.588480 0.595971 2.133831
C -5.490590 0.450376 -1.231941
H -4.711730 1.105760 -1.638140
H -5.706635 -0.320364 -1.982129
H -6.403370 1.052161 -1.111944
C -6.196824 -1.089421 0.629374
H -7.133136 -0.524294 0.743730
H -6.398933 -1.912474 -0.067628
H -5.960775 -1.527920 1.606796

Ts3'-5b'$_{CO}$

Zero-point correction= 0.474238 (Hartree/Particle)
Thermal correction to Energy= 0.506246
Thermal correction to Enthalpy= 0.507191
Thermal correction to Gibbs Free Energy= 0.409682
Sum of electronic and zero-point Energies= -2222.373050
Sum of electronic and thermal Energies= -2222.341042
Sum of electronic and thermal Enthalpies= -2222.340098
Sum of electronic and thermal Free Energies= -2222.437606
HF (M06/6-311++g(d,p) and SDD, SMD(cyclohexane): -2222.67518457

C -0.494914 0.726707 0.412452
H -1.137917 1.337041 1.052566
C -1.253478 -0.313206 -0.352985
H -1.074557 -1.261387 0.178578
C 0.456063 1.808034 -1.260575
C -0.685325 -0.419834 -1.781354
C -0.383409 0.998927 -2.271584
H -1.416903 -0.922586 -2.420379
H 0.226382 -1.024112 -1.770372
H 0.155805 0.961103 -3.224240
H -1.334159 1.516413 -2.441094
C -0.033595 3.213499 -1.060890
H -0.403069 3.688910 -1.969539
C 0.864555 1.020877 0.284995
C 1.430289 2.115347 1.253916
C 2.799136 2.638490 0.769181
H 3.200606 3.342837 1.507425
H 3.517212 1.823582 0.650442
H 2.727988 3.164981 -0.187099
C 1.614315 1.504407 2.659489
H 2.357024 0.703204 2.657468
H 1.950541 2.285332 3.352588
H 0.679800 1.083362 3.046813
Pt 2.173757 -0.667931 -0.028732
Cl 3.290845 0.314185 -1.910742
Cl 1.035484 -1.787838 1.774415
C 3.372512 -2.167212 -0.156773
O 4.088237 -3.055389 -0.217633
H 1.503123 1.796601 -1.587862
C -0.021762 3.895450 0.085531
H -0.403635 4.914782 0.097523
C 0.465796 3.327587 1.389219
H -0.398184 3.066866 2.022722
H 0.989486 4.110551 1.953440
O -2.626319 0.040247 -0.370293
Si -3.883676 -0.944303 0.203064
C -3.644820 -1.240709 2.053888
H -2.685315 -1.732903 2.256432
H -3.663740 -0.306460 2.626726
H -4.431102 -1.892199 2.454370
C -3.834051 -2.607690 -0.694181
H -4.622723 -3.276367 -0.328238
H -3.964951 -2.498438 -1.776698
H -2.878159 -3.118944 -0.525252
C -5.466305 0.050762 -0.184244
C -5.415456 1.420050 0.528637
H -4.553392 2.013154 0.203171
H -6.322555 1.999817 0.304417
H -5.359960 1.313598 1.619041
C -5.584072 0.282781 -1.706295
H -4.724019 0.837785 -2.097614
H -5.656191 -0.660802 -2.260615
H -6.488645 0.864819 -1.934216
C -6.704240 -0.731246 0.308424
H -7.622114 -0.168720 0.085779
H -6.796904 -1.708984 -0.180596
H -6.681770 -0.898836 1.392408

I1$_{CO}^{eq}$

Zero-point correction= 0.469552 (Hartree/Particle)
Thermal correction to Energy= 0.505467
Thermal correction to Enthalpy= 0.506411
Thermal correction to Gibbs Free Energy= 0.395754
Sum of electronic and zero-point Energies= -2222.372422
Sum of electronic and thermal Energies= -2222.336507

Sum of electronic and thermal Enthalpies= -2222.335563
Sum of electronic and thermal Free Energies= -2222.446220
HF (M06/6-311++g(d,p) and SDD, SMD(cyclohexane): -2222.65651657

C 1.659444 -0.615463 2.045113
C 0.866658 0.134220 1.220983
C 4.758792 3.962056 0.991861
C 2.146109 3.315467 -0.538111
C 0.147834 1.205645 0.946629
C -0.684841 1.494688 -0.283820
H -0.529248 0.691947 -1.017166
H 5.511347 4.264786 1.714480
C 3.159877 -0.446926 2.090388
H 3.667423 -1.416602 2.129252
H 3.393169 0.082298 3.025996
H 3.543101 0.127100 1.249099
C 1.064155 -1.477612 3.132720
H 1.299832 -0.984047 4.087267
H 1.523699 -2.470941 3.155340
H -0.014676 -1.581559 3.038382
C 1.058478 3.028444 -1.537618
C -0.357975 2.851596 -0.937280
H -0.555793 3.643279 -0.203567
H -1.091307 2.985452 -1.742181
H 1.011905 3.855651 -2.256749
H 1.321929 2.127712 -2.110047
Pt 1.097661 -1.586829 -0.203874
H 0.106044 1.976747 1.719290
Cl -0.765370 -2.764974 0.715809
Cl 2.895250 -0.443054 -1.287821
C 2.740418 4.510102 -0.386709
C 3.819039 4.815937 0.562244
H 2.449505 2.490784 0.102942
H 4.817183 2.941530 0.621151
H 3.851351 5.845389 0.922207
H 2.395477 5.345106 -0.999747
O -2.037520 1.514449 0.163255
Si -3.432470 0.979314 -0.620934
C -4.641653 0.552994 0.799629
C -5.976396 0.032698 0.223155
H -6.673144 -0.213484 1.037613
H -6.472066 0.777402 -0.412232
H -5.839512 -0.879299 -0.371053
C -4.912306 1.816967 1.644714
H -3.985939 2.226971 2.062625
H -5.396102 2.607998 1.058098
H -5.581396 1.579057 2.484861
C -4.023559 -0.533896 1.704523
H -3.835839 -1.465828 1.158771
H -3.069817 -0.206379 2.132235
H -4.704190 -0.769108 2.536190
C -4.127509 2.367826 -1.704693
H -3.455258 2.590545 -2.542317
H -5.098614 2.090866 -2.133653
H -4.265388 3.293998 -1.135606
C -3.042962 -0.511917 -1.714390
H -2.576396 -1.325220 -1.147968
H -3.960517 -0.900446 -2.173224
H -2.366702 -0.240507 -2.535171
C 1.090738 -2.837256 -1.646735
O 1.080390 -3.575180 -2.514669

I2$_{co}^{eq}$
Zero-point correction= 0.470909 (Hartree/Particle)
Thermal correction to Energy= 0.505938
Thermal correction to Enthalpy= 0.506882
Thermal correction to Gibbs Free Energy= 0.401143
Sum of electronic and zero-point Energies= -2222.368330
Sum of electronic and thermal Energies= -2222.333301
Sum of electronic and thermal Enthalpies= -2222.332357
Sum of electronic and thermal Free Energies= -2222.438096
HF (M06/6-311++g(d,p) and SDD, SMD(cyclohexane): -2222.65538778

C 1.613770 0.788777 2.072963
C 0.982348 0.538873 0.832951
C 3.675808 2.745941 0.830917
C 1.488226 2.999604 -1.263146
C 0.040144 1.457617 0.393859
C -0.906573 1.339812 -0.782243
H -0.605012 0.503199 -1.424432
H 4.426301 2.750993 1.616516
C 2.704377 -0.121996 2.546837
H 2.225103 -1.036079 2.931394
H 3.295312 0.321403 3.353633
H 3.353127 -0.438502 1.725610
C 1.144075 1.765972 3.114296
H 0.445064 2.523622 2.762652
H 1.994198 2.259643 3.593520
H 0.633999 1.182773 3.896847
C 0.337640 3.089992 -2.231451
C -0.990926 2.654256 -1.580203
H -1.331205 3.430602 -0.882213
H -1.772461 2.550833 -2.341413
H 0.220416 4.115607 -2.604288
H 0.552244 2.453683 -3.097432
Pt 1.356465 -1.243428 -0.154423
H -0.198649 2.322781 1.007471
Cl -0.079362 -2.261892 1.476244
Cl 2.916495 -0.215346 -1.663672
C 1.794955 3.930446 -0.325402
C 2.850634 3.803441 0.667908
H 2.116553 2.118925 -1.362195
H 3.676256 1.890859 0.161362
H 2.946020 4.640477 1.359198
H 1.194661 4.840067 -0.272085
O -2.165325 1.098395 -0.160343
Si -3.431714 0.096211 -0.682981
C -2.778230 -1.581599 -1.238337
H -2.130711 -1.487905 -2.119331
H -2.197257 -2.072378 -0.450778
H -3.609130 -2.241269 -1.518826
C -4.314628 0.922476 -2.142378
H -5.195373 0.343123 -2.446544
H -4.650360 1.937148 -1.900199
H -3.657437 0.988064 -3.018498
C -4.572998 -0.014337 0.845590
C -5.803026 -0.890904 0.519454
H -5.519339 -1.915715 0.250074
H -6.462896 -0.957525 1.396447
H -6.400138 -0.479085 -0.303970
C -5.052492 1.397144 1.248644
H -5.637375 1.875608 0.453293
H -5.696862 1.340287 2.138172
H -4.210008 2.055511 1.488791
C -3.804775 -0.642414 2.028337
H -3.453211 -1.655087 1.801050
H -2.926741 -0.047417 2.300859
H -4.456527 -0.707611 2.912187
C 1.624992 -2.960794 -1.033168
O 1.770327 -3.971773 -1.545466

Ts2-3$_{co}^{eq}$
Zero-point correction= 0.472276 (Hartree/Particle)
Thermal correction to Energy= 0.505640
Thermal correction to Enthalpy= 0.506584
Thermal correction to Gibbs Free Energy= 0.406214
Sum of electronic and zero-point Energies= -2222.365408
Sum of electronic and thermal Energies= -2222.332044
Sum of electronic and thermal Enthalpies= -2222.331100
Sum of electronic and thermal Free Energies= -2222.431469
HF (M06/6-311++g(d,p) and SDD, SMD(cyclohexane): -2222.65219053

C 1.710895 1.031731 1.956359
C 1.034272 0.673625 0.752137
C 3.385529 2.380433 0.875546
C 1.357964 2.812991 -1.256328
C 0.050809 1.533149 0.262786
C -0.955976 1.269328 -0.844158
H -0.631755 0.408609 -1.443414
H 4.093468 2.312841 1.695912
C 2.689226 0.059358 2.569729
H 2.104615 -0.730951 3.062297
H 3.3203 0.536776 3.326171
H 3.313929 -0.432774 1.820448
C 1.155455 2.022648 2.96011
H 0.634541 2.872869 2.519174
H 1.946537 2.403711 3.612334
H 0.437416 1.486304 3.597153
C 0.267088 2.98265 -2.28424
C -1.094061 2.530596 -1.718049
H -1.50936 3.318747 -1.076662
H -1.818682 2.358791 -2.521025
H 0.198499 4.028544 -2.608263
H 0.524652 2.381988 -3.163675
Pt 1.412184 -1.162773 -0.13166
H -0.261372 2.380794 0.868776
Cl -0.040883 -2.06871 1.545942
Cl 2.960998 -0.250557 -1.736633
C 1.756559 3.784555 -0.361259
C 2.727642 3.56902 0.651816
H 1.983908 1.93591 -1.384405
H 3.461614 1.60978 0.116526
H 2.863348 4.373161 1.373595
H 1.229782 4.739109 -0.354326
O -2.190494 1.014164 -0.190957
Si -3.451952 -0.00626 -0.675167
C -2.78534 -1.693541 -1.187621
H -2.174704 -1.623306 -2.096756
H -2.162034 -2.133113 -0.40222

H -3.608665 -2.385195 -1.406396
C -4.36536 0.761805 -2.149176
H -5.244176 0.16216 -2.417398
H -4.70982 1.780296 -1.936427
H -3.725031 0.804512 -3.03909
C -4.581636 -0.081742 0.865141
C -5.829033 -0.941703 0.563573
H -5.564967 -1.972281 0.295801
H -6.47666 -0.994053 1.450737
H -6.432239 -0.525729 -0.253164
C -5.033197 1.343226 1.252777
H -5.614141 1.821699 0.454324
H -5.672941 1.310028 2.146876
H -4.176945 1.988559 1.478461
C -3.81117 -0.705625 2.048448
H -3.494621 -1.733107 1.836324
H -2.910568 -0.132463 2.292208
H -4.44891 -0.733277 2.944524
C 1.67129 -2.939499 -0.894377
O 1.809774 -3.98485 -1.334563

I3$_{CO}^{eq}$
Zero-point correction= 0.476868 (Hartree/Particle)
Thermal correction to Energy= 0.509235
Thermal correction to Enthalpy= 0.510180
Thermal correction to Gibbs Free Energy= 0.411698
Sum of electronic and zero-point Energies= -2222.397268
Sum of electronic and thermal Energies= -2222.364901
Sum of electronic and thermal Enthalpies= -2222.363957
Sum of electronic and thermal Free Energies= -2222.462438
HF (M06/6-311++g(d,p) and SDD, SMD(cyclohexane): -2222.69728949

C 1.873621 1.305372 1.765804
C 1.117149 0.767451 0.576324
C 2.974964 2.315837 1.173854
C 1.143768 2.498490 -1.140738
C 0.181655 1.656284 -0.125136
C -0.945556 1.104304 -1.033567
H -0.589285 0.200739 -1.548411
H 3.648159 2.502676 2.016496
C 2.658805 0.214096 2.524845
H 1.981968 -0.537537 2.937645
H 3.212475 0.674640 3.351278
H 3.377552 -0.292162 1.873013
C 0.960089 2.051128 2.770523
H 0.518649 2.957142 2.350172
H 1.557175 2.343123 3.641483
H 0.155651 1.394983 3.118268
C 0.251534 2.730584 -2.394809
C -1.158304 2.248985 -2.041081
H -1.729798 3.036833 -1.534253
H -1.735668 1.934458 -2.915188
H 0.267507 3.784516 -2.693355
H 0.659127 2.151602 -3.229671
Pt 1.453591 -1.081213 -0.087832
H -0.285823 2.380868 0.546156
Cl -0.116634 -1.801345 1.589456
Cl 3.096664 -0.422414 -1.709601
C 1.660377 3.712568 -0.435307
C 2.477195 3.622208 0.623012
H 1.980851 1.856882 -1.426165
H 3.552468 1.764112 0.422743
H 2.777892 4.529866 1.142119
H 1.296334 4.685452 -0.763361
O -2.087708 0.834364 -0.255791
Si -3.423139 -0.121290 -0.661456
C -2.871827 -1.870969 -1.105750
H -2.217702 -1.868050 -1.987109
H -2.318630 -2.337793 -0.284685
H -3.734739 -2.503154 -1.349286
C -4.332812 0.615354 -2.154327
H -5.263481 0.066737 -2.345535
H -4.594087 1.668909 -2.003378
H -3.730502 0.548830 -3.068519
C -4.532020 -0.060753 0.896212
C -5.818401 -0.880539 0.653150
H -5.601278 -1.934923 0.442051
H -6.459247 -0.854626 1.546356
H -6.410925 -0.485275 -0.181383
C -4.916387 1.403014 1.203872
H -5.488010 1.858463 0.385547
H -5.543140 1.451481 2.106408
H -4.030020 2.022634 1.380604
C -3.781289 -0.648185 2.109990
H -3.513833 -1.699987 1.957504
H -2.854245 -0.103315 2.315457
H -4.413222 -0.594640 3.008994
C 1.680981 -2.964415 -0.678888
O 1.796449 -4.045841 -1.017479

Ts3-2b$_{CO}^{eq}$
Zero-point correction= 0.473072 (Hartree/Particle)
Thermal correction to Energy= 0.504710
Thermal correction to Enthalpy= 0.505654
Thermal correction to Gibbs Free Energy= 0.409402
Sum of electronic and zero-point Energies= -2222.370966
Sum of electronic and thermal Energies= -2222.339328
Sum of electronic and thermal Enthalpies= -2222.338384
Sum of electronic and thermal Free Energies= -2222.434636
HF (M06/6-311++g(d,p) and SDD, SMD(cyclohexane): -2222.67801185

C 3.035467 0.756815 0.700028
C 1.580723 0.623654 0.140302
C 3.740588 2.138839 0.513766
C 1.366563 3.105181 -0.72747
C 0.856864 1.686765 -0.42319
C -0.608609 1.60991 -0.918708
H -0.51447 1.245785 -1.956254
H 4.729329 2.046615 0.975362
C 3.922775 -0.285623 -0.022777
H 3.590908 -1.306138 0.185547
H 4.954335 -0.180929 0.334518
H 3.911312 -0.147891 -1.108108
C 3.019774 0.43479 2.212577
H 2.430289 1.168773 2.77473
H 4.047496 0.464288 2.594291
H 2.599721 -0.55122 2.41344
C 0.183752 3.836299 -1.404677
C -1.057821 3.082577 -0.928223
H -1.326314 3.370069 0.096102
H -1.932284 3.243006 -1.562701
H 0.166849 4.900101 -1.14906
H 0.275683 3.765871 -2.494375
Pt 0.835045 -1.323215 -0.085553
H 0.760987 1.266543 0.884899
Cl 0.165783 -1.537539 2.206608
Cl 1.352046 -1.036636 -2.423531
C 1.899375 3.781924 0.519093
C 3.013459 3.324457 1.093085
H 2.197395 2.987393 -1.436041
H 3.92463 2.30497 -0.557528
H 3.405955 3.801215 1.988496
H 1.346021 4.63125 0.914551
O -1.410591 0.767412 -0.146836
Si -2.962408 0.159527 -0.509522
C -4.065908 0.554912 1.004063
C -2.838677 -1.694311 -0.812214
H -3.820337 -2.116488 -1.06137
H -2.164069 -1.899138 -1.651433
H -2.45601 -2.219306 0.068704
C -3.619907 0.974971 -2.088391
H -2.893441 0.905637 -2.907568
H -4.522853 0.448732 -2.421143
H -3.886477 2.029696 -1.95998
C -3.571545 -0.229491 2.238968
H -3.647515 -1.31267 2.090439
H -2.526092 -0.007085 2.477763
H -4.182458 0.02472 3.117616
C -4.031107 2.064224 1.323332
H -3.023508 2.39222 1.60263
H -4.36611 2.677512 0.476654
H -4.696126 2.289119 2.169622
C -5.523102 0.143286 0.69174
H -6.166858 0.345818 1.559736
H -5.938982 0.69997 -0.157484
H -5.611913 -0.927212 0.468747
C 0.36812 -3.167418 -0.384072
O 0.141505 -4.274094 -0.558169

2b-[Pt]$_{CO}^{eq}$
Zero-point correction= 0.477543 (Hartree/Particle)
Thermal correction to Energy= 0.509639
Thermal correction to Enthalpy= 0.510583
Thermal correction to Gibbs Free Energy= 0.413754
Sum of electronic and zero-point Energies= -2222.424698
Sum of electronic and thermal Energies= -2222.392602
Sum of electronic and thermal Enthalpies= -2222.391657
Sum of electronic and thermal Free Energies= -2222.488487
HF (M06/6-311++g(d,p) and SDD, SMD(cyclohexane): -2222.72786559

C 1.114927 1.861977 1.786656
C 0.424251 0.918185 0.793242
C 1.917241 3.011998 1.116096
C 0.919151 2.071439 -1.496629

C 0.247323 1.056273 -0.570606
C -0.976127 0.443277 -1.299006
H -0.726330 -0.573320 -1.632998
H 2.359142 3.614221 1.918378
C 2.044112 1.083590 2.741186
H 1.527067 0.225131 3.185468
H 2.372901 1.738517 3.557230
H 2.933558 0.715789 2.220878
C -0.050001 2.460315 2.619838
H -0.769676 2.987097 1.984983
H 0.347549 3.172331 3.353076
H -0.585667 1.677308 3.168042
C 0.287827 1.788837 -2.874606
C -1.141885 1.353160 -2.537987
H -1.751375 2.218424 -2.250477
H -1.650517 0.839654 -3.359803
H 0.329739 2.660832 -3.535240
H 0.830849 0.974959 -3.370443
Pt 1.738339 -0.903146 -0.014715
H -0.324154 0.288459 1.271478
Cl -0.055642 -2.310238 0.700457
Cl 3.696228 0.299285 -0.701600
C 0.631288 3.472763 -0.975850
C 1.099445 3.895665 0.202339
H 2.001769 1.924345 -1.518060
H 2.753543 2.570623 0.561663
H 0.877520 4.909531 0.530569
H 0.028891 4.128301 -1.603426
O -2.091827 0.411911 -0.441120
Si -3.584047 -0.344114 -0.702525
C -4.406675 -0.399534 1.022948
C -3.322309 -2.061642 -1.442299
H -4.269586 -2.613187 -1.489441
H -2.932601 -2.004389 -2.466337
H -2.613918 -2.648375 -0.848305
C -4.621070 0.695981 -1.898934
H -4.132398 0.791424 -2.875485
H -5.601398 0.234850 -2.070490
H -4.792319 1.708308 -1.514876
C -3.674025 -1.402110 1.940493
H -3.730889 -2.426729 1.554028
H -2.613640 -1.155009 2.058226
H -4.131484 -1.403928 2.940815
C -4.362302 1.001548 1.671578
H -3.333065 1.349907 1.809824
H -4.890737 1.751306 1.069313
H -4.845285 0.977745 2.659487
C -5.881387 -0.840535 0.881507
H -6.354796 -0.897847 1.872178
H -6.468604 -0.135556 0.280959
H -5.974619 -1.832979 0.422071
C 2.786860 -2.465714 -0.189651
O 3.417695 -3.410834 -0.286713

Ts3^{eq} -3'$_{CO}$
Zero-point correction= 0.476528 (Hartree/Particle)
Thermal correction to Energy= 0.508268
Thermal correction to Enthalpy= 0.509212
Thermal correction to Gibbs Free Energy= 0.411798
Sum of electronic and zero-point Energies= -2222.388309
Sum of electronic and thermal Energies= -2222.356570
Sum of electronic and thermal Enthalpies= -2222.355625
Sum of electronic and thermal Free Energies= -2222.453040
HF (M06/6-311++g(d,p) and SDD, SMD(cyclohexane): -2222.68686741

C -0.043635 1.538161 -0.114629
H -0.508838 2.267059 0.556161
C -1.210205 0.768718 -0.788656
H -0.837429 -0.159882 -1.240831
C 0.659246 2.376707 -1.277105
C -1.672276 1.760445 -1.873778
C -0.387216 2.373864 -2.436904
H 0.000195 1.771053 -3.264687
H -0.546384 3.387149 -2.821515
C 1.073508 3.718956 -0.749551
H 0.975242 4.554432 -1.441888
C 1.073087 0.847054 0.53956
C 1.664133 1.518936 1.744344
C 2.982535 0.868877 2.218442
H 3.33113 1.369618 3.129421
H 2.844402 -0.191802 2.447931
H 3.760377 0.958161 1.454125
C 0.57093 1.235627 2.8437
H 0.347495 0.168473 2.921876
H 0.984011 1.575173 3.799787
H -0.358788 1.775534 2.649422
Pt 1.784936 -0.886961 -0.13128
Cl 3.411143 0.197398 -1.53217
Cl 0.330793 -2.137372 1.308812
C 2.483733 -2.621826 -0.821046
O 2.875436 -3.610848 -1.226255
H 1.551622 1.850849 -1.62874
C 1.555268 3.97443 0.470911
H 1.80939 5.01285 0.686355
C 1.902379 3.082389 1.644739
H 1.453947 3.534683 2.539849
H 2.983679 3.218215 1.781652
O -2.20786 0.505969 0.16942
Si -3.360272 -0.731302 0.253761
C -3.312217 -1.366453 2.026712
H -2.312349 -1.747932 2.256028
H -3.543305 -0.572343 2.746299
H -4.02987 -2.180087 2.185667
C -2.922849 -2.104399 -0.967508
H -3.678718 -2.898748 -0.940694
H -2.861175 -1.748252 -2.002706
H -1.959613 -2.555041 -0.70286
C -5.094763 0.01108 -0.123774
C -5.335692 1.258048 0.754442
H -4.590154 2.038147 0.562209
H -6.328441 1.685989 0.550542
H -5.298919 1.018709 1.82426
C -5.226246 0.413691 -1.607398
H -4.506409 1.191509 -1.885485
H -5.078248 -0.439369 -2.281109
H -6.230749 0.814979 -1.807436
C -6.179386 -1.043223 0.195126
H -7.178265 -0.64031 -0.027633
H -6.058992 -1.955288 -0.403381
H -6.174668 -1.333394 1.252164
H -2.289089 1.2791 -2.639131
H -2.287794 2.524052 -1.382482

Ts3^{eq} -4$_{CO}$
Zero-point correction= 0.473663 (Hartree/Particle)
Thermal correction to Energy= 0.505286
Thermal correction to Enthalpy= 0.506230
Thermal correction to Gibbs Free Energy= 0.409614
Sum of electronic and zero-point Energies= -2222.373276
Sum of electronic and thermal Energies= -2222.341653
Sum of electronic and thermal Enthalpies= -2222.340708
Sum of electronic and thermal Free Energies= -2222.437325
HF (M06/6-311++g(d,p) and SDD, SMD(cyclohexane): -2222.67695077

C -1.770074 1.861026 -1.475283
C -1.143689 1.038141 -0.276865
C -2.668496 3.015042 -0.944592
C -0.75436 2.11745 1.159704
C 0.225985 1.476248 0.222737
C 1.152074 0.542942 1.039748
H 0.856867 -0.499111 0.882926
H -3.01334 3.593458 -1.809778
C -2.674813 0.940894 -2.324646
H -2.097657 0.14143 -2.796329
H -3.14796 1.535125 -3.116603
H -3.469231 0.488516 -1.722558
C -0.678804 2.435674 -2.402493
H -0.119614 3.255891 -1.940816
H -1.152147 2.835082 -3.306501
H 0.026098 1.656259 -2.70923
C -0.549371 1.477305 2.546304
C 0.903792 0.969594 2.507381
H 1.598535 1.787165 2.734423
H 1.087211 0.16205 3.223411
H -0.736553 2.221129 3.326895
H -1.263279 0.662688 2.701929
Pt -1.707221 -1.00034 -0.04471
H 0.778887 2.12656 -0.444973
Cl -0.008074 -1.538427 -1.645163
Cl -3.45354 -0.3425 1.471029
C -1.186907 3.528407 1.007148
C -2.030055 3.943871 0.058142
H -1.822052 1.381999 0.718867
H -3.575752 2.581443 -0.494974
H -2.307123 4.994943 0.024489
H -0.772395 4.216082 1.741666
O 2.486118 0.748783 0.631243
Si 3.779291 -0.338622 0.686138
C 4.803958 0.036948 -0.88418
C 4.777811 0.002285 2.257178
H 5.110691 1.045285 2.307347
H 4.175545 -0.195726 3.15258
H 5.668279 -0.635831 2.316101
C 3.146454 -2.117376 0.720873
H 2.629511 -2.343968 1.661848
H 2.449452 -2.321621 -0.09915
H 3.983518 -2.821709 0.638287
C 3.955539 -0.259645 -2.139849
H 3.671936 -1.316736 -2.203772
H 3.031599 0.328959 -2.154031
H 4.523137 -0.015881 -3.049994
C 6.075619 -0.839018 -0.914879

H 6.659487 -0.630441 -1.823043
H 6.73141 -0.645899 -0.056857
H 5.838559 -1.910274 -0.92266
C 5.21586 1.525372 -0.895734
H 4.341735 2.185722 -0.869664
H 5.855668 1.781232 -0.041857
H 5.783088 1.757524 -1.809114
C -2.19138 -2.856154 0.104787
O -2.470915 -3.960329 0.1925

Ts3-5b$_{CO}^{eq}$
Zero-point correction= 0.474987 (Hartree/Particle)
Thermal correction to Energy= 0.506747
Thermal correction to Enthalpy= 0.507691
Thermal correction to Gibbs Free Energy= 0.410583
Sum of electronic and zero-point Energies= -2222.370852
Sum of electronic and thermal Energies= -2222.339092
Sum of electronic and thermal Enthalpies= -2222.338148
Sum of electronic and thermal Free Energies= -2222.435257
HF (M06/6-311++g(d,p) and SDD, SMD(cyclohexane): -2222.67196077

C -1.775992 1.864104 -1.45057
C -1.080359 1.044651 -0.295544
C -2.67118 3.020547 -0.87366
C -1.335868 1.956289 1.306286
C 0.291188 1.233342 -0.110778
C 1.186321 0.587809 0.909207
H 0.922402 -0.468407 1.022809
H -3.102512 3.567977 -1.71817
C -2.702724 0.951832 -2.284796
H -2.139104 0.149038 -2.76873
H -3.18976 1.546066 -3.068325
H -3.485565 0.501394 -1.66687
C -0.751398 2.496552 -2.42051
H -0.161911 3.293649 -1.952873
H -1.284673 2.944978 -3.265983
H -0.065166 1.743064 -2.823501
C -0.583086 1.36514 2.485794
C 0.922709 1.327413 2.249839
H 1.341448 2.337814 2.165996
H 1.460528 0.816997 3.056503
H -0.820772 1.977914 3.366308
H -0.969958 0.360738 2.683608
Pt -1.729264 -0.981317 -0.03895
H 0.825219 2.007373 -0.664732
Cl 0.0516 -1.544631 -1.557552
Cl -3.573286 -0.41718 1.388121
C -1.235433 3.417968 1.065852
C -1.915814 3.944342 0.038736
H -2.378206 1.627437 1.332291
H -3.513825 2.564195 -0.33508
H -1.877467 5.009946 -0.174179
H -0.60749 4.020413 1.719867
O 2.519755 0.753003 0.485264
Si 3.828381 -0.303981 0.706178
C 4.936479 -0.025603 -0.824917
C 4.72249 0.177236 2.30231
H 5.597426 -0.460541 2.477423
H 5.066811 1.217351 2.277785
H 4.062128 0.067446 3.171435
C 3.207807 -2.081589 0.837752
H 2.514636 -2.330702 0.026775
H 4.049441 -2.783819 0.792243
H 2.690611 -2.264954 1.787893
C 5.262166 1.47677 -0.97418
H 5.889824 1.642985 -1.861804
H 4.353422 2.077419 -1.091513
H 5.813323 1.86688 -0.10931
C 4.205363 -0.511283 -2.095431
H 3.988347 -1.585399 -2.059031
H 3.254455 0.012174 -2.244847
H 4.82843 -0.332256 -2.983795
C 6.256636 -0.813406 -0.670062
H 6.89216 -0.664566 -1.554715
H 6.834135 -0.48566 0.203139
H 6.085648 -1.893148 -0.574501
C -2.231603 -2.836907 0.086215
O -2.515535 -3.941225 0.161806

5b-[Pt]$_{CO}^{eq}$
Zero-point correction= 0.477395 (Hartree/Particle)
Thermal correction to Energy= 0.509498
Thermal correction to Enthalpy= 0.510442
Thermal correction to Gibbs Free Energy= 0.411692
Sum of electronic and zero-point Energies= -2222.424373
Sum of electronic and thermal Energies= -2222.392270
Sum of electronic and thermal Enthalpies= -2222.391325
Sum of electronic and thermal Free Energies= -2222.490075
HF (M06/6-311++g(d,p) and SDD, SMD(cyclohexane): -2222.72553758

C 2.038118 1.967289 1.489821
C 1.331651 1.574221 0.180551
C 3.285928 2.848437 1.189767
C 1.815921 2.223509 -1.105069
C 0.196846 0.777199 0.178837
C -0.863275 0.822154 -0.942939
H -0.802650 -0.081092 -1.566415
H 3.677267 3.233608 2.137249
C 2.483236 0.754852 2.333888
H 1.638899 0.131137 2.639038
H 2.981515 1.114403 3.242203
H 3.193319 0.126714 1.784997
C 1.027433 2.807109 2.321134
H 0.686700 3.687803 1.768970
H 1.516055 3.148648 3.241015
H 0.151878 2.215434 2.602846
C 0.836546 2.062297 -2.289137
C -0.622790 2.043739 -1.834955
H -0.867610 2.944038 -1.255565
H -1.300601 2.013427 -2.694962
H 1.008517 2.875991 -3.002553
H 1.064102 1.129912 -2.816902
Pt 1.279570 -1.295981 -0.016915
H -0.242925 0.537508 1.142947
Cl -0.186847 -1.966815 1.757100
Cl 2.842465 -0.833216 -1.771190
C 2.227707 3.665242 -0.843251
C 2.959265 3.961462 0.230912
H 2.737208 1.672096 -1.364971
H 4.075910 2.209829 0.764690
H 3.302618 4.973685 0.428981
H 1.937472 4.413645 -1.576981
O -2.123632 0.893333 -0.301320
Si -3.536001 0.069396 -0.733137
C -4.694530 0.305444 0.767736
C -4.265681 0.844268 -2.299606
H -5.188291 0.335326 -2.604725
H -4.500064 1.905684 -2.158344
H -3.563797 0.769539 -3.139637
C -3.147901 -1.749365 -1.066970
H -2.571153 -2.192259 -0.247522
H -4.072628 -2.328090 -1.184819
H -2.569700 -1.878045 -1.990515
C -4.810968 1.807424 1.107718
H -5.472991 1.951265 1.974228
H -3.835467 2.239904 1.355000
H -5.233248 2.385603 0.276069
C -4.127494 -0.445530 1.991906
H -4.078480 -1.527558 1.821982
H -3.117289 -0.106231 2.245791
H -4.768517 -0.279850 2.870235
C -6.098511 -0.249630 0.440480
H -6.764251 -0.134555 1.308036
H -6.566376 0.278324 -0.399563
H -6.073022 -1.318592 0.193375
C 1.806390 -3.086968 -0.145455
O 2.111422 -4.184667 -0.224129

1b-PtCl$_2$(ethene)

I1$_{et}$
Zero-point correction= 0.516637 (Hartree/Particle)
Thermal correction to Energy= 0.553012
Thermal correction to Enthalpy= 0.553956
Thermal correction to Gibbs Free Energy= 0.444258
Sum of electronic and zero-point Energies= -2187.597466
Sum of electronic and thermal Energies= -2187.561090
Sum of electronic and thermal Enthalpies= -2187.560146
Sum of electronic and thermal Free Energies= -2187.669845
HF (M06/6-311++g(d,p) and SDD, SMD(cyclohexane): -2187.91315005

C -3.199301 -1.528206 -1.536439
Si -3.711736 0.076059 -0.714617
C -4.269826 -0.217968 1.076233
C -4.859306 1.074082 1.643869
O -2.435491 1.168378 -0.737595
C -1.069710 0.839773 -0.872012
C -0.473485 1.645802 -2.024708
C -0.387619 3.152438 -1.781897
C 0.759288 3.536474 -0.904673
C 0.701909 4.388059 0.128380
C 1.824431 4.755773 0.990474
C 3.122139 4.524032 0.762267
C -0.391804 1.097688 0.446242

C 0.628260 0.445961 0.967467
Cl 0.041778 -2.737807 0.781668
C 1.538748 0.216678 1.961208
C 1.222342 -0.667247 3.123560
C 2.840631 0.945739 2.033475
Cl 3.085168 0.273797 -1.202024
C -5.069386 0.898978 -1.705492
C -5.332159 -1.317887 1.099597
C -3.084644 -0.651550 1.938344
H 3.881411 4.822416 1.480581
H 3.477634 4.044376 -0.150068
H 1.711656 3.051620 -1.142095
H -0.806863 1.929517 1.022319
H -0.947311 -0.230109 -1.121331
H 3.676626 0.259251 2.213275
H 2.778039 1.614266 2.905211
H 3.040344 1.549545 1.147894
H 0.259090 -1.170450 3.025052
H 1.205458 -0.025877 4.016491
H 2.011206 -1.412605 3.283612
H -1.335563 3.527027 -1.369476
H -0.261469 3.643114 -2.760043
H -1.101345 1.440130 -2.903276
H 0.531546 1.252780 -2.244822
H -0.265066 4.830905 0.379142
H 1.553689 5.275852 1.911959
H -4.084140 -2.153342 -1.713717
H -2.741118 -1.338164 -2.516335
H -2.489762 -2.120023 -0.941969
H -5.230841 1.933141 -1.380539
H -4.799536 0.926624 -2.768053
H -6.025804 0.367377 -1.622529
H -4.927565 -2.285067 0.772181
H -5.717184 -1.457926 2.122904
H -6.196956 -1.081807 0.462731
H -2.589382 -1.552088 1.547501
H -2.322895 0.136672 2.006413
H -3.417094 -0.878535 2.963710
H -4.137672 1.902956 1.602932
H -5.761088 1.390080 1.102728
H -5.144002 0.938775 2.699576
Pt 1.588985 -1.206901 -0.128383
C 2.630565 -2.827994 -1.147197
C 1.541950 -2.415017 -1.932517
H 3.631311 -2.470683 -1.369860
H 2.546777 -3.704536 -0.511723
H 1.697630 -1.739697 -2.768749
H 0.611454 -2.974545 -1.913415

$I2_{et}$

Zero-point correction= 0.517030 (Hartree/Particle)
Thermal correction to Energy= 0.552939
Thermal correction to Enthalpy= 0.553883
Thermal correction to Gibbs Free Energy= 0.446187
Sum of electronic and zero-point Energies= -2187.596471
Sum of electronic and thermal Energies= -2187.560562
Sum of electronic and thermal Enthalpies= -2187.559618
Sum of electronic and thermal Free Energies= -2187.667314
HF (M06/6-311++g(d,p) and SDD, SMD(cyclohexane): -2187.91138964

C -0.422440 0.785715 0.360661
H -1.037716 1.562614 0.805771
C -1.119378 0.041340 -0.739316
H -0.822155 -1.014758 -0.645511
C -0.002605 2.821679 -1.589773
C -0.714422 0.489676 -2.164855
C -0.930814 1.992402 -2.423554
H -1.310704 -0.107605 -2.864486
H 0.339883 0.233636 -2.318042
H -0.731640 2.175864 -3.490084
H -1.976711 2.261348 -2.236649
C -0.385030 3.792323 -0.731197
H -1.446707 4.036228 -0.668871
C 0.844612 0.518889 0.858462
C 1.258387 1.168320 2.032931
C 2.681632 1.087177 2.489403
H 2.921933 1.869741 3.216125
H 2.833400 0.114683 2.981944
H 3.371154 1.120984 1.641076
C 0.333421 1.827697 3.015806
H 0.326359 1.221659 3.934387
H 0.721260 2.812956 3.295729
H -0.698571 1.925332 2.680549
Cl 3.299965 0.929889 -1.116144
Cl 0.817275 -2.579773 0.985250
H 1.057060 2.590156 -1.695944
C 0.495888 4.547466 0.158915
H 0.035763 5.403744 0.652261
C 1.781815 4.264667 0.441391
H 2.349470 4.896962 1.118791
H 2.310866 3.425168 -0.002495
O -2.523638 0.206283 -0.579266
Si -3.551120 -0.921008 0.161173
C -3.039692 -1.170400 1.962853
H -2.012684 -1.551916 2.021818
H -3.090685 -0.240498 2.541747
H -3.687296 -1.904607 2.457935
C -3.429133 -2.575366 -0.743187
H -4.129949 -3.306217 -0.320921
H -3.650398 -2.479932 -1.812468
H -2.423104 -3.000723 -0.642594
C -5.282403 -0.124994 0.002358
C -5.286123 1.264424 0.675969
H -4.553845 1.936644 0.214732
H -6.276655 1.733061 0.580507
H -5.058990 1.201956 1.747606
C -5.651686 0.039976 -1.487648
H -4.925554 0.667752 -2.016326
H -5.700261 -0.925573 -2.005421
H -6.638982 0.514377 -1.586949
C -6.334913 -1.023131 0.688816
H -7.335299 -0.575702 0.598668
H -6.384704 -2.020732 0.234844
H -6.131351 -1.151695 1.759120
Pt 2.062798 -0.834154 -0.070954
C 3.781261 -2.318232 -0.502440
C 2.939088 -2.344009 -1.587658
H 4.668168 -1.691823 -0.502433
H 3.688474 -3.051695 0.292593
H 3.145123 -1.739808 -2.465847
H 2.163752 -3.099394 -1.671457

$Ts2\text{-}3_{et}$

Zero-point correction= 0.519327 (Hartree/Particle)
Thermal correction to Energy= 0.553107
Thermal correction to Enthalpy= 0.554051
Thermal correction to Gibbs Free Energy= 0.453197
Sum of electronic and zero-point Energies= -2187.590541
Sum of electronic and thermal Energies= -2187.556761
Sum of electronic and thermal Enthalpies= -2187.555816
Sum of electronic and thermal Free Energies= -2187.656671
HF (M06/6-311++g(d,p) and SDD, SMD(cyclohexane): -2187.90793500

C -0.42873 0.927515 0.153063
H -1.103023 1.621944 0.644179
C -1.152886 0.069393 -0.865412
H -0.848203 -0.974386 -0.710366
C 0.164368 2.572615 -1.499079
C -0.800471 0.466914 -2.314184
C -0.821012 1.997764 -2.467455
H -1.505677 -0.018842 -2.996641
H 0.205926 0.096291 -2.540492
H -0.520905 2.259452 -3.492928
H -1.828348 2.395331 -2.30087
C -0.033728 3.670879 -0.690277
H -0.993746 4.184865 -0.733924
C 0.84007 0.699758 0.683685
C 1.260174 1.449174 1.822325
C 2.592451 1.126349 2.456461
H 2.903226 1.899043 3.167334
H 2.483395 0.183089 3.011289
H 3.374826 0.969453 1.710243
C 0.279395 2.091899 2.78404
H -0.072091 1.316872 3.480338
H 0.767941 2.868451 3.379852
H -0.598636 2.526854 2.30546
Cl 3.285012 0.698173 -1.456236
Cl 0.778398 -2.290915 1.323761
H 1.165213 2.152444 -1.568992
C 0.874656 4.065967 0.326728
H 0.550708 4.877448 0.977074
C 2.031622 3.394155 0.65775
H 2.637365 3.761922 1.480773
H 2.525289 2.71232 -0.025985
O -2.555922 0.230922 -0.67602
Si -3.543442 -0.81827 0.213559
C -3.040552 -0.796155 2.035215
H -2.00235 -1.133024 2.146324
H -3.125294 0.204797 2.475006
H -3.668014 -1.473621 2.627628
C -3.362943 -2.576105 -0.454483
H -4.073879 -3.256589 0.030295
H -3.539232 -2.623286 -1.535023
H -2.357539 -2.968104 -0.258148
C -5.302151 -0.113406 -0.056101
C -5.358948 1.349497 0.4342
H -4.642955 1.981333 -0.103527
H -6.362858 1.769365 0.27399
H -5.14027 1.429643 1.506372
C -5.663279 -0.153646 -1.556375
H -4.956697 0.430405 -2.156802

H -5.670019 -1.178351 -1.947917
H -6.667363 0.26469 -1.720497
C -6.33071 -0.950992 0.735134
H -7.343569 -0.547774 0.590516
H -6.349181 -1.9979 0.407554
H -6.128457 -0.941076 1.813324
Pt 2.016154 -0.791922 -0.067776
C 3.688901 -2.38844 -0.297303
C 2.80061 -2.587644 -1.32397
H 4.58552 -1.794145 -0.444284
H 3.613504 -2.958872 0.623363
H 2.977303 -2.157242 -2.304947
H 2.004644 -3.320813 -1.23638

$I3_{et}$

Zero-point correction= 0.523686 (Hartree/Particle)
Thermal correction to Energy= 0.556718
Thermal correction to Enthalpy= 0.557662
Thermal correction to Gibbs Free Energy= 0.458726
Sum of electronic and zero-point Energies= -2187.626033
Sum of electronic and thermal Energies= -2187.593001
Sum of electronic and thermal Enthalpies= -2187.592056
Sum of electronic and thermal Free Energies= -2187.690993
HF (M06/6-311++g(d,p) and SDD, SMD(cyclohexane): -2187.95515978

C -0.278057 1.217702 -0.151864
H -0.962429 1.719020 0.534704
C -1.130666 0.189301 -0.972973
H -0.790351 -0.835529 -0.800974
C 0.186760 2.342180 -1.233780
C -0.976417 0.617923 -2.442440
C -0.828271 2.140345 -2.370201
H -1.827105 0.279274 -3.040216
H -0.061454 0.176632 -2.857542
H -0.468395 2.589152 -3.302654
H -1.788469 2.603719 -2.111982
C 0.267142 3.692209 -0.595434
H -0.442538 4.449563 -0.926047
C 0.960174 0.797727 0.519340
C 1.501967 1.652394 1.643673
C 2.666399 0.971253 2.394329
H 3.017692 1.629446 3.197979
H 2.342259 0.026544 2.839781
H 3.508898 0.766487 1.727197
C 0.407351 2.031866 2.672415
H -0.066071 1.134487 3.084105
H 0.875139 2.575682 3.500459
H -0.366861 2.674399 2.247843
Cl 3.270302 0.409368 -1.661813
Cl 0.636695 -2.077602 1.479631
H 1.172060 2.044744 -1.609114
C 1.117129 3.965038 0.403952
H 1.089776 4.950170 0.865528
C 2.100731 2.973973 0.967195
H 2.682605 3.449343 1.763658
H 2.816775 2.651625 0.201891
O -2.488746 0.347487 -0.586869
Si -3.455179 -0.724142 0.293529
C -3.053273 -0.602247 2.135339
H -2.011650 -0.893494 2.315906
H -3.196562 0.413033 2.523610
H -3.686230 -1.276539 2.725376
C -3.145824 -2.494329 -0.290819
H -3.834035 -3.192965 0.200905
H -3.279860 -2.602270 -1.373511
H -2.127707 -2.814648 -0.039624
C -5.237614 -0.135904 -0.078581
C -5.391817 1.350704 0.310976
H -4.685628 1.984760 -0.236717
H -6.407906 1.703245 0.079954
H -5.227717 1.513093 1.383510
C -5.542039 -0.289558 -1.584481
H -4.847546 0.295695 -2.197935
H -5.480700 -1.335001 -1.911039
H -6.560099 0.062807 -1.806547
C -6.250257 -0.976807 0.729518
H -7.277425 -0.649411 0.512416
H -6.191951 -2.044130 0.481593
H -6.099546 -0.875246 1.811298
Pt 1.921331 -0.778849 -0.088464
C 3.463116 -2.586892 -0.237688
C 2.513213 -2.804296 -1.195048
H 4.391120 -2.076486 -0.476007
H 3.377339 -3.037163 0.746649
H 2.663587 -2.472533 -2.217791
H 1.652240 -3.434662 -0.994428

$Ts3\text{-}2b_{et}$

Zero-point correction= 0.519733 (Hartree/Particle)
Thermal correction to Energy= 0.552186
Thermal correction to Enthalpy= 0.553130
Thermal correction to Gibbs Free Energy= 0.456628
Sum of electronic and zero-point Energies= -2187.594637
Sum of electronic and thermal Energies= -2187.562185
Sum of electronic and thermal Enthalpies= -2187.561241
Sum of electronic and thermal Free Energies= -2187.657742
HF (M06/6-311++g(d,p) and SDD, SMD(cyclohexane): -2187.92950375

C -2.042182 1.892069 -1.115646
C -1.092965 1.029235 -0.221692
C -2.024555 3.427089 -0.828508
C 0.214599 3.01793 0.947591
C -0.097741 1.55492 0.613881
C 0.918948 0.680463 1.389671
H 0.482987 -0.274949 1.689709
H -2.794432 3.873347 -1.467192
C -3.497777 1.420905 -0.888981
H -3.627625 0.376765 -1.18864
H -4.172987 2.036183 -1.496102
H -3.792368 1.505539 0.16125
C -1.671692 1.660783 -2.598673
H -0.66474 2.03174 -2.823341
H -2.379445 2.202608 -3.238072
H -1.705924 0.600769 -2.858213
C 1.422485 2.972719 1.906127
C 1.302397 1.590965 2.564288
H 2.218987 1.252449 3.052954
H 0.493425 1.580066 3.306351
H 2.357245 3.039707 1.339757
H 1.400301 3.799788 2.621951
H 0.048991 1.008564 -0.706583
Cl -0.554161 -1.671875 -1.999711
Cl -2.512857 -0.314223 2.147955
C 0.330804 3.931991 -0.248005
C -0.706895 4.118737 -1.064728
H -0.667759 3.323324 1.53714
H -2.356442 3.596206 0.206433
H -0.607011 4.771669 -1.929166
H 1.289854 4.417811 -0.413637
O 2.011522 0.509603 0.495481
Si 3.193774 -0.714767 0.521958
C 4.196655 -0.401616 -1.073318
C 2.36523 -2.406933 0.553913
H 3.112464 -3.207218 0.483142
H 1.812423 -2.562484 1.488865
H 1.658482 -2.515876 -0.275517
C 4.276347 -0.526104 2.064879
H 3.701276 -0.704048 2.981748
H 5.093773 -1.257619 2.053743
H 4.724954 0.471212 2.138429
C 3.299224 -0.590048 -2.315169
H 2.899862 -1.607744 -2.386053
H 2.443099 0.092746 -2.309776
H 3.876893 -0.396536 -3.23091
C 4.757994 1.037187 -1.070344
H 3.955392 1.782271 -1.030587
H 5.428476 1.217228 -0.220529
H 5.337339 1.220551 -1.986838
C 5.373929 -1.400567 -1.149387
H 5.95056 -1.23357 -2.070309
H 6.068974 -1.289879 -0.307716
H 5.03047 -2.442347 -1.168575
Pt -1.582747 -0.977367 0.039193
C -2.815777 -2.898146 0.060414
C -1.640846 -3.158709 0.731517
H -3.7155 -2.624784 0.603535
H -2.92474 -3.154397 -0.988958
H -1.595081 -3.094778 1.814199
H -0.80274 -3.623348 0.222071

$2b[Pt]_{et}$

Zero-point correction= 0.524376 (Hartree/Particle)
Thermal correction to Energy= 0.557218
Thermal correction to Enthalpy= 0.558162
Thermal correction to Gibbs Free Energy= 0.459272
Sum of electronic and zero-point Energies= -2187.646903
Sum of electronic and thermal Energies= -2187.614061
Sum of electronic and thermal Enthalpies= -2187.613117
Sum of electronic and thermal Free Energies= -2187.712007
HF (M06/6-311++g(d,p) and SDD, SMD(cyclohexane): -2187.98015289

C -0.712207 2.083322 -1.511649
C -0.324905 0.781500 -0.796562
C -0.975290 3.283625 -0.561846

C 0.039076 1.589161 1.672079
C 0.084586 0.590010 0.512906
C 0.955978 -0.596224 0.958971
H 0.696419 -1.529464 0.455645
H -1.280904 4.132118 -1.185560
C -1.960699 1.859426 -2.391626
H -1.842721 0.977297 -3.031731
H -2.122725 2.728867 -3.040443
H -2.857539 1.721125 -1.779132
C 0.486339 2.404571 -2.442529
H 1.411141 2.545390 -1.874405
H 0.283512 3.326125 -3.001738
H 0.647946 1.601066 -3.170607
C 0.733579 0.865198 2.859209
C 0.742240 -0.624286 2.473773
H 1.518614 -1.203540 2.982304
H -0.230135 -1.086121 2.689160
H 1.763282 1.223311 2.961759
H 0.219864 1.054976 3.806207
H 0.015567 0.020128 -1.497194
Cl -1.119022 -2.319786 -1.324231
Cl -3.313127 1.057612 1.223641
C 0.665647 2.919085 1.291996
C 0.203747 3.679776 0.296036
H -1.012518 1.766924 1.924383
H -1.835496 3.038118 0.072023
H 0.704171 4.620844 0.074295
H 1.530015 3.237045 1.872806
O 2.301484 -0.202802 0.682337
Si 3.446525 -1.056636 -0.221534
C 5.027134 0.005770 -0.055369
C 2.892485 -1.222207 -2.020358
H 3.623146 -1.795238 -2.604913
H 1.933787 -1.750674 -2.088392
H 2.770382 -0.246478 -2.504469
C 3.662853 -2.787249 0.509210
H 2.730905 -3.361959 0.440619
H 4.430514 -3.352267 -0.033802
H 3.955604 -2.753678 1.564590
C 4.753320 1.431561 -0.582957
H 4.485664 1.430133 -1.646961
H 3.938864 1.915648 -0.032556
H 5.651345 2.057332 -0.474282
C 5.455023 0.095720 1.425655
H 4.665114 0.531506 2.047750
H 5.707303 -0.887453 1.842044
H 6.347713 0.730280 1.526444
C 6.173113 -0.626917 -0.875251
H 7.087066 -0.022622 -0.782403
H 6.417837 -1.639113 -0.529165
H 5.931324 -0.687169 -1.943570
Pt -2.121447 -0.572980 -0.036734
C -4.058513 -1.617683 -0.294745
C -3.461460 -2.115532 0.861609
H -4.819469 -0.846058 -0.229709
H -3.970006 -2.157512 -1.232642
H -3.739634 -1.726622 1.836256
H -2.892062 -3.039350 0.834127

Ts3-3b$_{et}$

Zero-point correction= 0.521139 (Hartree/Particle)
Thermal correction to Energy= 0.553980
Thermal correction to Enthalpy= 0.554924
Thermal correction to Gibbs Free Energy= 0.456446
Sum of electronic and zero-point Energies= -2187.596095
Sum of electronic and thermal Energies= -2187.563254
Sum of electronic and thermal Enthalpies= -2187.562310
Sum of electronic and thermal Free Energies= -2187.660789
HF (M06/6-311++g(d,p) and SDD, SMD(cyclohexane): -2187.92803359

C -0.138743 1.504121 -0.043653
H -0.820629 2.051047 0.612996
C -1.092759 0.539244 -0.816632
H -0.681113 -0.468864 -0.895548
C 0.342563 2.557368 -1.085441
C -1.247982 1.190361 -2.216901
C -0.853343 2.666653 -2.040075
H -2.256642 1.04406 -2.612621
H -0.543515 0.711307 -2.909306
H -0.60465 3.162761 -2.984519
H -1.670704 3.2295 -1.568997
C 0.787336 3.77279 -0.329102
H 0.421592 4.758329 -0.612231
C 1.021706 0.920267 0.776541
C 0.889296 0.878872 2.194138
C 1.842274 0.112978 3.057935
H 2.091674 0.665712 3.971159
H 1.321424 -0.808193 3.352375
H 2.74277 -0.189791 2.519677
C -0.229632 1.566333 2.924002
H -1.170349 1.058277 2.676974
H -0.084514 1.544364 4.006673
H -0.339637 2.605493 2.593246
Cl 3.516711 0.633185 -1.392206
Cl 0.49127 -2.168151 1.037821
H 1.196159 2.139268 -1.637633
C 1.557811 3.612865 0.758302
H 1.830111 4.459958 1.384851
C 2.134311 2.287324 1.118974
H 2.574373 2.300301 2.118535
H 2.916001 1.956915 0.429796
O -2.339437 0.505558 -0.118317
Si -3.392406 -0.788242 0.121872
C -3.229693 -1.367956 1.91324
H -2.207508 -1.719225 2.094013
H -3.445543 -0.56081 2.624095
H -3.911592 -2.197306 2.137867
C -2.980999 -2.220022 -1.04097
H -3.698177 -3.039948 -0.911692
H -3.001151 -1.926577 -2.097062
H -1.984889 -2.61851 -0.816295
C -5.152002 -0.093443 -0.20354
C -5.414604 1.121866 0.712057
H -4.682085 1.919239 0.54185
H -6.414368 1.539229 0.520028
H -5.37553 0.850112 1.774282
C -5.285076 0.355198 -1.673818
H -4.566029 1.145098 -1.920179
H -5.126523 -0.475368 -2.372854
H -6.292085 0.754637 -1.865305
C -6.20973 -1.180964 0.086396
H -7.22117 -0.790995 -0.100369
H -6.080216 -2.063014 -0.553348
H -6.179528 -1.517329 1.129955
Pt 1.986421 -0.715299 -0.151657
C 3.317772 -2.534088 -0.606336
C 2.406497 -2.423535 -1.632396
H 4.3145 -2.114661 -0.701141
H 3.135336 -3.203804 0.228338
H 2.667951 -1.916342 -2.555871
H 1.488907 -3.00362 -1.623961

3b[Pt]$_{et}$

Zero-point correction= 0.524642 (Hartree/Particle)
Thermal correction to Energy= 0.557473
Thermal correction to Enthalpy= 0.558417
Thermal correction to Gibbs Free Energy= 0.459688
Sum of electronic and zero-point Energies= -2187.626790
Sum of electronic and thermal Energies= -2187.593959
Sum of electronic and thermal Enthalpies= -2187.593015
Sum of electronic and thermal Free Energies= -2187.691744
HF (M06/6-311++g(d,p) and SDD, SMD(cyclohexane): -2187.96257126

C -0.223230 1.953527 0.322600
H -0.846358 2.175534 1.200693
C -1.163409 1.121601 -0.611726
H -0.587783 0.377914 -1.170402
C -0.051042 3.308472 -0.421933
C -1.783144 2.179375 -1.577557
C -1.451247 3.559614 -0.979585
H -2.854135 2.004491 -1.705676
H -1.308867 2.088636 -2.562096
H -1.483676 4.364738 -1.721624
H -2.150979 3.817500 -0.173085
C 0.634254 4.297409 0.478406
H 0.217750 5.286918 0.654504
C 1.121176 1.455161 0.887304
C 1.190110 0.503641 1.901032
C 2.412994 0.350464 2.792030
H 2.374475 1.121415 3.575844
H 2.402177 -0.626473 3.277748
H 3.364738 0.447597 2.267250
C -0.058096 -0.084227 2.516960
H -0.925143 -0.049537 1.860878
H 0.109633 -1.111955 2.842951
H -0.282363 0.515878 3.413854
Cl 2.048796 0.736607 -2.094625
Cl 1.747493 -2.550170 1.356866
H 0.607242 3.122509 -1.283935
C 1.761906 3.871059 1.056146
H 2.344064 4.486527 1.737652
C 2.262657 2.475280 0.714809
H 3.125636 2.212883 1.324924
H 2.597697 2.470423 -0.328401
O -2.177631 0.475083 0.159725
Si -3.084723 -0.877590 -0.288746
C -2.330643 -2.421408 0.496459
H -1.259902 -2.496605 0.272402
H -2.426721 -2.414606 1.588086
H -2.815244 -3.333253 0.125823
C -3.075642 -1.094339 -2.170633
H -3.643300 -1.989296 -2.453669

H -3.513557 -0.242053 -2.701524
H -2.053890 -1.227875 -2.547236
C -4.847529 -0.550499 0.385297
C -4.784264 -0.292008 1.906939
H -4.147511 0.568229 2.142413
H -5.789652 -0.082189 2.300877
H -4.395369 -1.158098 2.456468
C -5.460102 0.688923 -0.301177
H -4.854891 1.586050 -0.126286
H -5.558280 0.552729 -1.385468
H -6.467239 0.887016 0.093993
C -5.749492 -1.774944 0.115718
H -6.762996 -1.595796 0.503121
H -5.846356 -1.987663 -0.956545
H -5.371084 -2.681123 0.604422
Pt 1.841065 -0.758192 -0.225423
C 3.165703 -2.087652 -1.375359
C 1.842111 -2.354559 -1.744413
H 3.784374 -1.438520 -1.986731
H 3.667801 -2.716675 -0.647399
H 1.427719 -1.916674 -2.646770
H 1.310778 -3.192778 -1.305383

Ts3-4b$_{et}$

Zero-point correction= 0.520183 (Hartree/Particle)
Thermal correction to Energy= 0.552576
Thermal correction to Enthalpy= 0.553520
Thermal correction to Gibbs Free Energy= 0.455730
Sum of electronic and zero-point Energies= -2187.595798
Sum of electronic and thermal Energies= -2187.563405
Sum of electronic and thermal Enthalpies= -2187.562461
Sum of electronic and thermal Free Energies= -2187.660251
HF (M06/6-311++g(d,p) and SDD, SMD(cyclohexane): -2187.93049817
C 1.639458 2.098484 1.256929
C 1.012566 1.025373 0.27103
C 2.01016 3.403718 0.496344
C -0.029352 1.842657 -1.019442
C -0.504076 1.018712 0.143981
C -1.257293 -0.197408 -0.416813
H -1.051317 -1.092114 0.178062
H 2.382307 4.124739 1.233587
C 2.948017 1.549809 1.867599
H 2.759002 0.662118 2.476532
H 3.392709 2.319822 2.511376
H 3.677926 1.29252 1.094016
C 0.684549 2.426525 2.424235
H -0.186265 3.010689 2.109976
H 1.223044 3.022765 3.169498
H 0.338362 1.510897 2.914554
C -0.369598 1.087876 -2.308984
C -0.758276 -0.336527 -1.869707
H -1.532341 -0.772365 -2.506669
H 0.118829 -0.989771 -1.90282
H -1.235636 1.620178 -2.724808
H 0.434348 1.11759 -3.048377
H -1.042809 1.529581 0.932758
Cl 1.031879 -1.656776 1.918002
Cl 3.131166 0.183319 -1.972732
C 0.000627 3.324752 -0.991358
C 0.901917 4.034464 -0.307776
H 1.284056 1.459998 -0.874946
H 2.859071 3.194444 -0.173309
H 0.86319 5.120287 -0.355849
H -0.767519 3.808506 -1.591482
O -2.643734 0.140426 -0.402155
Si -3.86192 -0.839758 0.235857
C -5.470252 0.139008 -0.098109
C -3.855148 -2.516368 -0.641558
H -4.022274 -2.419143 -1.720415
H -2.893773 -3.025657 -0.50003
H -4.631857 -3.179465 -0.241262
C -3.55505 -1.118244 2.079344
H -2.575827 -1.583546 2.247408
H -3.572498 -0.17923 2.644276
H -4.310698 -1.784155 2.513855
C -5.406738 1.512262 0.605735
H -5.318223 1.411817 1.694466
H -4.556519 2.106867 0.252919
H -6.322863 2.087166 0.405369
C -6.685032 -0.648684 0.439832
H -7.614534 -0.092821 0.249544
H -6.788636 -1.628346 -0.04317
H -6.622392 -0.813899 1.522675
C -5.643456 0.364563 -1.615724
H -4.802516 0.926541 -2.037545
H -5.72374 -0.581693 -2.164552
H -6.561554 0.936429 -1.815199
Pt 2.076733 -0.762747 -0.038146
C 3.701586 -2.340374 0.103511
C 2.68094 -2.86516 -0.663187
H 4.56736 -1.881069 -0.363534
H 3.765938 -2.561283 1.164643
H 2.726536 -2.826942 -1.747485
H 1.927603 -3.507878 -0.21829

I4$_{et}$

Zero-point correction= 0.522508 (Hartree/Particle)
Thermal correction to Energy= 0.555426
Thermal correction to Enthalpy= 0.556370
Thermal correction to Gibbs Free Energy= 0.457739
Sum of electronic and zero-point Energies= -2187.606952
Sum of electronic and thermal Energies= -2187.574034
Sum of electronic and thermal Enthalpies= -2187.573090
Sum of electronic and thermal Free Energies= -2187.671721
HF (M06/6-311++g(d,p) and SDD, SMD(cyclohexane): -2187.94132813

C 1.908824 2.029223 1.165419
C 1.275425 1.185148 0.009491
C 2.064586 3.523284 0.782974
C -0.407636 2.454953 -0.852533
C -0.320646 1.253237 -0.035391
C -1.084454 0.176422 -0.846472
H -0.734394 -0.831090 -0.612667
H 2.430630 4.063361 1.667328
C 3.345274 1.506738 1.411288
H 3.326206 0.515990 1.873685
H 3.876720 2.187661 2.090091
H 3.913820 1.435797 0.477770
C 1.137264 1.958111 2.499058
H 0.198048 2.524941 2.470376
H 1.747452 2.398328 3.297158
H 0.914458 0.924040 2.770456
C -0.859863 2.114904 -2.246275
C -0.824920 0.577735 -2.304789
H -1.577520 0.159240 -2.976869
H 0.164355 0.231309 -2.621724
H -1.898065 2.481778 -2.314675
H -0.288139 2.633698 -3.023526
H -0.678773 1.332648 0.988073
Cl 0.620578 -1.515737 1.867061
Cl 3.095473 -0.351063 -2.057917
C -0.134062 3.818950 -0.507224
C 0.906969 4.284252 0.220818
H 1.717179 1.514023 -0.939642
H 2.873088 3.637056 0.037460
H 1.010959 5.368206 0.263728
H -0.740023 4.549158 -1.043827
O -2.476772 0.323814 -0.584534
Si -3.440174 -0.637337 0.421709
C -5.223487 -0.238892 -0.150672
C -3.003525 -2.458023 0.179016
H -3.059688 -2.762895 -0.872480
H -1.988724 -2.662488 0.540314
H -3.685816 -3.100594 0.749000
C -3.166741 -0.165860 2.230174
H -2.131889 -0.380074 2.522502
H -3.362204 0.897380 2.414202
H -3.819854 -0.744081 2.895614
C -5.504492 1.271074 0.009055
H -5.420203 1.595496 1.053552
H -4.810793 1.875340 -0.586912
H -6.525161 1.508475 -0.325598
C -6.239392 -1.032748 0.699800
H -7.266544 -0.805119 0.379396
H -6.102238 -2.116672 0.599661
H -6.169504 -0.783324 1.765703
C -5.398498 -0.624944 -1.635142
H -4.689312 -0.089137 -2.276337
H -5.252364 -1.699704 -1.798910
H -6.413546 -0.377524 -1.979551
Pt 1.879632 -0.897151 -0.076095
C 3.142930 -2.746817 0.190042
C 2.064125 -3.104568 -0.599943
H 4.098423 -2.496095 -0.260590
H 3.130202 -2.936902 1.259013
H 2.152152 -3.126260 -1.681633
H 1.187449 -3.569473 -0.160022

Ts4-4b

Zero-point correction= 0.522226 (Hartree/Particle)
Thermal correction to Energy= 0.554515
Thermal correction to Enthalpy= 0.555459
Thermal correction to Gibbs Free Energy= 0.458302
Sum of electronic and zero-point Energies= -2187.606165
Sum of electronic and thermal Energies= -2187.573876
Sum of electronic and thermal Enthalpies= -2187.572931

Sum of electronic and thermal Free Energies= -2187.670089
HF (M06/6-311++g(d,p) and SDD, SMD(cyclohexane): -2187.94150353

C 0.387156 1.139204 -0.007359
H 0.715005 1.216245 -1.037443
C 1.096591 0.062744 0.838738
H 0.783096 -0.949429 0.568751
C 0.270442 2.312333 0.816571
C 0.722545 0.428855 2.285573
C 0.56962 1.961712 2.263075
H 1.494333 0.090134 2.980883
H -0.223685 -0.045219 2.562702
H -0.172087 2.354374 2.966359
H 1.523147 2.460129 2.494462
C 0.186936 3.723482 0.433719
H 1.020433 4.324622 0.799006
C -1.195561 1.270597 0.052127
C -1.917786 2.128744 -1.041585
C -3.341346 1.563008 -1.250422
H -3.91361 2.238463 -1.899713
H -3.310285 0.581767 -1.734947
H -3.880631 1.459659 -0.302899
C -1.190812 2.116617 -2.402054
H -0.99401 1.095069 -2.736839
H -1.823202 2.604711 -3.153157
H -0.243667 2.666666 -2.372525
Pt -1.880425 -0.910011 0.046557
Cl -3.080654 -0.441355 2.057787
Cl -0.668101 -1.440189 -1.944059
H -1.656862 1.393787 1.035873
C -0.846756 4.316319 -0.173372
H -0.807963 5.39362 -0.321391
C -2.099022 3.602409 -0.589928
H -2.571349 4.152978 -1.413328
H -2.818757 3.649454 0.243956
O 2.498489 0.231371 0.665431
Si 3.493305 -0.601512 -0.421336
C 3.213047 0.028821 -2.181072
H 2.195923 -0.208188 -2.515813
H 3.352695 1.113693 -2.25656
H 3.905241 -0.444639 -2.8884
C 3.100919 -2.448124 -0.35846
H 3.796301 -3.015884 -0.988906
H 3.168446 -2.851005 0.658752
H 2.090099 -2.642348 -0.736682
C 5.260735 -0.21036 0.196168
C 5.482268 1.317833 0.225874
H 4.762433 1.815221 0.885617
H 6.491663 1.550294 0.596194
H 5.390471 1.766205 -0.771413
C 5.456389 -0.769683 1.622217
H 4.732553 -0.342746 2.325671
H 5.350666 -1.861116 1.652804
H 6.4637 -0.528967 1.992733
C 6.302796 -0.853109 -0.745285
H 7.321105 -0.642603 -0.38746
H 6.196587 -1.944066 -0.795713
H 6.230983 -0.461908 -1.76753
C -2.051668 -3.081928 0.467168
C -3.151643 -2.680825 -0.290602
H -3.163846 -2.839415 -1.36481
H -4.100313 -2.462797 0.190542
H -1.196671 -3.549532 -0.011209
H -2.129254 -3.17185 1.546301

4b
Zero-point correction= 0.521627 (Hartree/Particle)
Thermal correction to Energy= 0.554557
Thermal correction to Enthalpy= 0.555501
Thermal correction to Gibbs Free Energy= 0.454527
Sum of electronic and zero-point Energies= -2187.621610
Sum of electronic and thermal Energies= -2187.588680
Sum of electronic and thermal Enthalpies= -2187.587736
Sum of electronic and thermal Free Energies= -2187.688709
HF (M06/6-311++g(d,p) and SDD, SMD(cyclohexane): -2187.95162869

C 0.610958 1.680392 0.030828
H 1.021618 1.703541 -0.970475
C 0.726335 0.391405 0.812502
H -0.162063 -0.327719 0.498825
C 0.837692 2.831196 1.021722
C 0.540068 0.764620 2.297307
C 1.082900 2.207839 2.397327
H 1.073352 0.051458 2.929091
H -0.515817 0.714754 2.572685
H 0.610666 2.774163 3.208793
H 2.163290 2.193887 2.591738
C 1.561976 4.069362 0.648129
H 2.630271 4.114326 0.858057
C -0.521664 2.614917 0.392805
C -1.073272 3.670971 -0.602334
C -2.611609 3.645882 -0.524948
H -3.048650 4.412976 -1.175703
H -3.001525 2.671834 -0.843744
H -2.962089 3.833943 0.497639
C -0.653847 3.392916 -2.060057
H -0.936762 2.380465 -2.366129
H -1.148810 4.104486 -2.732296
H 0.426357 3.506841 -2.202927
Pt -1.760809 -1.217401 0.042625
Cl -2.084426 -1.720124 2.324484
Cl -1.355914 -0.656803 -2.221798
H -1.290391 2.193395 1.040846
C 0.923395 5.110073 0.099556
H 1.472450 6.017640 -0.144929
C -0.561449 5.077417 -0.183826
H -0.812150 5.800634 -0.970469
H -1.105403 5.411775 0.713870
O 1.913656 -0.285443 0.628497
Si 2.653952 -1.162854 -0.626666
C 2.602116 -0.227957 -2.264628
H 1.570387 -0.107233 -2.613210
H 3.061692 0.764257 -2.194451
H 3.142806 -0.789624 -3.036931
C 1.761539 -2.814802 -0.806628
H 2.282029 -3.458120 -1.527296
H 1.702907 -3.353219 0.145760
H 0.741850 -2.669582 -1.181165
C 4.443719 -1.375617 0.014025
C 5.098028 0.007851 0.218521
H 4.544275 0.612395 0.945712
H 6.125046 -0.107501 0.594427
H 5.156483 0.576976 -0.717621
C 4.437964 -2.133079 1.359472
H 3.854520 -1.602121 2.119695
H 4.019561 -3.141980 1.259600
H 5.463931 -2.241917 1.740212
C 5.271210 -2.178423 -1.014408
H 6.299120 -2.316199 -0.649478
H 4.854136 -3.177758 -1.190953
H 5.337125 -1.666109 -1.982196
C -3.106575 -2.790487 -0.542085
C -3.837414 -1.593432 -0.383124
H -4.100598 -0.995961 -1.251185
H -4.392639 -1.410430 0.532235
H -2.807098 -3.117696 -1.533537
H -3.097985 -3.534258 0.249505

Ts3-5b$_{et}$
Zero-point correction= 0.521341 (Hartree/Particle)
Thermal correction to Energy= 0.553924
Thermal correction to Enthalpy= 0.554869
Thermal correction to Gibbs Free Energy= 0.457008
Sum of electronic and zero-point Energies= -2187.587746
Sum of electronic and thermal Energies= -2187.555162
Sum of electronic and thermal Enthalpies= -2187.554218
Sum of electronic and thermal Free Energies= -2187.652079
HF (M06/6-311++g(d,p) and SDD, SMD(cyclohexane): -2187.91737429

C 1.441753 2.002616 1.364026
C 0.832165 0.981318 0.342298
C 2.116524 3.189876 0.589151
C 0.51159 1.864943 -1.321744
C -0.516386 0.663487 0.450232
C -1.292511 -0.279332 -0.425673
H -1.149245 -1.282767 0.001639
H 2.618719 3.83593 1.316818
C 2.539825 1.339114 2.226484
H 2.152041 0.475985 2.774526
H 2.918389 2.068651 2.954039
H 3.384544 1.004794 1.615855
C 0.392529 2.590333 2.335282
H -0.420384 3.109445 1.815863
H 0.878251 3.318744 2.994597
H -0.042198 1.813932 2.97544
C -0.491755 1.192989 -2.250251
C -0.757456 -0.26375 -1.867384
H -1.443261 1.73776 -2.235364
H -0.091185 1.247439 -3.270626
H -1.152384 1.160546 1.184277
Cl 0.881143 -1.896462 1.666093
Cl 3.420424 0.341649 -1.72517
C 0.302447 3.30194 -1.055651
C 1.107725 3.959967 -0.209319
H 1.534133 1.649583 -1.629762
H 2.895845 2.774492 -0.063466
H 0.963166 5.021325 -0.020527
H -0.525764 3.798091 -1.559337
O -2.660163 0.112766 -0.403526
Si -3.929041 -0.840512 0.187275
C -5.491283 0.206008 -0.147248
C -3.958709 -2.489908 -0.7374

H -4.772954 -3.130059 -0.376161
H -4.094149 -2.35414 -1.816331
H -3.024911 -3.04613 -0.587767
C -3.65907 -1.175553 2.027033
H -3.664084 -0.252876 2.618673
H -4.438963 -1.833523 2.429446
H -2.695913 -1.672246 2.199038
C -5.641495 0.46208 -1.662759
H -6.532525 1.076116 -1.858687
H -4.7747 0.994813 -2.06988
H -5.758662 -0.470616 -2.227975
C -5.382116 1.564937 0.579171
H -5.307089 1.445454 1.667117
H -4.508207 2.133474 0.24173
H -6.274801 2.175514 0.380003
C -6.740693 -0.542845 0.367369
H -7.645101 0.053512 0.179803
H -6.879921 -1.508555 -0.134517
H -6.693954 -0.729547 1.447501
H 0.166301 -0.84861 -1.926803
H -1.499525 -0.725874 -2.525092
Pt 2.097075 -0.732072 -0.050152
C 3.767531 -2.234223 0.195055
C 2.898182 -2.725756 -0.763203
H 4.668781 -1.704043 -0.096945
H 3.691926 -2.557234 1.228628
H 3.105563 -2.586841 -1.819813
H 2.128867 -3.443538 -0.496194

5b[Pt]$_{et}$

Zero-point correction= 0.524325 (Hartree/Particle)
Thermal correction to Energy= 0.557123
Thermal correction to Enthalpy= 0.558067
Thermal correction to Gibbs Free Energy= 0.458441
Sum of electronic and zero-point Energies= -2187.650875
Sum of electronic and thermal Energies= -2187.618076
Sum of electronic and thermal Enthalpies= -2187.617132
Sum of electronic and thermal Free Energies= -2187.716758
HF (M06/6-311++g(d,p) and SDD, SMD(cyclohexane): -2187.98249753

C 0.939388 2.274255 1.511329
C 0.525441 1.629566 0.188133
C 1.926424 3.450485 1.278247
C 0.576649 2.463129 -1.077875
C -0.031762 0.354298 0.153567
C -0.981008 -0.094633 -0.967079
H -0.861875 -1.170026 -1.143823
H 2.074367 3.969989 2.232570
C 1.572445 1.302378 2.523961
H 0.911595 0.475677 2.795426
H 1.815020 1.850844 3.441806
H 2.499768 0.871593 2.130023
C -0.386721 2.828187 2.117378
H -0.876173 3.539766 1.447095
H -0.158260 3.346478 3.056260
H -1.087166 2.016045 2.333649
C -0.622082 2.168804 -2.008260
C -0.747346 0.668388 -2.272538
H -1.547423 2.545544 -1.555214
H -0.473912 2.713643 -2.948068
H -0.292660 -0.077436 1.114816
Cl 0.868988 -2.319660 1.584534
Cl 3.025438 0.278399 -1.778079
C 0.798914 3.939125 -0.849239
C 1.448416 4.404123 0.217377
H 1.473622 2.090706 -1.607825
H 2.908330 3.039121 0.998586
H 1.641845 5.467880 0.335545
H 0.451766 4.606605 -1.635603
O -2.310227 0.170405 -0.511296
Si -3.425575 -0.919576 0.138551
C -5.118561 -0.069537 -0.143501
C -3.306462 -2.581605 -0.758341
H -4.081586 -3.268542 -0.396920
H -3.430017 -2.482854 -1.843048
H -2.339783 -3.064248 -0.570858
C -3.083433 -1.193902 1.976178
H -3.097028 -0.253560 2.539862
H -3.830582 -1.860533 2.424636
H -2.100980 -1.658843 2.122454
C -5.361941 0.125280 -1.655020
H -6.327991 0.621920 -1.827818
H -4.582357 0.745991 -2.110938
H -5.386875 -0.831258 -2.191325
C -5.131049 1.311066 0.547864
H -4.995260 1.227103 1.633166
H -4.340015 1.962381 0.159618
H -6.093659 1.815934 0.378427
C -6.251430 -0.939481 0.443848
H -7.226344 -0.457646 0.280393
H -6.297638 -1.929897 -0.026175
H -6.140210 -1.086880 1.525168
H 0.169890 0.297596 -2.746219
H -1.582987 0.458012 -2.948527
Pt 1.894932 -0.941661 -0.077242
C 3.778148 -2.020266 0.290801
C 3.051623 -2.694891 -0.697881
H 4.581691 -1.343871 0.015954
H 3.737031 -2.350969 1.323976
H 3.291871 -2.552667 -1.747066
H 2.450037 -3.560429 -0.437884

Ts3-3'$_{et}$

Zero-point correction= 0.523488 (Hartree/Particle)
Thermal correction to Energy= 0.555794
Thermal correction to Enthalpy= 0.556738
Thermal correction to Gibbs Free Energy= 0.458729
Sum of electronic and zero-point Energies= -2187.616563
Sum of electronic and thermal Energies= -2187.584257
Sum of electronic and thermal Enthalpies= -2187.583313
Sum of electronic and thermal Free Energies= -2187.681322
HF (M06/6-311++g(d,p) and SDD, SMD(cyclohexane): -2187.94530576

C -0.215761 1.285076 -0.186951
H -0.846783 1.878437 0.482668
C -1.159478 0.25343 -0.903688
H -0.81586 -0.771788 -0.749439
C 0.270606 2.286726 -1.323263
C -1.129907 0.655724 -2.392199
C -0.852914 2.160524 -2.372458
H -2.061939 0.377317 -2.891668
H -0.303137 0.134742 -2.892312
H -0.538309 2.563033 -3.341806
H -1.743678 2.709931 -2.043639
C 0.529997 3.660871 -0.793218
H 0.339161 4.475076 -1.491943
C 0.99471 0.819719 0.508635
C 1.440239 1.589951 1.724362
C 2.849402 1.184854 2.210111
H 3.09506 1.740078 3.12334
H 2.898158 0.116653 2.440324
H 3.604141 1.408983 1.450686
C 0.410804 1.124773 2.817986
H 0.386453 0.035531 2.906164
H 0.740139 1.544319 3.774866
H -0.599981 1.485804 2.610225
Cl 3.425447 0.552129 -1.460876
Cl 0.607233 -2.216537 1.247189
H 1.188028 1.88831 -1.773743
C 0.967259 3.986566 0.426684
H 1.085883 5.051991 0.628903
C 1.39467 3.169802 1.626228
H 0.811573 3.532363 2.484498
H 2.41996 3.503089 1.834758
O -2.466393 0.434379 -0.377959
Si -3.488632 -0.728355 0.301261
C -3.202995 -0.81071 2.166725
H -2.178882 -1.140731 2.376968
H -3.352085 0.16352 2.646985
H -3.883044 -1.5259 2.645878
C -3.139436 -2.424227 -0.454542
H -3.845829 -3.169753 -0.068967
H -3.225324 -2.420588 -1.547339
H -2.131597 -2.768502 -0.194048
C -5.251959 -0.106004 -0.108156
C -5.448663 1.320755 0.449966
H -4.719083 2.021777 0.029047
H -6.45322 1.693645 0.201004
H -5.352622 1.351215 1.542437
C -5.45849 -0.07347 -1.637798
H -4.727922 0.579787 -2.128774
H -5.373397 -1.071292 -2.086059
H -6.460975 0.308516 -1.880753
C -6.303784 -1.04473 0.522512
H -7.31897 -0.691661 0.289785
H -6.222872 -2.070412 0.141038
H -6.217237 -1.085841 1.615255
Pt 1.953363 -0.757205 -0.101725
C 3.519889 -2.546003 -0.323212
C 2.624769 -2.676776 -1.346482
H 4.454608 -2.012048 -0.462443
H 3.383466 -3.08365 0.610227
H 2.827841 -2.249687 -2.323817
H 1.758675 -3.324531 -1.252506

I3'$_{et}$

Zero-point correction= 0.523688 (Hartree/Particle)
Thermal correction to Energy= 0.556688
Thermal correction to Enthalpy= 0.557632

Thermal correction to Gibbs Free Energy= 0.458376
Sum of electronic and zero-point Energies= -2187.623401
Sum of electronic and thermal Energies= -2187.590401
Sum of electronic and thermal Enthalpies= -2187.589457
Sum of electronic and thermal Free Energies= -2187.688713
HF (M06/6-311++g(d,p) and SDD, SMD(cyclohexane): -2187.95310782

C -0.262683 1.234272 -0.201756
H -0.945253 1.760468 0.472911
C -1.129744 0.210635 -1.008157
H -0.777669 -0.814265 -0.862204
C 0.238362 2.321536 -1.267080
C -1.018961 0.663308 -2.475959
C -0.818976 2.179108 -2.384321
H -1.902780 0.362930 -3.045139
H -0.136288 0.201259 -2.936259
H -0.468353 2.633176 -3.317777
H -1.752618 2.671607 -2.087657
C 0.426855 3.693828 -0.692795
H 0.428478 4.500449 -1.426190
C 0.965129 0.827129 0.491785
C 1.449949 1.713043 1.623003
C 2.966010 2.005649 1.507266
H 3.280490 2.587631 2.381244
H 3.547009 1.081335 1.475041
H 3.193638 2.577850 0.604707
C 1.201027 0.896449 2.931166
H 1.808379 -0.009169 2.960856
H 1.469425 1.539511 3.777628
H 0.152156 0.603460 3.040107
Cl 3.297404 0.424431 -1.633187
Cl 0.632019 -2.158381 1.386779
H 1.192031 1.980691 -1.692645
C 0.627203 4.005158 0.592345
H 0.755046 5.058294 0.838060
C 0.676324 3.061801 1.776363
H -0.343113 2.858435 2.134746
H 1.161417 3.586435 2.607785
O -2.476781 0.353294 -0.577284
Si -3.432606 -0.751145 0.272077
C -3.026151 -0.673590 2.115853
H -1.983804 -0.968433 2.286114
H -3.170255 0.332948 2.526422
H -3.656569 -1.361034 2.693210
C -3.110995 -2.501139 -0.363229
H -3.789156 -3.219890 0.113094
H -3.252205 -2.579344 -1.447540
H -2.088045 -2.818811 -0.128996
C -5.221473 -0.167411 -0.075691
C -5.387623 1.303710 0.364928
H -4.689345 1.962652 -0.163197
H -6.407712 1.654627 0.149570
H -5.221180 1.430903 1.441835
C -5.528894 -0.271380 -1.585167
H -4.840382 0.340039 -2.179611
H -5.461232 -1.304443 -1.947999
H -6.550031 0.081250 -1.792228
C -6.224639 -1.044320 0.705514
H -7.254991 -0.717041 0.503964
H -6.159492 -2.101613 0.419349
H -6.070670 -0.980540 1.789749
Pt 1.936920 -0.766547 -0.067010
C 3.516749 -2.542967 -0.211161
C 2.591031 -2.768210 -1.190399
H 4.437691 -2.009339 -0.424218
H 3.421350 -3.009276 0.764801
H 2.753965 -2.416221 -2.204371
H 1.739856 -3.418710 -1.015331

Ts3'-2b'$_{et}$
Zero-point correction= 0.519262 (Hartree/Particle)
Thermal correction to Energy= 0.552120
Thermal correction to Enthalpy= 0.553065
Thermal correction to Gibbs Free Energy= 0.454480
Sum of electronic and zero-point Energies= -2187.596104
Sum of electronic and thermal Energies= -2187.563246
Sum of electronic and thermal Enthalpies= -2187.562301
Sum of electronic and thermal Free Energies= -2187.660886
HF (M06/6-311++g(d,p) and SDD, SMD(cyclohexane): -2187.92893672

C 0.06444 1.525491 -0.482597
H 0.166645 1.013473 0.847048
C -1.093619 0.671554 -1.057008
H -0.751783 -0.314864 -1.378833
C -0.23985 2.988961 -0.792422
C -1.601093 1.567571 -2.19504
C -1.583039 2.966429 -1.562254
H -2.587609 1.250882 -2.542069
H -0.904505 1.510322 -3.041869
H -1.638558 3.777296 -2.294879
H -2.420196 3.07571 -0.865935
C -0.178764 3.966625 0.354363
H -0.87133 4.801522 0.259819
C 1.199674 1.006987 0.145497
C 2.272268 1.948685 0.767251
C 2.996821 2.733703 -0.35338
H 3.8903 3.209506 0.06724
H 3.312897 2.057904 -1.153963
H 2.385651 3.529788 -0.78454
C 3.341341 1.117915 1.514609
H 3.880489 0.461898 0.824262
H 4.070413 1.794683 1.976923
H 2.896846 0.495565 2.295759
Cl 2.325253 -0.448075 -2.330107
Cl 0.881662 -1.514192 2.104349
H 0.539065 3.248001 -1.529274
C 0.611529 3.920651 1.429952
H 0.487543 4.723054 2.157554
C 1.658025 2.909052 1.824517
H 1.263108 2.301977 2.654954
H 2.495926 3.467331 2.265089
O -2.064057 0.595034 -0.026688
Si -3.030627 -0.695762 0.519358
C -2.933531 -0.602847 2.395877
H -1.894134 -0.73565 2.715484
H -3.286899 0.364585 2.771599
H -3.533626 -1.386608 2.872972
C -2.347989 -2.334314 -0.116771
H -2.995522 -3.161968 0.198566
H -2.271904 -2.376127 -1.2095
H -1.353014 -2.510542 0.305261
C -4.834096 -0.417218 -0.083069
C -5.289662 1.021566 0.240974
H -4.669007 1.767831 -0.26832
H -6.329529 1.177338 -0.081814
H -5.246954 1.232324 1.316517
C -4.961547 -0.655001 -1.602554
H -4.327218 0.026661 -2.181759
H -4.69327 -1.680315 -1.883936
H -5.997883 -0.48705 -1.930285
C -5.766004 -1.412935 0.646099
H -6.800501 -1.292124 0.293121
H -5.482281 -2.456918 0.461787
H -5.771871 -1.253718 1.730542
Pt 1.65009 -0.992175 -0.100551
C 2.882028 -2.91656 -0.161682
C 1.636625 -3.215687 -0.667195
H 3.705879 -2.671539 -0.825257
H 3.120859 -3.109853 0.879704
H 1.454859 -3.21272 -1.737284
H 0.872437 -3.652829 -0.032304

2b'[Pt]$_{et}$
Zero-point correction= 0.524493 (Hartree/Particle)
Thermal correction to Energy= 0.557337
Thermal correction to Enthalpy= 0.558282
Thermal correction to Gibbs Free Energy= 0.459751
Sum of electronic and zero-point Energies= -2187.639740
Sum of electronic and thermal Energies= -2187.606896
Sum of electronic and thermal Enthalpies= -2187.605952
Sum of electronic and thermal Free Energies= -2187.704482
HF (M06/6-311++g(d,p) and SDD, SMD(cyclohexane): -2187.97413555

C 0.048682 0.921364 -0.479845
H 0.059929 0.410418 1.544575
C -1.107228 -0.017605 -0.867443
H -1.051006 -0.988780 -0.369508
C 0.293769 1.877272 -1.635912
C -0.976109 -0.082508 -2.392978
C -0.640724 1.368155 -2.777767
H -1.889338 -0.457822 -2.864042
H -0.148315 -0.752748 -2.656665
H -0.161083 1.447338 -3.757739
H -1.558139 1.964467 -2.798907
C 0.074641 3.338691 -1.308303
H -0.147526 3.940627 -2.189975
C 0.565131 1.014256 0.794768
C 1.335232 2.202396 1.387266
C 2.708913 2.489496 0.752207
H 3.151332 3.366027 1.241638
H 3.389729 1.644358 0.890893
H 2.650336 2.697386 -0.316754
C 1.546136 1.916029 2.889265
H 2.140723 1.006831 3.031937
H 2.072788 2.748328 3.369575
H 0.591002 1.775141 3.409831
Cl 3.127891 0.090608 -1.754510

Cl 0.692672 -2.023491 1.754329
H 1.332028 1.747999 -1.968310
C 0.126867 3.978826 -0.134634
H -0.080918 5.048647 -0.162678
C 0.417152 3.452668 1.253782
H -0.534959 3.248391 1.768807
H 0.886925 4.262568 1.829632
O -2.310738 0.673548 -0.536735
Si -3.571996 0.238557 0.499090
C -4.596507 1.816910 0.602846
H -3.992798 2.629270 1.023855
H -4.939674 2.140477 -0.385787
H -5.478267 1.691814 1.242344
C -2.899855 -0.208642 2.207073
H -3.712292 -0.486973 2.889384
H -2.185511 -1.038987 2.182676
H -2.385966 0.654081 2.648594
C -4.598444 -1.210498 -0.236366
C -5.165481 -0.813586 -1.616564
H -4.370560 -0.561458 -2.328314
H -5.743658 -1.644469 -2.046783
H -5.837436 0.050633 -1.550149
C -3.734601 -2.481237 -0.394756
H -2.917962 -2.337840 -1.112331
H -3.291990 -2.804031 0.555341
H -4.347827 -3.314348 -0.768684
C -5.775975 -1.530867 0.712677
H -6.387809 -2.344448 0.296674
H -5.431688 -1.857733 1.701256
H -6.438601 -0.668284 0.854926
Pt 1.858654 -0.846798 0.028641
C 3.524748 -2.273521 0.297760
C 2.638568 -2.828696 -0.625113
H 4.415561 -1.754139 -0.041558
H 3.484013 -2.569274 1.341768
H 2.825585 -2.735107 -1.690208
H 1.893143 -3.550688 -0.307443

Ts3'-4'$_{et}$

Zero-point correction= 0.520115 (Hartree/Particle)
Thermal correction to Energy= 0.552499
Thermal correction to Enthalpy= 0.553443
Thermal correction to Gibbs Free Energy= 0.455330
Sum of electronic and zero-point Energies= -2187.602524
Sum of electronic and thermal Energies= -2187.570139
Sum of electronic and thermal Enthalpies= -2187.569195
Sum of electronic and thermal Free Energies= -2187.667309
HF (M06/6-311++g(d,p) and SDD, SMD(cyclohexane): -2187.93691720

C -0.558146 0.937651 0.071929
H -1.160558 1.429593 0.829706
C -1.245042 -0.304761 -0.519582
H -1.033837 -1.193406 0.082779
C -0.068516 1.78418 -1.088706
C -0.676984 -0.429542 -1.946624
C -0.339574 1.00836 -2.381333
H -1.400911 -0.909064 -2.610482
H 0.230956 -1.039921 -1.93385
H 0.485083 1.067815 -3.09611
H -1.217225 1.496157 -2.825435
C -0.098774 3.264404 -1.071841
H -0.298787 3.748408 -2.024498
C 0.937218 0.990758 0.283658
C 1.429943 2.086049 1.278697
C 2.855635 2.550458 0.917363
H 3.209316 3.270806 1.664624
H 3.550627 1.707476 0.89475
H 2.891867 3.031852 -0.065551
C 1.438225 1.462602 2.692663
H 2.162306 0.64958 2.769137
H 1.703655 2.23891 3.420703
H 0.458679 1.056411 2.963827
Cl 3.214752 0.376241 -1.88808
Cl 1.050829 -1.828803 1.766377
H 1.212408 1.488557 -0.886564
C 0.161352 3.979308 0.029748
H 0.144048 5.065309 -0.029578
C 0.49989 3.34642 1.349988
H -0.427124 3.089853 1.881827
H 1.001898 4.080329 1.990124
O -2.643514 -0.028444 -0.583228
Si -3.821668 -0.85156 0.302647
C -3.462049 -0.68475 2.151618
H -2.466753 -1.08017 2.39066
H -3.493917 0.358696 2.486621
H -4.186634 -1.248415 2.75205
C -3.793309 -2.68514 -0.156951
H -4.547304 -3.249146 0.405462
H -3.982799 -2.843825 -1.224573
H -2.818217 -3.130593 0.075797
C -5.458959 -0.002628 -0.201142
C -5.419735 1.490677 0.191191
H -4.587512 2.013372 -0.293912
H -6.350721 1.990248 -0.11467
H -5.318592 1.628411 1.274847
C -5.657302 -0.110023 -1.729038
H -4.827439 0.35144 -2.275809
H -5.739335 -1.152515 -2.060698
H -6.583506 0.400966 -2.030547
C -6.647672 -0.682541 0.513191
H -7.592052 -0.19541 0.230274
H -6.737452 -1.742663 0.245372
H -6.564661 -0.618317 1.605409
Pt 2.150604 -0.690523 -0.023858
C 3.898281 -2.13507 0.154529
C 2.98247 -2.706539 -0.704122
H 4.746032 -1.575933 -0.229384
H 3.913556 -2.405415 1.206031
H 3.091786 -2.603059 -1.779398
H 2.260896 -3.431875 -0.341726

I4'$_{et}$

Zero-point correction= 0.523106 (Hartree/Particle)
Thermal correction to Energy= 0.555888
Thermal correction to Enthalpy= 0.556832
Thermal correction to Gibbs Free Energy= 0.458733
Sum of electronic and zero-point Energies= -2187.616271
Sum of electronic and thermal Energies= -2187.583489
Sum of electronic and thermal Enthalpies= -2187.582545
Sum of electronic and thermal Free Energies= -2187.680644
HF (M06/6-311++g(d,p) and SDD, SMD(cyclohexane): -2187.94960365

C 0.365392 1.200295 0.035902
H 0.725204 1.239330 -0.990744
C 1.103002 0.112372 0.857226
H 0.745479 -0.890511 0.619584
C 0.511534 2.415611 0.854290
C 0.836319 0.519282 2.312695
C 0.916392 2.055046 2.258702
H 1.568513 0.076975 2.991989
H -0.164769 0.197329 2.618416
H 0.332083 2.582478 3.020970
H 1.959787 2.392396 2.367039
C 0.275134 3.764110 0.490326
H 0.546891 4.523770 1.220568
C -1.223039 1.186201 0.034411
C -1.903213 2.079206 -1.043437
C -3.129780 2.766363 -0.405119
H -3.681227 3.355749 -1.148055
H -3.806508 2.013538 0.010397
H -2.837703 3.433991 0.413942
C -2.369825 1.295497 -2.294937
H -3.144056 0.570172 -2.030162
H -2.795764 1.991542 -3.028971
H -1.550836 0.743999 -2.761990
Pt -1.939337 -0.871487 0.057024
Cl -3.322592 -0.261171 1.900428
Cl -0.515826 -1.558212 -1.749484
H -1.590040 1.486758 1.020772
C -0.381724 4.142182 -0.642656
H -0.590545 5.203178 -0.769339
C -0.936495 3.199332 -1.638127
H -0.124979 2.679411 -2.163475
H -1.494972 3.752543 -2.398505
O 2.501110 0.244930 0.613630
Si 3.474546 -0.698564 -0.397623
C 3.191050 -0.229241 -2.206156
H 2.157407 -0.452692 -2.495140
H 3.378225 0.835572 -2.390430
H 3.847578 -0.801762 -2.873134
C 3.072353 -2.526784 -0.154558
H 3.750941 -3.157682 -0.741785
H 3.156181 -2.833489 0.894451
H 2.052486 -2.744153 -0.493045
C 5.253719 -0.266756 0.166196
C 5.504937 1.248017 0.003444
H 4.805086 1.839708 0.604769
H 6.523813 1.505234 0.328811
H 5.405536 1.569749 -1.040578
C 5.444080 -0.648351 1.649694
H 4.727857 -0.126343 2.294368
H 5.319777 -1.725711 1.814313
H 6.455947 -0.381258 1.988865
C 6.279666 -1.041854 -0.689516
H 7.304193 -0.794716 -0.375101
H 6.163388 -2.128114 -0.588180
H 6.199218 -0.794457 -1.755164
C -2.272022 -3.047786 0.573462
C -3.246673 -2.655180 -0.331397
H -3.131556 -2.864025 -1.390794
H -4.232916 -2.360127 0.013870
H -1.378156 -3.561473 0.233403

H -2.477558 -3.056331 1.639199

Ts4'-4b'$_{et}$

Zero-point correction= 0.522602 (Hartree/Particle)
Thermal correction to Energy= 0.554985
Thermal correction to Enthalpy= 0.555929
Thermal correction to Gibbs Free Energy= 0.457414
Sum of electronic and zero-point Energies= -2187.610811
Sum of electronic and thermal Energies= -2187.578427
Sum of electronic and thermal Enthalpies= -2187.577483
Sum of electronic and thermal Free Energies= -2187.675998
HF (M06/6-311++g(d,p) and SDD, SMD(cyclohexane): -2187.94588635

C 0.384373 1.146771 -0.042719
H 0.692364 1.197348 -1.081798
C 1.10494 0.089299 0.814635
H 0.78619 -0.929747 0.574605
C 0.27798 2.350462 0.772081
C 0.756013 0.48729 2.260258
C 0.632217 2.023223 2.215123
H 1.529901 0.143174 2.950597
H -0.19188 0.027915 2.559061
H -0.0793 2.430472 2.941514
H 1.603891 2.497036 2.412281
C 0.291575 3.732612 0.312712
H 0.796757 4.437626 0.970604
C -1.142989 1.368636 0.141011
C -2.001373 2.238732 -0.821757
C -3.021347 3.013723 0.042742
H -3.678018 3.622388 -0.590556
H -3.648977 2.314078 0.605573
H -2.525738 3.679176 0.756361
C -2.792426 1.41263 -1.86347
H -3.494148 0.723747 -1.379112
H -3.38351 2.090213 -2.493061
H -2.131381 0.828609 -2.508375
Pt -1.902523 -0.936012 0.017813
Cl -3.174844 -0.513389 1.988674
Cl -0.618669 -1.404698 -1.939407
H -1.565402 1.267464 1.138535
C -0.308853 4.161249 -0.808513
H -0.256979 5.21481 -1.072699
C -1.133161 3.242182 -1.653422
H -0.496869 2.668507 -2.342989
H -1.806769 3.825162 -2.291515
O 2.503772 0.247214 0.619412
Si 3.508307 -0.633984 -0.415066
C 3.278347 -0.062764 -2.201741
H 2.266194 -0.298127 -2.552217
H 3.43218 1.01738 -2.308742
H 3.982091 -0.567443 -2.87549
C 3.091755 -2.473397 -0.296846
H 3.782044 -3.068826 -0.906891
H 3.150068 -2.846419 0.732384
H 2.079949 -2.666309 -0.673074
C 5.266823 -0.24521 0.229072
C 5.527949 1.275644 0.161976
H 4.800577 1.835749 0.760431
H 6.53038 1.508092 0.550813
H 5.481419 1.655878 -0.86605
C 5.403181 -0.708793 1.695803
H 4.668235 -0.216792 2.342719
H 5.268267 -1.792754 1.797735
H 6.404347 -0.466946 2.081888
C 6.320464 -0.977685 -0.63046
H 7.333024 -0.757717 -0.261974
H 6.194064 -2.067177 -0.597629
H 6.284017 -0.667525 -1.682069
C -2.050542 -3.077201 0.397531
C -3.134766 -2.675012 -0.399334
H -3.108989 -2.829698 -1.474019
H -4.105006 -2.489773 0.051959
H -1.180398 -3.540346 -0.057704
H -2.173503 -3.199113 1.469459

4b'

Zero-point correction= 0.523017 (Hartree/Particle)
Thermal correction to Energy= 0.555830
Thermal correction to Enthalpy= 0.556774
Thermal correction to Gibbs Free Energy= 0.455790
Sum of electronic and zero-point Energies= -2187.620571
Sum of electronic and thermal Energies= -2187.587758
Sum of electronic and thermal Enthalpies= -2187.586814
Sum of electronic and thermal Free Energies= -2187.687798
HF (M06/6-311++g(d,p) and SDD, SMD(cyclohexane): -2187.95494825

C 0.822467 1.443933 -0.034564
H 1.161002 1.421931 -1.066250
C 1.367697 0.377517 0.907908
H 0.840898 -0.581786 0.796191
C 0.751091 2.769327 0.727075
C 1.159044 0.968389 2.321568
C 1.240711 2.502002 2.148806
H 1.910373 0.574454 3.011010
H 0.175462 0.675563 2.706258
H 0.660034 3.036803 2.910449
H 2.281990 2.839019 2.230780
C 1.050515 4.059270 0.061099
H 1.810400 4.689061 0.521369
C -0.519554 2.050742 0.292164
C -1.414340 2.697889 -0.769029
C -2.470242 3.560286 -0.046211
H -3.168871 4.006538 -0.764794
H -3.051541 2.958783 0.661734
H -1.989559 4.372144 0.509212
C -2.107438 1.599442 -1.592875
H -2.718536 0.947990 -0.910776
H -2.846445 1.995536 -2.300671
H -1.395568 0.979358 -2.141764
Pt -2.351528 -0.981957 -0.077101
Cl -3.655353 -0.027857 1.642855
Cl -1.011075 -1.841862 -1.816760
H -1.099470 1.577636 1.086182
C 0.434812 4.452228 -1.060372
H 0.698285 5.399047 -1.526706
C -0.596376 3.591619 -1.749055
H -0.097056 2.952889 -2.493933
H -1.293943 4.216054 -2.321853
O 2.764011 0.193627 0.683869
Si 3.493694 -0.962662 -0.296332
C 3.177632 -0.596268 -2.125276
H 2.107473 -0.672258 -2.353751
H 3.512488 0.409055 -2.405715
H 3.697717 -1.314256 -2.771505
C 2.793364 -2.677783 0.095932
H 3.331405 -3.455888 -0.459396
H 2.864436 -2.919156 1.162913
H 1.739206 -2.744737 -0.199849
C 5.351049 -0.828543 0.143384
C 5.846454 0.608164 -0.131146
H 5.287362 1.344599 0.456405
H 6.909910 0.703595 0.134283
H 5.749594 0.879993 -1.189578
C 5.557399 -1.149523 1.639338
H 4.981446 -0.470688 2.278008
H 5.257924 -2.176381 1.883694
H 6.618368 -1.045666 1.911087
C 6.175317 -1.819600 -0.706658
H 7.242606 -1.745367 -0.451901
H 5.873896 -2.860872 -0.535986
H 6.084152 -1.616382 -1.780921
C -2.112341 -2.763595 1.044945
C -3.263988 -2.875006 0.216889
H -3.210022 -3.425607 -0.718075
H -4.252753 -2.710511 0.635985
H -1.182171 -3.237755 0.744779
H -2.225450 -2.519523 2.097473

Ts3'-5b'$_{et}$

Zero-point correction= 0.521127 (Hartree/Particle)
Thermal correction to Energy= 0.553748
Thermal correction to Enthalpy= 0.554692
Thermal correction to Gibbs Free Energy= 0.456661
Sum of electronic and zero-point Energies= -2187.590085
Sum of electronic and thermal Energies= -2187.557464
Sum of electronic and thermal Enthalpies= -2187.556519
Sum of electronic and thermal Free Energies= -2187.654550
HF (M06/6-311++g(d,p) and SDD, SMD(cyclohexane): -2187.92279199

C -0.519389 0.68626 0.363887
H -1.178389 1.282491 1.000596
C -1.254775 -0.342913 -0.440741
H -1.083939 -1.304823 0.066702
C 0.455106 1.811216 -1.263446
C -0.661016 -0.410403 -1.860179
C -0.359258 1.021794 -2.309764
H -1.380662 -0.90108 -2.522103
H 0.254862 -1.007745 -1.84706
H 0.198698 1.010946 -3.2524
H -1.310122 1.537164 -2.485323
C -0.045771 3.209077 -1.043444
H -0.397394 3.703222 -1.949327
C 0.841354 0.989507 0.278043
C 1.375437 2.070117 1.28024

C 2.748635 2.616954 0.836405
H 3.125633 3.311569 1.596694
H 3.475761 1.810355 0.717387
H 2.692849 3.159918 -0.111546
C 1.535542 1.433761 2.677344
H 2.284967 0.63889 2.673449
H 1.849917 2.204607 3.391903
H 0.597729 0.995945 3.036628
Cl 3.324048 0.345702 -1.858084
Cl 0.992085 -1.833124 1.709883
H 1.509301 1.808691 -1.566682
C -0.063687 3.865601 0.117729
H -0.450775 4.88276 0.143597
C 0.396186 3.270491 1.419334
H -0.480942 2.986366 2.024092
H 0.898262 4.043962 2.015511
O -2.631896 -0.005137 -0.492001
Si -3.863875 -0.836814 0.321821
C -3.616287 -0.655179 2.187479
H -2.646759 -1.06592 2.496868
H -3.652187 0.392042 2.509642
H -4.388531 -1.19933 2.745033
C -3.784066 -2.670658 -0.127677
H -4.58179 -3.231241 0.374771
H -3.887871 -2.835793 -1.20602
H -2.833281 -3.118131 0.187276
C -5.467323 -0.001361 -0.290426
C -5.439884 1.505873 0.046493
H -4.584045 2.008204 -0.418227
H -6.353782 1.994086 -0.321849
H -5.390148 1.685429 1.127641
C -5.593959 -0.168354 -1.820737
H -4.740452 0.273645 -2.346954
H -5.661458 -1.222937 -2.11493
H -6.504636 0.329746 -2.183772
C -6.690325 -0.651924 0.39355
H -7.618325 -0.175861 0.045989
H -6.770609 -1.721964 0.16475
H -6.659489 -0.543047 1.484797
Pt 2.153366 -0.667903 -0.039223
C 3.927093 -2.054331 0.259358
C 3.081765 -2.662818 -0.647487
H 4.781693 -1.477578 -0.080801
H 3.887947 -2.314383 1.312692
H 3.255933 -2.570495 -1.715007
H 2.362365 -3.406859 -0.320473

5b'[Pt]$_{et}$

Zero-point correction= 0.524709 (Hartree/Particle)
Thermal correction to Energy= 0.557420
Thermal correction to Enthalpy= 0.558364
Thermal correction to Gibbs Free Energy= 0.459057
Sum of electronic and zero-point Energies= -2187.653628
Sum of electronic and thermal Energies= -2187.620917
Sum of electronic and thermal Enthalpies= -2187.619973
Sum of electronic and thermal Free Energies= -2187.719279
HF (M06/6-311++g(d,p) and SDD, SMD(cyclohexane): -2187.98445552

C -0.084590 0.313296 0.168757
H -0.297422 -0.131229 1.134738
C -0.978986 -0.222809 -0.952220
H -0.816414 -1.303003 -1.059717
C 0.417253 2.436340 -1.102875
C -0.714145 0.473234 -2.287065
C -0.688837 1.988707 -2.094335
H -1.502802 0.187525 -2.991719
H 0.242691 0.127160 -2.693461
H -0.522913 2.497389 -3.051164
H -1.662826 2.321098 -1.716225
C 0.275880 3.918506 -0.837602
H 0.247745 4.547286 -1.726029
C 0.435870 1.600295 0.165543
C 0.972941 2.275780 1.429531
C 2.475917 2.614576 1.243789
H 2.836193 3.146549 2.132118
H 3.064490 1.699783 1.126671
H 2.654585 3.247419 0.371760
C 0.812721 1.438697 2.708653
H 1.365598 0.496237 2.662171
H 1.197646 2.011349 3.560222
H -0.237334 1.204761 2.916942
Cl 2.944316 0.343114 -1.863057
Cl 1.106843 -2.214326 1.711309
H 1.386569 2.260156 -1.598993
C 0.126537 4.449045 0.375506
H -0.027319 5.520149 0.492004
C 0.173668 3.603749 1.616988
H -0.847126 3.373349 1.959290
H 0.644931 4.157910 2.439364
O -2.331297 0.026094 -0.553675
Si -3.457130 -1.107822 -0.007322
C -2.956249 -1.777203 1.686319
H -1.958757 -2.232094 1.651943
H -2.929621 -0.987573 2.446301
H -3.657111 -2.547528 2.031507
C -3.555681 -2.549611 -1.230235
H -4.313368 -3.278347 -0.916808
H -3.811979 -2.215701 -2.242140
H -2.601362 -3.087350 -1.289090
C -5.093742 -0.119533 0.070423
C -4.923909 1.095544 1.008251
H -4.125658 1.761996 0.663072
H -5.854822 1.680255 1.049119
H -4.686936 0.790696 2.035157
C -5.472194 0.384803 -1.338469
H -4.690656 1.027206 -1.759423
H -5.638757 -0.443735 -2.037653
H -6.402031 0.971004 -1.298787
C -6.227191 -1.019349 0.609509
H -7.171639 -0.457792 0.653933
H -6.400342 -1.893434 -0.030775
H -6.017607 -1.382436 1.623289
Pt 1.961545 -0.854623 -0.056000
C 3.930367 -1.755133 0.308776
C 3.233056 -2.541502 -0.618300
H 4.668462 -1.034345 -0.029534
H 3.947899 -2.030489 1.358720
H 3.433727 -2.440376 -1.680464
H 2.712159 -3.436486 -0.292393

1b-PtCl$_2$(PC$_6$F$_5$)

I1$_p$

Zero-point correction= 0.614557 (Hartree/Particle)
Thermal correction to Energy= 0.678931
Thermal correction to Enthalpy= 0.679875
Thermal correction to Gibbs Free Energy= 0.506198
Sum of electronic and zero-point Energies= -4633.587700
Sum of electronic and thermal Energies= -4633.523326
Sum of electronic and thermal Enthalpies= -4633.522382
Sum of electronic and thermal Free Energies= -4633.696059
HF (M06/6-311++g(d,p) and SDD, SMD(cyclohexane): -4633.63400975

C 3.418160 -3.011350 0.628087
Si 4.993763 -1.980205 0.450962
C 5.800623 -2.217125 -1.274289
C 7.037178 -1.300559 -1.396624
O 4.651558 -0.350835 0.700412
C 3.406048 0.341019 0.684009
C 3.287988 1.194392 1.962744
C 4.430759 2.198385 2.209740
C 4.443544 3.384277 1.285596
C 5.530007 3.850806 0.646549
C 5.583278 5.036226 -0.219062
C 4.754498 6.090276 -0.188309
C 3.318085 1.148813 -0.595042
C 2.240017 1.410424 -1.309006
Pt 0.199877 0.811954 -0.828783
Cl 0.429925 -1.274460 -1.996196
C 1.614024 1.976835 -2.396617
C 1.598123 1.280511 -3.739778
C 1.213854 3.435291 -2.429654
Cl -0.003764 2.730964 0.575581
C 6.209419 -2.443774 1.819642
C 6.244133 -3.687070 -1.446938
C 4.801472 -1.864811 -2.396957
H 4.862098 6.913496 -0.888765
H 3.951275 6.172443 0.539844
H 3.487677 3.892380 1.149342
H 4.262853 1.562239 -0.946653
H 2.571736 -0.371444 0.695474
H 0.231607 3.566512 -2.896339
H 1.950580 3.954314 -3.060557
H 1.207193 3.890158 -1.441771
H 1.896729 0.236477 -3.671132
H 2.305086 1.817861 -4.388936
H 0.610165 1.341656 -4.208064
H 5.395074 1.678907 2.173908
H 4.312586 2.566735 3.241298
H 3.250794 0.494462 2.807798
H 2.324257 1.716194 1.932464
H 6.466003 3.299901 0.751909
H 6.398265 5.045866 -0.944157
H 3.639066 -4.076023 0.483152
H 3.001719 -2.901160 1.636602
H 2.645061 -2.731108 -0.096896
H 7.103323 -1.810295 1.795448
H 5.739439 -2.312253 2.801512
H 6.536342 -3.487809 1.744249

H 5.397769 -4.382709 -1.386605
H 6.710855 -3.830287 -2.432495
H 6.981273 -3.988690 -0.692742
H 3.905756 -2.496510 -2.367245
H 4.469159 -0.822361 -2.336170
H 5.270946 -2.005704 -3.382024
H 6.771738 -0.244652 -1.269386
H 7.803502 -1.543950 -0.650336
H 7.500714 -1.411273 -2.388154
P -1.765955 -0.169916 0.077368
C -1.248561 -1.732625 0.897546
C -2.718342 0.833983 1.295378
C -3.106310 -0.565106 -1.116954
C -1.551729 -3.030640 0.474217
C -0.300811 -1.614089 1.922096
C -3.204422 2.061087 0.823746
C -2.983220 0.525246 2.632745
C -3.097576 -0.100473 -2.437506
C -4.254799 -1.246725 -0.692967
C -0.974212 -4.150868 1.069767
F -2.392875 -3.265398 -0.539108
C 0.292349 -2.712968 2.525312
F 0.064490 -0.392909 2.341124
C -3.896059 2.953385 1.632765
F -3.023740 2.392485 -0.462578
C -3.670513 1.405614 3.466101
F -2.604144 -0.640106 3.173444
C -4.161135 -0.347240 -3.305566
F -2.090672 0.630077 -2.917314
C -5.325086 -1.504623 -1.538209
F -4.338325 -1.685775 0.572183
C -0.047037 -3.993375 2.094147
F -1.295238 -5.374083 0.642244
F 1.211102 -2.549972 3.482409
C -4.124185 2.623206 2.966964
F -4.340253 4.111938 1.142630
F -3.908620 1.075965 4.738043
C -5.273176 -1.052463 -2.856763
F -4.122632 0.108816 -4.559011
F -6.394558 -2.172683 -1.100266
F 0.520915 -5.058240 2.654535
F -4.787484 3.462873 3.758845
F -6.292400 -1.286479 -3.679158

$I2_p$

Zero-point correction= 0.614965 (Hartree/Particle)
Thermal correction to Energy= 0.678857
Thermal correction to Enthalpy= 0.679802
Thermal correction to Gibbs Free Energy= 0.509462
Sum of electronic and zero-point Energies= -4633.583289
Sum of electronic and thermal Energies= -4633.519397
Sum of electronic and thermal Enthalpies= -4633.518452
Sum of electronic and thermal Free Energies= -4633.688792
HF (M06/6-311++g(d,p) and SDD, SMD(cyclohexane): -4633.63400365

C 3.117017 -1.420579 0.552528
H 4.058530 -1.900877 0.805443
C 3.274051 -0.289354 -0.420469
H 2.551115 0.485662 -0.125381
C 3.391893 -3.119202 -1.745941
C 2.949488 -0.660513 -1.888305
C 3.779792 -1.841206 -2.424543
H 3.130779 0.239303 -2.488492
H 1.882836 -0.895549 -1.956970
H 3.579492 -1.922099 -3.503489
H 4.850196 -1.638129 -2.306254
C 4.236846 -3.944450 -1.090964
H 5.300759 -3.702367 -1.093280
C 1.935087 -1.818636 1.157601
C 1.983995 -2.774991 2.185100
C 0.725755 -3.405152 2.693935
H 0.926986 -4.313777 3.270011
H 0.219552 -2.688121 3.357852
H 0.030065 -3.610682 1.874834
C 3.215987 -3.125178 2.968176
H 3.075047 -2.762955 3.997780
H 3.325493 -4.213052 3.033293
H 4.138776 -2.687133 2.589090
Pt 0.153948 -0.968015 0.613149
Cl -0.302164 -2.846718 -0.799898
Cl 0.735863 0.897126 2.023982
H 2.330965 -3.365020 -1.786182
C 3.856254 -5.144257 -0.345605
H 4.683579 -5.784907 -0.039822
C 2.608500 -5.499841 0.014096
H 2.433143 -6.419553 0.565617
H 1.732729 -4.909943 -0.244031
O 4.610385 0.193111 -0.345962
Si 5.109671 1.526249 0.575129
C 4.952785 1.127570 2.415911
H 3.905164 0.927516 2.673767
H 5.549661 0.253625 2.702633
H 5.282450 1.971693 3.034191
C 4.014310 3.014807 0.180712
H 4.374610 3.912090 0.698699
H 3.987963 3.238157 -0.892024
H 2.985614 2.840309 0.519463
C 6.926727 1.787701 0.040472
C 7.747248 0.512921 0.333721
H 7.345685 -0.356215 -0.199358
H 8.791004 0.647643 0.014344
H 7.763948 0.273975 1.404440
C 6.990981 2.088937 -1.472551
H 6.565498 1.271148 -2.064881
H 6.449555 3.007432 -1.730806
H 8.034685 2.225399 -1.791425
C 7.539037 2.972584 0.819621
H 8.584832 3.127422 0.517239
H 7.004950 3.911855 0.629438
H 7.537049 2.799181 1.902920
P -1.790790 0.254890 -0.039374
C -1.119003 1.758229 -0.872691
C -2.986274 -0.541117 -1.204158
C -2.977717 0.828508 1.248748
C -1.077883 3.045681 -0.331208
C -0.361442 1.546442 -2.031189
C -3.519975 -1.761878 -0.770984
C -3.392194 -0.091718 -2.463416
C -2.962351 0.298180 2.543756
C -4.003318 1.732505 0.946813
C -0.340404 4.071203 -0.922734
F -1.728184 3.355560 0.797013
C 0.390622 2.545307 -2.633307
F -0.338568 0.326034 -2.590496
C -4.380876 -2.523339 -1.551897
F -3.226910 -2.211663 0.457600
C -4.249650 -0.838647 -3.269028
F -2.986256 1.088244 -2.951909
C -3.902724 0.680200 3.501054
F -2.067043 -0.618227 2.913999
C -4.949311 2.129511 1.882039
F -4.087839 2.255370 -0.286639
C 0.399241 3.821423 -2.073486
F -0.332864 5.290647 -0.377034
F 1.110584 2.286556 -3.730532
C -4.741013 -2.059108 -2.814708
F -4.867123 -3.681560 -1.099109
F -4.614836 -0.378440 -4.469733
C -4.893841 1.598412 3.170553
F -3.863474 0.155872 4.728970
F -5.905194 3.005591 1.559320
F 1.115243 4.794637 -2.636906
F -5.568338 -2.772100 -3.578676
F -5.796531 1.964009 4.079339

$Ts2\text{-}3_p$

Zero-point correction= 0.617424 (Hartree/Particle)
Thermal correction to Energy= 0.679108
Thermal correction to Enthalpy= 0.680052
Thermal correction to Gibbs Free Energy= 0.517420
Sum of electronic and zero-point Energies= -4633.576983
Sum of electronic and thermal Energies= -4633.515299
Sum of electronic and thermal Enthalpies= -4633.514355
Sum of electronic and thermal Free Energies= -4633.676988
HF (M06/6-311++g(d,p) and SDD, SMD(cyclohexane): -4633.63172636

C 3.085695 -1.599851 0.268167
H 4.04735 -1.976859 0.602782
C 3.237603 -0.344322 -0.570652
H 2.517992 0.397996 -0.202766
C 3.12424 -3.016069 -1.671375
C 2.948317 -0.603734 -2.063748
C 3.642342 -1.898183 -2.519759
H 3.274595 0.263844 -2.647133
H 1.866877 -0.711609 -2.194436
H 3.386763 -2.090728 -3.572272
H 4.731977 -1.808403 -2.448966
C 3.873182 -4.02343 -1.100277
H 4.951354 -4.026847 -1.25886
C 1.912171 -2.073992 0.852727
C 1.978367 -3.127823 1.81294
C 0.706776 -3.558836 2.50642
H 0.835683 -4.507228 3.038644
H 0.447139 -2.790389 3.248739
H -0.135252 -3.630276 1.814213
C 3.228056 -3.411192 2.625026
H 3.246376 -2.712405 3.473777
H 3.206319 -4.424028 3.03795
H 4.159682 -3.283325 2.072889
Pt 0.135681 -1.139197 0.444066
Cl -0.458654 -2.777302 -1.205655
Cl 0.793987 0.479367 2.102941
H 2.039765 -3.094055 -1.643959

C 3.344229 -4.954448 -0.170526
H 4.058809 -5.62561 0.303958
C 2.0479 -4.949012 0.302812
H 1.75516 -5.690085 1.040667
H 1.236057 -4.470964 -0.233915
O 4.575185 0.129298 -0.439201
Si 5.069496 1.39234 0.573473
C 4.957094 0.857848 2.38255
H 3.918451 0.620369 2.64421
H 5.571649 -0.025708 2.591553
H 5.287445 1.659048 3.055281
C 3.950331 2.895102 0.319053
H 4.313586 3.752151 0.8996
H 3.891398 3.206978 -0.730353
H 2.933773 2.679095 0.67006
C 6.872394 1.723804 0.028578
C 7.715695 0.441666 0.199258
H 7.314252 -0.385713 -0.396833
H 8.751052 0.617979 -0.127848
H 7.756673 0.114173 1.24555
C 6.902112 2.147976 -1.455808
H 6.473779 1.374815 -2.103512
H 6.344383 3.076792 -1.627845
H 7.937296 2.323608 -1.783591
C 7.485796 2.850123 0.889318
H 8.524517 3.041604 0.583221
H 6.93822 3.794927 0.783333
H 7.504351 2.591554 1.955299
P -1.760464 0.259893 -0.023551
C -0.993454 1.812722 -0.664743
C -3.005771 -0.290947 -1.275959
C -2.909719 0.741253 1.335274
C -0.860742 3.012406 0.038866
C -0.24678 1.698397 -1.844116
C -3.621014 -1.52032 -1.00849
C -3.383434 0.355039 -2.456407
C -2.926329 0.048678 2.551208
C -3.872157 1.742734 1.162096
C -0.040302 4.046133 -0.413392
F -1.494142 3.221306 1.199385
C 0.586921 2.704778 -2.30987
F -0.309811 0.560532 -2.556237
C -4.536154 -2.105788 -1.875133
F -3.353905 -2.154683 0.141889
C -4.293746 -0.212802 -3.345809
F -2.897886 1.560836 -2.783073
C -3.837083 0.365497 3.559652
F -2.093791 -0.96512 2.788571
C -4.787615 2.077527 2.150541
F -3.921814 2.424771 0.006764
C 0.691383 3.890428 -1.585338
F 0.057818 5.178635 0.288507
F 1.299155 2.535522 -3.42971
C -4.868 -1.447389 -3.056767
F -5.099956 -3.279851 -1.580051
F -4.629723 0.431857 -4.467791
C -4.764967 1.382221 3.359592
F -3.830668 -0.313189 4.710174
F -5.683245 3.049859 1.954347
F 1.499149 4.863128 -2.00912
F -5.745931 -1.989644 -3.90061
F -5.639561 1.687026 4.317213

$I3_p$

Zero-point correction= 0.621489 (Hartree/Particle)
Thermal correction to Energy= 0.682569
Thermal correction to Enthalpy= 0.683513
Thermal correction to Gibbs Free Energy= 0.520481
Sum of electronic and zero-point Energies= -4633.611224
Sum of electronic and thermal Energies= -4633.550144
Sum of electronic and thermal Enthalpies= -4633.549200
Sum of electronic and thermal Free Energies= -4633.712232
HF (M06/6-311++g(d,p) and SDD, SMD(cyclohexane): -4633.67994674

C 3.089150 -1.821072 -0.175210
H 3.993677 -2.026827 0.399975
C 3.249451 -0.383563 -0.778218
H 2.478197 0.292294 -0.400262
C 3.125455 -2.824972 -1.459394
C 3.164531 -0.569668 -2.302437
C 3.780691 -1.951185 -2.540962
H 3.676284 0.242922 -2.825726
H 2.111771 -0.570189 -2.609365
H 3.580989 -2.350773 -3.541382
H 4.867314 -1.912972 -2.395228
C 3.786579 -4.116546 -1.098295
H 4.743177 -4.343546 -1.567347
C 1.872300 -2.199328 0.555218
C 1.922361 -3.385689 1.490148
C 0.641799 -3.517139 2.342448
H 0.730067 -4.390095 3.000319
H 0.494531 -2.630546 2.965135
H -0.246329 -3.646655 1.717257
C 3.145293 -3.331518 2.440079
H 3.146545 -2.399877 3.015586
H 3.079326 -4.164480 3.148725
H 4.095845 -3.419066 1.909537
Pt 0.206398 -1.223740 0.263645
Cl -0.513293 -2.654318 -1.508171
Cl 0.867456 0.283774 2.039910
H 2.088014 -3.005239 -1.760137
C 3.284061 -4.943566 -0.170910
H 3.839841 -5.841361 0.092596
C 1.997746 -4.693857 0.570521
H 1.805963 -5.523366 1.259207
H 1.147101 -4.652685 -0.120037
O 4.547808 0.086273 -0.439138
Si 4.960576 1.340299 0.613822
C 4.858571 0.751113 2.406091
H 3.828960 0.467683 2.655231
H 5.505046 -0.114974 2.590424
H 5.157305 1.543302 3.103880
C 3.775301 2.795754 0.379509
H 4.095956 3.657905 0.977404
H 3.712970 3.121458 -0.665644
H 2.768135 2.525302 0.718048
C 6.754607 1.783370 0.117379
C 7.658440 0.538148 0.249095
H 7.304841 -0.283809 -0.383530
H 8.687281 0.778183 -0.057371
H 7.703941 0.171991 1.282277
C 6.788359 2.272603 -1.346360
H 6.413957 1.506681 -2.034939
H 6.185143 3.177646 -1.489573
H 7.818350 2.516090 -1.645819
C 7.295426 2.899845 1.037234
H 8.327423 3.157561 0.758252
H 6.701300 3.819210 0.963132
H 7.310875 2.594602 2.090804
P -1.739882 0.282395 -0.022584
C -0.984305 1.904787 -0.466688
C -2.978228 -0.134222 -1.328848
C -2.876372 0.573434 1.395162
C -0.922170 3.039793 0.346564
C -0.204395 1.928673 -1.629708
C -3.620189 -1.369470 -1.172859
C -3.322708 0.613915 -2.457786
C -2.849913 -0.244838 2.529995
C -3.877672 1.550687 1.339037
C -0.144809 4.147145 0.007894
F -1.585510 3.112583 1.507142
C 0.585131 3.012700 -1.985365
F -0.204088 0.859020 -2.441866
C -4.532937 -1.862729 -2.096960
F -3.376614 -2.103483 -0.077624
C -4.229891 0.139474 -3.403324
F -2.807733 1.831149 -2.677747
C -3.755705 -0.071736 3.576737
F -1.977213 -1.246585 2.645779
C -4.789761 1.742982 2.367585
F -3.968054 2.348373 0.263597
C 0.613572 4.133131 -1.157452
F -0.114577 5.213522 0.811467
F 1.325804 2.981361 -3.097029
C -4.833190 -1.102284 -3.224867
F -5.122157 -3.045350 -1.908322
F -4.534758 0.881080 -4.472131
C -4.723041 0.924804 3.495683
F -3.706812 -0.867553 4.647494
F -5.722812 2.695361 2.286434
F 1.375825 5.178022 -1.476477
F -5.707289 -1.554574 -4.122694
F -5.592580 1.093788 4.489602

$Ts3\text{-}2b_p$

Zero-point correction= 0.617500 (Hartree/Particle)
Thermal correction to Energy= 0.678028
Thermal correction to Enthalpy= 0.678973
Thermal correction to Gibbs Free Energy= 0.519574
Sum of electronic and zero-point Energies= -4633.582455
Sum of electronic and thermal Energies= -4633.521926
Sum of electronic and thermal Enthalpies= -4633.520982
Sum of electronic and thermal Free Energies= -4633.680381
HF (M06/6-311++g(d,p) and SDD, SMD(cyclohexane): -4633.64883356

C -2.17847 3.390257 0.926032
C -2.226783 2.039444 0.140109
C -3.162359 4.496407 0.425706
C -4.382921 2.547773 -1.31378
C -3.240164 1.685093 -0.760617
C -3.379483 0.281408 -1.40157
H -2.415262 -0.213024 -1.530433
H -2.944617 5.395249 1.012567

C -0.755757 3.985671 0.812095
H -0.016149 3.332393 1.281722
H -0.731463 4.9528 1.328812
H -0.462839 4.13706 -0.231062
C -2.472448 3.105945 2.417479
H -3.49458 2.737139 2.563415
H -2.366344 4.035672 2.989982
H -1.783951 2.36296 2.824545
C -5.154403 1.634875 -2.289958
C -4.106527 0.596111 -2.715317
H -4.533775 -0.303085 -3.16559
H -3.390408 1.02891 -3.426008
H -5.982963 1.141877 -1.771487
H -5.569428 2.202502 -3.128122
Pt -0.519194 0.848726 0.13579
H -3.144272 1.321311 0.599293
Cl -1.06169 -0.133555 2.240829
Cl -0.078031 1.815019 -2.036839
C -5.198825 3.266058 -0.26746
C -4.629015 4.166295 0.534934
H -3.843633 3.300562 -1.914335
H -2.911397 4.747795 -0.615352
H -5.222232 4.670602 1.294729
H -6.253785 3.011735 -0.192724
O -4.227982 -0.4276 -0.5066
Si -4.414509 -2.10823 -0.322036
C -5.561088 -2.262425 1.200703
C -2.740893 -2.928848 -0.067622
H -2.862979 -3.999969 0.137103
H -2.111173 -2.836601 -0.959519
H -2.193926 -2.476705 0.765262
C -5.229461 -2.827788 -1.873361
H -4.581907 -2.713236 -2.751319
H -5.414113 -3.90221 -1.751482
H -6.189275 -2.349717 -2.100532
C -4.850531 -1.722371 2.46068
H -3.932704 -2.276679 2.686697
H -4.57443 -0.667576 2.355683
H -5.51283 -1.808751 3.33464
C -6.859123 -1.459218 0.970419
H -6.65059 -0.393589 0.823281
H -7.416463 -1.818294 0.095941
H -7.524396 -1.551624 1.841272
C -5.920792 -3.748704 1.42594
H -6.564976 -3.85191 2.310937
H -6.466882 -4.177115 0.576324
H -5.03149 -4.366991 1.601038
P 1.619415 -0.167174 -0.015483
C 2.796869 1.243315 -0.189689
C 2.203898 -1.204416 1.401865
C 1.987923 -1.334277 -1.397049
C 3.494986 1.593892 -1.348785
C 2.834143 2.167138 0.861657
C 1.425745 -2.33465 1.682861
C 3.299974 -0.97893 2.240235
C 0.986087 -1.847168 -2.226897
C 3.283151 -1.82899 -1.594842
C 4.217431 2.782513 -1.442932
F 3.491116 0.815025 -2.438267
C 3.54389 3.357854 0.794507
F 2.15754 1.906663 1.991748
C 1.684108 -3.179027 2.755577
F 0.40928 -2.655287 0.868938
C 3.577718 -1.806275 3.326854
F 4.152985 0.03252 2.029098
C 1.263836 -2.786369 -3.21986
F -0.292621 -1.483551 -2.09218
C 3.586993 -2.761544 -2.577501
F 4.289361 -1.385754 -0.824964
C 4.243888 3.666556 -0.370136
F 4.87698 3.077193 -2.56696
F 3.556215 4.202751 1.82941
C 2.765436 -2.905395 3.589144
F 0.914523 -4.246459 2.982039
F 4.634276 -1.557574 4.106485
C 2.565879 -3.241591 -3.397199
F 0.280788 -3.257796 -3.992037
F 4.838621 -3.197846 -2.74287
F 4.933109 4.803994 -0.454802
F 3.033681 -3.70387 4.621572
F 2.838134 -4.139468 -4.342155

2b-[Pt]$_p$

Zero-point correction= 0.622086 (Hartree/Particle)
Thermal correction to Energy= 0.683049
Thermal correction to Enthalpy= 0.683993
Thermal correction to Gibbs Free Energy= 0.522946
Sum of electronic and zero-point Energies= -4633.635697
Sum of electronic and thermal Energies= -4633.574734
Sum of electronic and thermal Enthalpies= -4633.573790
Sum of electronic and thermal Free Energies= -4633.734837
HF (M06/6-311++g(d,p) and SDD, SMD(cyclohexane): -4633.69838624

C -2.539427 2.991491 0.376506
C -2.513855 1.460915 0.294613
C -2.644332 3.706501 -0.998416
C -3.015565 1.028699 -2.244887
C -2.793839 0.628053 -0.779785
C -3.329640 -0.805069 -0.619792
H -2.866371 -1.344602 0.207564
H -2.630962 4.786364 -0.807124
C -1.291922 3.513501 1.120645
H -1.132173 2.971228 2.059935
H -1.415737 4.577244 1.358466
H -0.394787 3.401671 0.504208
C -3.790078 3.324033 1.232798
H -4.706456 2.944278 0.770257
H -3.885591 4.411367 1.340122
H -3.706763 2.893979 2.237702
C -3.414011 -0.287899 -2.971423
C -3.058458 -1.421885 -1.992960
H -3.642691 -2.333206 -2.152226
H -1.994189 -1.677483 -2.063298
H -4.491679 -0.294415 -3.165007
H -2.904525 -0.388415 -3.934356
Pt -0.429524 0.425728 -0.093323
H -2.643370 1.003191 1.273829
Cl -0.940454 -0.835473 1.873926
Cl 0.302747 1.748447 -1.966011
C -4.043367 2.141282 -2.358114
C -3.869769 3.344807 -1.805128
H -2.069960 1.397592 -2.654096
H -1.737710 3.481383 -1.571658
H -4.647980 4.097584 -1.918953
H -4.951620 1.917166 -2.915233
O -4.741845 -0.666714 -0.432771
Si -5.666907 -1.362146 0.795598
C -7.461676 -0.892864 0.328573
C -5.166395 -0.663975 2.479297
H -5.740457 -1.132159 3.288626
H -4.104772 -0.854304 2.678433
H -5.326788 0.418663 2.539196
C -5.394895 -3.234483 0.809536
H -4.347029 -3.475609 1.027343
H -6.004597 -3.720915 1.580910
H -5.646558 -3.691632 -0.154091
C -7.601106 0.644191 0.274576
H -7.395178 1.106953 1.247586
H -6.917279 1.086431 -0.458711
H -8.626027 0.925059 -0.009425
C -7.815773 -1.476156 -1.056110
H -7.138938 -1.104951 -1.833744
H -7.768501 -2.572146 -1.064382
H -8.839873 -1.192340 -1.340233
C -8.442114 -1.454546 1.381501
H -9.476312 -1.184834 1.122660
H -8.398270 -2.549286 1.442298
H -8.244041 -1.055034 2.383928
P 1.830005 -0.130638 0.044249
C 2.693568 1.437070 0.466815
C 2.319448 -1.413230 1.276543
C 2.624367 -0.851722 -1.449853
C 3.465154 2.205622 -0.411086
C 2.402173 2.007700 1.712714
C 1.690349 -2.658191 1.139358
C 3.249220 -1.290014 2.313185
C 1.887124 -1.395653 -2.508576
C 4.016728 -0.995023 -1.508940
C 3.950854 3.461297 -0.051556
F 3.760853 1.780161 -1.643571
C 2.874788 3.256495 2.093864
F 1.637974 1.333695 2.582385
C 1.932945 -3.719227 2.001886
F 0.838369 -2.859000 0.124162
C 3.506694 -2.338202 3.194971
F 3.952069 -0.165510 2.497548
C 2.512930 -2.002171 -3.597576
F 0.554457 -1.390766 -2.511143
C 4.661946 -1.592852 -2.582828
F 4.775965 -0.537538 -0.500806
C 3.657177 3.988018 1.202469
F 4.691137 4.163342 -0.912725
F 2.581592 3.755605 3.296551
C 2.844221 -3.552776 3.042632
F 1.308786 -4.886811 1.836370
F 4.401164 -2.185216 4.174662
C 3.900398 -2.096350 -3.637059
F 1.782995 -2.509212 -4.592821
F 5.992906 -1.693760 -2.608485
F 4.119803 5.187315 1.548736
F 3.094156 -4.558387 3.878282
F 4.501031 -2.678042 -4.672057

Ts3-3b$_p$

Zero-point correction= 0.619519 (Hartree/Particle)
Thermal correction to Energy= 0.680238
Thermal correction to Enthalpy= 0.681182
Thermal correction to Gibbs Free Energy= 0.521866

Sum of electronic and zero-point Energies= -4633.582654
Sum of electronic and thermal Energies= -4633.521936
Sum of electronic and thermal Enthalpies= -4633.520991
Sum of electronic and thermal Free Energies= -4633.680307
HF (M06/6-311++g(d,p) and SDD, SMD(cyclohexane): -4633.65379786

C 2.979953 -2.059157 -0.20449
H 3.940318 -2.405123 0.188954
C 3.285865 -0.59432 -0.642987
H 2.474531 0.087526 -0.381767
C 2.770802 -2.865348 -1.513234
C 3.465585 -0.682127 -2.184113
C 3.721865 -2.167237 -2.496635
H 4.261527 -0.015644 -2.527928
H 2.533614 -0.364158 -2.668498
H 3.523658 -2.427223 -3.542103
H 4.764906 -2.432556 -2.276057
C 2.989262 -4.314198 -1.202954
H 3.571498 -4.93071 -1.885989
C 1.876062 -2.308452 0.824792
C 2.242597 -2.566356 2.172299
C 1.225346 -2.560181 3.274061
H 1.431477 -3.334744 4.021335
H 1.305188 -1.581369 3.765221
H 0.204809 -2.639436 2.89444
C 3.672473 -2.747687 2.612505
H 4.171792 -1.772968 2.547115
H 3.734686 -3.110808 3.641333
H 4.222854 -3.427614 1.955615
Pt 0.093952 -1.247809 0.460349
Cl -0.796178 -2.946558 -0.96239
Cl 0.962553 0.504134 1.885663
H 1.738989 -2.72288 -1.861959
C 2.543434 -4.833562 -0.049618
H 2.771168 -5.865244 0.213399
C 1.647133 -4.113376 0.904021
H 1.687398 -4.59099 1.888178
H 0.59955 -4.099809 0.599267
O 4.492049 -0.192911 0.012465
Si 4.964811 1.339503 0.523578
C 4.764013 1.43928 2.400271
H 3.715379 1.268821 2.669615
H 5.373099 0.687055 2.916511
H 5.054691 2.422774 2.789653
C 3.892517 2.672929 -0.281863
H 4.224806 3.674265 0.017858
H 3.912252 2.630923 -1.377195
H 2.852542 2.561996 0.046611
C 6.810407 1.513168 0.029971
C 7.628441 0.357453 0.64577
H 7.262074 -0.618754 0.30807
H 8.686141 0.436865 0.353655
H 7.593053 0.369743 1.742284
C 6.960742 1.464948 -1.505088
H 6.593588 0.517654 -1.917017
H 6.416791 2.280346 -1.998074
H 8.018707 1.560133 -1.791224
C 7.366207 2.857608 0.54831
H 8.424556 2.967831 0.270253
H 6.829421 3.715872 0.124875
H 7.308512 2.932583 1.64115
P -1.699747 0.241849 -0.03822
C -0.891322 1.700405 -0.831874
C -3.036454 -0.339758 -1.177926
C -2.757867 0.888342 1.327786
C -0.73737 2.970342 -0.26834
C -0.169842 1.451983 -2.006472
C -3.75974 -1.454475 -0.733991
C -3.388565 0.175257 -2.428278
C -2.739647 0.320379 2.606305
C -3.701925 1.896851 1.098507
C 0.063878 3.947733 -0.858293
F -1.333195 3.309513 0.881789
C 0.644838 2.401554 -2.606205
F -0.246544 0.24487 -2.5874
C -4.756668 -2.054421 -1.493048
F -3.511849 -1.960499 0.482652
C -4.38022 -0.411321 -3.212778
F -2.800723 1.270199 -2.93
C -3.593552 0.763808 3.61664
F -1.928853 -0.693978 2.910857
C -4.561528 2.35638 2.087019
F -3.78771 2.465532 -0.114424
C 0.761102 3.663122 -2.027177
F 0.177116 5.151777 -0.29014
F 1.330522 2.102918 -3.714747
C -5.063087 -1.530605 -2.746683
F -5.419623 -3.116536 -1.029154
F -4.689095 0.109979 -4.404201
C -4.502189 1.784334 3.357609
F -3.551868 0.200171 4.827112
F -5.437581 3.332396 1.832088
F 1.545541 4.58516 -2.583846
F -6.017844 -2.089053 -3.490201
F -5.321964 2.209633 4.317403

3b-[Pt]$_p$
Zero-point correction= 0.622106 (Hartree/Particle)
Thermal correction to Energy= 0.683263
Thermal correction to Enthalpy= 0.684207
Thermal correction to Gibbs Free Energy= 0.522255
Sum of electronic and zero-point Energies= -4633.624619
Sum of electronic and thermal Energies= -4633.563462
Sum of electronic and thermal Enthalpies= -4633.562518
Sum of electronic and thermal Free Energies= -4633.724470
HF (M06/6-311++g(d,p) and SDD, SMD(cyclohexane): -4633.68956373

C 3.231695 1.220152 -0.569915
H 4.028487 1.679648 -1.181754
C 4.046646 0.599140 0.593742
H 3.516220 -0.214645 1.085215
C 2.485810 2.425806 0.047717
C 4.213660 1.783286 1.603331
C 3.570144 3.028176 0.957694
H 5.267268 1.937737 1.845625
H 3.692898 1.535676 2.535431
H 3.168875 3.730216 1.696892
H 4.300302 3.574936 0.347080
C 1.917037 3.320412 -1.013609
H 1.587914 4.318228 -0.725309
C 2.417442 0.506911 -1.649298
C 2.290935 -0.868210 -1.897871
C 2.047901 -1.408582 -3.299071
H 3.020259 -1.747829 -3.686992
H 1.387271 -2.279635 -3.268752
H 1.627642 -0.694972 -4.001540
C 2.884349 -1.951461 -1.017531
H 2.880824 -1.718930 0.041091
H 2.329877 -2.885247 -1.157050
H 3.919231 -2.129363 -1.337604
Pt 0.184603 -0.258152 -0.909832
Cl -0.831302 0.031586 -3.050957
Cl 0.914982 -0.574620 1.372327
H 1.678891 2.047009 0.691529
C 1.801700 2.912942 -2.280720
H 1.403437 3.586028 -3.037895
C 2.147420 1.523535 -2.766193
H 3.059425 1.564714 -3.388586
H 1.347091 1.188169 -3.423976
O 5.288633 0.124675 0.070139
Si 6.437155 -0.854733 0.812087
C 5.670530 -2.487704 1.387331
H 4.805823 -2.315371 2.040038
H 5.332530 -3.109058 0.551024
H 6.397924 -3.071997 1.964340
C 7.202854 -0.012051 2.327209
H 8.006845 -0.629441 2.747386
H 7.629610 0.967676 2.084068
H 6.460779 0.135068 3.120816
C 7.754003 -1.128398 -0.552851
C 7.094351 -1.720860 -1.816381
H 6.326451 -1.050987 -2.218954
H 7.846401 -1.879954 -2.603217
H 6.625230 -2.692697 -1.616188
C 8.411168 0.219767 -0.918596
H 7.670704 0.944525 -1.275636
H 8.931424 0.664899 -0.061790
H 9.155314 0.081278 -1.716671
C 8.839930 -2.102832 -0.047155
H 9.602056 -2.263126 -0.823633
H 9.358769 -1.718075 0.839595
H 8.424320 -3.085669 0.207449
P -1.910063 -0.083027 0.109640
C -1.788417 1.450395 1.119558
C -3.411275 0.047697 -0.954617
C -2.443914 -1.469353 1.191784
C -1.678947 1.509237 2.512745
C -1.567643 2.644384 0.419040
C -3.651031 -1.038443 -1.807614
C -4.335399 1.095948 -0.997688
C -1.850232 -2.735926 1.128810
C -3.563000 -1.332476 2.022419
C -1.396037 2.702484 3.175062
F -1.820069 0.421990 3.277733
C -1.274541 3.842308 1.056716
F -1.634972 2.644155 -0.917012
C -4.724706 -1.076754 -2.687636
F -2.834300 -2.099967 -1.770236
C -5.418033 1.083148 -1.875355
F -4.238000 2.155558 -0.184409
C -2.316607 -3.797607 1.903668
F -0.839449 -2.994214 0.300806
C -4.044232 -2.374370 2.803513
F -4.206301 -0.155686 2.083792
C -1.190176 3.870267 2.447321
F -1.306952 2.723150 4.507546
F -1.061027 4.955404 0.349128

C -5.610791 -0.002165 -2.724810
F -4.912982 -2.129382 -3.485620
F -6.281417 2.102157 -1.888762
C -3.410115 -3.615112 2.744484
F -1.729459 -4.993549 1.826389
F -5.104002 -2.199499 3.596963
F -0.910532 5.010321 3.076604
F -6.648591 -0.021016 -3.558659
F -3.861373 -4.627120 3.481873

Ts3-4$_p$

Zero-point correction= 0.618357 (Hartree/Particle)
Thermal correction to Energy= 0.678667
Thermal correction to Enthalpy= 0.679612
Thermal correction to Gibbs Free Energy= 0.520162
Sum of electronic and zero-point Energies= -4633.582644
Sum of electronic and thermal Energies= -4633.522334
Sum of electronic and thermal Enthalpies= -4633.521390
Sum of electronic and thermal Free Energies= -4633.680840
HF (M06/6-311++g(d,p) and SDD, SMD(cyclohexane): -4633.65011195

C -1.6821 -3.738052 -1.133932
C -1.787724 -2.421794 -0.255828
C -1.881866 -5.010462 -0.261118
C -3.068859 -2.628145 1.064959
C -3.154253 -1.762758 -0.164654
C -3.310562 -0.303934 0.297013
H -2.727237 0.367259 -0.340349
H -1.835789 -5.880871 -0.925978
C -0.272752 -3.842313 -1.755338
H -0.079481 -3.015884 -2.442097
H -0.200721 -4.781929 -2.31845
H 0.507755 -3.844707 -0.988797
C -2.703169 -3.733377 -2.291717
H -3.734473 -3.864593 -1.949252
H -2.477415 -4.564555 -2.969163
H -2.636342 -2.804397 -2.867111
C -3.077255 -1.713469 2.294088
C -2.822621 -0.292836 1.761742
H -3.347987 0.468161 2.344471
H -1.754765 -0.069798 1.800656
H -4.092697 -1.805306 2.702684
H -2.370711 -2.026733 3.066198
Pt -0.071831 -1.21539 -0.068348
H -3.866707 -2.044559 -0.930734
Cl -0.696018 -0.186965 -2.156651
Cl 0.448224 -2.312717 1.999836
C -3.676297 -3.979997 1.135686
C -3.156776 -5.056268 0.540771
H -1.731668 -2.841686 0.94102
H -1.023721 -5.109323 0.422009
H -3.654247 -6.01637 0.657074
H -4.584509 -4.041268 1.731976
O -4.704387 -0.008473 0.217446
Si -5.357434 1.509646 -0.127169
C -7.238292 1.184871 -0.252414
C -4.957686 2.736863 1.2585
H -5.346133 2.399989 2.226658
H -3.878215 2.89111 1.374971
H -5.399497 3.719078 1.049042
C -4.639334 2.162092 -1.749833
H -3.551772 2.289531 -1.688647
H -4.837368 1.480313 -2.584368
H -5.066816 3.139517 -2.005787
C -7.522517 0.199427 -1.406705
H -7.216349 0.606812 -2.377939
H -6.999086 -0.752434 -1.26179
H -8.59907 -0.017045 -1.46858
C -7.987642 2.50848 -0.521057
H -9.068689 2.324491 -0.602285
H -7.842756 3.236334 0.286815
H -7.668372 2.98016 -1.458786
C -7.754412 0.570079 1.066942
H -7.250839 -0.376328 1.293753
H -7.605087 1.243376 1.92023
H -8.833264 0.367145 0.997798
P 1.737331 0.301905 0.001266
C 0.95894 1.97637 0.002189
C 2.89292 0.215458 1.442797
C 2.979475 0.293733 -1.360051
C 0.905298 2.849699 -1.087923
C 0.138385 2.29214 1.091695
C 3.538926 -1.015223 1.621099
C 3.183037 1.215926 2.374883
C 3.073503 -0.765183 -2.269521
C 3.945031 1.302995 -1.461394
C 0.09959 3.988121 -1.082623
F 1.60939 2.628004 -2.203613
C -0.683415 3.409774 1.116764
F 0.11987 1.479568 2.161145
C 4.392524 -1.266677 2.688449
F 3.366519 -1.988209 0.716227
C 4.03075 0.987801 3.457143
F 2.674959 2.450666 2.262257
C 4.061399 -0.797833 -3.254454
F 2.244263 -1.806986 -2.215345
C 4.936353 1.294142 -2.43285
F 3.920714 2.335831 -0.603622
C -0.701911 4.267159 0.018658
F 0.084215 4.801499 -2.14172
F -1.471267 3.653596 2.171268
C 4.632245 -0.257181 3.617618
F 4.986031 -2.454921 2.820309
F 4.282475 1.967201 4.330982
C 4.990509 0.233795 -3.337541
F 4.126856 -1.823458 -4.106737
F 5.830981 2.283614 -2.506305
F -1.485868 5.344669 0.024991
F 5.449977 -0.475532 4.646645
F 5.937765 0.207026 -4.273004

I4$_p$

Zero-point correction= 0.620177 (Hartree/Particle)
Thermal correction to Energy= 0.681202
Thermal correction to Enthalpy= 0.682146
Thermal correction to Gibbs Free Energy= 0.521158
Sum of electronic and zero-point Energies= -4633.593215
Sum of electronic and thermal Energies= -4633.532190
Sum of electronic and thermal Enthalpies= -4633.531246
Sum of electronic and thermal Free Energies= -4633.692234
HF (M06/6-311++g(d,p) and SDD, SMD(cyclohexane): -4633.66055104

C -1.710554 -3.830743 -0.974091
C -1.782751 -2.657721 0.059660
C -2.408475 -5.115657 -0.455632
C -3.849902 -2.692576 0.927699
C -3.150404 -1.828596 -0.006810
C -3.224443 -0.425707 0.633543
H -2.410933 0.216601 0.292618
H -2.401931 -5.855174 -1.268227
C -0.222679 -4.212003 -1.161519
H 0.314415 -3.430744 -1.701850
H -0.150040 -5.141979 -1.741798
H 0.277698 -4.365793 -0.199305
C -2.299460 -3.493999 -2.359424
H -3.395628 -3.448059 -2.348752
H -2.023573 -4.280410 -3.072504
H -1.912003 -2.544006 -2.734114
C -4.006075 -2.011568 2.262157
C -3.187638 -0.713980 2.141619
H -3.606005 0.108820 2.725967
H -2.155666 -0.884073 2.464945
H -5.082994 -1.795712 2.358193
H -3.738412 -2.658338 3.105015
Pt -0.116290 -1.254366 0.038185
H -3.494400 -1.822087 -1.037572
Cl -0.814791 -0.253617 -2.041861
Cl 0.479596 -2.163749 2.171366
C -4.388418 -4.009356 0.731347
C -3.792692 -5.047777 0.105531
H -1.601008 -3.067603 1.061521
H -1.795651 -5.575703 0.340987
H -4.313057 -6.003552 0.160774
H -5.298937 -4.210130 1.296057
O -4.501975 0.096226 0.267714
Si -4.894528 1.703666 -0.067881
C -6.740224 1.621015 -0.566601
C -4.648456 2.770005 1.476361
H -5.196589 2.369465 2.337127
H -3.593207 2.845547 1.762840
H -5.004812 3.793695 1.305931
C -3.810544 2.363642 -1.466727
H -2.755776 2.108968 -1.309912
H -4.092256 1.936045 -2.435322
H -3.885753 3.455359 -1.545056
C -6.917553 0.672792 -1.771996
H -6.367250 1.022079 -2.653864
H -6.570184 -0.340441 -1.541132
H -7.978643 0.607875 -2.054355
C -7.241243 3.030117 -0.953709
H -8.299065 2.990722 -1.251614
H -7.166730 3.739331 -0.119786
H -6.681432 3.447782 -1.799678
C -7.585942 1.090566 0.611494
H -7.267653 0.086405 0.915328
H -7.523481 1.743928 1.490425
H -8.646164 1.030267 0.324809
P 1.679134 0.260406 -0.002406
C 0.925818 1.946317 0.027692
C 2.907582 0.177323 1.379189
C 2.858941 0.237220 -1.421953
C 0.858147 2.834728 -1.049734

C 0.161523 2.275813 1.154136
C 3.556966 -1.055038 1.531448
C 3.243684 1.177970 2.295034
C 2.899279 -0.814234 -2.344095
C 3.836503 1.231267 -1.556537
C 0.101632 4.005073 -0.995472
F 1.505098 2.601717 -2.197671
C -0.599010 3.434111 1.232667
F 0.149329 1.449397 2.209671
C 4.460658 -1.305779 2.556513
F 3.333792 -2.033418 0.643432
C 4.142199 0.950653 3.335768
F 2.733571 2.414319 2.206833
C 3.845226 -0.853242 -3.369409
F 2.057814 -1.844860 -2.270008
C 4.787046 1.215804 -2.567846
F 3.865167 2.258815 -0.692143
C -0.633815 4.304588 0.145849
F 0.070603 4.831578 -2.044597
F -1.318981 3.701285 2.330254
C 4.748038 -0.294875 3.470292
F 5.054969 -2.496577 2.664458
F 4.437990 1.932180 4.193992
C 4.787220 0.163272 -3.482747
F 3.857964 -1.872204 -4.232570
F 5.693385 2.192468 -2.669768
F -1.369962 5.414513 0.199775
F 5.614334 -0.513064 4.459468
F 5.694608 0.129726 -4.457258

Ts4-4b$_p$

Zero-point correction= 0.619721 (Hartree/Particle)
Thermal correction to Energy= 0.680246
Thermal correction to Enthalpy= 0.681190
Thermal correction to Gibbs Free Energy= 0.520638
Sum of electronic and zero-point Energies= -4633.594330
Sum of electronic and thermal Energies= -4633.533804
Sum of electronic and thermal Enthalpies= -4633.532860
Sum of electronic and thermal Free Energies= -4633.693412
HF (M06/6-311++g(d,p) and SDD, SMD(cyclohexane): -4633.65791412

C -3.216321 1.644785 -0.131259
H -3.550088 1.66369 0.899516
C -3.268076 0.266773 -0.821636
H -2.491137 -0.409628 -0.45831
C -3.702782 2.60749 -1.08187
C -3.110887 0.599766 -2.315224
C -3.763416 1.98639 -2.465544
H -3.590116 -0.163392 -2.933186
H -2.051763 0.64368 -2.582243
H -3.318054 2.617028 -3.242188
H -4.835078 1.900135 -2.70104
C -4.347668 3.90457 -0.863481
H -5.369467 3.952195 -1.241988
C -1.914996 2.550639 -0.281215
C -1.74283 3.785246 0.667338
C -0.232444 4.045156 0.876223
H -0.097048 4.991405 1.416626
H 0.230701 3.24959 1.467208
H 0.299255 4.116768 -0.078727
C -2.393716 3.589529 2.051586
H -2.042906 2.669697 2.524999
H -2.122954 4.431644 2.699632
H -3.487717 3.563674 1.996678
Pt -0.230111 1.028726 -0.104206
Cl 0.598477 1.865691 -2.208666
Cl -1.051554 0.266602 2.006494
H -1.575613 2.771237 -1.297403
C -3.758474 5.008547 -0.391865
H -4.337993 5.929061 -0.36267
C -2.319292 5.077793 0.028256
H -1.713794 5.359249 -0.849139
H -2.191504 5.89789 0.746002
O -4.567998 -0.270445 -0.600996
Si -5.00558 -1.416946 0.563384
C -5.020449 -0.636368 2.284558
H -4.014062 -0.300348 2.561968
H -5.694799 0.226473 2.339319
H -5.344228 -1.358861 3.044225
C -3.784327 -2.858905 0.541611
H -4.104963 -3.647373 1.23396
H -3.70075 -3.306497 -0.455538
H -2.782059 -2.544709 0.853829
C -6.760479 -1.959456 0.021758
C -7.692295 -0.729924 -0.040072
H -7.322367 0.018832 -0.749506
H -8.700801 -1.027846 -0.362891
H -7.794474 -0.244458 0.938488
C -6.700907 -2.613248 -1.375372
H -6.294193 -1.924981 -2.125017
H -6.079798 -3.517431 -1.377651
H -7.708148 -2.908618 -1.704265
C -7.333061 -2.977078 1.032349
H -8.34004 -3.294924 0.725219
H -6.71541 -3.881239 1.101744
H -7.419889 -2.553007 2.040297
P 1.653922 -0.287491 -0.018986
C 3.079743 0.877341 0.058933
C 1.801169 -1.470274 1.393746
C 1.970339 -1.462847 -1.404063
C 3.97858 1.141698 -0.979139
C 3.144244 1.725518 1.17246
C 0.770888 -2.413549 1.506867
C 2.8012 -1.518805 2.369314
C 0.98708 -1.807523 -2.3387
C 3.188774 -2.149209 -1.48737
C 4.916471 2.169515 -0.895796
F 3.972648 0.433182 -2.114594
C 4.068221 2.755788 1.279721
F 2.282697 1.551223 2.185657
C 0.703481 -3.331942 2.546161
F -0.186229 -2.468681 0.566881
C 2.755305 -2.42797 3.424924
F 3.864631 -0.705354 2.32841
C 1.226159 -2.754652 -3.334998
F -0.235607 -1.277015 -2.302273
C 3.450408 -3.094663 -2.469375
F 4.160146 -1.891274 -0.596979
C 4.963336 2.97775 0.234928
F 5.763857 2.385242 -1.905511
F 4.100362 3.530604 2.367123
C 1.701924 -3.332578 3.517488
F -0.301661 -4.207974 2.614202
F 3.72978 -2.443836 4.338651
C 2.458842 -3.395166 -3.402769
F 0.267559 -3.061414 -4.212413
F 4.6319 -3.71536 -2.522978
F 5.857677 3.961573 0.318396
F 1.658392 -4.207372 4.520986
F 2.689745 -4.303117 -4.348713

4b

Zero-point correction= 0.619646 (Hartree/Particle)
Thermal correction to Energy= 0.680548
Thermal correction to Enthalpy= 0.681493
Thermal correction to Gibbs Free Energy= 0.518880
Sum of electronic and zero-point Energies= -4633.610340
Sum of electronic and thermal Energies= -4633.549438
Sum of electronic and thermal Enthalpies= -4633.548493
Sum of electronic and thermal Free Energies= -4633.711106
HF (M06/6-311++g(d,p) and SDD, SMD(cyclohexane): -4633.66025717

C -3.931079 1.069736 0.062891
H -4.210021 0.783581 1.069137
C -3.447322 -0.016563 -0.872870
H -2.304890 -0.211750 -0.676633
C -4.783647 2.037985 -0.768132
C -3.605681 0.541380 -2.301924
C -4.803365 1.512358 -2.204812
H -3.765230 -0.279740 -3.004067
H -2.695702 1.060237 -2.610763
H -4.749702 2.314926 -2.950103
H -5.744999 0.972518 -2.370379
C -5.991923 2.701916 -0.224185
H -6.954964 2.221388 -0.395298
C -3.447684 2.477216 -0.206522
C -3.411593 3.571520 0.894554
C -2.077865 4.333624 0.776754
H -2.037033 5.162233 1.494443
H -1.228904 3.672490 0.981565
H -1.948884 4.756391 -0.227785
C -3.515059 2.988183 2.318330
H -2.739835 2.235382 2.493704
H -3.389926 3.788080 3.058602
H -4.491177 2.525093 2.499645
Pt -0.429998 -0.154759 -0.333402
Cl -0.067059 0.080347 -2.674963
Cl -1.008629 -0.261279 1.959726
H -2.629183 2.560366 -0.921447
C -5.910930 3.867294 0.429317
H -6.814741 4.347283 0.800449
C -4.587809 4.560828 0.662626
H -4.359559 5.201196 -0.204261
H -4.662663 5.239122 1.522422
O -4.120243 -1.217383 -0.750563
Si -4.219583 -2.481888 0.379348
C -4.583608 -1.841304 2.116627
H -3.747783 -1.241874 2.493387
H -5.492037 -1.229364 2.150897
H -4.722072 -2.680432 2.810047
C -2.599078 -3.445549 0.367658
H -2.683246 -4.347708 0.986869
H -2.319767 -3.756433 -0.645229

H -1.780480 -2.843489 0.776144
C -5.673245 -3.526958 -0.300135
C -6.961115 -2.676627 -0.344934
H -6.841880 -1.799723 -0.991248
H -7.797986 -3.270651 -0.740429
H -7.254997 -2.323342 0.651249
C -5.349766 -4.021767 -1.726491
H -5.173164 -3.186082 -2.412646
H -4.461396 -4.664728 -1.745509
H -6.188342 -4.611020 -2.125738
C -5.906814 -4.748310 0.616888
H -6.737303 -5.358609 0.233450
H -5.025641 -5.399785 0.670623
H -6.168291 -4.452645 1.640527
P 1.784547 -0.033604 -0.040302
C 2.265616 1.654016 -0.576842
C 2.391006 -0.317383 1.672843
C 2.804550 -1.262911 -0.944189
C 2.920728 1.964765 -1.773471
C 1.744544 2.730150 0.154737
C 2.039156 -1.544848 2.253101
C 3.171985 0.546373 2.447658
C 2.276548 -2.420230 -1.531306
C 4.198688 -1.119464 -0.958373
C 3.078527 3.281855 -2.200256
F 3.410041 1.012212 -2.573278
C 1.882534 4.048927 -0.253774
F 1.073809 2.493516 1.290219
C 2.403924 -1.890041 3.547876
F 1.349591 -2.441650 1.536738
C 3.546333 0.223518 3.750405
F 3.614593 1.714700 1.967864
C 3.103044 -3.359725 -2.149667
F 0.976333 -2.696192 -1.499853
C 5.038047 -2.040260 -1.568319
F 4.759890 -0.049674 -0.370959
C 2.557509 4.325852 -1.441788
F 3.718484 3.541969 -3.341928
F 1.368001 5.041183 0.475128
C 3.157003 -0.993312 4.303356
F 2.048020 -3.067186 4.063277
F 4.292717 1.071076 4.462072
C 4.480722 -3.167717 -2.172152
F 2.575535 -4.452050 -2.703394
F 6.360389 -1.859041 -1.575710
F 2.703551 5.584240 -1.848077
F 3.521057 -1.308051 5.543558
F 5.270089 -4.064324 -2.756984

Ts3-5b$_p$

Zero-point correction= 0.619171 (Hartree/Particle)
Thermal correction to Energy= 0.679803
Thermal correction to Enthalpy= 0.680747
Thermal correction to Gibbs Free Energy= 0.520896
Sum of electronic and zero-point Energies= -4633.573044
Sum of electronic and thermal Energies= -4633.512412
Sum of electronic and thermal Enthalpies= -4633.511467
Sum of electronic and thermal Free Energies= -4633.671319
HF (M06/6-311++g(d,p) and SDD, SMD(cyclohexane): -4633.63566576

C -1.734092 -3.643053 -1.197139
C -1.897123 -2.368038 -0.299107
C -1.547037 -4.908616 -0.288092
C -2.542457 -2.884263 1.406565
C -2.998442 -1.542598 -0.503221
C -3.324584 -0.283301 0.250636
H -2.743507 0.514252 -0.234489
H -1.321152 -5.766487 -0.930186
C -0.479002 -3.547524 -2.092853
H -0.513024 -2.670475 -2.743297
H -0.422058 -4.443638 -2.724221
H 0.437942 -3.49416 -1.498647
C -2.94484 -3.879975 -2.128221
H -3.886728 -3.978916 -1.577603
H -2.79421 -4.807595 -2.692314
H -3.05157 -3.069637 -2.858627
C -3.246665 -1.801702 2.21484
C -2.904683 -0.394691 1.729873
H -4.333739 -1.94032 2.164637
H -2.945088 -1.921233 3.263543
Pt -0.079881 -1.196703 -0.061174
H -3.775226 -1.805782 -1.222903
Cl -0.791646 0.03426 -2.029633
Cl 0.669446 -2.401143 1.856964
C -3.272243 -4.162821 1.278234
C -2.768399 -5.163021 0.542376
H -1.522583 -3.031248 1.76104
H -0.667625 -4.743513 0.349071
H -3.295245 -6.110861 0.458511
H -4.225269 -4.257082 1.796493
O -4.721818 -0.049038 0.122408
Si -5.426513 1.472276 -0.118366
C -7.292325 1.093952 -0.283661
C -5.071687 2.603751 1.357687
H -5.532606 3.588377 1.209553
H -5.468925 2.191039 2.292372
H -3.99806 2.774386 1.504473
C -4.710544 2.25503 -1.682703
H -4.91544 1.647497 -2.571209
H -5.135075 3.252207 -1.852435
H -3.622026 2.373775 -1.616914
C -7.803415 0.400031 0.997806
H -8.875267 0.171763 0.906088
H -7.277091 -0.542974 1.18355
H -7.681069 1.034142 1.884516
C -7.535051 0.159511 -1.488877
H -7.227694 0.621415 -2.435038
H -6.990224 -0.785433 -1.383191
H -8.604725 -0.080386 -1.575801
C -8.077416 2.407427 -0.495667
H -9.151407 2.195512 -0.597202
H -7.96226 3.098498 0.348557
H -7.763636 2.933748 -1.405767
H -1.832482 -0.210374 1.829777
H -3.43413 0.36841 2.307316
P 1.738439 0.302744 0.010512
C 0.951764 1.968697 0.153
C 2.964775 0.142429 1.385903
C 2.908821 0.388155 -1.410576
C 0.885899 2.935866 -0.854308
C 0.128386 2.17736 1.266959
C 3.677752 -1.063331 1.422445
C 3.243428 1.063993 2.399213
C 2.928696 -0.58313 -2.417633
C 3.895987 1.380174 -1.469172
C 0.060356 4.05573 -0.750722
F 1.590311 2.827831 -1.986586
C -0.717747 3.270379 1.38483
F 0.127118 1.278015 2.263893
C 4.590623 -1.365658 2.425309
F 3.505557 -1.962542 0.444133
C 4.15004 0.783147 3.41979
F 2.666355 2.27315 2.429886
C 3.868685 -0.548711 -3.448472
F 2.069804 -1.601395 -2.423446
C 4.84134 1.435797 -2.483823
F 3.936667 2.336098 -0.527127
C -0.750307 4.220755 0.366108
F 0.032337 4.95838 -1.734607
F -1.516192 3.404429 2.451369
C 4.821303 -0.435799 3.436291
F 5.245702 -2.528597 2.421182
F 4.38942 1.689293 4.372625
C 4.823406 0.461972 -3.482256
F 3.86298 -1.491138 -4.394051
F 5.758227 2.407135 -2.511642
F -1.557279 5.276819 0.463108
F 5.694181 -0.705002 4.406203
F 5.724728 0.498264 -4.461684

5b-[Pt]$_p$

Zero-point correction= 0.621833 (Hartree/Particle)
Thermal correction to Energy= 0.682883
Thermal correction to Enthalpy= 0.683827
Thermal correction to Gibbs Free Energy= 0.520962
Sum of electronic and zero-point Energies= -4633.636706
Sum of electronic and thermal Energies= -4633.575656
Sum of electronic and thermal Enthalpies= -4633.574712
Sum of electronic and thermal Free Energies= -4633.737578
HF (M06/6-311++g(d,p) and SDD, SMD(cyclohexane): -4633.69428085

C 2.641269 -3.367303 1.028392
C 2.734000 -2.342069 -0.102559
C 2.310335 -4.781482 0.477327
C 3.056767 -2.829652 -1.502652
C 2.666842 -0.978181 0.157709
C 3.312587 0.056639 -0.765958
H 2.747541 0.994605 -0.704628
H 2.395770 -5.500925 1.300276
C 1.609513 -3.019556 2.116717
H 1.798991 -2.054175 2.593228
H 1.641443 -3.788132 2.898241
H 0.597245 -2.995719 1.701471
C 4.060260 -3.385920 1.674141
H 4.835953 -3.646073 0.948736
H 4.076673 -4.135967 2.474003
H 4.305009 -2.412189 2.108687
C 3.947913 -1.838669 -2.282538
C 3.377443 -0.421494 -2.217482
H 4.963501 -1.846749 -1.868324
H 4.017177 -2.179192 -3.322516
Pt 0.337412 -0.646564 0.000089

H 2.698798 -0.685323 1.203255
Cl 0.727243 0.841274 1.859789
Cl -0.136434 -1.994773 -1.901768
C 3.562569 -4.251689 -1.565898
C 3.197895 -5.171694 -0.673432
H 2.073777 -2.825823 -2.009916
H 1.255936 -4.798071 0.162261
H 3.532960 -6.202751 -0.760876
H 4.197272 -4.503008 -2.413537
O 4.644460 0.252750 -0.270500
Si 5.319348 1.718142 0.224664
C 7.143518 1.284847 0.602778
C 5.172602 2.991860 -1.169628
H 5.615991 3.952098 -0.878518
H 5.673352 2.656228 -2.084994
H 4.121831 3.184971 -1.419614
C 4.419669 2.371490 1.751341
H 4.569431 1.720285 2.620112
H 4.769175 3.375851 2.021210
H 3.338249 2.429725 1.579772
C 7.846451 0.775285 -0.673774
H 8.889799 0.505488 -0.453520
H 7.351076 -0.114437 -1.078712
H 7.867514 1.536871 -1.462984
C 7.205856 0.180264 1.680041
H 6.752150 0.503023 2.625124
H 6.689768 -0.729320 1.353036
H 8.251590 -0.085457 1.894457
C 7.881965 2.538817 1.120743
H 8.931333 2.298485 1.345358
H 7.887044 3.349251 0.380934
H 7.433762 2.929344 2.042817
H 2.368159 -0.404529 -2.647611
H 3.997783 0.276118 -2.790784
P -1.761693 0.260127 0.000651
C -1.535255 2.035895 -0.425929
C -3.013597 -0.458232 -1.150904
C -2.732775 0.165346 1.561535
C -1.631258 3.107094 0.468544
C -1.032560 2.325779 -1.701223
C -3.284137 -1.823469 -0.982186
C -3.728985 0.203742 -2.153119
C -2.401999 -0.695852 2.614687
C -3.928671 0.885086 1.685449
C -1.280105 4.404289 0.098966
F -2.050185 2.939128 1.726899
C -0.675968 3.609182 -2.092446
F -0.884031 1.336535 -2.591674
C -4.182636 -2.513736 -1.785279
F -2.681422 -2.500462 0.004854
C -4.632667 -0.467628 -2.975006
F -3.597271 1.519852 -2.360692
C -3.199612 -0.792246 3.755394
F -1.333657 -1.489131 2.565768
C -4.737090 0.806352 2.810867
F -4.323377 1.696979 0.690968
C -0.802188 4.657327 -1.182741
F -1.393326 5.403265 0.977606
F -0.212774 3.840251 -3.323300
C -4.856313 -1.829252 -2.794715
F -4.407007 -3.814847 -1.592321
F -5.297919 0.198102 -3.922613
C -4.364025 -0.038090 3.855971
F -2.857300 -1.622040 4.742938
F -5.860663 1.522959 2.895087
F -0.465935 5.895326 -1.539585
F -5.724992 -2.472123 -3.572269
F -5.129560 -0.131506 4.940600

Ts3-3'$_p$

Zero-point correction= 0.621230 (Hartree/Particle)
Thermal correction to Energy= 0.681588
Thermal correction to Enthalpy= 0.682532
Thermal correction to Gibbs Free Energy= 0.520773
Sum of electronic and zero-point Energies= -4633.602220
Sum of electronic and thermal Energies= -4633.541863
Sum of electronic and thermal Enthalpies= -4633.540918
Sum of electronic and thermal Free Energies= -4633.702677
HF (M06/6-311++g(d,p) and SDD, SMD(cyclohexane): -4633.66960708

C 3.048228 -1.899815 -0.213522
H 3.952103 -2.234749 0.305664
C 3.312735 -0.422372 -0.67384
H 2.545655 0.253608 -0.290816
C 2.972638 -2.760752 -1.549865
C 3.316902 -0.477319 -2.215302
C 3.781076 -1.898677 -2.540973
H 3.953996 0.306852 -2.63403
H 2.296299 -0.321867 -2.586052
H 3.586951 -2.198135 -3.576988
H 4.855804 -2.004477 -2.347364
C 3.455839 -4.16127 -1.344048
H 3.94385 -4.618886 -2.20434
C 1.842412 -2.227899 0.563806
C 1.939396 -3.344714 1.567305
C 0.564773 -3.769015 2.1302
H 0.706077 -4.541239 2.896118
H 0.044584 -2.924578 2.590269
H -0.073238 -4.173597 1.339298
C 2.742791 -2.672887 2.741573
H 2.265671 -1.74796 3.076063
H 2.748884 -3.381317 3.57716
H 3.777044 -2.456553 2.460962
Pt 0.196376 -1.206588 0.331796
Cl -0.599497 -2.782916 -1.283024
Cl 0.872827 0.445131 1.95806
H 1.933169 -2.774923 -1.899534
C 3.353983 -4.895369 -0.232004
H 3.781497 -5.898172 -0.274695
C 2.704619 -4.65377 1.112793
H 3.462108 -4.870057 1.879214
H 1.974078 -5.467282 1.215307
O 4.59743 -0.05444 -0.190186
Si 5.033187 1.351367 0.637847
C 4.891715 1.056704 2.497469
H 3.856502 0.806536 2.758548
H 5.533168 0.2322 2.829924
H 5.17033 1.94929 3.071062
C 3.883506 2.773358 0.151117
H 4.236367 3.72103 0.576295
H 3.812492 2.903023 -0.935251
H 2.874052 2.597732 0.541754
C 6.84421 1.673013 0.107078
C 7.707132 0.430932 0.418663
H 7.337023 -0.457732 -0.104645
H 8.747268 0.597724 0.101987
H 7.726985 0.205286 1.492155
C 6.904126 1.956336 -1.409173
H 6.510231 1.115429 -1.991678
H 6.332754 2.852265 -1.682476
H 7.943504 2.122861 -1.728145
C 7.414297 2.888364 0.870788
H 8.453538 3.077914 0.565121
H 6.846654 3.805919 0.670756
H 7.419622 2.727596 1.955825
P -1.758032 0.282302 -0.027478
C -1.003425 1.873717 -0.575642
C -3.002399 -0.209376 -1.301357
C -2.884598 0.658691 1.377692
C -0.958705 3.068301 0.148076
C -0.198448 1.809607 -1.7201
C -3.668812 -1.417147 -1.058045
C -3.327351 0.45858 -2.485362
C -2.836685 -0.07648 2.567363
C -3.900288 1.615602 1.261918
C -0.17435 4.147443 -0.259381
F -1.645668 3.230884 1.285528
C 0.600989 2.862155 -2.140552
F -0.178449 0.67833 -2.445148
C -4.588847 -1.959052 -1.94713
F -3.441412 -2.075489 0.087195
C -4.241307 -0.066328 -3.397072
F -2.785979 1.644932 -2.794155
C -3.737062 0.156241 3.607043
F -1.946377 -1.053437 2.747174
C -4.807868 1.865861 2.282016
F -4.009166 2.335891 0.135008
C 0.610821 4.044136 -1.40228
F -0.163496 5.27412 0.4578
F 1.369075 2.742522 -3.227645
C -4.870914 -1.278585 -3.129365
F -5.201245 -3.113059 -1.674114
F -4.527099 0.599407 -4.519803
C -4.7206 1.129755 3.463991
F -3.667218 -0.560618 4.73101
F -5.755548 2.796734 2.142437
F 1.376829 5.063979 -1.786017
F -5.751662 -1.778654 -3.994706
F -5.585438 1.355176 4.450695

I3'$_p$

Zero-point correction= 0.621357 (Hartree/Particle)
Thermal correction to Energy= 0.682458
Thermal correction to Enthalpy= 0.683402
Thermal correction to Gibbs Free Energy= 0.519874
Sum of electronic and zero-point Energies= -4633.609035
Sum of electronic and thermal Energies= -4633.547935
Sum of electronic and thermal Enthalpies= -4633.546990
Sum of electronic and thermal Free Energies= -4633.710518
HF (M06/6-311++g(d,p) and SDD, SMD(cyclohexane): -4633.67369361

C -3.173465 1.742120 -0.529302
H -4.088602 2.106475 -0.050455

C -3.438680 0.245521 -0.905462
H -2.647498 -0.405423 -0.525955
C -3.060554 2.526712 -1.917174
C -3.500681 0.221930 -2.447816
C -3.924519 1.639698 -2.841033
H -4.180465 -0.559650 -2.797645
H -2.501539 0.011618 -2.847326
H -3.743602 1.875084 -3.895920
H -4.988837 1.799799 -2.629601
C -3.438402 3.975939 -1.850728
H -3.632275 4.436866 -2.819640
C -1.978882 2.144581 0.226550
C -2.050161 3.441639 1.001762
C -0.764002 4.285795 0.839314
H -0.833133 5.166938 1.487764
H 0.122601 3.713025 1.120810
H -0.635778 4.618824 -0.193617
C -2.175887 3.008865 2.499110
H -1.280022 2.491862 2.844459
H -2.320696 3.919782 3.091983
H -3.033864 2.350059 2.666382
Pt -0.365378 1.039934 0.151978
Cl 0.553358 2.243324 -1.721293
Cl -1.092598 -0.236421 2.043885
H -2.025743 2.448817 -2.277244
C -3.524502 4.742947 -0.758483
H -3.809516 5.784280 -0.900424
C -3.294339 4.329676 0.679998
H -4.199110 3.850501 1.080264
H -3.173211 5.238206 1.281279
O -4.699335 -0.115774 -0.358820
Si -5.066157 -1.393308 0.684705
C -4.955093 -0.796764 2.472594
H -3.927491 -0.492195 2.702140
H -5.614518 0.059821 2.656349
H -5.231909 -1.587763 3.180674
C -3.863315 -2.826631 0.415116
H -4.120698 -3.669130 1.069092
H -3.880612 -3.193750 -0.617932
H -2.833539 -2.536548 0.653590
C -6.862793 -1.877790 0.226019
C -7.794259 -0.657882 0.395860
H -7.477022 0.180607 -0.234544
H -8.824308 -0.919481 0.111450
H -7.823209 -0.305789 1.434353
C -6.925145 -2.349338 -1.242260
H -6.591864 -1.564144 -1.930676
H -6.303184 -3.236213 -1.415809
H -7.956576 -2.615717 -1.516498
C -7.350572 -3.019121 1.144771
H -8.382381 -3.301593 0.889491
H -6.733577 -3.920789 1.044194
H -7.346563 -2.726771 2.202110
P 1.725372 -0.279165 -0.013708
C 3.084108 0.921859 0.309444
C 1.946302 -1.702412 1.144817
C 2.107153 -1.133573 -1.600614
C 3.963657 1.447417 -0.641072
C 3.097512 1.523367 1.573825
C 0.950837 -2.686238 1.082306
C 2.962479 -1.898674 2.084023
C 1.129162 -1.328010 -2.582090
C 3.357511 -1.721116 -1.829195
C 4.835593 2.491874 -0.337188
F 4.000021 0.985971 -1.897112
C 3.955155 2.564031 1.902971
F 2.250810 1.083488 2.517320
C 0.932084 -3.790491 1.924588
F -0.015795 -2.589319 0.155955
C 2.964599 -2.994778 2.945068
F 3.992782 -1.049159 2.191871
C 1.397077 -2.034818 -3.754060
F -0.116657 -0.875419 -2.423750
C 3.649836 -2.428501 -2.987606
F 4.327861 -1.601169 -0.910343
C 4.832726 3.051508 0.936211
F 5.667188 2.962096 -1.270687
F 3.939689 3.098513 3.126954
C 1.945653 -3.940008 2.868542
F -0.038225 -4.702288 1.830325
F 3.951646 -3.149364 3.832025
C 2.659726 -2.582095 -3.957927
F 0.441359 -2.202815 -4.671239
F 4.859994 -2.961333 -3.175572
F 5.663825 4.050039 1.231230
F 1.948953 -4.992949 3.684491
F 2.921001 -3.262215 -5.072181

Ts3'-2b'$_p$

Zero-point correction= 0.617637 (Hartree/Particle)
Thermal correction to Energy= 0.678349
Thermal correction to Enthalpy= 0.679293
Thermal correction to Gibbs Free Energy= 0.518665
Sum of electronic and zero-point Energies= -4633.582902
Sum of electronic and thermal Energies= -4633.522190
Sum of electronic and thermal Enthalpies= -4633.521246
Sum of electronic and thermal Free Energies= -4633.681875
HF (M06/6-311++g(d,p) and SDD, SMD(cyclohexane): -4633.64814815

C -3.188118 1.829934 -0.573884
H -2.949251 1.594705 0.793503
C -3.497013 0.398454 -1.073143
H -2.59055 -0.189265 -1.2299
C -4.29845 2.746782 -1.087538
C -4.29529 0.685046 -2.350702
C -5.227072 1.827478 -1.919168
H -4.817847 -0.207195 -2.703666
H -3.607821 1.015489 -3.140464
H -5.674806 2.366109 -2.759887
H -6.035015 1.437783 -1.292576
C -4.996917 3.616348 -0.073872
H -6.042144 3.816244 -0.304746
C -2.050431 2.196356 0.149151
C -1.886821 3.641365 0.702517
C -1.689625 4.635402 -0.46899
H -1.347474 5.59509 -0.064721
H -0.929985 4.266149 -1.164663
H -2.608139 4.833477 -1.025737
C -0.631291 3.733761 1.599567
H 0.275458 3.524954 1.025241
H -0.550162 4.749303 2.006245
H -0.671777 3.024432 2.42972
Pt -0.422179 0.923581 0.124378
Cl -0.080163 1.640337 -2.152967
Cl -0.885839 0.236213 2.367538
H -3.768135 3.389198 -1.809775
C -4.481073 4.153744 1.034732
H -5.159907 4.744428 1.6502
C -3.085745 4.059463 1.601011
H -3.1082 3.393987 2.479038
H -2.838315 5.048372 2.011866
O -4.34279 -0.166099 -0.082029
Si -4.440769 -1.751184 0.52943
C -4.281797 -1.598465 2.397972
H -3.309182 -1.164909 2.655013
H -5.060735 -0.950817 2.817155
H -4.359052 -2.575127 2.890973
C -3.044045 -2.799515 -0.181626
H -3.127497 -3.831601 0.180708
H -3.043768 -2.834826 -1.277056
H -2.071905 -2.415329 0.142558
C -6.162592 -2.464006 0.06171
C -7.281322 -1.524972 0.562378
H -7.204988 -0.52702 0.114626
H -8.269199 -1.931714 0.300516
H -7.257913 -1.403811 1.651955
C -6.304893 -2.640273 -1.464159
H -6.251104 -1.680858 -1.991767
H -5.532062 -3.298402 -1.879911
H -7.279518 -3.087534 -1.70884
C -6.332997 -3.846354 0.733942
H -7.31389 -4.272992 0.479235
H -5.572289 -4.564144 0.402198
H -6.280272 -3.783173 1.827212
P 1.644417 -0.233162 -0.033552
C 2.895295 1.09381 -0.314722
C 2.20591 -1.228361 1.421824
C 1.897784 -1.495089 -1.355121
C 3.533108 1.370656 -1.527335
C 3.06231 2.036499 0.707147
C 1.339048 -2.255218 1.816314
C 3.368488 -1.067694 2.181457
C 0.82887 -2.035219 -2.077828
C 3.165766 -2.033557 -1.60707
C 4.324073 2.505433 -1.700935
F 3.40491 0.566632 -2.590173
C 3.844243 3.174277 0.560802
F 2.448097 1.847725 1.884722
C 1.577042 -3.057238 2.925315
F 0.250349 -2.520201 1.077904
C 3.628555 -1.853783 3.30268
F 4.30165 -0.162949 1.857605
C 1.01995 -3.034574 -3.03217
F -0.429063 -1.640923 -1.869075
C 3.382739 -3.026732 -2.552519
F 4.229677 -1.5767 -0.927721
C 4.48186 3.409114 -0.655765
F 4.924375 2.729836 -2.873258
F 3.982832 4.039107 1.569707
C 2.728716 -2.846392 3.679469
F 0.721798 -4.025869 3.26145
F 4.749462 -1.669001 4.006231
C 2.298104 -3.527447 -3.272299
F -0.022669 -3.529015 -3.705073
F 4.610701 -3.503601 -2.774326
F 5.237502 4.495034 -0.816211
F 2.978797 -3.606099 4.745074
F 2.48692 -4.483213 -4.180273

2b'-[Pt]$_p$

Zero-point correction= 0.622360 (Hartree/Particle)
Thermal correction to Energy= 0.683200
Thermal correction to Enthalpy= 0.684145
Thermal correction to Gibbs Free Energy= 0.523654
Sum of electronic and zero-point Energies= -4633.630339
Sum of electronic and thermal Energies= -4633.569499
Sum of electronic and thermal Enthalpies= -4633.568555
Sum of electronic and thermal Free Energies= -4633.729045
HF (M06/6-311++g(d,p) and SDD, SMD(cyclohexane): -4633.69372364

C -2.812960 0.760248 -0.753525
H -2.642799 0.836951 1.327604
C -3.330202 -0.686688 -0.816489
H -2.801794 -1.359816 -0.137156
C -3.098199 1.420277 -2.097172
C -3.147816 -1.033809 -2.297028
C -3.574218 0.254229 -3.021851
H -3.738729 -1.909383 -2.582098
H -2.089947 -1.251467 -2.485732
H -3.147685 0.334698 -4.026144
H -4.664382 0.280634 -3.115768
C -4.113638 2.544128 -2.024580
H -4.629189 2.707447 -2.971649
C -2.485696 1.412670 0.419477
C -2.478840 2.923947 0.668079
C -1.499811 3.754069 -0.182468
H -1.621515 4.814217 0.072470
H -0.464373 3.470165 0.023577
H -1.665656 3.647352 -1.254531
C -2.134497 3.150853 2.155521
H -1.133249 2.767558 2.382656
H -2.155994 4.219461 2.398273
H -2.845554 2.640096 2.816056
Pt -0.439370 0.374670 -0.098021
Cl 0.245760 1.495389 -2.114120
Cl -0.923564 -0.880578 1.880673
H -2.161783 1.822031 -2.502252
C -4.454981 3.346570 -1.008431
H -5.236202 4.077414 -1.218809
C -3.935772 3.407728 0.411802
H -4.618925 2.849181 1.071066
H -3.998470 4.451721 0.750821
O -4.725633 -0.634552 -0.517698
Si -5.557509 -1.442433 0.707204
C -5.131486 -0.719126 2.401311
H -4.066607 -0.852372 2.627445
H -5.354486 0.352769 2.457111
H -5.698764 -1.217677 3.197308
C -5.086571 -3.274387 0.695127
H -5.641386 -3.828892 1.461946
H -5.292392 -3.745529 -0.272686
H -4.019362 -3.408273 0.910260
C -7.395189 -1.163578 0.257013
C -7.704771 0.349730 0.229457
H -7.068821 0.880799 -0.487821
H -8.752303 0.518720 -0.060844
H -7.562712 0.814583 1.213233
C -7.689458 -1.758070 -1.137110
H -7.065992 -1.296252 -1.910580
H -7.515831 -2.840978 -1.167018
H -8.741477 -1.589048 -1.410226
C -8.304415 -1.848654 1.300814
H -9.362715 -1.695672 1.044075
H -8.136086 -2.931993 1.346550
H -8.153818 -1.443114 2.309054
P 1.828970 -0.145636 0.027427
C 2.664684 1.483230 0.215961
C 2.391978 -1.242288 1.400010
C 2.582554 -1.036263 -1.392650
C 3.435643 2.126587 -0.757895
C 2.341432 2.232628 1.354931
C 1.860105 -2.539470 1.403062
C 3.283762 -0.928868 2.430882
C 1.810799 -1.697897 -2.355327
C 3.972306 -1.184985 -1.481428
C 3.894593 3.431347 -0.586330
F 3.751508 1.531962 -1.912901
C 2.784574 3.533955 1.548179
F 1.571381 1.686734 2.307984
C 2.159310 -3.470183 2.389691
F 1.049945 -2.924656 0.407969
C 3.595629 -1.843354 3.435200
F 3.900690 0.258174 2.493492
C 2.400889 -2.423906 -3.389359
F 0.478907 -1.700242 -2.304018
C 4.582452 -1.902001 -2.501662
F 4.762724 -0.612819 -0.559629
C 3.570623 4.136946 0.567926
F 4.635398 4.008591 -1.535041
F 2.461277 4.204016 2.656474
C 3.029104 -3.114467 3.418079
F 1.626493 -4.692745 2.354230
F 4.452080 -1.507664 4.403171
C 3.786868 -2.521403 -3.465162
F 1.639758 -3.043055 -4.293666
F 5.912161 -2.005405 -2.562112
F 4.005903 5.383852 0.734798
F 3.331589 -3.993164 4.371122
F 4.354123 -3.217450 -4.447092

Ts3'-4'$_p$

Zero-point correction= 0.618017 (Hartree/Particle)
Thermal correction to Energy= 0.678376
Thermal correction to Enthalpy= 0.679320
Thermal correction to Gibbs Free Energy= 0.519777
Sum of electronic and zero-point Energies= -4633.590315
Sum of electronic and thermal Energies= -4633.529956
Sum of electronic and thermal Enthalpies= -4633.529012
Sum of electronic and thermal Free Energies= -4633.688556
HF (M06/6-311++g(d,p) and SDD, SMD(cyclohexane): -4633.65681679

C 3.279525 -1.566556 -0.018816
H 4.030072 -1.877608 0.701918
C 3.440461 -0.097713 -0.449282
H 2.898397 0.568984 0.227778
C 3.136027 -2.398742 -1.282426
C 2.877884 -0.03674 -1.882949
C 3.109808 -1.437313 -2.475387
H 3.375144 0.747984 -2.45925
H 1.807788 0.184807 -1.857162
H 2.374589 -1.718051 -3.233418
H 4.110881 -1.511173 -2.920222
C 3.727933 -3.75086 -1.419191
H 4.100877 -4.008813 -2.407275
C 1.917715 -2.197591 0.129614
C 1.866996 -3.511728 0.96635
C 0.724021 -4.425624 0.478371
H 0.663584 -5.313382 1.11925
H -0.237726 -3.908518 0.514378
H 0.881025 -4.759124 -0.552823
C 1.611284 -3.116424 2.438904
H 0.628894 -2.660133 2.567111
H 1.662061 -4.018932 3.060382
H 2.357508 -2.403793 2.804393
Pt 0.161067 -1.059296 -0.012089
Cl -0.390767 -2.179448 -2.058165
Cl 0.817927 0.186242 1.947802
H 1.84726 -2.620603 -1.11166
C 3.760431 -4.632372 -0.412812
H 4.193601 -5.615205 -0.585329
C 3.202477 -4.33198 0.949854
H 3.961449 -3.811563 1.550972
H 3.009992 -5.269991 1.482259
O 4.838777 0.188615 -0.464919
Si 5.5898 1.315118 0.543076
C 5.269096 0.868527 2.352447
H 4.192075 0.82312 2.557722
H 5.697019 -0.105327 2.618087
H 5.698382 1.615995 3.030829
C 4.881396 3.036874 0.207331
H 5.373532 3.798968 0.823784
H 4.995607 3.329863 -0.842557
H 3.811318 3.071419 0.447066
C 7.440594 1.191383 0.08067
C 7.941916 -0.25031 0.314527
H 7.378908 -0.973938 -0.285513
H 9.002255 -0.336227 0.034675
H 7.858685 -0.54837 1.367028
C 7.633998 1.550386 -1.408683
H 7.05587 0.885965 -2.060685
H 7.329502 2.581639 -1.625135
H 8.693224 1.457052 -1.690305
C 8.268058 2.163001 0.95033
H 9.333905 2.097187 0.68789
H 7.963361 3.2072 0.806575
H 8.182751 1.933066 2.019818
P -1.776708 0.288864 0.000882
C -1.215705 2.039863 -0.15231
C -3.039329 -0.010782 -1.316915
C -2.875254 0.191954 1.478339
C -1.22157 2.998869 0.864872
C -0.527356 2.379309 -1.3235
C -3.553095 -1.313189 -1.376494
C -3.5236 0.89662 -2.263472
C -2.750464 -0.820199 2.436835
C -3.954584 1.072075 1.626649
C -0.605614 4.240098 0.709947
F -1.803371 2.76943 2.048157
C 0.095364 3.606727 -1.503548
F -0.452684 1.489071 -2.326221
C -4.46825 -1.715099 -2.34165
F -3.183807 -2.212942 -0.454121
C -4.436617 0.517438 -3.245714

F -3.146857 2.182624 -2.261566
C -3.633349 -0.921833 3.512294
F -1.805605 -1.75782 2.350499
C -4.845698 0.992432 2.687953
F -4.146194 2.046843 0.723416
C 0.05342 4.546692 -0.475574
F -0.639701 5.132237 1.703633
F 0.730156 3.887098 -2.645332
C -4.906454 -0.791926 -3.288053
F -4.931373 -2.966837 -2.361145
F -4.875492 1.412534 -4.135732
C -4.678709 -0.013335 3.639625
F -3.488021 -1.89974 4.409764
F -5.853476 1.861894 2.801671
F 0.643472 5.731689 -0.62784
F -5.786037 -1.156093 -4.220158
F -5.526579 -0.108659 4.661951

I4'$_p$

Zero-point correction= 0.620661 (Hartree/Particle)
Thermal correction to Energy= 0.681644
Thermal correction to Enthalpy= 0.682588
Thermal correction to Gibbs Free Energy= 0.520550
Sum of electronic and zero-point Energies= -4633.603827
Sum of electronic and thermal Energies= -4633.542845
Sum of electronic and thermal Enthalpies= -4633.541901
Sum of electronic and thermal Free Energies= -4633.703938
HF (M06/6-311++g(d,p) and SDD, SMD(cyclohexane): -4633.66848819

C 3.255481 1.752676 0.195905
H 3.613107 1.784396 -0.832236
C 3.363791 0.325294 0.790881
H 2.569680 -0.328509 0.431403
C 3.943354 2.600043 1.184260
C 3.303902 0.560376 2.306232
C 4.105184 1.860439 2.485505
H 3.726603 -0.281755 2.858829
H 2.266010 0.700600 2.624608
H 3.831565 2.464972 3.357548
H 5.182216 1.643700 2.573741
C 4.372934 3.945225 1.061008
H 4.950885 4.351366 1.888729
C 1.852192 2.495642 0.285274
C 1.700581 3.755798 -0.612208
C 0.903228 4.819300 0.172920
H 0.717043 5.706160 -0.445336
H -0.060832 4.408128 0.487232
H 1.434650 5.136792 1.077767
C 0.980649 3.485440 -1.954995
H -0.033977 3.116578 -1.789052
H 0.917550 4.417296 -2.531715
H 1.501727 2.734391 -2.552470
Pt 0.241084 1.041667 0.106799
Cl -0.669845 1.973405 2.130935
Cl 1.167759 0.119993 -1.903995
H 1.660419 2.780835 1.325397
C 3.996217 4.776252 0.048547
H 4.310655 5.816722 0.112361
C 3.096261 4.385915 -1.058068
H 3.590624 3.646196 -1.701051
H 2.884299 5.254769 -1.687520
O 4.654649 -0.186127 0.465555
Si 5.014853 -1.451121 -0.597556
C 4.990717 -0.829512 -2.380872
H 3.989087 -0.467782 -2.640990
H 5.700738 -0.008800 -2.537874
H 5.246207 -1.629626 -3.086779
C 3.761503 -2.849797 -0.392537
H 4.031316 -3.704064 -1.025895
H 3.713023 -3.207581 0.642771
H 2.754477 -2.535042 -0.687840
C 6.776795 -1.995804 -0.074523
C 7.751745 -0.804307 -0.190562
H 7.436790 0.035439 0.439578
H 8.761641 -1.101753 0.128659
H 7.830993 -0.438572 -1.221786
C 6.764872 -2.490551 1.387315
H 6.425215 -1.707474 2.074945
H 6.109466 -3.360165 1.519213
H 7.775433 -2.793130 1.699406
C 7.265969 -3.139158 -0.990157
H 8.277526 -3.457239 -0.698216
H 6.618283 -4.022433 -0.927185
H 7.313109 -2.832537 -2.042387
P -1.682473 -0.284296 0.019693
C -3.097440 0.888104 -0.139977
C -1.818824 -1.519409 -1.352400
C -2.056811 -1.403385 1.438583
C -4.027976 1.197333 0.856425
C -3.112869 1.701983 -1.279965
C -0.801098 -2.481408 -1.401977
C -2.786547 -1.585103 -2.358816
C -1.103629 -1.704568 2.418114
C -3.279219 -2.082209 1.516973
C -4.947998 2.234399 0.708647
F -4.071899 0.526717 2.014085
C -4.017076 2.740875 -1.451898
F -2.219386 1.484939 -2.257482
C -0.715742 -3.435509 -2.407562
F 0.123910 -2.520942 -0.429899
C -2.722107 -2.529484 -3.382067
F -3.837021 -0.753393 -2.381123
C -1.375040 -2.604204 3.449537
F 0.119878 -1.175126 2.394380
C -3.572933 -2.980994 2.533374
F -4.224377 -1.862313 0.588917
C -4.944658 3.007658 -0.446911
F -5.826752 2.493123 1.681476
F -3.999542 3.481952 -2.563843
C -1.682048 -3.453467 -3.410276
F 0.276066 -4.329965 -2.413456
F -3.666830 -2.560382 -4.327016
C -2.610930 -3.239136 3.509284
F -0.444366 -2.871262 4.370048
F -4.758004 -3.596562 2.581083
F -5.821582 4.000930 -0.592071
F -1.620965 -4.362370 -4.383062
F -2.873272 -4.101902 4.489710

Ts4'-4b'$_p$

Zero-point correction= 0.620162 (Hartree/Particle)
Thermal correction to Energy= 0.680770
Thermal correction to Enthalpy= 0.681714
Thermal correction to Gibbs Free Energy= 0.520566
Sum of electronic and zero-point Energies= -4633.598584
Sum of electronic and thermal Energies= -4633.537977
Sum of electronic and thermal Enthalpies= -4633.537032
Sum of electronic and thermal Free Energies= -4633.698181
HF (M06/6-311++g(d,p) and SDD, SMD(cyclohexane): -4633.65868315

C 3.209314 1.639169 0.124717
H 3.529874 1.645877 -0.911327
C 3.260524 0.267827 0.825572
H 2.472849 -0.408669 0.483886
C 3.722678 2.617571 1.076594
C 3.134534 0.612242 2.320633
C 3.818288 1.986571 2.457518
H 3.60668 -0.160265 2.932556
H 2.080465 0.671121 2.606373
H 3.3961 2.611806 3.251859
H 4.889695 1.870253 2.672341
C 4.466901 3.833576 0.779319
H 5.243398 4.092283 1.497137
C 2.017742 2.600315 0.386237
C 1.76853 3.893001 -0.441543
C 1.279868 4.982544 0.539918
H 1.064492 5.914809 0.003847
H 0.359071 4.658018 1.036775
H 2.025515 5.198708 1.311324
C 0.695393 3.728926 -1.542132
H -0.276295 3.461874 -1.114845
H 0.573801 4.681007 -2.074988
H 0.967397 2.956346 -2.264541
Pt 0.166317 1.03887 0.10909
Cl -0.738716 1.932258 2.152303
Cl 1.069461 0.253655 -1.956421
H 1.575345 2.620484 1.380406
C 4.213558 4.636281 -0.266085
H 4.814376 5.531117 -0.410451
C 3.058897 4.382403 -1.182672
H 3.324447 3.641363 -1.950429
H 2.809288 5.298145 -1.730482
O 4.55037 -0.2874 0.592405
Si 4.991858 -1.418679 -0.581234
C 5.00302 -0.628314 -2.298653
H 3.994453 -0.300936 -2.577864
H 5.668178 0.242099 -2.344143
H 5.338283 -1.342522 -3.061213
C 3.785669 -2.874342 -0.571191
H 4.107407 -3.647798 -1.279832
H 3.718497 -3.339047 0.419378
H 2.776443 -2.566958 -0.86624
C 6.751273 -1.955412 -0.04755
C 7.678889 -0.722517 0.010003
H 7.306924 0.027263 0.717127
H 8.688798 -1.016204 0.332476
H 7.778264 -0.239553 -0.970072
C 6.699931 -2.608822 1.350074
H 6.294929 -1.921057 2.100969
H 6.081134 -3.514682 1.355667
H 7.709473 -2.901605 1.674342
C 7.323331 -2.971593 -1.059841

H 8.333185 -3.28482 -0.757306
H 6.709266 -3.878501 -1.125536
H 7.403688 -2.548118 -2.068627
P -1.67482 -0.274731 0.005221
C -3.117021 0.855186 -0.160706
C -1.739755 -1.513924 -1.361102
C -1.992832 -1.398504 1.42977
C -4.049478 1.143336 0.841303
C -3.167103 1.651664 -1.312782
C -0.688034 -2.439938 -1.395721
C -2.70361 -1.624519 -2.367856
C -1.030105 -1.69076 2.40357
C -3.201731 -2.103113 1.505254
C -5.006225 2.144911 0.686614
F -4.059599 0.484583 2.00547
C -4.110302 2.65454 -1.490394
F -2.273945 1.450581 -2.290916
C -0.564458 -3.398965 -2.391793
F 0.236045 -2.433075 -0.4225
C -2.601574 -2.577202 -3.380212
F -3.783133 -0.832832 -2.399256
C -1.283801 -2.602388 3.429
F 0.185109 -1.144454 2.381321
C -3.47681 -3.013677 2.515866
F -4.150164 -1.897345 0.577069
C -5.038057 2.901773 -0.480025
F -5.88594 2.385552 1.661855
F -4.12943 3.379661 -2.611191
C -1.527353 -3.461963 -3.396663
F 0.460913 -4.253172 -2.387241
F -3.541971 -2.65306 -4.325461
C -2.507847 -3.26033 3.487958
F -0.345972 -2.85936 4.343176
F -4.649128 -3.65139 2.559634
F -5.950198 3.85992 -0.630934
F -1.430514 -4.376692 -4.359153
F -2.751071 -4.13401 4.461916

4b'

Zero-point correction= 0.620698 (Hartree/Particle)
Thermal correction to Energy= 0.681668
Thermal correction to Enthalpy= 0.682613
Thermal correction to Gibbs Free Energy= 0.519817
Sum of electronic and zero-point Energies= -4633.611816
Sum of electronic and thermal Energies= -4633.550845
Sum of electronic and thermal Enthalpies= -4633.549901
Sum of electronic and thermal Free Energies= -4633.712697
HF (M06/6-311++g(d,p) and SDD, SMD(cyclohexane): -4633.65822445

C 3.819342 1.696406 -0.078962
H 4.170330 1.601330 -1.102670
C 3.740973 0.420619 0.749687
H 2.828602 -0.157157 0.541619
C 4.344639 2.821779 0.819494
C 3.770862 0.903550 2.219379
C 4.565284 2.229423 2.209248
H 4.226325 0.140290 2.856266
H 2.750701 1.061941 2.581735
H 4.254989 2.904198 3.016919
H 5.636960 2.031839 2.340406
C 5.270372 3.855531 0.300239
H 6.209662 3.992447 0.834226
C 2.916321 2.842291 0.294644
C 2.512466 3.937876 -0.697943
C 1.963013 5.133784 0.107658
H 1.618045 5.931788 -0.561695
H 1.116249 4.829356 0.733276
H 2.739486 5.548367 0.758755
C 1.433441 3.410360 -1.658983
H 0.524330 3.120014 -1.064311
H 1.063835 4.181899 -2.345381
H 1.775243 2.552522 -2.239693
Pt -0.528486 1.368096 -0.720665
Cl -1.375551 2.799999 0.988469
Cl 0.355749 0.178611 -2.555658
H 2.128186 2.629429 1.017595
C 4.992172 4.596312 -0.779235
H 5.707056 5.333604 -1.138301
C 3.719036 4.407895 -1.566664
H 3.893574 3.676909 -2.371256
H 3.442539 5.340373 -2.075476
O 4.901750 -0.374874 0.498142
Si 4.991083 -1.760513 -0.447170
C 4.411031 -1.412165 -2.213668
H 3.381418 -1.032741 -2.224479
H 5.042191 -0.668227 -2.713633
H 4.426714 -2.324327 -2.823356
C 3.898836 -3.123680 0.287343
H 4.033390 -4.069124 -0.252976
H 4.133149 -3.305561 1.342623
H 2.836312 -2.866258 0.217120
C 6.842691 -2.238865 -0.378725
C 7.698212 -1.084523 -0.944007
H 7.536246 -0.155139 -0.387201
H 8.767931 -1.333588 -0.880529
H 7.472242 -0.887139 -1.999169
C 7.258862 -2.496604 1.085666
H 7.090110 -1.613327 1.711521
H 6.703880 -3.333354 1.528093
H 8.328267 -2.748782 1.141225
C 7.098568 -3.514407 -1.210031
H 8.163086 -3.788516 -1.171865
H 6.529580 -4.373247 -0.832296
H 6.836738 -3.377628 -2.266749
P -1.904448 -0.205723 0.007652
C -3.603645 0.448770 -0.190263
C -1.772287 -1.831365 -0.839284
C -1.653884 -0.725580 1.749328
C -4.432818 0.876497 0.853307
C -4.031087 0.731052 -1.495624
C -0.516013 -2.453909 -0.794464
C -2.792023 -2.515601 -1.510130
C -0.525389 -0.390025 2.507807
C -2.572019 -1.608604 2.334460
C -5.644319 1.518161 0.606426
F -4.095154 0.704625 2.134974
C -5.233260 1.370147 -1.764942
F -3.260269 0.378773 -2.530693
C -0.262821 -3.669890 -1.414205
F 0.483266 -1.880022 -0.109315
C -2.560495 -3.735623 -2.142442
F -4.042916 -2.043506 -1.557229
C -0.351690 -0.870245 3.805764
F 0.449402 0.375956 2.021322
C -2.420409 -2.098193 3.623749
F -3.651135 -1.998175 1.637021
C -6.045265 1.766294 -0.703021
F -6.415774 1.903178 1.624274
F -5.609525 1.607594 -3.021797
C -1.293262 -4.310478 -2.100315
F 0.947063 -4.225962 -1.350684
F -3.556089 -4.361385 -2.772480
C -1.300396 -1.720460 4.365351
F 0.732138 -0.528478 4.502650
F -3.327349 -2.922681 4.150143
F -7.201523 2.377645 -0.941351
F -1.071100 -5.477965 -2.695935
F -1.136753 -2.182623 5.600695

Ts3'-5b'$_p$

Zero-point correction= 0.618950 (Hartree/Particle)
Thermal correction to Energy= 0.679664
Thermal correction to Enthalpy= 0.680608
Thermal correction to Gibbs Free Energy= 0.519492
Sum of electronic and zero-point Energies= -4633.577021
Sum of electronic and thermal Energies= -4633.516307
Sum of electronic and thermal Enthalpies= -4633.515363
Sum of electronic and thermal Free Energies= -4633.676479
HF (M06/6-311++g(d,p) and SDD, SMD(cyclohexane): -4633.64240074

C 3.146515 -1.40754 0.286332
H 3.972098 -1.797943 0.888066
C 3.453733 -0.082636 -0.344958
H 2.929731 0.669503 0.264501
C 2.660352 -2.576746 -1.524251
C 2.893886 -0.04325 -1.780075
C 3.142637 -1.413464 -2.414975
H 3.397556 0.755454 -2.332901
H 1.823973 0.177898 -1.756755
H 2.630857 -1.477865 -3.381381
H 4.218265 -1.522923 -2.593231
C 3.630279 -3.720363 -1.460796
H 4.140149 -3.922105 -2.403049
C 1.996703 -2.172796 0.084488
C 1.88673 -3.498311 0.912321
C 0.794675 -4.425888 0.338229
H 0.69506 -5.309805 0.979724
H -0.173057 -3.920105 0.298741
H 1.032449 -4.77328 -0.67163
C 1.520875 -3.161254 2.374028
H 0.535149 -2.699702 2.450216
H 1.517907 -4.084762 2.966482
H 2.24173 -2.469424 2.823916
Pt 0.168078 -1.061353 -0.065063
Cl -0.495429 -2.121348 -2.098819
Cl 0.856017 0.177559 1.901507
H 1.680704 -2.909998 -1.886942
C 3.877913 -4.486193 -0.397326
H 4.604623 -5.292223 -0.483514
C 3.23043 -4.282349 0.942934
H 3.94584 -3.793423 1.625134
H 3.036122 -5.258632 1.406296
O 4.859319 0.117896 -0.347078

Si 5.658437 1.304052 0.561728
C 5.384105 0.972097 2.402237
H 4.314072 0.966267 2.645475
H 5.799529 0.006536 2.713466
H 5.85132 1.74897 3.019703
C 4.943056 3.001229 0.133739
H 5.450313 3.795514 0.694698
H 5.039808 3.230848 -0.933315
H 3.877982 3.059911 0.390639
C 7.48815 1.128968 0.046958
C 7.986116 -0.299387 0.359241
H 7.401449 -1.056487 -0.175272
H 9.036337 -0.411401 0.052846
H 7.934947 -0.527709 1.430989
C 7.634538 1.387813 -1.468668
H 7.027299 0.690824 -2.057049
H 7.337037 2.407488 -1.742486
H 8.682371 1.260375 -1.777056
C 8.350889 2.148666 0.822889
H 9.406483 2.054004 0.530701
H 8.050134 3.183863 0.618504
H 8.299811 1.991892 1.907552
P -1.780265 0.270916 -0.000139
C -1.208532 2.018619 -0.16904
C -3.084324 -0.011067 -1.282204
C -2.847229 0.191288 1.50222
C -1.185202 2.980865 0.844949
C -0.543064 2.350588 -1.355905
C -3.622117 -1.304423 -1.321635
C -3.582744 0.902152 -2.215287
C -2.712816 -0.822325 2.457357
C -3.912571 1.083995 1.674853
C -0.565021 4.217971 0.672911
F -1.740874 2.759698 2.042172
C 0.083784 3.573384 -1.552639
F -0.492807 1.457527 -2.356746
C -4.576059 -1.692148 -2.25423
F -3.234282 -2.20962 -0.412504
C -4.534992 0.537193 -3.165343
F -3.182312 2.181155 -2.231419
C -3.570725 -0.913325 3.553825
F -1.782457 -1.771229 2.345842
C -4.779071 1.015208 2.757054
F -4.115028 2.060545 0.775704
C 0.070259 4.516939 -0.527216
F -0.571106 5.112814 1.664921
F 0.697852 3.845515 -2.708118
C -5.029611 -0.763317 -3.187973
F -5.060763 -2.935876 -2.255542
F -4.986941 1.438205 -4.042947
C -4.601546 0.008007 3.705345
F -3.41612 -1.892766 4.447947
F -5.773668 1.896618 2.893961
F 0.665803 5.697282 -0.695802
F -5.946386 -1.113927 -4.089015
F -5.426119 -0.076432 4.747585

5b'-[Pt]$_p$

Zero-point correction= 0.622347 (Hartree/Particle)
Thermal correction to Energy= 0.683319
Thermal correction to Enthalpy= 0.684263
Thermal correction to Gibbs Free Energy= 0.520528
Sum of electronic and zero-point Energies= -4633.640933
Sum of electronic and thermal Energies= -4633.579960
Sum of electronic and thermal Enthalpies= -4633.579016
Sum of electronic and thermal Free Energies= -4633.742752
HF (M06/6-311++g(d,p) and SDD, SMD(cyclohexane): -4633.69902525

C 2.701959 -0.978195 0.118322
H 2.710682 -0.646460 1.150573
C 3.347190 0.012397 -0.849319
H 2.793840 0.958882 -0.816601
C 3.020463 -2.913979 -1.467200
C 3.375315 -0.517466 -2.282007
C 3.904285 -1.950872 -2.302412
H 4.013287 0.138923 -2.884098
H 2.362953 -0.481803 -2.698970
H 3.954877 -2.330069 -3.329938
H 4.925065 -1.964897 -1.902269
C 3.692885 -4.266360 -1.392809
H 3.975748 -4.696027 -2.352544
C 2.667139 -2.346125 -0.102303
C 2.378058 -3.356483 1.011314
C 1.106539 -4.175840 0.663805
H 0.953564 -4.942974 1.432359
H 0.224415 -3.529346 0.641419
H 1.187346 -4.676447 -0.303686
C 2.192173 -2.730033 2.403231
H 1.326715 -2.064179 2.449092
H 2.035211 -3.531405 3.134504
H 3.075126 -2.163914 2.720834
Pt 0.358204 -0.611585 -0.056819
Cl -0.058547 -1.762354 -2.094767
Cl 0.708869 0.733305 1.919533
H 2.066821 -3.028364 -2.007754
C 3.992961 -4.889926 -0.254171
H 4.527586 -5.837852 -0.270793
C 3.602691 -4.322600 1.081499
H 4.458177 -3.797937 1.534781
H 3.346252 -5.130630 1.779268
O 4.693134 0.229717 -0.409299
Si 5.282709 1.502483 0.527283
C 4.894460 1.220252 2.355592
H 3.810847 1.209596 2.525477
H 5.299634 0.267486 2.716045
H 5.315042 2.018378 2.980095
C 4.484525 3.129275 -0.019153
H 4.938146 3.979240 0.505423
H 4.596076 3.304242 -1.095345
H 3.413040 3.143661 0.214430
C 7.167876 1.481214 0.194811
C 7.750444 0.107216 0.591520
H 7.277603 -0.706848 0.031024
H 8.830177 0.074432 0.383495
H 7.619393 -0.100318 1.660757
C 7.439303 1.724645 -1.305358
H 6.959689 0.962783 -1.929917
H 7.076199 2.706435 -1.634152
H 8.519835 1.692286 -1.508670
C 7.866712 2.584163 1.019479
H 8.950549 2.570083 0.833521
H 7.506807 3.586825 0.756301
H 7.721351 2.448065 2.098216
P -1.743511 0.278772 -0.011822
C -1.535754 2.091438 -0.242675
C -2.961764 -0.329776 -1.256823
C -2.731039 0.000574 1.516262
C -1.672537 3.060923 0.756322
C -1.007923 2.520313 -1.467501
C -3.214500 -1.708646 -1.240955
C -3.666203 0.426179 -2.198849
C -2.395710 -0.960338 2.477992
C -3.943372 0.679436 1.697040
C -1.336065 4.394692 0.533420
F -2.117847 2.754273 1.979041
C -0.665491 3.843142 -1.713451
F -0.822087 1.631256 -2.451885
C -4.084966 -2.320996 -2.133048
F -2.621357 -2.479382 -0.319128
C -4.541271 -0.165620 -3.108147
F -3.551297 1.758561 -2.261784
C -3.205524 -1.192496 3.589955
F -1.309640 -1.723920 2.363008
C -4.764315 0.466298 2.795690
F -4.341167 1.584428 0.788187
C -0.832208 4.787787 -0.702342
F -1.487002 5.294107 1.508560
F -0.177876 4.209282 -2.900999
C -4.747240 -1.541603 -3.079218
F -4.292858 -3.638034 -2.084714
F -5.196312 0.588316 -3.994593
C -4.387179 -0.476500 3.751454
F -2.858330 -2.114661 4.489738
F -5.903150 1.148238 2.938289
F -0.509688 6.061234 -0.918186
F -5.588235 -2.109078 -3.940959
F -5.164180 -0.698514 4.808532

1d-$PtCl_2$(CO)

$I2_m$

Zero-point correction= 0.364088 (Hartree/Particle)
Thermal correction to Energy= 0.395606
Thermal correction to Enthalpy= 0.396551
Thermal correction to Gibbs Free Energy= 0.296992
Sum of electronic and zero-point Energies= -2076.360042
Sum of electronic and thermal Energies= -2076.328524
Sum of electronic and thermal Enthalpies= -2076.327580
Sum of electronic and thermal Free Energies= -2076.427138
HF (M06/6-311++g(d,p) and SDD, SMD(cyclohexane): -2076.57523004

C -1.471951 1.986787 -1.323878
C -0.907025 0.824192 -0.771830
C -0.634575 3.826507 1.546341
C 1.300292 1.441045 1.694175
C 0.478938 0.705771 -0.784321
C 1.237664 -0.532100 -0.446820
H 0.601273 -1.235615 0.097384
H -1.222735 4.736558 1.463407
C -2.953495 2.190664 -1.251015
H -3.440554 1.447963 -1.900198
H -3.255678 3.189722 -1.577916

H -3.319382 1.992834 -0.237581
C -0.746571 3.026338 -2.129410
H 0.337513 2.927027 -2.158811
H -1.006805 4.026990 -1.767961
H -1.117861 2.965427 -3.163741
C 2.299171 0.315502 1.732677
C 2.565188 -0.324493 0.330698
H 3.257916 0.647919 2.142661
H 1.936910 -0.485301 2.382306
Pt -2.100113 -0.706417 -0.066418
H 1.093144 1.509223 -1.171865
Cl -1.759566 -1.757392 -2.190314
Cl -2.381840 0.466459 2.013827
C 1.625211 2.734906 1.464602
C 0.702051 3.864641 1.386000
H 0.266368 1.178285 1.910701
H -1.175454 2.916372 1.791279
H 1.167566 4.824819 1.165186
H 2.676491 2.980600 1.306011
C -3.211053 -2.183894 0.550318
O -3.860299 -3.055260 0.904113
H 1.470839 -1.003083 -1.414666
C 3.207669 -1.714820 0.528753
O 3.276679 -2.311035 1.577739
O 3.649698 -2.200080 -0.647416
C 4.230725 -3.517709 -0.600356
H 4.516613 -3.745141 -1.627055
H 5.104000 -3.522860 0.056677
H 3.498967 -4.241249 -0.233300
C 3.553035 0.533026 -0.475730
O 3.312179 1.112302 -1.514012
O 4.752363 0.577106 0.134892
C 5.773393 1.331797 -0.543025
H 6.658651 1.253664 0.087783
H 5.963775 0.908164 -1.532218
H 5.467706 2.375354 -0.652910

Ts2-3$_m$

Zero-point correction= 0.366056 (Hartree/Particle)
Thermal correction to Energy= 0.395673
Thermal correction to Enthalpy= 0.396618
Thermal correction to Gibbs Free Energy= 0.303051
Sum of electronic and zero-point Energies= -2076.355045
Sum of electronic and thermal Energies= -2076.325427
Sum of electronic and thermal Enthalpies= -2076.324483
Sum of electronic and thermal Free Energies= -2076.418049
HF (M06/6-311++g(d,p) and SDD, SMD(cyclohexane): -2076.57141777

C -1.376317 2.217593 -0.995423
C -0.799031 1.009588 -0.542878
C -1.087345 3.314395 1.220716
C 1.218849 1.432997 1.48125
C 0.602901 0.864843 -0.580915
C 1.323116 -0.448957 -0.446392
H 0.698704 -1.167751 0.093054
H -1.860083 4.055457 1.037423
C -2.879094 2.341957 -1.053811
H -3.228198 1.815839 -1.9543
H -3.20065 3.386001 -1.130037
H -3.365466 1.86596 -0.199019
C -0.651549 3.225466 -1.863253
H 0.416827 3.308602 -1.662227
H -1.099478 4.219166 -1.767982
H -0.768576 2.916517 -2.912215
C 2.416815 0.520212 1.606979
C 2.674855 -0.282565 0.290563
H 3.316037 1.081951 1.87927
H 2.240187 -0.210636 2.400847
Pt -1.992917 -0.595592 -0.012218
H 1.194268 1.615731 -1.091103
Cl -1.956235 -1.121594 -2.34959
Cl -1.986751 0.004892 2.32169
C 1.330556 2.807474 1.325408
C 0.23413 3.693482 1.187925
H 0.281645 1.028132 1.852957
H -1.41707 2.380236 1.661357
H 0.470725 4.720091 0.913253
H 2.325751 3.225631 1.171355
C -3.110015 -2.150529 0.364495
O -3.763065 -3.065763 0.5692
H 1.493505 -0.850633 -1.452591
C 3.244698 -1.675393 0.612724
O 3.327228 -2.164333 1.715687
O 3.598479 -2.305328 -0.523013
C 4.103332 -3.644706 -0.362856
H 4.320722 -3.99503 -1.371656
H 5.008678 -3.637596 0.249348
H 3.351564 -4.278927 0.113001
C 3.691691 0.46765 -0.582714
O 3.444672 1.062182 -1.609949
O 4.919893 0.414632 -0.03125
C 5.963191 1.087606 -0.759268
H 6.869338 0.938147 -0.17244
H 6.071187 0.652902 -1.756005
H 5.736324 2.152517 -0.855633

I3$_m$

Zero-point correction= 0.370183 (Hartree/Particle)
Thermal correction to Energy= 0.399082
Thermal correction to Enthalpy= 0.400027
Thermal correction to Gibbs Free Energy= 0.307119
Sum of electronic and zero-point Energies= -2076.387420
Sum of electronic and thermal Energies= -2076.358521
Sum of electronic and thermal Enthalpies= -2076.357577
Sum of electronic and thermal Free Energies= -2076.450484
HF (M06/6-311++g(d,p) and SDD, SMD(cyclohexane): -2076.61587985

C -1.376088 2.428400 -0.600539
C -0.748130 1.091761 -0.361855
C -1.340040 3.126011 0.852238
C 1.139706 1.372910 1.250554
C 0.719258 0.989015 -0.260303
C 1.368215 -0.391710 -0.436423
H 0.791113 -1.147213 0.106905
H -2.026074 3.973017 0.749937
C -2.863282 2.331214 -1.003466
H -2.972715 1.794695 -1.949855
H -3.273004 3.340589 -1.126220
H -3.454696 1.811057 -0.243996
C -0.632246 3.309499 -1.631556
H 0.383178 3.561247 -1.320551
H -1.183884 4.247087 -1.761064
H -0.589763 2.807280 -2.603656
C 2.555068 0.750294 1.394531
C 2.766755 -0.243291 0.214353
H 3.323960 1.529254 1.389382
H 2.647469 0.208992 2.339009
Pt -1.868896 -0.536298 -0.118850
H 1.222363 1.703585 -0.916301
Cl -1.579003 -0.774688 -2.500912
Cl -2.107832 -0.235251 2.247545
C 1.078832 2.846455 1.522328
C -0.004268 3.612587 1.334145
H 0.446152 0.838295 1.908445
H -1.793690 2.431297 1.567636
H 0.085301 4.681534 1.518165
H 2.001484 3.320616 1.853819
C -2.971296 -2.181852 -0.026010
O -3.602847 -3.129345 0.012165
H 1.419876 -0.689118 -1.484332
C 3.276212 -1.607537 0.694024
O 3.386980 -1.957367 1.846991
O 3.540238 -2.399807 -0.363024
C 3.992288 -3.729114 -0.047734
H 4.148527 -4.218429 -1.009069
H 4.924014 -3.687949 0.522236
H 3.236854 -4.259627 0.537252
C 3.763883 0.351957 -0.786499
O 3.475770 0.869901 -1.843424
O 5.021118 0.279469 -0.306820
C 6.044304 0.840804 -1.148445
H 6.978098 0.699292 -0.604267
H 6.074062 0.320686 -2.109153
H 5.855704 1.903310 -1.322574

Ts3-2d$_m$

Zero-point correction= 0.366053 (Hartree/Particle)
Thermal correction to Energy= 0.394366
Thermal correction to Enthalpy= 0.395310
Thermal correction to Gibbs Free Energy= 0.304386
Sum of electronic and zero-point Energies= -2076.369307
Sum of electronic and thermal Energies= -2076.340994
Sum of electronic and thermal Enthalpies= -2076.340050
Sum of electronic and thermal Free Energies= -2076.430973
HF (M06/6-311++g(d,p) and SDD, SMD(cyclohexane): -2076.60028072

C 1.631648 2.392079 -0.255045
C 0.819678 1.064886 -0.231086
C 0.904113 3.606459 -0.911027
C -1.483204 1.99912 -1.17555
C -0.516878 0.934199 -0.631524
C -1.253189 -0.388299 -0.614305
H -1.055287 -0.862075 -1.585926
H 1.610246 4.443708 -0.898493

C 2.922027 2.14837 -1.07163
H 3.54718 1.380253 -0.607827
H 3.49874 3.080151 -1.113266
H 2.703723 1.822669 -2.092593
C 2.024654 2.769577 1.191872
H 1.143439 2.972345 1.810461
H 2.643623 3.67483 1.172676
H 2.589563 1.969838 1.674654
C -2.854202 1.286922 -1.315751
C -2.748828 -0.019306 -0.485093
H -3.685136 1.919632 -0.990562
H -3.055655 1.010369 -2.353527
Pt 1.841874 -0.730167 0.131637
H -0.058484 1.108037 0.676508
Cl 1.547009 -0.480967 2.492468
Cl 1.89973 -1.011439 -2.257637
C -1.49016 3.275913 -0.361135
C -0.386022 4.01547 -0.248751
H -1.101141 2.238518 -2.179678
H 0.724139 3.379461 -1.972245
H -0.403274 4.925587 0.346671
H -2.419565 3.555056 0.128899
C 2.826998 -2.372059 0.392461
O 3.415073 -3.339837 0.542336
H -0.89073 -1.070846 0.155637
C -3.659278 -1.125494 -1.016044
O -4.420113 -1.015351 -1.950795
O -3.465443 -2.261477 -0.322513
C -4.259331 -3.388997 -0.73763
H -3.964664 -4.208217 -0.082244
H -5.322828 -3.16438 -0.623877
H -4.052854 -3.63538 -1.781998
C -3.055216 0.314675 0.9766
O -2.233514 0.778209 1.74223
O -4.343911 0.119237 1.285178
C -4.728075 0.468317 2.631174
H -5.790618 0.236265 2.6968
H -4.155389 -0.120408 3.351296
H -4.550888 1.53127 2.812131

2d-[Pt]$_m$

Zero-point correction= 0.370910 (Hartree/Particle)
Thermal correction to Energy= 0.399524
Thermal correction to Enthalpy= 0.400468
Thermal correction to Gibbs Free Energy= 0.309187
Sum of electronic and zero-point Energies= -2076.412953
Sum of electronic and thermal Energies= -2076.384340
Sum of electronic and thermal Enthalpies= -2076.383396
Sum of electronic and thermal Free Energies= -2076.474677
HF (M06/6-311++g(d,p) and SDD, SMD(cyclohexane): -2076.64588157

C 1.517284 2.379551 0.269991
C 0.883989 0.990419 0.146220
C 0.920563 3.443925 -0.687254
C -1.201160 1.438507 -1.378052
C -0.289812 0.594747 -0.470378
C -1.047492 -0.669690 -0.054207
H -0.798741 -1.507705 -0.713793
H 1.482656 4.372959 -0.536834
C 3.042534 2.298488 0.047499
H 3.490795 1.502391 0.653028
H 3.511864 3.247040 0.334937
H 3.283415 2.104775 -1.002541
C 1.257701 2.790705 1.744671
H 0.188813 2.793792 1.978826
H 1.656973 3.796651 1.922013
H 1.757450 2.104920 2.438213
C -2.466035 0.568805 -1.553084
C -2.535291 -0.302476 -0.277879
H -3.370970 1.161654 -1.706826
H -2.364346 -0.104020 -2.409169
Pt 1.743393 -0.404485 -1.588746
H 1.227140 0.320895 0.933928
Cl 2.091150 -2.012969 0.150246
Cl 1.514218 1.092356 -3.442647
C -1.497799 2.803562 -0.772657
C -0.553078 3.701875 -0.486705
H -0.713834 1.591949 -2.346728
H 1.110483 3.129073 -1.720067
H -0.851609 4.662901 -0.071639
H -2.546190 3.040620 -0.597842
C 2.835977 -1.465861 -2.702910
O 3.503986 -2.106571 -3.369077
H -0.825205 -0.967365 0.970402
C -3.381115 -1.561939 -0.484117
O -3.735890 -1.994924 -1.556743
O -3.634080 -2.163174 0.694594
C -4.386331 -3.388346 0.620353
H -4.493797 -3.726049 1.651027
H -5.364346 -3.206413 0.167759
H -3.847571 -4.129750 0.025097
C -3.063952 0.492874 0.922357
O -2.418141 0.798087 1.900704
O -4.353023 0.839297 0.735083
C -4.958019 1.581092 1.809318
H -5.982567 1.772715 1.490283
H -4.943237 0.994412 2.731310
H -4.422177 2.519422 1.973973

Ts3-3d$_m$

Zero-point correction= 0.368070 (Hartree/Particle)
Thermal correction to Energy= 0.396610
Thermal correction to Enthalpy= 0.397554
Thermal correction to Gibbs Free Energy= 0.306040
Sum of electronic and zero-point Energies= -2076.367864
Sum of electronic and thermal Energies= -2076.339324
Sum of electronic and thermal Enthalpies= -2076.338380
Sum of electronic and thermal Free Energies= -2076.429894
HF (M06/6-311++g(d,p) and SDD, SMD(cyclohexane): -2076.59876818

C -1.333093 2.261728 -1.023108
C -0.868348 1.263891 -0.125316
C -1.448276 2.502751 1.071899
C 1.089532 1.280043 1.572296
C 0.645378 1.119194 0.089951
C 1.295664 -0.21741 -0.303346
H 0.748139 -1.050385 0.150697
H -2.270731 3.145586 0.754078
C -2.748908 2.279197 -1.51999
H -2.728193 1.844441 -2.528203
H -3.137827 3.300621 -1.597993
H -3.411771 1.654134 -0.918292
C -0.433733 3.306409 -1.626883
H 0.235481 3.751736 -0.884514
H -1.005596 4.095929 -2.120593
H 0.202005 2.815585 -2.376235
C 2.561054 0.81376 1.574913
C 2.717705 -0.12199 0.326995
H 3.242131 1.668916 1.501464
H 2.823883 0.262367 2.480001
Pt -1.939736 -0.565879 -0.06098
H 1.178697 1.890031 -0.474285
Cl -1.489506 -0.719082 -2.417655
Cl -2.353504 -0.437715 2.297744
C 0.825826 2.688425 2.014471
C -0.341344 3.270127 1.699436
H 0.488415 0.585376 2.176405
H -1.882822 1.739472 1.725829
H -0.526539 4.316634 1.932135
H 1.606885 3.253187 2.5203
C -2.848127 -2.275159 -0.110885
O -3.385001 -3.282636 -0.153566
H 1.331219 -0.384387 -1.379751
C 3.217884 -1.516379 0.716058
O 3.376064 -1.926845 1.843653
O 3.414161 -2.262671 -0.38942
C 3.843733 -3.615514 -0.158832
H 3.937789 -4.063467 -1.148152
H 4.803869 -3.626549 0.363821
H 3.104353 -4.15396 0.439441
C 3.696296 0.519599 -0.660889
O 3.389708 1.139518 -1.656809
O 4.969206 0.365788 -0.242721
C 5.976051 0.968017 -1.073792
H 6.926073 0.747188 -0.586869
H 5.948177 0.538409 -2.078433
H 5.820039 2.047885 -1.142859

3d-[Pt]$_m$

Zero-point correction= 0.370776 (Hartree/Particle)
Thermal correction to Energy= 0.399734
Thermal correction to Enthalpy= 0.400678
Thermal correction to Gibbs Free Energy= 0.307754
Sum of electronic and zero-point Energies= -2076.399176
Sum of electronic and thermal Energies= -2076.370218
Sum of electronic and thermal Enthalpies= -2076.369274
Sum of electronic and thermal Free Energies= -2076.462197
HF (M06/6-311++g(d,p) and SDD, SMD(cyclohexane): -2076.63204616

C -1.325368 2.007249 -1.075170
C -0.786304 1.672401 0.163138
C -1.432477 2.150950 1.470334
C 1.216941 1.404798 1.757825
C 0.701151 1.334537 0.300278

C 1.315784 0.004826 -0.174850
H 0.775791 -0.831696 0.276015
H -2.379953 2.655490 1.282629
C -2.640149 2.756576 -1.218059
H -3.071494 2.572443 -2.203904
H -2.443615 3.835314 -1.130100
H -3.388034 2.484950 -0.471270
C -0.439254 2.127507 -2.299554
H -0.064703 3.162958 -2.320925
H -1.002579 1.958369 -3.217304
H 0.426783 1.467462 -2.296687
C 2.710651 1.083933 1.596762
C 2.770616 0.073526 0.394599
H 3.274217 1.994076 1.360377
H 3.153592 0.634535 2.487438
Pt -2.054995 -0.354450 -0.751152
H 1.225441 2.133758 -0.244208
Cl -2.666251 -0.086306 -3.064226
Cl -1.703073 -1.126342 1.507602
C 0.796202 2.700230 2.394373
C -0.477685 3.067276 2.223621
H 0.751407 0.574863 2.310469
H -1.653838 1.286081 2.106693
H -0.874756 3.990103 2.639288
H 1.505396 3.306955 2.953308
C -2.840296 -2.046932 -0.977164
O -3.317470 -3.073617 -1.115871
H 1.325554 -0.133198 -1.256201
C 3.228502 -1.316085 0.846896
O 3.452421 -1.656885 1.986111
O 3.307434 -2.145365 -0.214464
C 3.689368 -3.499820 0.082940
H 3.702023 -4.016125 -0.877094
H 4.678350 -3.523795 0.547929
H 2.964577 -3.960387 0.759119
C 3.727971 0.609278 -0.672552
O 3.397290 1.147617 -1.707490
O 5.009706 0.461057 -0.284665
C 6.000297 0.970439 -1.194789
H 6.961612 0.759641 -0.726106
H 5.923333 0.467703 -2.162191
H 5.869249 2.046016 -1.339536

Ts3-4d$_m$

Zero-point correction= 0.367081 (Hartree/Particle)
Thermal correction to Energy= 0.395077
Thermal correction to Enthalpy= 0.396022
Thermal correction to Gibbs Free Energy= 0.306347
Sum of electronic and zero-point Energies= -2076.359113
Sum of electronic and thermal Energies= -2076.331117
Sum of electronic and thermal Enthalpies= -2076.330173
Sum of electronic and thermal Free Energies= -2076.419848
HF (M06/6-311++g(d,p) and SDD, SMD(cyclohexane): -2076.59512763

C 1.71814 2.4291 0.458235
C 0.775773 1.173025 0.262977
C 1.530212 3.444153 -0.705404
C -0.838444 1.634979 -0.484186
C -0.595567 1.225272 0.935785
C -1.413205 -0.044803 1.21849
H -0.770873 -0.926277 1.247801
H 2.142674 4.325967 -0.4835
C 3.194586 1.976354 0.433907
H 3.416092 1.303431 1.266574
H 3.842682 2.857432 0.524029
H 3.445672 1.466969 -0.501597
C 1.465458 3.132167 1.808363
H 0.510193 3.666628 1.838021
H 2.255 3.872623 1.978735
H 1.494832 2.415898 2.635927
C -1.683883 0.541228 -1.146544
C -2.423335 -0.138779 0.039274
H -2.357338 0.968177 -1.894506
H -1.066375 -0.202518 -1.65964
Pt 1.673049 -0.73158 -0.073213
H -0.699248 2.00428 1.680524
Cl 1.816952 -0.973831 2.304734
Cl 1.567167 -0.327535 -2.441225
C -0.93857 3.055122 -0.896314
C 0.111615 3.876292 -0.981468
H 0.426297 1.231187 -0.921344
H 1.951776 3.011835 -1.626484
H -0.051407 4.901773 -1.304787
H -1.944821 3.390934 -1.13798
C 2.497549 -2.447566 -0.329556
O 2.981283 -3.472172 -0.475055
H -1.932179 0.029134 2.174849
C -2.792312 -1.587818 -0.279994
O -2.486721 -2.18556 -1.286094
O -3.476 -2.128596 0.746969
C -3.85087 -3.508981 0.584304
H -4.386898 -3.773827 1.49561
H -4.493391 -3.627075 -0.291923
H -2.961718 -4.13291 0.46427
C -3.683211 0.675242 0.362131
O -3.770307 1.501273 1.24457
O -4.669031 0.406534 -0.51518
C -5.890919 1.144437 -0.329193
H -6.562814 0.79613 -1.113434
H -6.310446 0.940561 0.658995
H -5.707472 2.217699 -0.425762

I4$_m$

Zero-point correction= 0.368572 (Hartree/Particle)
Thermal correction to Energy= 0.397174
Thermal correction to Enthalpy= 0.398119
Thermal correction to Gibbs Free Energy= 0.306556
Sum of electronic and zero-point Energies= -2076.373103
Sum of electronic and thermal Energies= -2076.344500
Sum of electronic and thermal Enthalpies= -2076.343556
Sum of electronic and thermal Free Energies= -2076.435119
HF (M06/6-311++g(d,p) and SDD, SMD(cyclohexane): -2076.60715947

C 1.788668 2.377642 0.348392
C 1.089104 1.017022 0.033775
C 1.684318 3.336641 -0.858807
C -1.168601 1.795560 -0.864911
C -0.462807 1.038000 0.187353
C -1.187823 -0.340076 0.211808
H -0.678202 -1.031127 -0.468500
H 2.146520 4.301046 -0.591697
C 3.303617 2.153550 0.568669
H 3.480449 1.634115 1.514311
H 3.830012 3.117493 0.607259
H 3.739723 1.547725 -0.232209
C 1.225359 3.108553 1.585415
H 0.200832 3.471593 1.428713
H 1.843044 3.986019 1.815088
H 1.224514 2.450287 2.456626
C -2.385010 1.069130 -1.334694
C -2.619970 -0.060753 -0.310762
H -3.241506 1.729732 -1.513118
H -2.167514 0.594953 -2.308293
Pt 1.891911 -0.674540 1.069940
H -0.693480 1.521121 1.154521
Cl 0.759143 -0.051115 3.092888
Cl 2.933371 -1.279627 -1.008132
C -0.825950 3.012943 -1.495760
C 0.385541 3.654321 -1.498542
H 1.309126 0.770161 -1.011582
H 2.316400 2.977681 -1.695745
H 0.434138 4.514260 -2.169021
H -1.586996 3.425116 -2.156072
C 2.692885 -2.212955 1.934106
O 3.179296 -3.117767 2.439032
H -1.183042 -0.769117 1.211937
C -3.203885 -1.297432 -0.996039
O -3.270922 -1.449593 -2.196983
O -3.568825 -2.214805 -0.090307
C -4.069875 -3.457689 -0.620616
H -4.295588 -4.072662 0.250009
H -4.969620 -3.279903 -1.214853
H -3.311279 -3.934844 -1.245495
C -3.545244 0.437400 0.805849
O -3.193437 0.767007 1.914408
O -4.816098 0.522562 0.359333
C -5.781419 0.991135 1.320046
H -6.737226 0.989997 0.796179
H -5.811970 0.321576 2.182972
H -5.526037 1.998670 1.658198

Ts4-5$_m$

Zero-point correction= 0.369013 (Hartree/Particle)
Thermal correction to Energy= 0.396932
Thermal correction to Enthalpy= 0.397877
Thermal correction to Gibbs Free Energy= 0.308606
Sum of electronic and zero-point Energies= -2076.365887
Sum of electronic and thermal Energies= -2076.337967
Sum of electronic and thermal Enthalpies= -2076.337023
Sum of electronic and thermal Free Energies= -2076.426294
HF (M06/6-311++g(d,p) and SDD, SMD(cyclohexane): -2076.60178619

C -0.436503 1.402105 0.986672
H 0.110738 1.808887 1.829931

C -1.366329 0.228031 1.303323
H -0.851633 -0.726043 1.407623
C -1.108341 2.262688 0.058728
C -2.450195 0.204368 0.18932
C -2.344546 1.592311 -0.503964
H -2.339101 1.48566 -1.592858
H -3.193781 2.243528 -0.255606
C -0.973067 3.705413 -0.183129
H -1.860027 4.276105 0.093937
C 0.567378 1.311892 -0.263045
C 1.700988 2.383673 -0.437026
C 2.894651 1.739609 -1.1798
H 3.624778 2.518387 -1.433879
H 3.4057 0.999093 -0.555885
H 2.582645 1.242923 -2.103117
C 2.217082 2.938959 0.907423
H 2.529062 2.135861 1.579275
H 3.086337 3.580457 0.720484
H 1.469502 3.552187 1.421971
Cl 1.180629 -1.27424 -2.177187
Cl 1.882037 -0.31593 2.464639
H 0.154251 0.966552 -1.214089
C 0.035233 4.305203 -0.82149
H -0.037421 5.372698 -1.017984
C 1.245563 3.575277 -1.32077
H 2.084013 4.278191 -1.39912
H 1.055296 3.227646 -2.34911
Pt 1.510274 -0.763886 0.138339
C 2.337786 -2.434863 0.364888
O 2.849627 -3.449471 0.494044
H -1.858678 0.444292 2.256392
C -2.263388 -0.910004 -0.858192
O -2.266076 -0.734346 -2.055342
O -2.134856 -2.105073 -0.262827
C -1.973406 -3.228088 -1.15569
H -1.894012 -4.100645 -0.507156
H -2.842364 -3.311869 -1.813316
H -1.06877 -3.097593 -1.752862
C -3.851593 0.047884 0.810358
O -4.131684 0.284039 1.964075
O -4.749956 -0.329197 -0.116565
C -6.105482 -0.47119 0.34792
H -6.67818 -0.787246 -0.523714
H -6.157982 -1.222053 1.140043
H -6.478481 0.481795 0.731709

I5$_m$

Zero-point correction= 0.370092 (Hartree/Particle)
Thermal correction to Energy= 0.398744
Thermal correction to Enthalpy= 0.399688
Thermal correction to Gibbs Free Energy= 0.308919
Sum of electronic and zero-point Energies= -2076.378453
Sum of electronic and thermal Energies= -2076.349801
Sum of electronic and thermal Enthalpies= -2076.348857
Sum of electronic and thermal Free Energies= -2076.439626
HF (M06/6-311++g(d,p) and SDD, SMD(cyclohexane): -2076.61501683

C -0.194396 1.024882 0.961884
H 0.147266 1.591688 1.823584
C -1.313502 -0.015562 1.200166
H -0.986792 -1.057198 1.198436
C -0.923735 2.163230 0.000452
C -2.421418 0.178279 0.128410
C -2.340027 1.668332 -0.270217
H -2.607728 1.806131 -1.321771
H -3.035679 2.258770 0.336904
C -0.783857 3.602731 0.317140
H -1.478376 4.045813 1.028049
C 0.242248 1.456631 -0.511808
C 1.522753 2.283564 -0.864174
C 2.251091 1.579462 -2.024597
H 3.123167 2.165846 -2.337980
H 2.592512 0.583342 -1.727713
H 1.593042 1.463631 -2.894165
C 2.509990 2.480914 0.301516
H 2.943704 1.530155 0.627996
H 3.337579 3.120083 -0.029104
H 2.049795 2.953839 1.173711
Cl 1.398709 -1.730981 -0.452059
Cl 1.764623 0.741281 3.624291
H 0.054355 0.644184 -1.206225
C 0.118902 4.336963 -0.344419
H 0.185975 5.409807 -0.176570
C 1.051368 3.688426 -1.337491
H 1.929282 4.320996 -1.511605
H 0.542731 3.601607 -2.310263
Pt 1.592960 -0.465556 1.568435
C 2.846255 -1.672758 2.191855
O 3.618025 -2.421409 2.580567
H -1.748538 0.179561 2.184376
C -2.196930 -0.736265 -1.088193
O -1.923466 -0.361556 -2.208021
O -2.334592 -2.022887 -0.733693
C -2.072143 -2.990849 -1.768434
H -2.283724 -3.959960 -1.317105
H -2.720816 -2.811216 -2.629030
H -1.025515 -2.929043 -2.074367
C -3.805898 -0.136488 0.716505
O -4.053914 -0.300174 1.888948
O -4.735633 -0.148235 -0.258882
C -6.085194 -0.406096 0.170273
H -6.689088 -0.375005 -0.736564
H -6.150956 -1.387992 0.645588
H -6.412697 0.358057 0.879735

Ts3-5d$_m$

Zero-point correction= 0.368696 (Hartree/Particle)
Thermal correction to Energy= 0.396773
Thermal correction to Enthalpy= 0.397717
Thermal correction to Gibbs Free Energy= 0.308670
Sum of electronic and zero-point Energies= -2076.355738
Sum of electronic and thermal Energies= -2076.327661
Sum of electronic and thermal Enthalpies= -2076.326717
Sum of electronic and thermal Free Energies= -2076.415764
HF (M06/6-311++g(d,p) and SDD, SMD(cyclohexane): -2076.58953558

C 1.179334 2.4506 0.604084
C 0.504188 1.049397 0.345897
C 0.940349 3.417453 -0.608391
C -0.673832 1.204067 -1.064254
C -0.571397 0.687793 1.165142
C -1.34233 -0.588668 1.08651
H -0.683417 -1.429382 0.864184
H 1.438653 4.36796 -0.391501
C 2.708351 2.298034 0.770257
H 2.954797 1.653927 1.619163
H 3.15422 3.28461 0.949981
H 3.172282 1.877781 -0.12756
C 0.643252 3.142361 1.878294
H -0.416449 3.41101 1.801004
H 1.201055 4.070425 2.046882
H 0.780224 2.512115 2.764548
C -1.563293 -0.005374 -1.310169
C -2.373023 -0.45267 -0.079173
H -2.23828 0.22883 -2.141407
H -0.947994 -0.849187 -1.630635
Pt 1.84959 -0.578894 -0.059666
H -1.007361 1.415742 1.846963
Cl 1.752101 -1.000049 2.309471
Cl 2.011151 -0.101642 -2.402961
C -1.303125 2.550668 -1.051532
C -0.520132 3.62502 -0.890016
H 0.149244 1.172378 -1.783982
H 1.441352 2.993909 -1.490254
H -0.937629 4.628984 -0.894981
H -2.378138 2.634266 -1.192832
C 3.074747 -2.045927 -0.287496
O 3.793131 -2.925538 -0.413837
H -1.864648 -0.768521 2.028302
C -3.025832 -1.822851 -0.33381
O -2.81535 -2.524192 -1.294784
O -3.840133 -2.151757 0.68637
C -4.485101 -3.436325 0.579577
H -5.08924 -3.533046 1.481315
H -5.112607 -3.471492 -0.31437
H -3.737805 -4.231653 0.526607
C -3.471083 0.549947 0.303033
O -3.503347 1.195545 1.328288
O -4.398575 0.634374 -0.667891
C -5.501806 1.523176 -0.4035
H -6.140403 1.461891 -1.284304
H -6.040834 1.199944 0.490296
H -5.141736 2.544366 -0.255995

5d-[Pt]$_m$

Zero-point correction= 0.370183 (Hartree/Particle)
Thermal correction to Energy= 0.399082
Thermal correction to Enthalpy= 0.400027
Thermal correction to Gibbs Free Energy= 0.307120
Sum of electronic and zero-point Energies= -2076.387420
Sum of electronic and thermal Energies= -2076.358520
Sum of electronic and thermal Enthalpies= -2076.357576
Sum of electronic and thermal Free Energies= -2076.450482
HF (M06/6-311++g(d,p) and SDD, SMD(cyclohexane): -2076.61589053

C 1.412445 2.425607 0.722266
C 0.783191 1.082802 0.525467
C 1.526765 3.010498 -0.775216
C -0.939927 1.263619 -1.274442
C -0.670062 0.991305 0.293895
C -1.359980 -0.363416 0.510961
H -0.749774 -1.165614 0.082948
H 2.216378 3.854463 -0.671619
C 2.853089 2.340411 1.270854
H 2.862548 1.876284 2.260771
H 3.269522 3.350898 1.356153
H 3.502628 1.756327 0.611999
C 0.593038 3.392384 1.609132
H -0.383455 3.632871 1.185085
H 1.148864 4.329887 1.719994
H 0.449475 2.966364 2.607574
C -2.348313 0.651018 -1.503929
C -2.688453 -0.247654 -0.278530
H -3.098257 1.438479 -1.628409
H -2.364045 0.041318 -2.410362
Pt 1.889386 -0.573419 0.510559
H -1.217793 1.760438 0.843897
Cl 1.372538 -0.624795 2.865490
Cl 2.354030 -0.455957 -1.838405
C -0.823719 2.710876 -1.649738
C 0.252098 3.475239 -1.417679
H -0.199365 0.670623 -1.821796
H 2.032288 2.257874 -1.390237
H 0.201887 4.527754 -1.690121
H -1.701184 3.169915 -2.102881
C 2.962370 -2.235127 0.644206
O 3.575743 -3.190902 0.735692
H -1.515183 -0.579079 1.568609
C -3.176968 -1.638045 -0.701540
O -3.185984 -2.072965 -1.830583
O -3.554150 -2.344520 0.381692
C -4.000265 -3.688305 0.124732
H -4.255364 -4.101280 1.100631
H -4.873496 -3.679153 -0.532585
H -3.203732 -4.270894 -0.344795
C -3.763053 0.433918 0.576396
O -3.565023 1.026757 1.614531
O -4.971119 0.340704 -0.013388
C -6.057417 0.976737 0.683587
H -6.938730 0.806329 0.065222
H -6.187238 0.530944 1.672923
H -5.865115 2.046883 0.795855

Ts3-3'$_m$

Zero-point correction= 0.369998 (Hartree/Particle)
Thermal correction to Energy= 0.398216
Thermal correction to Enthalpy= 0.399160
Thermal correction to Gibbs Free Energy= 0.307344
Sum of electronic and zero-point Energies= -2076.378837
Sum of electronic and thermal Energies= -2076.350620
Sum of electronic and thermal Enthalpies= -2076.349676
Sum of electronic and thermal Free Energies= -2076.441491
HF (M06/6-311++g(d,p) and SDD, SMD(cyclohexane): -2076.60735582

C -0.629162 0.986842 0.105483
H -1.112045 1.796179 0.662251
C -1.371389 -0.329404 0.390792
H -0.830853 -1.165812 -0.063282
C -0.962591 1.250839 -1.413385
C -2.741238 -0.139185 -0.314891
C -2.447129 0.79447 -1.528366
H -2.621281 0.250619 -2.459635
H -3.113734 1.66265 -1.522302
C -0.744449 2.671091 -1.832861
H -1.328836 2.983617 -2.698074
C 0.834208 1.018735 0.29089
C 1.453343 2.312695 0.723348
C 2.995309 2.251355 0.791653
H 3.384634 3.21797 1.133238
H 3.330613 1.483617 1.495155
H 3.42343 2.032732 -0.190885
C 0.92558 2.510504 2.19317
H 1.112536 1.623952 2.805952
H 1.480515 3.350257 2.624814
H -0.141124 2.744403 2.2244
Pt 1.919341 -0.613405 0.038465
Cl 2.364215 -0.001447 -2.241079
Cl 1.532971 -1.228871 2.330458
C 3.005396 -2.267933 -0.211674
O 3.619713 -3.21551 -0.355543
H -0.340013 0.583088 -2.02049
C 0.049783 3.591972 -1.277309
H 0.025572 4.579339 -1.740527
C 1.059259 3.569088 -0.15252
H 0.798138 4.379236 0.542651
H 1.9956 3.897305 -0.622431
H -1.473259 -0.530237 1.457449
C -3.300694 -1.49761 -0.752511
O -3.394386 -1.891898 -1.892683
O -3.63093 -2.230857 0.328271
C -4.132177 -3.551823 0.055687
H -4.339212 -3.991091 1.031484
H -5.043386 -3.495656 -0.545346
H -3.383752 -4.140081 -0.481157
C -3.732782 0.549893 0.628767
O -3.442881 1.111394 1.663049
O -4.981031 0.507666 0.124288
C -5.99426 1.161659 0.909062
H -6.922562 1.029691 0.35324
H -6.066421 0.700529 1.897272
H -5.761249 2.223237 1.025468

I3'$_m$

Zero-point correction= 0.370321 (Hartree/Particle)
Thermal correction to Energy= 0.399179
Thermal correction to Enthalpy= 0.400123
Thermal correction to Gibbs Free Energy= 0.307415
Sum of electronic and zero-point Energies= -2076.386352
Sum of electronic and thermal Energies= -2076.357495
Sum of electronic and thermal Enthalpies= -2076.356551
Sum of electronic and thermal Free Energies= -2076.449259
HF (M06/6-311++g(d,p) and SDD, SMD(cyclohexane): -2076.61672222

C -0.547945 1.024352 -0.065012
H -0.777325 1.677819 0.784831
C -1.188675 -0.347804 0.179874
H -0.864256 -1.054254 -0.590293
C -1.388359 1.563457 -1.295870
C -2.716108 -0.073396 0.045333
C -2.834901 1.183220 -0.876068
H -3.456518 0.956016 -1.745171
H -3.295210 2.018735 -0.338867
C -1.209756 3.010006 -1.652492
H -1.845049 3.349359 -2.470483
C 0.874071 1.124757 -0.434919
C 1.566169 2.418293 -0.121218
C 2.689095 2.764807 -1.122715
H 3.213698 3.663882 -0.779901
H 3.414764 1.950784 -1.201352
H 2.282678 2.949712 -2.120310
C 2.215898 2.144702 1.283157
H 2.971620 1.359827 1.231911
H 2.687284 3.082976 1.598346
H 1.473198 1.861592 2.035483
Pt 1.794258 -0.395080 -1.311585
Cl 1.286188 0.477284 -3.492278
Cl 2.289481 -1.375345 0.823947
C 2.713291 -1.930170 -2.187854
O 3.239829 -2.807003 -2.687545
H -1.111308 0.954683 -2.165665
C -0.365928 3.889825 -1.101561
H -0.375667 4.904574 -1.495198
C 0.601853 3.637318 0.036087
H 0.054313 3.559554 0.984628
H 1.244625 4.516580 0.153692
H -0.925475 -0.763847 1.152517
C -3.422921 -1.293092 -0.554808
O -3.949597 -1.344285 -1.643123
O -3.334187 -2.338466 0.290137
C -3.929371 -3.564730 -0.170707
H -3.751733 -4.290186 0.623138
H -5.000921 -3.427588 -0.337263
H -3.460041 -3.889494 -1.102686
C -3.316048 0.260275 1.414431
O -2.680669 0.599904 2.389201
O -4.660520 0.199858 1.379275
C -5.333787 0.549933 2.602125
H -6.397553 0.448821 2.387246
H -5.035747 -0.126325 3.407222
H -5.093444 1.576774 2.889486

Ts3'-2d'$_m$

Zero-point correction= 0.366131 (Hartree/Particle)
Thermal correction to Energy= 0.394617
Thermal correction to Enthalpy= 0.395561
Thermal correction to Gibbs Free Energy= 0.304103
Sum of electronic and zero-point Energies= -2076.370413
Sum of electronic and thermal Energies= -2076.341927

Sum of electronic and thermal Enthalpies= -2076.340983
Sum of electronic and thermal Free Energies= -2076.432441
HF (M06/6-311++g(d,p) and SDD, SMD(cyclohexane): -2076.60132888

C -0.529589 0.878695 -0.63619
H -0.077208 1.043617 0.672105
C -1.249934 -0.452048 -0.62028
H -1.046697 -0.926637 -1.590512
C -1.48285 1.928086 -1.213832
C -2.746838 -0.090312 -0.497761
C -2.8589 1.205406 -1.34168
H -3.062214 0.917299 -2.376016
H -3.691258 1.835467 -1.016723
C -1.559408 3.253716 -0.488836
H -2.522183 3.750884 -0.595386
C 0.801584 1.030513 -0.245359
C 1.522729 2.400792 -0.322688
C 1.644448 2.843872 -1.800216
H 2.308197 3.714243 -1.858505
H 2.078243 2.042492 -2.406108
H 0.688548 3.138952 -2.239851
C 2.954803 2.277109 0.246838
H 3.552925 1.57644 -0.343759
H 3.447922 3.256161 0.20949
H 2.947041 1.930945 1.284165
Pt 1.886211 -0.704622 0.14496
Cl 2.076695 -0.947921 -2.236958
Cl 1.516908 -0.366881 2.487133
C 2.925232 -2.304927 0.456908
O 3.539044 -3.251664 0.636062
H -1.103738 2.112782 -2.230826
C -0.613988 3.879325 0.216961
H -0.900797 4.833985 0.658263
C 0.802206 3.475306 0.535858
H 0.845488 3.162774 1.591099
H 1.417917 4.384416 0.487683
H -0.883109 -1.126263 0.154741
C -3.649174 -1.208232 -1.018924
O -4.377438 -1.127944 -1.982108
O -3.486303 -2.319746 -0.278936
C -4.273516 -3.457237 -0.679509
H -4.007094 -4.253406 0.015202
H -5.338665 -3.222488 -0.610524
H -4.033439 -3.743199 -1.706459
C -3.060992 0.249767 0.961734
O -2.23098 0.644099 1.754926
O -4.369148 0.139315 1.233257
C -4.763499 0.499914 2.572919
H -5.841075 0.342248 2.608712
H -4.252838 -0.13519 3.300378
H -4.516974 1.545708 2.771675

2d'-[Pt]$_m$
Zero-point correction= 0.370907 (Hartree/Particle)
Thermal correction to Energy= 0.399574
Thermal correction to Enthalpy= 0.400519
Thermal correction to Gibbs Free Energy= 0.308656
Sum of electronic and zero-point Energies= -2076.408120
Sum of electronic and thermal Energies= -2076.379452
Sum of electronic and thermal Enthalpies= -2076.378508
Sum of electronic and thermal Free Energies= -2076.470370
HF (M06/6-311++g(d,p) and SDD, SMD(cyclohexane): -2076.64174162

C -0.307463 0.560108 -0.489078
H 1.127805 0.352196 1.002765
C -1.067325 -0.706622 -0.091489
H -0.811570 -1.539738 -0.756240
C -1.183582 1.404935 -1.414624
C -2.548841 -0.331177 -0.337595
C -2.453759 0.534726 -1.614705
H -2.331173 -0.139890 -2.466707
H -3.355515 1.126541 -1.786830
C -1.534740 2.780520 -0.873221
H -2.412769 3.202072 -1.363294
C 0.833143 0.976635 0.162468
C 1.406295 2.395893 0.241069
C 1.870211 3.015818 -1.089566
H 2.212068 4.041365 -0.903619
H 2.706046 2.452178 -1.513814
H 1.081619 3.056855 -1.841690
C 2.611198 2.356409 1.205316
H 3.393767 1.690718 0.824783
H 3.041788 3.357306 1.320799
H 2.319213 1.997218 2.199522
Pt 1.782817 -0.510679 -1.442620
Cl 1.311201 0.581801 -3.520422
Cl 2.324219 -1.826415 0.486771
C 2.955535 -1.613575 -2.423592
O 3.678498 -2.274794 -3.007208
H -0.682512 1.537725 -2.381577
C -0.939740 3.539762 0.053769
H -1.408060 4.504082 0.251284
C 0.291690 3.270654 0.885902
H -0.013644 2.815269 1.840466
H 0.743290 4.236589 1.149885
H -0.858340 -1.011983 0.934065
C -3.404289 -1.582557 -0.551893
O -3.764643 -2.004595 -1.626988
O -3.660004 -2.190608 0.622893
C -4.420177 -3.410300 0.540637
H -4.525488 -3.756720 1.568628
H -5.398996 -3.218584 0.093813
H -3.888530 -4.149497 -0.063753
C -3.084463 0.472110 0.855498
O -2.454231 0.750079 1.851993
O -4.359170 0.849707 0.641123
C -4.960679 1.623233 1.694233
H -5.977807 1.829015 1.360456
H -4.967055 1.055354 2.627963
H -4.406542 2.553471 1.843548

Ts3'-4'$_m$
Zero-point correction= 0.367031 (Hartree/Particle)
Thermal correction to Energy= 0.394994
Thermal correction to Enthalpy= 0.395938
Thermal correction to Gibbs Free Energy= 0.306847
Sum of electronic and zero-point Energies= -2076.366172
Sum of electronic and thermal Energies= -2076.338210
Sum of electronic and thermal Enthalpies= -2076.337266
Sum of electronic and thermal Free Energies= -2076.426357
HF (M06/6-311++g(d,p) and SDD, SMD(cyclohexane): -2076.60109858

C -0.607318 1.333861 0.722889
H -0.75077 2.226078 1.325783
C -1.413693 0.110653 1.190071
H -0.780258 -0.764129 1.341866
C -0.839016 1.502953 -0.766756
C -2.415652 -0.173919 0.034291
C -1.665527 0.30039 -1.238348
H -1.01364 -0.49312 -1.614738
H -2.345548 0.593463 -2.039719
C -0.974834 2.838662 -1.393958
H -1.708289 2.916232 -2.190288
C 0.776074 1.195499 0.121397
C 1.651885 2.481052 0.114823
C 2.6364 2.453281 -1.072579
H 3.298605 3.325662 -1.024132
H 3.254381 1.551866 -1.053594
H 2.114597 2.474729 -2.035344
C 2.448919 2.517666 1.438482
H 3.157675 1.690189 1.506186
H 3.007421 3.460291 1.488189
H 1.791138 2.460047 2.311411
Pt 1.717171 -0.702914 0.05082
Cl 1.572275 -0.723902 -2.350731
Cl 1.803647 -0.698638 2.441968
C 2.602621 -2.412986 0.046197
O 3.129533 -3.425717 0.052425
H 0.380283 1.108005 -1.110186
C -0.219437 3.882694 -1.031385
H -0.358972 4.832465 -1.542745
C 0.825293 3.811176 0.047794
H 0.355486 3.999344 1.023953
H 1.542507 4.629115 -0.083514
H -1.926154 0.301972 2.135958
C -2.791147 -1.655495 -0.059916
O -2.317328 -2.548038 0.602754
O -3.708885 -1.838092 -1.031973
C -4.121852 -3.200636 -1.246589
H -4.85761 -3.158452 -2.049713
H -3.266714 -3.815606 -1.537937
H -4.565231 -3.610902 -0.335837
C -3.678963 0.674944 0.221367
O -3.940556 1.680176 -0.404824
O -4.443747 0.188642 1.214965
C -5.64528 0.928162 1.500089
H -6.122885 0.39899 2.324466
H -5.402167 1.954045 1.788052
H -6.296875 0.946697 0.622866

I4'$_m$
Zero-point correction= 0.369618 (Hartree/Particle)
Thermal correction to Energy= 0.398185
Thermal correction to Enthalpy= 0.399129

Thermal correction to Gibbs Free Energy= 0.307536
Sum of electronic and zero-point Energies= -2076.379787
Sum of electronic and thermal Energies= -2076.351220
Sum of electronic and thermal Enthalpies= -2076.350275
Sum of electronic and thermal Free Energies= -2076.441869
HF (M06/6-311++g(d,p) and SDD, SMD(cyclohexane): -2076.61256910

C -0.591272 1.066138 0.133658
H -0.621821 1.562753 1.110002
C -1.184204 -0.370047 0.240684
H -0.617667 -1.073751 -0.376073
C -1.441613 1.737373 -0.881136
C -2.617361 -0.267039 -0.341573
C -2.423980 0.770294 -1.468627
H -1.954384 0.277760 -2.335261
H -3.341515 1.251068 -1.815812
C -1.350647 3.051021 -1.373513
H -2.055568 3.341620 -2.148813
C 0.894314 1.137131 -0.400724
C 1.635028 2.496618 -0.287671
C 2.362548 2.785931 -1.617424
H 2.921327 3.728812 -1.566608
H 3.068033 1.977901 -1.834016
H 1.662572 2.845131 -2.459353
C 2.670250 2.574535 0.863005
H 3.477395 1.856017 0.694624
H 3.114969 3.577322 0.897752
H 2.222955 2.348669 1.833726
Pt 2.004402 -0.507842 0.472641
Cl 2.801356 -0.968784 -1.737733
Cl 1.140992 -0.009392 2.667929
C 3.041499 -1.968309 1.167272
O 3.669089 -2.834834 1.573027
H 0.860004 0.849381 -1.455786
C -0.394757 3.953392 -0.983141
H -0.374313 4.906323 -1.510415
C 0.633358 3.709121 0.036673
H 0.165866 3.463707 0.998318
H 1.235346 4.609419 0.182645
H -1.157122 -0.746583 1.262558
C -3.154068 -1.601629 -0.855180
O -2.567667 -2.656982 -0.823269
O -4.379980 -1.429842 -1.395830
C -4.996604 -2.622244 -1.917219
H -5.957915 -2.301550 -2.318802
H -4.375688 -3.061203 -2.702136
H -5.136157 -3.355968 -1.119402
C -3.541353 0.335617 0.718642
O -3.744779 1.528042 0.835974
O -4.028568 -0.600574 1.541773
C -4.830071 -0.122092 2.640123
H -5.126520 -1.014290 3.190646
H -4.240934 0.545094 3.273731
H -5.706166 0.412591 2.265188

Ts4'-4d'$_m$
Zero-point correction= 0.368931 (Hartree/Particle)
Thermal correction to Energy= 0.397195
Thermal correction to Enthalpy= 0.398140
Thermal correction to Gibbs Free Energy= 0.306815
Sum of electronic and zero-point Energies= -2076.370474
Sum of electronic and thermal Energies= -2076.342209
Sum of electronic and thermal Enthalpies= -2076.341265
Sum of electronic and thermal Free Energies= -2076.432590
HF (M06/6-311++g(d,p) and SDD, SMD(cyclohexane): -2076.60625093

C -0.596481 1.204228 0.698072
H -0.409848 1.829986 1.564559
C -1.333906 -0.120817 0.96584
H -0.707218 -1.003649 0.831903
C -1.127302 1.792282 -0.530375
C -2.491426 -0.159959 -0.074456
C -1.993677 0.746887 -1.232217
H -1.423553 0.156184 -1.957225
H -2.823789 1.216107 -1.762622
C -1.310316 3.212617 -0.823668
H -2.220913 3.462013 -1.362067
C 0.573865 1.304239 -0.318924
C 1.539069 2.521925 -0.372573
C 1.942506 2.730622 -1.849652
H 2.649627 3.564002 -1.936915
H 2.427916 1.833098 -2.24719
H 1.074789 2.955148 -2.478443
C 2.824774 2.31968 0.46031
H 3.421792 1.482909 0.081092
H 3.446064 3.221774 0.394998
H 2.606364 2.123074 1.512999
Pt 1.794288 -0.720552 0.146645
Cl 1.859104 -1.13498 -2.21448
Cl 1.703739 -0.321928 2.502657
C 2.768634 -2.272043 0.458882
O 3.372069 -3.223785 0.650589
H 0.531776 0.726818 -1.243397
C -0.428432 4.163632 -0.483283
H -0.638948 5.20036 -0.734442
C 0.872321 3.827877 0.175427
H 0.73961 3.729073 1.263151
H 1.583791 4.650625 0.041658
H -1.701916 -0.156071 1.993707
C -2.789401 -1.584837 -0.54888
O -2.170116 -2.576904 -0.241987
O -3.831786 -1.579713 -1.404972
C -4.193442 -2.863048 -1.948378
H -5.039896 -2.671457 -2.607891
H -3.356326 -3.289088 -2.506995
H -4.475314 -3.549385 -1.14593
C -3.758646 0.456368 0.534257
O -4.201103 1.55254 0.266967
O -4.297706 -0.369048 1.450147
C -5.478094 0.11806 2.114268
H -5.769454 -0.672845 2.805189
H -5.257044 1.041585 2.655404
H -6.271435 0.309218 1.387314

4d'-[Pt]$_m$
Zero-point correction= 0.371410 (Hartree/Particle)
Thermal correction to Energy= 0.399467
Thermal correction to Enthalpy= 0.400411
Thermal correction to Gibbs Free Energy= 0.309690
Sum of electronic and zero-point Energies= -2076.415134
Sum of electronic and thermal Energies= -2076.387077
Sum of electronic and thermal Enthalpies= -2076.386133
Sum of electronic and thermal Free Energies= -2076.476854
HF (M06/6-311++g(d,p) and SDD, SMD(cyclohexane): -2076.64283488

C -0.139745 1.948460 0.722086
H 0.423615 2.658439 1.321606
C -0.749312 0.759214 1.445143
H -0.037323 -0.054120 1.606648
C -1.139481 2.462042 -0.315503
C -1.981396 0.312990 0.594126
C -2.384081 1.587499 -0.228602
H -2.818328 1.324438 -1.195251
H -3.151080 2.134349 0.334820
C -1.296825 3.912537 -0.584117
H -2.298620 4.331134 -0.497479
C 0.170600 1.813615 -0.741880
C 1.217481 2.671846 -1.460501
C 0.929911 2.599616 -2.975828
H 1.687736 3.154734 -3.542143
H 0.945140 1.561452 -3.330184
H -0.051190 3.024882 -3.212327
C 2.624806 2.116150 -1.174937
H 2.718177 1.079113 -1.519408
H 3.391940 2.709403 -1.688452
H 2.846261 2.130470 -0.101706
Pt -0.622285 -2.945807 1.926075
Cl 1.613154 -2.213454 1.552801
Cl -2.859629 -3.724842 2.169288
C -0.113626 -3.841463 3.442596
O 0.199236 -4.387955 4.396723
H 0.111892 0.808832 -1.160320
C -0.259355 4.695676 -0.904758
H -0.412267 5.759927 -1.070658
C 1.146314 4.155636 -0.999969
H 1.641545 4.253776 -0.021496
H 1.743558 4.767377 -1.688342
H -1.128341 1.065776 2.424292
C -1.676447 -0.907423 -0.268604
O -1.200190 -1.979018 0.136943
O -1.964883 -0.787269 -1.548045
C -1.744619 -1.944212 -2.392523
H -2.059229 -1.627720 -3.385720
H -0.687671 -2.216796 -2.381989
H -2.347048 -2.781109 -2.034677
C -3.182440 -0.065782 1.492473
O -3.301746 0.243508 2.653363
O -4.114609 -0.707224 0.769291
C -5.306504 -1.095457 1.486598
H -5.941778 -1.580043 0.745681
H -5.043330 -1.790844 2.285137
H -5.797376 -0.212532 1.902802

Ts3'-5d'$_m$

Zero-point correction= 0.368275 (Hartree/Particle)
Thermal correction to Energy= 0.396420
Thermal correction to Enthalpy= 0.397364
Thermal correction to Gibbs Free Energy= 0.307890
Sum of electronic and zero-point Energies= -2076.357114
Sum of electronic and thermal Energies= -2076.328970
Sum of electronic and thermal Enthalpies= -2076.328026
Sum of electronic and thermal Free Energies= -2076.417499
HF (M06/6-311++g(d,p) and SDD, SMD(cyclohexane): -2076.59077221

C -0.570084 1.012407 0.969688
H -0.991736 1.912715 1.425185
C -1.3491 -0.234967 1.20722
H -0.696464 -1.106997 1.228546
C -0.650465 1.067774 -1.223703
C -2.343699 -0.424127 0.021513
C -1.530639 -0.185185 -1.269015
H -0.881747 -1.047849 -1.445088
H -2.212729 -0.09751 -2.120386
C -1.349208 2.383621 -1.434542
H -2.197947 2.344614 -2.112774
C 0.52393 1.137201 0.101386
C 1.210578 2.544932 0.039924
C 2.073763 2.691544 -1.231191
H 2.623796 3.638969 -1.187363
H 2.798879 1.878721 -1.31658
H 1.472839 2.702775 -2.145907
C 2.128676 2.717421 1.269026
H 2.953039 2.00037 1.261477
H 2.551442 3.729703 1.263629
H 1.583325 2.577798 2.208499
Pt 1.833099 -0.554754 0.051995
Cl 1.860345 -0.709526 -2.342458
Cl 1.777703 -0.490497 2.454138
C 3.068776 -2.034684 0.127808
O 3.801956 -2.908666 0.183284
H 0.130777 0.922751 -1.983264
C -0.975948 3.547055 -0.897106
H -1.540523 4.444495 -1.144298
C 0.172 3.702377 0.061594
H -0.218758 3.853241 1.082121
H 0.706952 4.634915 -0.162282
H -1.89082 -0.175754 2.153095
C -2.860177 -1.880178 0.053811
O -2.426094 -2.754361 0.766436
O -3.838229 -2.052234 -0.851329
C -4.363674 -3.391193 -0.952457
H -5.134902 -3.340907 -1.720521
H -3.572295 -4.086696 -1.241915
H -4.786947 -3.705342 0.004707
C -3.574733 0.498776 0.090354
O -4.063762 1.081912 -0.84996
O -4.074934 0.541051 1.341053
C -5.277764 1.31744 1.502807
H -5.537397 1.233651 2.557895
H -5.096957 2.359768 1.228988
H -6.075203 0.914845 0.873536

5d'-[Pt]$_m$

Zero-point correction= 0.371388 (Hartree/Particle)
Thermal correction to Energy= 0.399891
Thermal correction to Enthalpy= 0.400835
Thermal correction to Gibbs Free Energy= 0.309224
Sum of electronic and zero-point Energies= -2076.412207
Sum of electronic and thermal Energies= -2076.383704
Sum of electronic and thermal Enthalpies= -2076.382760
Sum of electronic and thermal Free Energies= -2076.474371
HF (M06/6-311++g(d,p) and SDD, SMD(cyclohexane): -2076.64521934

C -0.092096 0.475950 0.967944
H 0.222421 0.848360 1.937006
C -1.126120 -0.643006 1.019656
H -0.667843 -1.630196 0.906241
C -0.589591 1.027158 -1.437643
C -2.209046 -0.514262 -0.069946
C -1.531320 -0.209444 -1.426633
H -0.937520 -1.090056 -1.690497
H -2.297535 -0.080996 -2.195491
C -1.264314 2.284171 -1.964714
H -1.936920 2.129805 -2.804691
C 0.101543 1.307253 -0.119389
C 0.869770 2.631316 -0.034972
C 1.958455 2.697325 -1.136202
H 2.493118 3.650228 -1.053480
H 2.683995 1.886005 -1.022161
H 1.533128 2.638757 -2.141135
C 1.532582 2.893751 1.326766
H 2.292804 2.146119 1.570680
H 2.022179 3.873622 1.300029
H 0.805960 2.914853 2.146355
Pt 1.970269 -0.655816 0.644116
Cl 1.912163 -1.095796 -1.708881
Cl 2.200234 -0.387317 3.015644
C 3.503401 -1.720914 0.709188
O 4.439033 -2.372992 0.759592
H 0.204384 0.766989 -2.155504
C -1.070159 3.504032 -1.467225
H -1.593525 4.354111 -1.900298
C -0.175476 3.764394 -0.289712
H -0.785680 3.910399 0.615284
H 0.381427 4.701170 -0.426616
H -1.582414 -0.643443 2.012877
C -2.933379 -1.869660 -0.203709
O -2.498202 -2.932356 0.177475
O -4.105415 -1.728594 -0.852158
C -4.844104 -2.944111 -1.074081
H -5.748072 -2.641639 -1.602597
H -4.257262 -3.640615 -1.678037
H -5.092175 -3.417688 -0.120874
C -3.268276 0.544509 0.276939
O -3.665579 1.414720 -0.463493
O -3.736787 0.362233 1.530823
C -4.784836 1.259178 1.935591
H -5.040395 0.968465 2.954693
H -4.435257 2.294448 1.905778
H -5.649629 1.155997 1.275038

1b-[Au-P(C_6F_5)]$^+$

I3$_{Au7}$

Zero-point correction= 0.618350 (Hartree/Particle)
Thermal correction to Energy= 0.676232
Thermal correction to Enthalpy= 0.677176
Thermal correction to Gibbs Free Energy= 0.520884
Sum of electronic and zero-point Energies= -3729.244854
Sum of electronic and thermal Energies= -3729.186972
Sum of electronic and thermal Enthalpies= -3729.186028
Sum of electronic and thermal Free Energies= -3729.342319
HF (M06/6-311++g(d,p) and SDD, SMD(dichloromethane): -3729.43395718

C -3.317186 2.127858 -0.465334
H -4.257677 2.491476 -0.042665
C -3.598260 0.760734 -1.135112
H -2.646088 0.338048 -1.488748
C -2.974764 3.073142 -1.738511
C -4.474447 1.155142 -2.338544
C -3.873155 2.471546 -2.868380
H -5.497570 1.307206 -1.977404
H -4.509089 0.367837 -3.097005
H -3.261764 2.308527 -3.761121
H -4.658341 3.182432 -3.143387
C -3.197737 4.522176 -1.428424
H -3.912614 5.046834 -2.059764
C -2.187798 2.270505 0.440735
C -2.195525 3.344798 1.463972
C -1.162624 3.118840 2.588222
H -1.186395 3.959382 3.289840
H -1.397021 2.207717 3.149116
H -0.143744 3.030194 2.198818
C -3.571587 3.666542 2.090562
H -3.975931 2.785601 2.600552
H -3.452802 4.458205 2.837042
H -4.302884 4.010726 1.357319
H -1.921956 2.898460 -1.987838
C -2.643185 5.186687 -0.402613
H -2.935600 6.223056 -0.249648
C -1.679019 4.618363 0.597582
H -1.452764 5.366746 1.364129
H -0.723716 4.345516 0.134212
O -4.210227 -0.094085 -0.208088
Si -4.469865 -1.770417 -0.319514
C -2.883318 -2.607206 -0.928152
H -2.579868 -2.233781 -1.914031
H -2.049124 -2.456161 -0.234669
H -3.042163 -3.687532 -1.029809
C -5.860835 -2.127537 -1.545004
H -6.135436 -3.189253 -1.526801
H -6.762561 -1.549725 -1.314312
H -5.567311 -1.890530 -2.574550
C -4.937537 -2.285615 1.458939
C -3.856496 -1.826496 2.461464
H -3.731535 -0.737218 2.446506
H -4.142627 -2.114184 3.482921
H -2.878716 -2.279562 2.259761
C -6.285277 -1.637149 1.846881
H -6.238480 -0.542664 1.800636

H -7.102411 -1.967325 1.194937
H -6.557596 -1.913777 2.875074
C -5.074746 -3.823516 1.532493
H -5.366503 -4.129617 2.546527
H -5.842618 -4.204985 0.848335
H -4.132074 -4.333186 1.298416
Au -0.511606 1.130556 0.143159
P 1.521926 -0.180193 -0.116201
C 1.506023 -1.443435 -1.437569
C 2.941654 0.947018 -0.382259
C 1.859607 -1.130525 1.419367
C 2.466423 -2.464178 -1.502604
C 0.475699 -1.486896 -2.385178
C 3.116775 1.975875 0.553005
C 3.825181 0.925373 -1.467571
C 0.769268 -1.739014 2.056110
C 3.110953 -1.283429 2.030678
C 2.394237 -3.493009 -2.433716
F 3.503754 -2.455255 -0.657553
C 0.373482 -2.510857 -3.321466
F -0.462808 -0.527062 -2.431157
C 4.110900 2.937159 0.436175
F 2.297765 2.035116 1.621128
C 4.831075 1.880473 -1.611480
F 3.731797 -0.005850 -2.423904
C 0.892925 -2.451591 3.241812
F -0.457805 -1.649638 1.506584
C 3.262901 -1.986520 3.224030
F 4.212146 -0.759246 1.484473
C 1.335293 -3.518941 -3.344487
F 3.322678 -4.443901 -2.464363
F -0.641381 -2.526492 -4.184086
C 4.976310 2.886462 -0.658223
F 4.238777 3.895249 1.351024
F 5.649450 1.831848 -2.658638
C 2.152092 -2.571758 3.831263
F -0.173702 -3.012735 3.806971
F 4.465010 -2.107258 3.779685
F 1.251174 -4.496953 -4.233388
F 5.930988 3.796137 -0.790790
F 2.293164 -3.246968 4.962571

Ts3-3b$_{Au7}$

Zero-point correction= 0.616415 (Hartree/Particle)
Thermal correction to Energy= 0.674347
Thermal correction to Enthalpy= 0.675292
Thermal correction to Gibbs Free Energy= 0.518623
Sum of electronic and zero-point Energies= -3729.232665
Sum of electronic and thermal Energies= -3729.174733
Sum of electronic and thermal Enthalpies= -3729.173789
Sum of electronic and thermal Free Energies= -3729.330457
HF (M06/6-311++g(d,p) and SDD, SMD(dichloromethane): -3729.42478868

C -3.236002 2.255835 -0.581643
H -4.205232 2.635628 -0.240359
C -3.533711 0.881097 -1.213033
H -2.583708 0.40488 -1.49286
C -2.822291 3.108097 -1.79967
C -4.319546 1.26681 -2.495657
C -3.843839 2.694413 -2.891674
H -5.387535 1.262294 -2.255934
H -4.163142 0.536282 -3.29513
H -3.39331 2.726502 -3.887862
H -4.689546 3.390754 -2.903496
C -2.786782 4.554452 -1.407843
H -3.181179 5.2931 -2.10323
C -2.221088 2.268006 0.534659
C -2.617677 2.612691 1.844416
C -1.729461 2.329079 3.029241
H -1.841353 3.082507 3.81565
H -2.052794 1.366488 3.44921
H -0.67689 2.231097 2.751874
C -4.030396 3.023011 2.201433
H -4.655581 2.121152 2.195006
H -4.075453 3.463775 3.200403
H -4.464048 3.724006 1.485038
H -1.816523 2.78973 -2.115036
C -2.371992 4.961317 -0.198991
H -2.459483 6.012081 0.071527
C -1.728338 4.111568 0.845944
H -1.847838 4.573616 1.830587
H -0.664671 3.926683 0.710279
O -4.23438 0.060162 -0.305341
Si -4.510995 -1.608915 -0.436449
C -2.933263 -2.468244 -1.038636
H -2.62325 -2.102584 -2.025356
H -2.096636 -2.32691 -0.345711
H -3.106399 -3.546734 -1.136915
C -5.899106 -1.935988 -1.673301
H -6.170796 -2.998435 -1.692838
H -6.802809 -1.367552 -1.427082
H -5.601599 -1.660142 -2.691911
C -4.998444 -2.150252 1.331559
C -3.909542 -1.740213 2.346477
H -3.760076 -0.65332 2.354509
H -4.202136 -2.044695 3.361415
H -2.941057 -2.207765 2.133567
C -6.331676 -1.480006 1.731087
H -6.262713 -0.385517 1.702988
H -7.15457 -1.779034 1.071638
H -6.612959 -1.768705 2.753699
C -5.172398 -3.685498 1.373417
H -5.475362 -4.00689 2.379541
H -5.945925 -4.033301 0.678001
H -4.241175 -4.211833 1.131058
Au -0.469069 1.159219 0.193161
P 1.535856 -0.140111 -0.109294
C 1.510802 -1.366104 -1.467805
C 2.974155 0.973567 -0.340208
C 1.870374 -1.146719 1.394071
C 2.451847 -2.403014 -1.555324
C 0.48765 -1.363211 -2.424183
C 3.149707 1.985718 0.612902
C 3.872717 0.958361 -1.413211
C 0.780698 -1.777037 2.011281
C 3.122051 -1.324318 1.998259
C 2.366953 -3.404068 -2.515136
F 3.484373 -2.438421 -0.704647
C 0.372578 -2.359157 -3.389109
F -0.429977 -0.383891 -2.452173
C 4.157183 2.93614 0.524525
F 2.317261 2.042099 1.671055
C 4.891797 1.903306 -1.529148
F 3.782984 0.042859 -2.385005
C 0.906619 -2.529019 3.172612
F -0.448212 -1.672658 1.469709
C 3.275855 -2.067451 3.16691
F 4.225118 -0.786842 1.468432
C 1.314632 -3.384672 -3.433511
F 3.277779 -4.371578 -2.565928
F -0.635983 -2.33118 -4.25911
C 5.036642 2.89239 -0.558556
F 4.283838 3.87853 1.456572
F 5.723705 1.860827 -2.566189
C 2.165767 -2.671145 3.756247
F -0.160478 -3.107254 3.721142
F 4.479419 -2.208823 3.715302
F 1.218578 -4.336294 -4.349974
F 6.00421 3.792515 -0.663866
F 2.307216 -3.38419 4.864678

3b-$_{[Au7]}$

Zero-point correction= 0.619654 (Hartree/Particle)
Thermal correction to Energy= 0.677265
Thermal correction to Enthalpy= 0.678209
Thermal correction to Gibbs Free Energy= 0.524506
Sum of electronic and zero-point Energies= -3729.275357
Sum of electronic and thermal Energies= -3729.217746
Sum of electronic and thermal Enthalpies= -3729.216802
Sum of electronic and thermal Free Energies= -3729.370505
HF (M06/6-311++g(d,p) and SDD, SMD(dichloromethane): -3729.47131434

C -3.443522 2.421909 -0.055234
H -4.236607 2.509072 0.700920
C -3.738990 1.099949 -0.823462
H -2.885131 0.881054 -1.481185
C -3.759481 3.481295 -1.149137
C -4.993293 1.469975 -1.683746
C -5.116223 3.015387 -1.682247
H -5.876356 1.002143 -1.243295
H -4.890565 1.076294 -2.699410
H -5.339745 3.425289 -2.671583
H -5.916710 3.341334 -1.007473
C -3.590313 4.876967 -0.620530
H -4.369320 5.623179 -0.756213
C -2.124812 2.749492 0.670100
C -1.867623 2.299385 1.975444
C -0.898270 2.985412 2.925183
H -1.455086 3.742696 3.495775
H -0.500453 2.268215 3.648786
H -0.054750 3.481021 2.444738
C -2.814494 1.356209 2.682192
H -3.402314 0.750455 1.994902
H -2.273996 0.698183 3.369999
H -3.497867 1.961912 3.297491
H -3.020243 3.336814 -1.957651
C -2.444002 5.135302 0.015830
H -2.204513 6.104356 0.444238
C -1.428781 4.008738 0.118317
H -0.572268 4.300884 0.724697
H -1.041137 3.792031 -0.888693
O -3.955003 -0.003090 0.042640
Si -4.280161 -1.621623 -0.381482

C -2.760559 -2.339699 -1.254090
H -2.572961 -1.825858 -2.204392
H -1.861292 -2.261156 -0.634138
H -2.916197 -3.400249 -1.486414
C -5.748360 -1.769311 -1.562992
H -5.935199 -2.827509 -1.782654
H -6.671530 -1.354180 -1.143990
H -5.563285 -1.271805 -2.520967
C -4.663209 -2.510587 1.268789
C -3.419961 -2.583394 2.180385
H -3.024777 -1.590101 2.420327
H -3.678072 -3.072289 3.130351
H -2.609439 -3.164688 1.727412
C -5.795886 -1.770852 2.015326
H -5.512006 -0.746090 2.279563
H -6.714990 -1.719125 1.419354
H -6.043380 -2.298589 2.946908
C -5.129585 -3.953778 0.962697
H -5.325618 -4.491439 1.900528
H -6.056767 -3.974631 0.379143
H -4.372875 -4.528864 0.414122
Au -0.457726 1.085834 0.506639
P 1.485878 -0.145218 -0.138559
C 1.348218 -1.112462 -1.678631
C 2.874200 1.036936 -0.298446
C 1.941461 -1.358776 1.157160
C 2.262998 -2.125176 -2.006622
C 0.279411 -0.915541 -2.561460
C 3.126547 1.878698 0.793769
C 3.673040 1.221250 -1.434019
C 0.908775 -2.097531 1.750619
C 3.240453 -1.600783 1.624409
C 2.105974 -2.928006 -3.129704
F 3.339149 -2.326426 -1.237576
C 0.094744 -1.710046 -3.687870
F -0.615734 0.062772 -2.349893
C 4.111921 2.855731 0.777909
F 2.393085 1.735246 1.914019
C 4.667825 2.197414 -1.477680
F 3.506686 0.475088 -2.532032
C 1.133075 -3.020594 2.764075
F -0.357633 -1.925350 1.329612
C 3.492778 -2.515516 2.644186
F 4.289881 -0.962205 1.098938
C 1.009550 -2.722739 -3.970945
F 2.990949 -3.879170 -3.409348
F -0.955514 -1.508624 -4.481071
C 4.890023 3.014336 -0.370551
F 4.313023 3.632031 1.839359
F 5.403387 2.348175 -2.574682
C 2.437415 -3.226900 3.215500
F 0.119482 -3.699436 3.295242
F 4.736769 -2.718361 3.066716
F 0.845821 -3.484579 -5.040892
F 5.834788 3.941938 -0.407475
F 2.674047 -4.102176 4.180775

Ts3-3'$_{Au7}$

Zero-point correction= 0.618097 (Hartree/Particle)
Thermal correction to Energy= 0.675296
Thermal correction to Enthalpy= 0.676240
Thermal correction to Gibbs Free Energy= 0.521034
Sum of electronic and zero-point Energies= -3729.236727
Sum of electronic and thermal Energies= -3729.179527
Sum of electronic and thermal Enthalpies= -3729.178583
Sum of electronic and thermal Free Energies= -3729.333790
HF (M06/6-311++g(d,p) and SDD, SMD(dichloromethane): -3729.42609518

C -3.26397 2.163839 -0.558069
H -4.195098 2.603827 -0.184987
C -3.591364 0.784743 -1.193108
H -2.646354 0.325911 -1.517832
C -2.840649 3.01037 -1.824498
C -4.433454 1.181097 -2.427601
C -3.883068 2.546701 -2.89627
H -5.479026 1.263722 -2.114216
H -4.386128 0.41322 -3.205521
H -3.398296 2.493193 -3.875817
H -4.684968 3.287587 -2.970607
C -2.825948 4.485422 -1.572066
H -2.935778 5.094534 -2.468737
C -2.167566 2.267254 0.391528
C -2.303476 3.22054 1.531888
C -1.077782 3.214509 2.469379
H -1.222148 3.934736 3.282087
H -0.931184 2.227385 2.921589
H -0.16191 3.486025 1.934084
C -3.54603 2.752387 2.366695
H -3.466399 1.698234 2.650067
H -3.572015 3.347737 3.284966
H -4.487881 2.897762 1.834462
H -1.844579 2.671953 -2.140845
C -2.729967 5.138114 -0.406981
H -2.782427 6.225104 -0.471129
C -2.533843 4.711853 1.03135
H -3.369866 5.121966 1.613435
H -1.652297 5.2689 1.372922
O -4.245827 -0.036074 -0.265704
Si -4.498914 -1.715858 -0.363837
C -2.902417 -2.552207 -0.94833
H -2.598901 -2.204604 -1.943594
H -2.070607 -2.376735 -0.257366
H -3.052163 -3.636287 -1.020535
C -5.876706 -2.082434 -1.600201
H -6.132379 -3.14895 -1.599283
H -6.789582 -1.523622 -1.366436
H -5.581718 -1.823785 -2.624104
C -4.978673 -2.225351 1.412702
C -3.884611 -1.797889 2.414802
H -3.730734 -0.712057 2.400771
H -4.176178 -2.078466 3.436608
H -2.918845 -2.275154 2.210719
C -6.309833 -1.546224 1.805265
H -6.237083 -0.453002 1.764391
H -7.134955 -1.853009 1.151925
H -6.588562 -1.821943 2.831972
C -5.153143 -3.759848 1.48053
H -5.447162 -4.062978 2.494779
H -5.933605 -4.118781 0.79866
H -4.2246 -4.29172 1.239401
Au -0.492261 1.139057 0.125059
P 1.54737 -0.170728 -0.113276
C 1.520362 -1.4539 -1.414756
C 2.969027 0.947911 -0.398784
C 1.877534 -1.095772 1.438752
C 2.455258 -2.499522 -1.451683
C 0.50034 -1.487159 -2.374143
C 3.12267 2.016506 0.49534
C 3.879231 0.877964 -1.460019
C 0.785804 -1.696296 2.08098
C 3.126681 -1.234897 2.05765
C 2.36702 -3.541757 -2.366517
F 3.483188 -2.50366 -0.595468
C 0.382291 -2.52389 -3.294215
F -0.411496 -0.503469 -2.448049
C 4.119917 2.972258 0.35955
F 2.279855 2.121841 1.540404
C 4.887847 1.826845 -1.622385
F 3.810877 -0.097376 -2.37338
C 0.906711 -2.387551 3.279552
F -0.439812 -1.62019 1.525262
C 3.275605 -1.916307 3.263889
F 4.228582 -0.718411 1.50565
C 1.318126 -3.556415 -3.289017
F 3.271154 -4.516244 -2.370482
F -0.62278 -2.528317 -4.168422
C 5.010541 2.873982 -0.711033
F 4.227846 3.96884 1.23474
F 5.731527 1.73254 -2.646083
C 2.163703 -2.493858 3.876398
F -0.160602 -2.941765 3.850312
F 4.475599 -2.024279 3.826465
F 1.218924 -4.546985 -4.162292
F 5.968562 3.777231 -0.861135
F 2.301453 -3.148732 5.019987

I3'$_{Au7}$

Zero-point correction= 0.618489 (Hartree/Particle)
Thermal correction to Energy= 0.676305
Thermal correction to Enthalpy= 0.677249
Thermal correction to Gibbs Free Energy= 0.521316
Sum of electronic and zero-point Energies= -3729.246103
Sum of electronic and thermal Energies= -3729.188288
Sum of electronic and thermal Enthalpies= -3729.187344
Sum of electronic and thermal Free Energies= -3729.343277
HF (M06/6-311++g(d,p) and SDD, SMD(dichloromethane): -3729.43592299

C -3.348148 2.088835 -0.486620
H -4.264323 2.440004 0.002392
C -3.638450 0.721323 -1.133175
H -2.701635 0.322987 -1.551020
C -3.113897 3.038354 -1.741959
C -4.605992 1.090149 -2.280971
C -4.199118 2.508154 -2.745842
H -5.625155 1.087637 -1.881448
H -4.572491 0.355867 -3.090676
H -3.788207 2.518392 -3.759746
H -5.058091 3.185547 -2.735330
C -3.205984 4.510847 -1.458271
H -3.210805 5.134182 -2.352266
C -2.163686 2.300155 0.330937
C -2.195083 3.393663 1.341445

C -0.830614 4.093016 1.526289
H -0.887716 4.792875 2.366629
H -0.030061 3.377035 1.734229
H -0.564296 4.660226 0.628668
C -2.541277 2.588872 2.650223
H -1.737593 1.902408 2.929226
H -2.661803 3.328349 3.450212
H -3.474375 2.024745 2.558333
H -2.124682 2.809730 -2.163963
C -3.295520 5.115794 -0.267120
H -3.384753 6.200043 -0.267105
C -3.303394 4.462825 1.101138
H -4.292680 4.036534 1.314434
H -3.161547 5.237668 1.861875
O -4.161485 -0.154124 -0.167311
Si -4.429510 -1.828050 -0.301692
C -2.853377 -2.662657 -0.938616
H -2.545461 -2.257300 -1.910418
H -2.016952 -2.545030 -0.241798
H -3.024801 -3.736631 -1.079007
C -5.832090 -2.168636 -1.519756
H -6.106692 -3.230472 -1.508243
H -6.732282 -1.593325 -1.277016
H -5.546944 -1.923749 -2.549609
C -4.888733 -2.370028 1.471372
C -3.807500 -1.925876 2.480043
H -3.685607 -0.836259 2.484788
H -4.091367 -2.233032 3.496484
H -2.828684 -2.371853 2.268987
C -6.237200 -1.731230 1.872854
H -6.193420 -0.635969 1.843076
H -7.055298 -2.053312 1.218160
H -6.506045 -2.024007 2.897451
C -5.022587 -3.909311 1.520496
H -5.311754 -4.232291 2.530026
H -5.790796 -4.281728 0.831759
H -4.079114 -4.412867 1.276711
Au -0.503201 1.142199 0.084850
P 1.539258 -0.158577 -0.123782
C 1.570906 -1.404364 -1.460190
C 2.951879 0.988221 -0.333409
C 1.848763 -1.127232 1.406519
C 2.577401 -2.378555 -1.539740
C 0.539704 -1.483852 -2.404651
C 3.111537 1.978588 0.645020
C 3.839983 1.020597 -1.414467
C 0.746902 -1.744737 2.013897
C 3.088763 -1.289538 2.038662
C 2.552961 -3.395660 -2.485694
F 3.612194 -2.332435 -0.692621
C 0.485220 -2.497759 -3.356150
F -0.446954 -0.572978 -2.432121
C 4.098886 2.951271 0.576015
F 2.281875 1.987199 1.706884
C 4.839589 1.988178 -1.510639
F 3.755157 0.132702 -2.412225
C 0.848711 -2.477759 3.189072
F -0.469896 -1.643934 1.444355
C 3.218533 -2.013462 3.222338
F 4.199297 -0.753146 1.524835
C 1.494727 -3.457638 -3.395772
F 3.524774 -4.301425 -2.531148
F -0.528518 -2.549413 -4.218235
C 4.971627 2.953044 -0.513828
F 4.213773 3.870166 1.531465
F 5.663677 1.991727 -2.554427
C 2.096924 -2.608854 3.799109
F -0.228405 -3.047754 3.725199
F 4.409901 -2.142940 3.798562
F 1.455813 -4.424769 -4.299421
F 5.920302 3.874328 -0.601148
F 2.217265 -3.303348 4.921007

1b-[Au-IPr']$^+$

I3$_{Au1}$

Zero-point correction= 0.595138 (Hartree/Particle)
Thermal correction to Energy= 0.630431
Thermal correction to Enthalpy= 0.631376
Thermal correction to Gibbs Free Energy= 0.523147
Sum of electronic and zero-point Energies= -1509.445022
Sum of electronic and thermal Energies= -1509.409729
Sum of electronic and thermal Enthalpies= -1509.408784
Sum of electronic and thermal Free Energies= -1509.517013
HF (M06/6-311++g(d,p) and SDD, SMD(dichloromethane): -1509.87105848

C 0.926685 2.013582 0.340345
H 1.697331 2.615571 -0.149793
C 1.634992 0.885893 1.125297
H 0.863291 0.232085 1.562798
C 0.314345 2.910015 1.528500
C 2.361668 1.655712 2.245173
C 1.410752 2.807270 2.636935
H 3.300534 2.043260 1.835307
H 2.618129 1.008004 3.089028
H 0.931195 2.635697 3.605641
H 1.954145 3.754085 2.714321
C -0.026364 4.304043 1.090651
H 0.423080 5.110729 1.667225
C -0.183839 1.665963 -0.543595
C -0.521204 2.586317 -1.661644
C -1.391653 1.920147 -2.748317
H -1.653097 2.652873 -3.519123
H -0.844913 1.104564 -3.234198
H -2.321894 1.515747 -2.335497
C 0.665566 3.311154 -2.335794
H 1.364369 2.586982 -2.768502
H 0.290442 3.938370 -3.150901
H 1.214684 3.957133 -1.648715
H -0.590523 2.394000 1.872507
C -0.781148 4.626329 0.029659
H -0.903965 5.681970 -0.202391
C -1.461593 3.666705 -0.905414
H -1.924348 4.220633 -1.729156
H -2.269430 3.120608 -0.404044
O 2.470183 0.161214 0.263361
Si 3.182363 -1.358796 0.518226
C 1.932254 -2.475786 1.398896
H 1.713272 -2.117942 2.412757
H 0.984577 -2.539190 0.850616
H 2.327451 -3.493709 1.499670
C 4.727127 -1.180293 1.586743
H 5.229039 -2.147192 1.713113
H 5.450206 -0.487308 1.142338
H 4.485141 -0.809088 2.589761
C 3.594866 -1.977397 -1.239248
C 2.297223 -2.152152 -2.058188
H 1.736891 -1.211905 -2.134403
H 2.532659 -2.482101 -3.079795
H 1.633536 -2.906682 -1.616847
C 4.504931 -0.952245 -1.952393
H 4.025919 0.030382 -2.030525
H 5.460195 -0.819157 -1.430633
H 4.736686 -1.293723 -2.971046
C 4.328105 -3.335511 -1.159702
H 4.564926 -3.698093 -2.169499
H 5.275832 -3.260417 -0.613423
H 3.719937 -4.108678 -0.673391
Au -1.363481 0.044360 -0.113649
C -2.542516 -1.626042 0.291762
N -3.081107 -2.491074 -0.607276
N -2.941396 -2.090228 1.505129
C -3.804578 -3.481043 0.034731
C -2.929341 -2.418224 -2.060489
C -3.718167 -3.227342 1.366240
C -2.625461 -1.483158 2.797133
H -4.308812 -4.268818 -0.503615
H -2.326749 -1.544719 -2.307714
H -2.429175 -3.317970 -2.428595
H -3.911650 -2.327171 -2.531599
H -4.135931 -3.748318 2.214002
H -2.126834 -2.214578 3.438508
H -1.961820 -0.634969 2.631461
H -3.542219 -1.136479 3.281899

Ts3-3b$_{Au1}$

Zero-point correction= 0.593899 (Hartree/Particle)
Thermal correction to Energy= 0.628974
Thermal correction to Enthalpy= 0.629918
Thermal correction to Gibbs Free Energy= 0.523139
Sum of electronic and zero-point Energies= -1509.430760
Sum of electronic and thermal Energies= -1509.395685
Sum of electronic and thermal Enthalpies= -1509.394741
Sum of electronic and thermal Free Energies= -1509.501519
HF (M06/6-311++g(d,p) and SDD, SMD(dichloromethane): -1509.85808232

C -0.812219 2.011494 -0.407999
H -1.643415 2.634781 -0.059787
C -1.463109 0.896253 -1.248741
H -0.68699 0.172664 -1.541677
C -0.057316 2.836081 -1.465691
C -1.963757 1.665279 -2.504754
C -1.083329 2.943834 -2.622256
H -3.015382 1.926171 -2.352453
H -1.911251 1.040339 -3.401807
H -0.587998 3.028849 -3.593979
H -1.696165 3.843493 -2.497392
C 0.431205 4.115327 -0.857171
H 0.41758 5.018878 -1.464161
C 0.059883 1.551309 0.736574
C -0.367334 1.796974 2.060364
C 0.286434 1.105405 3.230313
H 0.334654 1.750742 4.11384

H -0.347348 0.24641 3.490955
H 1.281604 0.723355 2.990406
C -1.650856 2.524894 2.404946
H -2.492524 1.859373 2.177026
H -1.690637 2.779665 3.467046
H -1.790765 3.435827 1.818981
H 0.80451 2.24595 -1.815052
C 0.814467 4.208608 0.423489
H 1.080533 5.184173 0.827939
C 0.991385 3.09029 1.404762
H 0.826885 3.475352 2.416881
H 1.977677 2.629571 1.401201
O -2.471782 0.24326 -0.506817
Si -3.235925 -1.217478 -0.904894
C -1.942883 -2.433363 -1.563979
H -1.530419 -2.10398 -2.525562
H -1.104654 -2.560265 -0.868451
H -2.38957 -3.420889 -1.730949
C -4.552585 -0.929196 -2.225946
H -5.083365 -1.859416 -2.46154
H -5.29828 -0.193997 -1.90313
H -4.110662 -0.562996 -3.15999
C -4.005988 -1.815194 0.739335
C -2.896176 -2.105733 1.772793
H -2.286715 -1.214806 1.970688
H -3.335822 -2.428423 2.727149
H -2.223946 -2.905698 1.437615
C -4.949646 -0.732021 1.306707
H -4.420834 0.209849 1.49536
H -5.781075 -0.515191 0.625707
H -5.387496 -1.066379 2.257829
C -4.816237 -3.108769 0.496036
H -5.256004 -3.465161 1.437897
H -5.642969 -2.949397 -0.206149
H -4.193152 -3.921695 0.102493
Au 1.493214 0.070705 0.27882
C 2.861919 -1.412667 -0.188277
N 2.892624 -2.686525 0.284829
N 3.930967 -1.325498 -1.022959
C 3.96644 -3.383518 -0.244308
C 1.943029 -3.266878 1.232963
C 4.620811 -2.525943 -1.068238
C 4.33185 -0.136231 -1.772511
H 4.164695 -4.414444 0.005575
H 2.446604 -3.496235 2.176403
H 1.143961 -2.548072 1.413436
H 1.517388 -4.183066 0.815334
H 5.50151 -2.662848 -1.676679
H 4.42368 -0.382053 -2.833669
H 3.568702 0.631041 -1.644202
H 5.289719 0.238175 -1.400383

3b-$_{[Au1]}$
Zero-point correction= 0.596255 (Hartree/Particle)
Thermal corr. to Energy= 0.631370
Thermal corr. to Enthalpy= 0.632314
Thermal correction to Gibbs Free Energy= 0.527587
Sum of electronic and zero-point Energies= -1509.479876
Sum of electronic and thermal Energies= -1509.444761
Sum of electronic and thermal Enthalpies= -1509.443817
Sum of electronic and thermal Free Energies= -1509.548544
HF (M06/6-311++g(d,p) and SDD, SMD(dichloromethane): -1509.91589598

C -2.609468 0.178380 -0.027667
H -3.147685 -0.282266 0.812210
C -1.925176 -0.984356 -0.792517
H -1.317723 -0.548449 -1.601393
C -3.686944 0.594536 -1.067512
C -3.143329 -1.747729 -1.401584
C -4.334566 -0.748147 -1.428178
H -3.364210 -2.610906 -0.767800
H -2.907375 -2.130248 -2.399383
H -4.841447 -0.717893 -2.397098
H -5.086293 -1.019933 -0.678180
C -4.511115 1.746528 -0.567639
H -5.597348 1.716078 -0.603266
C -1.871174 1.400371 0.544527
C -1.284437 1.373048 1.812169
C -1.002583 2.619611 2.635517
H -1.863909 2.801910 3.294073
H -0.135159 2.465304 3.284612
H -0.831658 3.524186 2.051311
C -1.245092 0.102955 2.637615
H -1.260821 -0.800337 2.029803
H -0.359702 0.081774 3.281302
H -2.120385 0.098868 3.305075
H -3.143382 0.944242 -1.963684
C -3.832211 2.794523 -0.089706
H -4.314800 3.687422 0.297498
C -2.312773 2.723512 -0.105757
H -1.869365 3.590022 0.382829
H -1.968053 2.744254 -1.151009
O -1.094509 -1.788904 0.027853
Si -0.108737 -3.068351 -0.510080
C 0.973853 -2.437648 -1.932954
H 0.367654 -2.166075 -2.806126
H 1.560200 -1.558632 -1.639792
H 1.675009 -3.213968 -2.261420
C -1.141990 -4.523452 -1.127554
H -0.491858 -5.364724 -1.396367
H -1.845944 -4.881008 -0.367756
H -1.720060 -4.266971 -2.021779
C 0.938330 -3.575473 1.009238
C 1.837656 -2.408696 1.468796
H 1.246645 -1.531991 1.759015
H 2.437622 -2.710099 2.339682
H 2.535582 -2.100969 0.679459
C 0.017550 -3.996868 2.175862
H -0.632784 -3.177697 2.502491
H -0.623979 -4.843227 1.904131
H 0.618258 -4.310278 3.041217
C 1.839861 -4.772450 0.626587
H 2.452650 -5.073529 1.487508
H 1.256558 -5.649585 0.324461
H 2.528998 -4.528902 -0.191654
Au 0.479781 1.279778 0.236941
C 2.366148 1.297338 -0.560714
N 3.540983 1.148298 0.101473
N 2.706217 1.468380 -1.863436
C 4.607123 1.222374 -0.779750
C 3.700300 0.970622 1.545469
C 4.082129 1.420930 -2.015922
C 1.771281 1.623507 -2.978284
H 5.631488 1.135931 -0.451576
H 4.187768 1.848583 1.977901
H 2.716554 0.841098 1.995064
H 4.303195 0.080687 1.740797
H 4.558757 1.532546 -2.977592
H 1.645849 0.671803 -3.502144
H 0.808543 1.955774 -2.589485
H 2.157630 2.375660 -3.669452

Ts3-3'$_{Au1}$
Zero-point correction= 0.595390 (Hartree/Particle)
Thermal correction to Energy= 0.629786
Thermal correction to Enthalpy= 0.630730
Thermal correction to Gibbs Free Energy= 0.525335
Sum of electronic and zero-point Energies= -1509.436926
Sum of electronic and thermal Energies= -1509.402530
Sum of electronic and thermal Enthalpies= -1509.401586
Sum of electronic and thermal Free Energies= -1509.506981
HF (M06/6-311++g(d,p) and SDD, SMD(dichloromethane): -1509.86335789

C 0.93601 1.897038 0.531622
H 1.705678 2.566482 0.132938
C 1.64702 0.697033 1.207836
H 0.873869 -0.011946 1.543996
C 0.293983 2.640385 1.763994
C 2.329742 1.354039 2.430518
C 1.420304 2.533924 2.84483
H 3.316336 1.709033 2.116429
H 2.486998 0.632811 3.238443
H 0.970724 2.395611 3.833009
H 1.98585 3.470238 2.876235
C -0.131517 4.0413 1.451404
H -0.204118 4.694419 2.320528
C -0.145229 1.633584 -0.413743
C -0.258887 2.548028 -1.592809
C -1.421411 2.164346 -2.532394
H -1.476225 2.863337 -3.374329
H -1.278136 1.158959 -2.944367
H -2.382023 2.193415 -2.00619
C 1.072962 2.416966 -2.407772
H 1.303682 1.371869 -2.637702
H 0.939839 2.949117 -3.355219
H 1.928217 2.851858 -1.887287
H -0.571364 2.054091 2.103216
C -0.398871 4.589751 0.259934
H -0.6545 5.649463 0.276636
C -0.466033 4.061989 -1.156806
H 0.215908 4.66951 -1.766976
H -1.470662 4.33112 -1.507292
O 2.522993 0.078067 0.305256
Si 3.202853 -1.475132 0.424895
C 1.855823 -2.680199 0.993741
H 1.546897 -2.48146 2.027773
H 0.964927 -2.627437 0.35619
H 2.225423 -3.712138 0.964813
C 4.608546 -1.468821 1.683671
H 5.097351 -2.44933 1.731534
H 5.37571 -0.728759 1.430013
H 4.247633 -1.239316 2.693341
C 3.822107 -1.861753 -1.337979

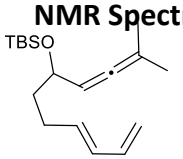
C 2.633422 -1.908452 -2.321952
H 2.090717 -0.955507 -2.345137
H 2.989578 -2.111206 -3.34161
H 1.917113 -2.698562 -2.064394
C 4.813763 -0.768986 -1.796173
H 4.349283 0.22361 -1.805023
H 5.697604 -0.719524 -1.149007
H 5.168748 -0.981226 -2.814373
C 4.538352 -3.231552 -1.349386
H 4.894838 -3.463104 -2.362519
H 5.413142 -3.24607 -0.688597
H 3.873631 -4.050402 -1.046601
Au -1.44968 0.100276 -0.090326
C -2.786762 -1.467476 0.219667
N -3.696579 -1.963318 -0.660351
N -2.939415 -2.221691 1.340425
C -4.403618 -3.011269 -0.099481
C -3.921243 -1.47851 -2.022172
C -3.92662 -3.173957 1.162455
C -2.170905 -2.079529 2.576153
H -5.175039 -3.540952 -0.637121
H -3.24875 -0.643063 -2.212774
H -3.718576 -2.27802 -2.739759
H -4.956044 -1.143007 -2.130457
H -4.201967 -3.872923 1.937273
H -1.550419 -2.965555 2.73583
H -1.532565 -1.200779 2.490981
H -2.852116 -1.951392 3.421303

I3'$_{Au1}$

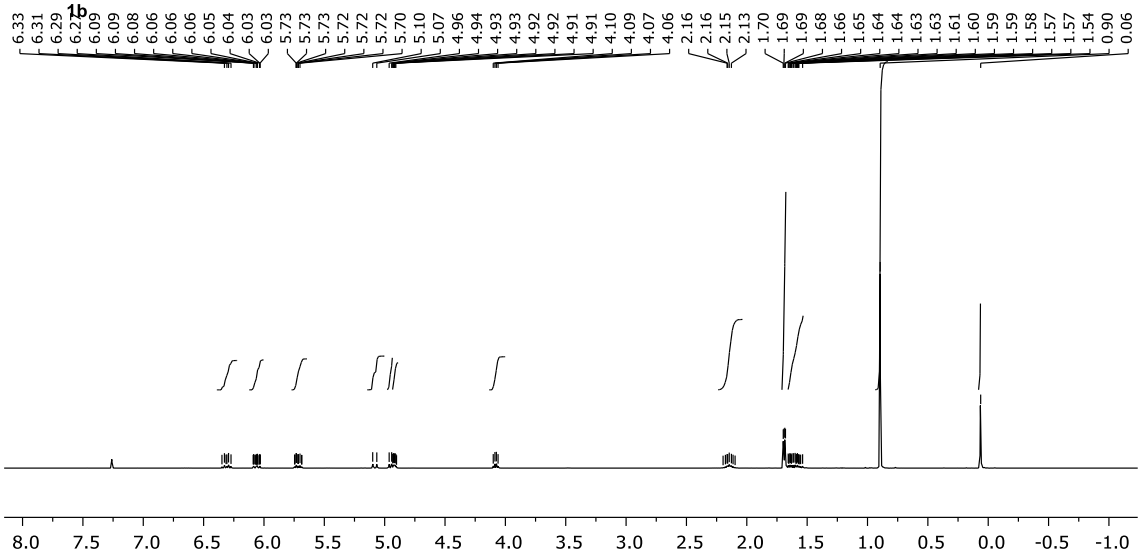
Zero-point correction= 0.595613 (Hartree/Particle)
Thermal corr. to Energy= 0.630722
Thermal corr. to Enthalpy= 0.631666
Thermal correction to Gibbs Free Energy= 0.525370
Sum of electronic and zero-point Energies= -1509.445912
Sum of electronic and thermal Energies= -1509.410804
Sum of electronic and thermal Enthalpies= -1509.409860
Sum of electronic and thermal Free Energies= -1509.516155
HF (M06/6-311++g(d,p) and SDD, SMD(dichloromethane): -1509.87388360

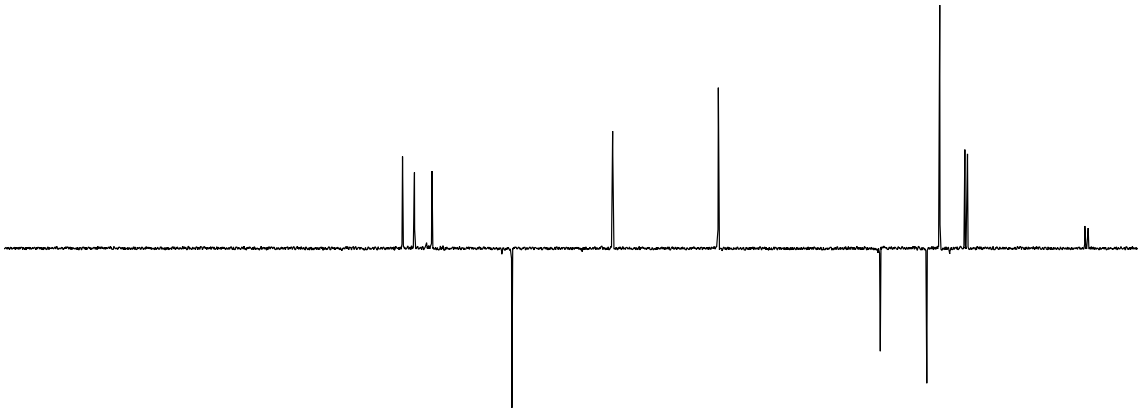
C 0.806302 2.037364 0.317168
H 1.550158 2.644123 -0.212785
C 1.552482 0.972902 1.140739
H 0.808861 0.308337 1.608790
C 0.175588 2.968335 1.437653
C 2.257063 1.814818 2.229728
C 1.334080 3.028299 2.493371
H 3.225705 2.140349 1.837092
H 2.452043 1.229439 3.133201
H 0.909514 3.025565 3.501773
H 1.880549 3.968429 2.373496
C -0.298979 4.314343 0.968708
H -0.587956 4.989051 1.774450
C -0.324373 1.667730 -0.528388
C -0.640048 2.571855 -1.672311
C -2.151960 2.661361 -1.974847
H -2.310426 3.221659 -2.902543
H -2.600046 1.670144 -2.094750
H -2.677857 3.183413 -1.169063
C 0.073171 1.821392 -2.857930
H -0.390469 0.852564 -3.061286
H -0.040698 2.454193 -3.745661
H 1.142063 1.673385 -2.675505
H -0.665692 2.426020 1.893497
C -0.386251 4.760911 -0.290395
H -0.727956 5.784217 -0.431404
C -0.043639 4.007467 -1.560379
H 1.044889 3.977659 -1.701885
H -0.422963 4.572526 -2.418362
O 2.409471 0.237216 0.302970
Si 3.276319 -1.170651 0.690370
C 2.155149 -2.317065 1.696314
H 1.924945 -1.895214 2.682475
H 1.203585 -2.511192 1.186967
H 2.642563 -3.283844 1.870276
C 4.806930 -0.735132 1.703927
H 5.400090 -1.630372 1.926205
H 5.457651 -0.029913 1.174823
H 4.537572 -0.280291 2.664311
C 3.731517 -1.911850 -1.009252
C 2.449047 -2.302241 -1.775930
H 1.788627 -1.437940 -1.922095
H 2.702644 -2.699924 -2.768815
H 1.882889 -3.081107 -1.248666
C 4.517101 -0.874305 -1.841615
H 3.934981 0.039861 -2.005205
H 5.458610 -0.589246 -1.357371
H 4.772175 -1.289963 -2.826575
C 4.604323 -3.172432 -0.815836
H 4.860854 -3.610315 -1.790497
H 5.547741 -2.945906 -0.305662
H 4.088271 -3.949642 -0.238094
C -4.049698 -3.173869 1.094444
C -3.366472 -3.831120 0.122655
H -4.844485 -3.502234 1.746372
H -3.453379 -4.842867 -0.242473
Au -1.421723 -0.015214 -0.145242
C -2.538234 -1.734092 0.234071
N -2.443578 -2.935475 -0.391568
N -3.529575 -1.891245 1.148753
C -1.538860 -3.250817 -1.497310
H -2.080958 -3.236922 -2.447303
H -0.736644 -2.513407 -1.524263
H -1.107057 -4.241838 -1.339776
C -3.998533 -0.869674 2.084427
H -3.817794 -1.193336 3.113106
H -3.454971 0.055996 1.895586
H -5.067923 -0.696171 1.938399

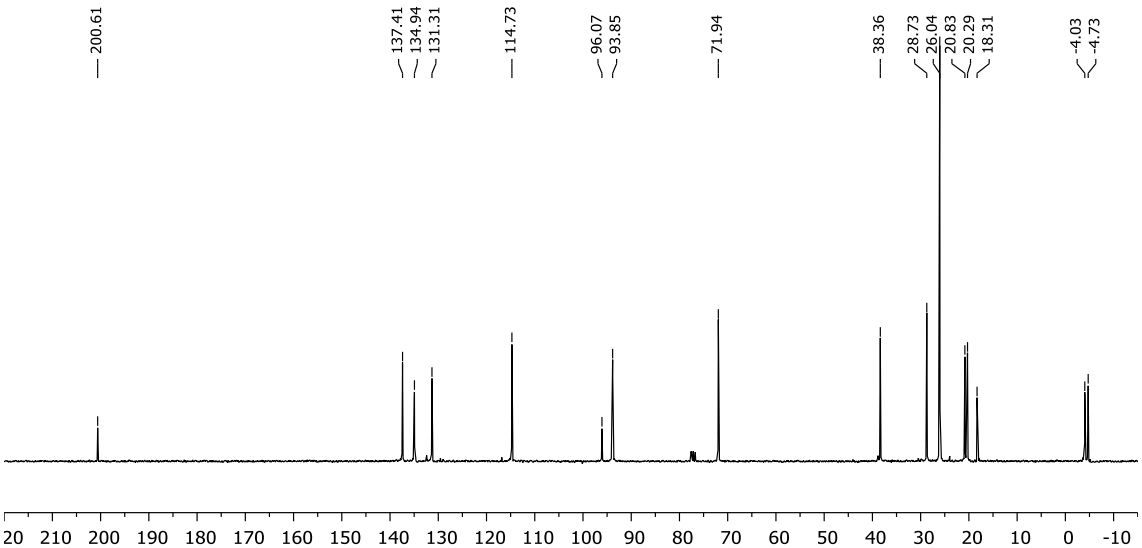
NMR Spectra

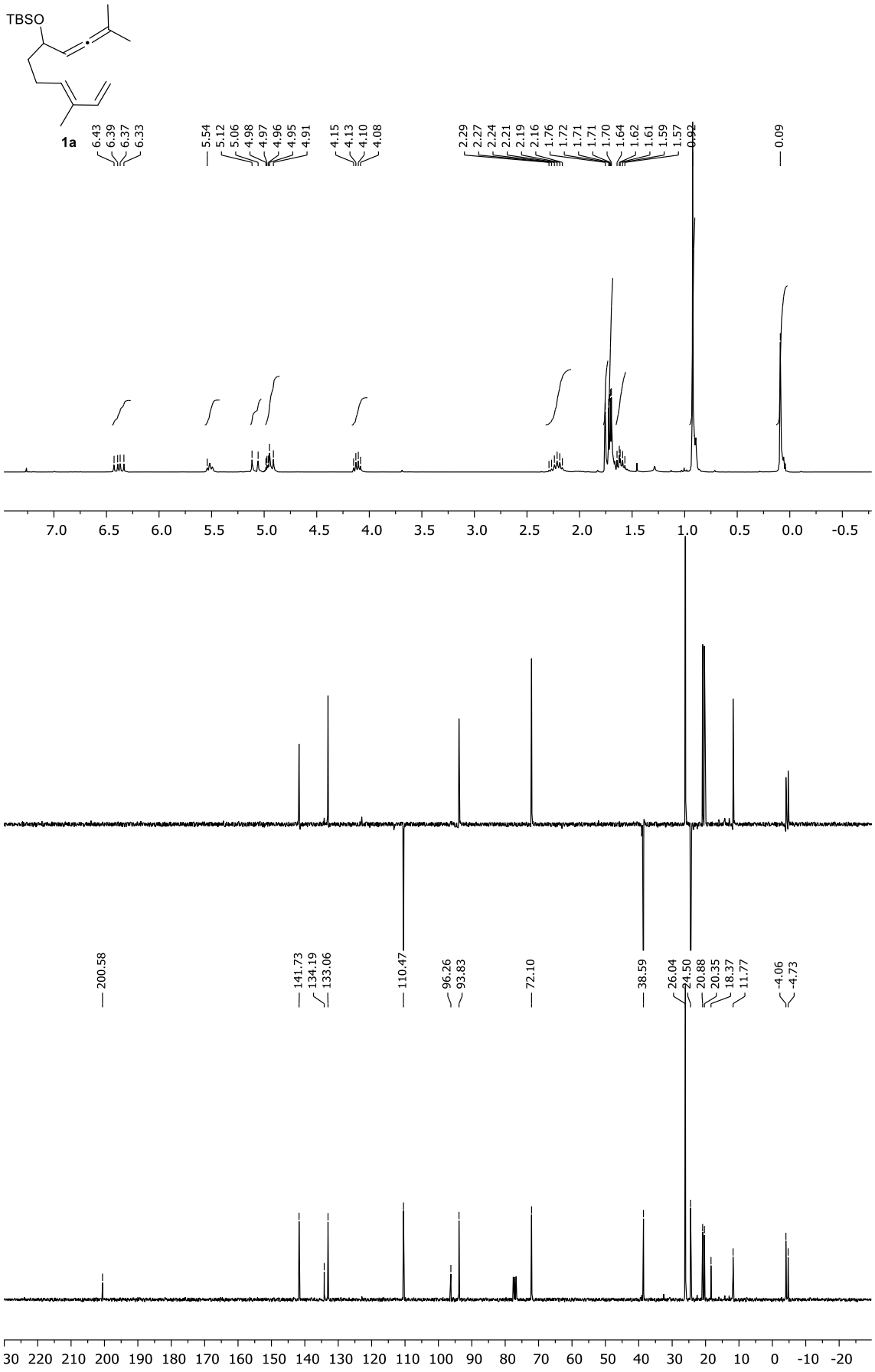


1b





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1a
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4.95
4.91
4.15
4.13
4.10
4.08
2.29
2.27
2.24
2.21
2.19
2.16
1.76
1.72
1.71
1.71
1.70
1.64
1.62
1.61
1.59
1.57
0.92
0.09
7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
200.58
141.73
134.19
133.06
110.47
96.26
93.83
72.10
38.59
26.04
24.50
20.88
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11.77
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-4.73
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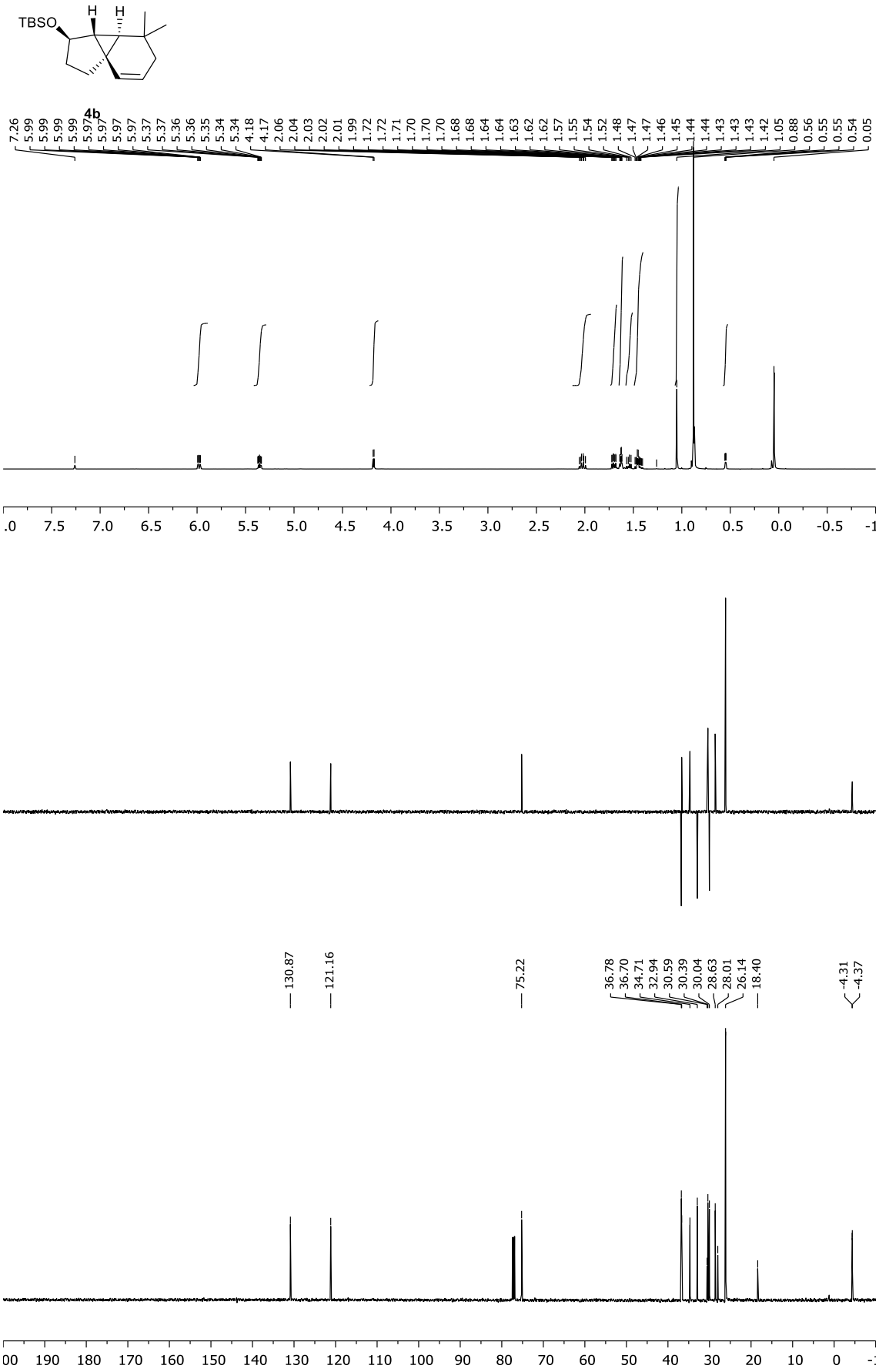
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H
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4.18
4.17
2.06
2.04
2.03
2.02
2.01
1.99
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1.47
1.46
1.45
1.44
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1.43
1.43
1.43
1.42
1.05
0.88
0.56
0.55
0.55
0.54
0.05
.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
130.87
121.16
75.22
36.78
36.70
34.71
32.94
30.59
30.39
30.04
28.63
28.01
26.14
18.40
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-4.37
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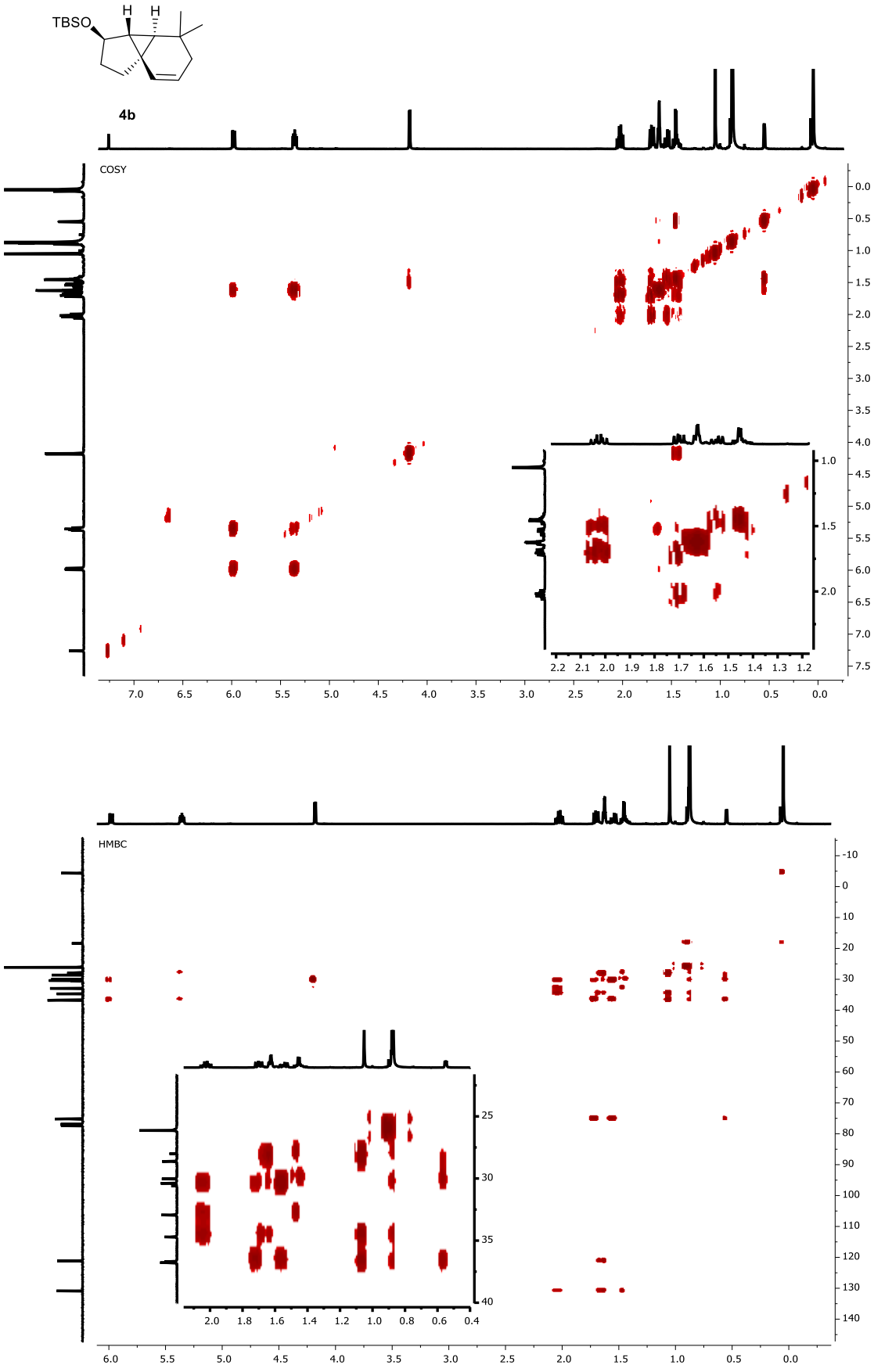
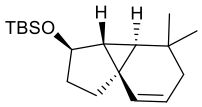
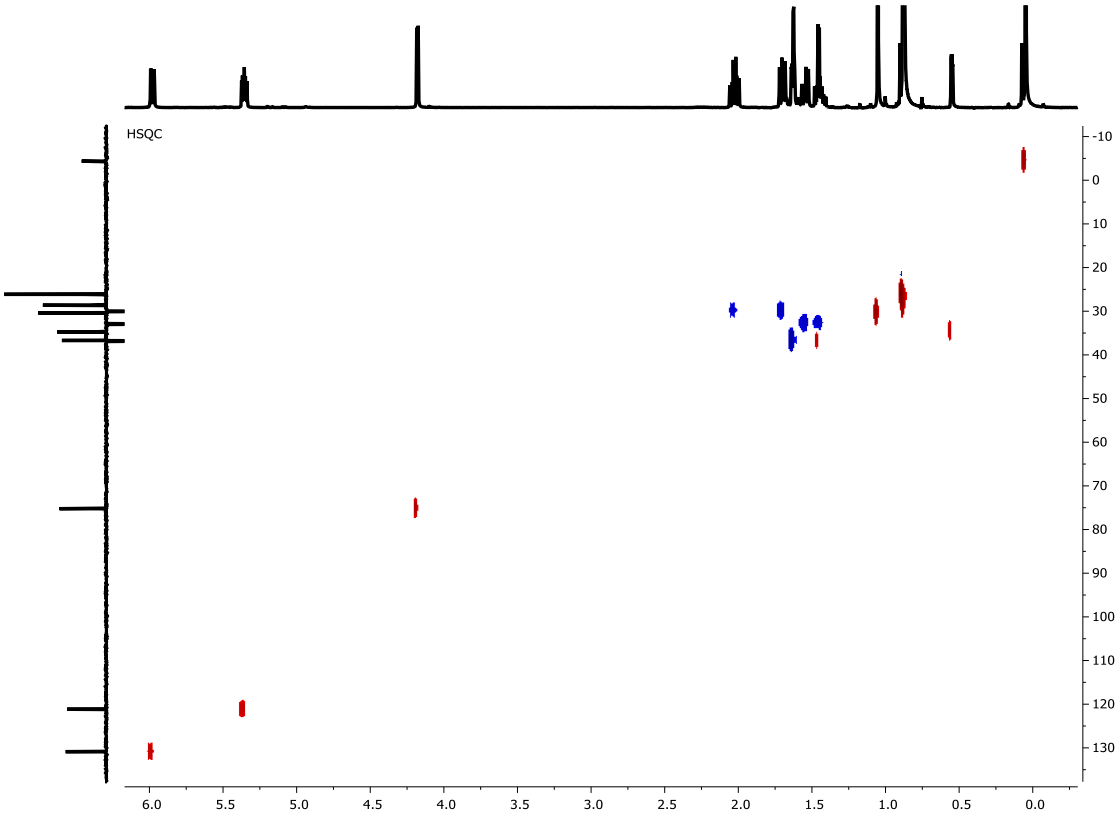

TBSO
H
H
4b
COSY
HMBC


TBSO
H
H

4b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90
100
110
120
130
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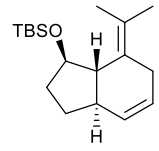
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0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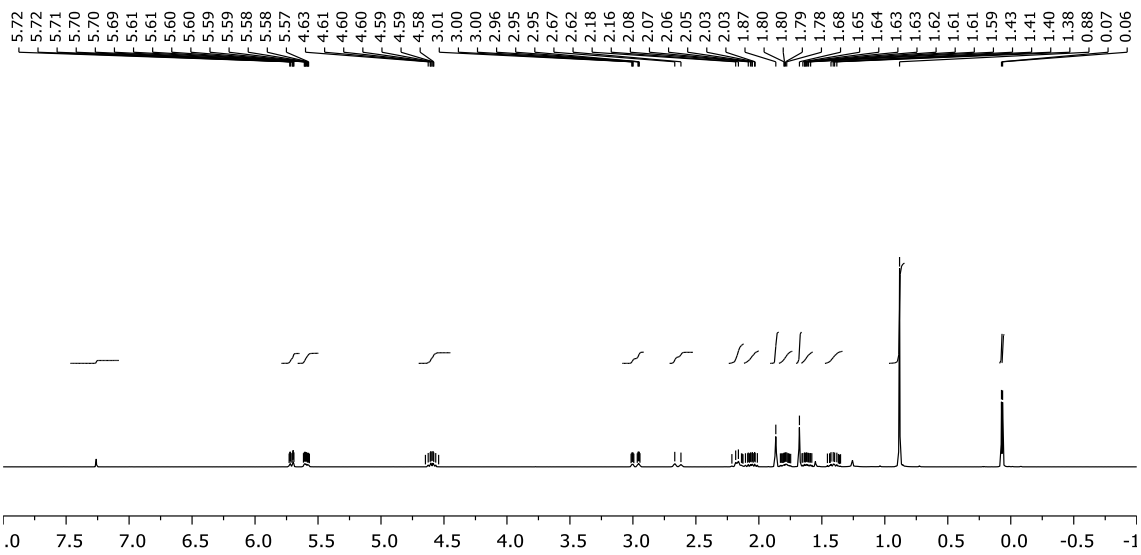
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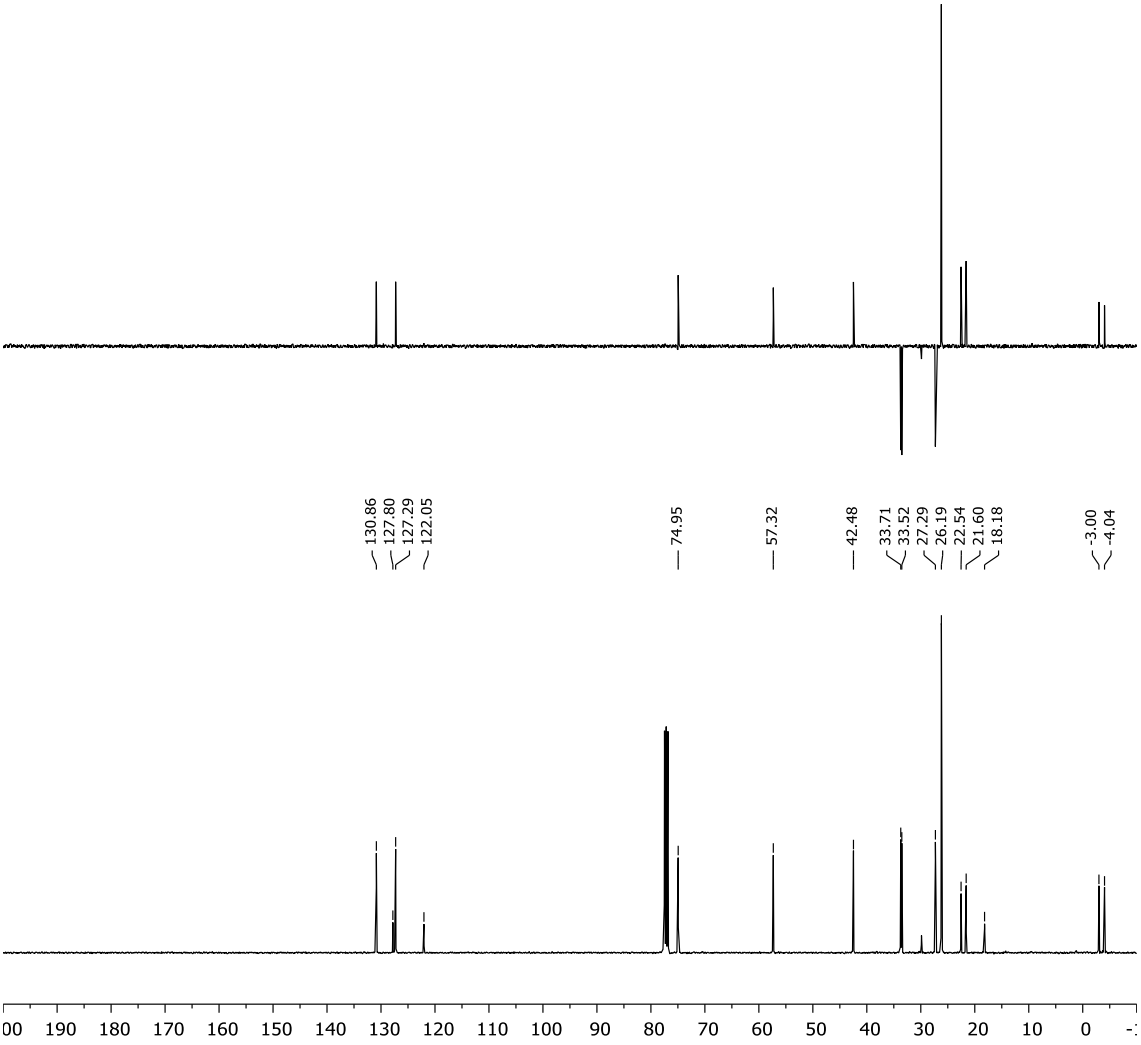
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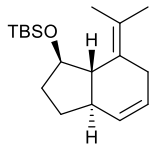

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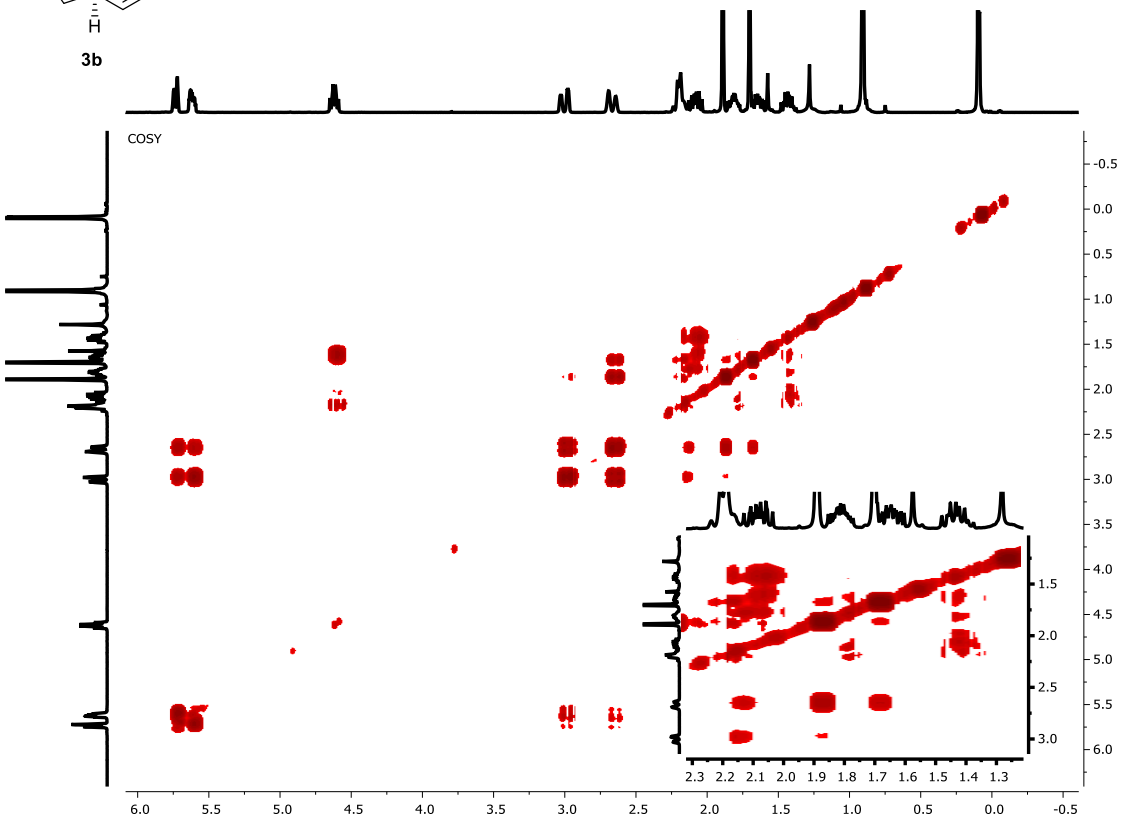

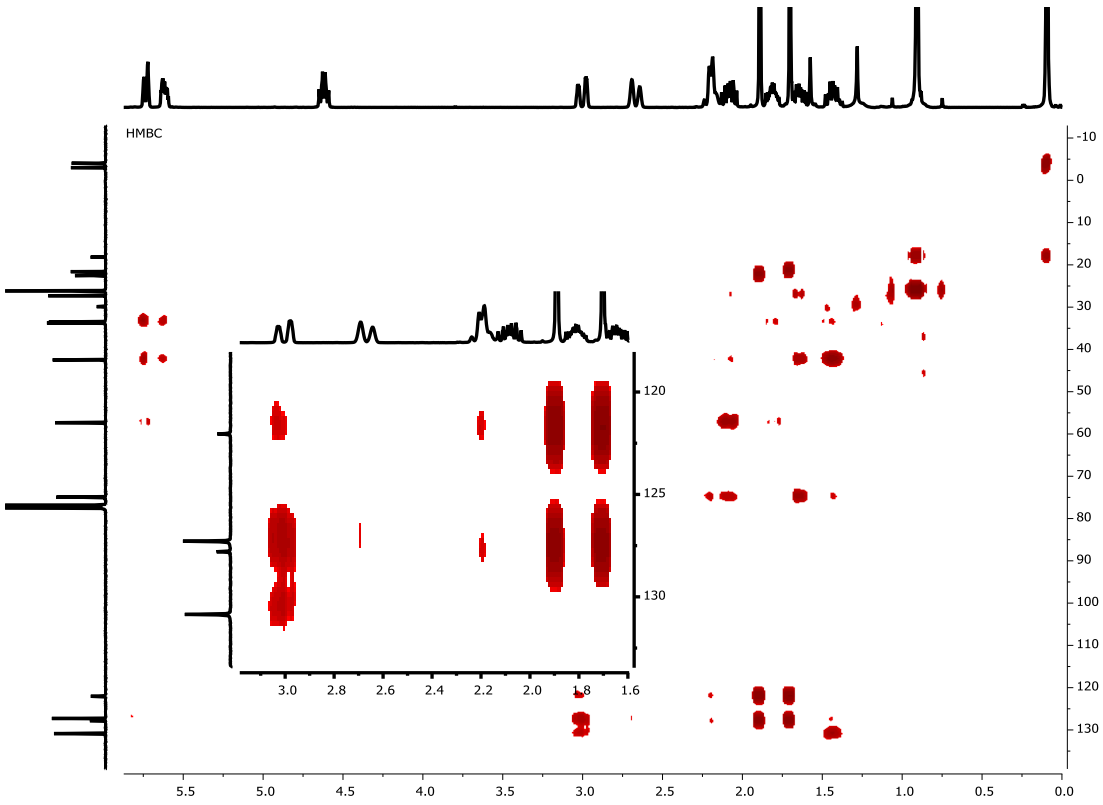

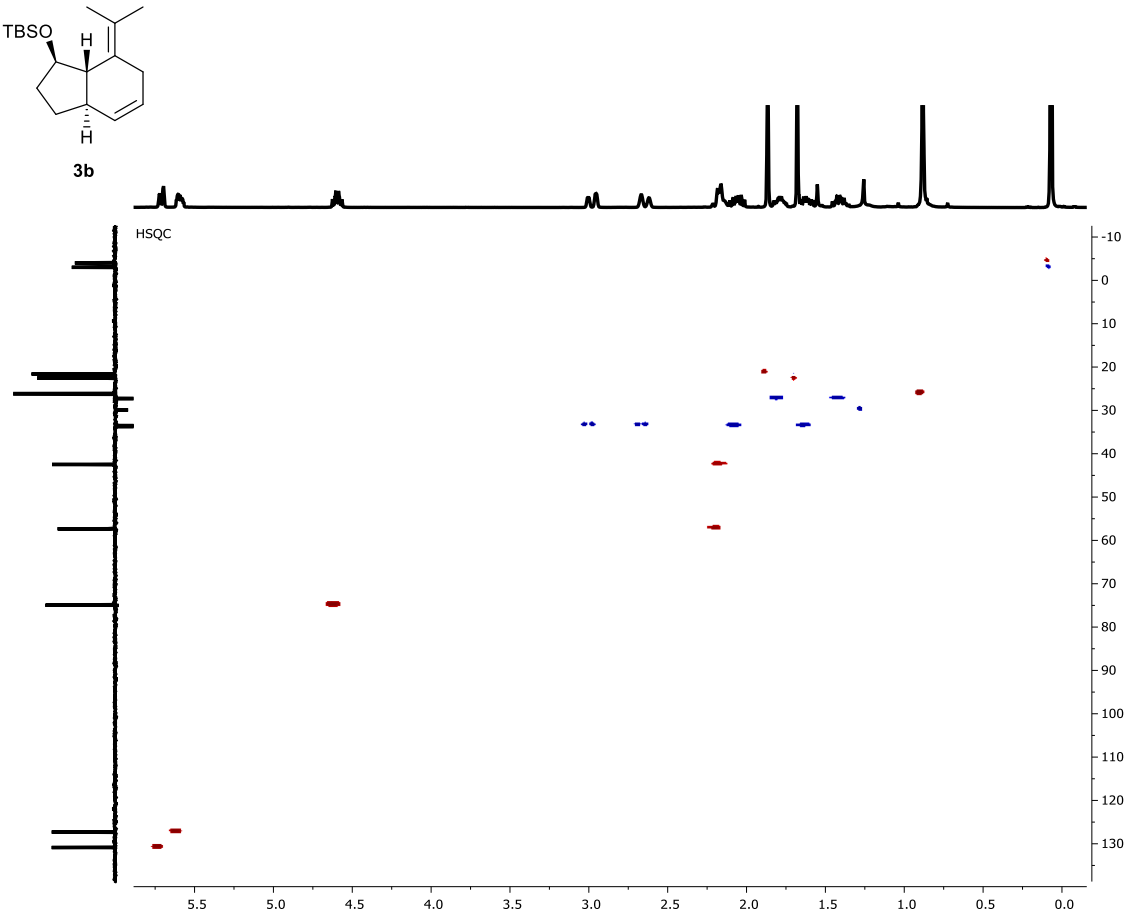
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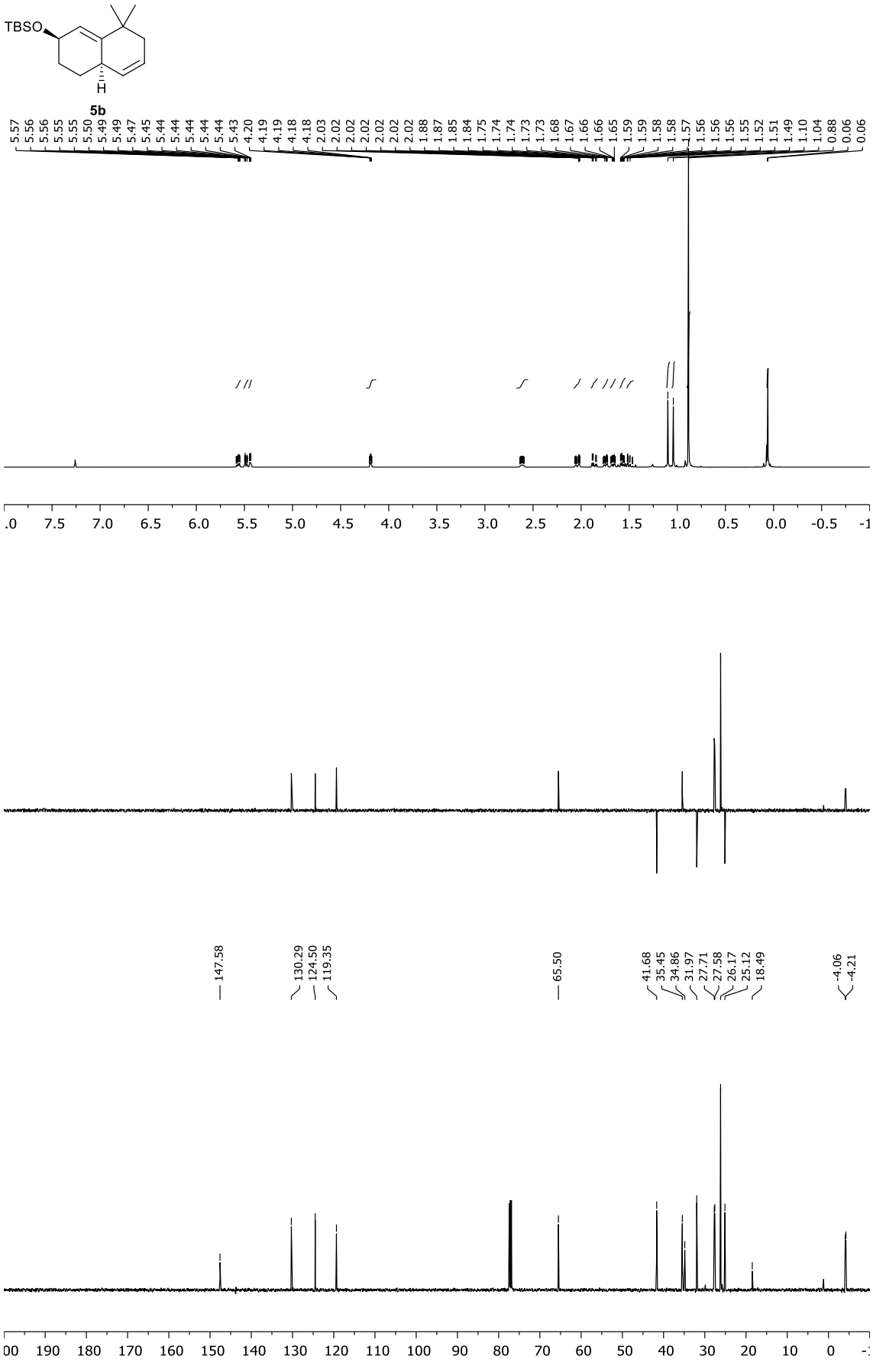
TBSO
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.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
147.58 130.29 124.50 119.35 65.50 41.68 35.45 34.86 31.97 27.71 27.58 26.17 25.12 18.49 -4.06 -4.21
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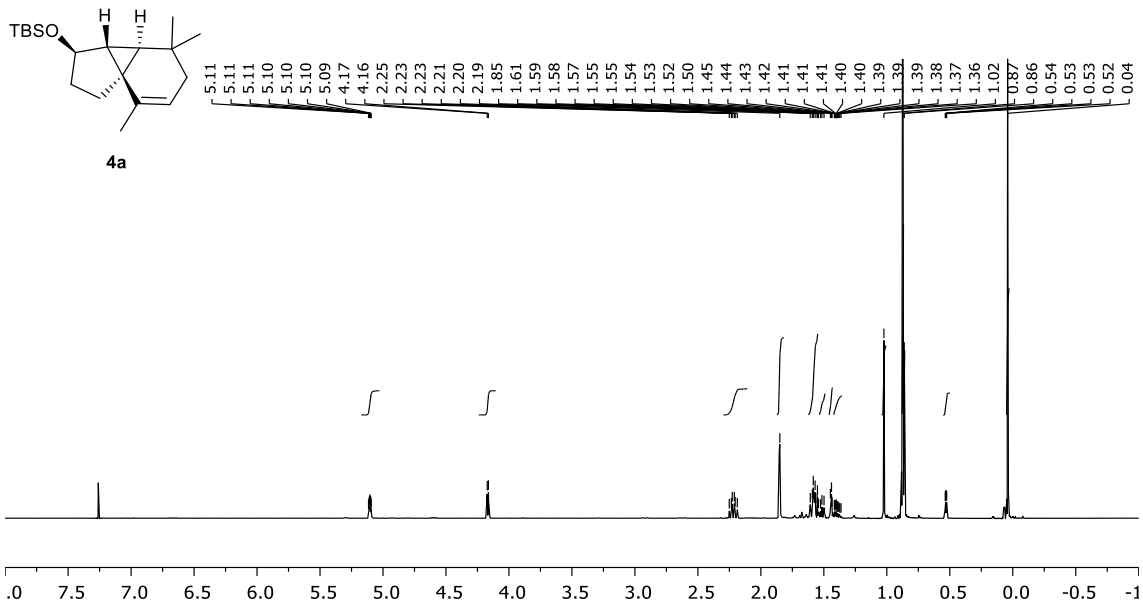
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1.39
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1.36
1.02
0.87
0.86
0.54
0.53
0.53
0.52
0.04
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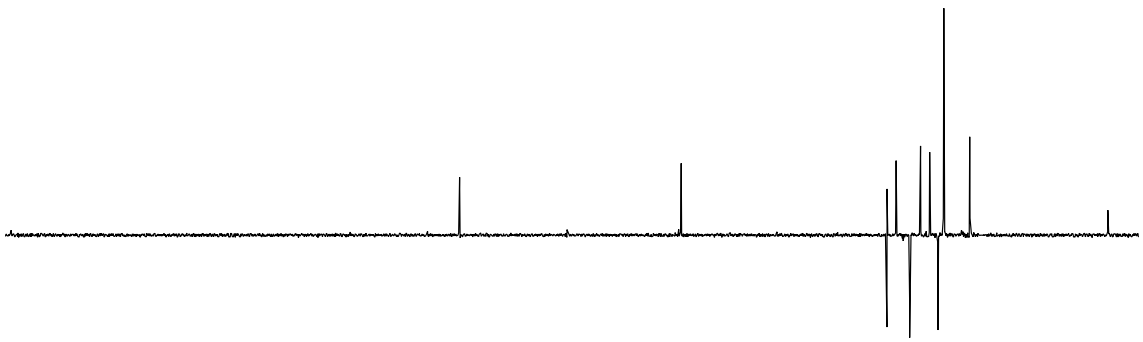

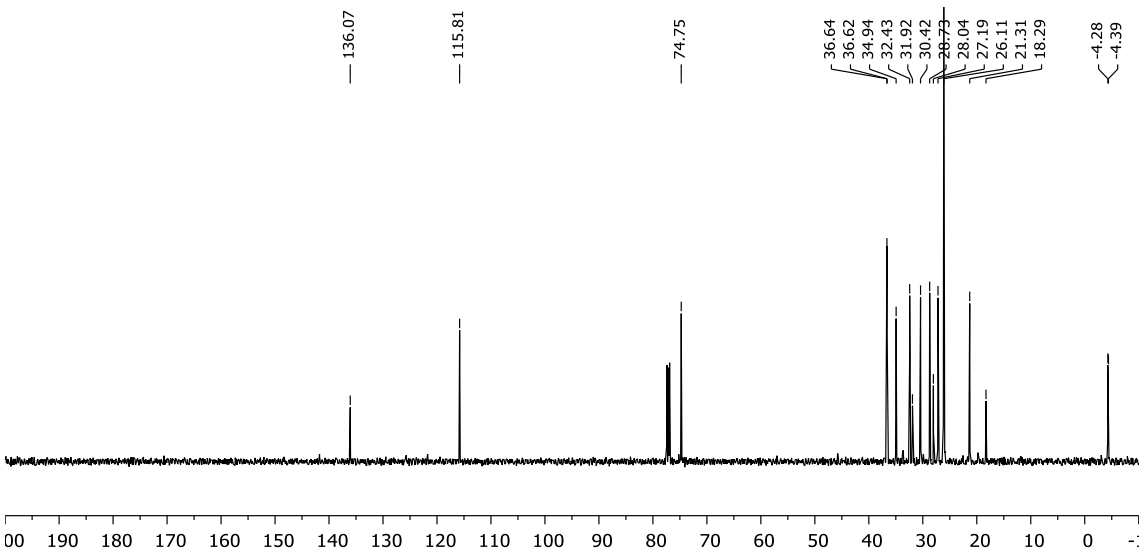
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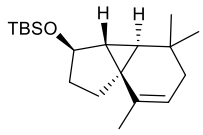
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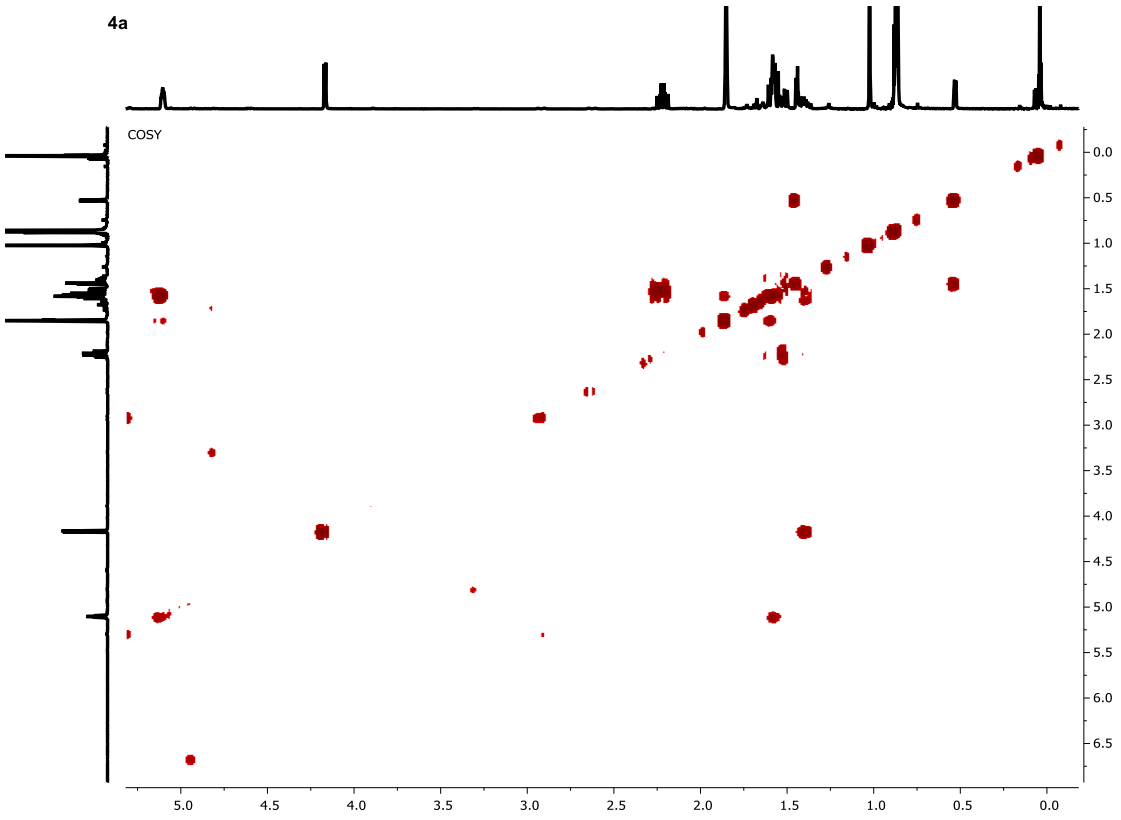
4a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0.0
0.5
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4.5
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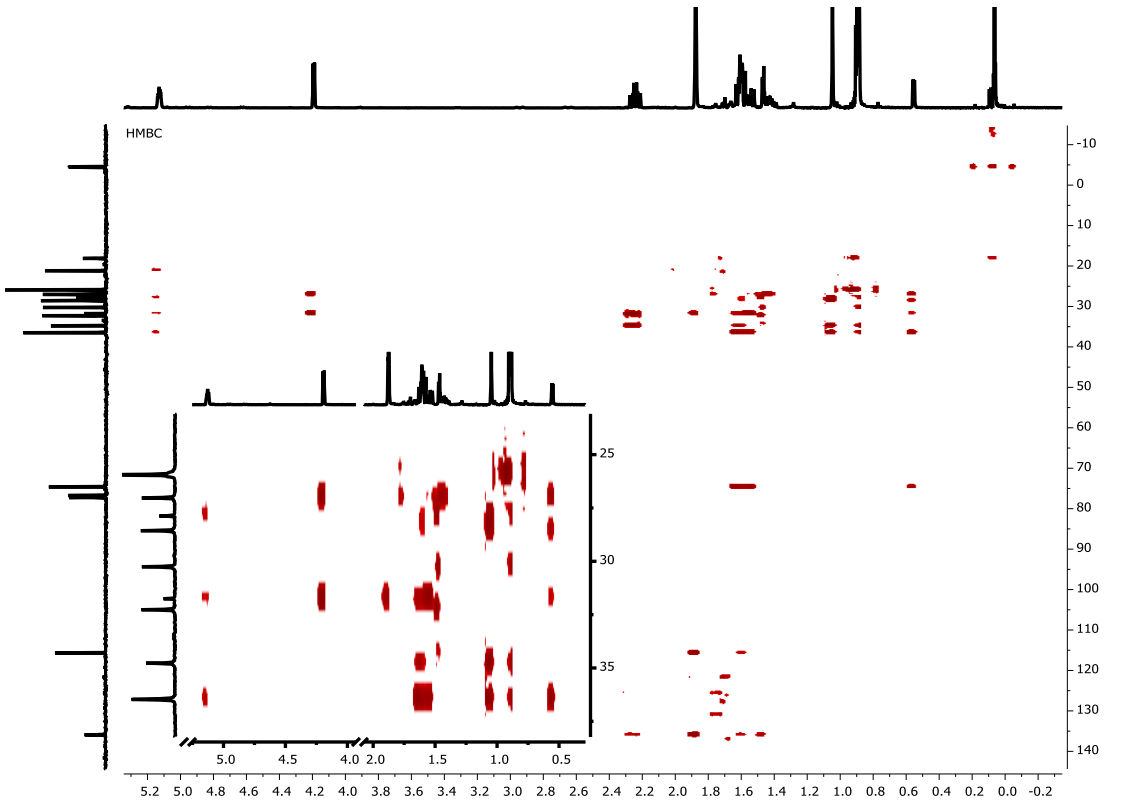
6.5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3.6
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3.0
2.8
2.6
2.4
2.2
2.0
1.8
1.6
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
-0.2
-10
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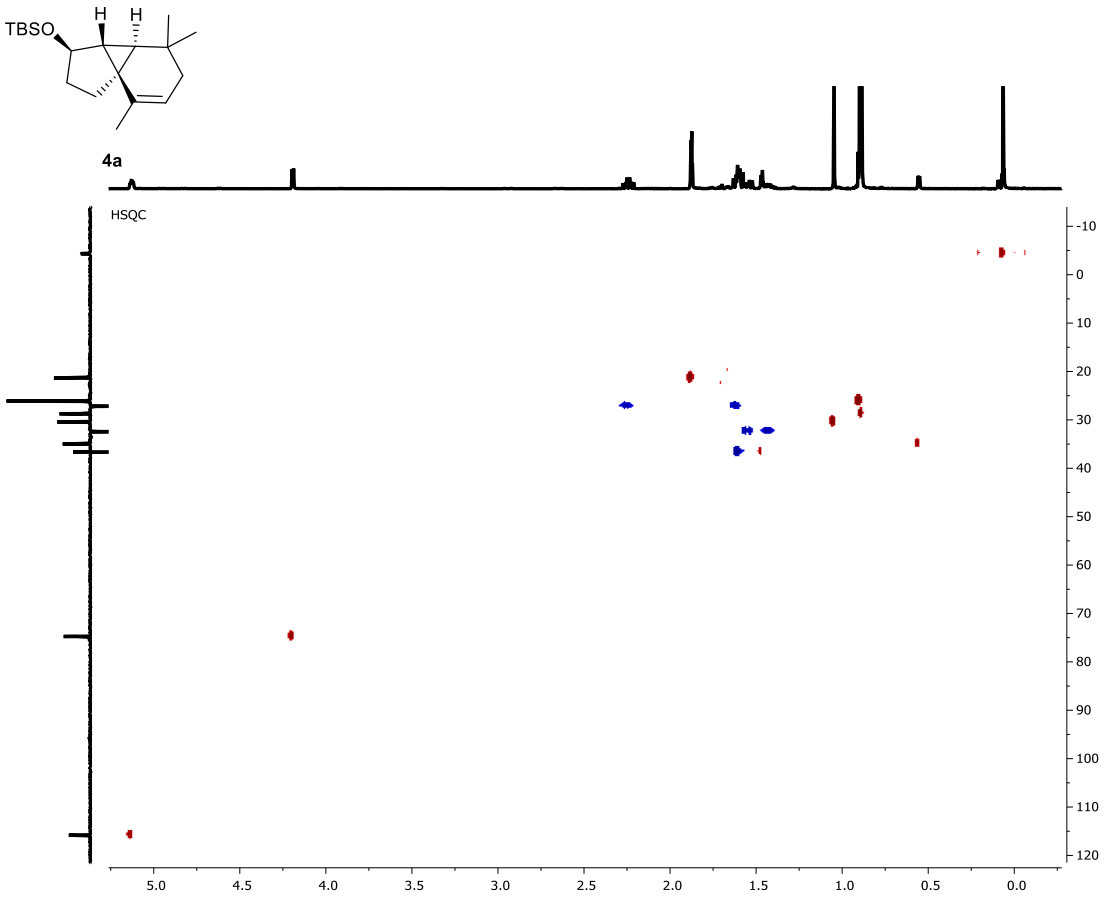
TBSO
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H
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HSQC
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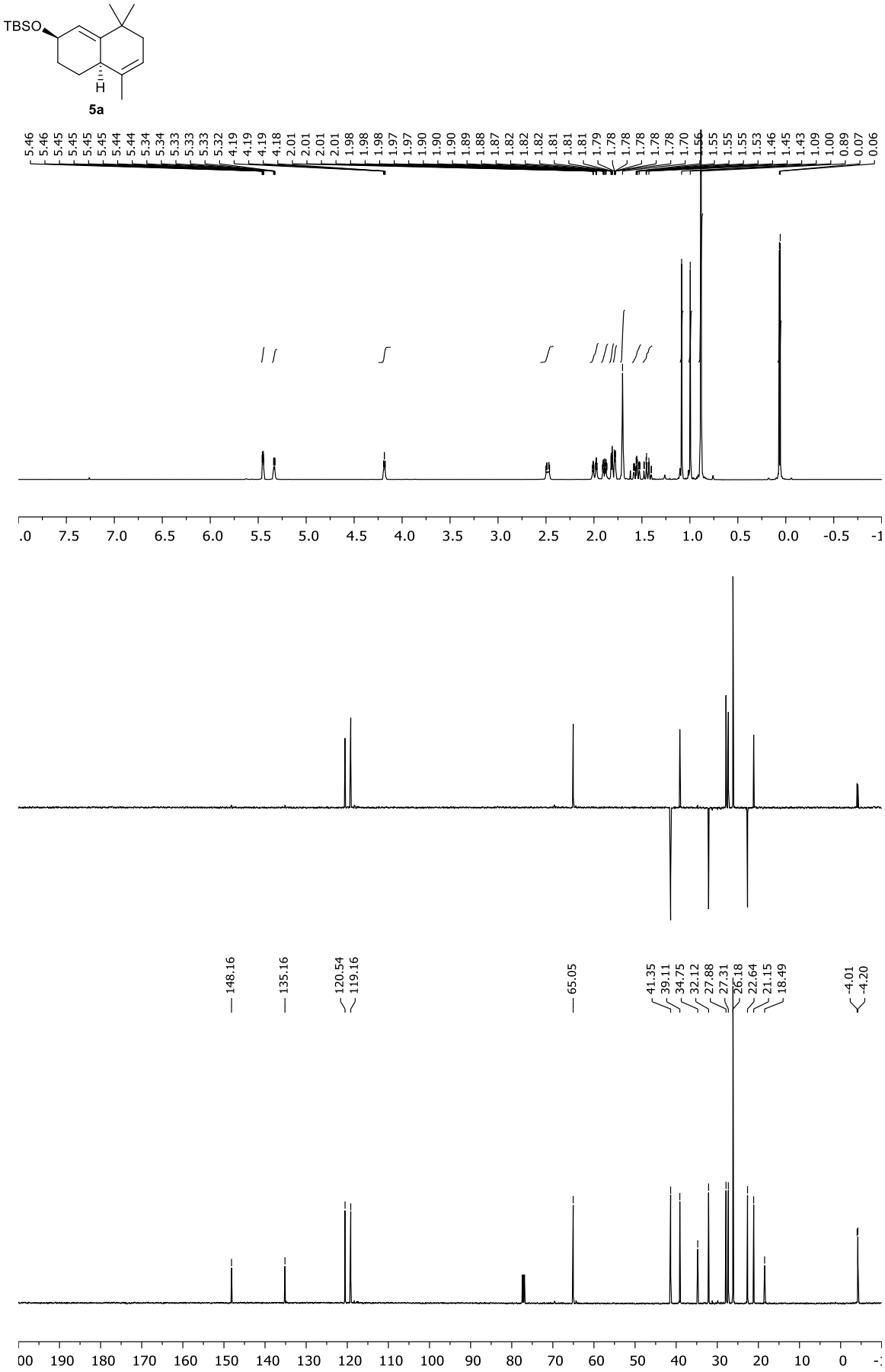
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H
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.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
148.16 135.16 120.54 119.16 65.05 41.35 39.11 34.75 32.12 27.88 27.31 26.18 22.64 21.15 18.49 -4.01 -4.20
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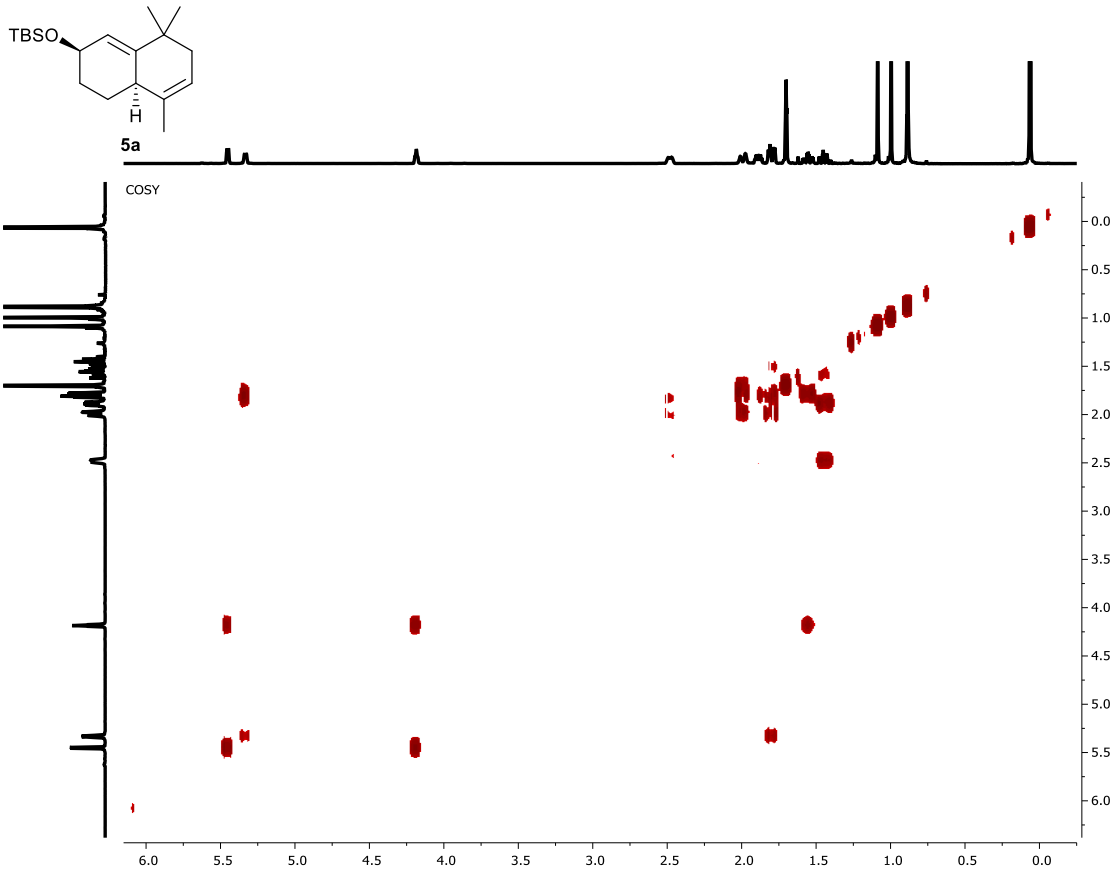
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3.0
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4.0
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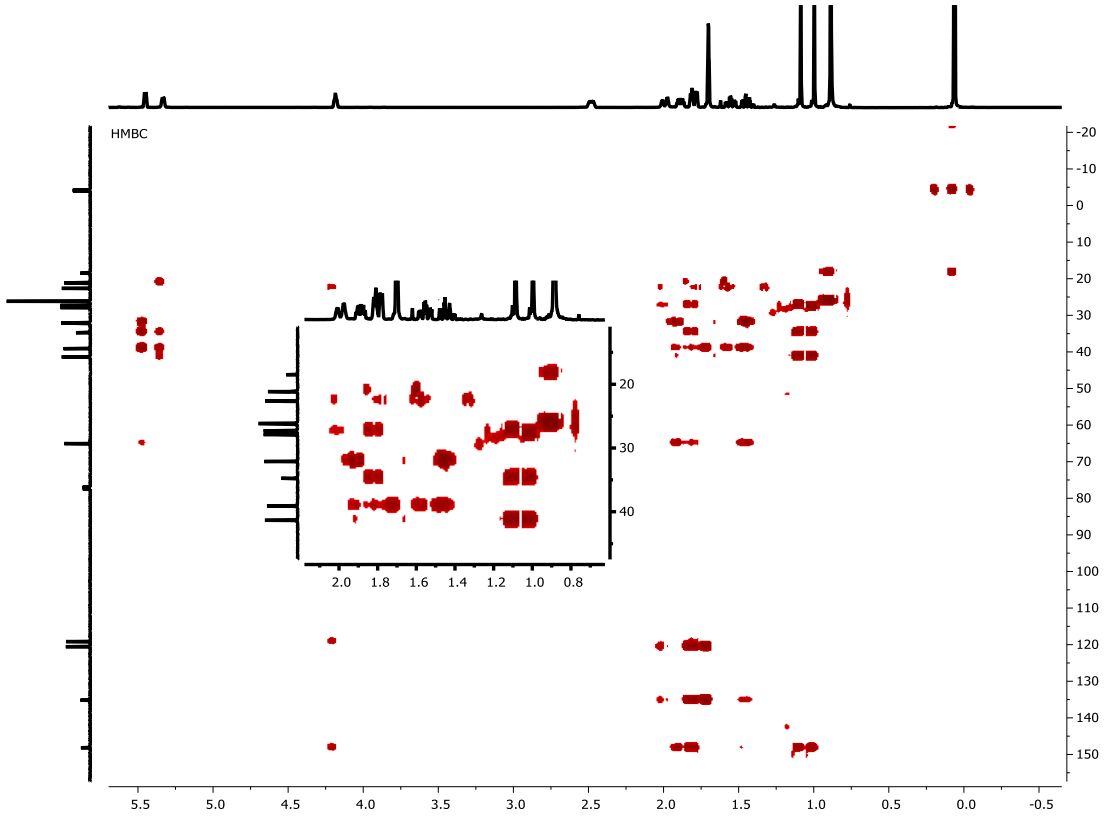
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20
30
40
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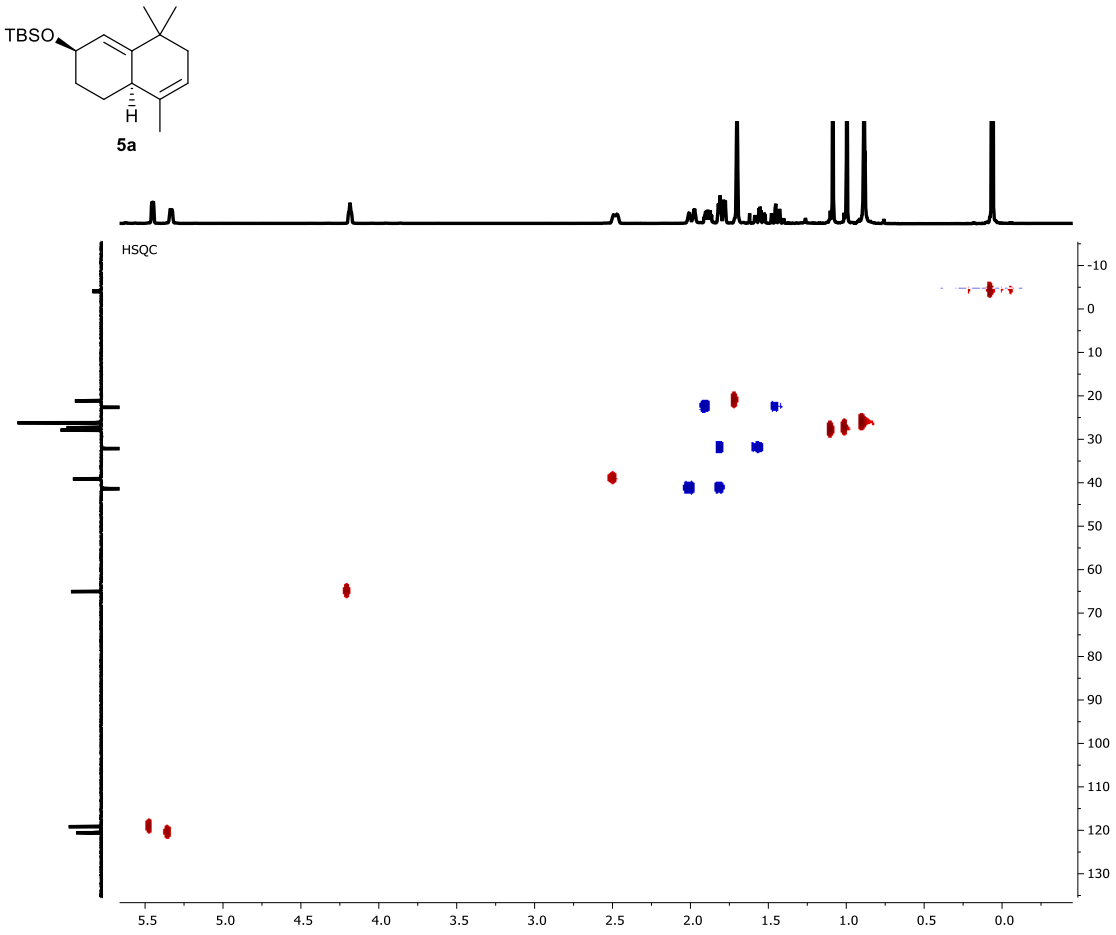
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HSQC
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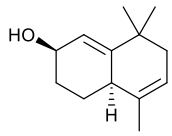
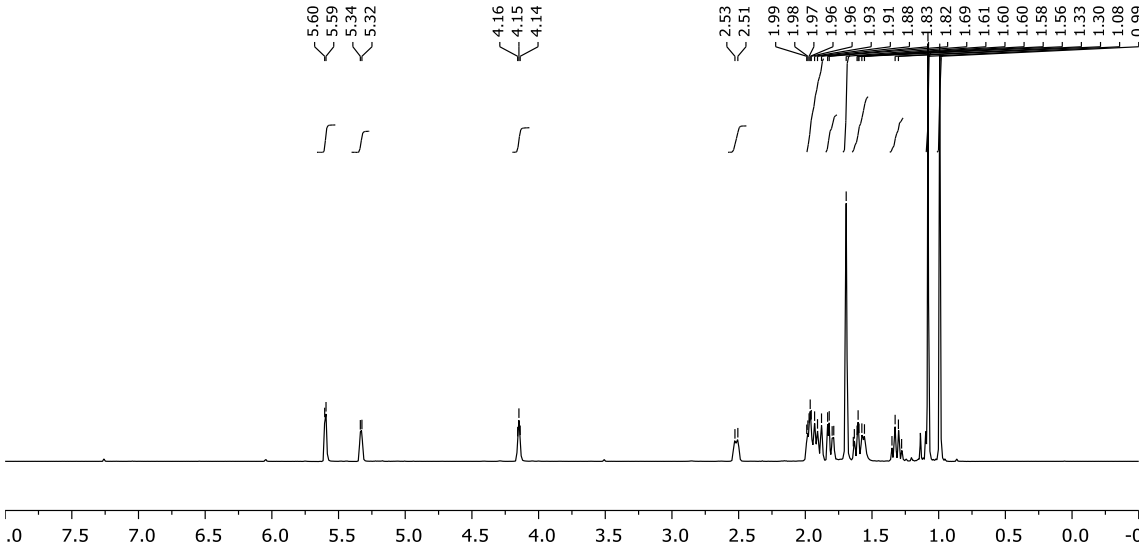

HO
H

5a´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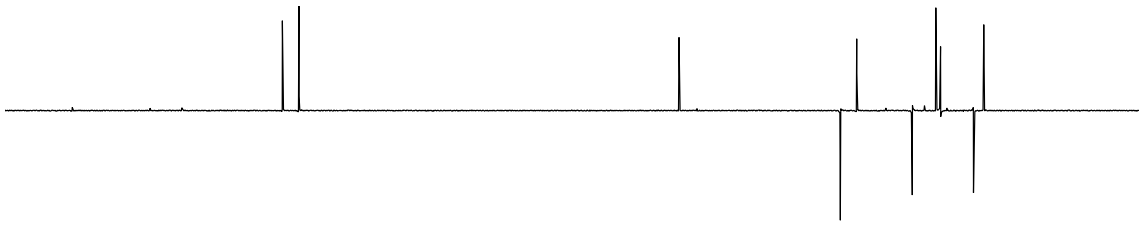

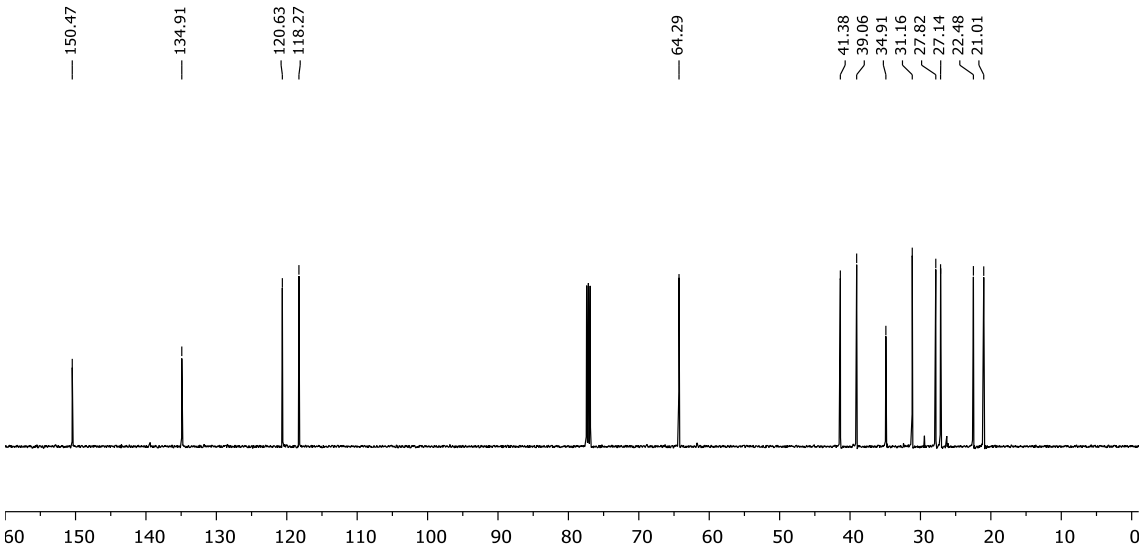
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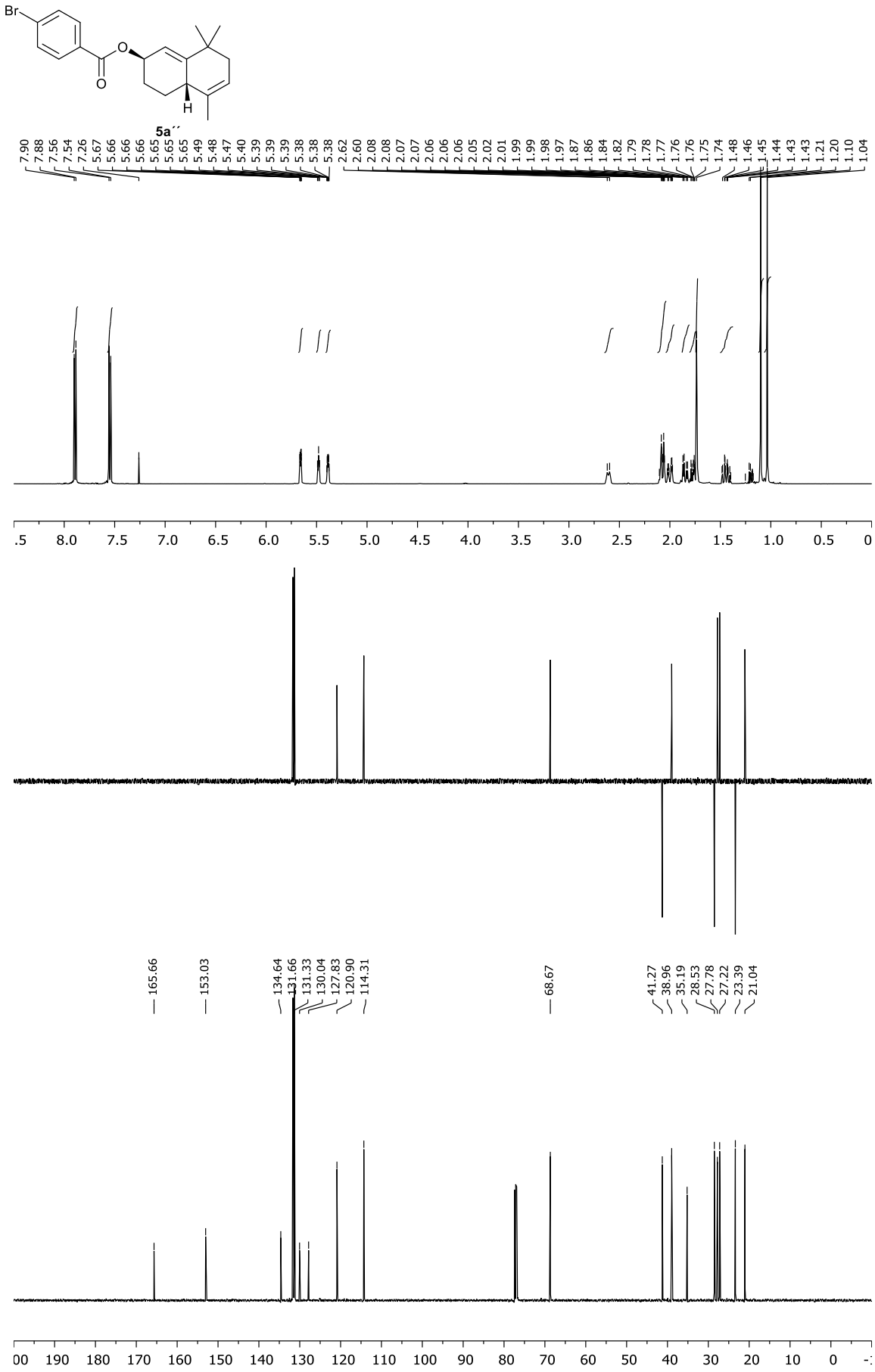
Br
O
O
H
5a´´
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2.62 2.60 2.08 2.08 2.07 2.07 2.06 2.06 2.06 2.05 2.02 2.01 1.99 1.99 1.98 1.97 1.87 1.86 1.84 1.82 1.79 1.78 1.77 1.76 1.76 1.75 1.74 1.48 1.46 1.45 1.44 1.43 1.43 1.21 1.20 1.10 1.04
.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0
165.66 153.03 134.64 131.66 131.33 130.04 127.83 120.90 114.31 68.67 41.27 38.96 35.19 28.53 27.78 27.22 23.39 21.04
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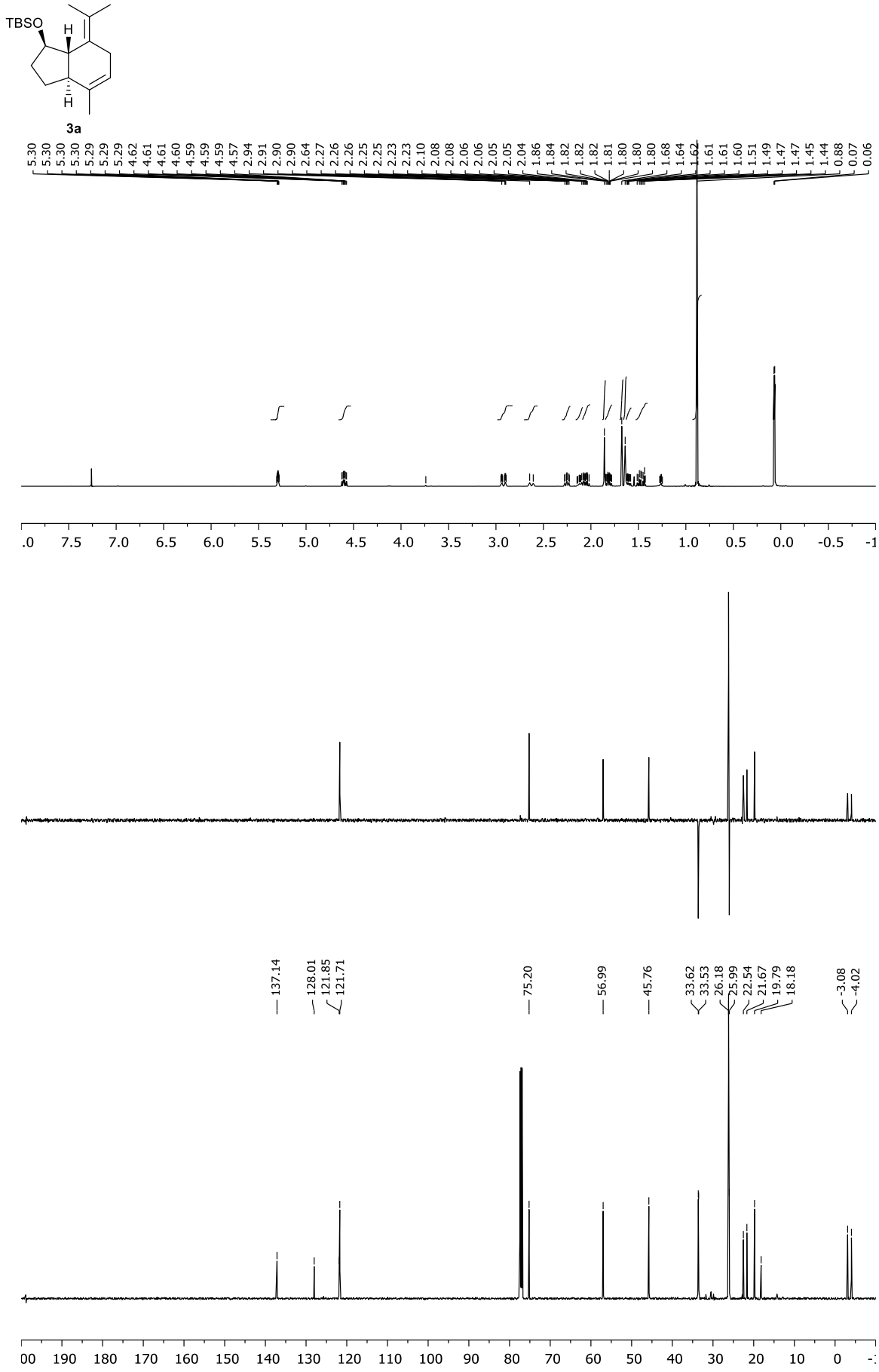
TBSO
H
H
3a
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.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
137.14 128.01 121.85 121.71 75.20 56.99 45.76 33.62 33.53 26.18 25.99 22.54 21.67 19.79 18.18 -3.08 -4.02
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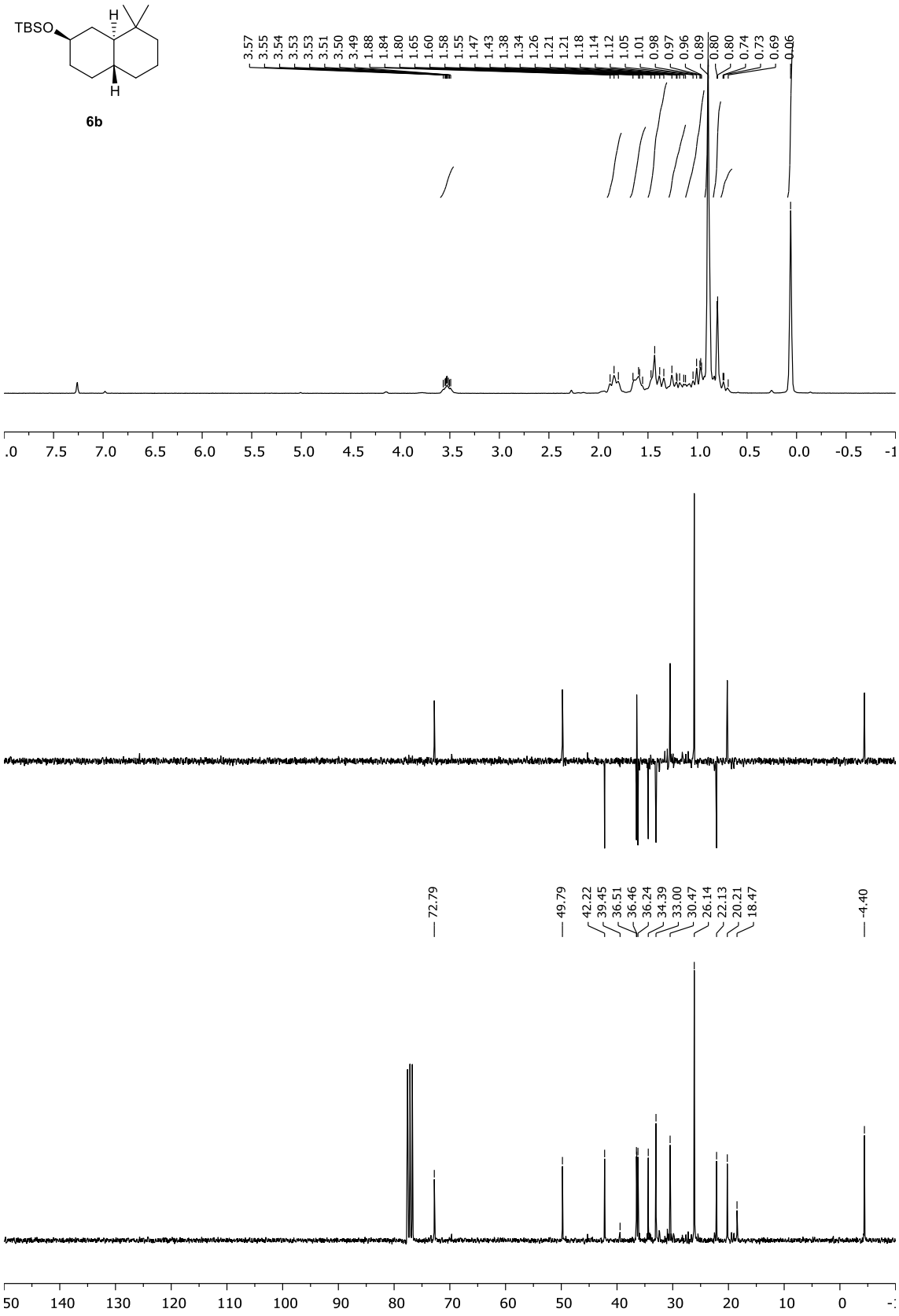
TBSO
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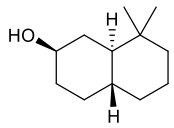
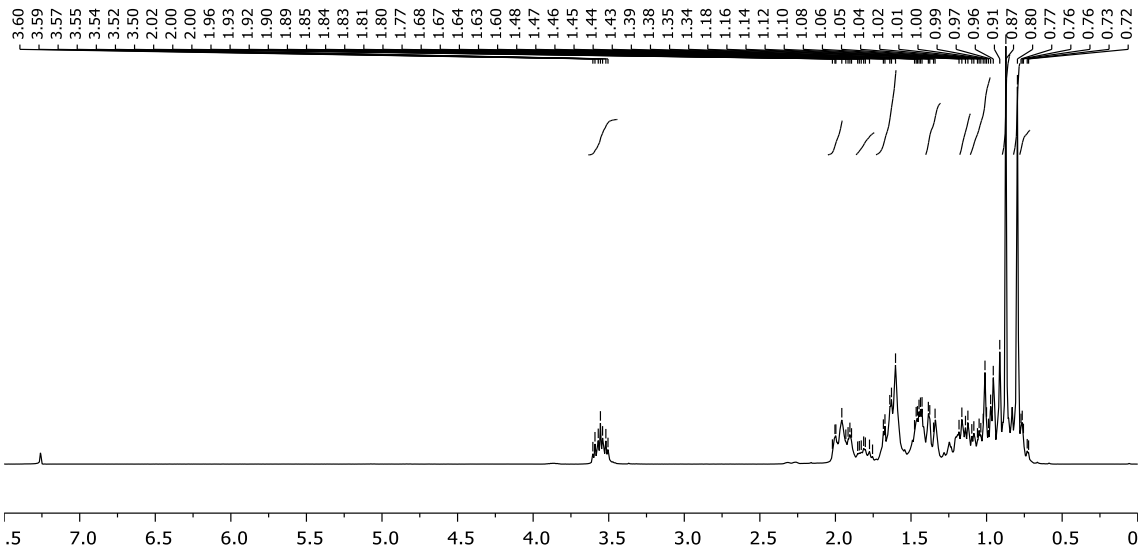

HO
H
H

6b´


3.60 3.59 3.57 3.55 3.54 3.52 3.50 2.02 2.00 2.00 1.96 1.93 1.92 1.90 1.89 1.85 1.84 1.83 1.81 1.80 1.77 1.68 1.67 1.64 1.63 1.60 1.48 1.47 1.46 1.45 1.44 1.43 1.39 1.38 1.35 1.34 1.18 1.16 1.14 1.12 1.10 1.08 1.06 1.05 1.04 1.02 1.01 1.00 0.99 0.97 0.96 0.91 0.87 0.80 0.77 0.76 0.76 0.73 0.72
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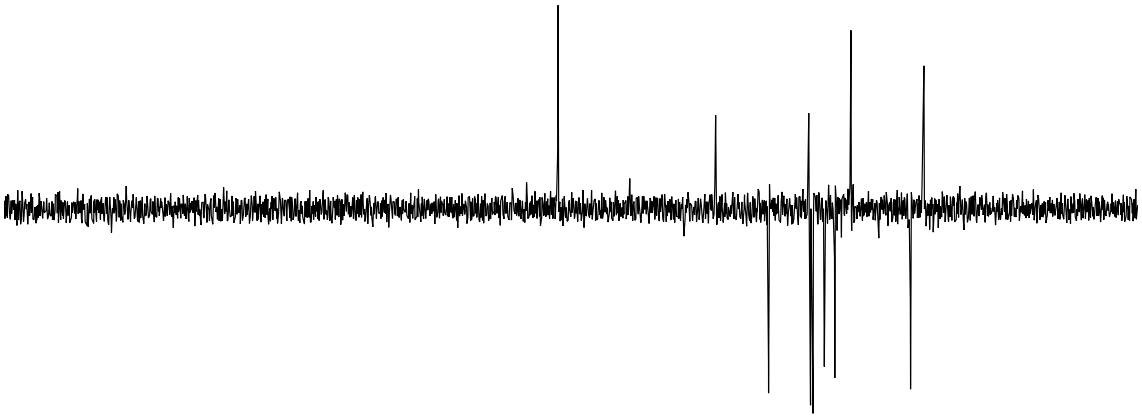

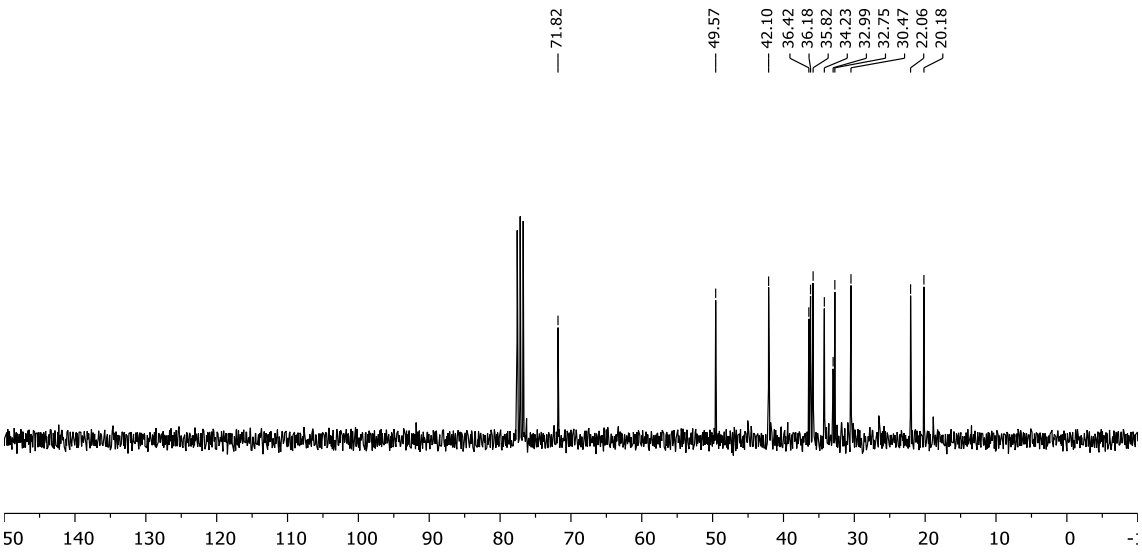
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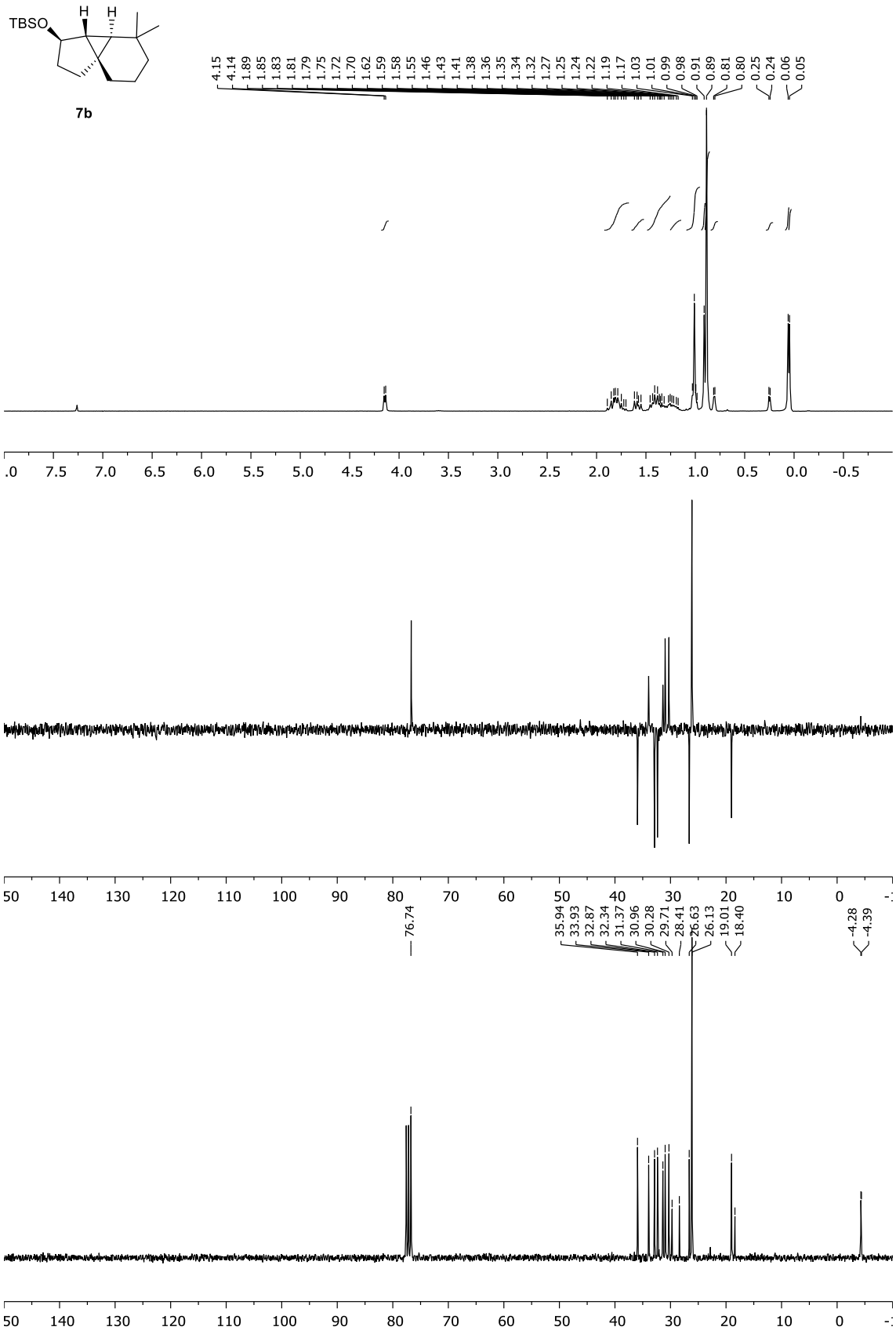
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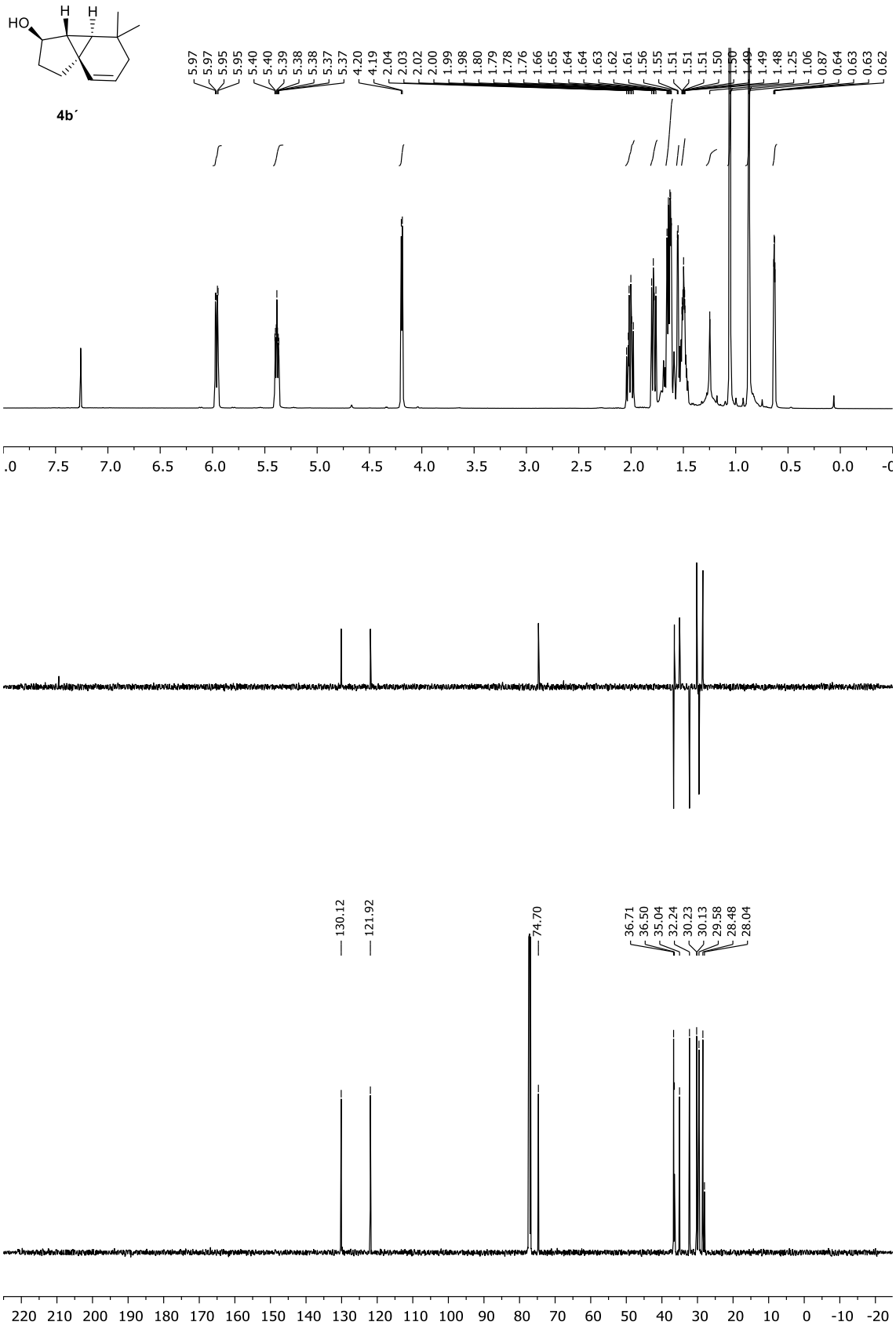
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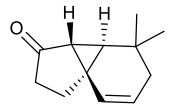
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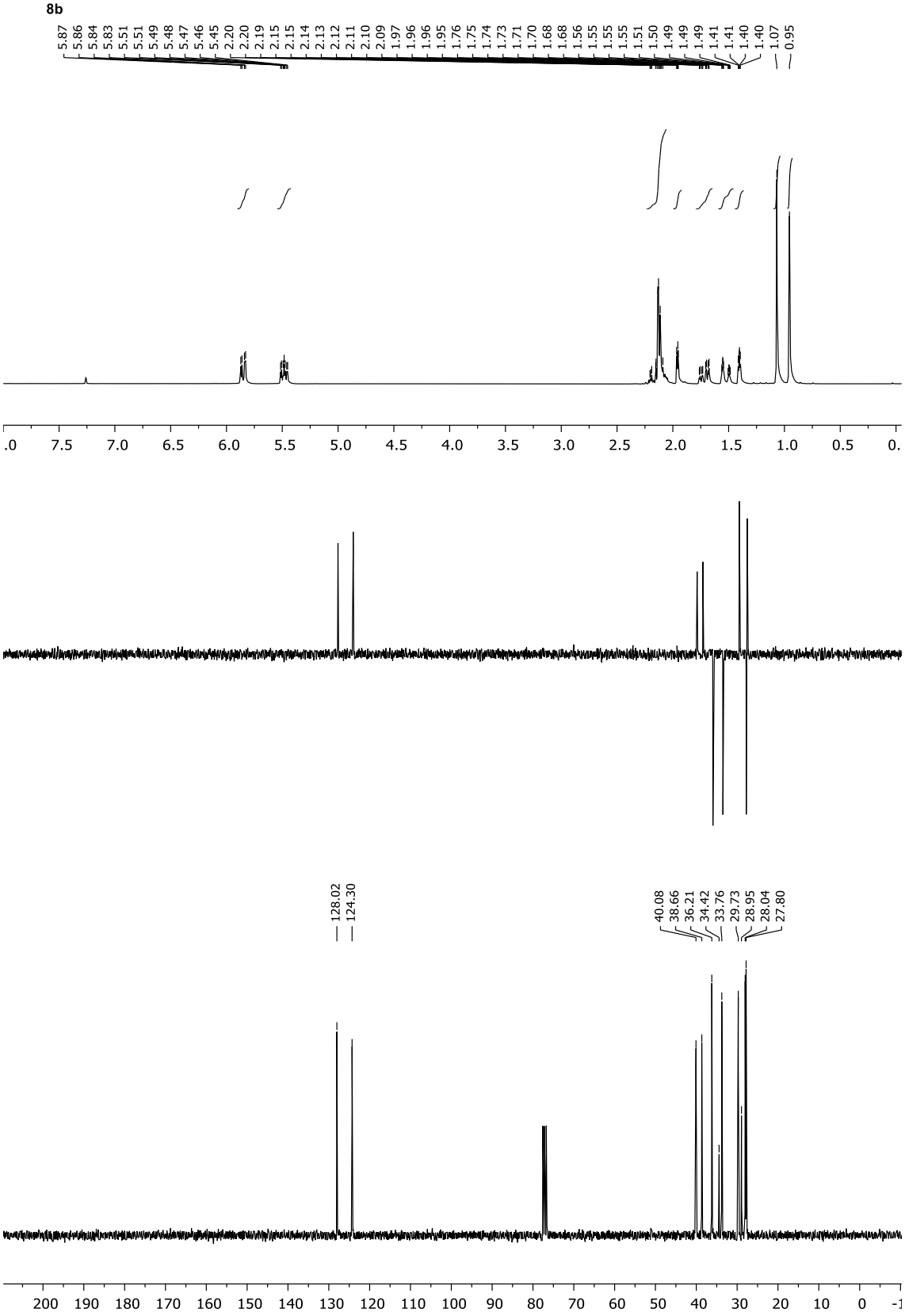
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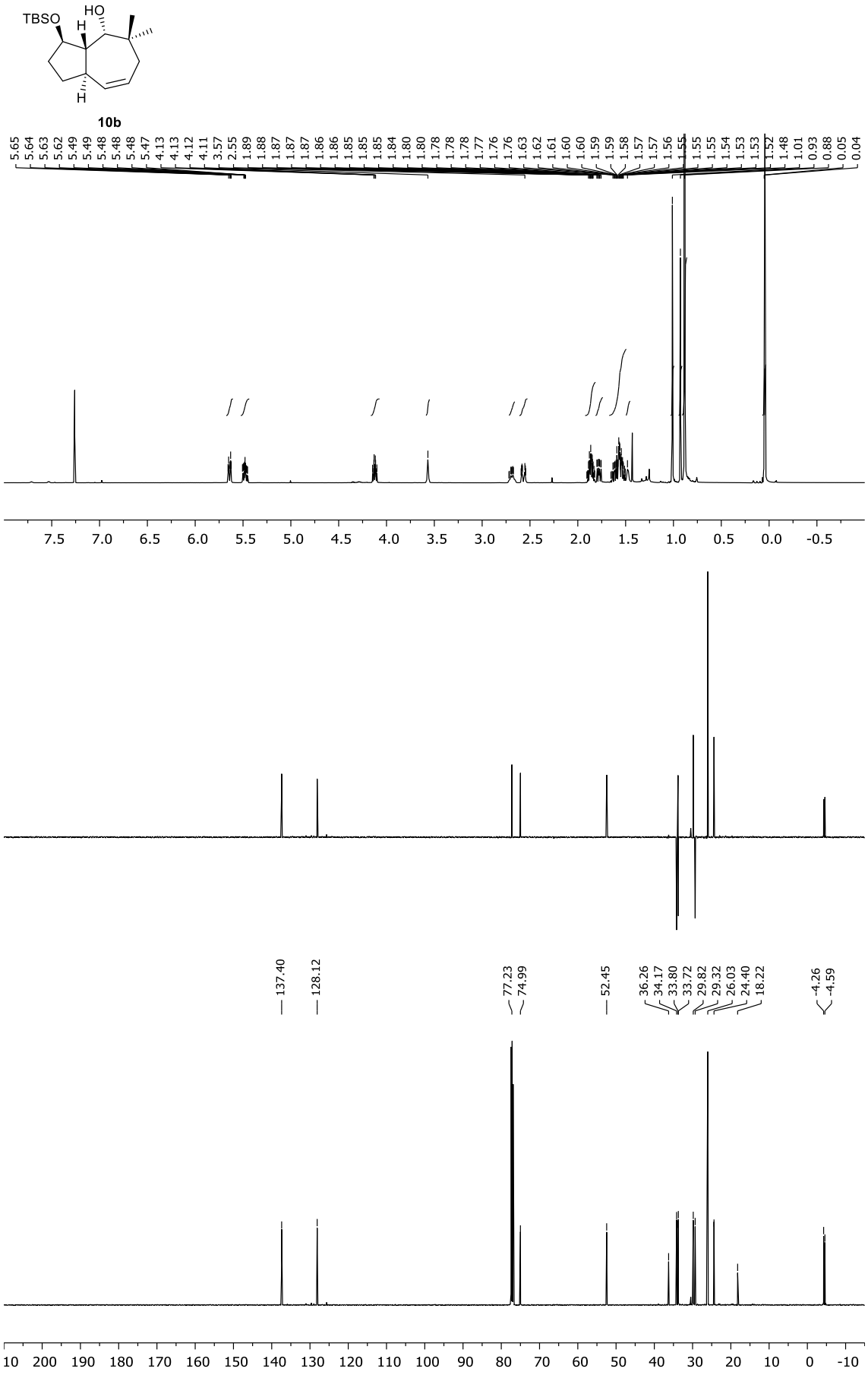
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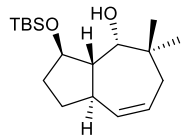

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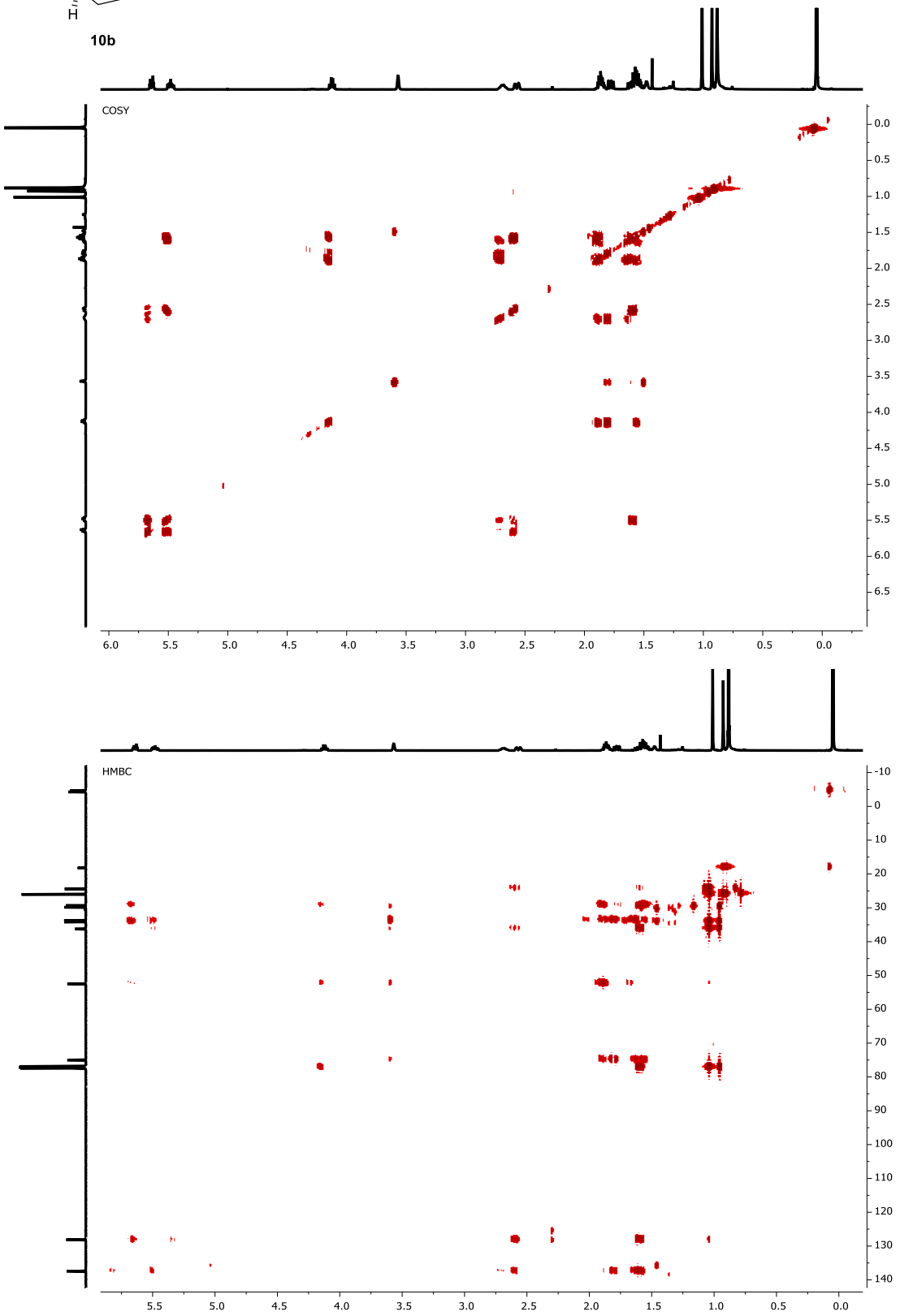

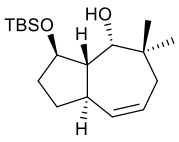
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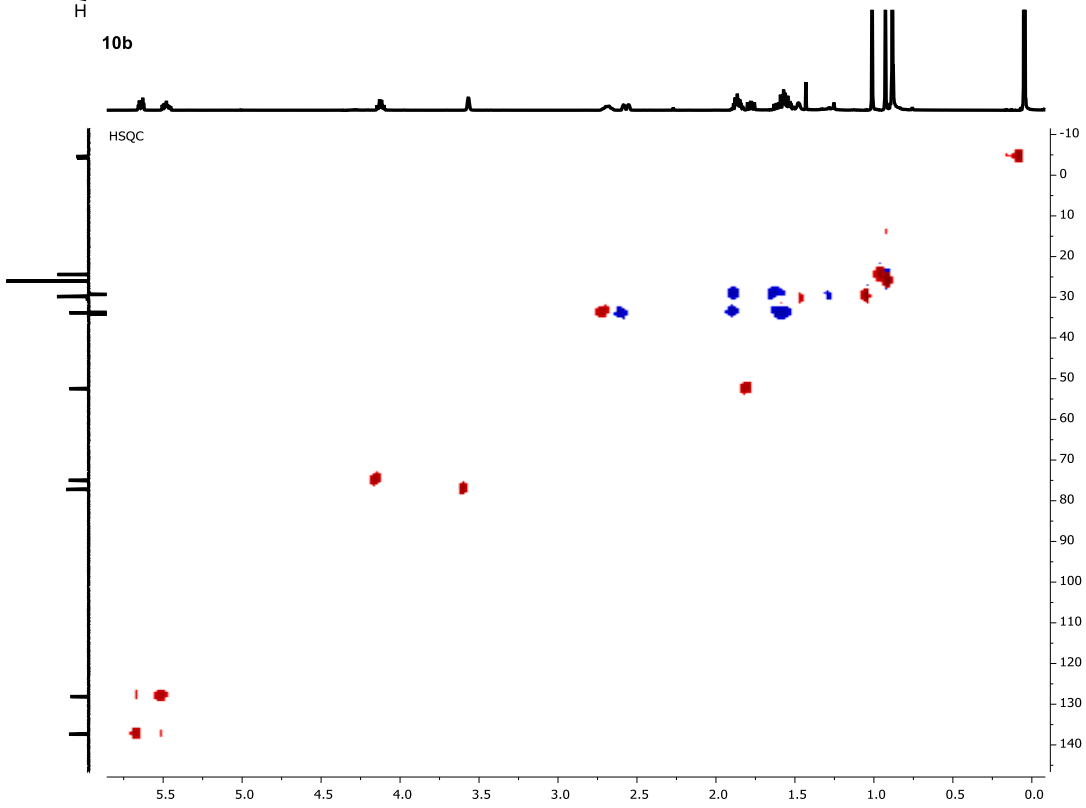
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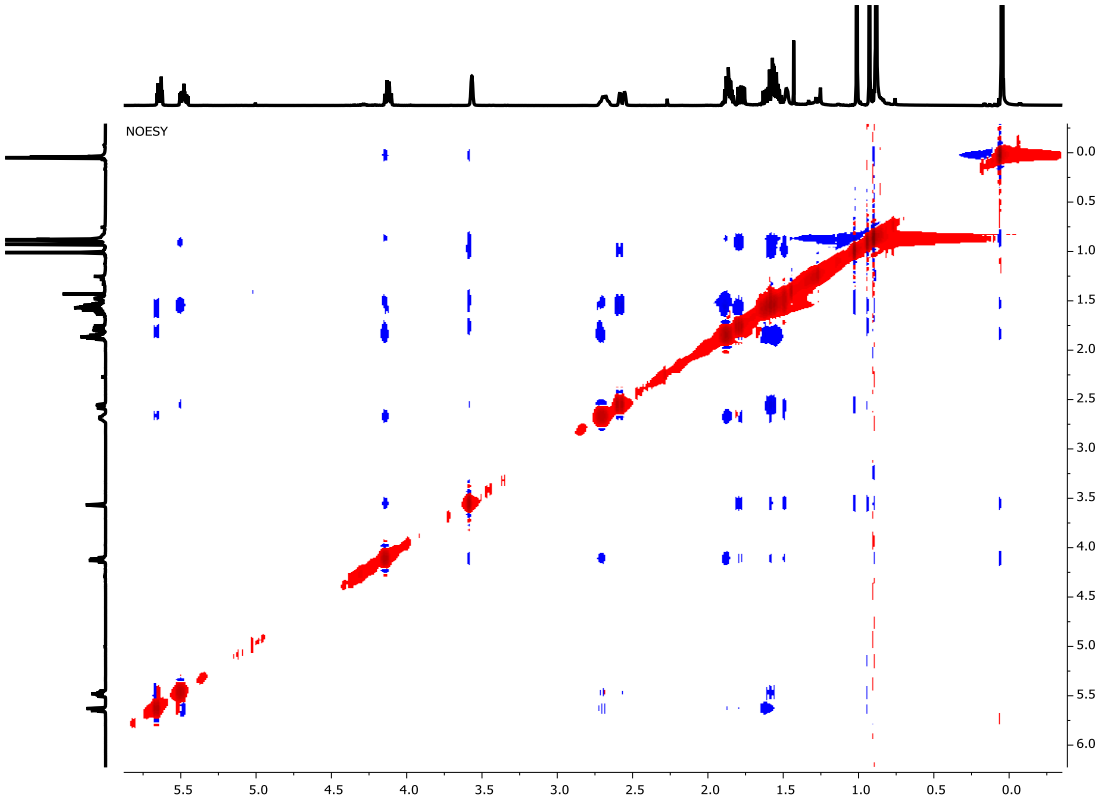
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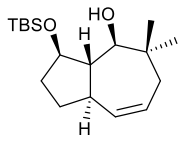
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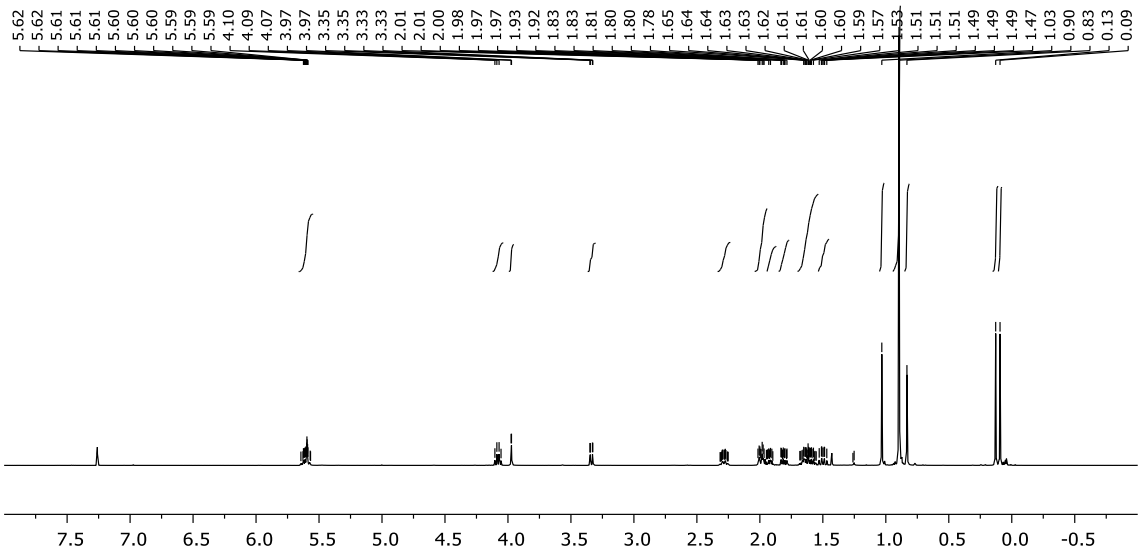
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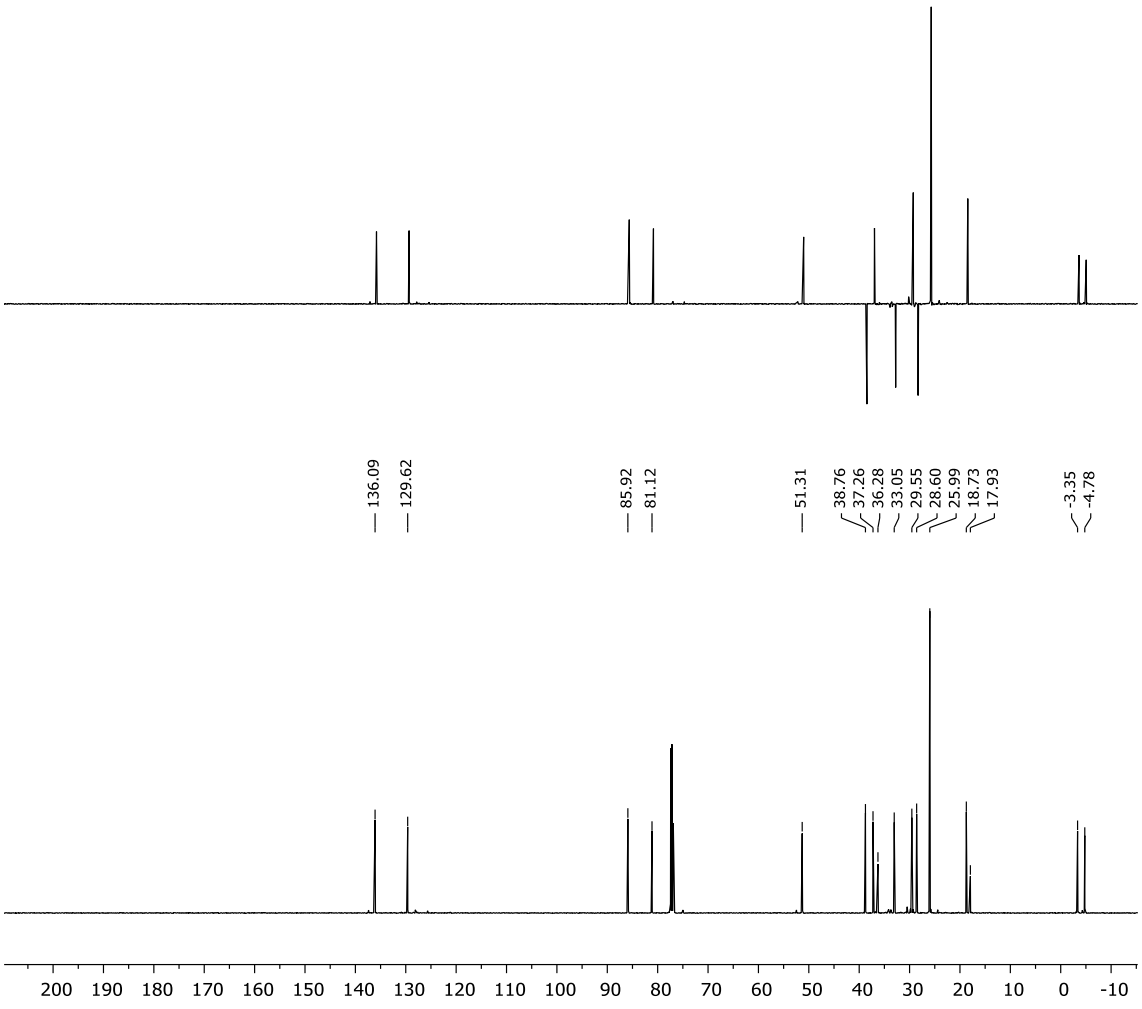
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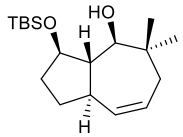
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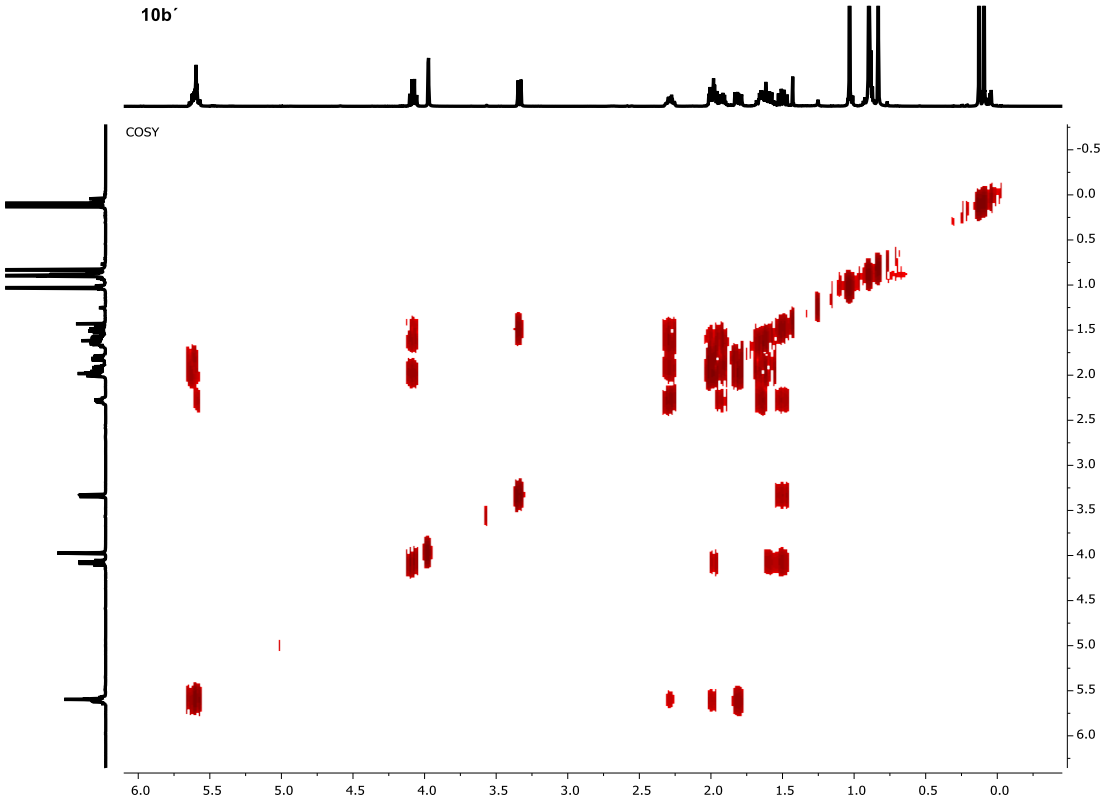
10b´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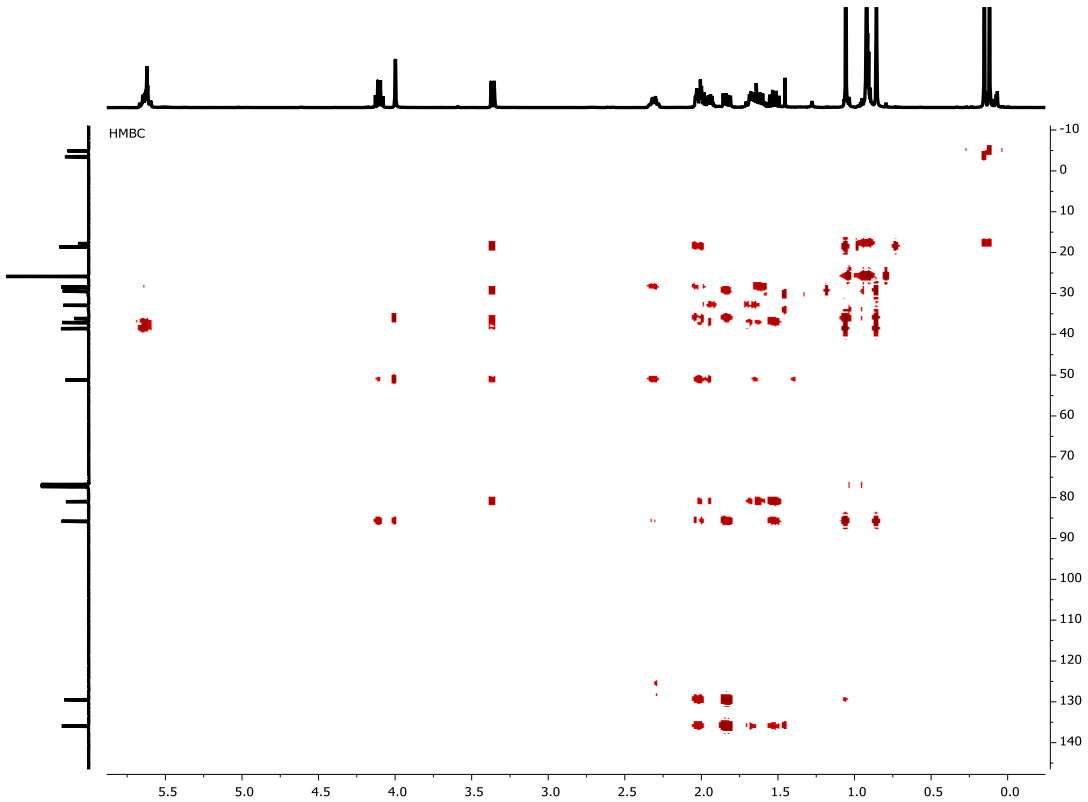
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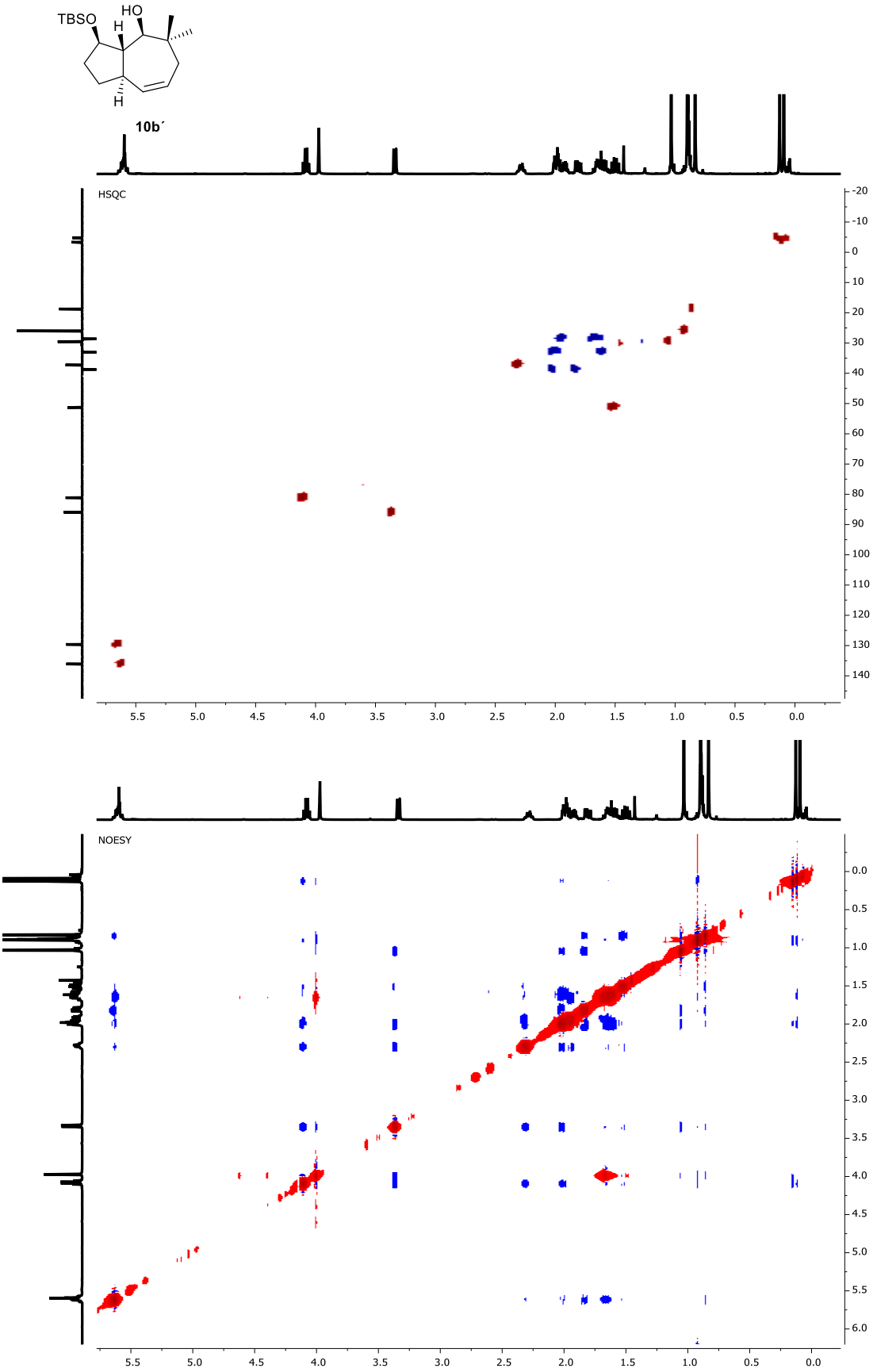
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10b´
HSQC
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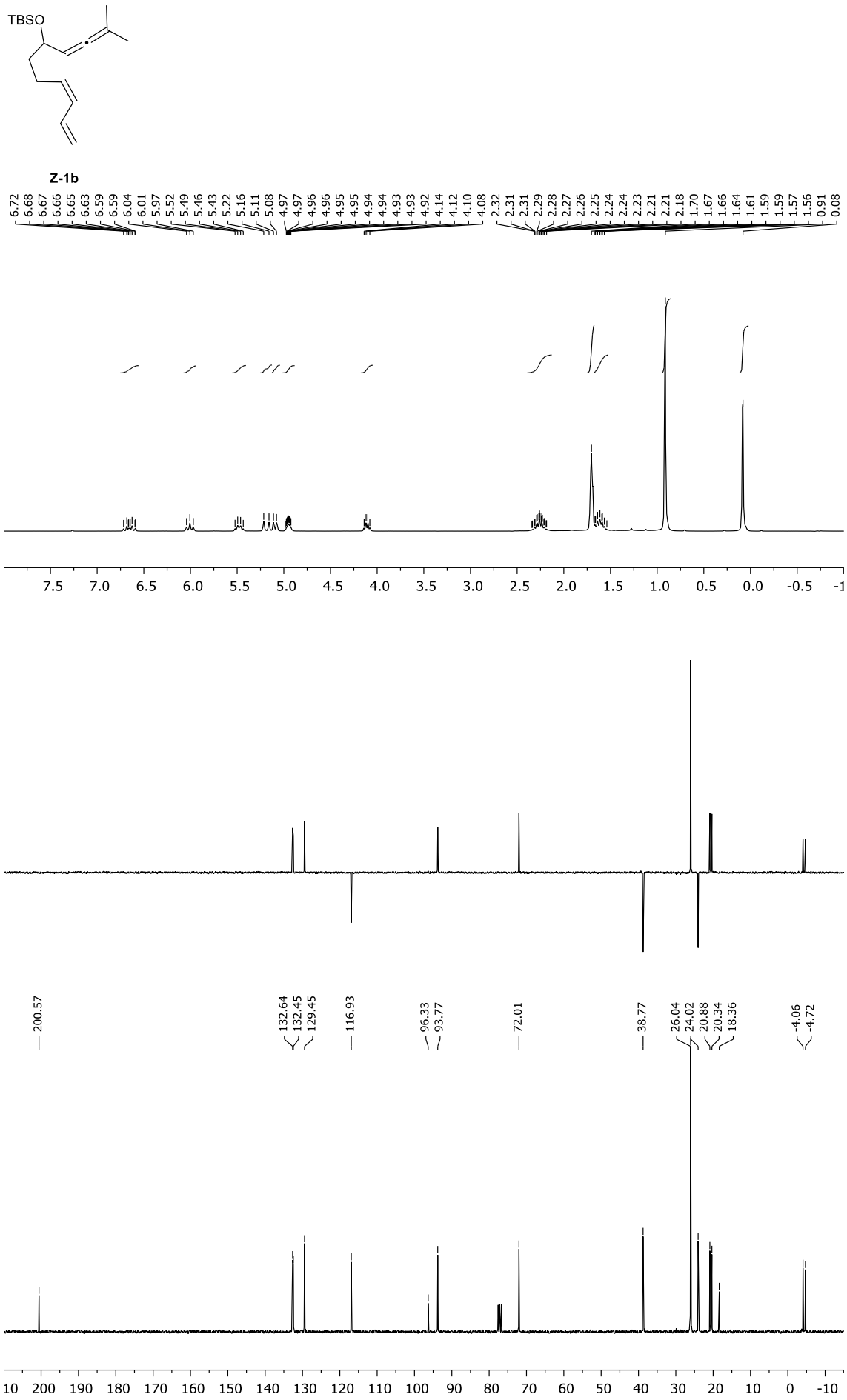
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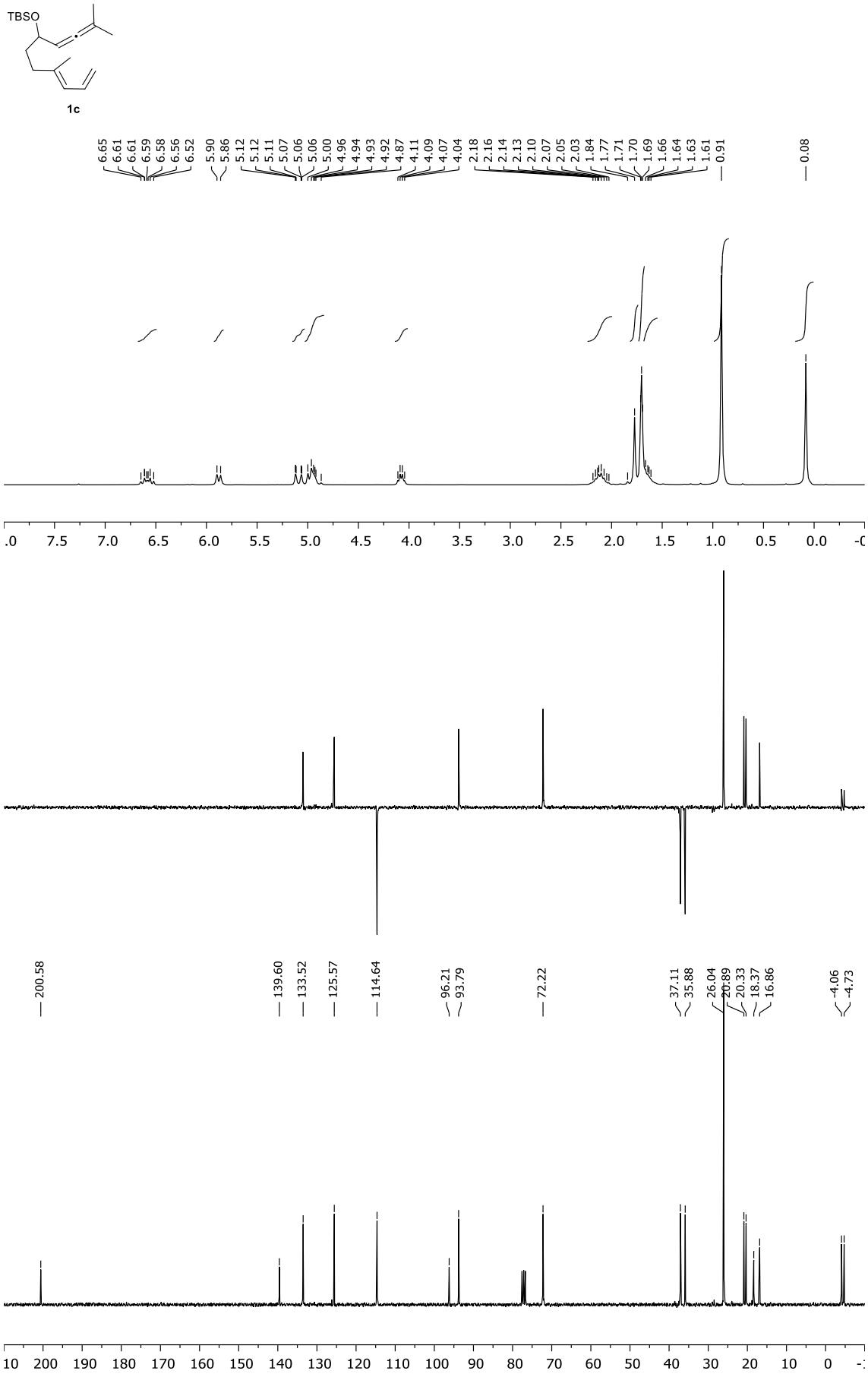
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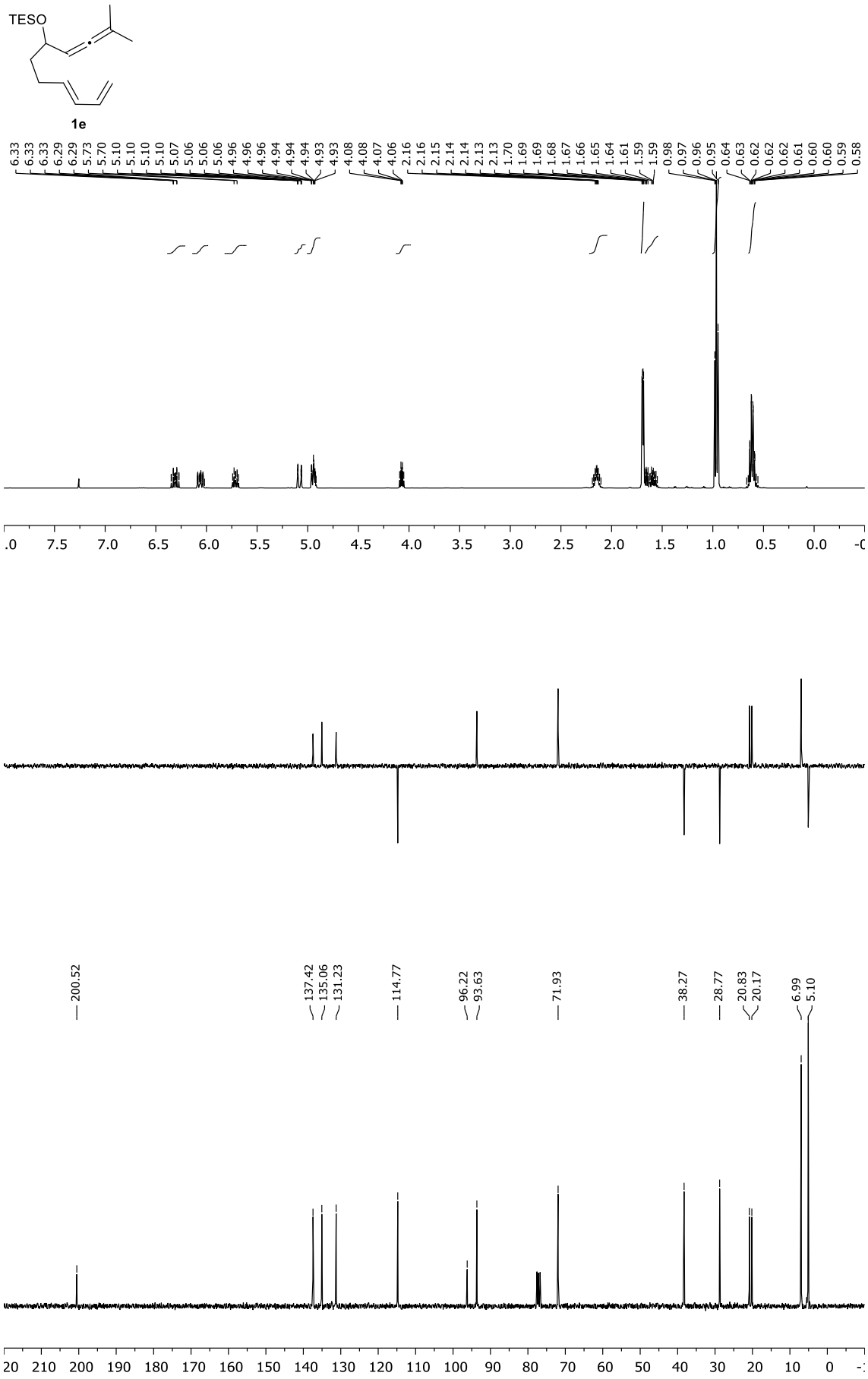
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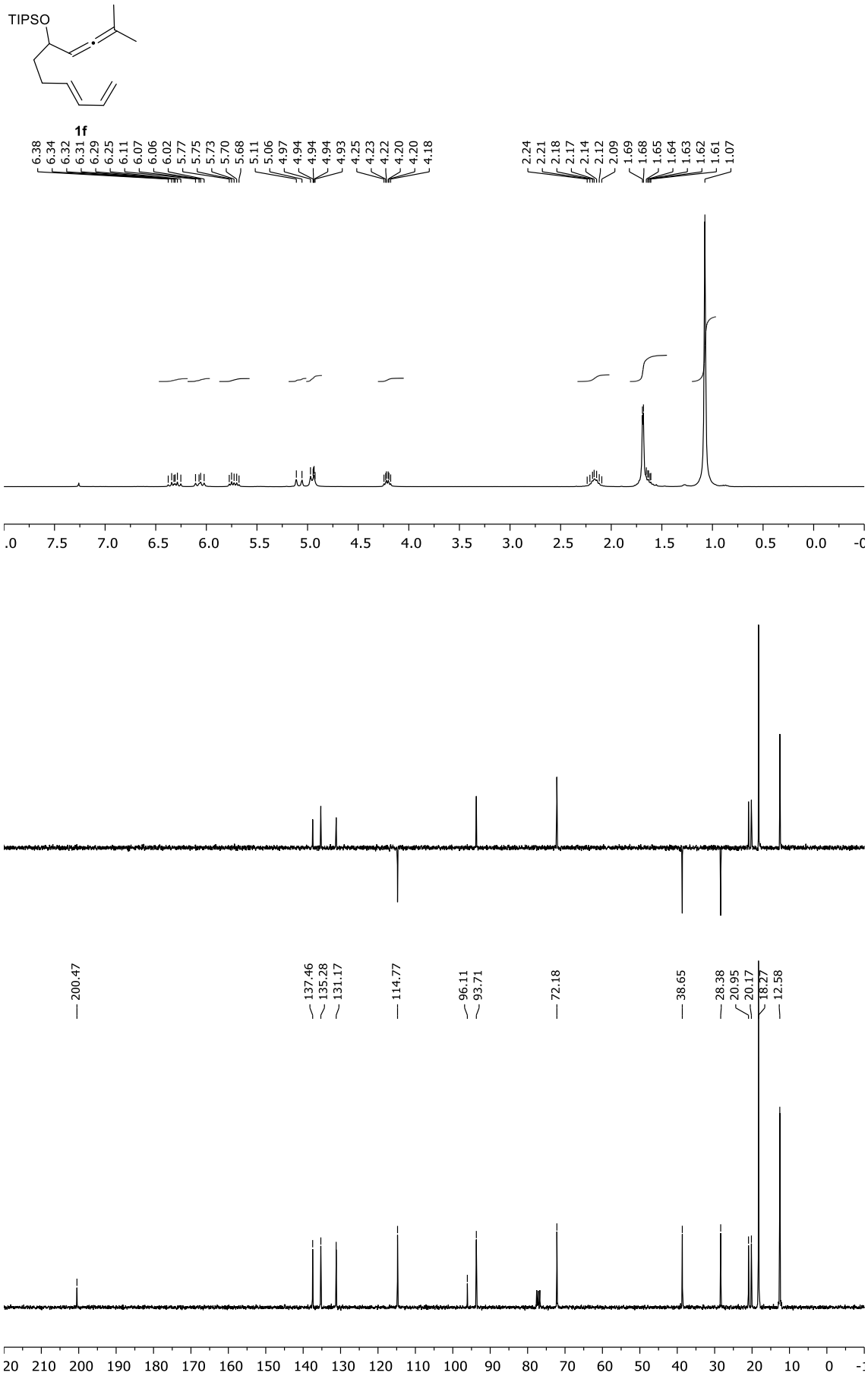
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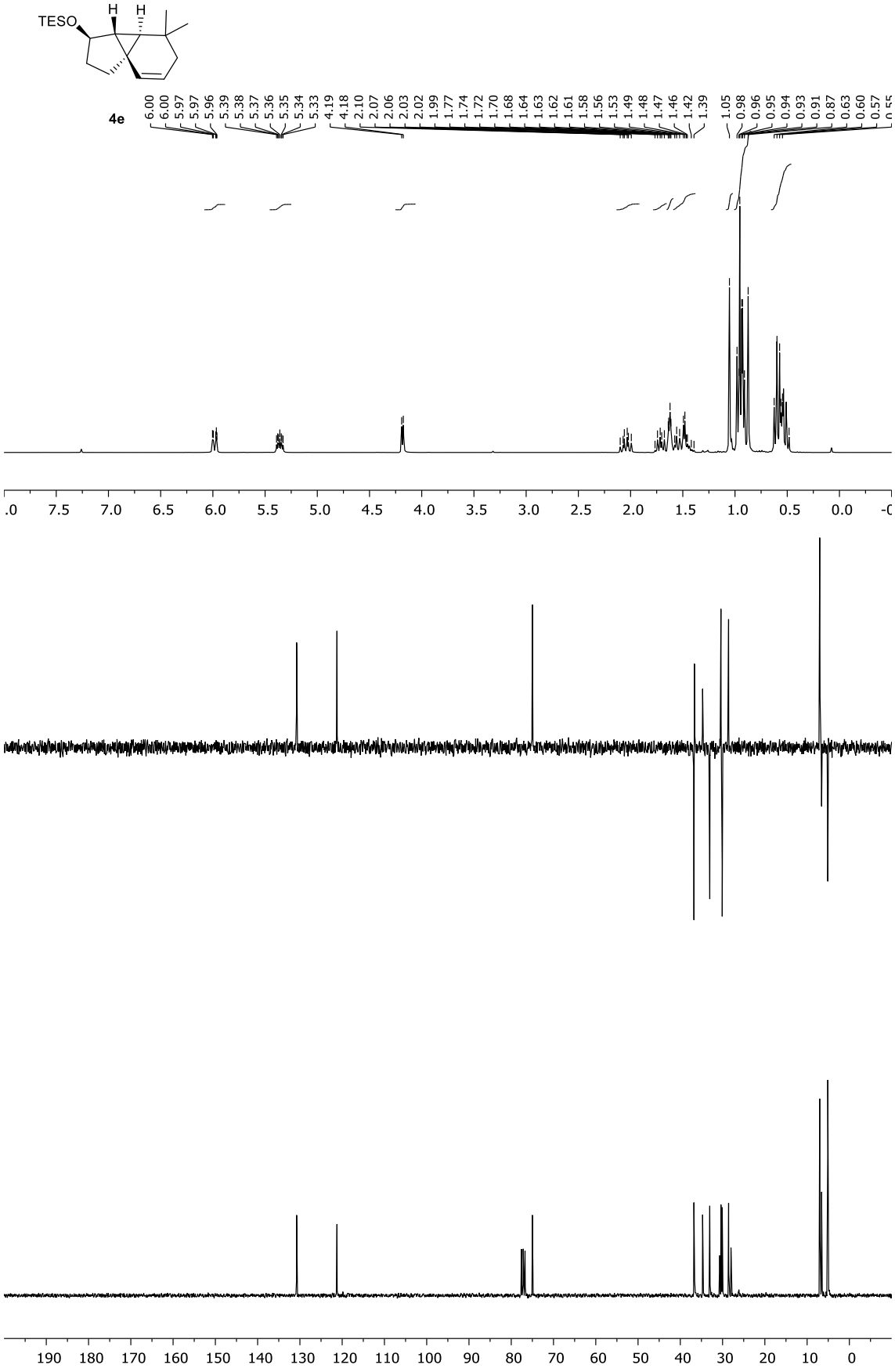
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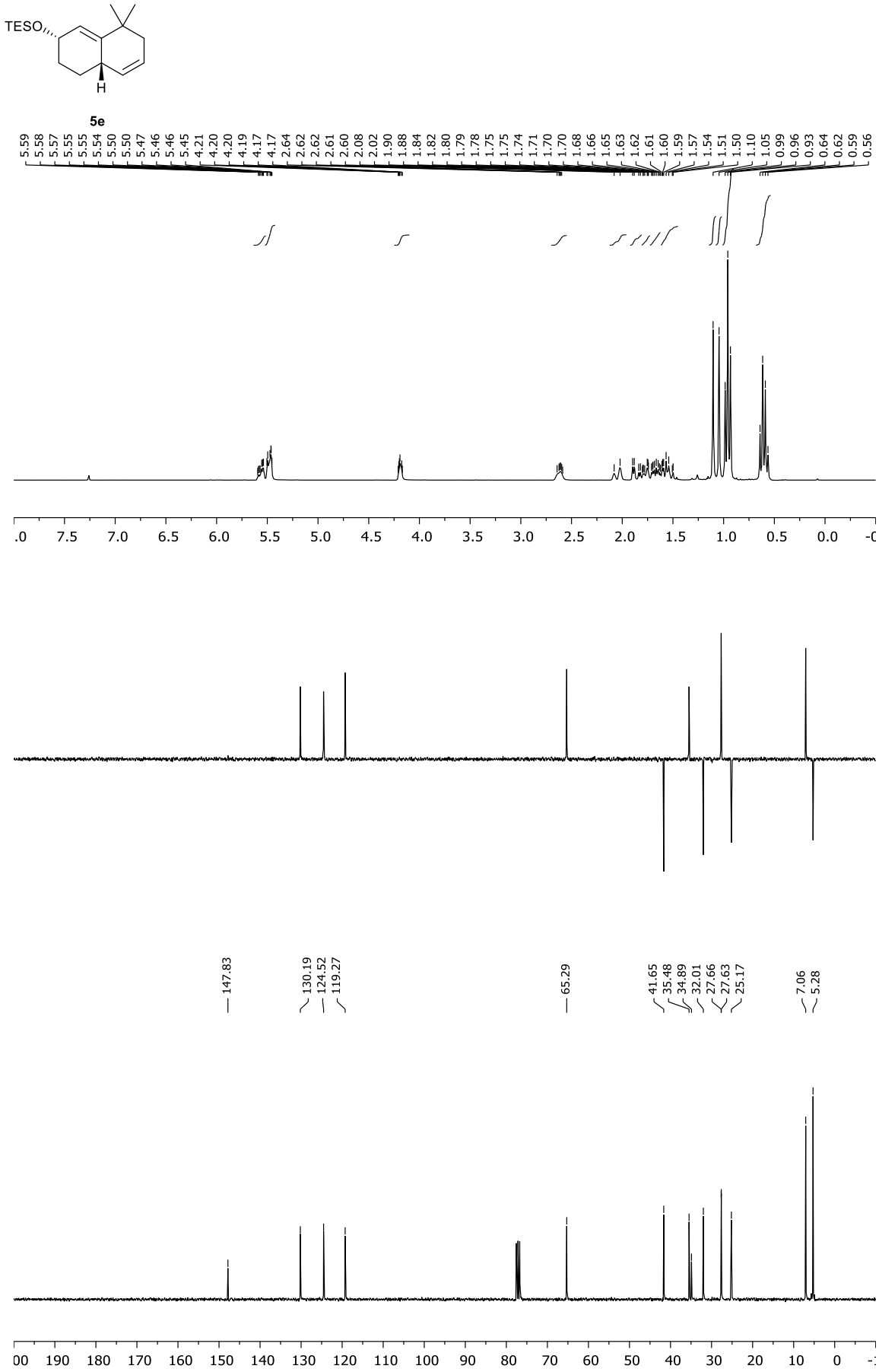
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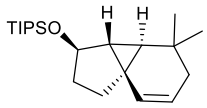
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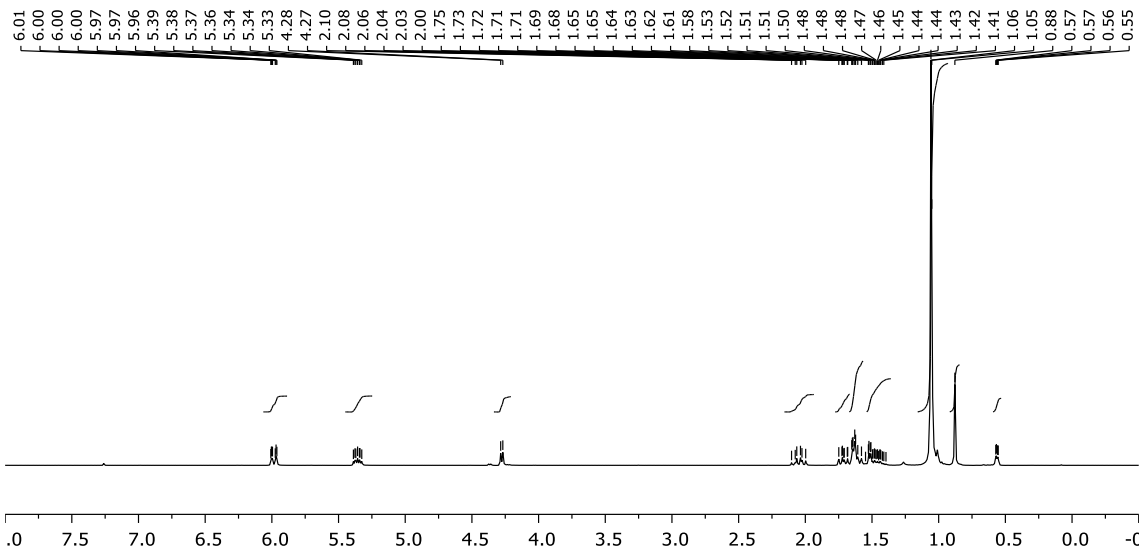
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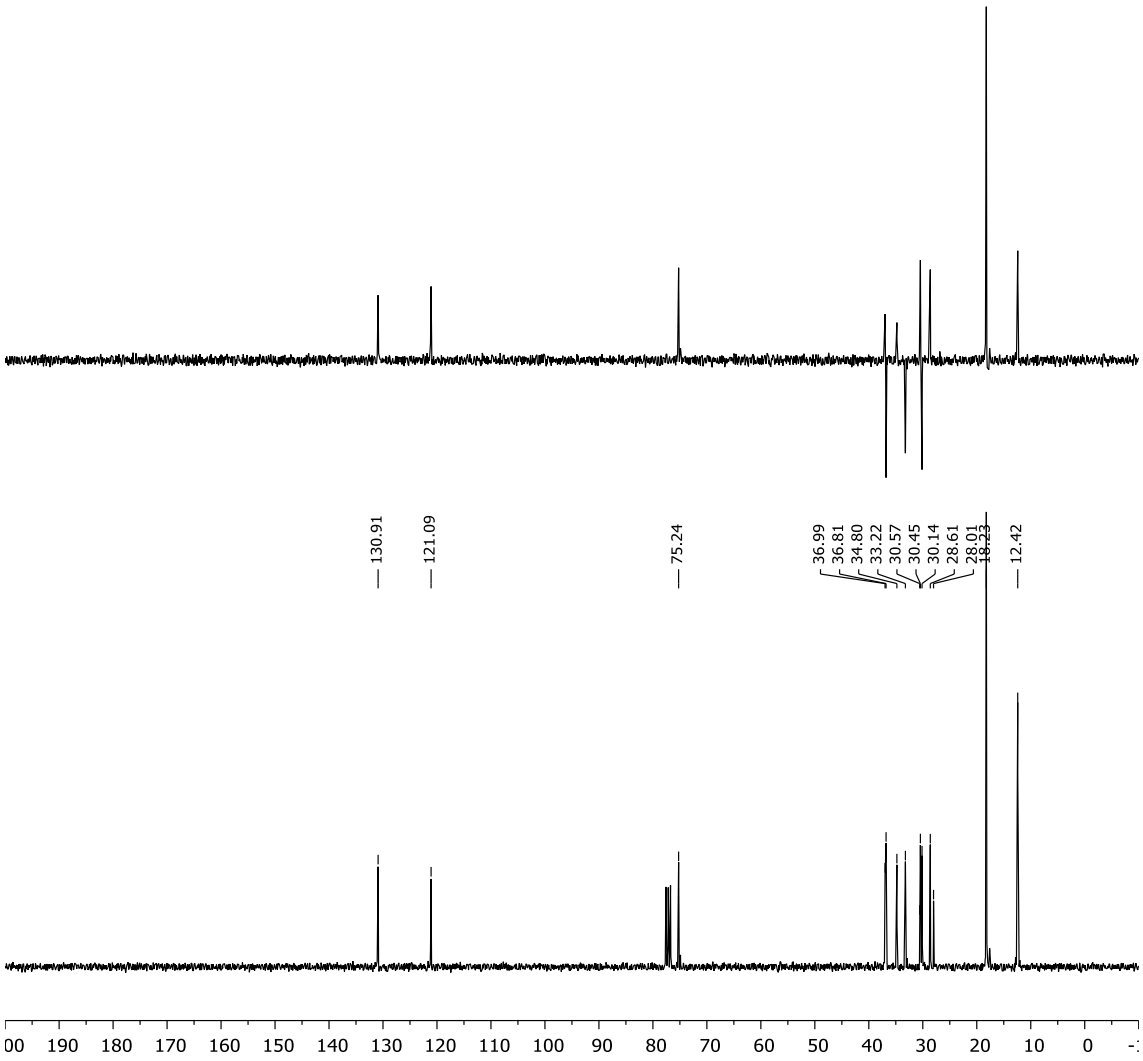
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121.09
75.24
36.99
36.81
34.80
33.22
30.57
30.45
30.14
28.61
28.01
18.23
12.42
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
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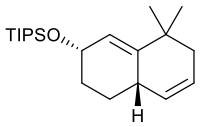
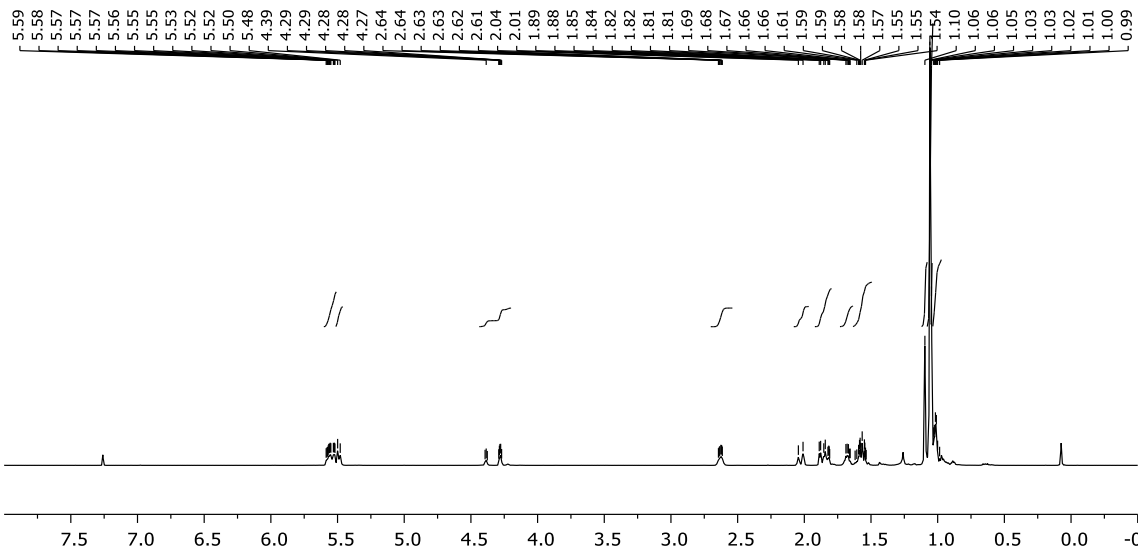
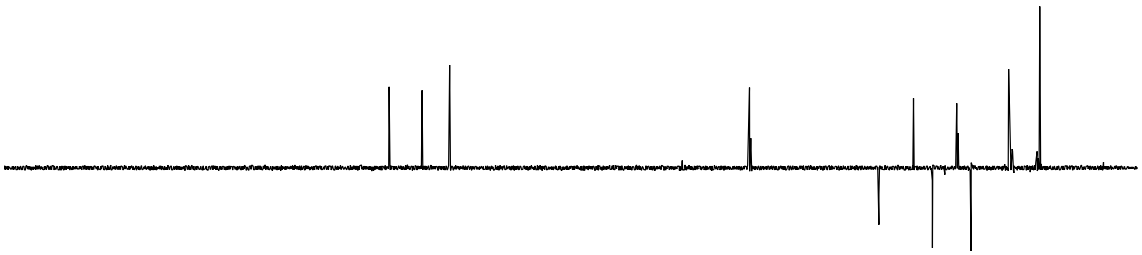
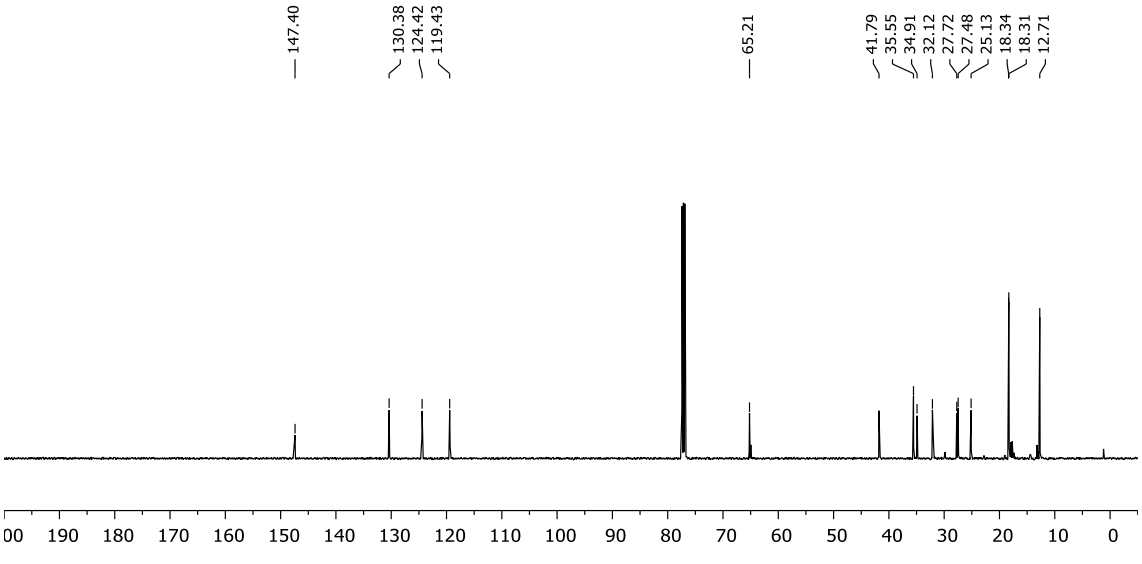

TIPSO
H

5f


5.59 5.58 5.57 5.57 5.57 5.56 5.55 5.55 5.53 5.52 5.52 5.50 5.48 4.39 4.29 4.29 4.28 4.28 4.27 2.64 2.64 2.63 2.63 2.62 2.61 2.04 2.01 1.89 1.88 1.85 1.84 1.82 1.82 1.81 1.81 1.69 1.68 1.67 1.66 1.66 1.61 1.59 1.59 1.58 1.58 1.57 1.55 1.55 1.54 1.10 1.06 1.06 1.05 1.03 1.03 1.02 1.01 1.00 0.99
7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0




147.40
130.38
124.42
119.43
65.21
41.79
35.55
34.91
32.12
27.72
27.48
25.13
18.34
18.31
12.71
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

9. References

[1] Compound **S1** was synthesized following a slightly modified procedure described in: A. G. Ross, X. Li and S. J. Danishefsky, *J. Am. Chem. Soc.*, 2012, **134**, 16080–16084.

[2] (*E*)-*N*-Methoxy-*N*,5-dimethylhepta-4,6-dienamide is known and was synthesized as described in: R. Nelson, M. Gulías, J. L. Mascareñas and F. López, *Angew. Chemie - Int. Ed.*, 2016, **55**, 14359–14363.

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