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The Effect of the C5-Substituent on Regioselectivity in the Rh(I)-Catalyzed Intermolecular Transannulation of 1,2,3-Thiadiazoles with Phenylacetylene

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Table of Contents

1. General Information

1.1. Reagents and Solvents

In general, all compounds were commercially available (Sigma Aldrich/Merck, Alfa Aesar and Combi Blocks) and used as received unless otherwise stated. Ethyl 1,2,3-thiadiazole-4-carboxylates **1** were prepared by the previously reported methods.[1] For all air - or moisture-sensitive procedures the solvents were degassed using the freeze-pump-thaw method, and stored under an inert atmosphere in glass ampoules fitted with a J. Young's Teflon valve. Chlorobenzene and 2-methyltetrahydrofuran were purchased from Aldrich, refluxed over CaH_2 prior to distillation and degassed using the freeze-pump-thaw method. Tetrahydrofuran was obtained from an LC Technology solvent purification system (SPS) and degassed using the freeze-pump-thaw method, and then distilled from sodium–benzophenone ketyl, which was prepared from commercial sodium dispersion and benzophenone.[2] Deuterated solvents were purchased from Cambridge Stable Isotopes and used as received. The compressed argon (>99.999%) used for the glovebox was obtained from Air Liquide and used as received. The nitrogen gas for the Schlenk line is from in-house liquid nitrogen boil-off. Solvents for columns such as *n*-hexane, and ethyl acetate were technical grade.

1.2. Experimental Techniques

Whether an inert or air atmosphere was used for a reaction is specified in the experimental section. All manipulations that were performed under an inert atmosphere were done so using standard Schlenk techniques or in a glovebox (LC Technology Solutions Inc.). The work-up of all reactions and the isolation of products were carried out in a fume hood using standard techniques. The term 'under reduced pressure' refers to use of a rotary evaporator. Components of reactions were visualized using short wavelength UV light (254 nm) on aluminum backed silica gel plates (Sorbfil UV–254).

1.3. Characterization

^{1}H, ^{13}C{^{1}H}, and ^{19}F{^{1}H} NMR spectra were recorded on either a Bruker 400 or 500 MHz (^{1}H) NMR spectrometer. ^{1}H and ^{13}C{^{1}H} NMR chemical shifts were referenced internally using the residual solvent resonance ($CDCl_3$: δ_H = 7.26 ppm; δ_C = 54.0 ppm). ^{19}F{^{1}H} NMR spectra are not calibrated by an internal reference. Coupling constants are represented by *J* in hertz (Hz). Unless otherwise stated, spectra were recorded at 298 K, and chemical shifts (δ) are quoted in parts per million (ppm). Multiplicity is abbreviated as: s (singlet); d (doublet); t (triplet); q (quartet); m (multiplet) and br (broad).

High resolution mass spectrometry (HRMS) analyses were performed on a Q Exactive™ Plus (Thermo Scientific) instrument, with a spray voltage of 4.5 kV.

Melting points were determined using the Stuart SMP10 melting point apparatus in open capillaries and are uncorrected.

The **X-ray data** for the single crystals of **4a**, **6a, 6j** and **8a'** were collected on a SuperNova, Dual, Cu or Mo at home/near, Atlas or Saxi-CrysAlisPro-abstract goniometer imported SAXI images diffractometer. The crystal **4a** was kept at 100.01(10) K, the crystal **6a** was kept at 99.9(3) K and the crystals **6j** was kept at 150.01 (10) K and **8a'** were kept at 150.00(10) K during data collection. In all cases, using Olex2[3], the structure was solved with the olex2.solve[4] structure solution program using Charge Flipping and refined with the SHELXL[5] refinement package using Least Squares minimization.

2. Abbreviations and Structural Formulas of the Precatalysts and Ligands Used

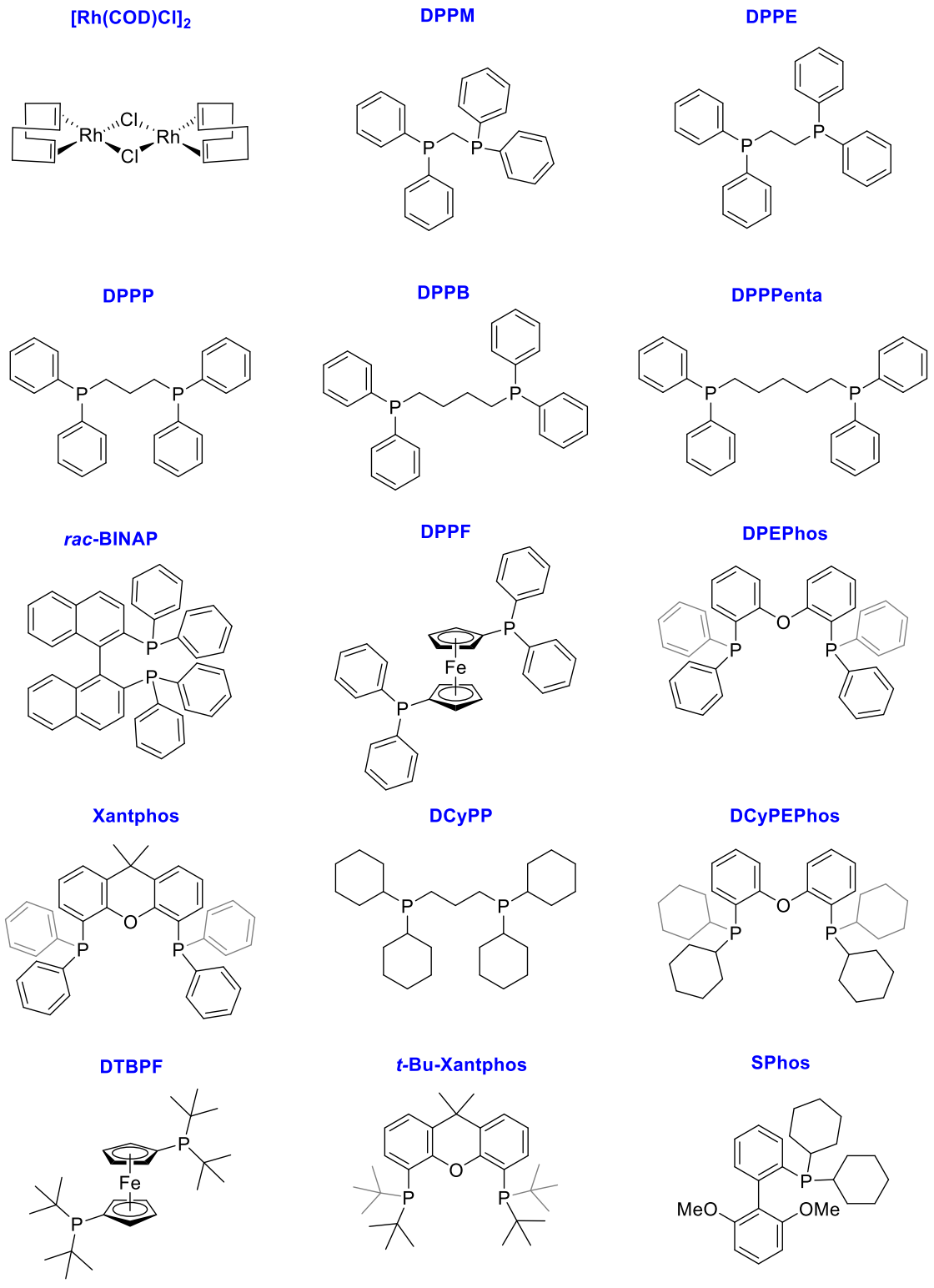


Figure S1. Abbreviations and structural formulas of the precatalysts and ligands used.

3. Differentiation and Assignment of 2,3,4- and 2,3,5-Substituted Thiophene Products

3.1. Assignment of the Thiophenes 3a and 4a

Since 2D NMR spectroscopy does not allow the obtained regioisomeric thiophenes to be distinguished, for unambiguous proof of the formation of 2,3,4-substituted thiophene **4a** as the main product in the case of pyrrolidinyl-derived 1,2,3-thiadiazole **1a**, the reaction products obtained under optimized reaction conditions were isolated as an inseparable regioisomeric mixture (93% **4a** and 7% **3a**) which was further recrystallized from hexane to obtain the crystals of the individual regioisomer. Differentiation of two regioisomers was elucidated by comparison of ^{1}H NMR spectrum of the crude reaction mixture and ^{1}H NMR spectrum of the grown crystals.

The synthetic procedure and full characterization of the mixture of **3a** and **4a** as well as additional crystallographic data for thiophene **4a** are provided on the pages S31 and S53.

3.1.1. X-Ray Crystallographic data of thiophene 4a

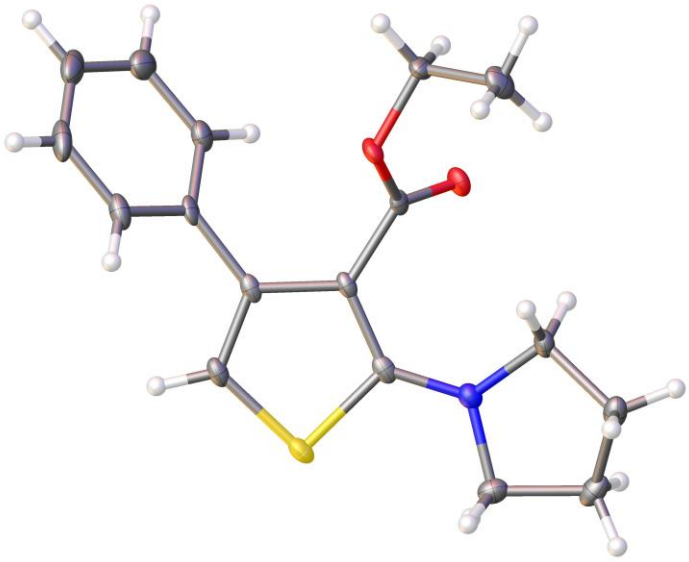
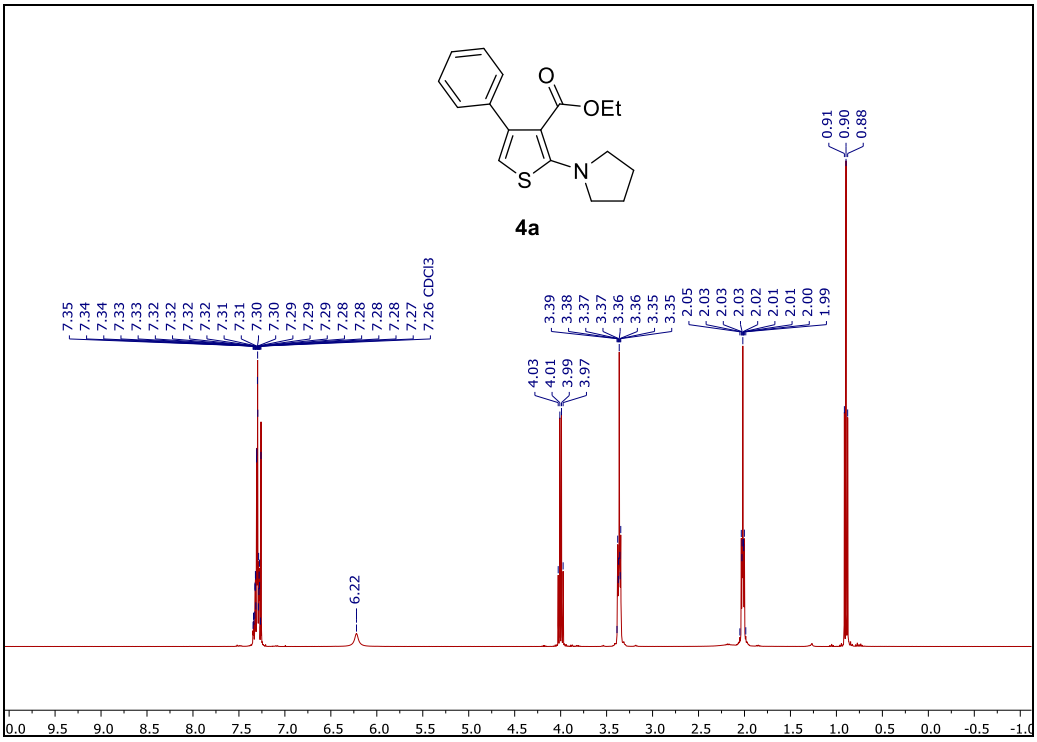


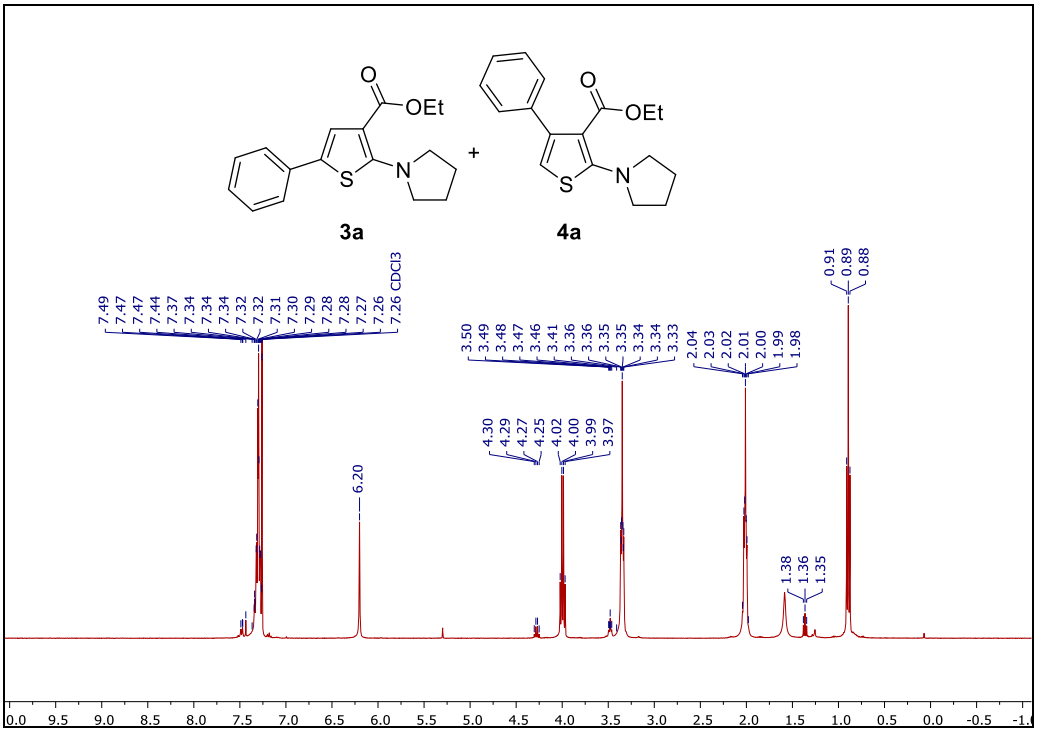
Figure S2. Solid state structure of 2,3,4-substituted thiophene **4a** (grown from *n*-hexane solution). Displacement ellipsoids depicted at the 50% probability level, CCDC: 2219742.

3.1.2. Comparison of the ^{1}H NMR spectra of the isolated crystals of the 2,3,4-substituted thiophene 4a and the purified mixture of 3a and 4a

^{1}H NMR Spectrum of the isolated crystals of 2,3,4-substituted thiophene **4a** (400 MHz, $CDCl_3$)



^{1}H NMR Spectrum of the purified regioisomeric mixture of **3a** and **4a** (400 MHz, $CDCl_3$)



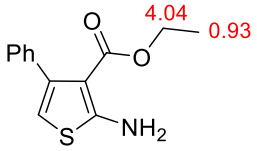
Thus, the combination of ^{1}H NMR spectroscopic and crystallographic data indicates that the Rh(I)-catalyzed intermolecular transannulation of pyrrolidinyl-substituted 1,2,3-thiadiazole **1a** with phenylacetylene leads predominantly to the formation of 2,3,4-substituted thiophene **4a**, which is the opposite of the results earlier reported by Gevorgyan when 2,3,5-substituted regioisomer was the major product.[6]

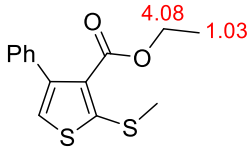
3.2. Assignment of Other Thiophenes

Differentiation of two regioisomers in the case of other thiophene mixtures was elucidated by comparison of their crude ^{1}H NMR spectra through comparison with reported ^{1}H NMR spectra of the corresponding thiophenes, and the data obtained for the pyrrolidinyl-substituted products **3a** and **4a**. Examples of assignment of several obtained thiophenes based on comparison of our experimental and previously reported data are provided on pages S23-26.

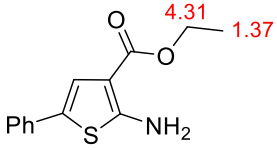
In general, there is a clear trend for thiophenes synthesized from 1,2,3-thiadiazole-4-carboxylates and phenylacetylene − the resonance due to the ester group of 2,3,4-substitued thiophenes **4** always come upfield relative to the 2,3,5-substitued thiophenes **3**. This trend could be additionally supported by comparison of previously reported data for different regioisomeric thiophenes.[7-9]

2,3,4-subsituted thiophenes **4**





2,3,5-subsituted thiophenes **3**

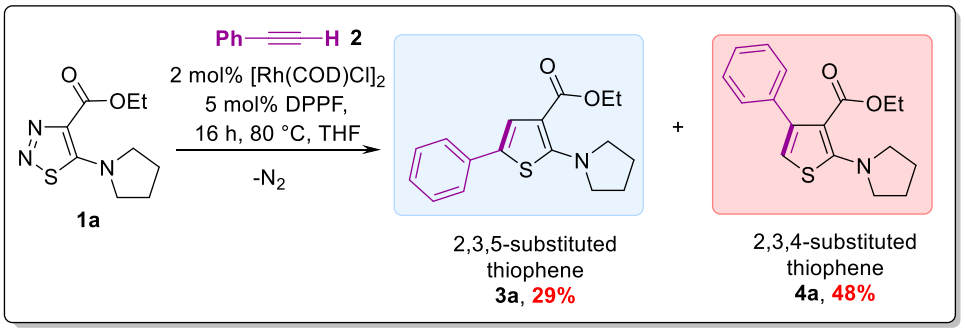


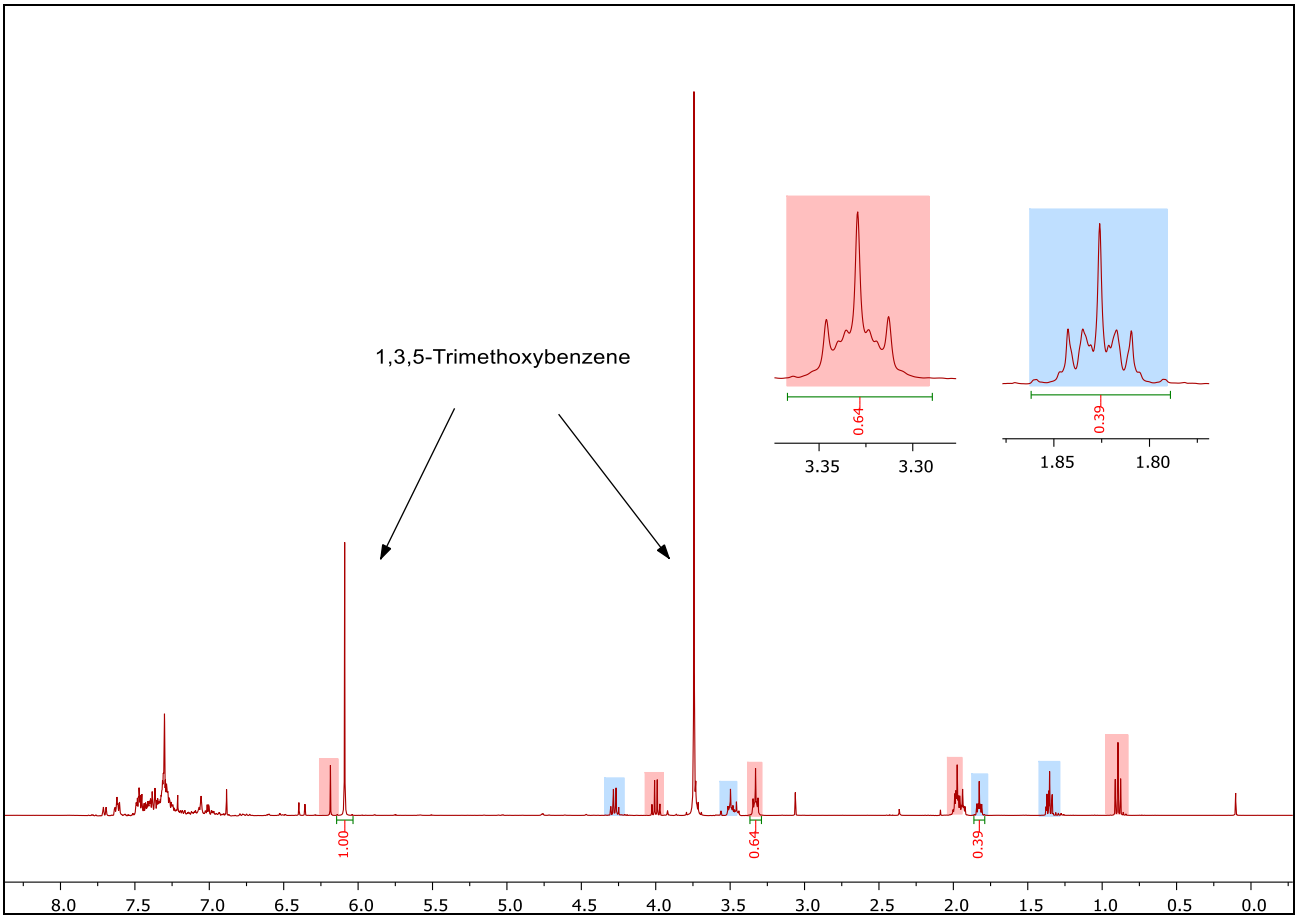
4. General Procedures and Representative ^{1}H NMR Spectra

In a glovebox under Ar atmosphere, a 4 mL vial was charged with 1,2,3-thiadiazole **1** (0.1 mmol, 1.0 equiv), $[Rh(COD)Cl]_2$ (2 mol%, 0.002 mmol) and ligand (5 mol%, 0.005 mmol). Dry degassed THF (0.5 mL) was added to the mixture, followed by phenylacetylene **2** (0.2 mmol, 2 equiv). The vial was capped, removed from the glovebox and placed into an aluminum heating block pre-warmed to 80 °C. The reaction mixture was heated at 80 °C for 16 h. After 16 h, the mixture was allowed to cool to room temperature and 1,3,5-trimethoxybenzene internal standard (0.1 mmol, 1 equiv) was added to the crude reaction mixture. The mixture was concentrated carefully under a flow of N_2 and additionally dried under vacuum to remove the majority of the solvent used. The dried sample was then dissolved in $CDCl_3$ and analyzed using ^{1}H NMR spectroscopy.

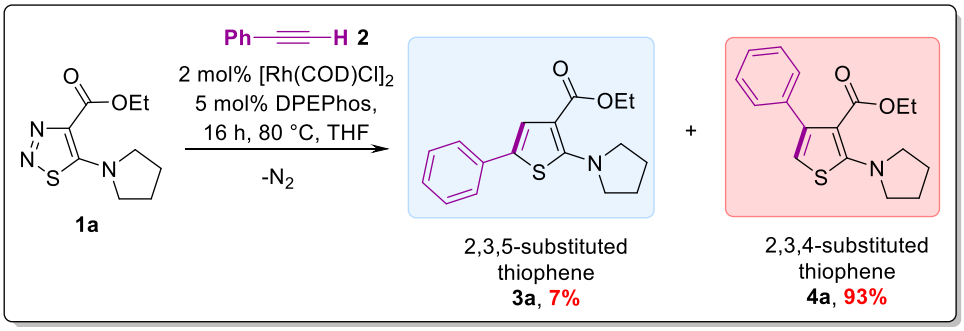
When analyzing the spectra for quantification, the resonances used were selected so that there was the least possible overlap with other resonances.

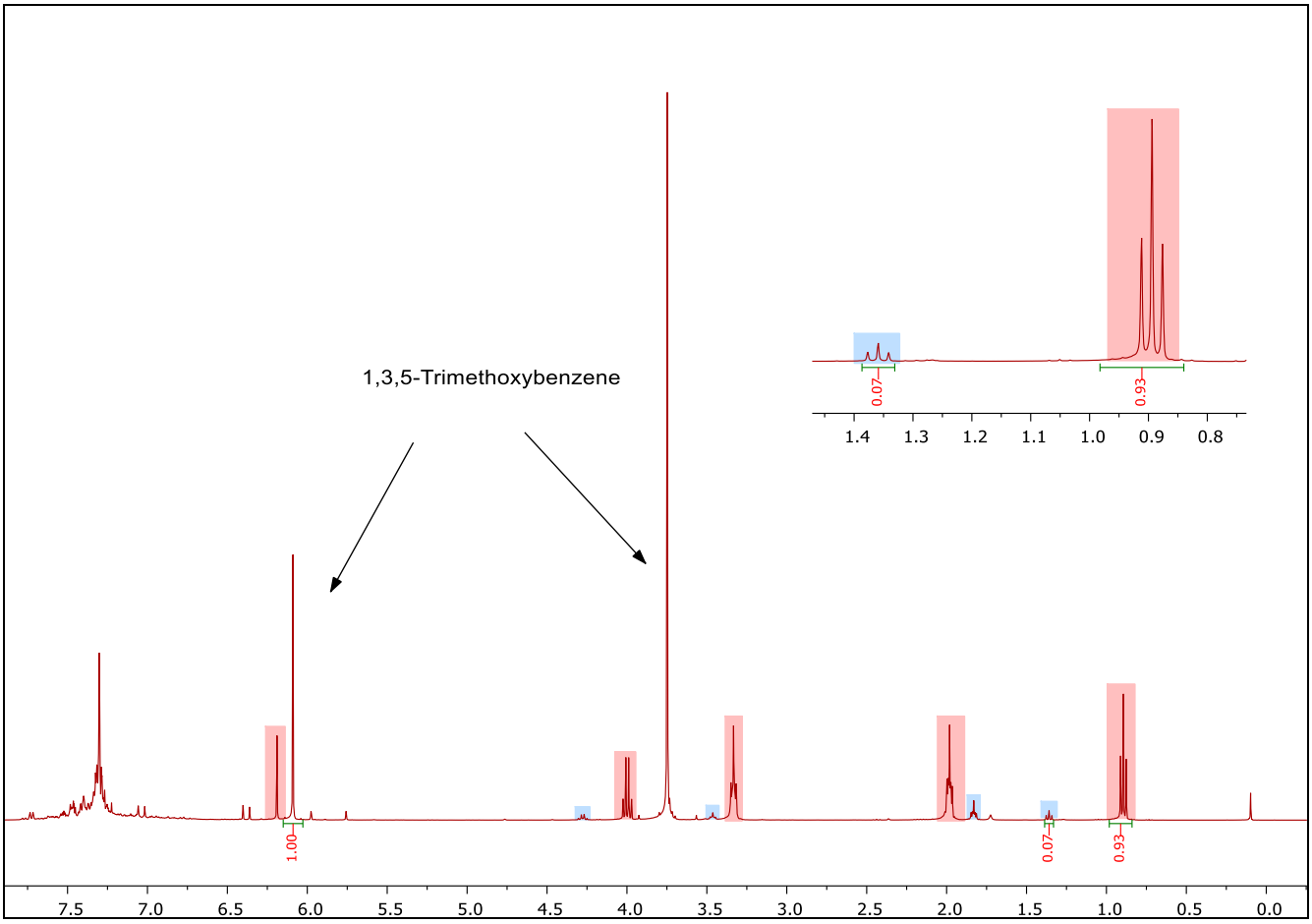
^{1}H NMR spectrum of the crude reaction mixture of **3a** and **4a** (400 MHz, $CDCl_3$)





^{1}H NMR spectrum of the crude reaction mixture of **3a** and **4a** (400 MHz, $CDCl_3$)

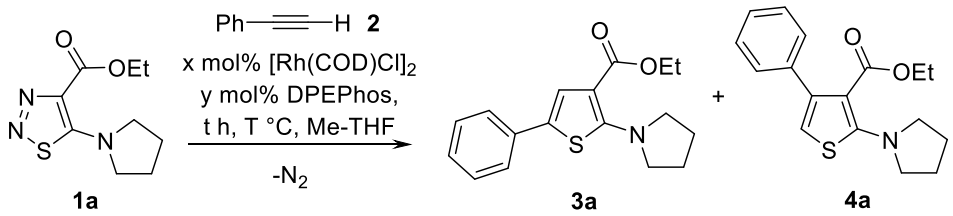




5. Additional Optimization Studies of Transannulation of 1,2,3-Thiadiazoles with Phenylacetylene

5.1. Optimization of The Transannulation of 1,2,3-Thiaidazole with Phenylacetylene

Table S1. Screening of Temperature, Reaction Time and Rh:DPEPhos Ratio

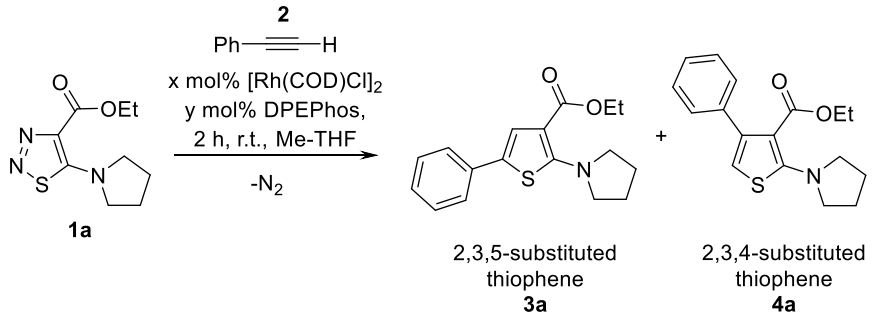


Reaction conditions: 1a (0.1 mmol, 1.0 equiv), $[Rh(COD)Cl]_2$ (mol% indicated below), DPEPhos (mol% indicated below) and phenylacetylene **2** (0.2 mmol, 2.0 equiv) in dry degassed Me-THF (0.5 mL) were left at the specified temperature in a 4 mL vial under an Ar atmosphere for 2, 6 or 16 h. At the end of the specified time, the mixture was allowed to cool to room temperature and 1,3,5-trimethoxybenzene internal standard (0.1 mmol, 1 equiv) was added to the crude reaction mixture. The mixture was concentrated carefully under a flow of N_2 and additionally dried under vacuum to remove the majority of the solvent used. The dried sample was then dissolved in $CDCl_3$ and analyzed using ^1H NMR spectroscopy. When analyzing the spectra for quantification, the resonances used were selected so that there was the least possible overlap with other resonances.

Entry	$[Rh(COD)Cl]_2$, mol %	DPEPhos, mol%	T, °C	Time, h	3a, %	4a, %	1a, %
1	2	5	80	16	4	96	0
2	2	5	80	6	5	95	0
2	2	5	80	2	7	93	0
3	2	5	60	6	5	95	0
4	2	5	60	2	5	95	0
5	2	5	r.t.	2	4	96	0
6[a]	2	5	r.t.	2	5	95	0
7	1	2.5	r.t.	2	7	93	0

[a] Reaction was performed using different order of mixing. **1a** was added to pre-prepared Me-THF solution of $[Rh(COD)Cl]_2$ and DPEPhos.

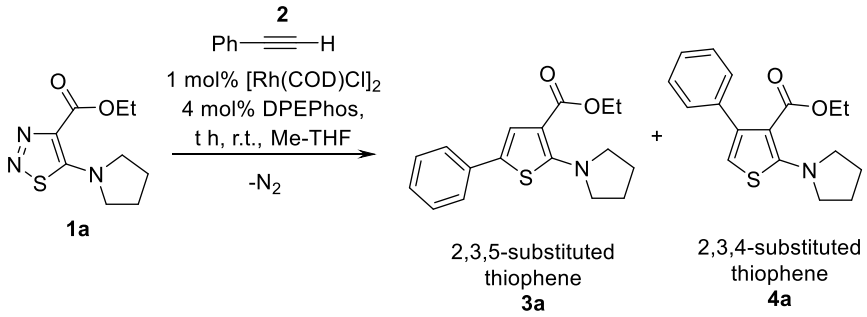
Table S2. Additional Screening of Rh:DPEPhos Ratio using Large Scale Reactions



Reaction conditions: 1a (0.4 mmol, 1.0 equiv), $[Rh(COD)Cl]_2$ (mol% indicated below), DPEPhos (mol% indicated below) and phenylacetylene **2** (0.8 mmol, 2.0 equiv) in dry degassed Me-THF (2.0 mL) were left at room temperature in an 18 mL vial under an Ar atmosphere for 2 h. After 2 h, 1,3,5-trimethoxybenzene internal standard (0.1 mmol, 0.25 equiv) was added to the crude reaction mixture. An aliquot of the reaction mixture was collected and concentrated carefully to dryness under a flow of N_2 and additionally dried under vacuum to remove the majority of the solvent used. The dried sample was then dissolved in $CDCl_3$ and analyzed using ^1H NMR spectroscopic analysis. When analyzing the spectra for quantification, the resonances used were selected so that there was the least possible overlap with other resonances.

Entry	$[Rh(COD)Cl]_2$, mol %	DPEPhos, mol%	Time, h	3a, %	4a, %	1a, %
1	1	2.5	2	4	67	29
2	1	3.0	2	6	82	12
3	1	4.0	2	7	92	0

Table S3. Additional Screening of Reaction Time Using Large Scale Reactions

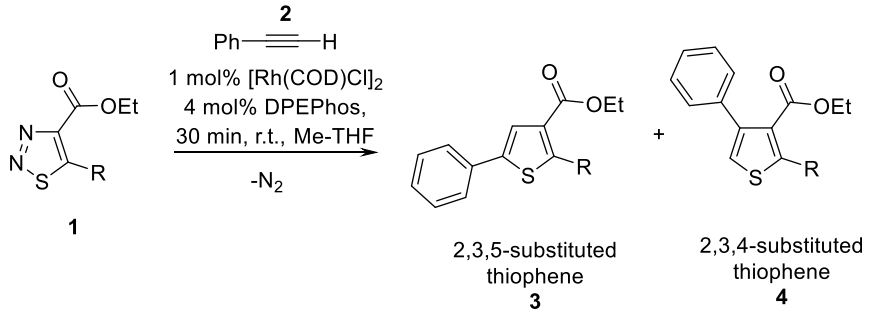


Reaction conditions: 1a (0.4 mmol, 1.0 equiv), $[Rh(COD)Cl]_2$ (1 mol%, 0.004 mmol), DPEPhos (4 mol%, 0.016 mmol) and phenylacetylene **2** (0.8 mmol, 2.0 equiv) in dry degassed Me-THF (2.0 mL) were left at room temperature in an 18 mL vial under an Ar atmosphere for different periods of time. At the end of the specified time, 1,3,5-trimethoxybenzene internal standard (0.1 mmol, 0.25 equiv) was added to the crude reaction mixture. An aliquot of the reaction mixture was collected and concentrated carefully to dryness under a flow of N_2 and additionally dried under vacuum to remove the majority of the solvent used. The dried sample was then dissolved in $CDCl_3$ and analyzed using ^1H NMR spectroscopic analysis. When analyzing the spectra for quantification, the resonances used were selected so that there was the least possible overlap with other resonances.

Entry	Time, h	3a, %	4a, %	1a, %
1	0.25	6	80	11
2	0.5	6	93	0
3	1.0	6	93	0
4	2.0	6	94	0

5.2. Transannulations of Different C5-Substituted 1,2,3-Thiadiazoles

Table S4. Transannulations of Different C5-Substituted 1,2,3-Thiadiazoles with Phenylacetylene Under Reaction Conditions Optimized for 5-Pyrrolidinyl-substituted Thiadiazole 1a



Reaction conditions: 1 (0.1 mmol, 1.0 equiv), $[Rh(COD)Cl]_2$ (1 mol%, 0.001 mmol), DPEPhos (4 mol%, 0.004 mmol) and phenylacetylene **2** (0.2 mmol, 2.0 equiv) in dry degassed Me-THF (0.5 mL) were left at room temperature in a 4 mL vial under an Ar atmosphere for 30 min. At the end of the specified time, the mixture was allowed to cool to room temperature and 1,3,5-trimethoxybenzene internal standard (0.1 mmol, 1 equiv) was added to the crude reaction mixture. The mixture was concentrated carefully under a flow of N_2 and additionally dried under vacuum to remove the majority of the solvent used. The dried sample was then dissolved in $CDCl_3$ and analyzed using ^1H NMR spectroscopy. When analyzing the spectra for quantification, the resonances used were selected so that there was the least possible overlap with other resonances.

Entry	C5-substituent	3, %	4, %	1, %
1	 (**a**)	6	93	0
2	 (**b**)	3	8	87
3	 (**c**)	12	36	47
4	NMe_2 (**d**)	4	26	63
5	SEt (**e**)	5	45	47
6	OEt (**f**)	7	92	0

Thus, experiments with other ethyl 1,2,3-thiadiazole-4-carboxylates revealed that the reaction conditions optimized using pyrrolidinyl-substituted substrate **1a** are not general and substrates demonstrate different reactivity depending on the nature of the substituent at the C5-position of the heterocycle.

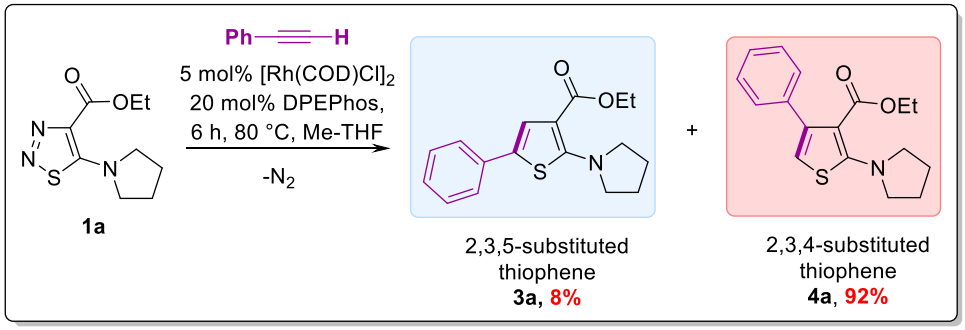
6. General Procedure and ^{1}H NMR Spectra for Regioselectivity Studies

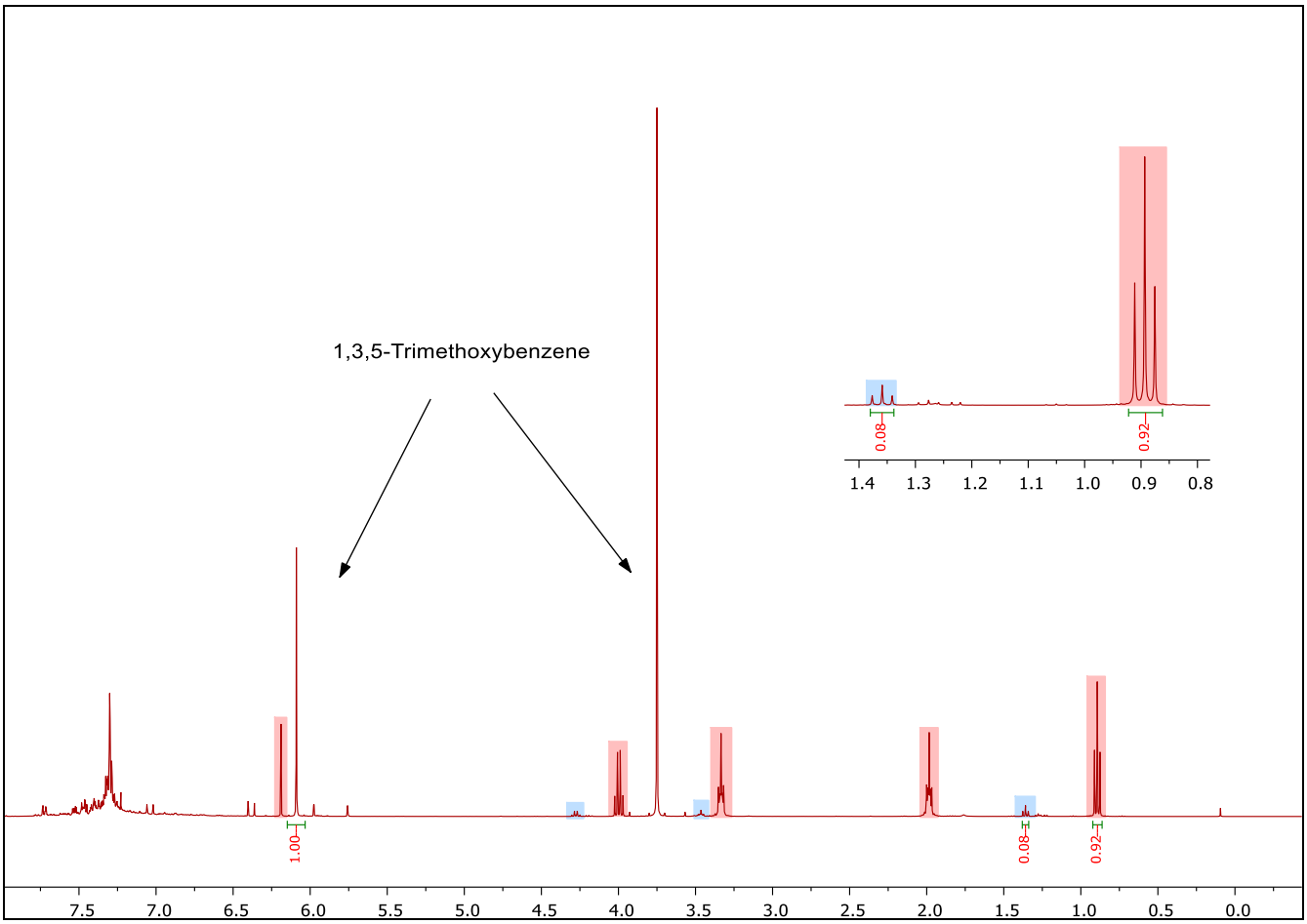
In a glovebox under Ar atmosphere, a 4 mL vial was charged with 1,2,3-thiadiazole **1** (0.1 mmol, 1.0 equiv), $[Rh(COD)Cl]_2$ (5 mol%, 0.005 mmol) and DPEPhos (20 mol%, 0.02 mmol). Dry degassed Me-THF (0.5 mL) was added to the mixture, followed by phenylacetylene **2** (0.2 mmol, 2 equiv). 1,2,3-Thiadiazoles **1k** and **1l** were added as 0.2 M Me-THF solutions. The vial was capped and placed into an aluminum heating block pre-warmed to 80 °C. The reaction mixture was heated at 80 °C for 6 h. After 6 h, the mixture was allowed to cool to room temperature and 1,3,5-trimethoxybenzene internal standard (0.1 mmol, 1 equiv) was added to the crude reaction mixture. The mixture was concentrated carefully under a flow of N_2 and additionally dried under vacuum to remove the majority of the solvent used. The dried sample was then dissolved in $CDCl_3$ and analyzed using ^{1}H NMR spectroscopy. When analyzing the spectra for quantification, the resonances used were selected so that there was the least possible overlap with other resonances.

Given all obtained crude reaction mixtures were clean and easy to analyze (see S17-30), quantitative ^{1}H NMR spectroscopic analysis with a long delay time (20 seconds) and 1,3,5-trimethoxybenzene as an internal standard was used as a reliable and sufficient method for determining the ratio of regioisomers and identifying general experimental regioselectivity trends.

The ^{1}H NMR spectra of purified regioisomeric mixtures **3a** and **4a**, **3b** and **4b** with indicated regioisomeric ratios are included on pages S44−45 to additionally show that analysis of the crude and the purified mixtures provides close regioisomeric ratios and quantitative ^{1}H NMR possesses the required accuracy and precision.

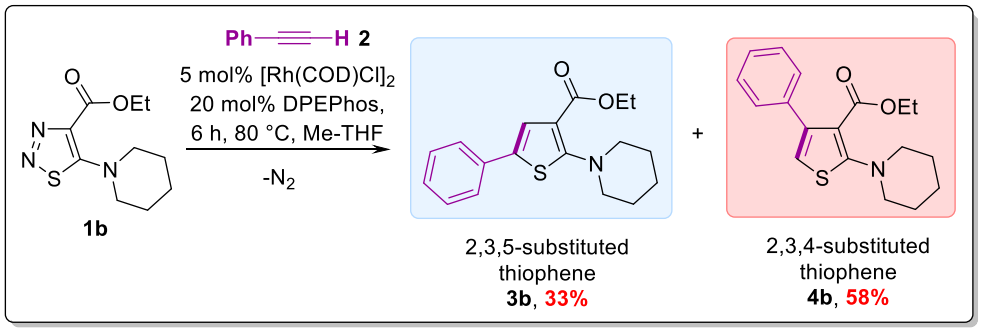
^{1}H NMR Spectrum of the crude reaction mixture of **3a** and **4a** (400 MHz, $CDCl_3$)[b]

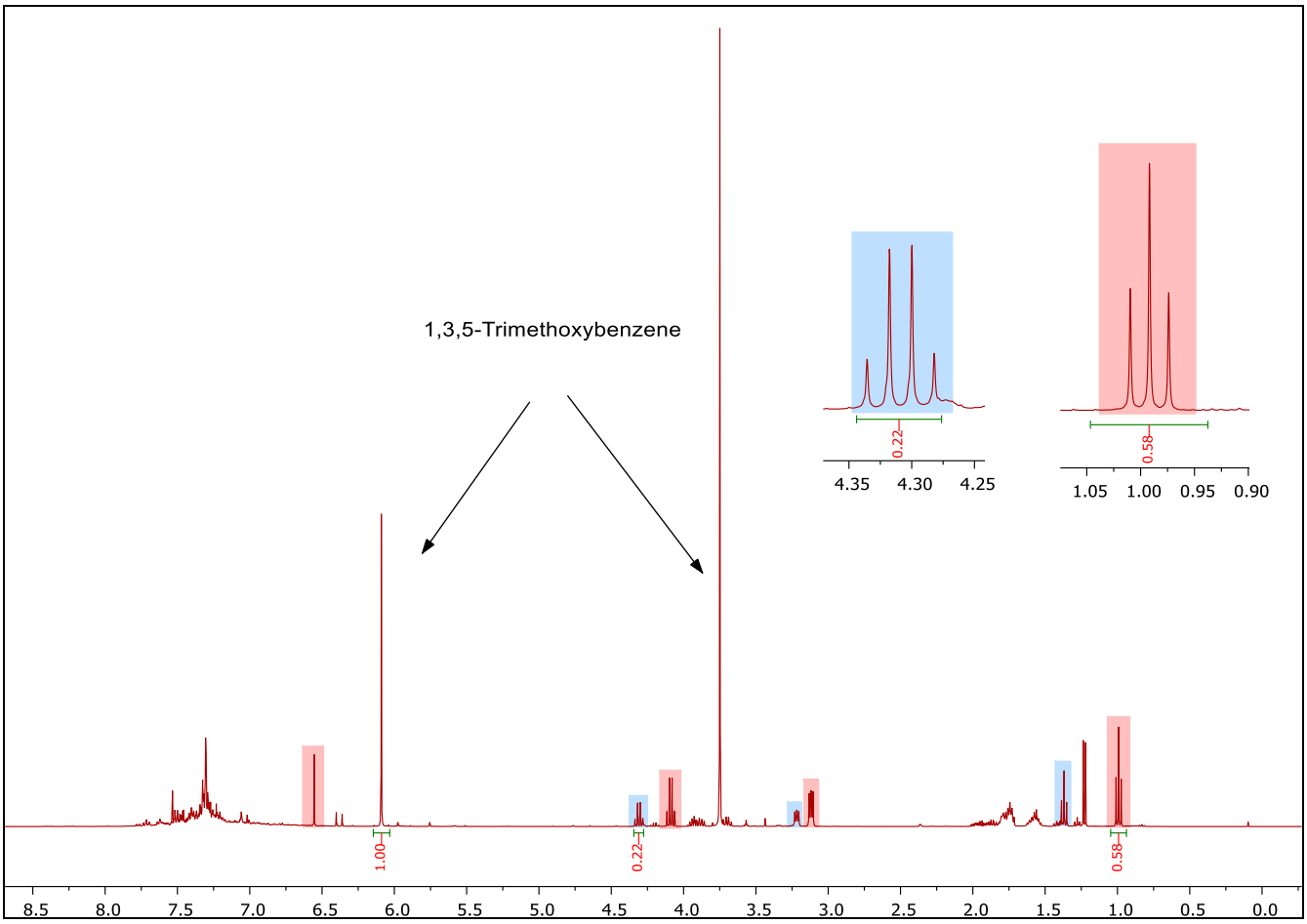




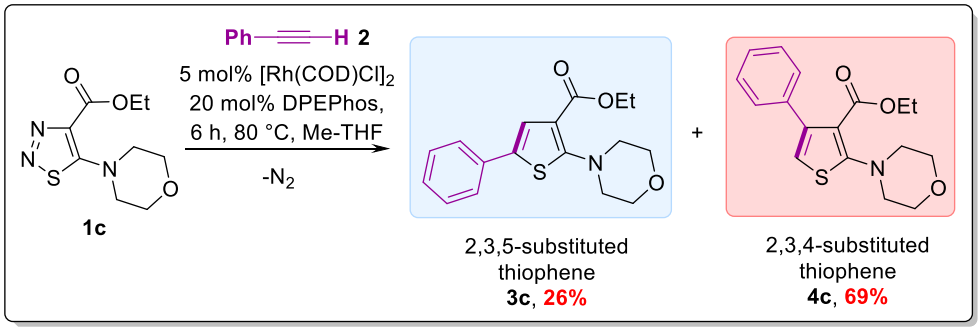
[b] Aromatic protons of the phenyl substituent were observed in all cases in the range from 7.19 to 7.56 and were not highlighted because they cannot be used to differentiate the two regioisomers. The resonances of the starting phenylacetylene are absent in all spectra.

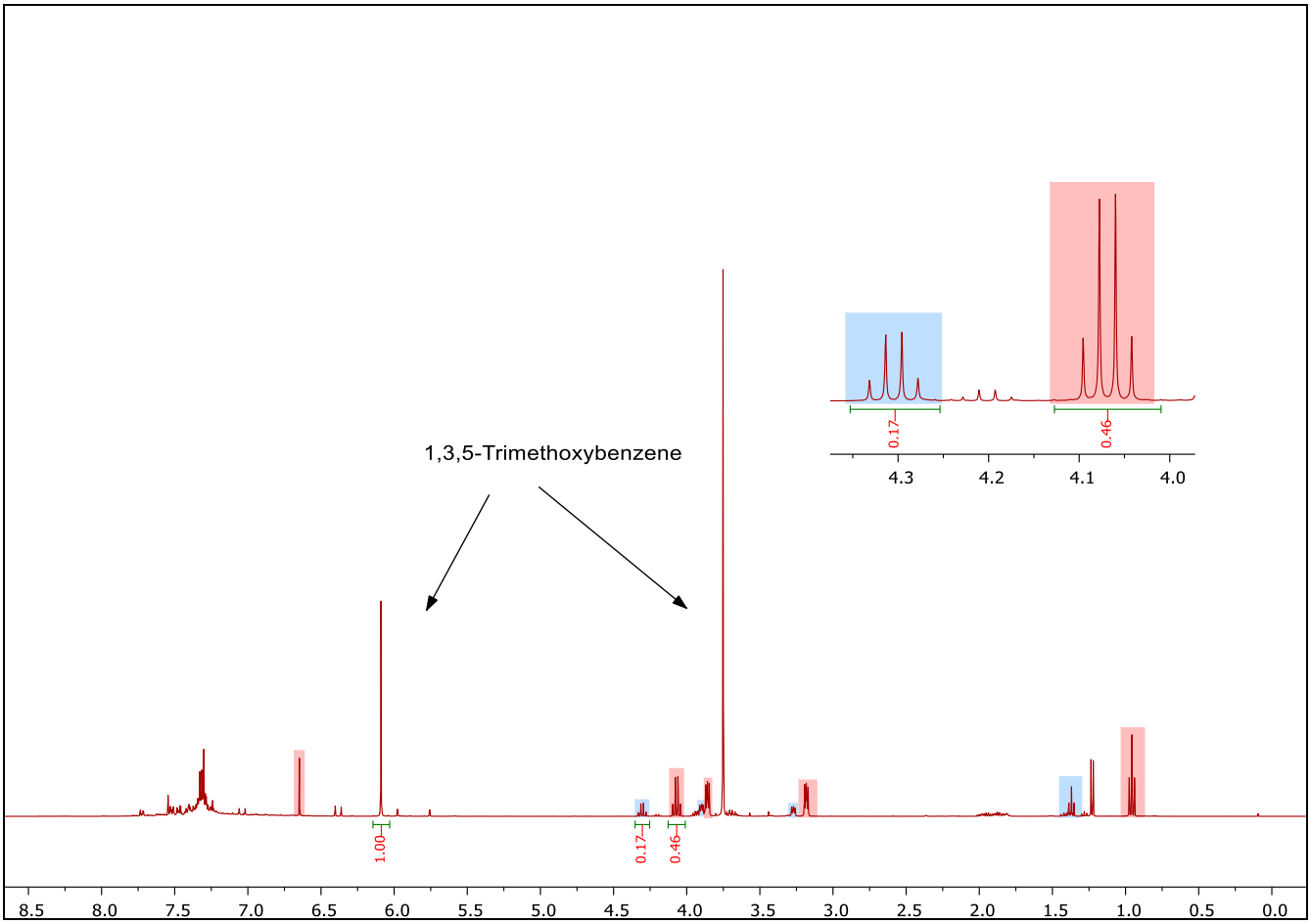
^{1}H NMR Spectrum of the crude reaction mixture of **3b** and **4b** (400 MHz, $CDCl_3$)



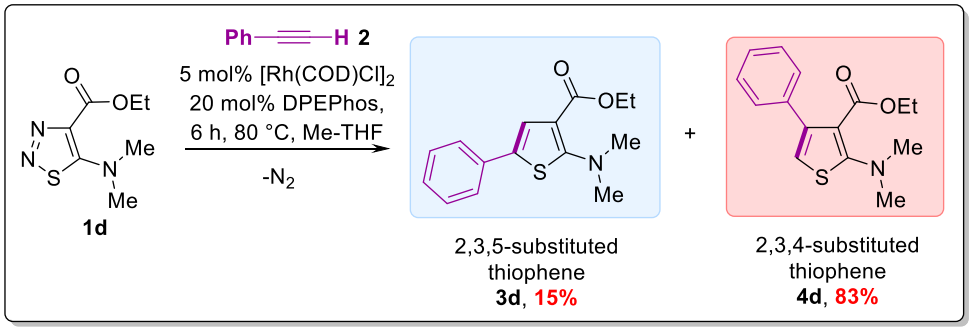


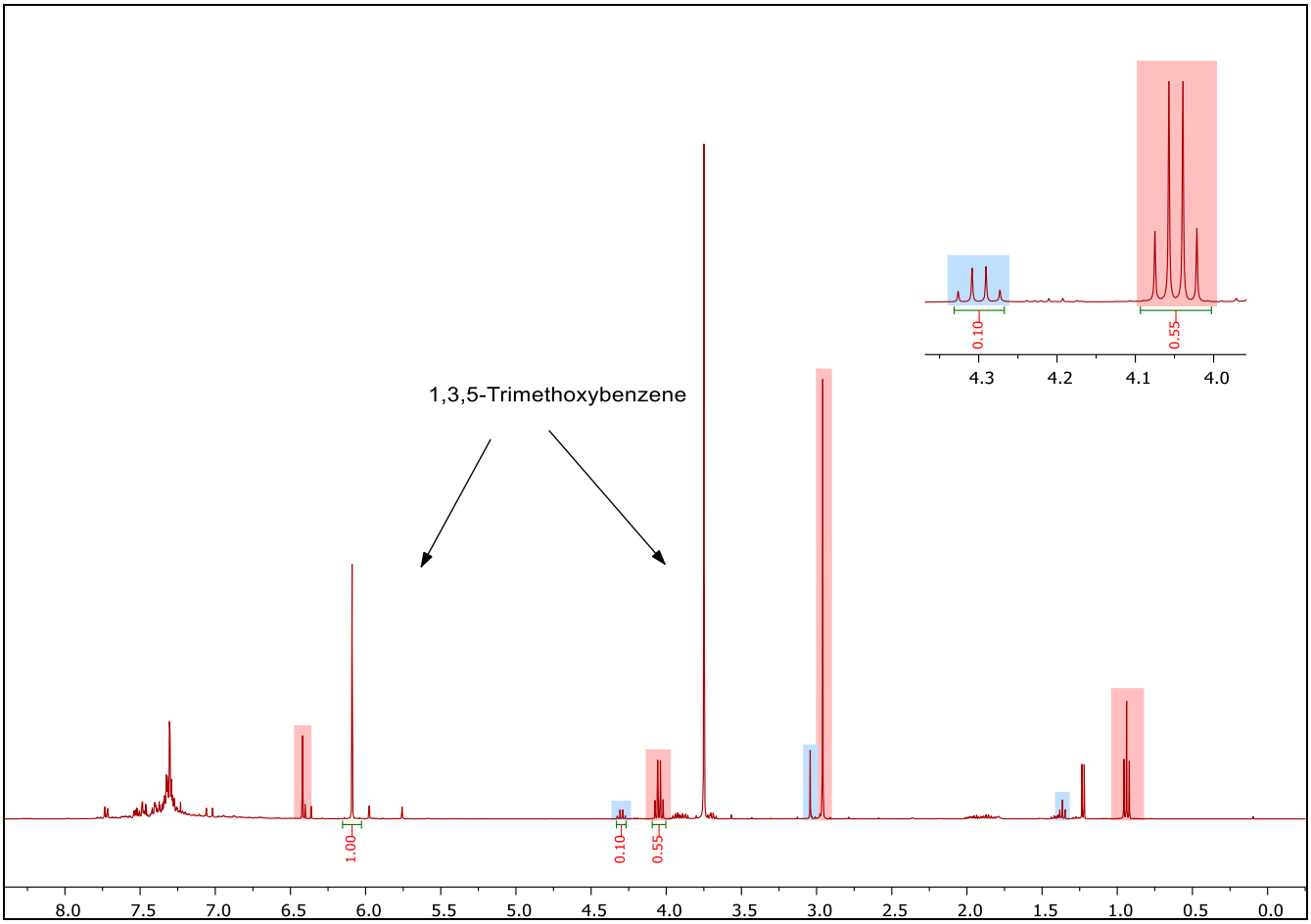
^{1}H NMR Spectrum of the crude reaction mixture of **3c** and **4c** (400 MHz, $CDCl_3$)



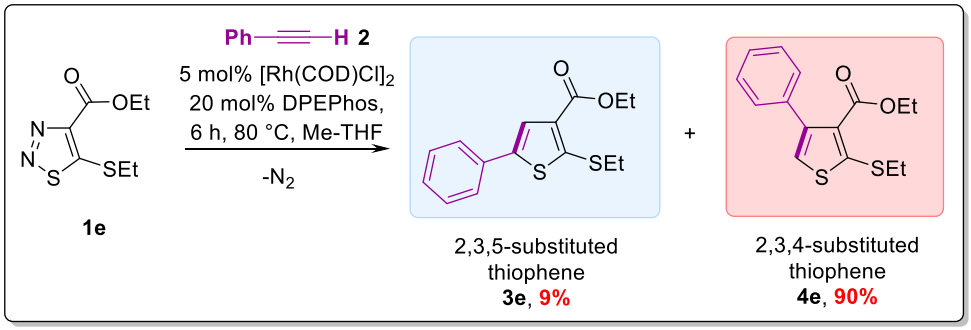


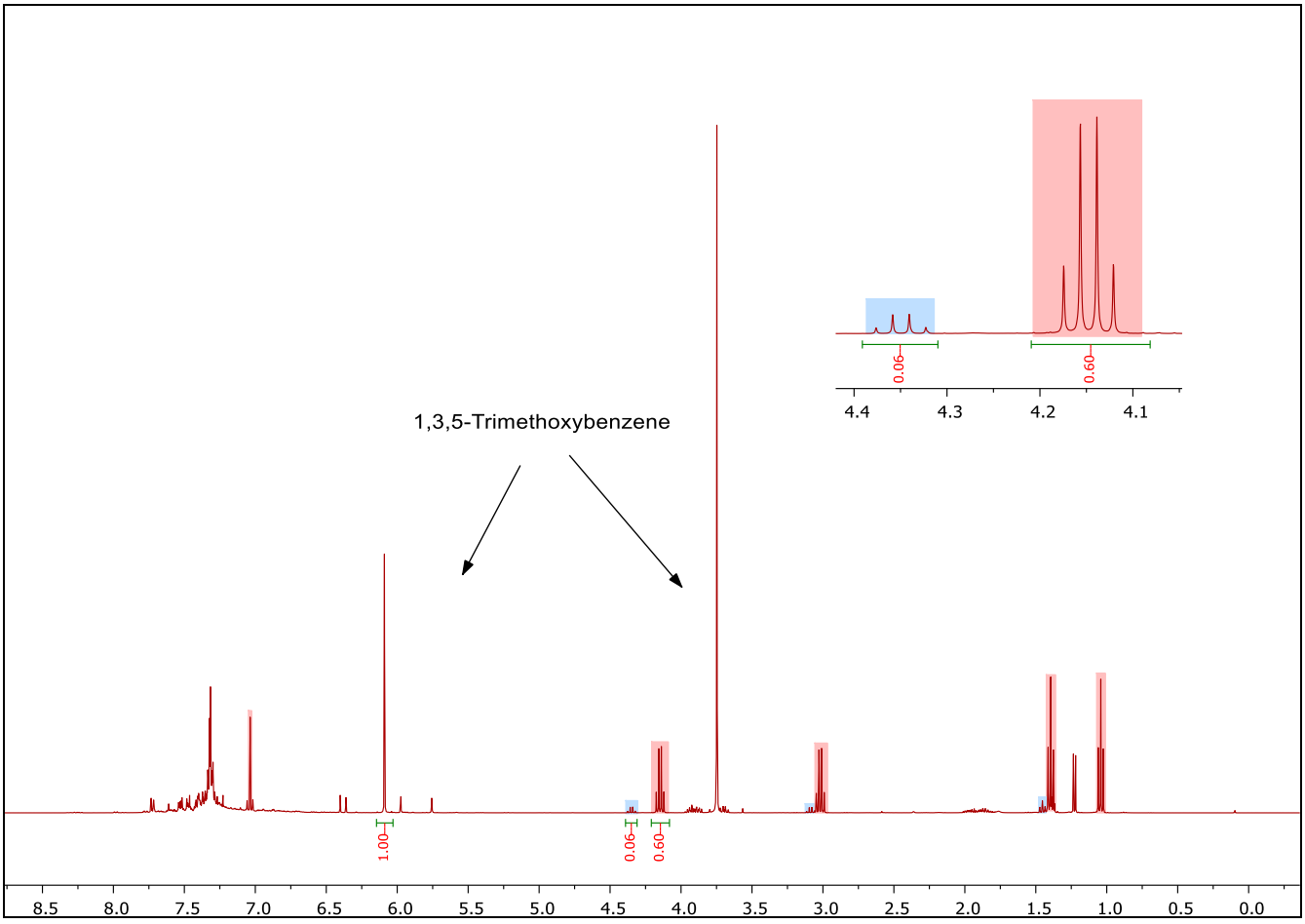
^{1}H NMR Spectrum of the crude reaction mixture of **3d** and **4d** (400 MHz, $CDCl_3$)



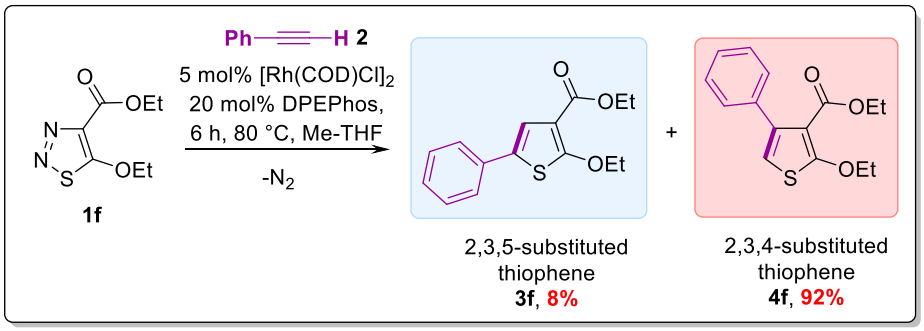


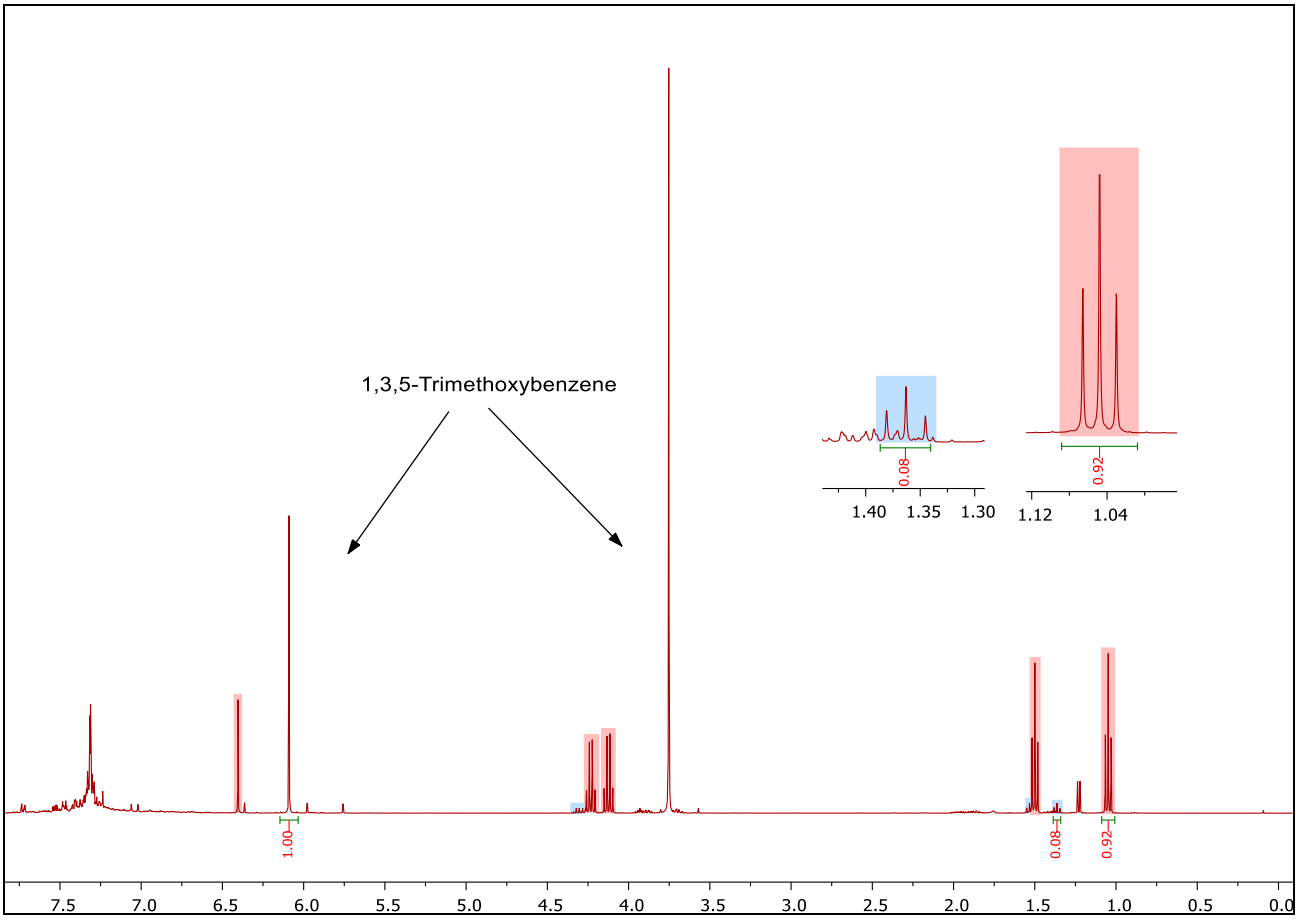
^{1}H NMR Spectrum of the crude reaction mixture of **3e** and **4e** (400 MHz, $CDCl_3$)



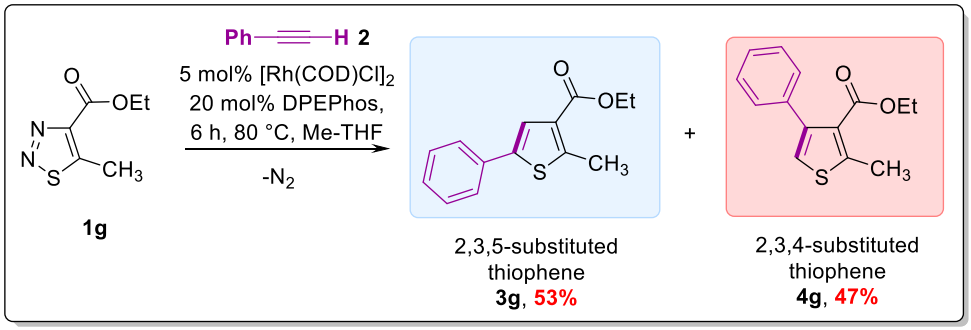


^{1}H NMR Spectrum of the crude reaction mixture of **3f** and **4f** (400 MHz, $CDCl_3$)





^{1}H NMR Spectrum of the crude reaction mixture of **3g** and **4g** (400 MHz, $CDCl_3$)



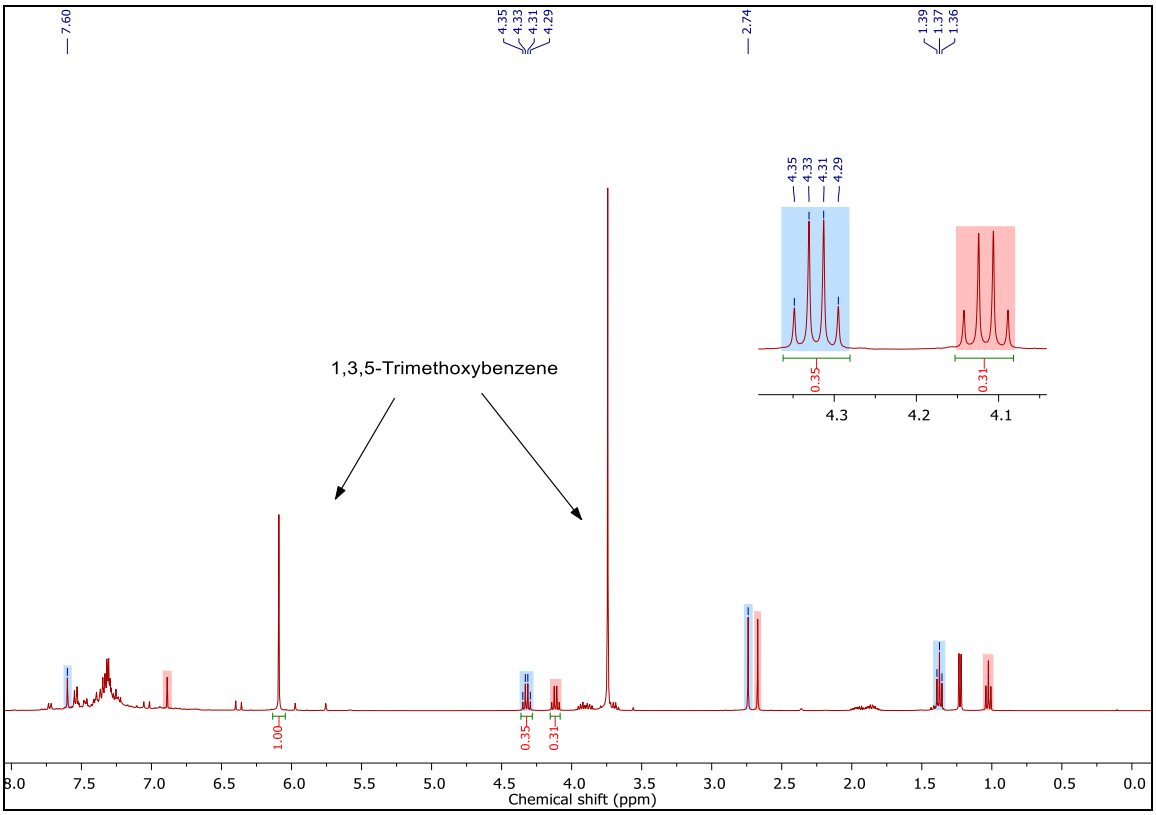
3g

Experimental data.

^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.60 (s, 1H, CH), 4.32 (q, J = 7.1 Hz, 2H, OCH_2), 2.74 (s, 3H), 1.37 (t, J = 7.1 Hz, 3H, CH_3).[c]

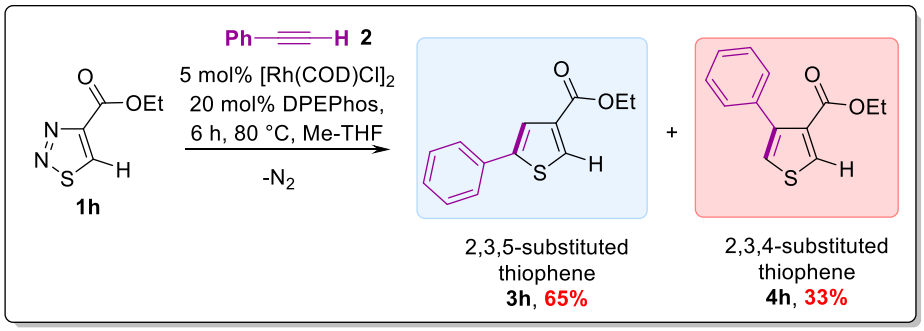
Literature data.

^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.59 (s, 1H, CH), 4.33 (q, J = 7.2 Hz, 2H, OCH_2), 2.75 (s, 3H), 1.39 (t, J = 7.2 Hz, 3H, CH_3).[10, 11]



[c] Only those signals that were used for comparison were listed.

^{1}H NMR Spectrum of the crude reaction mixture of **3h** and **4h** (400 MHz, $CDCl_3$)



3h

Experimental data.

^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.01 (d, *J*=1.3 Hz, 1H, CH), 7.72 (d, *J*=1.3 Hz, 1H, CH), 4.34 (q, *J*=7.1 Hz, 2H, OCH_2), 1.37 (t, *J*=7.1 Hz, 3H, CH_3).

Literature data.

^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.03 (s, 1H, CH), 7.72 (s, 1H, CH), 4.35 (q, *J*=7.1 Hz, 2H, OCH_2), 1.39 (t, *J*=7.2 Hz, 3H, CH_3).[12]

^{1}H NMR ($CDCl_3$, 200 MHz) δ 8.02 (d, *J*=1.0 Hz, 1H, CH), 7.71 (d, *J*=1.0 Hz, 1H, CH), 4.35 (q, *J*=7.0 Hz, 2H, OCH_2), 1.40 (t, *J*=7.0 Hz, 3H, CH_3).[13]

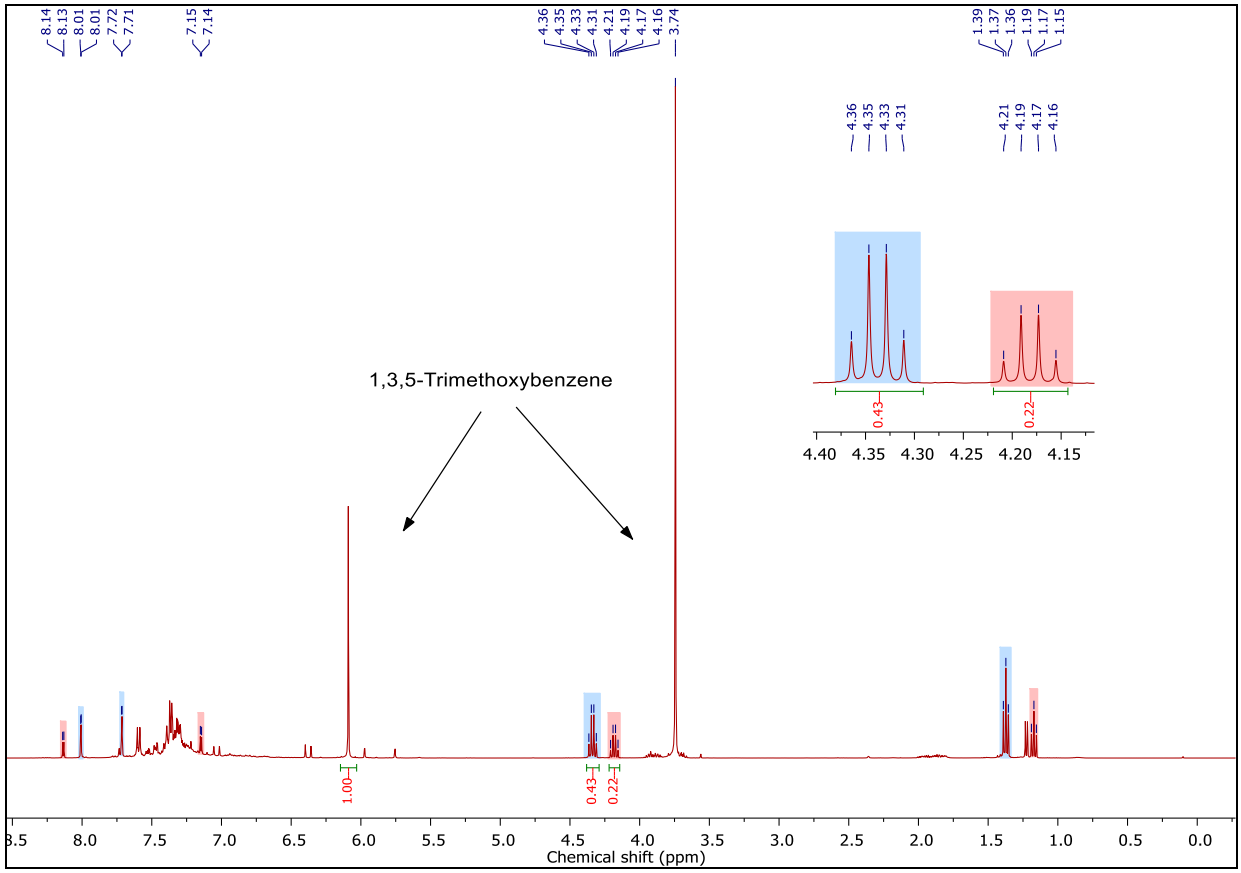
4h

Experimental data.

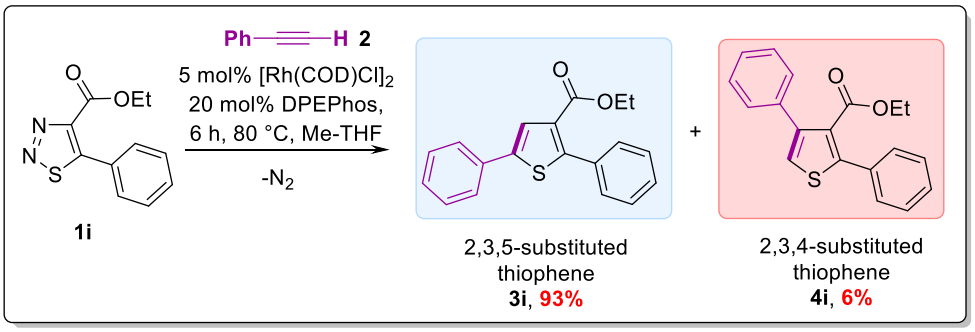
^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.14 (d, *J*=3.5 Hz, 1H, CH), 7.15 (d, *J*=3.5 Hz, 1H, CH), 4.18 (q, *J* = 7.1 Hz, 2H, OCH_2), 1.17 (t, *J* = 7.1 Hz, 3H, CH_3).

Literature data.

^{1}H NMR ($CDCl_3$, 600 MHz) δ 8.16 (d, *J*=3.5 Hz, 1H, CH), 7.18 (d, *J*=3.5 Hz, 1H, CH), 4.20 (q, *J* = 7.1 Hz, 2H, OCH_2), 1.19 (t, *J* = 7.1 Hz, 3H, CH_3).[14]


8.14
8.13
8.01
8.01
7.72
7.71
7.15
7.14
4.36
4.35
4.33
4.31
4.21
4.19
4.17
4.16
3.74
1.39
1.37
1.36
1.19
1.17
1.15
1,3,5-Trimethoxybenzene
1.00
0.43
0.22
Chemical shift (ppm)

[1]NMR Spectrum of the crude reaction mixture of **3i** and **4i** (400 MHz, $CDCl_3$)



3i

Experimental data.

^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.72 (s, 1H, CH), 4.21 (q, *J*=7.1 Hz, 2H, OCH_2), 1.20 (t, *J*=7.1 Hz, 3H, CH_3).

Literature data.

^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.74 (s, 1H, CH), 4.25 (q, *J*=7.1 Hz, 2H, OCH_2), 1.23 (t, *J*=7.1 Hz, 3H, CH_3).[11]

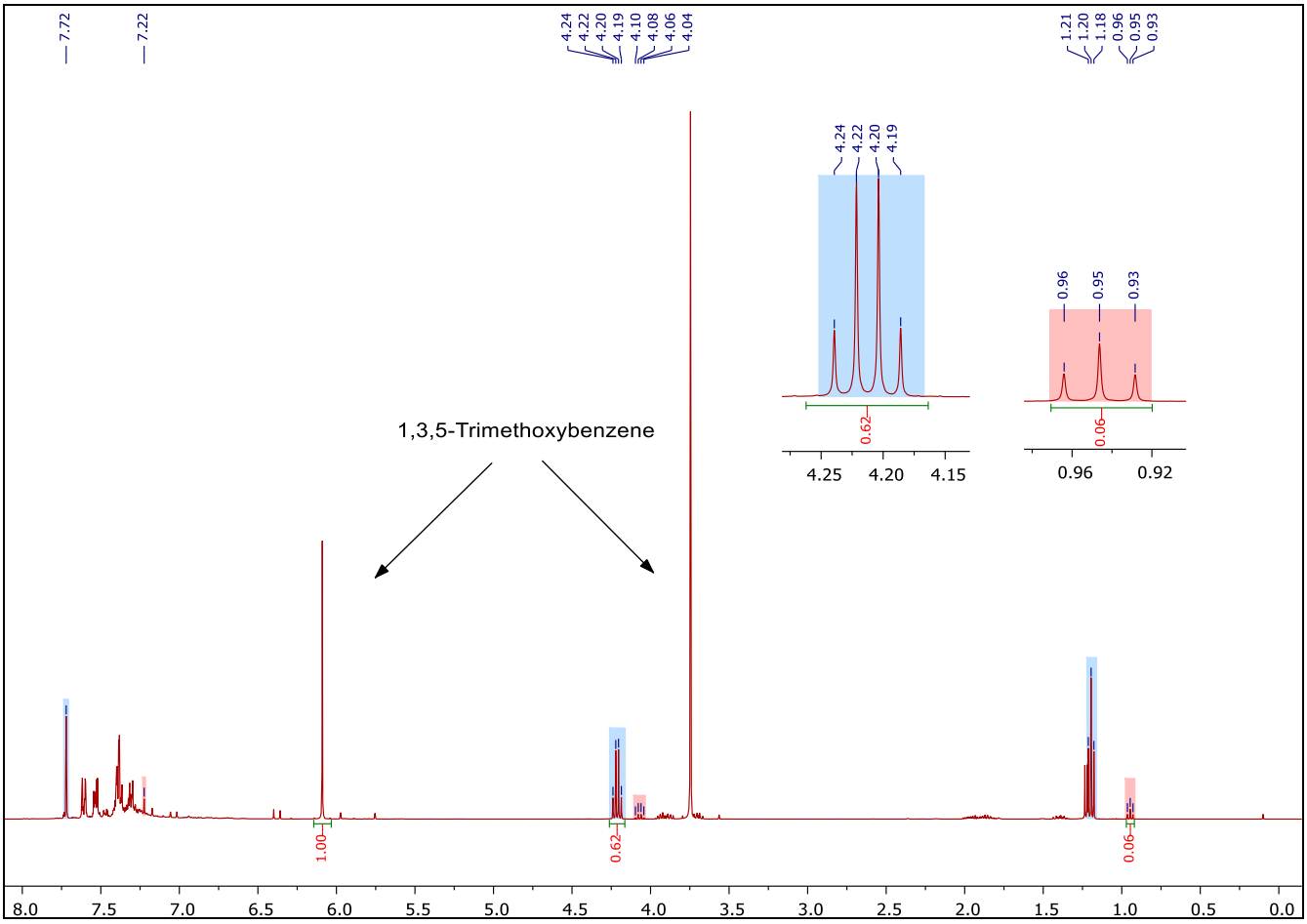
4i

Experimental data.

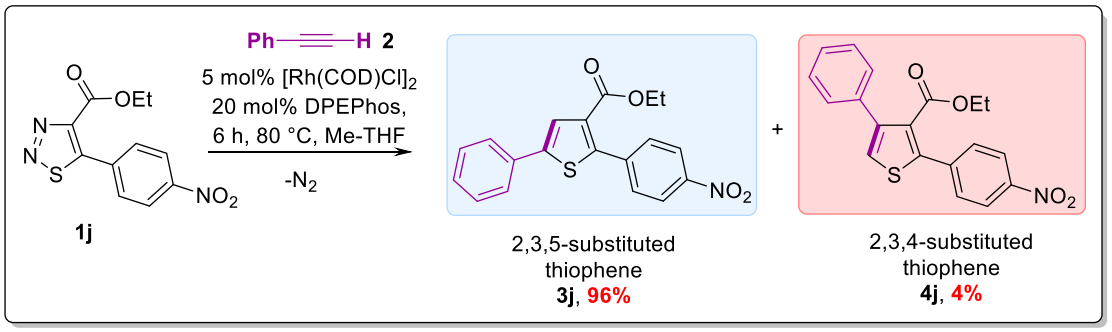
^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.22 (s, 1H, CH), 4.07 (q, *J*=7.1 Hz, 2H, OCH_2), 0.95 (t, *J*=7.1 Hz, 3H, CH_3).

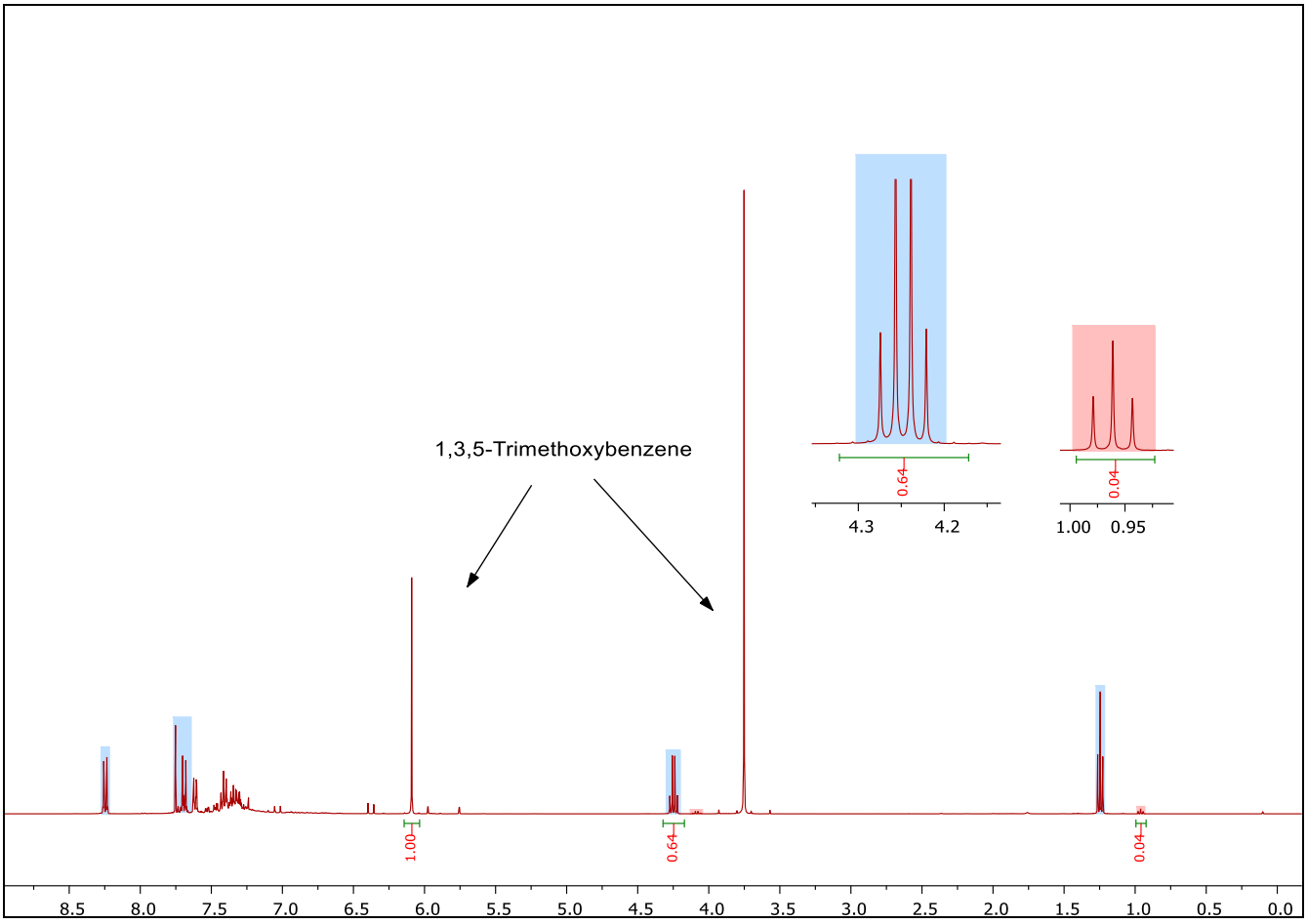
Literature data.

^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.20 (s, 1H, CH), 4.07 (q, *J*=7.1 Hz, 2H, OCH_2), 0.95 (t, *J*=7.1 Hz, 3H CH_3).[15]

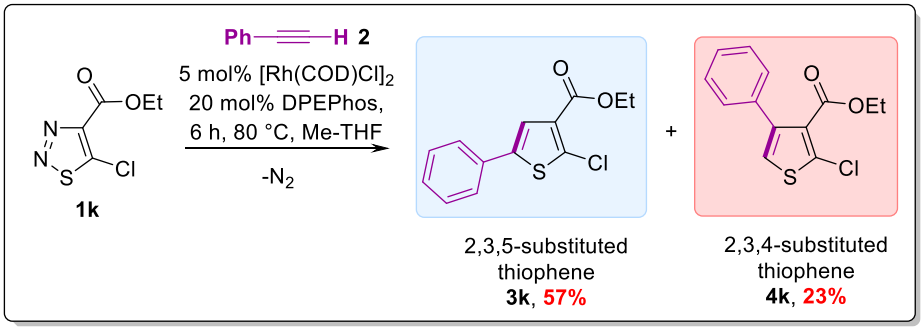

7.72
7.22
4.24
4.22
4.20
4.19
4.10
4.08
4.06
4.04
1.21
1.20
1.18
0.96
0.95
0.93
1,3,5-Trimethoxybenzene
1.00
0.62
0.06
4.25
4.20
4.15
0.96
0.92
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0

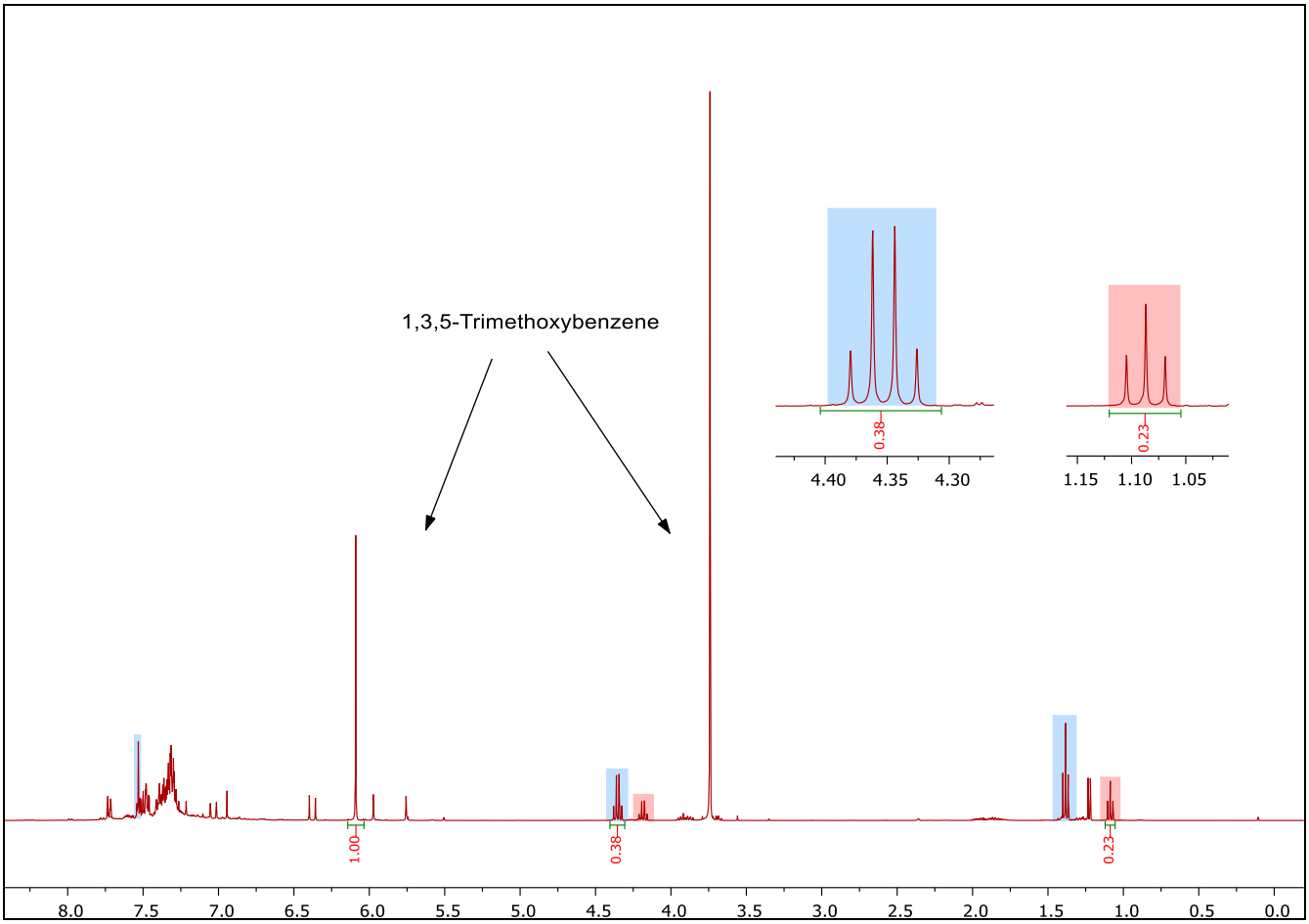
^{1}NMR Spectrum of the crude reaction mixture of **3j** and **4j** (400 MHz, $CDCl_3$)



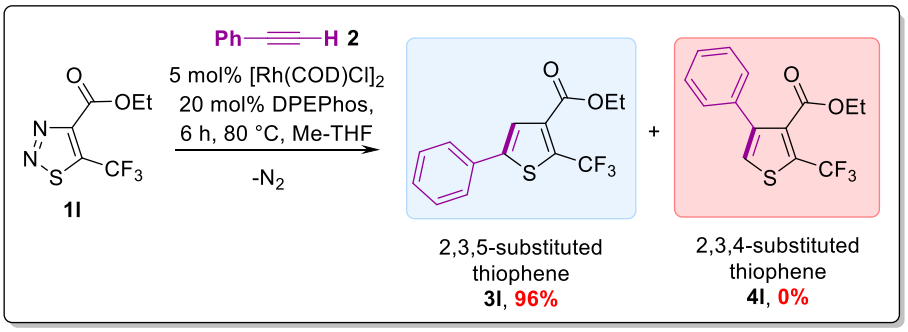


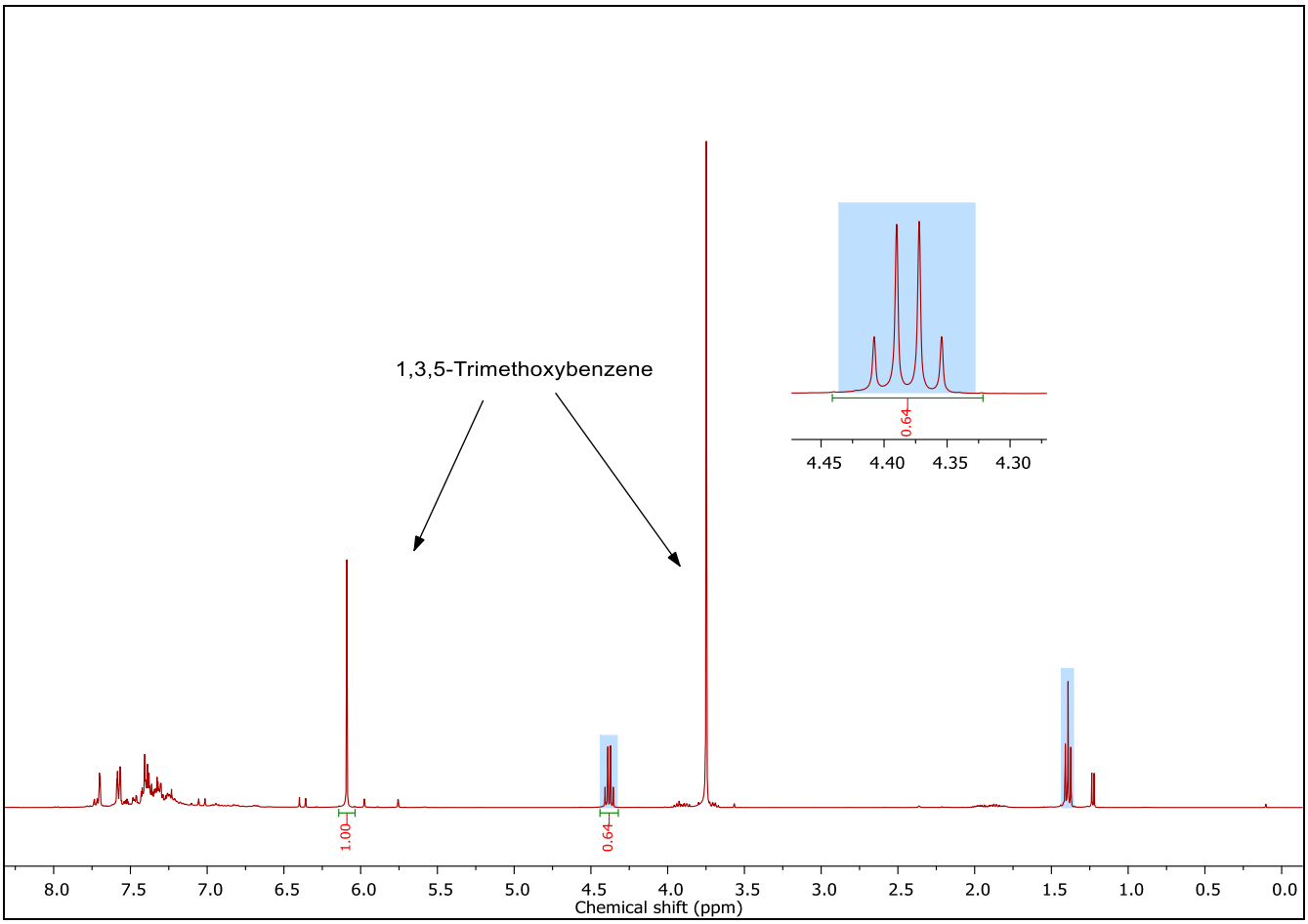
^{1}NMR Spectrum of the crude reaction mixture of **3k** and **4k** (400 MHz, $CDCl_3$)





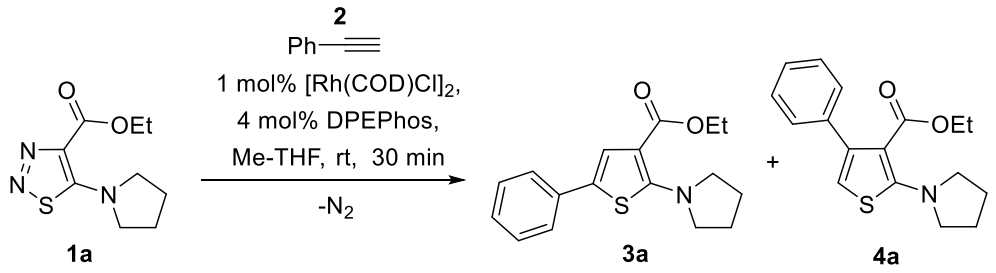
^{1}H NMR Spectrum of the crude reaction mixture of **3l** and **4l** (400 MHz, $CDCl_3$)



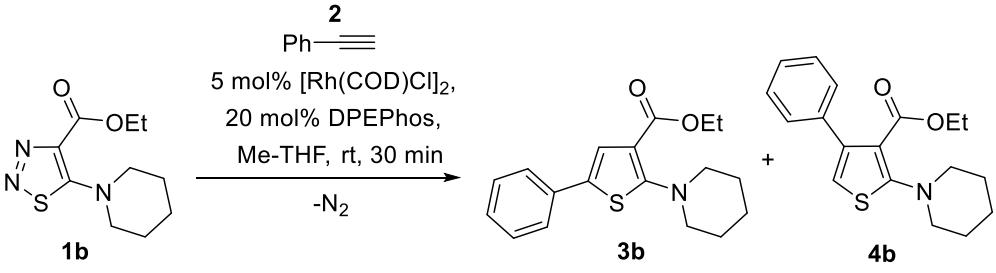


7. **Characterization data**

7.1. Thiophenes 3a and 4a, 3b and 4b



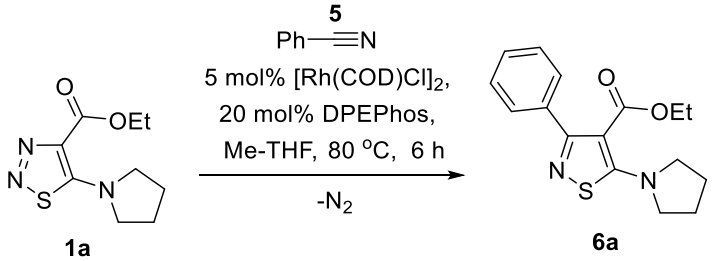
In a glovebox under Ar atmosphere, an 18 mL vial was charged with 1,2,3-thiadiazole (0.4 mmol, 1.0 equiv), $[Rh(COD)Cl]_2$ (0.004 mmol, 1 mol %) and DPEPhos (0.016 mmol, 4 mol %). Dry degassed Me-THF (2.0 mL) was added to the mixture, followed by phenylacetylene **2** (0.8 mmol, 2 equiv). The vial was capped and left at room temperature with stirring for 30 min. At the end of the specified time, the reaction mixture was concentrated under reduced pressure, and the product was purified by column chromatography on silica gel using 1:20 ethyl acetate/*n*-hexane as eluent to afford the corresponding mixture of inseparable isomers **3a** and **4a**. **Yield:** 80 mg (89%) of white powder. $\boldsymbol{R_f}$ = 0.21 (ethyl acetate/*n*-hexane 1:20). **^{1}H NMR (400 MHz, $CDCl_3$):** δ 7.15−7.52 (overlapped m, 5H, H_{Ar}; m, 5H, H_{Ar}; s, 1H, CH), 6.20 (s, 1H, CH), 4.28 (q, *J*=7.1 Hz, 2H, OCH_2), 4.00 (q, *J*=7.1 Hz, 2H, OCH_2), 3.45−3.50 (m, 4H, $N(CH_2)_2$), 3.24−3.42 (m, 4H, $2CH_2$), 1.93−2.11 (overlapped m, 4H, $2CH_2$; m, 4H, $2CH_2$), 1.36 (t, *J*=7.1 Hz, 3H, CH_3), 0.89 (t, *J*=7.1 Hz, 3H, CH_3). **^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$):** 165.8 (**4a**), 163.5 (**3a**), 162.2 (**3a**), 160.1 (**4a**), 142.8 (**4a**), 138.6 (**4a**), 134.5 (**3a**), 128.9 (**3a**), 128.4 (**4a**), 127.8 (**4a**), 126.9 (**4a**), 126.3 (**3a**), 125.0 (**3a**), 124.7 (**3a**), 124.5 (**3a**), 108.3 (**3a**), 107.8 (**4a**), 106.1 (**4a**), 60.2 (**4a**), 59.9 (**3a**), 54.4 **(3a**), 53.2 (**4a**), 26.3 (**3a**), 26.2 (**4a**), 14.7 (**3a**), 13.7 (**4a**). **HRMS (ESI)** calc. for $C_{17}H_{19}NO_2S$ [M]+H: 302.12148, found: 302.12038.



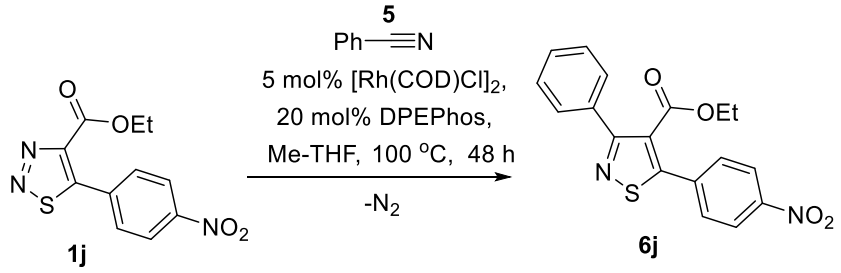
In a glovebox under Ar atmosphere, an 18 mL vial was charged with 1,2,3-thiadiazole (0.4 mmol, 1.0 equiv), $[Rh(COD)Cl]_2$ (0.02 mmol, 5 mol %) and DPEPhos (0.08 mmol, 20 mol %). Dry degassed

Me-THF (2.0 mL) was added to the mixture, followed by phenylacetylene **2** (0.8 mmol, 2 equiv). The vial was capped and left at room temperature with stirring for 30 min. At the end of the specified time, the reaction mixture was concentrated under reduced pressure, and the product was purified by column chromatography on silica gel using 1:50 ethyl acetate/*n*-hexane as eluent to afford the corresponding mixture of inseparable isomers **3b** and **4b**. **Yield:** 107 mg (85%) of light yellow oil. R_f = 0.12 (ethyl acetate/*n*-hexane 1:50). **^{1}H NMR (400 MHz, CDCl$_3$):** δ 7.50−7.53 (overlapped m, 1H, H_{Ar}; m, 1H, H_{Ar}), 7.20−7.36 (overlapped m, 3H, H_{Ar}; m, 3H, H_{Ar}; s, 1H, CH), 6.57 (s, 1H, CH), 4.31 (q, *J*=7.1 Hz, 2H, OCH_2), 4.09 (q, *J*=7.1 Hz, 2H, OCH_2), 3.20−3.26 (m, 4H, $N(CH_2)_2$), 3.09−3.16 (m, 4H, $N(CH_2)_2$), 1.49−1.85 (m, 12H, $6CH_2$), 1.74 (t, *J*=7.1 Hz, 3H, CH_3), 0.99 (t, *J*=7.1 Hz, 3H, CH_3). **^{13}C{^{1}H} NMR (101 MHz, CDCl$_3$):** 166.7, 165.1, 164.9, 162.8, 142.2, 138.1, 134.2, 129.5, 128.8, 128.3, 127.9, 127.0, 126.9, 124.9, 124.4, 117.0, 115.0, 112.0, 60.3, 60.1, 55.7, 55.2, 25.8, 25.6, 23.8 (2C), 14.6, 13.7. **HRMS (ESI)** calc. for $C_{18}H_{21}NO_2S$ [M]+H: 316.13713, found: 316.13620.

7.2. Isothiazoles 6a and 6j

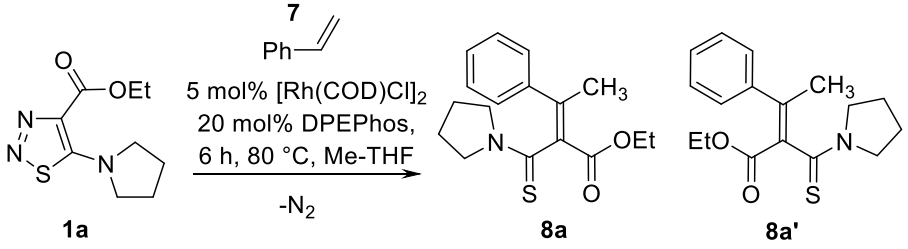


In a glovebox under Ar atmosphere, an 18 mL vial was charged with 1,2,3-thiadiazole (0.4 mmol, 1.0 equiv), $[Rh(COD)Cl]_2$ (0.02 mmol, 5 mol %) and DPEPhos (0.08 mmol, 20 mol %). Dry degassed Me-THF (2.0 mL) was added to the mixture, followed by benzonitrile **5** (0.8 mmol, 2 equiv). The vial was capped and placed into an aluminum heating block pre-warmed to 80 °C. The reaction mixture was heated at 80 °C for 6 h. At the end of the specified time, the reaction mixture was allowed to cool to room temperature and was concentrated under reduced pressure. The product was purified by column chromatography on silica gel using 1:7 ethyl acetate/*n*-hexane as eluent to afford the corresponding isothiazole **6a**. **Yield:** 104 mg (86 %) of white powder. R_f = 0.20 (ethyl acetate/*n*-hexane 1:7). **Mp** 82−84 °C. **^{1}H NMR (400 MHz, CDCl$_3$):** δ 7.44−7.49 (m, 2H, H_{Ar}), 7.34−7.37 (m, 3H, H_{Ar}), 4.06 (q, *J*=7.2 Hz, 2H, OCH_2), 3.18−3.56 (m, 4H, $N(CH_2)_2$), 1.95−2.14 (m, 4H, $2CH_2$), 0.97 (t, *J*=7.2 Hz, 3H, CH_3). **^{13}C{^{1}H} NMR (101 MHz, CDCl$_3$):** δ 174.3, 168.2, 165.5, 137.5, 128.5, 128.2, 127.9, 106.7, 60.9, 52.7, 26.2, 13.8. **HRMS (ESI)** calc. for $C_{16}H_{18}N_2O_2S$ [M]+H: 303.11674, found: 303.1188.



In a glovebox under Ar atmosphere, an 18 mL vial was charged with 1,2,3-thiadiazole (0.4 mmol, 1.0 equiv), $[Rh(COD)Cl]_2$ (0.02 mmol, 5 mol %) and DPEPhos (0.08 mmol, 20 mol %). Dry degassed Me-THF (2.0 mL) was added to the mixture, followed by benzonitrile **5** (4.0 mmol, 10 equiv). The vial was capped and placed into an aluminum heating block pre-warmed to 100 °C. The reaction mixture was heated at 100 °C for 48 h. At the end of the specified time, the reaction mixture was allowed to cool to room temperature and was concentrated under reduced pressure. The product was purified by column chromatography on silica gel using 1:10 ethyl acetate/*n*-hexane as eluent to afford the corresponding isothiazole **6j**. **Yield:** 119 mg (84%) of white powder. $\boldsymbol{R_f}$ = 0.27 (ethyl acetate/*n*-hexane 1:10). **Mp** 76−78 °C. **^{1}H NMR (400 MHz, $CDCl_3$):** δ 8.29−8.38 (m, 2H, H_{Ar}), 7.70−7.77 (m, 2H, H_{Ar}), 7.61−7.69 (m, 2H, H_{Ar}), 7.42−7.52 (m, 3H, H_{Ar}), 4.16 (q, *J*=7.2 Hz, 2H, OCH_2), 1.03 (t, *J*=7.2 Hz, 3H, CH_3). **^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$):** δ 168.4, 167.1, 164.2, 148.7, 136.4, 135.0, 129.9, 129.7, 128.6, 128.4, 128.2, 124.1, 62.1, 13.8. **HRMS (ESI)** calc. for $C_{18}H_{14}N_2O_4S$ [M]+H: 355.07528, found: 355.07438.

7.3. Alkenylation Products 8a and 8a'



In a glovebox under Ar atmosphere, an 18 mL vial was charged with 1,2,3-thiadiazole (0.4 mmol, 1.0 equiv), $[Rh(COD)Cl]_2$ (0.02 mmol, 5 mol %) and DPEPhos (0.08 mmol, 20 mol %). Dry degassed Me-THF (2.0 mL) was added to the mixture, followed by styrene **7** (0.8 mmol, 2 equiv). The vial was capped and placed into an aluminum heating block pre-warmed to 80 °C. The reaction mixture was heated at 80 °C for 6 h. At the end of the specified time, the reaction mixture was allowed to cool to room temperature and was concentrated under reduced pressure. The products was purified by column

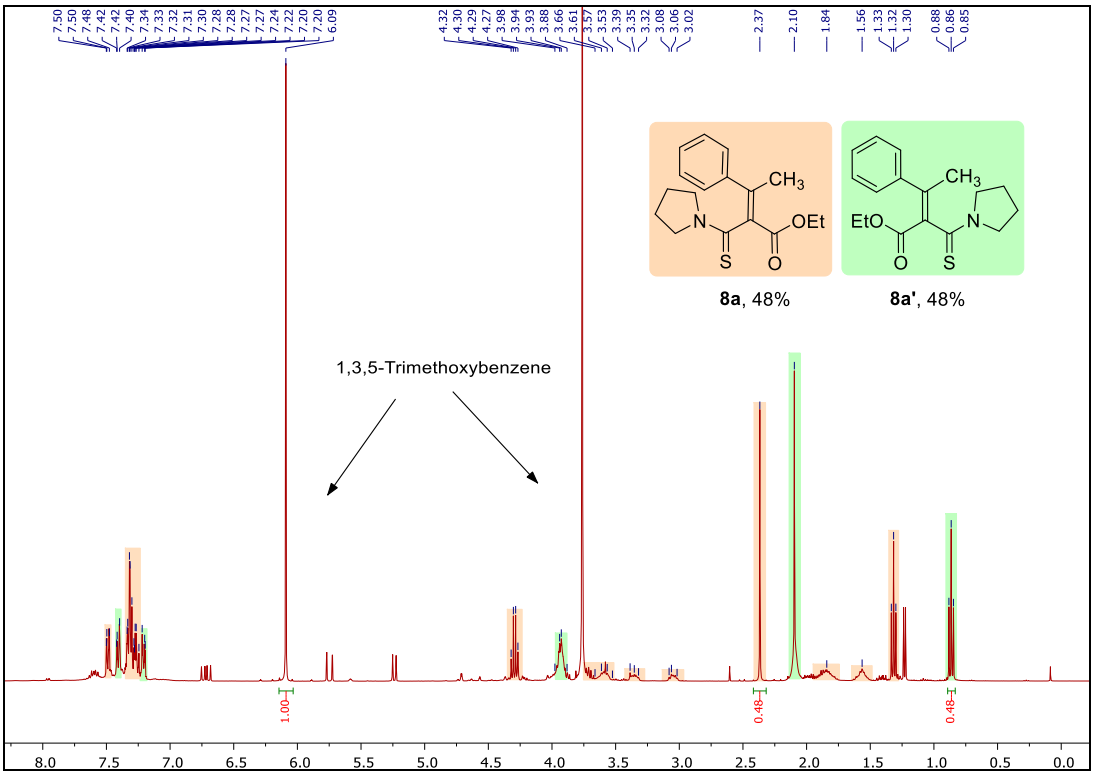
chromatography on silica gel using 1:8 ethyl acetate/*n*-hexane as eluent to afford the corresponding alkenylation products **8a** and **8a'**. Because of difficulty in separation of the obtained *E*, *Z*-isomeric mixture by column chromatography, both isolated products have insignificant amounts of the second isomer.

***Z*-Isomer 8a:** yellow-green oil. R_f = 0.18 (ethyl acetate/*n*-hexane 1:8). **^{1}H NMR (400 MHz, $CDCl_3$):** δ 7.45−7.50 (m, 2H, H_{Ar}), 7.26−7.34 (m, 3H, H_{Ar} overlapped with $CDCl_3$ signal), 4.29 (q, *J*=7.1 Hz, 2H, OCH_2), 3.71−3.80 (m, 1H, NCH), 3.51−3.62 (m, 1H, NCH), 3.29−3.40 (m, 1H, NCH), 2.98−3.09 (m, 1H, NCH), 2.36 (s, 3H, CH_3), 1.74−1.92 (m, 2H, 2CH), 1.49−1.63 (m, 2H, 2CH), 1.31 (t, *J*=7.1 Hz, 3H, CH_3). **^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$):** δ 191.9, 165.6, 142.2, 140.9, 132.8, 128.4, 128.2, 127.5, 61.3, 52.2, 52.1, 25.9, 24.4, 21.9, 14.3. **HRMS (ESI)** calc. for $C_{17}H_{21}NO_2S$ [M]+H: 304.13713, found: 304.13606.

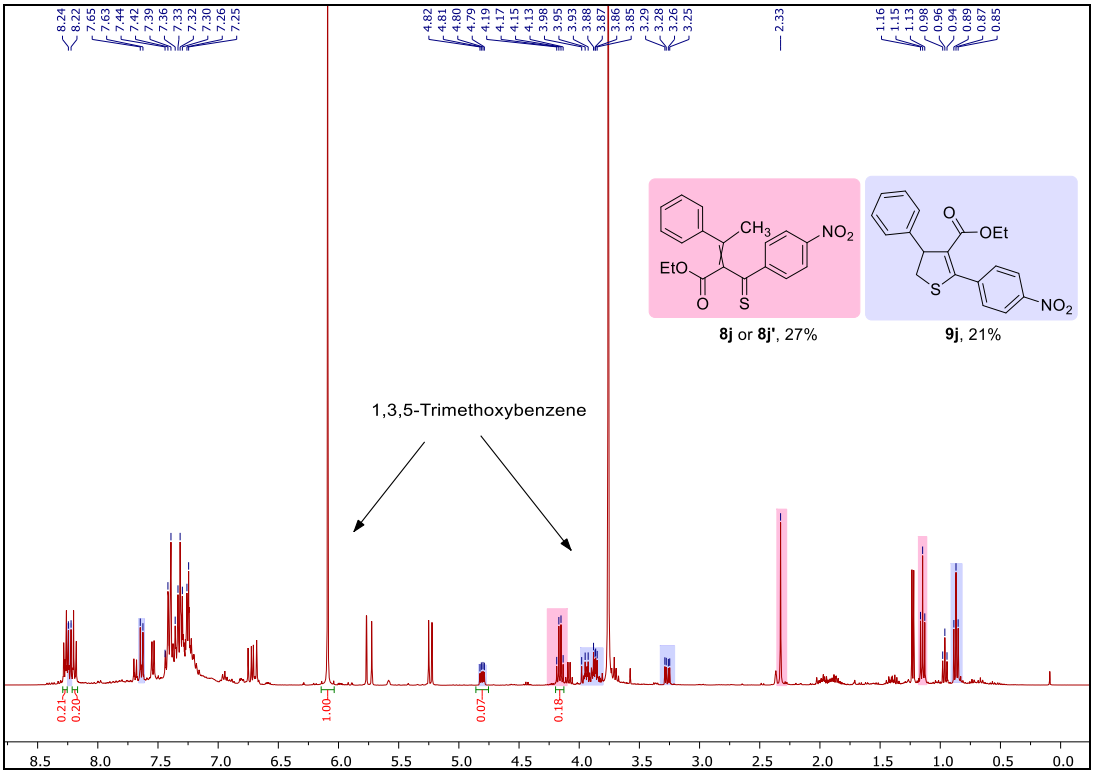
***E*-Isomer 8a':** white powder. R_f = 0.12 (ethyl acetate/*n*-hexane 1:8). **^{1}H NMR (400 MHz, $CDCl_3$):** δ 7.27−7.38 (m, 3H, H_{Ar}), 7.16−7.25 (m, 2H, H_{Ar}), 3.80−4.22 (overlapped d, *J*=7.1 Hz, 2H, OCH_2; m, 3H, 3NCH), 3.47−3.76 (m, 1H, NCH), 1.87−2.32 (overlapped s, 3H, CH_3; m, 4H, $2CH_2$), 0.86 (t, *J*=7.1 Hz, 3H, CH_3). **^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$):** δ 192.2, 165.3, 143.6, 141.6, 133.7, 128.2, 128.0, 126.9, 61.1, 52.4, 52.0, 26.3, 24.7. **HRMS (ESI)** calc. for $C_{17}H_{21}NO_2S$ [M]+H: 304.13713, found: 304.13612.

8. ^{1}H NMR Spectra of the Crude Reaction Mixtures from Scheme 6

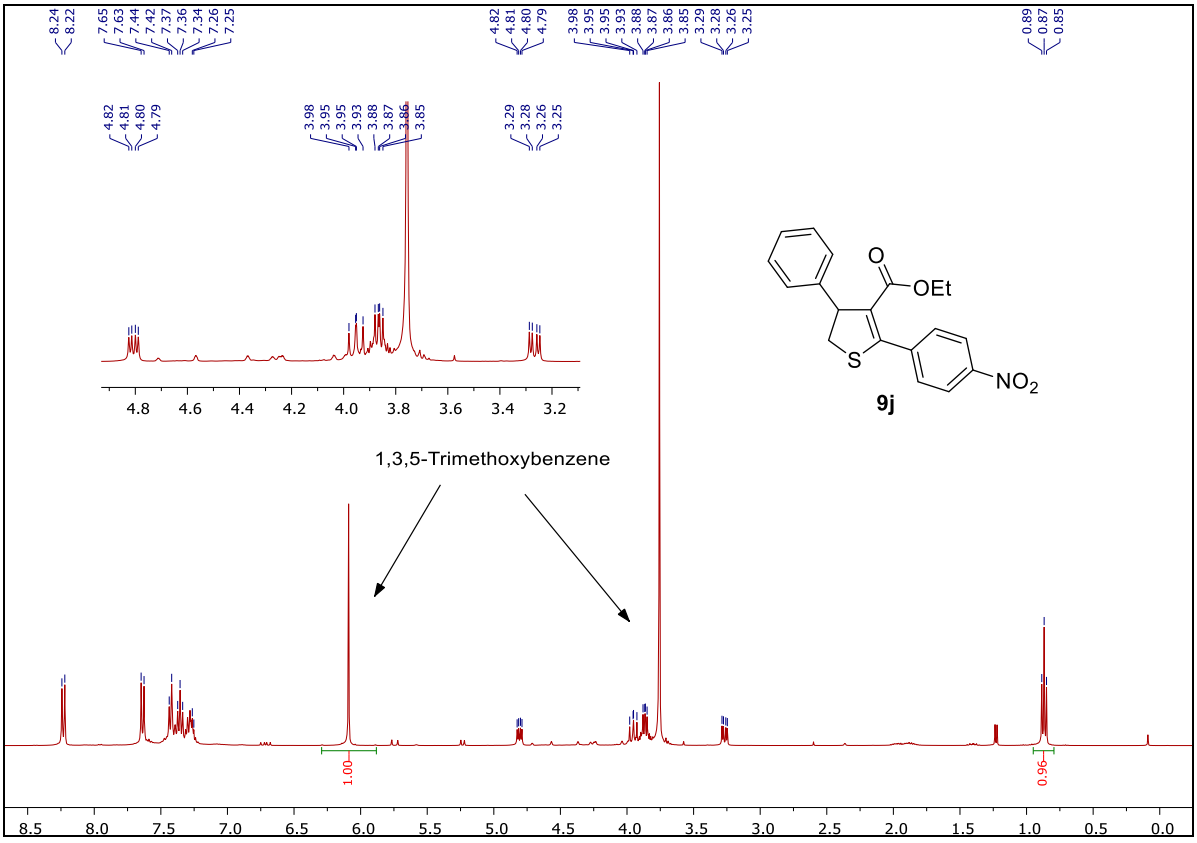
^{1}H NMR Spectra of the Crude Reaction Mixture from Scheme **6b)** (400 MHz, $CDCl_3$)



^{1}H NMR Spectrum of the Crude Reaction Mixture from Scheme **6c)** (400 MHz, $CDCl_3$)



^{1}H NMR Spectrum of the Crude Reaction Mixture from Scheme **6d)** (400 MHz, $CDCl_3$)



9j

Experimental data.

^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.23 (d, J = 8.8 Hz, 2H, H_{Ar}), 7.64 (d, J = 8.8 Hz, 2H, H_{Ar}), 7.44−7.25 (m, 5H, H_{Ar}), 4.81 (dd, J = 10.1, 4.5 Hz, 1H, CH_2), 3.95 (dd, J = 11.4, 10.2 Hz, 1H, CH), 3.88-3.85 (m, 2H, OCH_2), 3.27 (dd, J = 11.5, 4.6 Hz, 1H, CH_2), 0.87 (t, J = 7.1 Hz, 3H, CH_3).

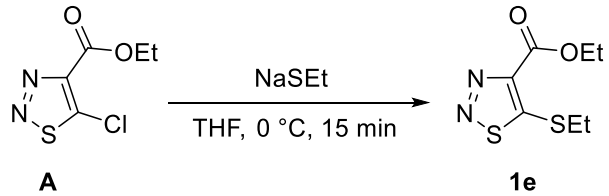
Literature data.

^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.24 (d, J = 8.9 Hz, 2H, H_{Ar}), 7.64 (d, J = 8.9 Hz, 2H, H_{Ar}), 7.43 (d, J = 7.0 Hz, 2H, H_{Ar}), 7.36 (t, J = 7.4 Hz, 2H, H_{Ar}), 7.29 (t, J = 7.2 Hz, 1H, H_{Ar}), 4.81 (dd, J = 10.1, 4.6 Hz, 1H, CH_2), 3.97 (dd, J = 11.5, 10.1 Hz, 1H, CH), 3.88-3.85 (m, 2H, OCH_2), 3.28 (dd, J = 11.5, 4.6 Hz, 1H, CH_2), 0.87 (t, J = 7.1 Hz, 3H, CH_3).[15]

9. Synthesis and Characterization of New Ethyl 1,2,3-thiadiazole-4-carboxylates

9.1. Synthesis of Ethyl 5-(ethylthio)-1,2,3-thiadiazole-4-carboxylate 1e

Ethyl 5-chloro-1,2,3-thiadiazole-4-carboxylate **A** was prepared according to a reported procedure.[16]

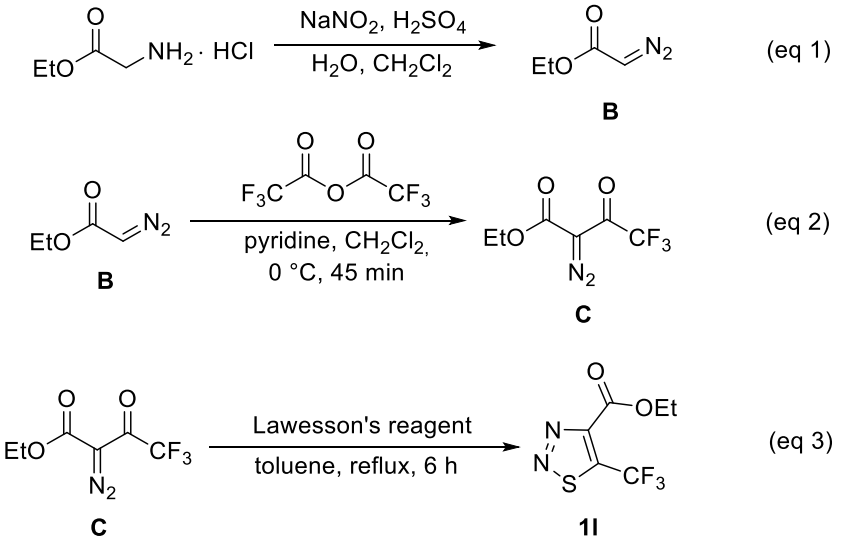


A **1e**

Ethyl 5-chloro-1,2,3-thiadiazole-4-carboxylate **A** (5.0 mmol, 1.0 equiv) was added to freshly prepared solution of sodium ethanethiolate (6.0 mmol, 1.2 equiv) in THF (10 mL) with constant stirring in an ice bath (0 °C) under an N_2 atmosphere. The resulting mixture was stirred for 15 min with the ice bath in place and then was concentrated under reduced pressure. The residue was purified by column chromatography on silica gel using 1:7 ethyl acetate/*n*-hexane as eluent. **Yield:** 0.971 g (89%) of white powder. $\boldsymbol{R_f}$ = 0.24 (ethyl acetate/*n*-hexane 1:7). **Mp** 54–56 °C. **^{1}H NMR (400 MHz, $CDCl_3$):** δ 4.50 (q, *J*=7.1 Hz, 2H, OCH_2), 3.07 (q, *J*=7.4 Hz, 2H, SCH_2), 1.32 (m, 6H, $2CH_3$). **^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$):** δ 165.8, 160.8, 146.2, 62.1, 32.8, 14.4, 13.4. **HRMS (ESI)** calc. for $C_{17}H_{10}N_2O_2S_2$ [M]+H: 219.02621, found: 219.02519.

9.2. Synthesis of Ethyl 5-(trifluoromethyl)-1,2,3-thiadiazole-4-carboxylate 1l

Ethyl diazoacetate **B**[17] and ethyl 2-diazo-4,4,4-trifluoro-3-oxobutanoate **C**[18] were prepared according to reported procedures.



Ethyl 2-diazo-4,4,4-trifluoro-3-oxobutanoate (5.0 mmol, 1.0 equiv) was dissolved in toluene (30 mL) and treated with Lawesson's reagent (6 mmol, 1.2 equiv). The reaction was heated at reflux for 6 hours, then cooled to room temperature and concentrated *in vacuo*. The resulting crude mixture was purified by column chromatography using 1:50 ethyl acetate/*n*-hexane as eluent. **Yield:** 0.509 g (45%) of bright yellow oil. $\boldsymbol{R_f}$ = 0.17 (ethyl acetate/*n*-hexane 1:50). **^{1}H NMR (400 MHz, $CDCl_3$):** δ 4.55 (q, *J*=7.2 Hz, 2H, CH_2), 1.46 (t, *J*=7.2 Hz, 3H, CH_3). **$^{13}C\{^1H\}$ NMR (101 MHz, $CDCl_3$):** δ 158.1, 151.9, 148.7 (q, *J*=41.1 Hz), 120.8 (q, *J*=272.1 Hz), 63.3, 14.0. **$^{19}F\{^1H\}$ NMR (376 MHz, DMSO-d_6):** δ -52.1. **HRMS (ESI)** calc. for $C_6H_5F_3N_2O_2S$ [M]+H: 227.01021, found: 227.00933.

10.Computational Details and Additional Data

Approximate molecular structures were prepared using GaussView.[19] All calculations were then performed using the Gaussian 16 software,[20] which was accessed through the Australian National Computational Infrastructure (NCI). The structure optimizations and frequency calculations were performed in the gas phase using the ωB97XD[21] functional and a combination of the 6-31G(d)[22] (for C, H, N, O, P, F and S) and SDD[23] (for Rh and Fe) basis sets. The obtained frequencies were used to confirm whether the calculated structure is a local minimum or a transition state. Single point energy calculations were then performed using the M06 functional and the DFT-D3 dispersion correction, along with the def2TZVP[24] basis set and the CPCM[25] solvation model to incorporate the solvent effects of THF. Transition states were verified by visualising the located imaginary frequency in GaussView,[19] and by carrying out intrinsic reaction coordinate (IRC)[26, 27] calculations to confirm that the located transition state connects the correct minima. The 3D structures of the optimized intermediates or transition states were visualised using the CYLView20[28] software.

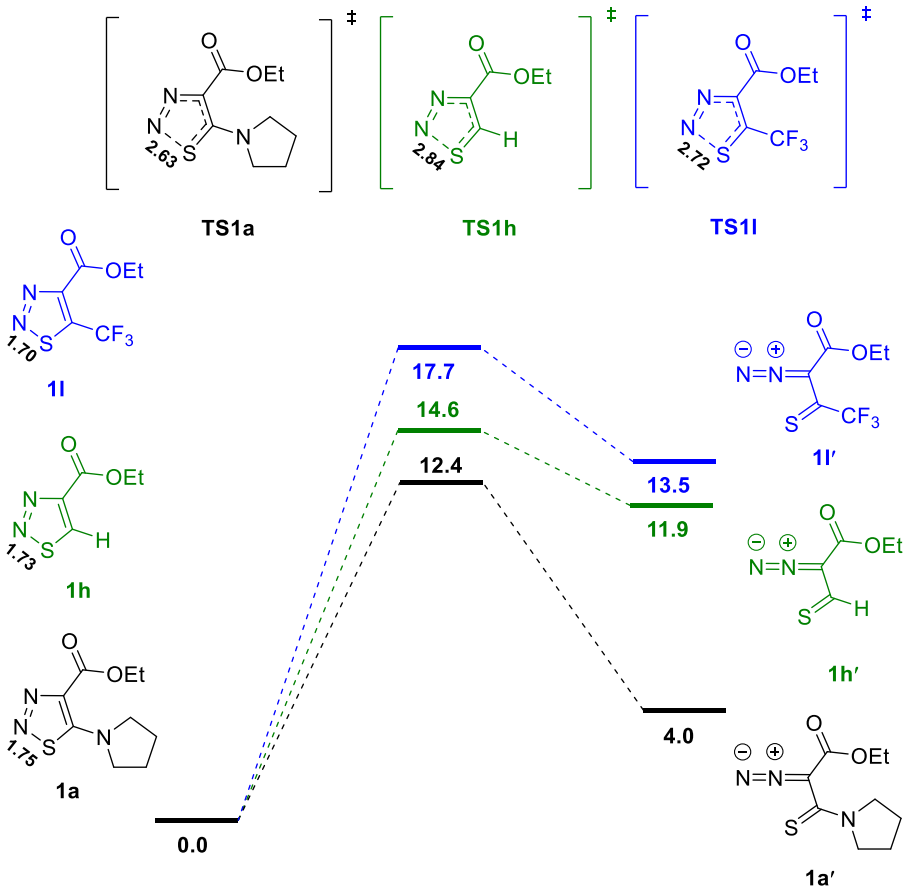
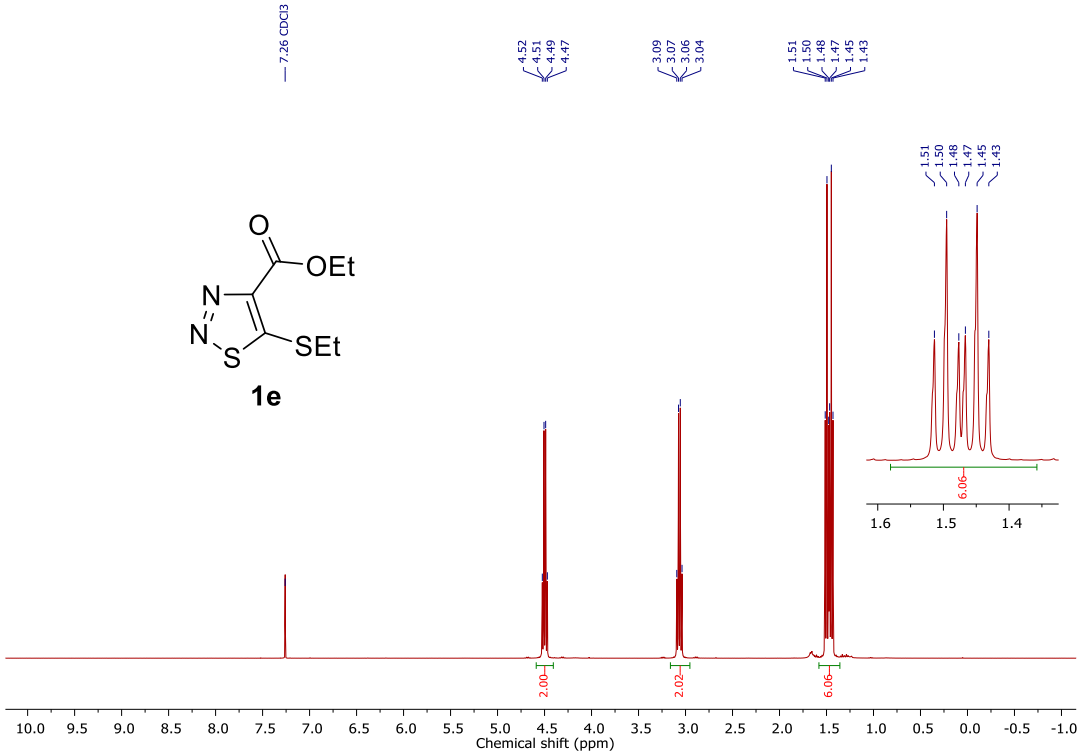


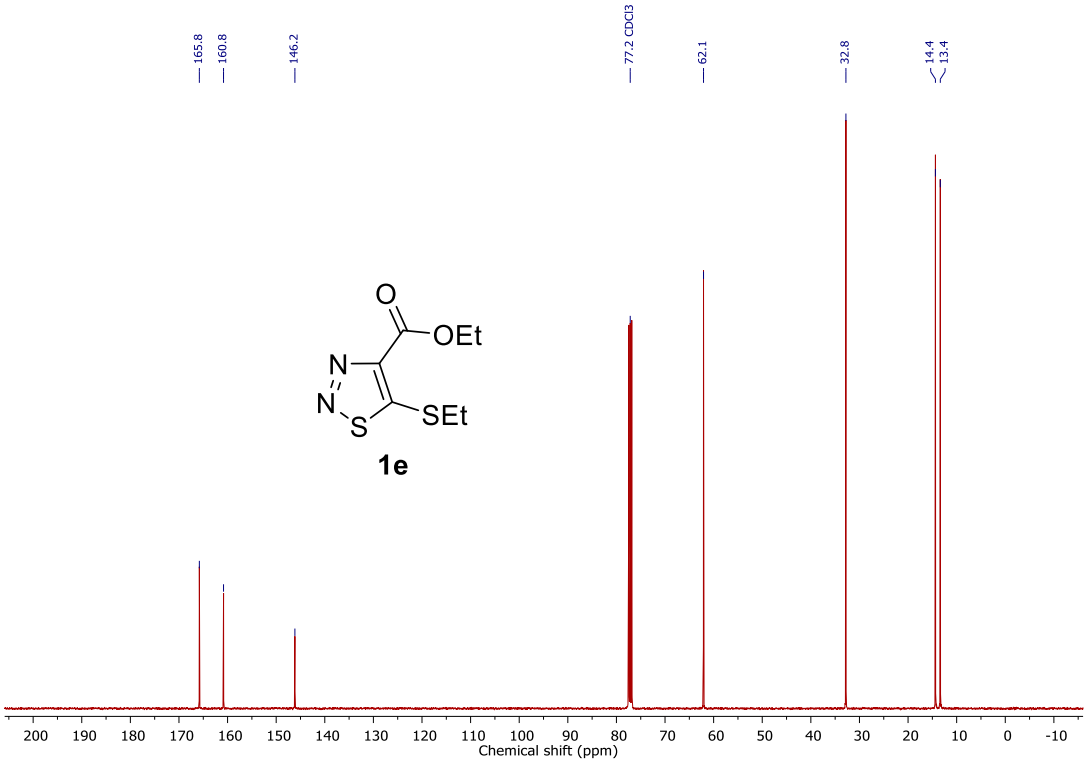
Figure S3. Energy profiles for the ring-opening of 1,2,3-thiadiazoles **1a, 1h** and **1l** to afford the corresponding diazothiones **1′**. Gibbs free energies are given in kcal mol^{-1}. Bond lengths are shown in Å.

11.NMR Spectra of Starting Materials and Products

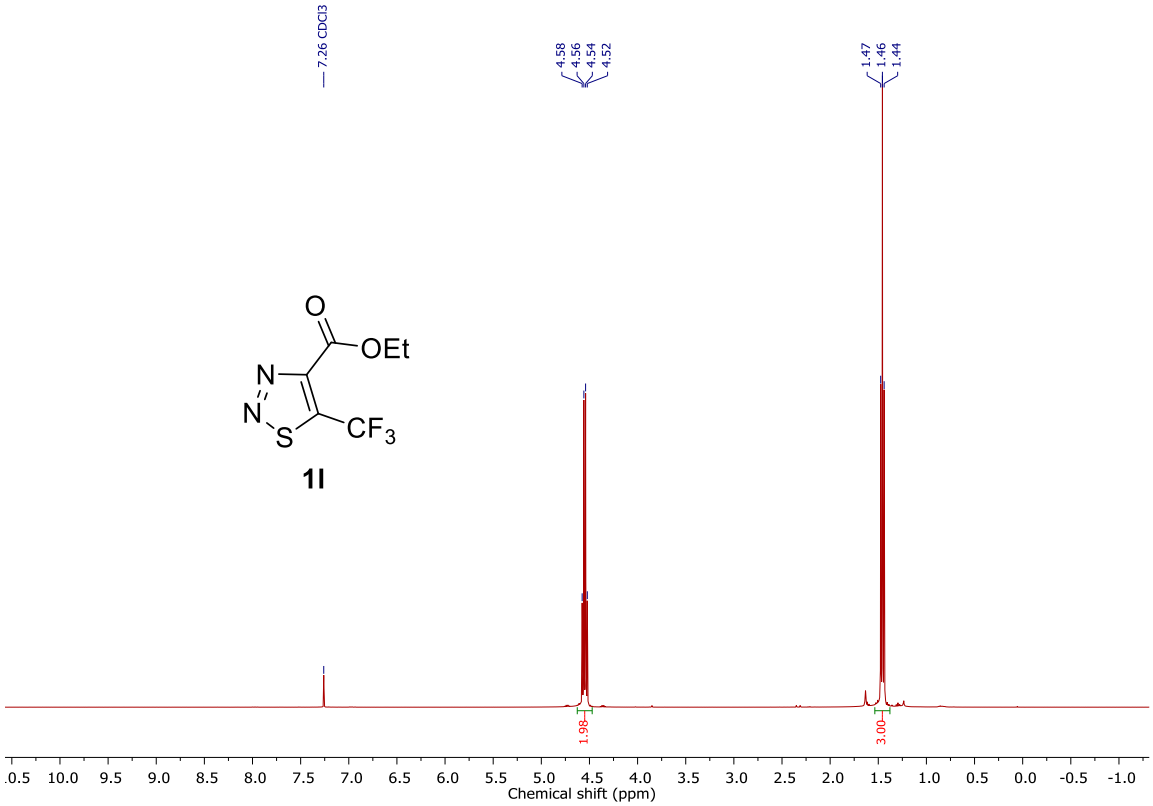
^{1}H NMR Spectrum of **1e** (400 MHz, $CDCl_3$)



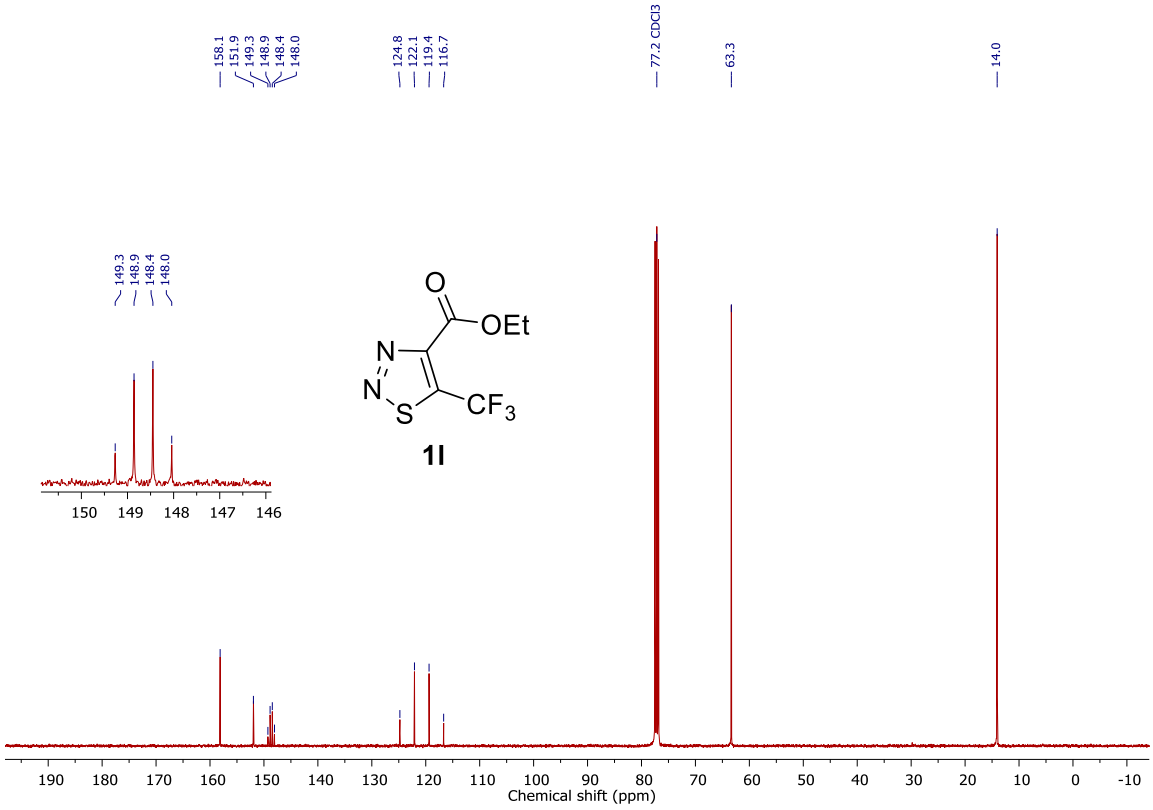
^{13}C NMR Spectrum of **1e** (400 MHz, $CDCl_3$)



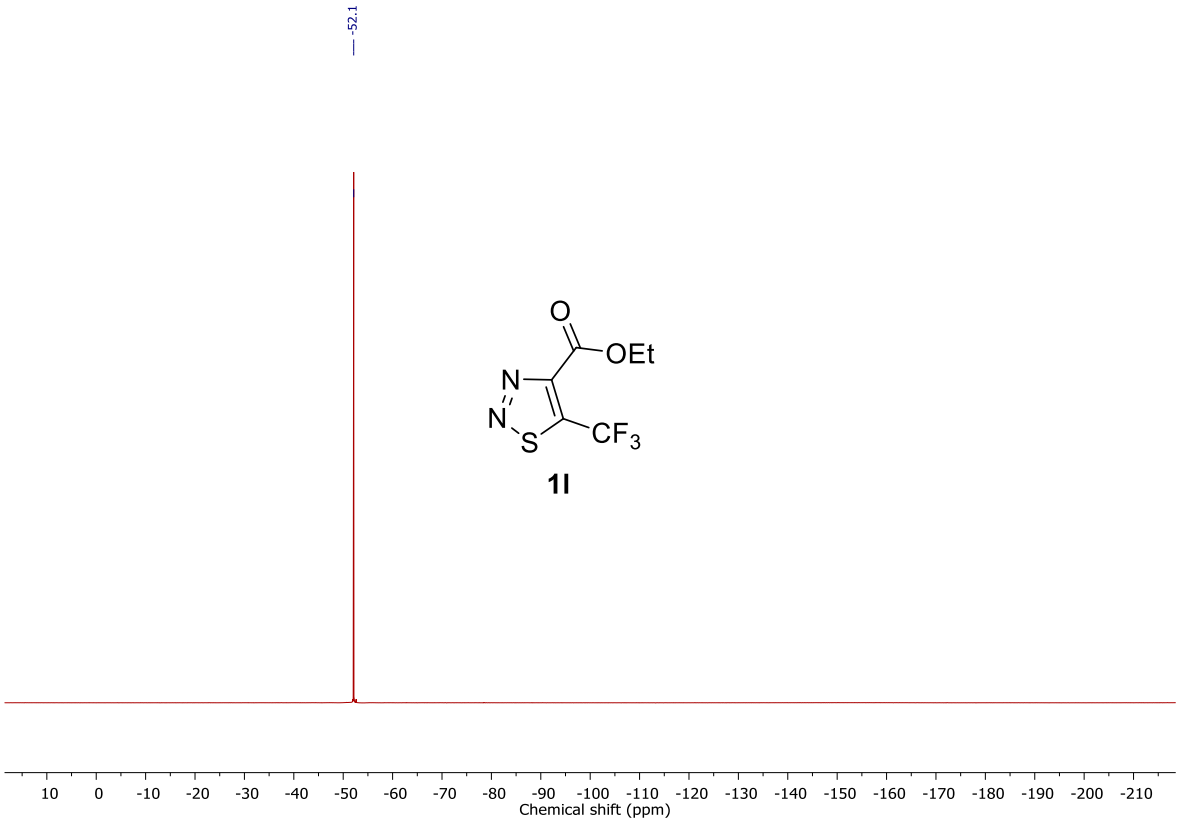
^{1}H NMR Spectrum of **1l** (400 MHz, $CDCl_3$)



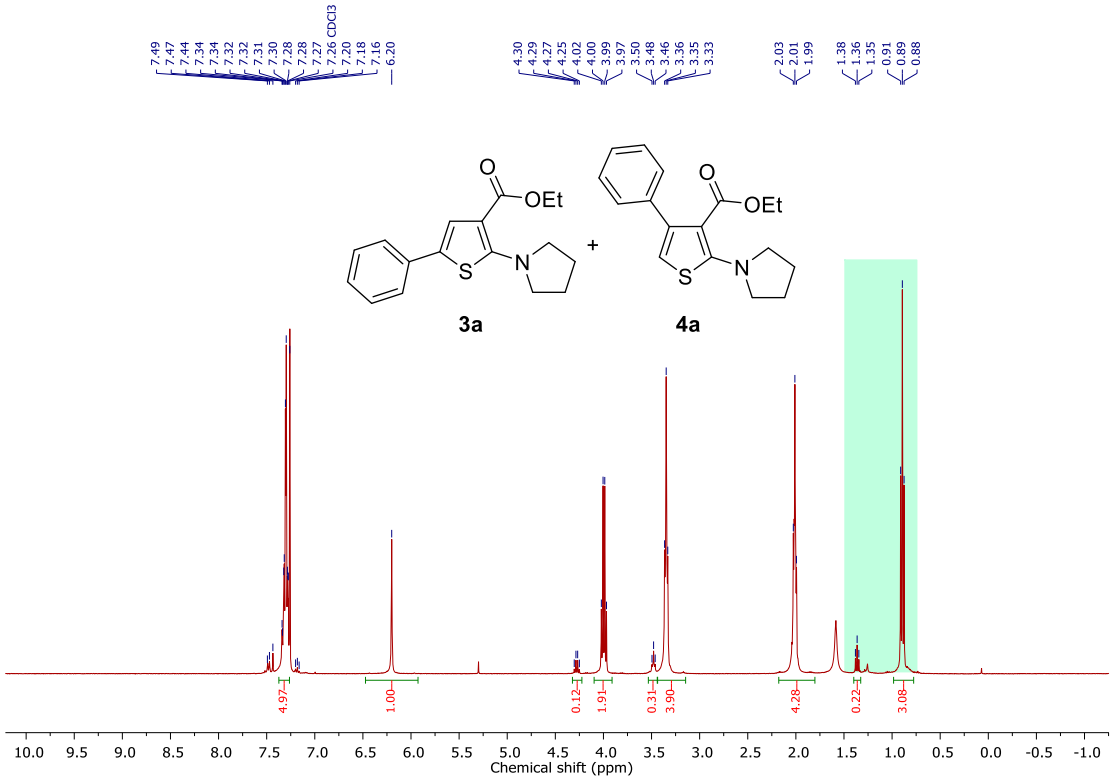
^{13}C NMR Spectrum of **1l** (400 MHz, $CDCl_3$)



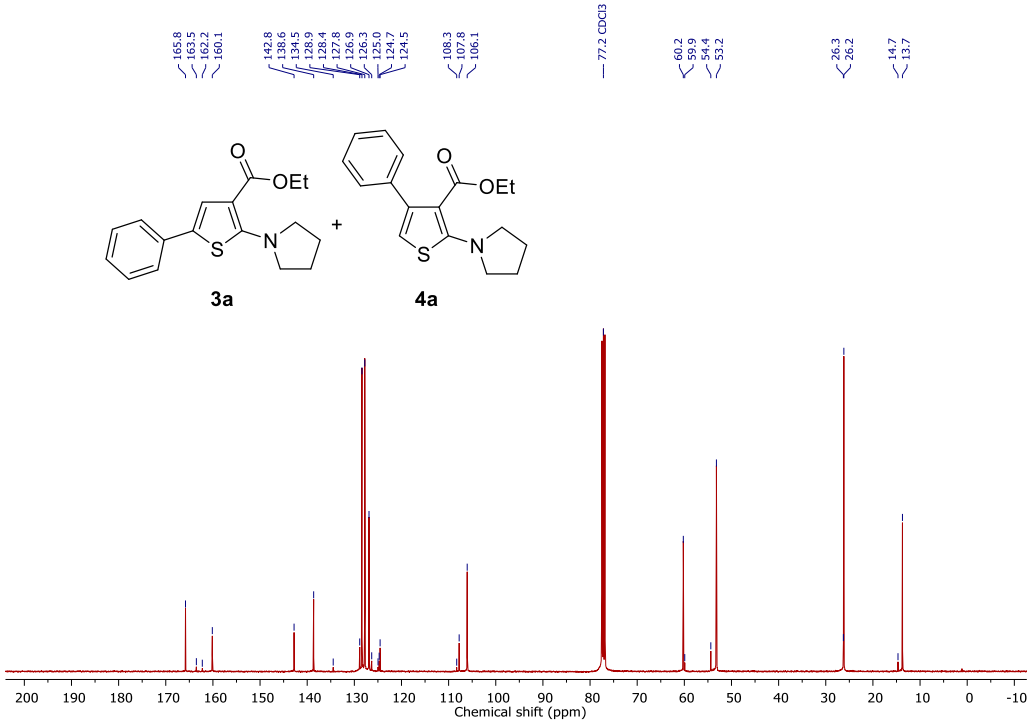
^{19}F NMR Spectrum of **1l** (400 MHz, $CDCl_3$)



^{1}H NMR Spectrum of regioisomeric mixture of **3a** and **4a** (**3a**:**4a**=1:14) (400 MHz, $CDCl_3$)[d]

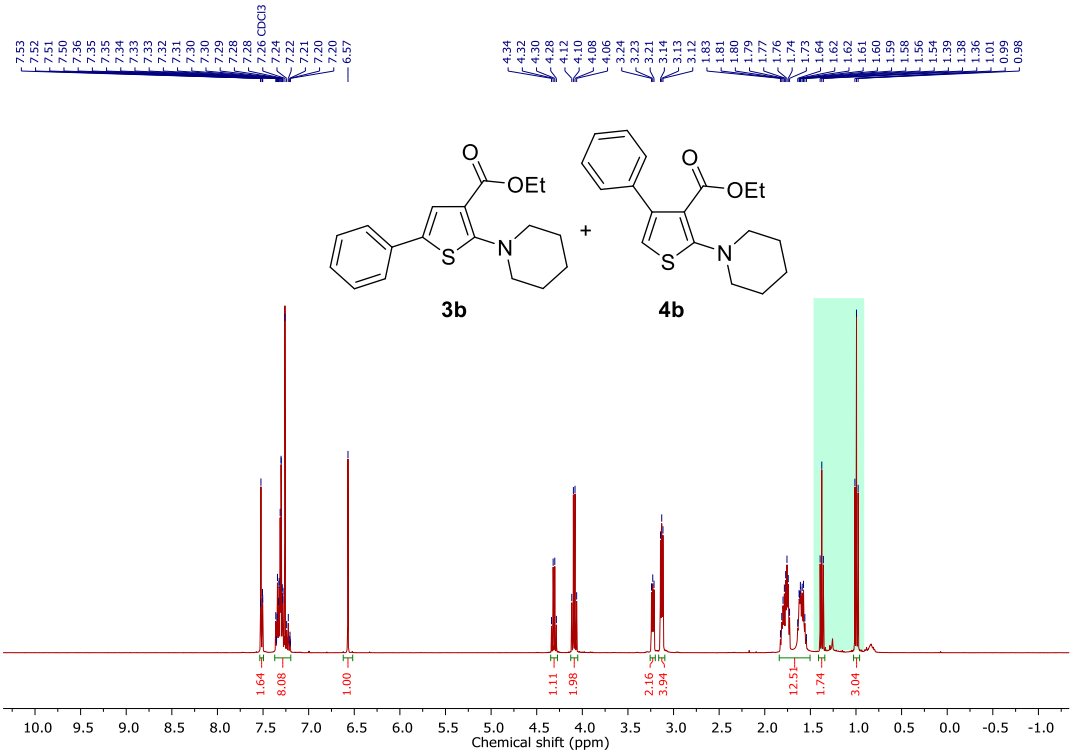


^{13}C NMR Spectrum of regioisomeric mixture of **3a** and **4a** (400 MHz, $CDCl_3$)

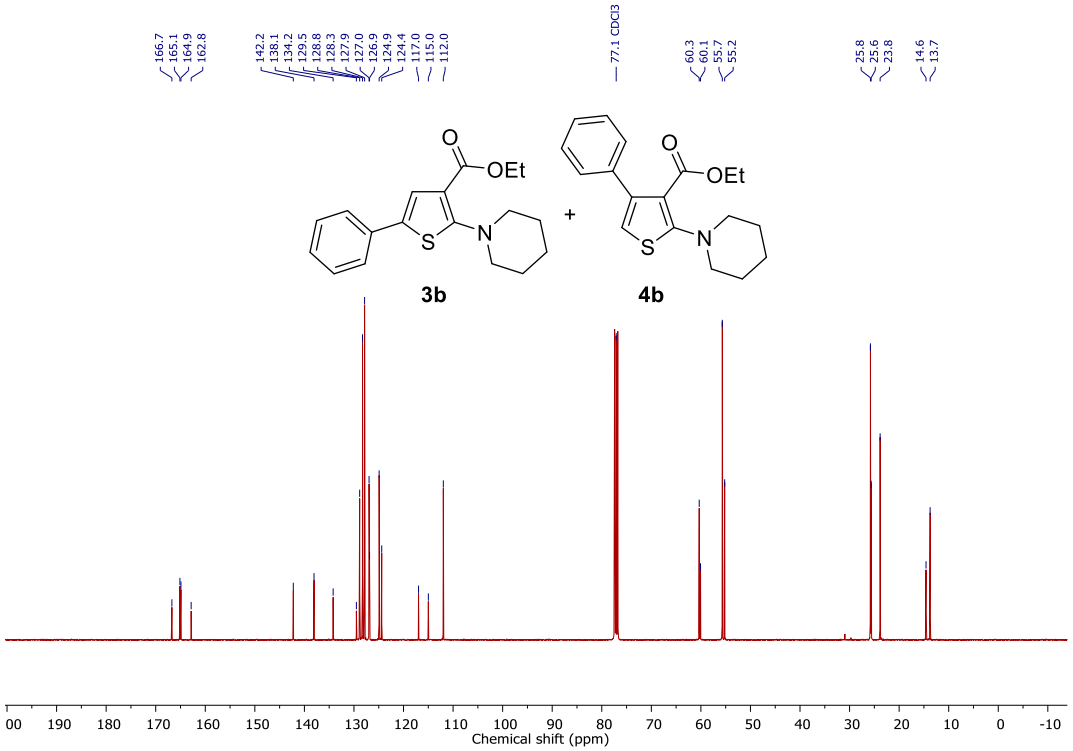


[d] The signals used for the calculation of regioisomeric ratio of the purified mixture are highlighted.

^{1}H NMR Spectrum of regioisomeric mixture of **3b** and **4b** (**3b**:**4b**=1:1.7) (400 MHz, $CDCl_3$)[e]

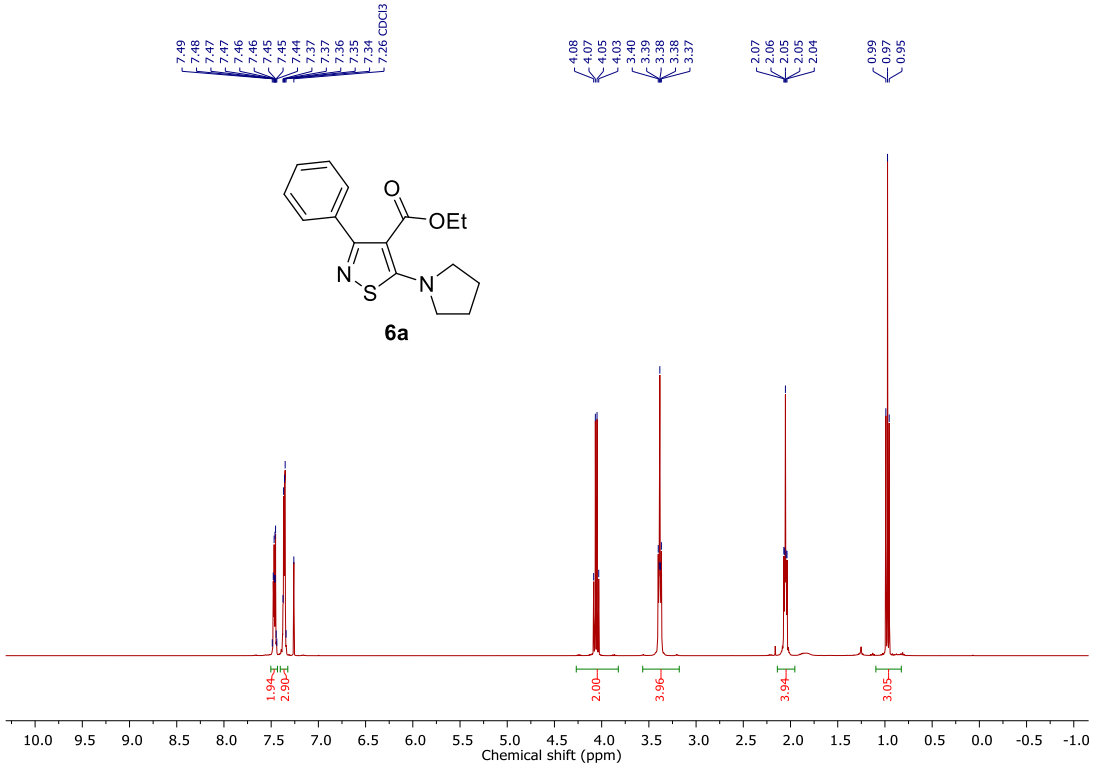


^{13}C NMR Spectrum of regioisomeric mixture of **3b** and **4b** (400 MHz, $CDCl_3$)

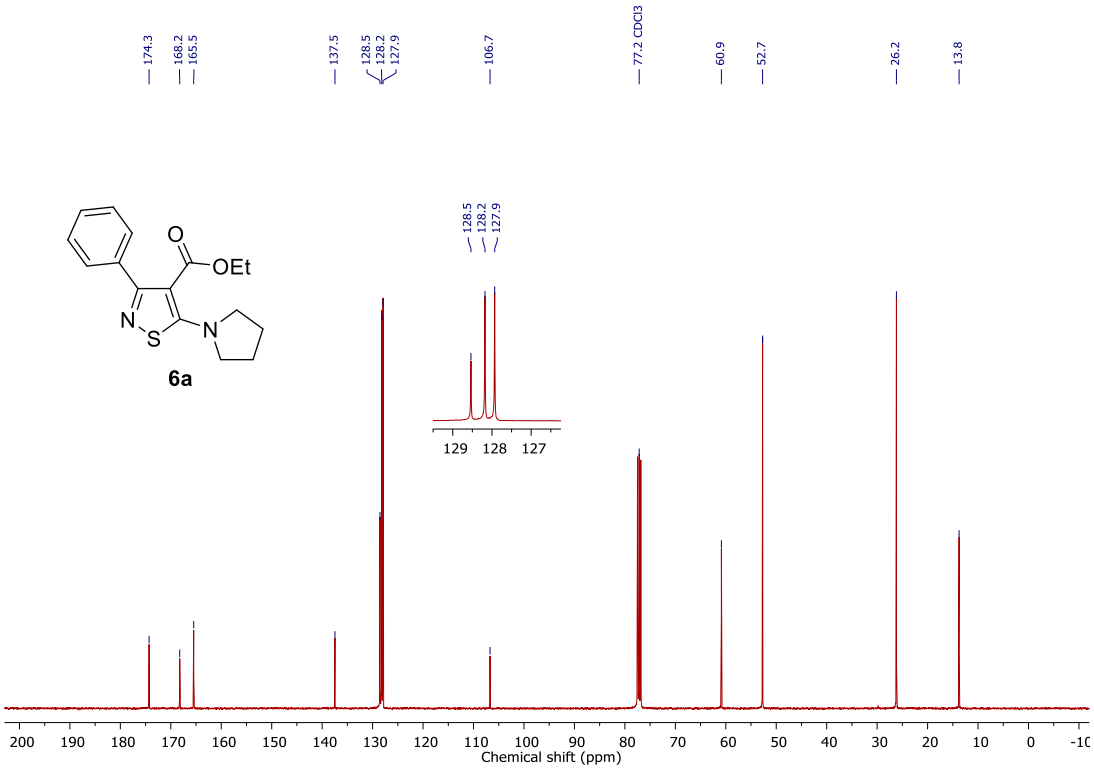


[e] The signals used for the calculation of regioisomeric ratio of the purified mixture are highlighted.

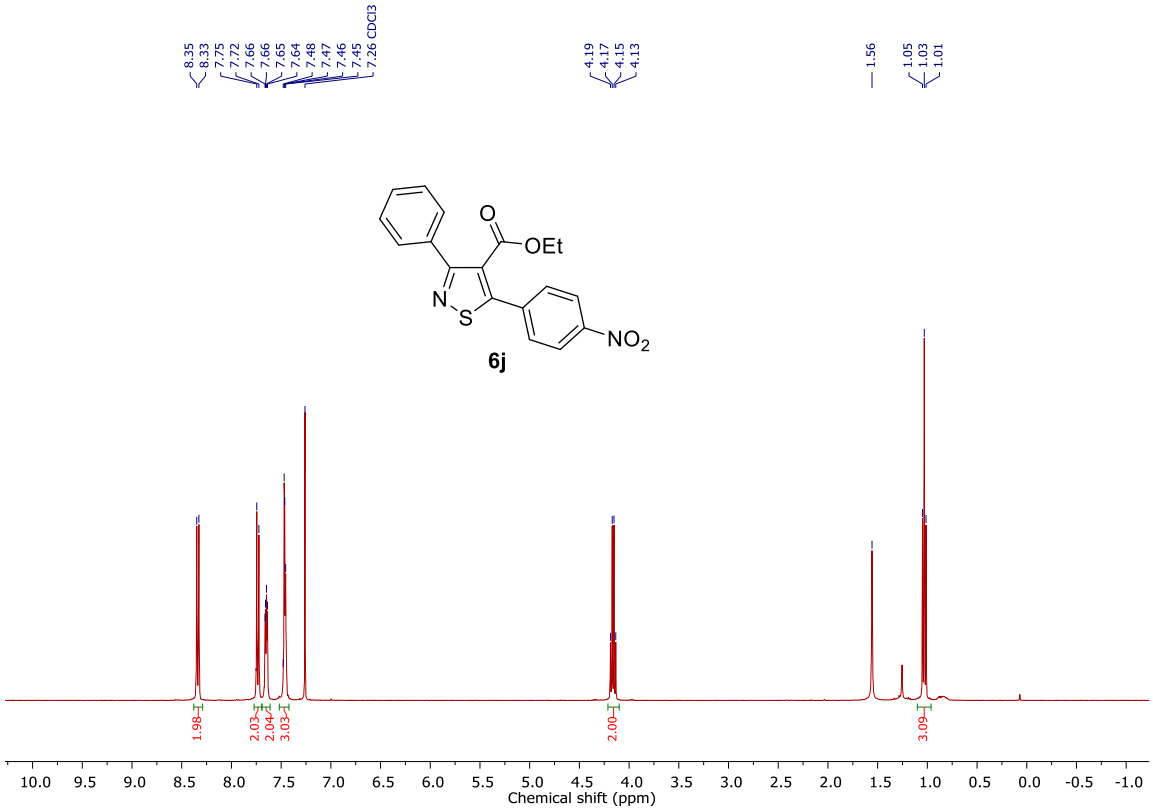
^{1}H NMR Spectrum of **6a** (400 MHz, $CDCl_3$)



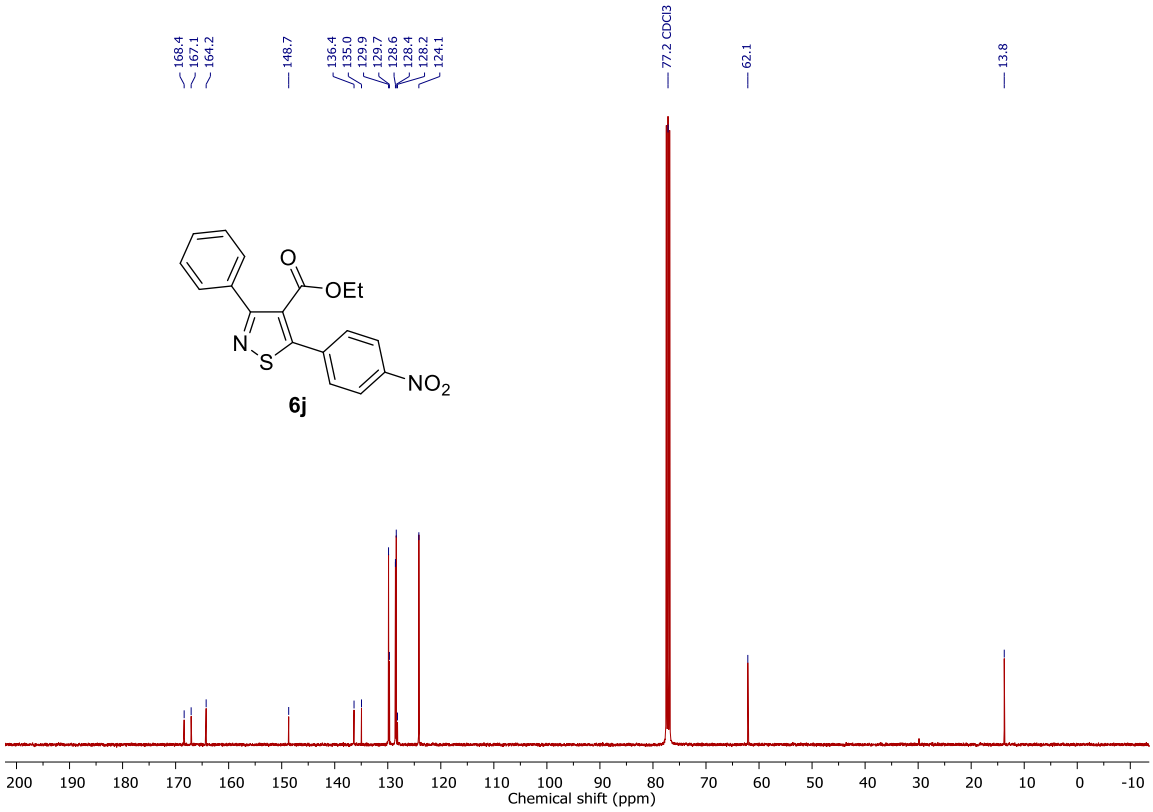
^{13}C NMR Spectrum of **6a** (400 MHz, $CDCl_3$)



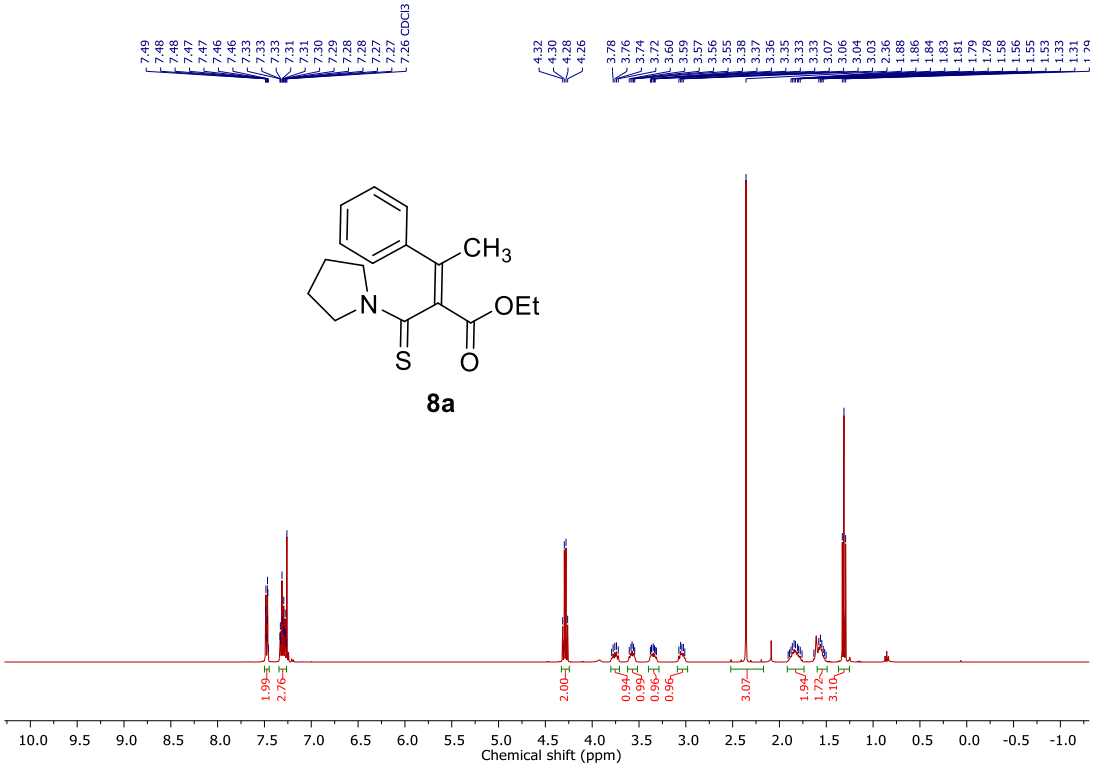
^{1}H NMR Spectrum of **6j** (400 MHz, $CDCl_3$)



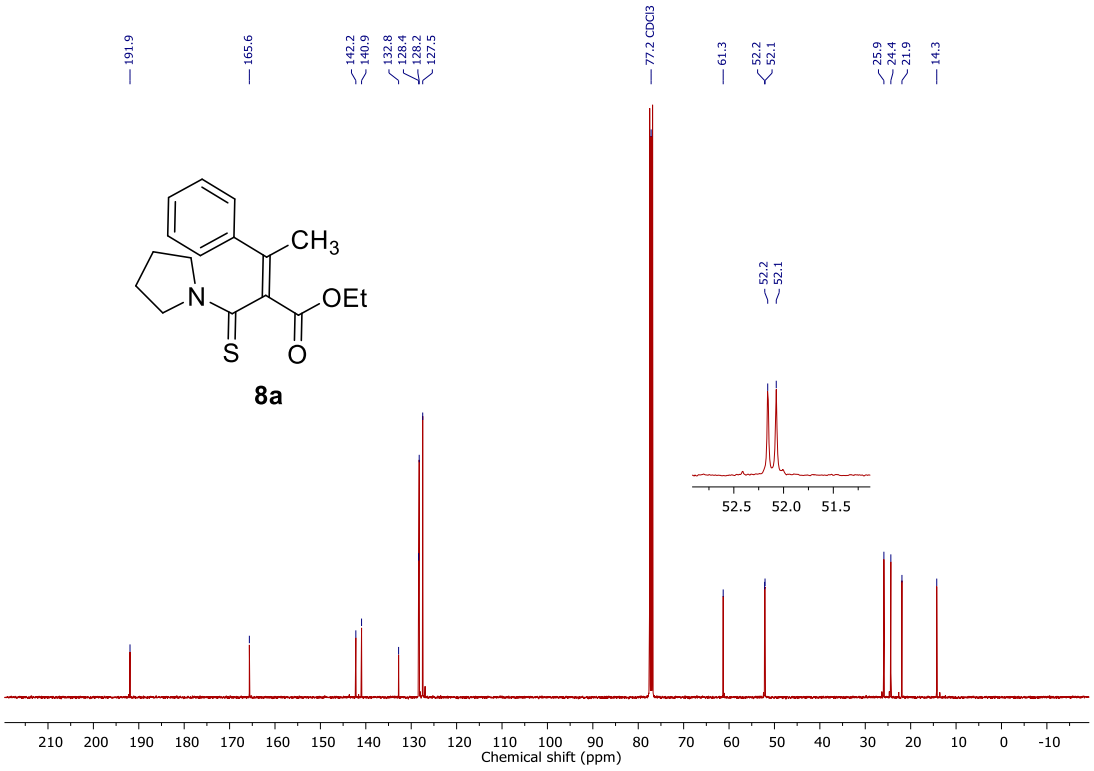
^{13}C NMR Spectrum of **6j** (400 MHz, $CDCl_3$)



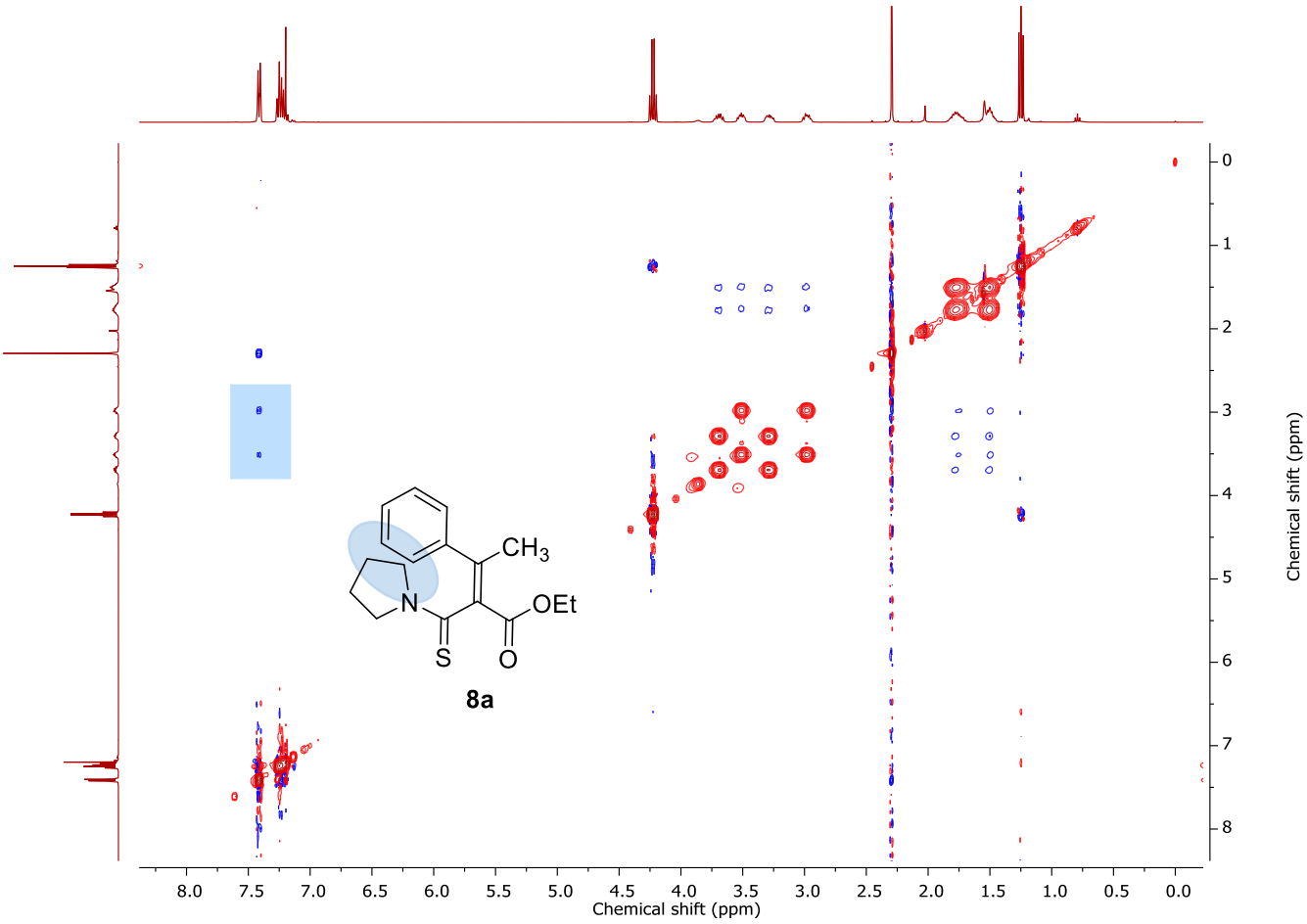
^{1}H NMR Spectrum of **8a** (400 MHz, $CDCl_3$)



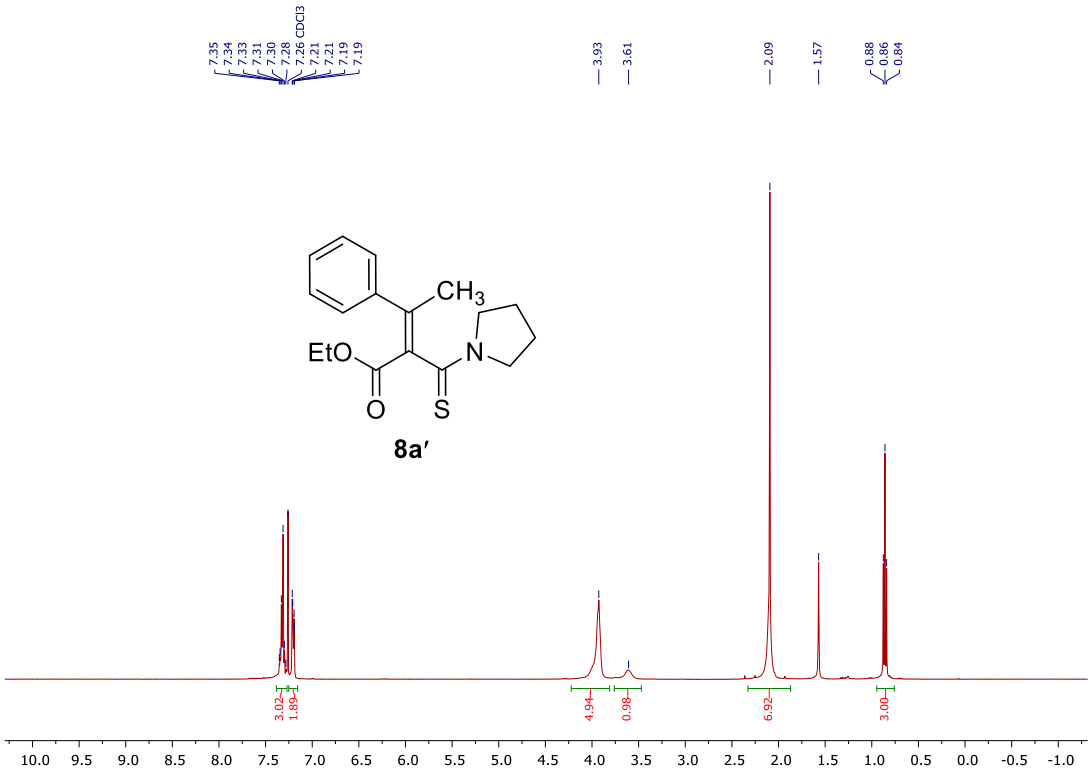
^{13}C NMR Spectrum of **8a** (400 MHz, $CDCl_3$)



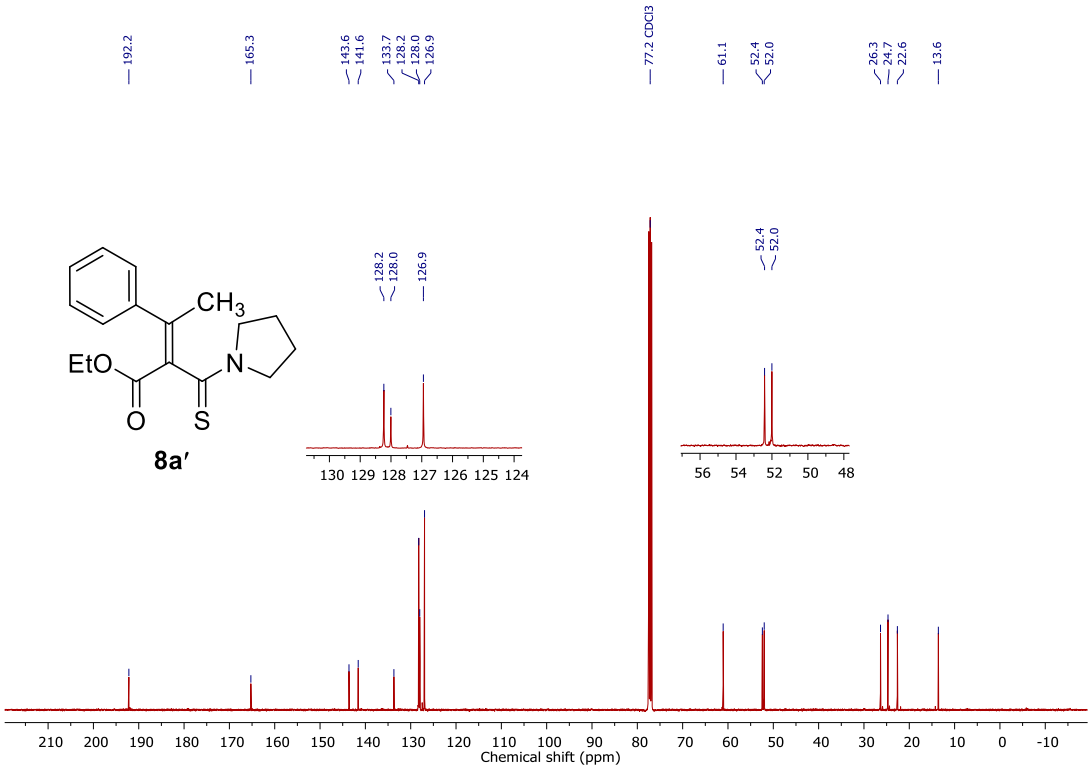
NOESY Spectrum of **8a** (400 MHz, $CDCl_3$)



^{1}H NMR Spectrum of **8a'** (400 MHz, $CDCl_3$)



^{13}C NMR Spectrum of **8a'** (400 MHz, $CDCl_3$)



12. X-Ray Crystallographic Data

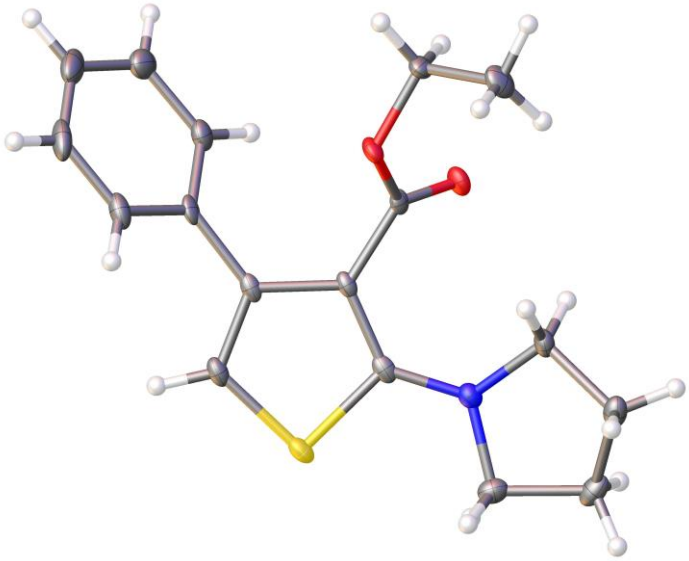


Figure S4. Solid state structure of **4a** (grown from *n*-hexane solution at -20 °C). Displacement ellipsoids depicted at the 50% probability level, CCDC: .2219742.

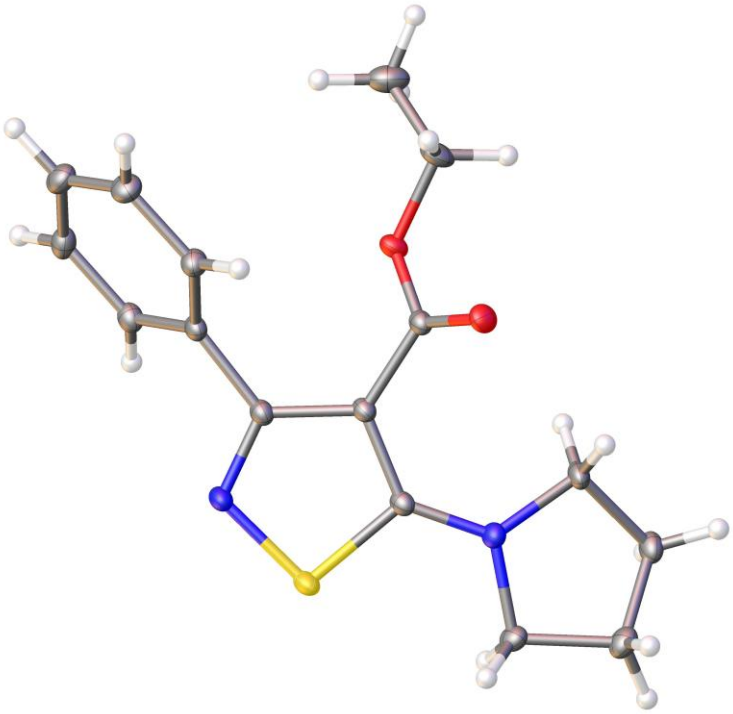


Figure S5. Solid state structure of **6a** (grown by slow evaporation of *n*-hexane solution). Displacement ellipsoids depicted at the 50% probability level, CCDC: 2219743.

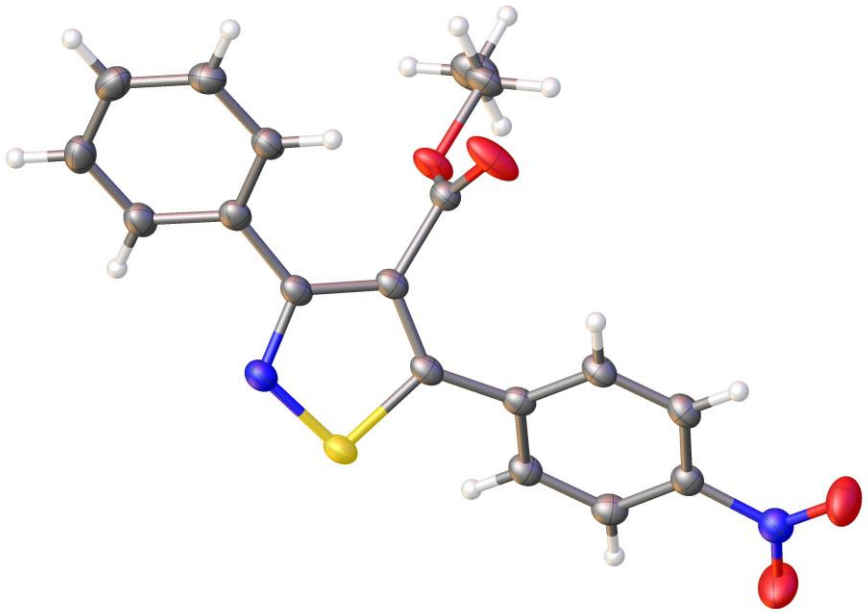


Figure S6. Solid state structure of **6j** (grown by slow evaporation of *n*-hexane solution). Displacement ellipsoids depicted at the 50% probability level, CCDC: 2219745.

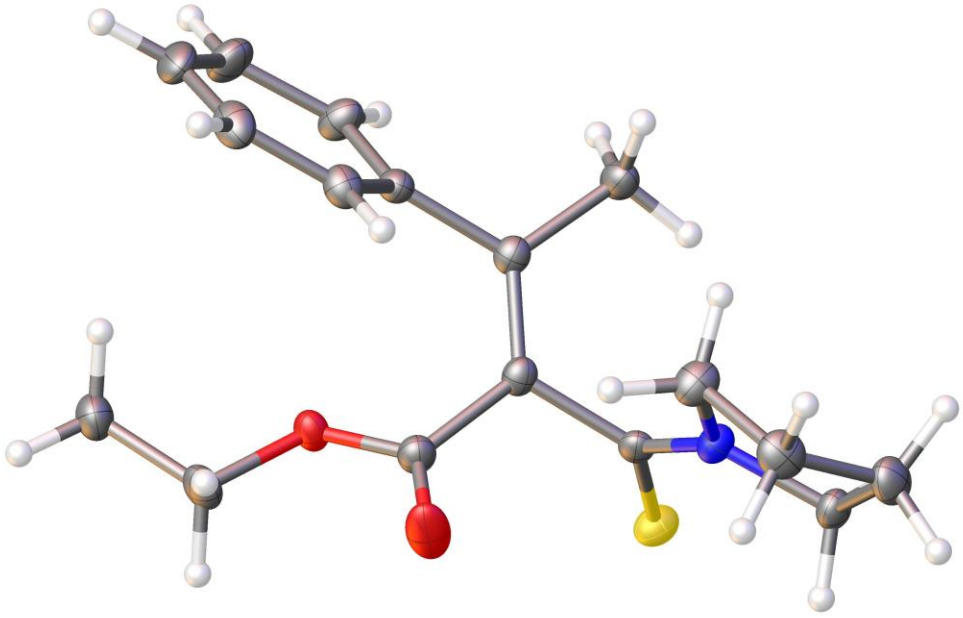


Figure S7. Solid state structure of **8a'** (grown by slow evaporation of ethyl acetate:*n*-hexane=1:8 solution). Displacement ellipsoids depicted at the 50% probability level, CCDC: 2219744.

Table S5. Crystallographic data for compounds **4a** and **6a**

Compound	**4a**	**6a**
CCDC number	2219742	2219743
Empirical formula	$C_{17}H_{19}NO_2S$	$C_{16}H_{18}N_2O_2S$
Formula weight	301.39	302.38
Temperature/K	100.01(10)	99.9(3)
Crystal system	monoclinic	monoclinic
Space group	$P2_1/c$	$P2_1/n$
a/Å	12.8925(4)	11.0494(2)
b/Å	7.8461(2)	10.37004(19)
c/Å	15.2747(5)	26.5033(5)
α/°	90	90
β/°	100.851(3)	100.2575(19)
γ/°	90	90
Volume/Å^3	1517.50(8)	2988.29(10)
Z	4	8
ρ_{calc}g/cm^3	1.319	1.344
μ/mm^{-1}	1.922	0.223
F(000)	640.0	1280.0
Crystal size/mm^3	0.319 × 0.244 × 0.122	0.4 × 0.2 × 0.05
Radiation	Cu Kα (λ = 1.54184)	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	12.532 to 145.128	3.794 to 91.696
Index ranges	-15 ≤ h ≤ 15, -7 ≤ k ≤ 9, -18 ≤ l ≤ 18	-22 ≤ h ≤ 16, -16 ≤ k ≤ 15, -39 ≤ l ≤ 51
Reflections collected	13345	187266
Independent reflections	2926 [R_{int} = 0.0437, R_{sigma} = 0.0287]	15899 [R_{int} = 0.0738, R_{sigma} = 0.0690]
Data/restraints/parameters	2926/0/191	15899/0/381
Goodness-of-fit on F^2	1.060	1.174
Final R indexes [I>=2σ (I)]	R_1 = 0.0369, wR_2 = 0.0980	R_1 = 0.0927, wR_2 = 0.1795
Final R indexes [all data]	R_1 = 0.0410, wR_2 = 0.1026	R_1 = 0.1463, wR_2 = 0.1954
Largest diff. peak/hole / e Å^{-3}	0.30/-0.32	1.11/-0.60

Table S6. Crystallographic data for compounds **6j** and **8a'**

Compound	**6j**	**8a'**
CCDC number	2219745	2219744
Empirical formula	$C_{18}H_{14}N_2O_4S$	$C_{17}H_{21}NO_2S$
Formula weight	354.380	303.428
Temperature/K	150.01(10)	150.00(10)
Crystal system	triclinic	monoclinic
Space group	P-1	$P2_1/n$
a/Å	8.8717(4)	9.7409(1)
b/Å	8.9788(4)	7.7066(1)
c/Å	10.5747(4)	21.1913(2)
α/°	100.966(4)	90
β/°	100.107(4)	91.380(1)
γ/°	93.879(4)	90
Volume/Å^3	809.68(6)	1590.35(3)
Z	4	4
ρ_{calc}g/cm^3	1.454	1.267
μ/mm^{-1}	0.226	1.835
F(000)	368.0	651.1
Crystal size/mm^3	0.38 × 0.28 × 0.21	0.55 × 0.4 × 0.15
Radiation	Mo Kα (λ = 0.71073)	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	3.998 to 59.008	8.34 to 144.84
Index ranges	$-12 \le h \le 12$, $-12 \le k \le 12$, $-14 \le l \le 14$	$-11 \le h \le 12$, $-8 \le k \le 9$, $-26 \le l \le 26$
Reflections collected	18033	21419
Independent reflections	4052 [R_{int} = 0.0267, R_{sigma} = 0.0266]	3130 [R_{int} = 0.0349, R_{sigma} = 0.0170]
Data/restraints/parameters	4052/0/227	3130/0/192
Goodness-of-fit on F^2	1.071	1.080
Final R indexes [I>=2σ (I)]	R_1 = 0.0386, wR_2 = 0.0845	R_1 = 0.0330, wR_2 = 0.1184
Final R indexes [all data]	R_1 = 0.0482, wR_2 = 0.0905	R_1 = 0.0351, wR_2 = 0.1224
Largest diff. peak/hole / e Å^{-3}	0.26/-0.32	0.35/-0.18

13. References

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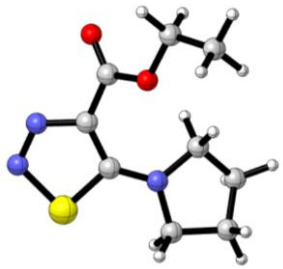
14. Cartesian Coordinates and Energies

All energies are given in Hartree.

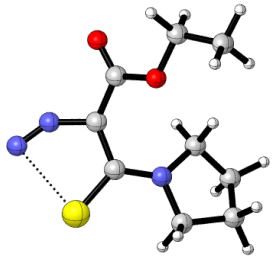
1a



C	0.09865700	1.38405100	-0.18717400
C	-0.94744700	0.50042600	0.10394400
S	-2.35042600	1.46072300	0.42492000
C	1.54133400	1.12664700	-0.38893100
N	-0.28036200	2.69840100	-0.17245700
N	-1.47623200	2.94456900	0.13780300
C	-2.24233200	-1.54831100	0.43523500
C	-0.07925000	-1.70738700	-0.65632300
C	-1.92132700	-3.01292300	0.14123500
H	-3.07070700	-1.18971700	-0.19567900
H	-2.50782100	-1.36530600	1.48185100
C	-0.94217900	-2.91274600	-1.03234600
H	0.76240900	-1.99442000	-0.02108100
H	0.31780900	-1.17233100	-1.52460600
H	-1.43215600	-3.47268900	1.00661400
H	-2.81818700	-3.59144000	-0.09085800
H	-0.34590600	-3.81720000	-1.17439500
H	-1.48715600	-2.71319600	-1.96149400
N	-1.00643800	-0.84467400	0.08616300
O	1.96005200	0.05375700	0.31394800
O	2.27813500	1.81300000	-1.05391100
C	3.35297100	-0.26091200	0.17799700
H	3.94216500	0.60688800	0.48747100
H	3.57636300	-0.45180600	-0.87666000
C	3.63448800	-1.46963600	1.04561700
H	4.69840300	-1.72074700	0.99627900
H	3.37482300	-1.26646200	2.08840100
H	3.06302100	-2.34052100	0.70905000

Zero-point correction = 0.227944
Thermal correction to Energy = 0.242361
Thermal correction to Enthalpy = 0.243305
Thermal correction to Gibbs Free Energy = 0.184959
Sum of electronic and zero-point Energies = -1063.193088
Sum of electronic and thermal Energies = -1063.178670
Sum of electronic and thermal Enthalpies = -1063.177726
Sum of electronic and thermal Free Energies = -1063.236072
E(RM06) = -1063.48024773

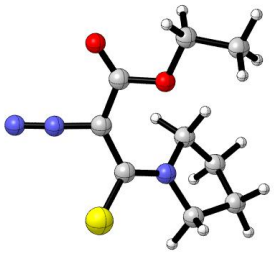
TS1a



C	-1.04868200	-0.56892900	-0.16258100
C	0.12603000	-1.33207500	0.30399300
S	-2.39179300	-1.39966700	-0.76466400
N	-0.98762100	-3.40004600	0.21276000
N	-0.16762900	-2.62973700	0.40905900
C	-2.16256000	1.57749400	-0.53507000
C	-0.19551500	1.54720400	0.87793900
C	-1.85771200	2.98713100	-0.02991400
H	-3.09610400	1.18492000	-0.11361100
H	-2.23276300	1.49847700	-1.62290300
C	-1.09127100	2.72081500	1.26775900
H	0.70174000	1.89525700	0.36217900
H	0.11127200	0.92510100	1.72320200
H	-1.21974800	3.52228500	-0.74215600
H	-2.76832700	3.57246900	0.11597300
H	-0.51203200	3.57937600	1.61638100
H	-1.78275200	2.42494200	2.06435700
N	-1.04053000	0.76646600	-0.03969500
C	3.28685800	0.40664600	-0.31731800
H	3.85003000	-0.42247800	-0.75458300
H	3.62250500	0.52704700	0.71721700
C	3.44569800	1.68089600	-1.11928700
H	4.50333600	1.95706900	-1.16777100
H	3.07579100	1.54554700	-2.13946000
H	2.89774400	2.50868000	-0.65819600
O	2.37140900	-1.74365000	0.92595300
O	1.89083400	0.06973200	-0.32194500
C	1.56223900	-1.03409100	0.36898700

Zero-point correction = 0.226843
Thermal correction to Energy = 0.241214
Thermal correction to Enthalpy = 0.242158
Thermal correction to Gibbs Free Energy = 0.184098
Sum of electronic and zero-point Energies = -1063.175107
Sum of electronic and thermal Energies = -1063.160735
Sum of electronic and thermal Enthalpies = -1063.159791
Sum of electronic and thermal Free Energies = -1063.217851
E(RM06) = -1063.45965361

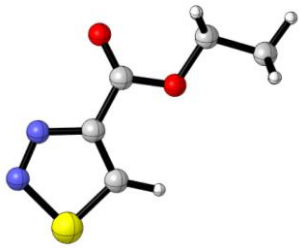
1a'



C	0.70390600	1.11744800	-0.27964700
C	-0.65049300	0.98547900	0.30183200
S	-1.26362400	2.17912900	1.30256000
N	1.07785100	2.34133400	-0.60758000
N	1.41676200	3.36668400	-0.91681400
C	-2.66721300	-0.38340400	0.52718300
C	-1.02381000	-1.03891200	-1.13261700
C	-3.09689800	-1.68455700	-0.15213200
H	-3.33556800	0.45134500	0.28532500
H	-2.60573200	-0.44445600	1.61701600
C	-2.38735100	-1.61629000	-1.50764600
H	-0.34958800	-1.82287500	-0.77599900
H	-0.52953900	-0.50322700	-1.94732700
H	-2.73768700	-2.54925500	0.41717300
H	-4.18324400	-1.76252700	-0.23572900
H	-2.30078100	-2.58609900	-2.00377400
H	-2.91705800	-0.93242600	-2.17996300
N	-1.33985700	-0.11229800	-0.03662200
C	1.83122200	0.17440700	-0.27762700
C	2.56985300	-1.94723000	0.41228000
H	2.91628800	-2.17052800	-0.60115300
H	3.41004200	-1.51874700	0.96586300
C	2.00069200	-3.16805600	1.10267500
H	1.16946600	-3.59087200	0.52979800
H	2.77625500	-3.93395300	1.19761100
H	1.63925600	-2.91421800	2.10301000
O	1.51762800	-0.97118100	0.34283800
O	2.92026500	0.42223500	-0.74927600

Zero-point correction = 0.227438
Thermal correction to Energy = 0.242681
Thermal correction to Enthalpy = 0.243625
Thermal correction to Gibbs Free Energy = 0.183325
Sum of electronic and zero-point Energies = -1063.187281
Sum of electronic and thermal Energies = -1063.172038
Sum of electronic and thermal Enthalpies = -1063.171094
Sum of electronic and thermal Free Energies = -1063.231395
E(RM06) = -1063.47217486

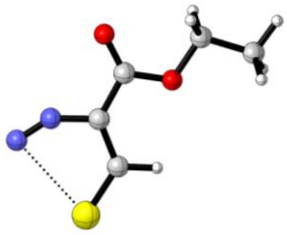
1h



C	-0.63389500	0.31587200	0.00007200
C	-1.05497900	-0.98752500	0.00026400
S	-2.74370200	-1.00578800	0.00002900
C	0.77468200	0.79241400	0.00013500
N	-1.65996400	1.22704000	-0.00025900
N	-2.81987300	0.71994700	-0.00033700
O	1.62000300	-0.24928100	0.00034600
O	1.11012200	1.94892800	0.00002300
C	3.01823000	0.08607500	0.00026700
H	3.23398200	0.69324800	0.88428500
H	3.23366900	0.69417800	-0.88318200
C	3.79481200	-1.21286200	-0.00052700
H	4.86804400	-1.00024200	-0.00041300
H	3.56102600	-1.80718600	0.88749700
H	3.56099500	-1.80613600	-0.88924100
H	-0.43372100	-1.87119000	0.00055000

Zero-point correction = 0.115886
Thermal correction to Energy = 0.125402
Thermal correction to Enthalpy = 0.126346
Thermal correction to Gibbs Free Energy = 0.079417
Sum of electronic and zero-point Energies = -851.965843
Sum of electronic and thermal Energies = -851.956327
Sum of electronic and thermal Enthalpies = -851.955383
Sum of electronic and thermal Free Energies = -852.002312
E(RM06) = -852.161643552

TS1h

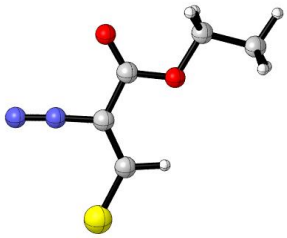


C	-1.13671900	-0.95538200	0.00011800
C	-0.61540700	0.35251700	-0.00015800
S	-2.79254700	-1.29422200	0.00013800
N	-2.72972700	1.33724700	-0.00028000
N	-1.58792200	1.31317900	-0.00029200
C	3.01862300	0.04990500	0.00022800
H	3.24445900	0.65231800	0.88474400
H	3.24465900	0.65314100	-0.88367400
C	3.76905100	-1.26399700	-0.00030500

H	4.84608700	-1.07166600	-0.00056300
H	3.52384400	-1.85322900	0.88787100
H	3.52334600	-1.85270600	-0.88869500
O	1.13507400	1.95052400	0.00033000
O	1.61302600	-0.25987100	-0.00005700
C	0.78723100	0.79284100	0.00006600
H	-0.39957500	-1.75381300	0.00023900

Zero-point correction = 0.114183
Thermal correction to Energy = 0.123979
Thermal correction to Enthalpy = 0.124923
Thermal correction to Gibbs Free Energy = 0.077281
Sum of electronic and zero-point Energies = -851.942491
Sum of electronic and thermal Energies = -851.932695
Sum of electronic and thermal Enthalpies = -851.931751
Sum of electronic and thermal Free Energies = -851.979393
E(RM06) = -852.136259180

1h'



C	0.68925600	0.29601600	-0.00009400
C	1.18075400	-1.04516200	-0.00011700
S	2.74682500	-1.52314000	0.00013900
N	1.57885100	1.28614300	-0.00000400
N	2.36475100	2.08365400	0.00008300
C	-0.71219400	0.75610300	-0.00017500
C	-2.95436300	0.05113300	-0.00020100
H	-3.16939000	0.65727100	0.88431500
H	-3.17040100	0.65681800	-0.88478000
C	-3.72281500	-1.25202200	0.00055300
H	-3.48472900	-1.84414800	0.88862900
H	-4.79692500	-1.04402300	0.00146100
H	-3.48625600	-1.84434500	-0.88779700
O	-1.55221500	-0.28007400	-0.00094700
O	-1.03562700	1.92262100	0.00043800
H	0.37218600	-1.77670800	-0.00033200

Zero-point correction = 0.114555
Thermal correction to Energy = 0.125225
Thermal correction to Enthalpy = 0.126169
Thermal correction to Gibbs Free Energy = 0.076568
Sum of electronic and zero-point Energies = -851.946494
Sum of electronic and thermal Energies = -851.935824
Sum of electronic and thermal Enthalpies = -851.934880
Sum of electronic and thermal Free Energies = -851.984481
E(RM06) = -852.139788402

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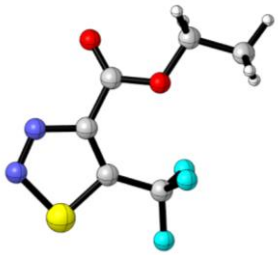
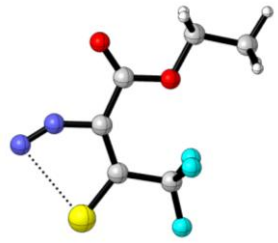


C	0.48408500	-1.08201800	0.00591200
C	1.05934700	0.16676600	0.00256800
S	2.74433200	-0.02975600	0.09929000
C	-0.96215300	-1.45253500	-0.08233900
N	1.39645900	-2.10138600	0.08384200
N	2.60884100	-1.72408700	0.14540400
O	-1.72892400	-0.38889800	0.14907500
O	-1.35883000	-2.56119200	-0.33019200
C	-3.14993200	-0.57814200	0.03218600
H	-3.46847000	-1.30033000	0.78947100
H	-3.36634300	-1.00297200	-0.95218400
C	-3.78978000	0.77941200	0.22536300
H	-4.87664100	0.69284900	0.13657400
H	-3.55172100	1.18281600	1.21341000
H	-3.43156900	1.48316400	-0.53093600
C	0.43500700	1.53799500	-0.08189400
F	1.40529700	2.46501500	-0.19043800
F	-0.27499300	1.83021800	1.00724700
F	-0.35353500	1.65707100	-1.15142400

Zero-point correction = 0.120950
Thermal correction to Energy = 0.134036
Thermal correction to Enthalpy = 0.134980
Thermal correction to Gibbs Free Energy = 0.078840
Sum of electronic and zero-point Energies = -1188.902793
Sum of electronic and thermal Energies = -1188.889707
Sum of electronic and thermal Enthalpies = -1188.888763
Sum of electronic and thermal Free Energies = -1188.944903
E(RM06) = -1189.22977596

TS1l



C	1.25357300	-0.17893000	0.00005900
C	0.45724300	1.01680300	0.00010600
S	2.90046500	-0.16781700	0.00024100
N	2.31658200	2.49029100	0.00040100
N	1.25227200	2.10157100	0.00026700

C	-3.18801200	0.52329900	-0.00002000
H	-3.44276900	1.11280600	-0.88523400
H	-3.44296900	1.11297500	0.88502400
C	-3.85701500	-0.83369100	0.00003300
H	-4.94393900	-0.70998600	-0.00011900
H	-3.56984200	-1.40506600	-0.88682600
H	-3.57007200	-1.40489100	0.88708000
O	-1.36790200	2.50102300	-0.00020300
O	-1.76870100	0.28415100	0.00016500
C	-0.98755300	1.35141800	-0.00000700
C	0.51123300	-1.52909800	-0.00020800
F	-0.25631600	-1.63908900	-1.09028500
F	-0.25628200	-1.63954100	1.08984100
F	1.34994900	-2.55959200	-0.00043900

Zero-point correction = 0.119187
Thermal correction to Energy = 0.132468
Thermal correction to Enthalpy = 0.133413
Thermal correction to Gibbs Free Energy = 0.076726
Sum of electronic and zero-point Energies = -1188.873259
Sum of electronic and thermal Energies = -1188.859978
Sum of electronic and thermal Enthalpies = -1188.859034
Sum of electronic and thermal Free Energies = -1188.915720
E(RM06) = -1189.19943544

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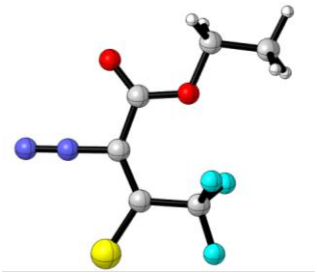
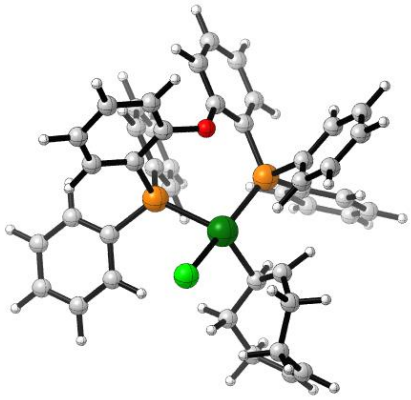


C	-0.49437800	0.98703200	0.00012400
C	-1.29674400	-0.20706200	0.00021200
S	-2.93745400	-0.18913700	-0.00021200
N	-1.20030100	2.12547600	-0.00003000
N	-1.78151300	3.07994700	-0.00012300
C	0.96053900	1.30531000	0.00004100
C	3.14831500	0.44546900	-0.00028200
H	3.41170900	1.03081600	-0.88563300
H	3.41210000	1.03056500	0.88512200
C	3.79375200	-0.92274100	-0.00060700
H	3.49632300	-1.48869800	-0.88747900
H	4.88261100	-0.81752000	-0.00082000
H	3.49669600	-1.48894100	0.88623600
O	1.72454100	0.22871100	0.00001700
O	1.35511800	2.45120200	-0.00024400
C	-0.55702900	-1.56005100	0.00032900
F	-1.40099800	-2.58403600	0.00060500
F	0.21222200	-1.67474700	1.09096200
F	0.21194500	-1.67511000	-1.09046100

Zero-point correction = 0.119547
Thermal correction to Energy = 0.133647
Thermal correction to Enthalpy = 0.134591
Thermal correction to Gibbs Free Energy = 0.075821
Sum of electronic and zero-point Energies = -1188.878875
Sum of electronic and thermal Energies = -1188.864774
Sum of electronic and thermal Enthalpies = -1188.863830
Sum of electronic and thermal Free Energies = -1188.922600
E(RM06) = -1189.20519417

[Rh(COD)DPEPhos]Cl

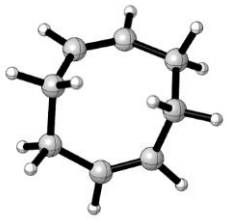


Cl	-0.03619000	2.49110200	-2.22222100
C	2.04318700	1.85614800	0.51147200
C	2.66614300	1.35323400	-0.64513000
C	3.19208600	2.10038200	-1.86236900
C	3.42655400	3.61381000	-1.69840000
C	4.37296400	3.96192600	-0.57717100
C	4.10649100	4.14444000	0.71892800
C	2.79408500	4.06867400	1.45978200
C	1.64724200	3.28603100	0.79748400
H	2.22410500	1.29064900	1.42720700
H	3.23337300	0.44039000	-0.46590300
H	2.52736400	1.96032100	-2.72056600
H	4.15102000	1.63373400	-2.12557800
H	3.85465900	3.97916700	-2.63985600
H	2.46630000	4.12077500	-1.59558300
H	5.41932300	4.05110700	-0.87114300
H	4.95274200	4.39406700	1.35998800
H	2.44372600	5.08894800	1.67662500
H	2.99602100	3.61723700	2.44174500
H	0.79880800	3.27621500	1.49427200
H	1.29375500	3.78565100	-0.10299100
Rh	0.50164500	0.82200700	-0.56065600
C	-2.78124400	-0.17868700	-1.37967100
C	-2.29134000	-1.35991200	-1.95734300
C	-2.91523400	-1.95905700	-3.04323500
C	-4.06740100	-1.38780800	-3.57390600
C	-4.57372900	-0.21645000	-3.02195500
C	-3.93084400	0.38318500	-1.94233300
O	-1.10583800	-1.90598400	-1.50430100
C	2.78529800	-2.08350900	-3.53016500

C	3.26312700	-3.38027400	-3.37057900
C	3.10659300	-4.03339200	-2.14900200
C	2.47629700	-3.38720900	-1.09191700
C	2.01014100	-2.07587600	-1.23919800
P	1.13790800	-1.23212200	0.14822900
C	-0.09742100	-2.54360900	0.53002500
P	-1.79021700	0.64172100	-0.06247500
C	-2.71987100	2.18699500	0.32848400
C	-2.20913900	-0.27458900	1.47910500
C	2.33017500	-1.33038500	1.54149300
H	-2.47668500	-2.85621900	-3.46813000
H	-4.55704200	-1.85137300	-4.42469300
H	-5.46212400	0.24572900	-3.44042900
H	-4.31768000	1.31580800	-1.54689600
H	2.34550800	-3.90588100	-0.14551000
H	3.47031900	-5.04877300	-2.02181100
H	3.75212800	-3.88626300	-4.19800000
H	2.89340700	-1.57312700	-4.48234900
C	-0.06295600	-3.38613600	1.64117800
C	-1.02417900	-4.37831100	1.81738700
C	-2.02490000	-4.55168000	0.86788700
C	-2.07466300	-3.73138600	-0.25393800
H	0.72080700	-3.26812400	2.38172300
H	-0.98443500	-5.01612700	2.69451400
H	-2.77200400	-5.32920600	0.99588700
H	-2.85364200	-3.85009500	-0.99978600
C	1.87780400	-1.03045900	2.83328100
C	2.76517400	-0.97378300	3.90116300
C	4.12525200	-1.19386600	3.69135200
C	4.58680400	-1.47695300	2.41072100
C	3.69577100	-1.54782400	1.34155400
H	0.82163400	-0.84568200	3.00258500
H	2.39514800	-0.74922100	4.89726800
H	4.82127300	-1.14020700	4.52309800
H	5.64559600	-1.64298800	2.23657800
H	4.07206100	-1.77219400	0.34865700
C	-1.51294000	0.10571500	2.63113400
C	-1.78892400	-0.49305100	3.85466800
C	-2.76056600	-1.48873500	3.93971400
C	-3.46458600	-1.86319600	2.80059200
C	-3.19930600	-1.25002200	1.57782200
H	-0.74849200	0.87691600	2.55920400
H	-1.24276200	-0.18534300	4.74218500
H	-2.97007700	-1.96642600	4.89220500
H	-4.22397700	-2.63735500	2.85842500
H	-3.75983100	-1.54567600	0.69604700
C	-4.01355200	2.10794700	0.86527600
C	-4.70475800	3.25833700	1.22348300
C	-4.10513400	4.50749400	1.06996800
C	-2.81712800	4.59414200	0.55538400
C	-2.12617500	3.44166100	0.18432200
H	-4.48286200	1.13966100	1.01528900
H	-5.70765200	3.17888800	1.63270900
H	-4.64167800	5.40756100	1.35609100
H	-2.34067100	5.56234200	0.43395400
H	-1.13271300	3.51806000	-0.23954600
C	2.16082300	-1.43219900	-2.46911700
H	1.78042500	-0.42222200	-2.59766500
C	-1.12145300	-2.73273800	-0.40563100

Zero-point correction = 0.729774
Thermal correction to Energy = 0.773426
Thermal correction to Enthalpy = 0.774370
Thermal correction to Gibbs Free Energy = 0.652256
Sum of electronic and zero-point Energies = -3028.182685
Sum of electronic and thermal Energies = -3028.139034
Sum of electronic and thermal Enthalpies = -3028.138089
Sum of electronic and thermal Free Energies = -3028.260204
E(RM06) = -3028.84717130

COD



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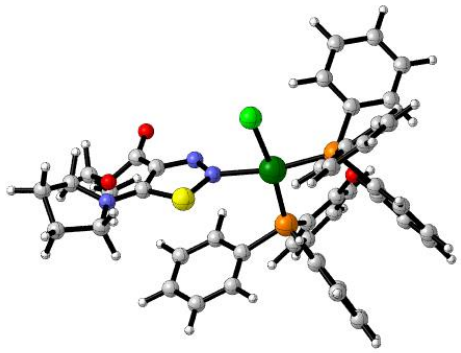
H	1.77210800	1.84794500	-1.19535400
C	-0.04563500	1.68942700	-0.23174600
C	1.18287600	1.24485900	-0.50393500
H	-1.79568100	1.87594900	0.96256800
H	2.70941200	0.35157500	0.68366900
C	-1.09614000	1.08461300	0.66912800
C	1.91722400	0.02652300	-0.00714000
H	-0.66132900	0.71920900	1.60155700
H	2.44512400	-0.41078900	-0.86590100
C	-1.91722300	-0.02650900	-0.00714400
C	1.09615300	-1.08462400	0.66910800
H	-2.44509300	0.41082000	-0.86591700
H	0.66136000	-0.71925200	1.60156000
C	-1.18288500	-1.24485500	-0.50392600
H	-2.70943600	-0.35155300	0.68363900
C	0.04562700	-1.68943000	-0.23174900
H	1.79570700	-1.87596200	0.96251200
H	-1.77213100	-1.84795200	-1.19532500
H	0.35488000	-2.60003000	-0.74428800

Zero-point correction = 0.183052
Thermal correction to Energy = 0.190436
Thermal correction to Enthalpy = 0.191380
Thermal correction to Gibbs Free Energy = 0.151532
Sum of electronic and zero-point Energies = -311.750173
Sum of electronic and thermal Energies = -311.742788
Sum of electronic and thermal Enthalpies = -311.741844
Sum of electronic and thermal Free Energies = -311.781692
E(RM06) = -311.888699040

INT1a



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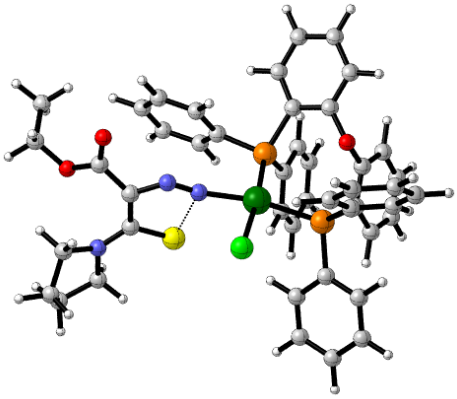
C	-4.12021500	-1.18016700	-0.23553800
C	-3.84828400	-0.67515900	1.04373800
S	-2.59897900	-1.42255200	-1.02022400
N	-1.75815100	-0.82430500	0.33520000
N	-2.51982400	-0.52391400	1.30016800
C	-4.75947700	-0.10431500	2.05619700
O	-4.51255000	-0.00975000	3.23337500
O	-5.89055800	0.37068600	1.48774400
C	-6.83820000	0.97378800	2.38183500
C	-6.49453300	2.42937200	2.64171700
H	-6.86280400	0.40413700	3.31379700
H	-7.79897600	0.87510000	1.87052500
H	-7.25874100	2.88463200	3.28014200
H	-5.53012400	2.50566400	3.15019900
H	-6.45121600	2.99127100	1.70321300
C	-5.27122300	-1.98947100	-2.22606300
C	-6.50914000	-1.88792500	-0.13709800
C	-6.72044500	-2.41146000	-2.46508500
H	-4.58856600	-2.84711900	-2.33638200
H	-4.93134100	-1.19084400	-2.89468800
C	-7.15936700	-2.90104800	-1.08094200
H	-7.13825700	-1.00497500	0.00312500
H	-6.27515600	-2.30053400	0.84884000
H	-7.31958000	-1.54674900	-2.77075500
H	-6.80305300	-3.17580000	-3.24087400
H	-8.24484800	-2.93681300	-0.96112300
H	-6.76035600	-3.90367800	-0.89222400
N	-5.27067700	-1.52453300	-0.83734600
Rh	0.34256300	-0.78249300	0.25658200
P	2.59738300	-1.04994200	0.43486200
P	0.35551100	1.34238900	-0.53440900
C	3.19152100	-1.29264300	2.16096900
C	3.70704400	0.30201800	-0.13562600
C	3.28785200	-2.48027800	-0.49052000
C	0.75663500	2.79882800	0.54613500
C	-1.31512300	1.82064700	-1.16911400
C	1.39010500	1.63506100	-2.03102900
C	4.48994700	-0.93429600	2.54222100
C	2.33070700	-1.84183500	3.11538300
C	4.62192200	0.18301700	-1.18266000
C	3.55816600	1.55464700	0.46274600
C	2.58672300	-2.96280100	-1.59835800
C	4.51695300	-3.05855700	-0.16103300
C	1.80678100	2.72862900	1.47326900
C	0.00181200	3.97884600	0.53493100
C	-1.61324500	1.81500900	-2.53365300
C	-2.35556100	2.04825500	-0.25769600
C	1.63151800	0.54944600	-2.87805800
C	1.87780500	2.89364100	-2.38740600
C	4.92385900	-1.13177200	3.84911900
H	5.16743900	-0.48742800	1.81981500
C	2.76797800	-2.03604200	4.42293600
H	1.32244700	-2.12428300	2.83131200
C	5.35994200	1.28068700	-1.61639300
H	4.74519000	-0.77425800	-1.67775300
O	2.64739400	1.64077200	1.49455300
C	4.30132500	2.65625100	0.05648100
C	3.11600300	-3.98593600	-2.37863500
H	1.60421700	-2.55744400	-1.81919800
C	5.04346200	-4.08653600	-0.93743300
H	5.06591400	-2.71156500	0.70900700
C	2.03586400	3.73587800	2.40341800
C	0.23994200	5.00872800	1.44033300
H	-0.79900500	4.09272700	-0.18714200
C	-2.92097800	2.01208500	-2.97580800
H	-0.82769500	1.64586300	-3.26272300
C	-3.65960100	2.24040000	-0.69746300
H	-2.14705100	2.04996800	0.80833600
C	2.34228400	0.71705100	-4.06172700
H	1.26296000	-0.43146400	-2.58987000
C	2.59679600	3.06093600	-3.56744900
H	1.70740900	3.74633400	-1.73665400
C	4.06221500	-1.68390000	4.79329300
H	5.93438600	-0.84833700	4.12958000
H	2.08749600	-2.46288300	5.15371600
C	5.20237100	2.51369400	-0.99287100
H	6.05301500	1.17048900	-2.44425800
H	4.15909100	3.61450300	0.54517800
C	4.34700000	-4.54754000	-2.05176800
H	2.55541300	-4.35767200	-3.23140400
H	5.99709400	-4.53080000	-0.66731000
C	1.24398900	4.87822300	2.39371900
H	2.84478300	3.60686900	3.11503000
H	-0.36977000	5.90616900	1.40474000
C	-3.94831200	2.21588800	-2.06125500
H	-3.13158100	2.00363800	-4.04154900
H	-4.45505600	2.38438700	0.02760300
C	2.82792600	1.97524200	-4.40762300
H	2.52647100	-0.13820000	-4.70528500
H	2.98044800	4.04303600	-3.82841200
H	4.39845900	-1.83486100	5.81528100
H	5.77727200	3.37287300	-1.32530700
H	4.75746300	-5.35184300	-2.65569300
H	1.42260200	5.66695200	3.11809700
H	-4.96849700	2.36054000	-2.40536600
H	3.39096100	2.10878900	-5.32690500

Zero-point correction = 0.774400

Thermal correction to Energy = 0.825518
Thermal correction to Enthalpy = 0.826462
Thermal correction to Gibbs Free Energy = 0.683851
Sum of electronic and zero-point Energies = -3779.623452
Sum of electronic and thermal Energies = -3779.572334
Sum of electronic and thermal Enthalpies = -3779.571390
Sum of electronic and thermal Free Energies = -3779.714002
E(RM06) = -3780.44779481

TS1a



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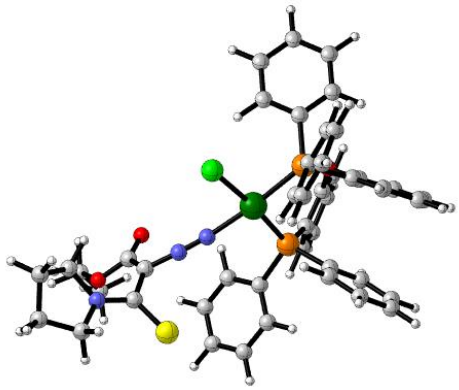
C	-3.92474100	-0.47016700	0.93335700
S	-2.60036600	-1.19149600	-1.30267800
N	-1.63477800	-0.32186000	0.74909500
N	-2.65777100	-0.20345600	1.29815600
C	-4.92860400	0.27461900	1.69238100
O	-4.72762100	0.79539900	2.76991300
O	-6.09758700	0.38335700	1.02563100
C	-7.14138400	1.09995900	1.69565600
C	-7.04095800	2.59143100	1.43260600
H	-7.09407300	0.88716700	2.76611100
H	-8.06646500	0.68737600	1.28454500
H	-7.88774200	3.11110100	1.89304200
H	-6.11707600	2.98725000	1.86188000
H	-7.05218400	2.79335400	0.35713200
C	-5.20909400	-2.46828900	-2.02541400
C	-6.16929200	-2.27811400	0.19011700
C	-6.50362200	-3.27779500	-1.94427600
H	-4.33134500	-3.11590600	-2.14840200
H	-5.19632700	-1.73250400	-2.83428100
C	-6.61020400	-3.59286100	-0.44986500
H	-6.99503300	-1.56413200	0.23078400
H	-5.75848700	-2.38926000	1.19696300
H	-7.35804700	-2.67045100	-2.26401800
H	-6.46589800	-4.16922000	-2.57476600
H	-7.61627600	-3.88415700	-0.13762800
H	-5.91764300	-4.39773600	-0.18004800
N	-5.12096600	-1.79575400	-0.72235300
Rh	0.31976200	-0.53165000	0.61828800
P	2.52861500	-1.20570500	0.43002400
P	0.48484400	1.55822700	-0.32668300
C	3.51630900	-1.32077400	1.97153100
C	3.60757300	-0.20967600	-0.66789500
C	2.66592100	-2.85786200	-0.35672100
C	1.44116000	2.93444000	0.47463500
C	-1.18294100	2.33228900	-0.42791600
C	1.05496900	1.62363100	-2.07244200
C	4.91007200	-1.19848800	1.94722400
C	2.86787000	-1.52648600	3.19181900
C	4.11761000	-0.64742600	-1.88979000
C	3.81453000	1.12167500	-0.30547700
C	1.65445900	-3.27867800	-1.22509600
C	3.78921400	-3.66815000	-0.17487800
C	2.71252900	2.71797700	1.02180500
C	0.91951200	4.23059200	0.58524500
C	-1.86231600	2.48961900	-1.63502100
C	-1.83713200	2.65853700	0.76757600
C	0.97343900	0.45748100	-2.83655800
C	1.49315800	2.80542100	-2.67704500
C	5.64579300	-1.29266800	3.12387800
H	5.42534500	-1.01842500	1.00751300
C	3.60843200	-1.61812200	4.36727300
H	1.78754600	-1.62623500	3.21561800
C	4.79557500	0.23153600	-2.73047500
H	3.96229400	-1.67614700	-2.19786400
O	3.31193800	1.48628200	0.92225700
C	4.49756800	2.00993700	-1.12514300
C	1.77523400	-4.47967400	-1.91602500
H	0.75483100	-2.67909600	-1.33039200
C	3.90505200	-4.87374900	-0.86103600
H	4.57505100	-3.36524800	0.51013700
C	3.40275900	3.71216500	1.70521100
C	1.60982200	5.24272800	1.24529800
H	-0.05186700	4.45282100	0.15871600
C	-3.17296100	2.96582600	-1.64694200
H	-1.38088700	2.22843000	-2.57157500
C	-3.14063400	3.13585600	0.75539400
H	-1.32999300	2.51512200	1.71859700
C	1.32029600	0.47084800	-4.18454700
H	0.64033700	-0.46284100	-2.36389200
C	1.84339400	2.81794000	-4.02258500
H	1.56668800	3.71880300	-2.09364600
C	4.99498300	-1.50306200	4.33706200
H	6.72727500	-1.19639100	3.09241300
H	3.09426700	-1.77922600	5.31004900
C	4.97977200	1.55629000	-2.34897800
H	5.16941800	-0.11817800	-3.68731800
H	4.62959200	3.04223100	-0.81821300
C	2.90158400	-5.27853100	-1.73694000
H	0.97777200	-4.79941900	-2.58010800
H	4.77939500	-5.49898800	-0.70573100
C	2.84706000	4.98031100	1.82361000
H	4.37163700	3.46964300	2.12907600
H	1.17055500	6.23285300	1.31482400
C	-3.81374000	3.28782600	-0.45656800
H	-3.69294700	3.07556000	-2.59391300

H	-3.63608300	3.35982500	1.69472300
C	1.75630100	1.65084500	-4.77869900
H	1.25564600	-0.44412100	-4.76570400
H	2.18630300	3.74065100	-4.48160900
H	5.56853500	-1.57351200	5.25691500
H	5.49985700	2.24635500	-3.00631500
H	2.99190300	-6.22072600	-2.26984400
H	3.38364100	5.75953400	2.35596700
H	-4.83679900	3.65141300	-0.46763500
H	2.03150900	1.66226200	-5.82939900

Zero-point correction = 0.773149 (Hartree/Particle)
Thermal correction to Energy = 0.824206
Thermal correction to Enthalpy = 0.825150
Thermal correction to Gibbs Free Energy = 0.683626
Sum of electronic and zero-point Energies = -3779.596747
Sum of electronic and thermal Energies = -3779.545690
Sum of electronic and thermal Enthalpies = -3779.544746
Sum of electronic and thermal Free Energies = -3779.686270
E(RM06) = -3780.42289576

INT2a



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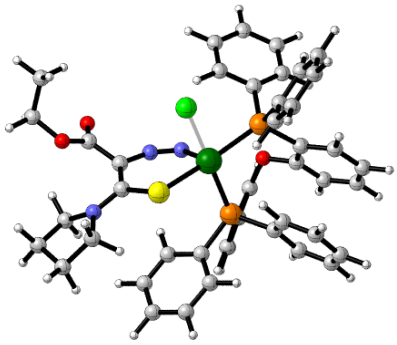
C	-4.81201400	-0.80581000	-0.86690600
C	-4.07664000	-0.38048900	0.34432600
S	-4.28102100	-0.34665400	-2.38773100
N	-1.63377100	-0.37835200	0.27695100
N	-2.76056700	-0.39667300	0.26586100
C	-4.56523200	0.32938500	1.52501600
O	-3.85415700	0.72647100	2.42868600
O	-5.89551600	0.52340200	1.47652700
C	-6.48051700	1.19154000	2.60356200
C	-6.31449200	2.69800500	2.51499800
H	-6.03462500	0.80123400	3.52196700
H	-7.53424400	0.90658500	2.56359500
H	-6.89345800	3.18269300	3.30810800
H	-5.26421600	2.97168200	2.64019200
H	-6.67234400	3.06761300	1.54909000
Rh	0.31199000	-0.63775400	0.32404800
P	2.52965200	-1.32087900	0.34679800
P	0.65595100	1.52830100	-0.35019600
C	3.21507300	-1.73469200	2.00007700
C	3.79713800	-0.16735100	-0.30578300
C	2.82174400	-2.80572400	-0.68749700
C	1.41755800	2.77983800	0.78601900
C	-0.94189600	2.34810900	-0.75408100
C	1.59607000	1.71252200	-1.91541300
C	4.59085500	-1.65510500	2.24652100
C	2.35864900	-2.12909200	3.03111800
C	4.57147300	-0.40103700	-1.44229100
C	3.93532700	1.05861300	0.34606200
C	1.96455200	-3.06231200	-1.76092400
C	3.91723600	-3.64645400	-0.47316100
C	2.52678700	2.46417000	1.58288600
C	0.87721100	4.06423400	0.93215200
C	-1.28910100	2.70439300	-2.05730300
C	-1.87144100	2.54663200	0.27653600
C	1.50968200	0.67714100	-2.85106700
C	2.32273100	2.86088600	-2.23429900
C	5.10277000	-1.97744700	3.49887100
H	5.26871400	-1.32984800	1.46218700
C	2.87554500	-2.44772300	4.28408200
H	1.29162400	-2.19754400	2.84852300
C	5.45792500	0.56617600	-1.90796500
H	4.46888800	-1.33971400	-1.97650600
O	3.14744400	1.24265000	1.46105800
C	4.82987000	2.02632300	-0.09210400
C	2.21136900	-4.12892600	-2.61905000
H	1.08223100	-2.44543300	-1.90055200
C	4.15927100	-4.71712300	-1.32844700
H	4.58147400	-3.47375000	0.36786400
C	3.02839900	3.34794600	2.53078500
C	1.38763400	4.96936100	1.85781400
H	0.03147600	4.35920800	0.32153100
C	-2.54661300	3.24062400	-2.32877700
H	-0.58822000	2.55559500	-2.87170200
C	-3.12117800	3.08602900	0.00277400
H	-1.62762000	2.26351500	1.29762200
C	2.14010900	0.78711800	-4.08559600
H	0.94256700	-0.21595000	-2.60271600
C	2.95973700	2.96750700	-3.46711200
H	2.39998300	3.67191200	-1.51603300
C	4.24464900	-2.37474100	4.52109200
H	6.17237300	-1.91229800	3.67619300
H	2.19943700	-2.75308500	5.07698200
C	5.58968500	1.77316000	-1.22922300
H	6.04099400	0.37577700	-2.80309300
H	4.91270000	2.96881800	0.43896300
C	3.31036400	-4.95645500	-2.40584800
H	1.53194100	-4.32333500	-3.44338700
H	5.00962400	-5.36802400	-1.14797400
C	2.45293200	4.60505700	2.67414700
H	3.87101100	3.03201700	3.13702500
H	0.94029700	5.95426600	1.94645600
C	-3.46396400	3.43018800	-1.30366700
H	-2.80970900	3.49570700	-3.35052000
H	-3.83161300	3.22351700	0.81141100
C	2.86883300	1.93289400	-4.39401200

H	2.06541300	-0.02486700	-4.80259400
H	3.53027000	3.86128700	-3.70194000
H	4.64321700	-2.62300300	5.50060900
H	6.28224400	2.52848000	-1.58815300
H	3.49843200	-5.79434500	-3.07088900
H	2.84363100	5.29814000	3.41275800
H	-4.44864300	3.83269600	-1.52037100
H	3.36701500	2.01889000	-5.35529800
C	-6.72410900	-2.02928300	-1.78656100
C	-6.23623800	-2.27297500	0.57779600
C	-7.77615400	-2.92074200	-1.12370900
H	-6.09979800	-2.58327700	-2.49775400
H	-7.13691600	-1.16810300	-2.31936900
C	-7.03456800	-3.48226700	0.09356500
H	-6.84896300	-1.62252800	1.20956700
H	-5.32772100	-2.53346000	1.12657500
H	-8.63412100	-2.32137100	-0.79792100
H	-8.14259500	-3.69465200	-1.80245100
H	-7.70035000	-3.87311200	0.86723300
H	-6.35448200	-4.28484500	-0.21239800
N	-5.88896300	-1.57775400	-0.66959500

Zero-point correction = 0.773785
Thermal correction to Energy = 0.825746
Thermal correction to Enthalpy = 0.826690
Thermal correction to Gibbs Free Energy = 0.681975
Sum of electronic and zero-point Energies = -3779.608054
Sum of electronic and thermal Energies = -3779.556093
Sum of electronic and thermal Enthalpies = -3779.555149
Sum of electronic and thermal Free Energies = -3779.699863
E(RM06) = -3780.43158597

INT3a



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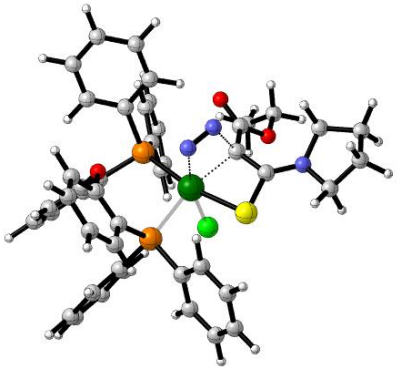
S	-2.10957000	-0.10473300	1.61922900
N	-0.86265600	0.96780100	-1.26177100
N	-2.01425800	1.18272200	-1.27374900
C	-4.10174600	2.18465800	-1.09452000
O	-3.99515100	2.77788500	-2.14750800
O	-5.03312200	2.49819600	-0.16272900
C	-5.86669300	3.62502800	-0.46091300
C	-5.17062200	4.92772000	-0.10905200
H	-6.75901800	3.47240600	0.15136400
H	-6.14282500	3.59969100	-1.51825700
H	-5.85376200	5.76986600	-0.26379400
H	-4.85196400	4.92209600	0.93735300
H	-4.29305200	5.07033100	-0.74424800
Rh	-0.03765300	0.45133200	0.62340000
C	-5.68273400	-0.35302500	-0.19895900
C	-4.85921700	-1.06166100	1.97119900
C	-6.84548500	-0.90051700	0.62382600
H	-5.38418500	-1.04300700	-0.99970100
H	-5.92369200	0.60932800	-0.63808600
C	-6.15964400	-1.80052400	1.65214700
H	-4.95003700	-0.40336300	2.84296000
H	-4.02295500	-1.74418400	2.15095900
H	-7.35747000	-0.07174200	1.12542200
H	-7.57612100	-1.42612500	0.00351800
H	-6.76420700	-1.97287800	2.54590100
H	-5.92961000	-2.77484600	1.20752900
N	-4.58597500	-0.25185000	0.77612900
P	2.14713600	1.23688800	0.23343200
P	0.26871100	-1.71364500	-0.15048600
C	2.33120000	2.57172300	-1.01432000
C	3.41587700	0.03184700	-0.31548100
C	2.93952700	1.89424700	1.75231800
C	0.51917300	-2.04219100	-1.96225400
C	-1.17403200	-2.81622400	0.16513000
C	1.63632000	-2.61109200	0.67883200
C	3.52253400	2.72966400	-1.73227700
C	1.26736900	3.44395600	-1.25887000
C	4.54546300	-0.34127900	0.41315900
C	3.17858100	-0.60179000	-1.53420100
C	2.53723000	1.40437600	2.99749200
C	3.98789100	2.81580800	1.69180200
C	1.29313400	-1.19481700	-2.76752700
C	-0.11268100	-3.11496300	-2.60805800
C	-1.14618400	-3.82008500	1.13053000
C	-2.36007200	-2.59402200	-0.54800700
C	1.93297000	-2.26545100	2.00078400
C	2.35007500	-3.64302000	0.06753200
C	3.64961200	3.74513800	-2.67430500
H	4.35633500	2.05397700	-1.56375300
C	1.39778000	4.45652900	-2.20508600
H	0.34411600	3.33904400	-0.70059300
C	5.41031500	-1.31856700	-0.07238700
H	4.74322100	0.12650000	1.37189600
O	2.04638200	-0.19495000	-2.20579800
C	4.04149100	-1.56272800	-2.04557800
C	3.18479900	1.81004200	4.15936400
H	1.68822400	0.73086200	3.06011500
C	4.63144400	3.22750200	2.85541600
H	4.30088200	3.22153600	0.73476300
C	1.34469400	-1.33321000	-4.14966300
C	-0.03763400	-3.28890500	-3.98611800
H	-0.68920700	-3.82468800	-2.02715700
C	-2.28287000	-4.58917800	1.38347900
H	-0.23992100	-4.00870000	1.69667500

C	-3.48173500	-3.37575600	-0.31427200
H	-2.40394600	-1.80820900	-1.29841100
C	2.92826500	-2.93825100	2.70106000
H	1.37941900	-1.46048800	2.47695500
C	3.35134500	-4.31113500	0.76596900
H	2.13522400	-3.91719600	-0.96095700
C	2.58507400	4.61008200	-2.91402500
H	4.57994900	3.85596400	-3.22391700
H	0.56117300	5.12394600	-2.38796900
C	5.16152900	-1.92007900	-1.30200800
H	6.27738800	-1.60863700	0.51220900
H	3.82897400	-2.03290900	-3.00001000
C	4.23543200	2.72112000	4.09014000
H	2.85365500	1.42935400	5.12091500
H	5.44023200	3.94980500	2.79549400
C	0.66799100	-2.37836300	-4.76524600
H	1.93364000	-0.61931000	-4.71573400
H	-0.54550600	-4.12975100	-4.44764100
C	-3.44917200	-4.37419200	0.66015700
H	-2.24635100	-5.36430200	2.14306700
H	-4.38727400	-3.20422300	-0.88916300
C	3.64152700	-3.96123100	2.08169500
H	3.15130600	-2.65583200	3.72546700
H	3.90992200	-5.10377500	0.27707900
H	2.68120700	5.39999300	-3.65349800
H	5.83819100	-2.67763500	-1.68595600
H	4.73598400	3.04569400	4.99777700
H	0.70913200	-2.49006500	-5.84426100
H	-4.32957900	-4.98200400	0.84856900
H	4.42592500	-4.48252300	2.62248100

Zero-point correction = 0.773268
Thermal correction to Energy = 0.824717
Thermal correction to Enthalpy = 0.825661
Thermal correction to Gibbs Free Energy = 0.684974
Sum of electronic and zero-point Energies = -3779.616851
Sum of electronic and thermal Energies = -3779.565402
Sum of electronic and thermal Enthalpies = -3779.564458
Sum of electronic and thermal Free Energies = -3779.705146
E(RM06) = -3780.44089862

TS2a



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C	-2.51001200	-0.71953000	-0.35761000
S	-1.14624800	-2.82076600	0.07266400
N	-0.71585700	-0.60075200	-2.02666300
N	-1.86831200	-0.63952800	-2.18289900
C	-3.47487600	0.33297500	-0.05844200
O	-3.53747800	1.42062300	-0.60560600
O	-4.30325700	-0.01212900	0.94963500
C	-5.29397100	0.95110900	1.33673500
C	-4.71510900	1.99979400	2.26466200
H	-6.06265200	0.35522000	1.83578300
H	-5.71839400	1.40969700	0.43902100
H	-5.51510700	2.64431800	2.64571600
H	-4.21008200	1.52502600	3.11048000
H	-3.99503900	2.61956100	1.72877200
C	-5.10907800	-2.31918300	-0.70705700
C	-3.80688300	-4.29933000	-0.16595100
C	-5.99560700	-3.56604500	-0.80060100
H	-4.97317400	-1.82887300	-1.67946300
H	-5.49894300	-1.58537200	-0.00350900
C	-5.00210500	-4.70940800	-1.02481200
H	-3.91854600	-4.61856800	0.87775800
H	-2.85557200	-4.69075400	-0.53836500
H	-6.52867500	-3.71388300	0.14511700
H	-6.74018700	-3.47963700	-1.59573500
H	-5.40056800	-5.68745800	-0.74395100
H	-4.70208000	-4.75103500	-2.07786000
N	-3.81389900	-2.83762900	-0.24773700
Rh	-0.45492700	-0.54772800	-0.00506600
P	-0.20816400	1.89099300	-0.14672100
P	1.94505300	-1.22010200	0.11702600
C	-0.43887900	2.76172800	-1.76612700
C	1.51990000	2.38181600	0.23876700
C	-1.16639200	2.95993000	1.00315100
C	2.90180100	-1.06518700	-1.45462700
C	2.02174900	-3.02242200	0.46040200
C	3.14808400	-0.57224100	1.35155700
C	0.44308600	3.78075300	-2.15018900
C	-1.52644400	2.47555200	-2.59517900
C	1.91526400	3.19341300	1.30100100
C	2.51137700	1.88349100	-0.61184000
C	-1.12192400	2.70647200	2.37935200
C	-1.86560900	4.08117600	0.54380700
C	2.81935400	0.13336900	-2.17214900
C	3.71580400	-2.07237100	-1.98615300
C	2.31732600	-3.48402800	1.74564300
C	1.67662700	-3.95030700	-0.53068500
C	2.69562000	0.11170000	2.47959100
C	4.51959000	-0.81294400	1.20031500
C	0.26054000	4.47021900	-3.34335000
H	1.27936900	4.05159500	-1.51523900
C	-1.70677800	3.16769200	-3.79029600
H	-2.26411800	1.74854300	-2.28710300
C	3.26270200	3.45885800	1.52966700
H	1.16737700	3.61216400	1.96484600
O	2.05476600	1.16732300	-1.69162400

C	3.85885200	2.14500500	-0.40329600
C	-1.73180100	3.57807100	3.27684800
H	-0.62300300	1.81682500	2.74649000
C	-2.48348300	4.94375500	1.44491400
H	-1.93270600	4.28663600	-0.51800100
C	3.46060800	0.31204600	-3.39137700
C	4.37975700	-1.90234700	-3.19734100
H	3.82724900	-3.00878000	-1.45061000
C	2.29271600	-4.84710600	2.02674000
H	2.56311200	-2.78006900	2.53361600
C	1.66923900	-5.31249600	-0.25104400
H	1.40889800	-3.60840400	-1.52647200
C	3.60432800	0.55299700	3.44033200
H	1.63218200	0.27724700	2.61464300
C	5.42192300	-0.36765200	2.15714900
H	4.88756300	-1.34426100	0.32777100
C	-0.81204100	4.15965600	-4.17449900
H	0.95892300	5.25499800	-3.61959300
H	-2.55921900	2.92590900	-4.41812800
C	4.23063800	2.92612600	0.68559100
H	3.55362400	4.07471800	2.37447200
H	4.60312000	1.72650900	-1.07243400
C	-2.40858900	4.70253200	2.81374800
H	-1.68410700	3.36628600	4.34087200
H	-3.02390400	5.80832200	1.07097400
C	4.24061400	-0.71498500	-3.90968900
H	3.33578400	1.25666900	-3.91002200
H	5.00043500	-2.70383000	-3.58538800
C	1.97824400	-5.76432300	1.02911600
H	2.52182100	-5.18966100	3.03125700
H	1.40787800	-6.01893600	-1.03323900
C	4.96466100	0.31891800	3.28138500
H	3.23887900	1.08550600	4.31331800
H	6.48334200	-0.55823400	2.02703800
H	-0.95405700	4.69563000	-5.10865200
H	5.28304900	3.11729700	0.86993500
H	-2.88635500	5.38100300	3.51468600
H	4.74484300	-0.58302500	-4.86197100
H	1.96587300	-6.82767000	1.24966500
H	5.67015300	0.66649900	4.03079400

Zero-point correction = 0.771698
Thermal correction to Energy = 0.822750
Thermal correction to Enthalpy = 0.823695
Thermal correction to Gibbs Free Energy = 0.685463
Sum of electronic and zero-point Energies = -3779.611385
Sum of electronic and thermal Energies = -3779.560333
Sum of electronic and thermal Enthalpies = -3779.559389
Sum of electronic and thermal Free Energies = -3779.697620
E(RM06) = -3780.41818464

N_2

N	0.00000000	0.00000000	0.55086000
N	0.00000000	0.00000000	-0.55086000

Zero-point correction = 0.005701
Thermal correction to Energy = 0.008061
Thermal correction to Enthalpy = 0.009005
Thermal correction to Gibbs Free Energy = -0.012742
Sum of electronic and zero-point Energies = -109.479351
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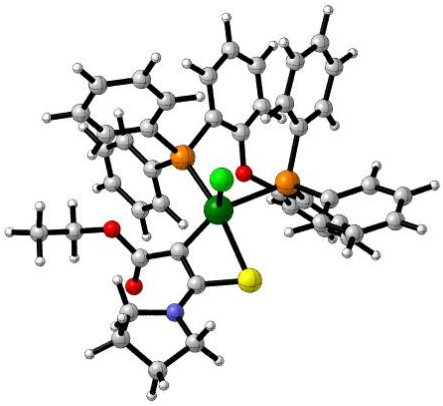
Sum of electronic and thermal Free Energies = -109.497794
E(RM06) = -109.506602411

INT4a



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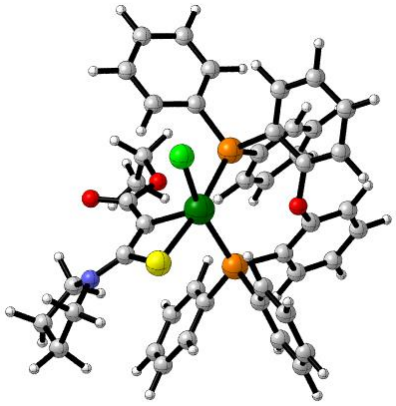
S	-0.36168000	3.16295900	0.75462800
N	-2.99590700	3.36104500	0.33010200
C	-2.83677900	4.80437600	0.11778000
C	-4.33457300	2.89388100	-0.06091800
C	-4.26753300	5.28905200	-0.11445000
H	-2.19668400	4.97481600	-0.75622600
H	-2.35249400	5.26273000	0.98412800
C	-4.92675600	4.09157700	-0.80564200
H	-4.91493400	2.64013900	0.83255600
H	-4.24922500	2.00366700	-0.69007100
H	-4.75864400	5.49035800	0.84431100
H	-4.29873300	6.20310700	-0.71219600
H	-6.01824700	4.10812900	-0.75470800
H	-4.63303000	4.05716500	-1.86048800
C	-4.87023600	-1.20662500	0.63912200
H	-5.20729800	-0.87564900	1.62231600
H	-4.54258800	-2.24891900	0.71346000
C	-3.24915300	0.46286500	1.13984500
O	-3.79674800	0.71639800	2.19557100
O	-3.71577200	-0.44446100	0.26167400
C	-5.93854300	-1.02454500	-0.42216100
H	-6.80350300	-1.65757100	-0.19861000
H	-6.27354400	0.01715400	-0.45607400
H	-5.55557200	-1.29263000	-1.41202200
Rh	-0.32964900	0.80463700	-0.14074300
P	-0.64632200	-1.49930000	-0.29403000
P	2.08554900	0.79466900	0.08633100

C	-1.64197300	-2.39896500	0.97621600
C	0.84949700	-2.56390900	-0.06475300
C	-1.31997300	-2.01511500	-1.91567000
C	2.49954800	0.56299500	1.86734300
C	3.00724300	2.31383900	-0.41211400
C	3.15481600	-0.41662700	-0.80214600
C	-2.09569700	-3.70004500	0.73004100
C	-1.82578000	-1.84914800	2.24569400
C	1.24743700	-3.59971600	-0.90964500
C	1.55068100	-2.39687100	1.13401100
C	-0.49189600	-1.93063300	-3.04075900
C	-2.66261500	-2.35907100	-2.09294500
C	1.96505600	-0.52716000	2.57482700
C	3.24041600	1.49569600	2.60114000
C	4.39961500	2.36825500	-0.24566200
C	2.36490000	3.37637800	-1.04797400
C	2.95026000	-0.57014200	-2.17797300
C	4.22508200	-1.07516200	-0.19589800
C	-2.77025600	-4.41216500	1.71663400
H	-1.91860100	-4.16554900	-0.23492400
C	-2.50482900	-2.56001500	3.23093600
H	-1.44233700	-0.85825700	2.46259700
C	2.31787300	-4.42423400	-0.57342300
H	0.71922400	-3.76944100	-1.84126400
O	1.09648700	-1.40488100	1.96835700
C	2.59830100	-3.22971300	1.49940700
C	-0.98686400	-2.22078700	-4.30691900
H	0.54405800	-1.62989600	-2.93042800
C	-3.15907400	-2.64092100	-3.36180100
H	-3.32661800	-2.40582400	-1.23963100
C	2.18553900	-0.69556100	3.93608800
C	3.46801900	1.33548200	3.96515300
H	3.63277100	2.37504000	2.10400800
C	5.12125000	3.48099100	-0.65634200
H	4.92877000	1.53154900	0.20121800
C	3.09300900	4.48862200	-1.46875900
H	1.30115000	3.32829800	-1.24424400
C	3.79034900	-1.38924800	-2.92382500
H	2.13782400	-0.03217100	-2.65965400
C	5.06620900	-1.89215200	-0.94678100
H	4.40327600	-0.96019800	0.86950100
C	-2.98553700	-3.83884700	2.96793300
H	-3.12280500	-5.41792400	1.50725300
H	-2.65966800	-2.10454000	4.20404000
C	2.98722000	-4.24364800	0.63203600
H	2.62119700	-5.21324300	-1.25402000
H	3.10817100	-3.06739500	2.44384000
C	-2.32202900	-2.57738100	-4.47156200
H	-0.32889000	-2.15017600	-5.16753000
H	-4.20465600	-2.91089200	-3.48015200
C	2.94711800	0.23470800	4.63468100
H	1.73097800	-1.54765700	4.43099400
H	4.04445700	2.08189300	4.50229000
C	4.46582700	4.54960800	-1.26663300
H	6.19720200	3.50844000	-0.51130700
H	2.57549600	5.30423600	-1.96444800
C	4.84917100	-2.05467300	-2.31064600
H	3.61933300	-1.50049900	-3.99071700
H	5.88979100	-2.40577400	-0.45912600
H	-3.51742400	-4.39164600	3.73679800
H	3.81554800	-4.89222000	0.90050800
H	-2.71018100	-2.79719000	-5.46176200
H	3.11593100	0.10578600	5.69928300
H	5.02960700	5.41798800	-1.59524700
H	5.50530400	-2.69354700	-2.89468900
Cl	0.02799200	1.29883800	-2.50845800

Zero-point correction = 0.764208
Thermal correction to Energy = 0.813710
Thermal correction to Enthalpy = 0.814654
Thermal correction to Gibbs Free Energy = 0.679028
Sum of electronic and zero-point Energies = -3670.154371
Sum of electronic and thermal Energies = -3670.104869
Sum of electronic and thermal Enthalpies = -3670.103925
Sum of electronic and thermal Free Energies = -3670.239551
E(RM06) = -3670.93581853

INT4a'



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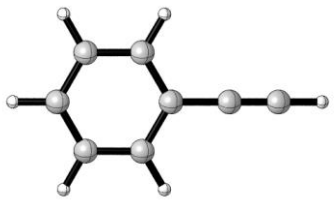
S	-2.34981500	0.13776100	-2.19855500
C	-1.02245200	-2.70688800	0.18213900
O	-1.56533500	-3.80400200	0.13282000
O	0.08387600	-2.52008900	0.96070300
C	0.59276600	-3.67046500	1.63700300
C	-0.12680500	-3.88586400	2.95734400
H	1.65447600	-3.45719700	1.78904600
H	0.49370300	-4.54209000	0.98660600
H	0.30030100	-4.74444700	3.48653100
H	-0.02704200	-3.00412400	3.60079000
H	-1.18774300	-4.07804900	2.77748300
Cl	0.71548900	-0.69569700	-3.32148800
Rh	-0.19190000	-0.05342000	-1.21240200
C	3.08129400	0.63558100	-1.18639800
C	2.74430800	1.99299400	-1.10507900
C	3.50744200	2.97452100	-1.71981200
C	4.64397900	2.60430100	-2.43389700

C	4.99166500	1.26165900	-2.53935900
C	4.21192500	0.28535700	-1.92367600
O	1.55104700	2.36117600	-0.50379100
C	-1.63419800	4.48756700	-2.34860700
C	-2.28859900	5.44102100	-1.57444600
C	-2.57538200	5.17062400	-0.23867300
C	-2.21077000	3.94922400	0.31697800
C	-1.57707700	2.97627400	-0.46301100
P	-1.00155700	1.41673900	0.32661500
C	0.24386500	2.16413700	1.44560000
P	1.97972700	-0.56497000	-0.33653100
C	2.64318800	-2.23777000	-0.71518900
C	2.56539400	-0.32958200	1.40492300
C	-2.37818800	0.85933600	1.39007300
H	3.19043400	4.00998400	-1.64941400
H	5.24509800	3.36582200	-2.92077500
H	5.86435900	0.96805900	-3.11389900
H	4.47414300	-0.76219900	-2.03045400
H	-2.42384400	3.75357700	1.36449400
H	-3.07802800	5.91277300	0.37435500
H	-2.57035800	6.39565200	-2.00890800
H	-1.40009900	4.69329500	-3.38853600
C	0.05818700	2.41883900	2.80356900
C	1.07132300	2.99557100	3.56300900
C	2.27892200	3.33549800	2.96217300
C	2.47281200	3.12785800	1.60070800
H	-0.87968200	2.14793900	3.27777500
H	0.91930000	3.17076100	4.62308200
H	3.07841600	3.77158800	3.55295400
H	3.40962900	3.39181000	1.12135700
C	-2.11855700	0.00652200	2.46855200
C	-3.15859200	-0.49341900	3.24258900
C	-4.47666200	-0.16100700	2.93610400
C	-4.74472800	0.66308200	1.84769500
C	-3.70313300	1.16665100	1.07150900
H	-1.09771300	-0.27111200	2.70624800
H	-2.93920400	-1.15304200	4.07656000
H	-5.29155700	-0.55160200	3.53823600
H	-5.76997000	0.91951900	1.59796400
H	-3.92375300	1.79218400	0.21311800
C	1.72727000	-0.61727000	2.48237500
C	2.17993800	-0.49746800	3.79212900
C	3.48504300	-0.08973100	4.04748200
C	4.33022600	0.20724300	2.98263100
C	3.87250200	0.09632400	1.67388100
H	0.72087600	-0.95758500	2.28028700
H	1.50593400	-0.72168100	4.61411700
H	3.84023000	0.00208600	5.06967600
H	5.34895400	0.53503500	3.16813100
H	4.54072800	0.35742800	0.85886600
C	3.88375800	-2.65367000	-0.21747000
C	4.34624300	-3.94472800	-0.45342900
C	3.56617900	-4.84285500	-1.17587600
C	2.32697700	-4.44094500	-1.66505600
C	1.86781200	-3.14727000	-1.44072500
H	4.49446800	-1.97853300	0.37258600
H	5.31241500	-4.24886000	-0.06175300
H	3.92132200	-5.85403800	-1.35217100
H	1.70578200	-5.13408200	-2.22346100
H	0.90356200	-2.84934700	-1.83339700
C	-1.27936000	3.25999200	-1.79731700
H	-0.76845000	2.52748300	-2.41479000
C	1.45456100	2.55080000	0.85566100
C	-4.19789600	-2.66054600	0.09408800
C	-4.97255100	-1.42920400	-1.84624000
C	-5.71898200	-2.79619600	-0.03019400
H	-3.90589200	-2.11163500	0.99964700
H	-3.67685400	-3.61776800	0.10732400
C	-6.13215900	-1.57933300	-0.86263400
H	-5.10770500	-2.06918700	-2.72830500
H	-4.84080800	-0.40088600	-2.19187400
H	-5.97222100	-3.71929100	-0.56392900
H	-6.20551900	-2.83182700	0.94863500
H	-7.09524500	-1.70302600	-1.36538900
H	-6.18669000	-0.68950500	-0.22593300
N	-3.80984800	-1.86733400	-1.07554800

Zero-point correction = 0.764205
Thermal correction to Energy = 0.813508
Thermal correction to Enthalpy = 0.814452
Thermal correction to Gibbs Free Energy = 0.679940
Sum of electronic and zero-point Energies = -3670.188581
Sum of electronic and thermal Energies = -3670.139279
Sum of electronic and thermal Enthalpies = -3670.138335
Sum of electronic and thermal Free Energies = -3670.272847
E(RM06) = -3670.97142583

Phenylacetylene



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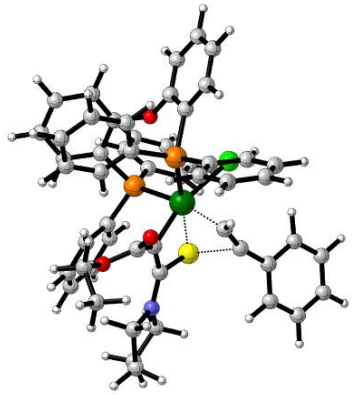
C	-1.50919300	-1.20547100	-0.00002700
C	-2.20669400	0.00009600	0.00033800
C	-1.50908600	1.20557000	0.00009900
C	-0.11957800	1.20946800	-0.00048600
C	0.58777400	-0.00005100	-0.00008100
H	0.42933700	-2.14559900	0.00007500
H	-2.04956900	-2.14723700	-0.00041800
H	-3.29253200	0.00016100	0.00081100
H	-2.04935400	2.14739800	0.00046300
H	0.42950400	2.14551900	-0.00054300
C	2.02165500	-0.00034600	0.00005400
C	3.22785000	0.00017300	0.00017200
H	4.29453500	0.00034200	0.00089700

Zero-point correction = 0.110968
Thermal correction to Energy = 0.117331

Thermal correction to Enthalpy = 0.118276
Thermal correction to Gibbs Free Energy = 0.080604
Sum of electronic and zero-point Energies = -308.167427
Sum of electronic and thermal Energies = -308.161063
Sum of electronic and thermal Enthalpies = -308.160119
Sum of electronic and thermal Free Energies = -308.197791
E(RM06) = -308.262192191

TS3a

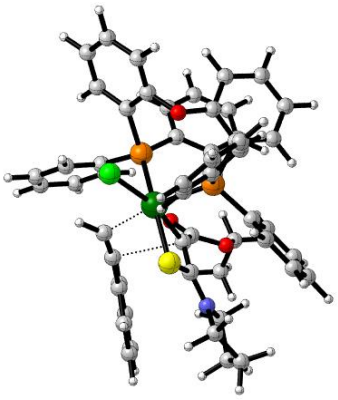


C	2.50619200	-0.32335800	0.88426900
C	1.23925300	-0.09246000	1.32100000
S	2.55794500	0.10210200	-0.83719500
C	0.71328600	-0.05173400	2.67696900
O	0.04647000	0.85538400	3.14711200
O	0.94907900	-1.18832500	3.39548900
C	0.44259500	-1.20738000	4.73475500
C	1.36527300	-0.47909700	5.69699700
H	0.37198000	-2.26958100	4.98383900
H	-0.55895100	-0.77014600	4.74266600
H	0.97351800	-0.54994700	6.71736500
H	2.36848400	-0.91711900	5.68237300
H	1.43404200	0.57784800	5.42691000
Cl	-0.44926100	1.75939100	-2.44800600
Rh	0.25242200	0.56437100	-0.34458500
C	-3.28901600	1.31006900	-0.74550800
C	-3.49913900	0.32922900	-1.71745900
C	-4.51949200	0.41716400	-2.65399600
C	-5.39463600	1.49618200	-2.61422600
C	-5.23568500	2.47020600	-1.63531300
C	-4.19353300	2.37675400	-0.71718400
O	-2.64003800	-0.73979100	-1.79280400
C	0.78850000	-1.30480400	-5.13601100
C	0.17964500	-2.41773600	-5.70673100
C	-0.54831000	-3.29510800	-4.90615500
C	-0.66259400	-3.05833700	-3.54086300
C	-0.05477100	-1.93869300	-2.96233100
P	-0.12791600	-1.68885500	-1.14652800
C	-1.68747300	-2.54338700	-0.69835400
P	-1.90431000	1.14031500	0.47786300
C	-1.91439200	2.81329900	1.22377200
C	-2.74567000	0.07538700	1.71996700
C	1.15765200	-2.86150400	-0.54609600
H	-4.60398600	-0.36111500	-3.40515500
H	-6.19438900	1.57288000	-3.34430300
H	-5.91528900	3.31534400	-1.58765600
H	-4.07960300	3.15885400	0.02445800
H	-1.22720600	-3.75075200	-2.92327500
H	-1.02795600	-4.16580000	-5.34386700
H	0.26795600	-2.60075800	-6.77392000
H	1.34856000	-0.60986300	-5.75421400
C	-1.80861800	-3.75380900	-0.01613800
C	-3.05951000	-4.21659800	0.38429700
C	-4.19943800	-3.46791400	0.10557000
C	-4.10900400	-2.27943800	-0.61182400
H	-0.92093000	-4.33070400	0.22000400
H	-3.14046400	-5.15468300	0.92424500
H	-5.17301200	-3.81353700	0.43954100
H	-4.99248200	-1.69513000	-0.84441900
C	1.25311600	-3.14903200	0.82097800
C	2.27949700	-3.94735000	1.31190700
C	3.23358300	-4.47135900	0.44286400
C	3.14882700	-4.19381000	-0.91796100
C	2.11917300	-3.39339000	-1.40904500
H	0.54456800	-2.72597400	1.52282800
H	2.33761700	-4.14491700	2.37827500
H	4.03928700	-5.09214800	0.82500300
H	3.88806100	-4.59511300	-1.60492700
H	2.07812700	-3.17270800	-2.47005700
C	-2.14976400	-1.10428400	2.15762700
C	-2.80399300	-1.94500700	3.05200000
C	-4.06708400	-1.60745600	3.52548800
C	-4.67461800	-0.42951000	3.09490600
C	-4.02099700	0.40308800	2.19400800
H	-1.17362100	-1.37805900	1.78049500
H	-2.32554000	-2.86761100	3.36631500
H	-4.58189100	-2.26172000	4.22316600
H	-5.66259700	-0.16079800	3.45708600
H	-4.50937100	1.31237400	1.85575100
C	-2.05728500	3.02580200	2.59436400
C	-1.99620400	4.31926000	3.11018000
C	-1.78845500	5.40385800	2.26476500
C	-1.62801600	5.19475800	0.89543700
C	-1.68320800	3.90697500	0.37597900
H	-2.18930900	2.18445500	3.26451400
H	-2.10521300	4.47386900	4.17950300
H	-1.74161100	6.41018700	2.67094600
H	-1.45026800	6.03427700	0.23005600
H	-1.52717600	3.73655100	-0.68752900
C	0.67213300	-1.06212800	-3.76979400
H	1.12423600	-0.17769200	-3.33943100
C	-2.85457800	-1.84614700	-1.02335900
C	3.83361900	-0.81996300	2.93645300
C	4.85569900	-1.08875400	0.75299700
C	5.34344600	-0.99844400	3.10019500
H	3.28430000	-1.69547800	3.30478300
H	3.44386200	0.05951900	3.46321100
C	5.72742900	-1.75141300	1.82221400

H	5.36472000	-0.22714300	0.29618000
H	4.58211500	-1.78203000	-0.04991500
H	5.83938000	-0.02108500	3.12682600
H	5.60306400	-1.53701800	4.01581900
H	6.79368700	-1.69616300	1.58703400
H	5.45039800	-2.80812800	1.91540300
N	3.67460100	-0.66377300	1.50036200
C	2.81447000	3.81619800	-2.29141700
C	3.79484400	4.43644900	-3.05766500
C	5.12607300	4.40198400	-2.64843300
C	5.48996400	3.73566600	-1.47615900
C	4.52290000	3.09804800	-0.71453600
C	3.17805700	3.14711600	-1.11282900
H	1.77092200	3.80904200	-2.59255000
H	3.51973500	4.94795700	-3.97477000
H	5.88818200	4.89201200	-3.24759300
H	6.53030900	3.70867200	-1.16683000
H	4.78501700	2.55313000	0.18715400
C	2.15410400	2.54192400	-0.32367300
C	1.06890800	2.39157200	0.30826300
H	0.56066300	3.03281800	1.01433500

Zero-point correction = 0.875847
Thermal correction to Energy = 0.932211
Thermal correction to Enthalpy = 0.933155
Thermal correction to Gibbs Free Energy = 0.783007
Sum of electronic and zero-point Energies = -3978.359101
Sum of electronic and thermal Energies = -3978.302737
Sum of electronic and thermal Enthalpies = -3978.301792
Sum of electronic and thermal Free Energies = -3978.451940
E(RM06) = -3979.22769541

TS4a



C	-2.36500900	0.97867600	-0.54399700
C	-1.59871500	0.00163300	0.05248100
S	-1.47765800	1.56967200	-1.94705300
C	-1.85141900	-0.86206400	1.18259700
O	-1.53619600	-2.04229900	1.25954700
O	-2.41068700	-0.23328200	2.25966600
C	-2.71076600	-1.05771400	3.38931400
C	-4.03172700	-1.78776600	3.21393900
H	-2.75413400	-0.36161700	4.23155900
H	-1.88985400	-1.76114800	3.54753300
H	-4.25123800	-2.38759800	4.10383200
H	-4.85294100	-1.07955200	3.06387300
H	-3.98140500	-2.45385500	2.34865100
C	-4.33932700	-1.19094200	-2.04224500
C	-5.66356800	-1.45307400	-1.71979300
C	-5.97315900	-2.48630600	-0.83568500
C	-4.96139400	-3.27930000	-0.29187000
C	-3.63412100	-3.03979000	-0.61977100
C	-3.31639600	-1.98043400	-1.48613000
H	-4.06993100	-0.38238500	-2.71419500
H	-6.45609500	-0.85179400	-2.15475800
H	-7.00985200	-2.68388400	-0.57873600
H	-5.21252500	-4.09027500	0.38494300
H	-2.82991000	-3.63653200	-0.20618200
C	-1.97319600	-1.71271400	-1.85409600
C	-0.85643600	-1.45224300	-2.33969100
H	-0.26720500	-1.67991200	-3.21223900
Cl	1.79609000	0.00382500	-2.96905000
Rh	0.12517500	0.01112000	-1.10836200
C	3.27283100	-1.73338900	-0.52502400
C	4.02061300	-0.55408300	-0.48518300
C	5.36984900	-0.52013600	-0.80751700
C	6.02176000	-1.69978000	-1.14783400
C	5.31407700	-2.89648100	-1.15773600
C	3.95574200	-2.90858700	-0.85339600
O	3.39695000	0.62669800	-0.16149300
C	2.25595700	4.21680400	-3.20773800
C	3.13332700	5.12339500	-2.62235300
C	3.37841900	5.06256800	-1.25245200
C	2.74612400	4.09876500	-0.47534500
C	1.86258700	3.18339300	-1.05915400
P	0.96157700	1.98706700	0.00115700
C	2.12904800	1.77534300	1.40511000
P	1.46973600	-1.69470100	-0.10470200
C	0.92939800	-3.35215000	-0.67128100
C	1.59201000	-1.86330800	1.72379000
C	-0.35081000	3.03603800	0.75053100
H	5.88467000	0.43473200	-0.79281300
H	7.07685900	-1.68139100	-1.40264600
H	5.81309300	-3.82580800	-1.41410000
H	3.42019400	-3.85067600	-0.88732300
H	2.94097400	4.06336100	0.59232300
H	4.06290500	5.76553700	-0.78660300
H	3.62925400	5.87398500	-3.23132700
H	2.06792000	4.24850100	-4.27649500
C	1.96800100	2.28802500	2.69306300
C	2.86157700	1.95373700	3.70680800
C	3.92782900	1.10034900	3.43887200
C	4.13810200	0.61495700	2.15285700
H	1.12939500	2.93940800	2.91258700
H	2.71630900	2.35074500	4.70650400
H	4.61183800	0.81609400	4.23270700
H	4.97429000	-0.03849600	1.92990400
C	-1.10496400	2.54728500	1.82145600
C	-2.16794400	3.28046500	2.33996700

C	-2.49328200	4.51799300	1.79448000
C	-1.74559700	5.01754700	0.73019100
C	-0.68538100	4.28164600	0.20996600
H	-0.88765000	1.57792800	2.25122200
H	-2.74447500	2.87170300	3.16467300
H	-3.32244800	5.09327000	2.19720300
H	-1.98976400	5.98319100	0.29721000
H	-0.12825600	4.67419000	-0.63352600
C	0.93994000	-0.96640900	2.56518700
C	1.07408100	-1.05662700	3.94636400
C	1.85916400	-2.06030600	4.50353700
C	2.51381900	-2.96716200	3.67259100
C	2.38567600	-2.86563000	2.29205300
H	0.33710500	-0.17887000	2.13403600
H	0.57050700	-0.33398800	4.58144500
H	1.96690600	-2.13430300	5.58187600
H	3.13080200	-3.75221600	4.09979700
H	2.91030100	-3.57076300	1.65388300
C	0.21522400	-4.22005000	0.15455200
C	-0.26648800	-5.42635400	-0.35050200
C	-0.03791100	-5.77542400	-1.67775300
C	0.67649500	-4.91206300	-2.50615300
C	1.15199900	-3.70473100	-2.00863300
H	0.00881400	-3.94527000	1.18181400
H	-0.82262700	-6.09460100	0.30098700
H	-0.41447000	-6.71693100	-2.06713200
H	0.85891300	-5.17470400	-3.54398700
H	1.69558400	-3.02404100	-2.66087400
C	1.62234000	3.24893600	-2.43260800
H	0.96470400	2.53063100	-2.90404500
C	3.24894800	0.97881000	1.14815300
C	-4.53048100	0.91184300	0.70421900
C	-4.16956400	2.58801900	-1.01387000
C	-5.86121800	1.57146500	0.34553000
H	-4.20097600	1.19106300	1.71070200
H	-4.56788600	-0.18165100	0.65417800
C	-5.42516100	2.92997600	-0.21079600
H	-4.41271500	2.31788600	-2.05191200
H	-3.44782200	3.40978200	-1.03880100
H	-6.36983600	0.98926300	-0.43114300
H	-6.53082800	1.64889300	1.20655600
H	-6.19004000	3.41815600	-0.82040600
H	-5.15935200	3.60357700	0.61218000
N	-3.61523700	1.43712000	-0.30179200

Zero-point correction = 0.876965
Thermal correction to Energy = 0.932652
Thermal correction to Enthalpy = 0.933596
Thermal correction to Gibbs Free Energy = 0.787945
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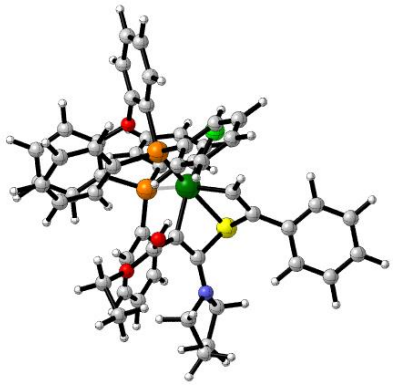
Sum of electronic and thermal Energies = -3978.317932
Sum of electronic and thermal Enthalpies = -3978.316988
Sum of electronic and thermal Free Energies = -3978.462640
E(RM06) = -3979.24555067

INT5a



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C	1.32008800	-0.03215500	1.01884900
S	2.39005700	-0.37800400	-1.26959100
C	1.06715200	0.40286900	2.40143600
O	0.87038400	1.55468200	2.73205900
O	1.02366600	-0.61287100	3.30150200
C	0.75414100	-0.24314900	4.66209800
C	2.00907800	0.22642400	5.37646300
H	0.35564000	-1.15380400	5.11615300
H	-0.01875700	0.52867800	4.67223500
H	1.77662200	0.45520400	6.42191400
H	2.78403300	-0.54637600	5.35786900
H	2.39766000	1.13262000	4.90485100
Cl	-0.71844300	0.98965000	-2.87542600
Rh	0.18800900	0.38075500	-0.65522700
C	-3.15875400	1.73814600	-0.71881900
C	-3.74760200	0.58839900	-1.25221900
C	-4.94948500	0.62671400	-1.94612200
C	-5.62235700	1.83445800	-2.08808800
C	-5.08137400	2.98880800	-1.53386200
C	-3.86401400	2.93754000	-0.86133400
O	-3.09305400	-0.61442900	-1.14412000
C	-0.46704100	-2.79397700	-4.72785700
C	-1.43153000	-3.77855400	-4.91927600
C	-2.21485000	-4.19862300	-3.84700300
C	-2.03018000	-3.63769400	-2.58769400
C	-1.06651600	-2.64406300	-2.39018400
P	-0.73794100	-1.96006900	-0.72206200
C	-2.28908600	-2.33140900	0.18018600
P	-1.56457700	1.63802900	0.22243900
C	-1.09059200	3.39867000	0.35172200
C	-2.26219300	1.20130100	1.86714600
C	0.44918600	-3.19171000	-0.03874800
H	-5.33405000	-0.29440300	-2.37162200
H	-6.56216100	1.87062400	-2.63016400
H	-5.59843900	3.93817900	-1.63163700
H	-3.45442300	3.85421000	-0.45292600
H	-2.63970600	-3.97705400	-1.75532900
H	-2.97026000	-4.96599900	-3.98930400
H	-1.57636000	-4.21553200	-5.90315900
H	0.13937100	-2.45198400	-5.56087200

C	-2.47322600	-3.29985300	1.16543000
C	-3.66987300	-3.36558200	1.87656700
C	-4.68992300	-2.45891600	1.60349400
C	-4.54312600	-1.50360700	0.60191700
H	-1.67216500	-3.99621300	1.39152800
H	-3.80038700	-4.11986800	2.64611900
H	-5.61576400	-2.49487000	2.16958500
H	-5.33542800	-0.79652900	0.38277600
C	0.77883300	-3.14269300	1.32241000
C	1.71713600	-4.01454900	1.86148300
C	2.35744500	-4.94514100	1.04521500
C	2.05266300	-4.99155300	-0.31120600
C	1.10352600	-4.12308100	-0.85005600
H	0.31732800	-2.40823300	1.97237600
H	1.95453000	-3.95552600	2.91988000
H	3.09400500	-5.62532400	1.46364200
H	2.54857600	-5.70901800	-0.95824500
H	0.87453100	-4.17864100	-1.90902400
C	-1.95923900	-0.02333600	2.45530700
C	-2.56973700	-0.41539400	3.64296200
C	-3.48718400	0.42565300	4.26175500
C	-3.79702900	1.65611900	3.68366700
C	-3.19605200	2.03758000	2.49044300
H	-1.25088900	-0.68441100	1.97475300
H	-2.32935600	-1.38315800	4.07213700
H	-3.96618800	0.12460600	5.18893800
H	-4.51500900	2.31711200	4.15999300
H	-3.45732100	2.99130700	2.04115700
C	-0.73461700	3.98204500	1.56787500
C	-0.28772500	5.30135300	1.60373100
C	-0.18798800	6.04199000	0.43094200
C	-0.52338100	5.45660000	-0.78905100
C	-0.96415300	4.13925600	-0.83239700
H	-0.77732000	3.40418600	2.48351600
H	-0.00960000	5.74508800	2.55493500
H	0.16115900	7.06995900	0.46362300
H	-0.43102700	6.02157100	-1.71172300
H	-1.18927400	3.66996600	-1.78743600
C	-0.28664900	-2.22414800	-3.47068600
H	0.44502200	-1.43605100	-3.33830800
C	-3.34971300	-1.46355600	-0.10806700
C	3.95927600	-0.86587900	2.49079900
C	4.46123400	-1.98881100	0.41101700
C	5.37347900	-1.43083400	2.57817900
H	3.25412300	-1.48715200	3.06027000
H	3.87304200	0.16448700	2.85307600
C	5.32823400	-2.55999600	1.54183000
H	5.07537700	-1.57483900	-0.39901500
H	3.80573800	-2.75347400	-0.02088900
H	6.10205600	-0.66662500	2.28507000
H	5.62524000	-1.77925600	3.58362500
H	6.31708400	-2.86860600	1.19266500
H	4.83289400	-3.43668300	1.97439900
N	3.68736300	-0.91868800	1.06199000
C	3.86624200	3.16087400	-2.59977100
C	5.06391800	3.77429900	-2.95249300
C	6.27370700	3.27962800	-2.47093800
C	6.27875400	2.17187700	-1.62567700
C	5.08244100	1.56304500	-1.26357800
C	3.86351300	2.05092300	-1.74803300
H	2.92111900	3.52588300	-2.99136200
H	5.05311700	4.63400300	-3.61640500
H	7.20876700	3.75437300	-2.75375100
H	7.21833000	1.78664500	-1.23949000
H	5.08043800	0.72311700	-0.57307000
C	2.58868900	1.43573400	-1.35184600
C	1.42339800	1.94247000	-0.95534900
H	1.22464100	3.00714400	-0.86724800

Zero-point correction = 0.878996
Thermal correction to Energy = 0.934904
Thermal correction to Enthalpy = 0.935848
Thermal correction to Gibbs Free Energy = 0.787606
Sum of electronic and zero-point Energies = -3978.390339
Sum of electronic and thermal Energies = -3978.334430
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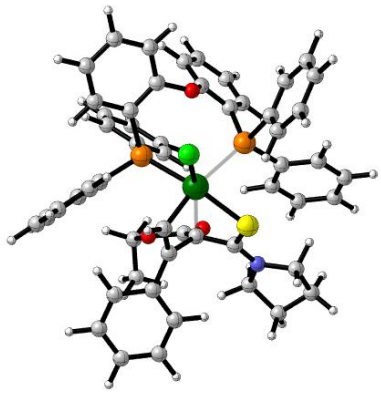
Sum of electronic and thermal Free Energies = -3978.481729
E(RM06) = -3979.25469202

INT6a

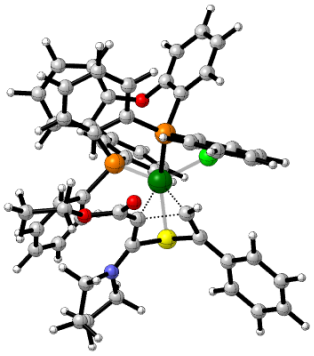


Rh	0.00997300	0.01878300	-1.10855700
Cl	1.29572100	-0.86567400	-2.96672600
C	-1.61554300	2.16807000	-0.68363400
C	-1.84688000	0.79851400	-0.17349200
S	-0.58121300	2.15171500	-2.04853200
C	-2.13955100	0.55047900	1.24920000
O	-1.89083900	1.28140800	2.19834900
O	-2.70849600	-0.65715500	1.41403700
C	-3.20963700	-0.97355300	2.71399900
C	-4.59152500	-0.36996400	2.89796900
H	-2.50613300	-0.62744000	3.47440700
H	-3.24905500	-2.06469000	2.73500100
H	-5.02805000	-0.70162500	3.84601200
H	-4.52934800	0.72221400	2.91152700
H	-5.24932200	-0.67473500	2.07784500
C	-4.88332700	0.97031800	-1.16289600
C	-6.27010300	0.86144300	-1.12073300
C	-6.87203600	-0.39472700	-1.11545200

C	-6.07599000	-1.53780200	-1.16506600
C	-4.68990300	-1.42714900	-1.20057700
C	-4.07488800	-0.17104800	-1.19373900
H	-4.42003200	1.95301700	-1.20521300
H	-6.88262800	1.75883800	-1.10276300
H	-7.95412100	-0.48196300	-1.07935200
H	-6.53689600	-2.52191300	-1.16487100
H	-4.06458300	-2.31442300	-1.20991900
C	-2.60124200	-0.07580300	-1.17559200
C	-1.68347700	-0.65561600	-1.93199500
H	-1.80093100	-1.29184200	-2.80232700
C	-1.72375700	4.60306600	-0.75588700
C	-3.11811900	3.44206900	0.85872100
C	-2.52008900	5.61226600	0.07288200
H	-2.00737600	4.62543300	-1.81504300
H	-0.64029400	4.73540100	-0.68923000
C	-3.73146100	4.80426100	0.54857000
H	-2.63573300	3.42171400	1.83875300
H	-3.83023000	2.61637300	0.81488500
H	-1.92424600	5.93754500	0.93203900
H	-2.79008700	6.49632300	-0.50939700
H	-4.22658900	5.23816600	1.42081100
H	-4.47141900	4.71267900	-0.25556000
N	-2.09942600	3.29645600	-0.19075400
C	1.78637400	-3.09737900	-0.51356100
C	3.05465300	-2.51312000	-0.45258200
C	4.21051300	-3.22083000	-0.75085700
C	4.12114500	-4.56544400	-1.09253800
C	2.87591500	-5.18199700	-1.13193800
C	1.72387500	-4.45327300	-0.84800100
O	3.16212100	-1.17874200	-0.15167400
C	4.12102900	2.26332600	-3.44665500
C	5.42121100	2.40529400	-2.97242100
C	5.69266900	2.18838600	-1.62356200
C	4.66574000	1.83427700	-0.75497400
C	3.35657800	1.68689700	-1.22557200
P	1.97336800	1.30531300	-0.08022400
C	2.85156300	0.55520000	1.34774900
P	0.29415700	-2.09217300	-0.07824900
C	-1.05729200	-3.25890100	-0.50206200
C	0.39386400	-2.19105500	1.75407200
C	1.57198900	2.97915500	0.58213000
H	5.16205800	-2.70049200	-0.71967900
H	5.02085400	-5.12510300	-1.32863600
H	2.79281500	-6.23218600	-1.39360300
H	0.76357000	-4.95338900	-0.89732400
H	4.88532000	1.67519700	0.29675800
H	6.70518900	2.29591400	-1.24508300
H	6.22295500	2.67982000	-3.65210200
H	3.90205900	2.41772400	-4.49878900
C	3.01990600	1.11578900	2.61265000
C	3.57103500	0.36739400	3.65062500
C	3.95490300	-0.95150800	3.42863100
C	3.82865500	-1.52414300	2.16616300
H	2.69970900	2.13616700	2.79619700
H	3.68747700	0.81199000	4.63397000
H	4.36215200	-1.54476800	4.24171600
H	4.12816600	-2.55026900	1.98300700
C	0.58951000	3.08485500	1.57234700
C	0.27228000	4.31879100	2.13187800
C	0.91526900	5.47348100	1.69175100
C	1.87630100	5.38219100	0.68855900
C	2.20796200	4.14409800	0.14176500
H	0.04367600	2.20908900	1.90731900
H	-0.48569500	4.37206900	2.90864900
H	0.66765000	6.43845300	2.12543400
H	2.37955100	6.27632700	0.33228900
H	2.96650200	4.09042000	-0.63169400
C	0.28830700	-1.03564100	2.52195000
C	0.39136500	-1.09034800	3.90914500
C	0.60477100	-2.30971400	4.54088500
C	0.72089400	-3.47361600	3.78121200
C	0.62088100	-3.41487900	2.39691200
H	0.14151900	-0.08194900	2.03375400
H	0.31292700	-0.17371700	4.48493400
H	0.68925800	-2.35653500	5.62278100
H	0.89496400	-4.42834200	4.26880400
H	0.72309000	-4.32481500	1.81225800
C	-1.97933400	-3.71773800	0.43699000
C	-3.00848700	-4.57624500	0.05346000
C	-3.12369900	-4.98174000	-1.27162500
C	-2.20912200	-4.52012400	-2.21834100
C	-1.18591700	-3.66049900	-1.83884600
H	-1.89644900	-3.41129000	1.47338200
H	-3.72114700	-4.92424500	0.79542800
H	-3.92511100	-5.65131800	-1.56990400
H	-2.29595700	-4.82555100	-3.25660500
H	-0.47818400	-3.29285400	-2.57901100
C	3.09287600	1.90268000	-2.57998600
H	2.09097900	1.76450800	-2.96689500
C	3.29457200	-0.75552800	1.14030400

Zero-point correction = 0.881068
Thermal correction to Energy =0.936263
Thermal correction to Enthalpy = 0.937207
Thermal correction to Gibbs Free Energy = 0.791918
Sum of electronic and zero-point Energies = -3978.445074
Sum of electronic and thermal Energies = -3978.389879
Sum of electronic and thermal Enthalpies = -3978.388934
Sum of electronic and thermal Free Energies =-3978.534223
E(RM06) = -3979.30950739

TS5a



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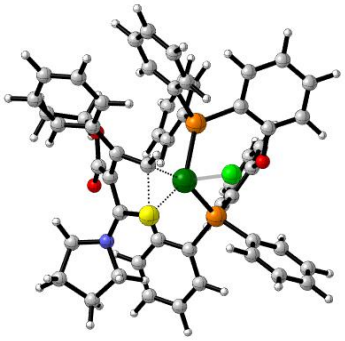
C	1.56596500	0.13250400	1.14900500
S	2.58036500	-0.22174900	-1.17776700
C	1.15383100	0.30827800	2.54357500
O	0.89455500	1.37066200	3.07122300
O	1.01248000	-0.86618600	3.20799700
C	0.61936200	-0.77059500	4.57978600
C	0.43689600	-2.18764700	5.08345400
H	-0.30571800	-0.19155500	4.64900500
H	1.39329500	-0.23544600	5.14039000
H	0.12062600	-2.17898500	6.13107100
H	-0.32713400	-2.70982900	4.49742600
H	1.37188500	-2.75274400	5.00975600
Rh	0.29296000	0.42316200	-0.51298200
C	3.90905700	3.70055900	-0.86436000
C	4.99968800	4.48970200	-1.19747600
C	6.08568600	3.94951800	-1.88704300
C	6.06135100	2.60243400	-2.23582000
C	4.97868600	1.80110000	-1.89067600
C	3.88197800	2.33070700	-1.19136500
H	3.05753500	4.14120000	-0.35306900
H	4.99724300	5.54250600	-0.92792700
H	6.93225300	4.57356200	-2.15696700
H	6.89434900	2.16670000	-2.78113500
H	4.97966400	0.75210400	-2.17579400
C	2.74730000	1.52749600	-0.78685400
C	1.72530800	1.71509400	0.10225700
H	1.59134400	2.61534400	0.69388300
C	3.58488100	-1.94406000	2.45507600
C	4.42161500	-2.20465900	0.18347700
C	4.97994600	-2.57400900	2.48233000
H	2.80992600	-2.62742600	2.81026400
H	3.53107100	-1.03097800	3.05461800
C	5.10933700	-3.21478000	1.09864400
H	5.11662200	-1.42365000	-0.15600300
H	3.97429400	-2.67781100	-0.69502200
H	5.74015500	-1.79512100	2.60852300
H	5.09037700	-3.28957800	3.30119200
H	6.14496700	-3.39824600	0.80248500
H	4.56675600	-4.16501200	1.06867400
N	3.37647400	-1.62783500	1.03945200
C	-2.88684800	2.02193300	-0.77671700
C	-3.50931100	1.01108000	-1.51405900
C	-4.60009100	1.26240800	-2.33394900
C	-5.11731000	2.55088300	-2.41189200
C	-4.53211800	3.57169600	-1.67217100
C	-3.42700100	3.30767100	-0.86748000
O	-2.98476000	-0.25828500	-1.49356000
C	-0.25377400	-2.21916300	-5.02919900
C	-1.07078100	-3.29969300	-5.34461600
C	-1.82759000	-3.91301100	-4.34719500
C	-1.76017100	-3.44797800	-3.03911000
C	-0.93830100	-2.36226900	-2.71570900
P	-0.76355000	-1.78987000	-0.98231500
C	-2.42090400	-2.14723800	-0.27789900
P	-1.45967700	1.63816800	0.33304500
C	-0.89391600	3.31192100	0.80771300
C	-2.38071400	1.00150000	1.78892600
C	0.28597100	-3.12252800	-0.26563000
H	-5.01814400	0.44363400	-2.91022600
H	-5.96911600	2.75397800	-3.05344400
H	-4.92462300	4.58221600	-1.72673300
H	-2.97324400	4.12153500	-0.31328800
H	-2.35000300	-3.93122000	-2.26496200
H	-2.47104700	-4.75410100	-4.58902900
H	-1.12536700	-3.66140200	-6.36754700
H	0.32547000	-1.72605600	-5.80395200
C	-2.77707300	-3.19604900	0.56926700
C	-4.03768100	-3.23360700	1.16103200
C	-4.95323500	-2.21587800	0.90982600
C	-4.63959400	-1.18136700	0.03357300
H	-2.05949300	-3.98057000	0.78640200
H	-4.29842300	-4.05142300	1.82556700
H	-5.92701000	-2.22812900	1.38996900
H	-5.35016700	-0.38974200	-0.17786600
C	0.36136000	-3.27779500	1.12460800
C	1.16008000	-4.26408100	1.69009100
C	1.94492800	-5.08001900	0.87854200
C	1.92124200	-4.89993500	-0.50110900
C	1.09064700	-3.93598200	-1.07020900
H	-0.20937400	-2.62703400	1.77778200
H	1.17423300	-4.38759900	2.76966900
H	2.56963700	-5.85196900	1.31934800
H	2.53410400	-5.52564800	-1.14364500
H	1.05988100	-3.82946600	-2.15001700
C	-2.03105700	-0.22258600	2.35210500
C	-2.77680400	-0.76355200	3.39538800
C	-3.87595700	-0.07372500	3.89434300
C	-4.23039600	1.15643700	3.34289800
C	-3.49291100	1.68708900	2.29151200
H	-1.17844200	-0.75977000	1.95565400
H	-2.50545300	-1.73239300	3.80422300
H	-4.46191700	-0.49487600	4.70607400
H	-5.08952400	1.69878500	3.72633000
H	-3.78984900	2.63559000	1.85316600
C	-0.88857900	3.76220400	2.12656200
C	-0.36609600	5.01826500	2.43214000
C	0.15256200	5.82506500	1.42600700
C	0.15834200	5.37300800	0.10581200

C	-0.35427900	4.12001000	-0.20470100
H	-1.26400400	3.12989800	2.92311000
H	-0.35741900	5.35734500	3.46360100
H	0.56145700	6.80178900	1.66834200
H	0.57485700	5.99106100	-0.68396100
H	-0.31520500	3.74576400	-1.22600600
C	-0.18749000	-1.74714800	-3.71953400
H	0.41616400	-0.87667400	-3.48620600
C	-3.38677500	-1.17537400	-0.56658100
Cl	-0.28098700	1.49682200	-2.70079100

Zero-point correction = 0.876615
Thermal correction to Energy = 0.932545
Thermal correction to Enthalpy = 0.933489
Thermal correction to Gibbs Free Energy = 0.784156
Sum of electronic and zero-point Energies = -3978.358085
Sum of electronic and thermal Energies = -3978.302156
Sum of electronic and thermal Enthalpies = -3978.301212
Sum of electronic and thermal Free Energies = -3978.450545
E(RM06) = -3979.23452396

TS6a

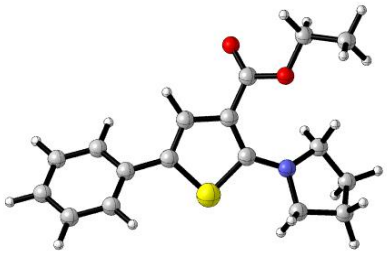


Rh	0.27240100	0.11957600	-1.07654300
Cl	0.87101400	-1.22704100	-2.98385700
C	-0.57436800	2.74088400	-0.75361000
C	-1.69640500	2.04325900	-0.17297700
S	-0.11283200	2.08334600	-2.29981800
C	-1.93958000	2.02816900	1.28014500
O	-1.30574000	2.64988700	2.11811300
O	-2.87865900	1.12587600	1.60729400
C	-3.27247100	1.04449800	2.97989200
C	-4.46312800	1.95220300	3.23174600
H	-2.42469600	1.30275000	3.61609100
H	-3.52402200	-0.00665200	3.13775700
H	-4.82001900	1.83117200	4.25984800
H	-4.17954700	2.99996700	3.08861200
H	-5.27966400	1.71199500	2.54416200
C	-4.70441200	2.05379100	-0.50337700
C	-6.08316000	2.01991500	-0.64838600
C	-6.67560800	1.15808400	-1.57109100
C	-5.86143900	0.34081600	-2.34824500
C	-4.48156400	0.36085100	-2.18823300
C	-3.86764900	1.19986400	-1.24768900
H	-4.26629000	2.76918400	0.18434500
H	-6.69931500	2.68955200	-0.05406400
H	-7.75467900	1.13813300	-1.69194100
H	-6.30076000	-0.33145300	-3.08004900
H	-3.87252700	-0.30628200	-2.78539700
C	-2.41158600	1.25951900	-1.12651500
C	-1.47858400	0.75509100	-2.07078100
H	-1.76449900	0.30172400	-3.01640600
C	1.10451800	4.50963100	-1.02788100
C	-0.74800500	4.87279000	0.49601500
C	1.20425900	5.90571300	-0.41390900
H	0.87681400	4.58012100	-2.10149600
H	2.01265800	3.91261100	-0.90547000
C	-0.24592800	6.21530100	-0.03409800
H	-0.51363300	4.73517800	1.55340400
H	-1.82594900	4.73097900	0.37236900
H	1.83420700	5.87591000	0.47973800
H	1.63378000	6.62744200	-1.11299800
H	-0.33740500	7.01090800	0.71007200
H	-0.81609000	6.51040600	-0.92260100
N	-0.02133000	3.88906200	-0.31973500
C	0.02030700	-3.49952000	-0.25893100
C	1.40179000	-3.68630700	-0.36701900
C	1.96330200	-4.91133000	-0.70495000
C	1.14076000	-6.01249700	-0.90582400
C	-0.23490900	-5.87442700	-0.75463600
C	-0.78151600	-4.63386500	-0.44201200
O	2.26041500	-2.63451400	-0.15050700
C	4.92116100	0.19994200	-3.42033900
C	6.08873200	-0.41419300	-2.97495600
C	6.16921700	-0.88861200	-1.66800800
C	5.08623600	-0.74342900	-0.80597700
C	3.91272000	-0.12784100	-1.24826100
P	2.48534800	0.16443600	-0.14566600
C	2.80324600	-0.90764600	1.31038300
P	-0.68822100	-1.81405100	0.08680000
C	-2.41760400	-2.13239000	-0.43306300
C	-0.76979700	-1.84716300	1.92572800
C	2.88541500	1.80239000	0.59470900
H	3.04186700	-4.97669800	-0.80184400
H	1.57374900	-6.97208100	-1.17112700
H	-0.89053600	-6.72848400	-0.89346200
H	-1.85891500	-4.54686100	-0.35813400
H	5.15595200	-1.10745000	0.21520800
H	7.07642700	-1.37229900	-1.31754000
H	6.93357700	-0.52965300	-3.64793900
H	4.84765600	0.55740900	-4.44295200
C	3.16377300	-0.46597000	2.58453400
C	3.17448500	-1.34423200	3.66422200
C	2.82174600	-2.67726900	3.47763400
C	2.49832500	-3.15114600	2.21085200
H	3.41194100	0.57776000	2.74362200
H	3.44117800	-0.98203800	4.65201100
H	2.80258000	-3.36013300	4.32150600
H	2.23000600	-4.19014000	2.05402900
C	1.94868200	2.38055300	1.45912400
C	2.23874000	3.55814800	2.13891000

C	3.46252800	4.19338800	1.94136000
C	4.38881000	3.64588500	1.05732400
C	4.10753600	2.45256400	0.39533400
H	0.97704000	1.92155300	1.60719200
H	1.49726200	3.97766300	2.81227900
H	3.69169900	5.11483800	2.46948300
H	5.34220700	4.13911700	0.89196700
H	4.84816500	2.02312500	-0.27159600
C	-0.36023900	-0.70978000	2.61865300
C	-0.35713200	-0.68137100	4.01059300
C	-0.77417700	-1.79851100	4.72523300
C	-1.19089900	-2.94221400	4.04385900
C	-1.18475500	-2.96826200	2.65422800
H	-0.02955100	0.15812500	2.05831500
H	-0.02303200	0.21327300	4.52744000
H	-0.77074700	-1.78416400	5.81141500
H	-1.51504400	-3.81822300	4.59839500
H	-1.49779300	-3.86800900	2.13222100
C	-3.51335900	-2.03689000	0.42332100
C	-4.78855300	-2.37620100	-0.02493100
C	-4.97515200	-2.82661800	-1.32637000
C	-3.88845900	-2.89588900	-2.19776300
C	-2.62170400	-2.52627600	-1.76376800
H	-3.37295400	-1.71208400	1.44868800
H	-5.63538300	-2.29140100	0.64936800
H	-5.96744300	-3.10504800	-1.66889500
H	-4.03010400	-3.22586100	-3.22304800
H	-1.77468400	-2.57036200	-2.44562100
C	3.83375700	0.33760800	-2.56351900
H	2.91103400	0.78324000	-2.92130200
C	2.51039600	-2.26312600	1.14055300

Zero-point correction = 0.878744
Thermal correction to Energy = 0.934049
Thermal correction to Enthalpy = 0.934993
Thermal correction to Gibbs Free Energy = 0.787532
Sum of electronic and zero-point Energies = -3978.383629
Sum of electronic and thermal Energies = -3978.328324
Sum of electronic and thermal Enthalpies = -3978.327380
Sum of electronic and thermal Free Energies = -3978.474841
E(RM06) = -3979.26064371

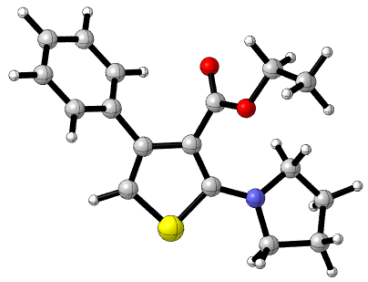
3a



C	0.47043100	-0.79475500	0.19719300
C	0.67451200	0.56241100	-0.02636800
S	-0.86600900	1.39016900	-0.18465500
C	1.44007200	-1.89893600	0.20688600
C	1.78167300	2.72039700	-0.39933300
C	2.98798400	0.98551800	0.78055000
C	3.18746300	3.21275600	-0.06134500
H	1.03379800	3.25302200	0.21069000
H	1.51510400	2.85291800	-1.45320500
C	3.54819900	2.35812600	1.15685200
H	3.71280300	0.40306400	0.20676900
H	2.68428500	0.38512900	1.64464100
H	3.87204100	3.00206400	-0.89030500
H	3.21080700	4.28682500	0.13743100
H	4.62161800	2.32520800	1.36011200
H	3.04279900	2.74508200	2.04886300
N	1.81678400	1.30168000	-0.04688700
O	2.62462900	-1.58950400	-0.35825000
O	1.18829800	-3.01296100	0.61967300
C	3.57605400	-2.65851800	-0.41439300
H	3.14332400	-3.48936900	-0.97954000
H	3.77454500	-3.01936700	0.59970000
C	4.82688000	-2.12107100	-1.07836600
H	5.56663700	-2.92131100	-1.17894000
H	4.59923700	-1.73232400	-2.07509400
H	5.27361400	-1.31645300	-0.48582800
C	-0.92116100	-1.12607500	0.27200900
H	-1.24496900	-2.15033900	0.41367700
C	-1.77112100	-0.08939600	0.05972900
C	-3.23835600	-0.10354200	-0.00266100
C	-3.95869100	-1.03901100	0.75220700
C	-3.95061200	0.79287400	-0.80910000
C	-5.34557700	-1.08770200	0.68602200
H	-3.42354000	-1.72074300	1.40657800
C	-5.33919500	0.75111600	-0.86301200
H	-3.41275200	1.51803900	-1.41423500
C	-6.04353700	-0.19142100	-0.11965100
H	-5.88444800	-1.82185700	1.27784600
H	-5.87190400	1.45411700	-1.49677300
H	-7.12786800	-0.22508400	-0.16439700

Zero-point correction = 0.334525
Thermal correction to Energy = 0.353870
Thermal correction to Enthalpy = 0.354815
Thermal correction to Gibbs Free Energy = 0.284517
Sum of electronic and zero-point Energies = -1262.025961
Sum of electronic and thermal Energies = -1262.006616
Sum of electronic and thermal Enthalpies = -1262.005672
Sum of electronic and thermal Free Energies =-1262.075969
E(RM06) = -1262.36371598

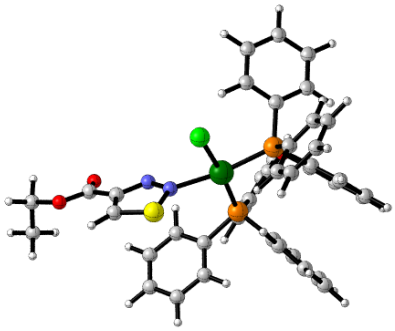
4a



C	0.05187800	-0.22638900	0.07242600
C	-1.08567500	-0.99185500	-0.13813700
S	-0.66394600	-2.64824100	-0.51758900
C	0.05202500	1.24032700	0.24798700
C	-3.45513800	-1.62669000	-0.30278600
C	-2.87371600	0.40847500	0.87124300
C	-4.72872700	-0.92470900	0.16731800
H	-3.29275900	-2.55777700	0.26507600
H	-3.47141900	-1.88066100	-1.36842200
C	-4.23283900	-0.09788100	1.35741500
H	-2.97441300	1.34834700	0.31865600
H	-2.15614400	0.57035800	1.68409300
H	-5.10863500	-0.26542600	-0.62086700
H	-5.51764800	-1.63374600	0.42917200
H	-4.90746200	0.71818400	1.62833400
H	-4.10543700	-0.74192900	2.23466500
N	-2.40131700	-0.65869100	-0.01326000
O	-0.81611100	1.84300800	-0.59181700
O	0.74959200	1.86810700	1.01530200
C	-0.91561000	3.26537700	-0.45913700
H	0.06884600	3.70995000	-0.63151100
H	-1.21220600	3.51097400	0.56648300
C	-1.93508100	3.74260400	-1.47236200
H	-2.03355200	4.83120000	-1.41738300
H	-1.62746600	3.47238600	-2.48644900
H	-2.91687600	3.29774800	-1.28153600
C	1.26898300	-1.00091300	-0.05858700
C	1.02576900	-2.29395600	-0.40050900
H	1.75537000	-3.06840100	-0.59009800
C	2.66062300	-0.49685200	0.05896700
C	3.12071900	0.13672200	1.21775700
C	3.55893000	-0.71720400	-0.99051900
C	4.44797900	0.53652100	1.32044300
H	2.42993400	0.32530500	2.03040300
C	4.88732800	-0.31657400	-0.88659700
H	3.20354300	-1.19609200	-1.89867700
C	5.33572100	0.31135000	0.27110300
H	4.79057000	1.02705200	2.22685500
H	5.56974100	-0.49134100	-1.71343100
H	6.37150800	0.62751900	0.35484800

Zero-point correction = 0.334294
Thermal correction to Energy = 0.353616
Thermal correction to Enthalpy = 0.354560
Thermal correction to Gibbs Free Energy = 0.284863
Sum of electronic and zero-point Energies = -1262.020684
Sum of electronic and thermal Energies = -1262.001363
Sum of electronic and thermal Enthalpies =-1262.000418
Sum of electronic and thermal Free Energies = -1262.070115
E(RM06) = -1262.35678468

INT1h

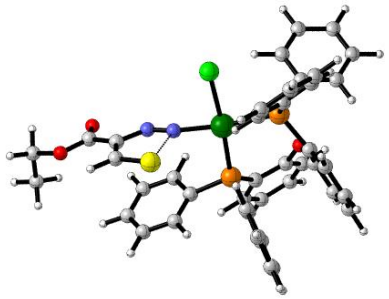


Cl	0.04769700	-3.31379300	-0.49531500
C	-4.22085800	-1.91567100	-1.39581300
C	-4.25159200	-1.57114300	-0.06914900
S	-2.63477600	-1.77016400	-1.95127400
N	-2.10629500	-1.25619700	-0.42288200
N	-3.03915100	-1.21051500	0.43979700
C	-5.45553200	-1.45447300	0.79036200
O	-5.46853200	-0.92812100	1.87592400
O	-6.52365300	-1.98222600	0.17616300
C	-7.77838200	-1.86597800	0.87016800
C	-8.40339800	-0.50019600	0.64926000
H	-7.61346100	-2.05989100	1.93246000
H	-8.39364400	-2.66232500	0.44775300
H	-9.39224700	-0.46609800	1.11771700
H	-7.78507100	0.28182200	1.09763200
H	-8.51993600	-0.29622000	-0.41945100
Rh	-0.05315600	-0.93432300	-0.15833300
P	2.20634500	-0.99242700	0.16795500
P	-0.30876100	1.32827400	-0.13869200
C	2.72961400	-1.73747800	1.76744400
C	3.14699200	0.58552800	0.17442400
C	3.13597200	-1.93949000	-1.10340500
C	-0.14250200	2.34659400	1.40789200
C	-2.00457400	1.81350000	-0.69145700
C	0.73259800	2.24624600	-1.35047400
C	3.94329700	-1.38856800	2.37130600
C	1.90069400	-2.66987000	2.39712400
C	4.11343000	0.93394100	-0.76971600
C	2.80122300	1.53219300	1.13946600
C	2.59906300	-2.04885700	-2.38864300
C	4.39319900	-2.49206900	-0.84466400
C	0.87088400	2.07578900	2.33809400
C	-1.03598900	3.37598800	1.73321800
C	-2.25426600	2.24389000	-1.99728000
C	-3.09086100	1.64152300	0.17756500
C	1.16563800	1.56314600	-2.49041000

C	1.04488700	3.60023800	-1.21280100
C	4.32637100	-1.96892700	3.57610900
H	4.59267600	-0.65209700	1.90600800
C	2.28671500	-3.24737900	3.60378800
H	0.95863300	-2.94899100	1.93732600
C	4.70881400	2.19203800	-0.74960300
H	4.38935900	0.22181100	-1.54018600
O	1.84525300	1.14804600	2.05547000
C	3.39899000	2.78548500	1.18679000
C	3.31462300	-2.67753700	-3.40249300
H	1.60027100	-1.66942300	-2.57974500
C	5.10619500	-3.12759800	-1.85700000
H	4.81876600	-2.43460900	0.15229300
C	0.93531900	2.71947800	3.56839700
C	-0.96426200	4.05160100	2.94774000
H	-1.81453300	3.64938700	1.03032600
C	-3.55736400	2.49257000	-2.42510400
H	-1.43146000	2.38877100	-2.68996500
C	-4.38988200	1.89437100	-0.24821100
H	-2.92632000	1.29175100	1.19196700
C	1.89237200	2.21960100	-3.47821100
H	0.93321900	0.50594900	-2.58720100
C	1.77901400	4.25604700	-2.19651600
H	0.72439200	4.14453900	-0.32935200
C	3.49750000	-2.90079100	4.19538500
H	5.27117600	-1.68794100	4.03265000
H	1.63251900	-3.97046300	4.08175700
C	4.35379700	3.11302800	0.23026500
H	5.44535900	2.45153400	-1.50317800
H	3.10471700	3.49800600	1.95023200
C	4.57109200	-3.21610500	-3.13931700
H	2.88081200	-2.76307400	-4.39449800
H	6.07954900	-3.55813100	-1.64064800
C	0.00794500	3.70632700	3.88028500
H	1.72672100	2.43981600	4.25602500
H	-1.67899400	4.83891500	3.16571200
C	-4.62790300	2.31796700	-1.55408100
H	-3.73093600	2.82827200	-3.44341600
H	-5.21309800	1.74574200	0.44465100
C	2.20158900	3.56892000	-3.33132000
H	2.22586700	1.67265200	-4.35521800
H	2.02390800	5.30703400	-2.07341500
H	3.79405800	-3.35197300	5.13806400
H	4.81632000	4.09524000	0.25091100
H	5.12708300	-3.71447300	-3.92827000
H	0.05706200	4.21261000	4.83938700
H	-5.64259200	2.51379500	-1.88885200
H	2.77557200	4.08331100	-4.09665900
H	-5.05115300	-2.22919800	-2.01140700

Zero-point correction = 0.662567
Thermal correction to Energy = 0.708696
Thermal correction to Enthalpy = 0.709640
Thermal correction to Gibbs Free Energy = 0.577953
Sum of electronic and zero-point Energies =- 3568.396057
Sum of electronic and thermal Energies = -3568.349927
Sum of electronic and thermal Enthalpies = -3568.348983
Sum of electronic and thermal Free Energies = -3568.480671
E(RM06) = -3569.12472966

TS1h

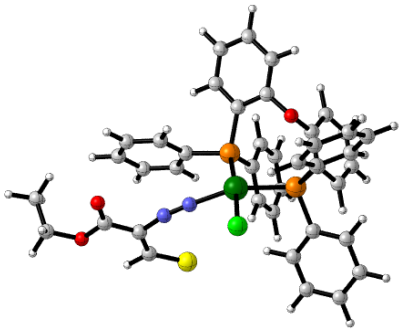


Cl	0.28877700	-3.25846000	0.92661300
C	-3.96675300	-1.98391400	-1.28119900
C	-4.13549800	-1.72471300	0.08021100
S	-2.48553400	-1.94651400	-2.01420400
N	-1.88088600	-1.33666500	0.35355900
N	-2.97708400	-1.43438000	0.73475600
C	-5.38358200	-1.63703000	0.84188200
O	-5.45585600	-1.34657900	2.01539000
O	-6.44101500	-1.90131300	0.05517200
C	-7.73137600	-1.77973800	0.67156000
C	-8.19153000	-0.33277700	0.69809400
H	-7.68510900	-2.19723500	1.67999100
H	-8.38645900	-2.39670300	0.05354000
H	-9.20816500	-0.27168100	1.09989600
H	-7.53250300	0.26283600	1.33553400
H	-8.19175400	0.08962900	-0.31162400
Rh	0.02336200	-0.94868300	0.37868700
P	2.35358000	-0.90380100	0.25193500
P	-0.42098400	1.27823700	-0.07870500
C	3.29034900	-1.06735700	1.81905600
C	3.10399200	0.57588600	-0.52404400
C	2.99094600	-2.23097600	-0.84127900
C	0.08448600	2.65490400	1.06143000
C	-2.24035600	1.56602400	-0.14955800
C	0.13526000	1.87877600	-1.72316300
C	4.58244400	-0.54439300	1.94194300
C	2.70680300	-1.71731000	2.90937300
C	3.74814700	0.58371800	-1.76086600
C	2.89529200	1.79512800	0.12057700
C	2.17766800	-2.70827700	-1.87317300
C	4.29524100	-2.71619000	-0.72044800
C	1.35309500	2.67977300	1.65457700
C	-0.78185800	3.70904500	1.38325500
C	-2.91611400	1.73903000	-1.35764400
C	-2.98110300	1.50313600	1.03894500
C	0.42875700	0.93461800	-2.70936900
C	0.20571700	3.23915100	-2.03838700
C	5.28542900	-0.67941500	3.13441400
H	5.04039000	-0.02036500	1.10731700
C	3.41390700	-1.84797400	4.10164900

H	1.70732200	-2.12975600	2.81770200
C	4.14892600	1.78390900	-2.34191300
H	3.91560300	-0.35167400	-2.28453400
O	2.27965100	1.71396300	1.34861600
C	3.29639600	3.00098400	-0.43817200
C	2.66748000	-3.64090000	-2.78094800
H	1.14652900	-2.37409200	-1.94195000
C	4.78164500	-3.65555700	-1.62525900
H	4.93416500	-2.36990600	0.08591000
C	1.71937700	3.65043400	2.57946300
C	-0.41945200	4.70287700	2.28723300
H	-1.76506500	3.75118500	0.92948200
C	-4.30542900	1.85863400	-1.37556400
H	-2.36533700	1.77311900	-2.29185600
C	-4.36372200	1.63616600	1.02199800
H	-2.47285600	1.33663700	1.98556200
C	0.78404800	1.34125300	-3.99245100
H	0.38063800	-0.12258700	-2.46292400
C	0.56467300	3.64502400	-3.31855700
H	-0.01406400	3.98505000	-1.27997000
C	4.70122500	-1.33215200	4.21717400
H	6.28796000	-0.26999500	3.21822600
H	2.95163600	-2.35602800	4.94259600
C	3.91810400	2.98692600	-1.68303300
H	4.63161400	1.77752300	-3.31375100
H	3.10684600	3.93355000	0.08284900
C	3.97117600	-4.11496100	-2.65955400
H	2.02173800	-4.01167700	-3.57116100
H	5.79441400	-4.03219400	-1.51663000
C	0.82652000	4.66438900	2.90396100
H	2.70796200	3.59383600	3.02287300
H	-1.11996900	5.50006100	2.51475500
C	-5.02994400	1.81358700	-0.18995300
H	-4.81781200	1.98680400	-2.32433000
H	-4.92053600	1.56765400	1.95063100
C	0.85323700	2.69655600	-4.29787100
H	1.01218100	0.59631600	-4.74868400
H	0.62022900	4.70418000	-3.55224800
H	5.24850800	-1.43534800	5.14975300
H	4.22099600	3.92495300	-2.13804000
H	4.35087500	-4.85050700	-3.36272500
H	1.10911400	5.42537400	3.62466600
H	-6.11186100	1.90585900	-0.20731400
H	1.13416200	3.01573300	-5.29730100
H	-4.87046900	-2.21732600	-1.83873000

Zero-point correction = 0.660663
Thermal correction to Energy = 0.706943
Thermal correction to Enthalpy = 0.707887
Thermal correction to Gibbs Free Energy = 0.577316
Sum of electronic and zero-point Energies = -3568.368320
Sum of electronic and thermal Energies = -3568.322041
Sum of electronic and thermal Enthalpies = -3568.321096
Sum of electronic and thermal Free Energies = -3568.451668
E(RM06) = -3569.10000643

INT2h



Cl	0.32198000	-2.97247300	1.75168200
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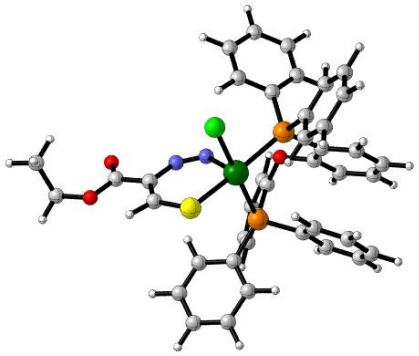
C	-4.12178100	-1.63626000	0.01322800
S	-2.89060100	-1.97650700	-2.42598400
N	-1.83922400	-1.18889700	0.77205300
N	-2.93291500	-1.38985500	0.57581400
C	-5.26012600	-1.49923800	0.92898600
O	-5.15699800	-1.23252000	2.10778800
O	-6.42313400	-1.69673300	0.29018100
C	-7.61134400	-1.55677000	1.08392100
C	-8.01322800	-0.09902300	1.22037400
H	-7.44109000	-2.01172300	2.06236600
H	-8.36617700	-2.13096500	0.54341800
H	-8.96209600	-0.02343800	1.76138400
H	-7.25254100	0.45275800	1.77899400
H	-8.13907900	0.35955900	0.23458000
Rh	0.04998900	-0.80513900	0.80001100
P	2.32799200	-0.89427300	0.31144200
P	-0.37827100	1.28845600	-0.07614800
C	3.50391900	-0.90351600	1.72122900
C	3.01244400	0.44330100	-0.73537100
C	2.71093600	-2.38490000	-0.68119800
C	0.24626700	2.80698100	0.78039400
C	-2.19187100	1.61233700	-0.08533800
C	0.07122300	1.53359600	-1.83496200
C	4.82512300	-0.47342200	1.54823900
C	3.08371600	-1.32901700	2.98377900
C	3.51460900	0.26504800	-2.02410500
C	2.95315600	1.73890300	-0.22188700
C	1.69694000	-2.96412600	-1.44999200
C	4.00304800	-2.91398100	-0.74166900
C	1.55641700	2.88314100	1.27395500
C	-0.58227400	3.91453800	1.00458400
C	-2.92372300	1.71892400	-1.26816500
C	-2.86926500	1.65667800	1.14173600
C	0.07440100	0.41136200	-2.66812200
C	0.31651500	2.79501600	-2.38165700
C	5.71490400	-0.48324300	2.61700100
H	5.16169400	-0.11791000	0.57831800
C	3.97721100	-1.33293000	4.05152800
H	2.06415700	-1.67033800	3.12616200
C	3.94289000	1.35725400	-2.77373200
H	3.55391600	-0.73176500	-2.45067400

O	2.44605700	1.85832700	1.05434500
C	3.39493800	2.83725700	-0.94684800
C	1.97692600	-4.04260200	-2.28256700
H	0.67923100	-2.59301400	-1.36918100
C	4.27908400	-3.99704200	-1.57067900
H	4.79684900	-2.48939400	-0.13500200
C	2.00053700	3.97055100	2.01654100
C	-0.14109200	5.02094100	1.72400600
H	-1.59625500	3.90924000	0.62141800
C	-4.30886500	1.87609100	-1.22472800
H	-2.42367600	1.66578500	-2.22899900
C	-4.24766900	1.81922400	1.18308400
H	-2.31485600	1.54567400	2.07077000
C	0.31491100	0.54925400	-4.03108100
H	-0.12684500	-0.56858200	-2.24555600
C	0.56605400	2.92985500	-3.74370400
H	0.32009800	3.67393700	-1.74342600
C	5.29162800	-0.91340900	3.87200200
H	6.73760300	-0.14895200	2.46895400
H	3.63891800	-1.66706900	5.02765800
C	3.88721000	2.63751900	-2.23254600
H	4.31455200	1.20599700	-3.78183700
H	3.33362700	3.83201100	-0.51788600
C	3.26822300	-4.55894800	-2.34618900
H	1.17811000	-4.48941500	-2.86644900
H	5.28468900	-4.40553400	-1.60460800
C	1.14663300	5.04237000	2.24876700
H	3.01736500	3.95675900	2.39475400
H	-0.81203600	5.85923100	1.88187400
C	-4.97125500	1.93051500	-0.00446300
H	-4.86650100	1.94648400	-2.15352900
H	-4.75830200	1.83219300	2.14035400
C	0.56333100	1.80866800	-4.56968600
H	0.30775500	-0.32946800	-4.66848900
H	0.76329600	3.91342400	-4.15974200
H	5.98499100	-0.91793500	4.70807300
H	4.22145800	3.49074300	-2.81484100
H	3.48452800	-5.40661300	-2.98982600
H	1.49169800	5.89354200	2.82741700
H	-6.05039600	2.04681500	0.02604500
H	0.75515900	1.91738000	-5.63318300
H	-5.17380800	-2.07693900	-1.73823300

Zero-point correction = 0.660756
Thermal correction to Energy = 0.708019
Thermal correction to Enthalpy = 0.708964
Thermal correction to Gibbs Free Energy = 0.575787
Sum of electronic and zero-point Energies = -3568.374083
Sum of electronic and thermal Energies = -3568.326820
Sum of electronic and thermal Enthalpies = -3568.325875
Sum of electronic and thermal Free Energies = -3568.459052
E(RM06) = -3569.10492763

INT3h



Cl	-0.24932400	-2.61797000	-2.06301500
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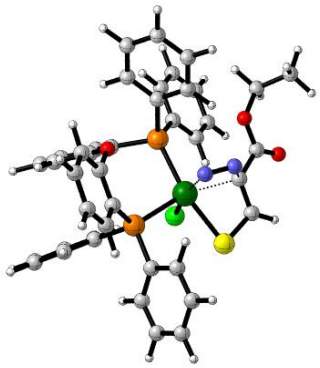
S	-2.16086600	-0.09548000	-2.27358300
N	-1.36556900	-1.17888800	0.70033200
N	-2.53621100	-1.33755500	0.68739900
C	-4.88976700	-1.58356000	0.42767400
O	-5.02513600	-2.03604900	1.54250400
O	-5.91324100	-1.39250100	-0.43131400
C	-7.20534900	-1.81610000	0.02201000
C	-7.40130700	-3.30811600	-0.18154300
H	-7.90800900	-1.23589200	-0.58039200
H	-7.32027700	-1.54510900	1.07444100
H	-8.42128800	-3.59124900	0.09934300
H	-7.24195500	-3.57872900	-1.22966900
H	-6.70209200	-3.87144300	0.44146000
Rh	-0.28758500	-0.51107900	-0.92336100
P	1.84251900	-1.20146400	-0.07293000
P	-0.27550300	1.66244800	-0.04241900
C	1.82734600	-2.58224700	1.13714800
C	2.87244000	0.04387300	0.79232700
C	2.98728400	-1.74483000	-1.39786000
C	-0.46912100	1.90887000	1.78289200
C	-1.62732400	2.73263200	-0.67789300
C	1.22398900	2.60321000	-0.51044400
C	2.82026300	-2.69081500	2.11821800
C	0.81609700	-3.54497800	1.08156000
C	4.12500600	0.49117600	0.37210400
C	2.31742100	0.61493500	1.93707000
C	2.82277800	-1.24490100	-2.69195700
C	4.06479900	-2.59353500	-1.12957800
C	0.15972900	1.06616300	2.71114300
C	-1.31302000	2.90123800	2.30162400
C	-1.38983300	3.80130400	-1.54157600
C	-2.94701900	2.42749400	-0.32034100
C	1.81866800	2.30800100	-1.74080300
C	1.75076400	3.62996500	0.27399700
C	2.80404800	-3.74570100	3.02471500
H	3.60932500	-1.94711400	2.18273700
C	0.80268700	-4.59709300	1.99269800
H	0.04831900	-3.47954700	0.31944600
C	4.80100200	1.47633700	1.08724400

H	4.57047000	0.07402300	-0.52487000
O	1.07811000	0.13416000	2.29608800
C	2.98599600	1.58254900	2.67581000
C	3.72991500	-1.56789900	-3.69543200
H	1.95951900	-0.63016600	-2.92704600
C	4.96915700	-2.92210700	-2.13507600
H	4.19690600	-3.00624900	-0.13408100
C	-0.11265300	1.13653700	4.07190200
C	-1.56578300	3.00518000	3.66548900
H	-1.79663300	3.59848800	1.62819500
C	-2.45411900	4.55303200	-2.03945600
H	-0.37648000	4.05688600	-1.83298800
C	-4.00399100	3.18244600	-0.80772800
H	-3.15134200	1.59391700	0.34658200
C	2.92735300	3.02292800	-2.17961400
H	1.40803100	1.51226100	-2.35709300
C	2.86436600	4.34142600	-0.16241700
H	1.29947100	3.86673800	1.23294800
C	1.79260300	-4.70065600	2.96474700
H	3.58091100	-3.81734200	3.78041100
H	0.00874500	-5.33574200	1.93997700
C	4.23536600	2.01211300	2.23990600
H	5.76936200	1.82343900	0.74174500
H	2.52801800	2.00166800	3.56558100
C	4.80666100	-2.40549700	-3.41771700
H	3.58244300	-1.18118300	-4.69925300
H	5.79855700	-3.58783600	-1.91568900
C	-0.98656400	2.10389900	4.55204400
H	0.37977700	0.43079200	4.73242300
H	-2.22989400	3.78293500	4.02844200
C	-3.75930600	4.24809800	-1.67342400
H	-2.25490900	5.38095800	-2.71312100
H	-5.02043900	2.93112200	-0.52052600
C	3.45346500	4.03989500	-1.38715000
H	3.38253600	2.77948400	-3.13472500
H	3.27555000	5.13016700	0.46036400
H	1.77622400	-5.52196300	3.67540800
H	4.76425400	2.77479000	2.80353200
H	5.51060400	-2.66592700	-4.20267900
H	-1.20049200	2.16082700	5.61470400
H	-4.58611100	4.83537200	-2.06153100
H	4.32429100	4.59529200	-1.72253700
H	-4.43979800	-0.57489000	-1.98123900

Zero-point correction = 0.661584
Thermal correction to Energy = 0.708016
Thermal correction to Enthalpy = 0.708960
Thermal correction to Gibbs Free Energy = 0.578592
Sum of electronic and zero-point Energies = -3568.393815
Sum of electronic and thermal Energies = -3568.347383
Sum of electronic and thermal Enthalpies = -3568.346439
Sum of electronic and thermal Free Energies = -3568.476807
E(RM06) = -3569.12204029

TS2h

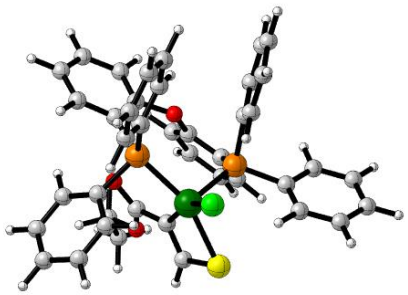


Cl	-0.13148200	1.22934300	-2.58256700
C	-1.00187700	3.69922100	-0.33558200
C	-1.70636100	2.61013600	0.15877600
S	0.66553800	3.46874700	-0.32408700
N	-0.36304800	1.51638000	1.85105100
N	-1.26673900	2.26287600	1.86105100
C	-3.17420300	2.54932000	0.01036700
O	-3.82905500	3.31581600	-0.66343300
O	-3.69369100	1.52683600	0.70297900
C	-5.09819800	1.27086300	0.56994900
C	-5.89335400	2.08145200	1.57586600
H	-5.19107300	0.19651500	0.74612000
H	-5.39960500	1.49239400	-0.45599500
H	-6.95496500	1.82166400	1.50819400
H	-5.55036400	1.87540500	2.59463800
H	-5.78453300	3.15049500	1.37437600
Rh	-0.10621300	1.19762400	-0.12942800
P	-1.41734100	-0.81809100	-0.17018200
P	2.17956900	0.28697000	0.08129000
C	-2.11602200	-1.56699100	1.37212700
C	-0.38621100	-2.17214000	-0.83250700
C	-2.90509000	-0.82546900	-1.25939800
C	2.58720800	-0.68743600	1.59800600
C	3.31134800	1.71974500	0.24632500
C	3.01890200	-0.74336700	-1.19416500
C	-2.14165400	-2.95781600	1.54071700
C	-2.67533500	-0.76589400	2.36940800
C	-0.50322000	-2.71260200	-2.11103500
C	0.65204500	-2.61631900	-0.00887500
C	-3.20802400	0.24669400	-2.10037400
C	-3.77938500	-1.92045900	-1.22142600
C	1.80537800	-1.79714000	1.93570900
C	3.70391400	-0.42544100	2.40061600
C	4.22678500	2.04958500	-0.75409600
C	3.19535400	2.55006500	1.36962800
C	2.49449900	-0.85581300	-2.48132000
C	4.21607800	-1.40428400	-0.88258200
C	-2.71196000	-3.52933700	2.67178200
H	-1.70754800	-3.60711600	0.78625600
C	-3.24416000	-1.34007100	3.50446000
H	-2.69271900	0.30818600	2.26072900

C	0.40386600	-3.67547900	-2.54687300
H	-1.29371800	-2.36597700	-2.76898100
O	0.65200100	-2.06200600	1.24535400
C	1.55811000	-3.58160600	-0.42274000
C	-4.36355700	0.23133700	-2.87757700
H	-2.53612700	1.09258200	-2.16520400
C	-4.92832800	-1.93802900	-2.00409500
H	-3.57496100	-2.76399000	-0.57061800
C	2.09623900	-2.60098900	3.03104100
C	4.01208700	-1.22571700	3.49671700
H	4.34463300	0.41738200	2.16638000
C	5.02658500	3.18354100	-0.62535700
H	4.31720800	1.42581300	-1.63736000
C	4.00613300	3.67049900	1.50197600
H	2.46619800	2.31888100	2.14207300
C	3.15416300	-1.62381100	-3.43997400
H	1.57267300	-0.34533400	-2.73507500
C	4.86694600	-2.17042200	-1.84008400
H	4.64133700	-1.32842000	0.11309100
C	-3.26491400	-2.72071500	3.66163500
H	-2.72099700	-4.61014800	2.77932900
H	-3.67052500	-0.69586800	4.26784400
C	1.42908000	-4.10250600	-1.70690700
H	0.31676500	-4.08270000	-3.54889700
H	2.36042600	-3.89536800	0.23684800
C	-5.22649200	-0.85801100	-2.83199100
H	-4.58318200	1.08251600	-3.51427300
H	-5.59374800	-2.79518000	-1.96056200
C	3.20624300	-2.31386100	3.81613400
H	1.43356700	-3.43004200	3.25570100
H	4.88298200	-0.99296000	4.10116300
C	4.92377600	3.98989300	0.50273800
H	5.73167400	3.43277800	-1.41244600
H	3.90957500	4.30292600	2.37908500
C	4.33454700	-2.28421800	-3.12409100
H	2.72917000	-1.70604000	-4.43572700
H	5.79222000	-2.67850000	-1.58426500
H	-3.70798800	-3.16580200	4.54768500
H	2.14454000	-4.84104000	-2.05431500
H	-6.12830600	-0.86773400	-3.43730700
H	3.43773400	-2.93673000	4.67448300
H	5.55052300	4.87113400	0.60148400
H	4.84357500	-2.88452100	-3.87289400
H	-1.48285200	4.56129700	-0.79638200

Zero-point correction = 0.659358
Thermal correction to Energy = 0.705511
Thermal correction to Enthalpy = 0.706455
Thermal correction to Gibbs Free Energy = 0.578961
Sum of electronic and zero-point Energies = -3568.372780
Sum of electronic and thermal Energies = -3568.326627
Sum of electronic and thermal Enthalpies = -3568.325683
Sum of electronic and thermal Free Energies = -3568.453176
E(RM06) = -3569.08502126

INT4h

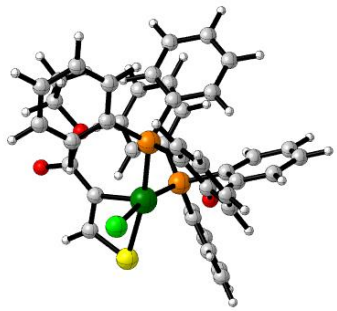


C	-0.32263600	-2.54414500	-2.19125700
C	0.25099900	-1.99449800	-1.10737900
S	-1.29934300	-1.34859600	-3.01998500
C	1.81697100	-4.84013400	0.55145100
H	1.78120000	-4.43327200	1.56634700
H	2.85491900	-4.77610600	0.20520700
C	1.14408300	-2.71317600	-0.21258300
O	1.94562700	-2.21474600	0.56274900
O	0.98586200	-4.05250300	-0.29862000
C	1.29222000	-6.26027400	0.49959100
H	1.89922300	-6.91025900	1.13814700
H	0.25562200	-6.29386400	0.84963500
H	1.32225000	-6.65092900	-0.52183400
Rh	-0.18643800	-0.01824900	-1.37858300
P	1.58044500	0.89971200	-0.10991500
P	-1.83950300	-0.06164400	0.11241300
C	2.87575600	0.35426200	-1.29008600
C	2.18798800	0.46464600	1.56857400
C	1.70622200	2.72609000	0.02990100
C	-1.67350600	-1.51853600	1.19837100
C	-3.54134800	-0.09336100	-0.56455400
C	-2.01353700	1.41378300	1.18896000
C	2.70812700	0.70263300	-2.64117800
C	3.90944600	-0.52102400	-0.93800200
C	3.47719300	0.83991200	1.95444800
C	1.36769700	-0.14117200	2.52167900
C	1.11666200	3.32593800	1.14785700
C	2.33699500	3.53161500	-0.91951900
C	-0.59073100	-1.53083300	2.08933000
C	-2.39903900	-2.69444600	1.00407400
C	-4.60173000	-0.46939300	0.26877600
C	-3.81259100	0.43108500	-1.82945600
C	-1.97653400	2.68023200	0.60351500
C	-2.32777000	1.28782700	2.54620500
C	3.58002800	0.20912000	-3.60879600
H	1.89241800	1.35379500	-2.94698500
C	4.77658300	-1.00555700	-1.91011000
H	4.01661600	-0.85319500	0.08689900
C	3.94968000	0.57259600	3.23482800
H	4.11810000	1.35290500	1.24310400
O	0.05753600	-0.33465100	2.17449300
C	1.81169900	-0.37585600	3.81838300
C	1.15161900	4.70587800	1.30860000

H	0.62390700	2.71846100	1.90188000
C	2.37524600	4.91280300	-0.75323000
H	2.80712300	3.09124500	-1.79074100
C	-0.25267700	-2.67832000	2.79596300
C	-2.07305000	-3.84764300	1.70931800
H	-3.19934100	-2.71685000	0.27194800
C	-5.91377300	-0.37323600	-0.18076700
H	-4.40948700	-0.83154600	1.27463500
C	-5.12891900	0.53713300	-2.26871800
H	-3.00164600	0.77447800	-2.46312900
C	-2.23739900	3.81008900	1.37461600
H	-1.72092600	2.78864100	-0.44683900
C	-2.57805200	2.42024900	3.31194400
H	-2.37898100	0.30817900	3.01088800
C	4.61760400	-0.64164000	-3.24566800
H	3.43346400	0.48768300	-4.64760600
H	5.57539900	-1.68250300	-1.62190300
C	3.11490000	-0.03715800	4.16598200
H	4.95927100	0.86050900	3.50931300
H	1.12807200	-0.78695200	4.55336100
C	1.78116700	5.50373200	0.35750000
H	0.68118400	5.15358800	2.17884800
H	2.86992900	5.52697700	-1.49954000
C	-1.00288500	-3.83364800	2.59882400
H	0.61084500	-2.68631200	3.44925500
H	-2.63941800	-4.75854200	1.54728600
C	-6.17867300	0.12517000	-1.45383400
H	-6.72835100	-0.68008400	0.46834900
H	-5.32846400	0.94321400	-3.25532300
C	-2.53192400	3.68506000	2.72755200
H	-2.19043800	4.79001400	0.91015400
H	-2.81367100	2.31362700	4.36671500
H	5.29476500	-1.03010600	-4.00058500
H	3.46594900	-0.22415400	5.17611000
H	1.81036100	6.58219900	0.48234200
H	-0.73301900	-4.73661900	3.13859300
H	-7.20357800	0.20244600	-1.80459700
H	-2.72972300	4.56836400	3.32798500
Cl	-0.59604600	2.09885400	-2.53215700
H	-0.19059900	-3.55744500	-2.56834600

Zero-point correction = 0.651628
Thermal correction to Energy = 0.696246
Thermal correction to Enthalpy = 0.697190
Thermal correction to Gibbs Free Energy = 0.572797
Sum of electronic and zero-point Energies = -3458.945460
Sum of electronic and thermal Energies =- 3458.900842
Sum of electronic and thermal Enthalpies = -3458.899898
Sum of electronic and thermal Free Energies = -3459.024291
E(RM06) = -3459.63199699

INT4h'



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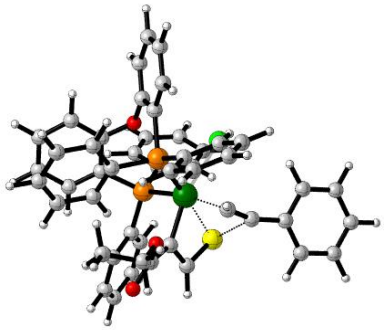
C	0.09881000	1.63027700	-2.05728900
S	1.64075400	0.07541000	-3.30987400
C	-0.64620800	2.79583900	-1.60230100
O	-0.60693000	3.88702000	-2.14203800
O	-1.40363900	2.56639600	-0.50181000
C	-2.28888400	3.62027400	-0.11109000
C	-1.60425700	4.61121000	0.81291000
H	-3.12227500	3.11208500	0.38414900
H	-2.66487900	4.11880900	-1.00743400
H	-2.32743800	5.35474300	1.16549300
H	-1.16935500	4.10511300	1.68142000
H	-0.80240800	5.12697800	0.27928000
Cl	-1.38240900	-1.16649400	-3.03677700
Rh	0.16695400	-0.27866100	-1.44213700
C	-1.90820600	-2.34655900	-0.00469300
C	-0.79819400	-3.14438300	-0.28744900
C	-0.91220800	-4.48963100	-0.59454900
C	-2.17303800	-5.07993500	-0.56556500
C	-3.29194000	-4.31814800	-0.24585500
C	-3.16098000	-2.95742400	0.01901500
O	0.45672400	-2.52991100	-0.33622300
C	5.33391300	-1.11289400	-1.66131800
C	6.26910500	-0.15294000	-1.27492000
C	5.86819300	0.92695000	-0.49902600
C	4.53535200	1.05514000	-0.10737500
C	3.59403700	0.10619400	-0.50318200
P	1.84104400	0.11986300	0.05437700
C	1.90966900	-1.34757900	1.15467900
P	-1.63628000	-0.53025100	0.10890600
C	-3.28349200	0.20462300	-0.21346500
C	-1.44882000	-0.24609600	1.91713900
C	1.73380100	1.60571500	1.10868300
H	-0.02685100	-5.05271100	-0.87047700
H	-2.27840600	-6.13262300	-0.80785000
H	-4.27603400	-4.77542900	-0.23313200
H	-4.04585100	-2.35841100	0.20758200
H	4.24402000	1.89921000	0.50806400
H	6.59020700	1.67700900	-0.19036200
H	7.30666800	-0.25008700	-1.58027300
H	5.63759200	-1.95798400	-2.27124700
C	2.74738700	-1.36946600	2.27632800
C	2.81389400	-2.47934700	3.10534900

C	2.06300500	-3.61033600	2.79358500
C	1.27182600	-3.63674900	1.65334300
H	3.35381800	-0.49625700	2.49796100
H	3.45587400	-2.46825700	3.97988600
H	2.10925800	-4.48998700	3.42818900
H	0.70553500	-4.52517800	1.40106300
C	1.50122300	1.58096100	2.48263700
C	1.46478100	2.77071100	3.20767900
C	1.65511200	3.98994400	2.56859900
C	1.86529100	4.02313100	1.19067600
C	1.89800600	2.84108200	0.46373000
H	1.32262700	0.64247600	2.99694100
H	1.27632000	2.73489800	4.27648300
H	1.62837500	4.91466500	3.13739000
H	1.99368800	4.97060300	0.67701100
H	2.05418700	2.87562900	-0.61037100
C	-1.61491400	1.04835300	2.42019500
C	-1.50500800	1.29967700	3.78225700
C	-1.18764200	0.26748400	4.66146100
C	-1.00268000	-1.02158900	4.16936100
C	-1.15128000	-1.27989600	2.80907100
H	-1.82838700	1.86171200	1.73932500
H	-1.64679400	2.31097100	4.15149600
H	-1.09059500	0.46498600	5.72505600
H	-0.76034000	-1.83686200	4.84436800
H	-1.04441300	-2.29790300	2.45204900
C	-4.26280100	0.21074500	0.78716600
C	-5.50845900	0.78605100	0.55183600
C	-5.78377900	1.36635900	-0.68308400
C	-4.81353100	1.36166200	-1.68192300
C	-3.56954800	0.78314200	-1.45315700
H	-4.05372000	-0.22330000	1.76047700
H	-6.25877100	0.78431200	1.33688800
H	-6.75244100	1.82239300	-0.86591700
H	-5.02009700	1.81320200	-2.64726200
H	-2.82127900	0.77665000	-2.23664400
C	4.00653400	-0.98270300	-1.28091300
H	3.28249900	-1.72825000	-1.59775100
C	1.20035900	-2.50906700	0.83664500
H	1.11452700	2.48301000	-3.78704900

Zero-point correction = 0.652435
Thermal correction to Energy = 0.696455
Thermal correction to Enthalpy = 0.697399
Thermal correction to Gibbs Free Energy = 0.575788
Sum of electronic and zero-point Energies = -3458.956577
Sum of electronic and thermal Energies = -3458.912557
Sum of electronic and thermal Enthalpies = -3458.911613
Sum of electronic and thermal Free Energies = -3459.033224
E(RM06) = -3459.64814383

TS3h

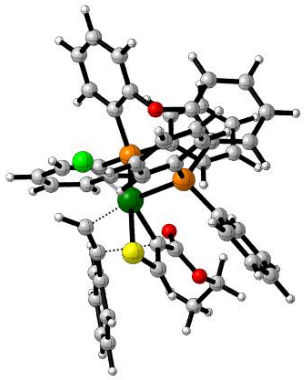


C	-1.84591700	0.12105600	2.58468600
C	-0.63717100	-0.30286300	2.18167600
S	-2.86045700	0.39692400	1.18426200
C	0.31992000	-0.81403100	3.17632600
O	0.50748800	-0.33823900	4.28002500
O	0.95001100	-1.93144400	2.74914500
C	1.73919800	-2.63334100	3.71714900
C	3.14328700	-2.07244900	3.85457900
H	1.75797600	-3.66212400	3.34886200
H	1.22042200	-2.60648900	4.67905800
H	3.71073600	-2.68409600	4.56483800
H	3.67347000	-2.07215900	2.89702000
H	3.10839100	-1.04728300	4.22918900
Cl	-1.44393400	-0.66384200	-2.23372100
Rh	-0.76066200	-0.31235700	0.15556100
C	1.85831500	-1.02173400	-2.27519900
C	1.77606300	0.22590700	-2.89758000
C	2.15427400	0.42249200	-4.21809900
C	2.66865100	-0.64223800	-4.94880000
C	2.79773700	-1.88813200	-4.34603400
C	2.39260500	-2.07320200	-3.02704000
O	1.25399400	1.28840400	-2.20370800
C	-3.19183100	3.14680800	-2.78656000
C	-2.68427600	4.32809800	-3.31794200
C	-1.45116300	4.80830200	-2.88378500
C	-0.73204000	4.10854200	-1.92116100
C	-1.23583200	2.91786600	-1.38655000
P	-0.32639200	2.05422200	-0.04891400
C	1.39903900	2.62146100	-0.31555300
P	1.32285600	-1.22724100	-0.51271200
C	1.34164700	-3.05645100	-0.39283100
C	2.85341400	-0.68021600	0.34317400
C	-0.80846100	3.01019200	1.44535700
H	2.02976300	1.40847700	-4.65322100
H	2.96563600	-0.49657900	-5.98272300
H	3.20337100	-2.72692900	-4.90294300
H	2.48552200	-3.05896400	-2.58615900
H	0.22493600	4.49497300	-1.58345000
H	-1.04729200	5.72969000	-3.29318000
H	-3.24618900	4.87312000	-4.07108500
H	-4.14789600	2.76022300	-3.12580800
C	2.10919600	3.50959500	0.49259200
C	3.45941800	3.75463400	0.25700800

C	4.11096900	3.10855700	-0.78941400
C	3.41390400	2.25321500	-1.63672600
H	1.61200200	3.99883600	1.32285700
H	4.00343300	4.43895800	0.90021000
H	5.16995500	3.27759900	-0.95925700
H	3.90860200	1.75672300	-2.46430400
C	-0.15875700	2.77605900	2.66354500
C	-0.52746000	3.46477800	3.81245800
C	-1.56328900	4.39454500	3.76459900
C	-2.22131400	4.63039400	2.56234600
C	-1.84739900	3.94357400	1.40977600
H	0.63249000	2.03833600	2.73470400
H	-0.01540100	3.25558200	4.74640200
H	-1.85907800	4.92820300	4.66318200
H	-3.03456100	5.34852000	2.51593100
H	-2.37802300	4.13285400	0.48326900
C	2.78303100	0.27102200	1.35748100
C	3.93776300	0.75601100	1.96205200
C	5.18084400	0.27477200	1.56858300
C	5.26509600	-0.68466700	0.56045600
C	4.11010400	-1.15068300	-0.05672900
H	1.81512200	0.64576000	1.66348200
H	3.85879300	1.50861000	2.74011800
H	6.08478500	0.64739900	2.04129600
H	6.23354200	-1.06197600	0.24567100
H	4.18815300	-1.87953500	-0.85847000
C	2.17582700	-3.75865500	0.47511900
C	2.10935000	-5.14935100	0.54458400
C	1.21163800	-5.84772500	-0.25579500
C	0.37519300	-5.15155500	-1.12774500
C	0.43418200	-3.76465100	-1.19467100
H	2.88182100	-3.22412200	1.10040800
H	2.76502600	-5.68412000	1.22571700
H	1.16147700	-6.93120500	-0.20137300
H	-0.33108800	-5.68853800	-1.75362000
H	-0.23180300	-3.21701700	-1.85920300
C	-2.47200400	2.44101400	-1.82665700
H	-2.86431200	1.51007600	-1.43829500
C	2.06110900	2.04163500	-1.40077200
C	-4.46562400	-2.50003000	-1.19026400
C	-5.77975900	-2.74582600	-1.57153100
C	-6.79120900	-2.77094400	-0.61417500
C	-6.49860700	-2.53597700	0.73091200
C	-5.19476800	-2.26972700	1.11926400
C	-4.16929100	-2.26449900	0.16126200
H	-3.65922800	-2.45174100	-1.91559300
H	-6.01425600	-2.91777600	-2.61740500
H	-7.81598900	-2.96805900	-0.91567800
H	-7.29265500	-2.55014800	1.47100300
H	-4.95123700	-2.05826200	2.15532400
C	-2.80604100	-2.05869600	0.53715700
C	-1.55593000	-2.23116800	0.59210200
H	-0.93769000	-3.10253200	0.74208000
H	-2.22542400	0.20149900	3.60089800

Zero-point correction = 0.764521
Thermal correction to Energy = 0.815532
Thermal correction to Enthalpy = 0.816476
Thermal correction to Gibbs Free Energy = 0.679359
Sum of electronic and zero-point Energies = -3767.128812
Sum of electronic and thermal Energies = -3767.077801
Sum of electronic and thermal Enthalpies = -3767.076857
Sum of electronic and thermal Free Energies = -3767.213974
E(RM06) = -3767.90548819

TS4h

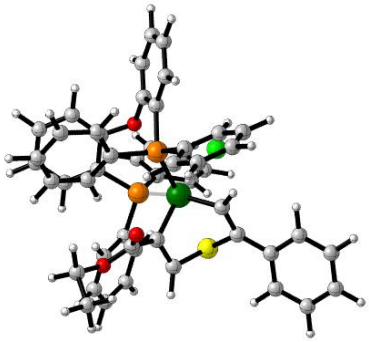


C	1.15513800	-2.69864800	-0.85285500
C	1.33627600	-1.52783900	-0.17578800
S	0.09344900	-2.44730700	-2.18068700
C	2.19379700	-1.37127600	0.99666100
O	2.58718900	-0.30964000	1.44887600
O	2.52556800	-2.55921300	1.55539100
C	3.38864500	-2.50802100	2.69617700
C	4.84393900	-2.37605900	2.28700500
H	3.20555100	-3.45068900	3.21815700
H	3.08503200	-1.67538500	3.33680500
H	5.48852400	-2.41940900	3.17173400
H	5.12789400	-3.18514800	1.60750000
H	5.00913100	-1.42256900	1.78001700
C	4.46969700	-2.16835700	-1.61069800
C	5.77900000	-2.52098400	-1.32053500
C	6.65221500	-1.57608000	-0.77905000
C	6.21425400	-0.27903700	-0.52189600
C	4.90342600	0.08315600	-0.80852200
C	4.02674500	-0.85878700	-1.36616400
H	3.77622400	-2.88932300	-2.03148600
H	6.12379500	-3.53126800	-1.51750700
H	7.67689300	-1.85599700	-0.55264900
H	6.89378600	0.45199100	-0.09495500
H	4.54328400	1.08612000	-0.61295700
C	2.71565200	-0.44863500	-1.75329700
C	1.73637400	0.11779100	-2.30084100
H	1.57003500	0.67052500	-3.21316800
Cl	-1.16090600	0.99241200	-2.94156600
Rh	0.01881500	-0.26585500	-1.15754600
C	-1.01599000	3.11052900	-0.42057500
C	-2.37689800	2.79068200	-0.40408300
C	-3.35857200	3.72045300	-0.71369500
C	-2.99224800	5.02609600	-1.02124900

C	-1.64872300	5.38218600	-1.01393300
C	-0.67408000	4.43210000	-0.71946900
O	-2.76027900	1.49915100	-0.13324600
C	-4.43300600	-1.76765600	-3.29387800
C	-5.68056600	-1.91858300	-2.69863500
C	-5.80424700	-1.81447900	-1.31465900
C	-4.68245300	-1.56237300	-0.53390700
C	-3.42294000	-1.41288200	-1.12757600
P	-1.94473700	-1.17503600	-0.06666300
C	-2.66321200	-0.27234400	1.36276300
P	0.22473000	1.80503000	0.00375300
C	1.80426600	2.65519000	-0.37735700
C	0.13733700	1.90426500	1.83851900
C	-1.67694000	-2.85059500	0.63936700
H	-4.39530500	3.40082300	-0.71967200
H	-3.75492400	5.75870200	-1.26628400
H	-1.35053400	6.39959200	-1.24694000
H	0.36808200	4.73036300	-0.73151900
H	-4.78906600	-1.48555200	0.54405700
H	-6.77513000	-1.92862800	-0.84135100
H	-6.55721800	-2.11233300	-3.31021700
H	-4.32885800	-1.83403400	-4.37242200
C	-2.92341000	-0.81077600	2.62344700
C	-3.37240500	0.00037400	3.66158000
C	-3.56223700	1.36210000	3.44597000
C	-3.35292400	1.91430700	2.18688300
H	-2.75675600	-1.86719000	2.80328000
H	-3.55867000	-0.42958200	4.64055600
H	-3.88582600	2.00323500	4.26024100
H	-3.50900400	2.97197900	2.00492800
C	-0.76767500	-3.02626200	1.68768800
C	-0.48817000	-4.29263800	2.18912300
C	-1.11259600	-5.40929900	1.64225300
C	-2.01747600	-5.24824700	0.59663100
C	-2.29654800	-3.97992600	0.09678800
H	-0.26178900	-2.17067100	2.12023100
H	0.22860300	-4.40233400	2.99714600
H	-0.89318800	-6.40108800	2.02681700
H	-2.50689800	-6.11397200	0.16059200
H	-2.99009900	-3.87349700	-0.73015200
C	0.09341800	0.75045000	2.61378600
C	-0.00047500	0.82543100	3.99935400
C	-0.04075200	2.06545000	4.62628900
C	0.00824700	3.22944900	3.86152000
C	0.09121700	3.14970900	2.47686900
H	0.12408100	-0.21051400	2.12164300
H	-0.05255000	-0.08790000	4.58421800
H	-0.11535500	2.12768500	5.70812500
H	-0.02467600	4.20194700	4.34380300
H	0.11574600	4.06330200	1.89041000
C	2.79908900	2.83335500	0.58396000
C	3.99076800	3.47466500	0.24693200
C	4.20269600	3.92658100	-1.05179800
C	3.21884700	3.73315400	-2.02090400
C	2.02789900	3.09983900	-1.68693800
H	2.65562900	2.45933500	1.59112200
H	4.75612000	3.61282100	1.00517800
H	5.13189700	4.42538100	-1.31154400
H	3.37782900	4.07780600	-3.03823700
H	1.25573700	2.95906200	-2.44039000
C	-3.30666100	-1.51501200	-2.51445100
H	-2.34707900	-1.36593500	-2.99208600
C	-2.92862700	1.08439600	1.15626100
H	1.57819100	-3.67204600	-0.60876900

Zero-point correction = 0.763394
Thermal correction to Energy = 0.814711
Thermal correction to Enthalpy = 0.815655
Thermal correction to Gibbs Free Energy = 0.677517
Sum of electronic and zero-point Energies = -3767.132008
Sum of electronic and thermal Energies = -3767.080691
Sum of electronic and thermal Enthalpies = -3767.079747
Sum of electronic and thermal Free Energies = -3767.217885
E(RM06) = -3767.90954354

INT5h



C	-1.92448500	1.51427900	1.71753200
C	-1.11399800	0.45911600	1.64927700
S	-2.29125500	2.03947700	0.02999800
C	-0.87422900	-0.39572300	2.83294200
O	-1.19637200	-1.56176800	2.90281900
O	-0.26018400	0.25885500	3.83943400
C	0.02072800	-0.51216700	5.01924500
C	-1.19232900	-0.59411400	5.92775100
H	0.84401200	0.02158000	5.49994800
H	0.36289000	-1.50548000	4.71764300
H	-0.92967900	-1.11809200	6.85276500
H	-1.54873200	0.40762600	6.18675400
H	-1.99930200	-1.14304900	5.43638100
Cl	-0.65170600	0.02403400	-2.78471800
Rh	-0.67833400	0.21151600	-0.32657100
C	1.37960400	-2.41332500	-1.71397100
C	2.37035000	-1.55492500	-2.19730100
C	3.21937100	-1.91528300	-3.23484400
C	3.12041700	-3.18420400	-3.79316300
C	2.17183300	-4.07553900	-3.30498700
C	1.31203900	-3.69045300	-2.28062000
O	2.47688100	-0.29069100	-1.67292800
C	0.71401500	3.85066900	-3.75281400
C	2.00055000	4.23568300	-4.11831600

C	3.08737400	3.84952900	-3.33810300
C	2.88683400	3.08367600	-2.19418500
C	1.59794300	2.68819200	-1.82613900
P	1.29350700	1.76371900	-0.27527300
C	2.94221600	1.07583400	0.13381200
P	0.28148600	-1.89928600	-0.31351100
C	-1.01128600	-3.19042200	-0.35564500
C	1.38445000	-2.35771700	1.08446500
C	1.09485500	3.12237500	0.94777800
H	3.94137700	-1.18859700	-3.59246200
H	3.78107900	-3.47187600	-4.60500600
H	2.08777100	-5.07207500	-3.72687100
H	0.56885700	-4.39677100	-1.92900700
H	3.73920600	2.79551200	-1.58604300
H	4.09405400	4.14652200	-3.61753800
H	2.15710200	4.83296500	-5.01198400
H	-0.13753700	4.13821800	-4.36165200
C	3.77898200	1.47993800	1.17285600
C	4.93243200	0.75783900	1.47235000
C	5.25454500	-0.37507700	0.73090200
C	4.45431500	-0.77882700	-0.33396300
H	3.52011400	2.35217200	1.76405100
H	5.57309100	1.07755200	2.28811000
H	6.14186700	-0.95119300	0.97509800
H	4.70244300	-1.65750000	-0.91888400
C	1.03515300	2.80820500	2.31105200
C	0.83587300	3.79974200	3.26363200
C	0.67381500	5.12525700	2.86751200
C	0.71811100	5.44828300	1.51543700
C	0.93096100	4.45571300	0.56077500
H	1.12760000	1.77966000	2.64184600
H	0.79028900	3.52958800	4.31443400
H	0.50912300	5.90121400	3.60942800
H	0.59031500	6.47818100	1.19565100
H	0.96797900	4.72769000	-0.48860000
C	1.85050000	-1.38799400	1.96834400
C	2.76073300	-1.71197900	2.96937500
C	3.20918400	-3.02138200	3.10111600
C	2.74976500	-4.00150600	2.22281200
C	1.85027400	-3.67094000	1.21638700
H	1.51334000	-0.36535700	1.86499300
H	3.12230100	-0.93379500	3.63441200
H	3.91941400	-3.28000400	3.88104400
H	3.09805800	-5.02561800	2.31788200
H	1.50994600	-4.44056400	0.52964900
C	-1.39280800	-3.89317500	0.78736000
C	-2.44972000	-4.79935600	0.72716500
C	-3.13277100	-5.00478600	-0.46662800
C	-2.76710800	-4.29035500	-1.60667200
C	-1.71774400	-3.38078300	-1.55220700
H	-0.88902900	-3.71663900	1.73034800
H	-2.74165500	-5.33894900	1.62297200
H	-3.95617400	-5.71178600	-0.50845500
H	-3.30600100	-4.43204000	-2.53864500
H	-1.45623300	-2.79579700	-2.43104400
C	0.51164300	3.07559200	-2.61501700
H	-0.49051900	2.75649100	-2.35329000
C	3.31739400	-0.03684500	-0.62844500
C	-5.53424000	-0.08175800	-1.40996400
C	-6.91143800	0.03704600	-1.54818200
C	-7.59969300	1.05477600	-0.89012000
C	-6.89661100	1.95208000	-0.09139000
C	-5.51864500	1.82917900	0.05508000
C	-4.81983400	0.80798700	-0.59621300
H	-4.99598800	-0.85894000	-1.94457700
H	-7.44909700	-0.66051000	-2.18409300
H	-8.67515900	1.15161100	-1.00574100
H	-7.42233900	2.75107500	0.42358400
H	-4.98037000	2.53213300	0.68567400
C	-3.36932800	0.63517200	-0.43330300
C	-2.58066400	-0.43263500	-0.53014300
H	-2.93377900	-1.43495300	-0.75273500
H	-2.42999900	1.97435900	2.56134100

Zero-point correction = 0.766388
Thermal correction to Energy = 0.817634
Thermal correction to Enthalpy = 0.818578
Thermal correction to Gibbs Free Energy = 0.678871
Sum of electronic and zero-point Energies = -3767.159947
Sum of electronic and thermal Energies = -3767.108702
Sum of electronic and thermal Enthalpies = -3767.107758
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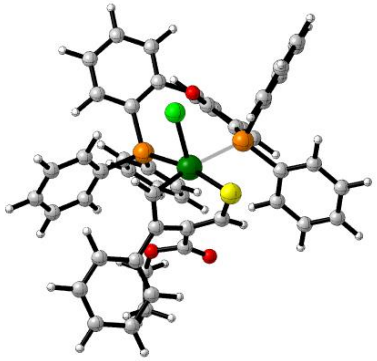
E(RM06) = -3767.93116789

INT6h



Rh	0.01099800	-0.45511100	-1.12484100
Cl	-0.80022100	0.89747500	-2.90735000
C	0.51574600	-2.59675800	-0.58855800
C	1.59913500	-1.80117300	-0.17892700
S	-0.09681300	-2.61606400	-2.19400000
C	1.92970000	-1.82650200	1.28084700
O	1.40822200	-2.55300500	2.10329100
O	2.88346400	-0.93807600	1.56907300
C	3.39005100	-0.93256900	2.91026900
C	4.46407600	-1.99272600	3.07335100
H	2.56172600	-1.07837800	3.60714000
H	3.79510700	0.07293100	3.04314500
H	4.91976700	-1.91394400	4.06587500
H	4.03131100	-2.99167400	2.97040900

H	5.24167000	-1.86763700	2.31410200
C	4.43101700	-2.79292200	-0.64264900
C	5.78504300	-3.11307700	-0.63997900
C	6.71206300	-2.23863700	-1.20174700
C	6.27271200	-1.04273000	-1.76744000
C	4.92134700	-0.72048600	-1.76404400
C	3.98203700	-1.59236400	-1.20336900
H	3.71366100	-3.48864200	-0.21283100
H	6.11558100	-4.05093100	-0.20242700
H	7.76938900	-2.48706500	-1.19898600
H	6.98886800	-0.35157200	-2.20335100
H	4.58280700	0.22599400	-2.17419000
C	2.55731600	-1.22840900	-1.17568000
C	1.83363800	-0.44999200	-1.97478900
H	2.10953000	0.06639000	-2.88765400
C	-0.37479600	3.11831500	-0.40335500
C	-1.77126300	3.08402000	-0.39941100
C	-2.54018100	4.20126300	-0.69393300
C	-1.91165200	5.41082900	-0.96645400
C	-0.52347400	5.48564800	-0.93825400
C	0.23393000	4.35040800	-0.66368700
O	-2.40714400	1.89602800	-0.14425300
C	-4.60113100	-0.91562400	-3.51579600
C	-5.85653900	-0.50265600	-3.08044800
C	-6.05201300	-0.17479200	-1.74088900
C	-4.99506600	-0.26225400	-0.84116900
C	-3.72976200	-0.67073100	-1.27415700
P	-2.34032700	-0.86853700	-0.09577900
C	-2.86285400	0.16798600	1.32762800
P	0.57942300	1.58320100	-0.01571900
C	2.28323300	2.11133700	-0.43456200
C	0.52987400	1.61525300	1.81778400
C	-2.62294000	-2.56668700	0.55680800
H	-3.62031900	4.10100900	-0.70895900
H	-2.50567200	6.28925300	-1.19841600
H	-0.02159200	6.42640900	-1.14113500
H	1.31472700	4.42991900	-0.66352900
H	-5.15808800	-0.01280000	0.20323100
H	-7.02955700	0.14729100	-1.39381300
H	-6.68175800	-0.43400900	-3.78349000
H	-4.43863100	-1.16586400	-4.55964800
C	-3.28081800	-0.28415800	2.57891900
C	-3.48762500	0.61227000	3.62470500
C	-3.27759200	1.97291100	3.42473000
C	-2.90342900	2.45517000	2.17400800
H	-3.42759700	-1.34549400	2.74695100
H	-3.80187300	0.24442200	4.59624500
H	-3.41442600	2.67235000	4.24382500
H	-2.74889200	3.51535200	2.00678900
C	-1.86802800	-3.01149700	1.65101900
C	-2.02360700	-4.29970600	2.14940100
C	-2.93371800	-5.17088400	1.55452100
C	-3.68202100	-4.74306400	0.46330400
C	-3.53051300	-3.44960700	-0.03252400
H	-1.13343800	-2.35969700	2.11540000
H	-1.42053100	-4.62280700	2.99230400
H	-3.05250100	-6.18038000	1.93682000
H	-4.38841400	-5.41738300	-0.01153000
H	-4.12044700	-3.13347800	-0.88599200
C	0.15468500	0.47413400	2.52093400
C	0.07431100	0.48796300	3.91025500
C	0.37365900	1.65215700	4.60866300
C	0.74883400	2.80214800	3.91458500
C	0.82177600	2.78655200	2.52724600
H	-0.09129900	-0.42904200	1.97658100
H	-0.23009300	-0.41097200	4.43694100
H	0.30944900	1.66908700	5.69266800
H	0.97898300	3.71488600	4.45606000
H	1.10279300	3.68972200	1.99294300
C	3.32921500	2.07285100	0.48539300
C	4.61379700	2.45782500	0.10625200
C	4.86026800	2.89068700	-1.19118300
C	3.82091400	2.91871700	-2.12123500
C	2.54274900	2.52011100	-1.75020700
H	3.14671300	1.74213800	1.50121800
H	5.42147000	2.41669100	0.83060800
H	5.86084500	3.19534900	-1.48337600
H	4.00698800	3.24399700	-3.14038300
H	1.73614300	2.52802300	-2.47994700
C	-3.53920400	-0.99599700	-2.61932800
H	-2.56036900	-1.30183200	-2.96898800
C	-2.72166600	1.54639400	1.13923600
H	-0.01435400	-3.14087400	0.18728800

Zero-point correction = 0.768240
Thermal correction to Energy = 0.819118
Thermal correction to Enthalpy = 0.820062
Thermal correction to Gibbs Free Energy = 0.682589
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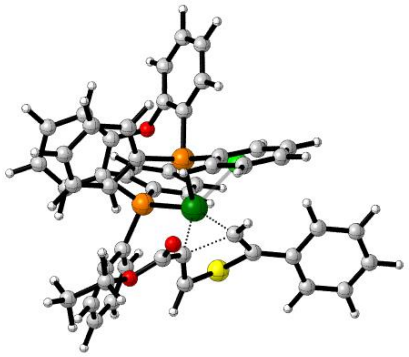
Sum of electronic and thermal Energies = -3767.145230
Sum of electronic and thermal Enthalpies = -3767.144286
Sum of electronic and thermal Free Energies = -3767.281759
E(RM06) = -3767.97117374

TS5h



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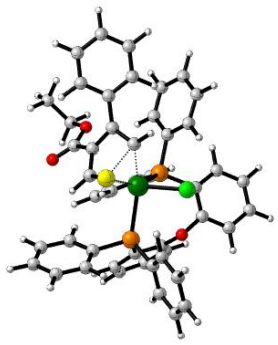
S	1.86197000	-2.48423400	0.93910900
C	0.37538100	0.47300300	3.10011600

O	0.78749700	1.60351100	3.23777900
O	-0.58939500	-0.05113600	3.88288500
C	-1.14286300	0.82619100	4.87186300
C	-2.34891900	0.12396800	5.45968900
H	-1.41411600	1.77238900	4.39465100
H	-0.38113800	1.03609900	5.62939300
H	-2.81722900	0.75504700	6.22137200
H	-3.08988200	-0.08509000	4.68056400
H	-2.06105600	-0.82384700	5.92478000
Rh	0.69157500	-0.35462500	0.02916900
C	5.13796000	-0.43206600	-0.37966000
C	6.45229500	-0.65013600	-0.77289200
C	7.08997100	-1.84633000	-0.45050700
C	6.40795000	-2.82346300	0.27149500
C	5.09804100	-2.60181900	0.67952500
C	4.45053300	-1.39988900	0.36600800
H	4.61648100	0.47597800	-0.66394100
H	6.97420200	0.10646200	-1.35129800
H	8.11350800	-2.02103600	-0.76921400
H	6.90023500	-3.75838400	0.52252500
H	4.57454100	-3.35996600	1.25527200
C	3.08782100	-1.11719200	0.81140500
C	2.44922800	0.03953200	1.05211500
H	2.92991600	1.00050300	1.19053700
C	-0.29706000	2.40658600	-2.00328100
C	-1.22285700	1.70466200	-2.77976700
C	-1.59010500	2.12567900	-4.05003800
C	-1.05300100	3.29921900	-4.56670200
C	-0.15352300	4.03519900	-3.80452500
C	0.22071800	3.58960500	-2.53992500
O	-1.74242700	0.52410200	-2.31070300
C	-0.24305500	-3.86848800	-3.71204600
C	-1.44990500	-4.20327500	-4.31777000
C	-2.64687500	-3.71092600	-3.80078600
C	-2.63408500	-2.89002400	-2.67871700
C	-1.42310700	-2.54958400	-2.06690600
P	-1.38128800	-1.54802000	-0.53510000
C	-2.92344100	-0.56355600	-0.64297900
P	0.15200300	1.83451000	-0.30266700
C	1.57943000	2.91222300	0.08235700
C	-1.25703000	2.53847900	0.64294700
C	-1.78401300	-2.79268500	0.75285100
H	-2.28551300	1.51673800	-4.61812100
H	-1.33528200	3.63230600	-5.56054900
H	0.27229200	4.95420900	-4.19468400
H	0.93825800	4.17018400	-1.97178400
H	-3.57039300	-2.51370100	-2.27599300
H	-3.59176300	-3.96716800	-4.27132600
H	-1.45973400	-4.84288500	-5.19576500
H	0.69415000	-4.23665300	-4.11796100
C	-4.07454100	-0.72297800	0.12707300
C	-5.10780000	0.20861100	0.05349600
C	-4.99280400	1.30930900	-0.79070900
C	-3.87056600	1.46980900	-1.59828000
H	-4.15618400	-1.56723900	0.80395400
H	-5.99596000	0.07939400	0.66404800
H	-5.78628500	2.04929800	-0.83178400
H	-3.77628700	2.31893800	-2.26644400
C	-2.03307800	-2.35943200	2.06094900
C	-2.27816300	-3.27050800	3.08153300
C	-2.24913600	-4.63731400	2.81654000
C	-1.97790200	-5.08165400	1.52587100
C	-1.74971800	-4.16724200	0.49975000
H	-2.01981700	-1.30150000	2.29850000
H	-2.47068400	-2.90766600	4.08703800
H	-2.43045600	-5.35281600	3.61337600
H	-1.94763200	-6.14566900	1.31055200
H	-1.54461900	-4.53016700	-0.50209400
C	-2.01207200	1.73253000	1.49070900
C	-3.12396200	2.24240600	2.15390500
C	-3.48537800	3.57381800	1.98127000
C	-2.73558100	4.39072700	1.13681200
C	-1.63313900	3.87515300	0.46601100
H	-1.73938700	0.69217800	1.61359800
H	-3.71261200	1.59077400	2.79277500
H	-4.35349100	3.97497100	2.49603800
H	-3.01472400	5.43039800	0.99433200
H	-1.06589700	4.51568200	-0.20320600
C	1.60192700	3.76400200	1.18528300
C	2.74950800	4.50209300	1.47213000
C	3.87459100	4.39266800	0.66317100
C	3.85850100	3.53377600	-0.43613100
C	2.72144400	2.78989400	-0.72389100
H	0.74149700	3.83609700	1.84003900
H	2.76085400	5.15654900	2.33832700
H	4.76718300	4.96795200	0.89123500
H	4.73743600	3.43525800	-1.06650800
H	2.71316500	2.09227000	-1.55931800
C	-0.22613400	-3.04120200	-2.59169500
H	0.71955500	-2.75189500	-2.14670300
C	-2.86136700	0.51811600	-1.52744900
Cl	1.65948200	-0.25230700	-2.30476900
H	0.82468200	-2.40407800	3.20647900

Zero-point correction = 0.764560
Thermal correction to Energy = 0.815549
Thermal correction to Enthalpy = 0.816493
Thermal correction to Gibbs Free Energy = 0.678070
Sum of electronic and zero-point Energies = -3767.128716
Sum of electronic and thermal Energies = -3767.077727
Sum of electronic and thermal Enthalpies = -3767.076783
Sum of electronic and thermal Free Energies = -3767.215206
E(RM06) = -3767.90722368

TS6h



Rh	-0.22758300	-0.46425800	-1.11604500
Cl	-0.91367900	0.96838200	-2.91809000
C	0.55786800	-2.43440600	-0.38189300
C	1.85065500	-1.91135100	-0.09028000
S	0.05372600	-2.55459100	-2.05934200
C	2.34325700	-2.06751200	1.31393900
O	1.91243300	-2.88989300	2.09489500
O	3.24722500	-1.13590300	1.62044000
C	3.80315200	-1.17508400	2.94146200
C	4.95017900	-2.16711100	3.00943000
H	3.01083900	-1.41747900	3.65365200
H	4.14392200	-0.15306000	3.11962800
H	5.43223300	-2.11501800	3.99104500
H	4.58289300	-3.18636400	2.86012300
H	5.69375400	-1.94136600	2.23916100
C	4.77861200	-2.31577600	-0.77692200
C	6.15063100	-2.34728400	-0.99065400
C	6.74730200	-1.43340600	-1.85732700
C	5.95338500	-0.49509500	-2.51045000
C	4.58302700	-0.45427500	-2.28252400
C	3.97111800	-1.35015400	-1.39886300
H	4.32627500	-3.06855000	-0.13707100
H	6.75325100	-3.10397900	-0.49592800
H	7.81884500	-1.46296800	-2.03162900
H	6.40271100	0.21861900	-3.19524400
H	3.98017800	0.30068200	-2.77342300
C	2.52177700	-1.29844200	-1.16286000
C	1.52886200	-0.82905700	-2.05299700
H	1.75028300	-0.46963000	-3.05724900
C	-0.34654000	3.09538700	-0.14358900
C	-1.74192400	3.15982200	-0.17639300
C	-2.42420800	4.34573400	-0.41358300
C	-1.70873400	5.52429700	-0.58752600
C	-0.31990900	5.50127600	-0.51620400
C	0.34909200	4.29973600	-0.30334900
O	-2.47937600	2.01465800	-0.00042900
C	-4.88048600	-0.60252000	-3.46269900
C	-6.11648700	-0.20561200	-2.96090000
C	-6.26380100	0.05125100	-1.59958100
C	-5.17808100	-0.09294700	-0.74228400
C	-3.93362700	-0.48644500	-1.24209400
P	-2.49946400	-0.76485700	-0.14201700
C	-2.91436500	0.18886100	1.37033700
P	0.50613400	1.46884400	0.09195300
C	2.20413100	1.93569600	-0.41571400
C	0.58971300	1.35844000	1.92378500
C	-2.75822700	-2.50589300	0.40320100
H	-3.50786500	4.32149200	-0.45843000
H	-2.23544300	6.45502600	-0.77403400
H	0.25025000	6.41656600	-0.64024500
H	1.43291200	4.30212300	-0.27743300
H	-5.29984700	0.10181400	0.31951500
H	-7.22617900	0.36225900	-1.20352600
H	-6.96462300	-0.09240800	-3.63010100
H	-4.75693400	-0.79455700	-4.52411700
C	-3.28456100	-0.33082200	2.61149000
C	-3.37375900	0.49288000	3.73042900
C	-3.09941100	1.85190300	3.61522200
C	-2.78376300	2.40540000	2.37877300
H	-3.48660400	-1.39116000	2.71368700
H	-3.64731200	0.06926400	4.69148600
H	-3.14397100	2.49413600	4.48948000
H	-2.58743300	3.46688300	2.27504100
C	-2.03664600	-3.00909000	1.49531800
C	-2.15348600	-4.33916000	1.88118300
C	-2.98845600	-5.19900000	1.17067900
C	-3.70340700	-4.71500000	0.08108900
C	-3.59230000	-3.37877000	-0.29934800
H	-1.37245500	-2.35752400	2.05656700
H	-1.58146300	-4.70366000	2.72902300
H	-3.07656800	-6.24062800	1.46448100
H	-4.35463100	-5.37731100	-0.48146700
H	-4.16033500	-3.02028200	-1.15118600
C	0.31786800	0.13579300	2.53576100
C	0.35808100	0.00583500	3.92106200
C	0.67077200	1.10785100	4.70976000
C	0.94154800	2.33701400	4.10942000
C	0.89868200	2.46297800	2.72581900
H	0.06429900	-0.71962000	1.91842800
H	0.14109700	-0.95583700	4.37607600
H	0.69920000	1.01369400	5.79142300
H	1.18236500	3.20080500	4.72215400
H	1.10081700	3.42661300	2.26670400
C	3.30286200	1.89341800	0.44032500
C	4.55564900	2.31285500	-0.00429500
C	4.71412900	2.79304400	-1.29869000
C	3.62237400	2.81940600	-2.16641600
C	2.37895100	2.37165000	-1.73769400
H	3.18478900	1.53769400	1.45771900
H	5.40692300	2.26675500	0.66809700
H	5.68859800	3.13109600	-1.63841100
H	3.74195800	3.17696100	-3.18507100
H	1.52947300	2.37716400	-2.41778400
C	-3.78908400	-0.73770200	-2.60903400
H	-2.82007000	-1.02031000	-3.00638300
C	-2.71647200	1.56956100	1.27018100
H	0.06004200	-3.04513200	0.35895200

Zero-point correction = 0.766606

Thermal correction to Energy = 0.817250
Thermal correction to Enthalpy = 0.818194
Thermal correction to Gibbs Free Energy = 0.679727
Sum of electronic and zero-point Energies = -3767.167774
Sum of electronic and thermal Energies = -3767.117130
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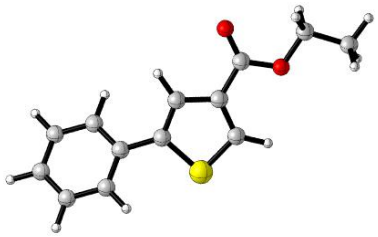
E(RM06) = -3767.94244112

3h



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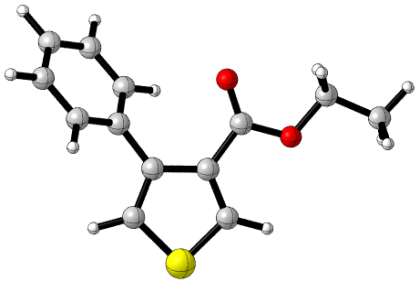
C	-1.17852200	1.35114500	-0.21454400
S	0.45261000	1.86852300	-0.30372200
C	-2.52505800	-0.76108300	0.12530300
O	-3.60753600	0.02428400	0.01149000
O	-2.57728000	-1.95668300	0.31033500
C	-4.87402500	-0.64006200	0.12275000
H	-4.92790100	-1.14081900	1.09421300
H	-4.94006900	-1.41035000	-0.65165700
C	-5.95143600	0.41215100	-0.03220900
H	-6.93835700	-0.05387200	0.04700300
H	-5.86544400	1.17419000	0.74780800
H	-5.87814200	0.90286600	-1.00708400
C	0.01280500	-0.62315500	0.09790900
H	0.13154500	-1.68219500	0.29195000
C	1.05201700	0.25208500	-0.03967600
C	2.49472700	-0.03549600	0.00010200
C	2.97289300	-1.26084600	-0.48004600
C	3.41050400	0.88754600	0.51794400
C	4.32931600	-1.55860900	-0.43118000
H	2.27569400	-1.97423200	-0.90924900
C	4.76856500	0.59237600	0.55455700
H	3.05594600	1.83594400	0.91272400
C	5.23274700	-0.63245200	0.08377200
H	4.68291700	-2.51369600	-0.80783200
H	5.46480300	1.31943000	0.96162800
H	6.29311900	-0.86350000	0.11590300
H	-1.99365200	2.05199600	-0.32494200

Zero-point correction = 0.222605
Thermal correction to Energy = 0.236982
Thermal correction to Enthalpy = 0.237926
Thermal correction to Gibbs Free Energy = 0.179230
Sum of electronic and zero-point Energies = -1050.804743
Sum of electronic and thermal Energies = -1050.790365
Sum of electronic and thermal Enthalpies = -1050.789421
Sum of electronic and thermal Free Energies = -1050.848118
E(RM06) = -1051.05113883

4h



C	-0.75012800	0.65979600	-0.03246000
C	-1.51835100	1.79226200	-0.09000800
S	-0.57128700	3.21376200	-0.16811100
C	-1.35514700	-0.68696500	0.11565100
O	-2.69799000	-0.63000700	0.04328500
O	-0.74806700	-1.71805200	0.29094200
C	-3.38185800	-1.87985600	0.20305600
H	-3.11439100	-2.31074600	1.17268600
H	-3.04156300	-2.57306200	-0.57228400
C	-4.86594400	-1.59890600	0.09859600
H	-5.42837400	-2.53044100	0.21430300
H	-5.18588300	-0.90319200	0.87981300
H	-5.11208400	-1.16524300	-0.87503300
C	0.66487900	0.94940000	-0.05563100
C	0.88586900	2.29636400	-0.12617500
H	1.84622900	2.78999300	-0.18712400
C	1.79532600	-0.01135300	-0.02789500
C	1.88289700	-1.06192600	-0.94572600
C	2.83543500	0.17445100	0.88647400
C	2.98632800	-1.90509200	-0.94745600
H	1.08024400	-1.21856600	-1.65832700
C	3.94090000	-0.67127100	0.88572800
H	2.76656100	0.97960000	1.61280400
C	4.01938200	-1.71289900	-0.03234300
H	3.04039300	-2.71705500	-1.66651300
H	4.73778400	-0.51722600	1.60737300
H	4.87971900	-2.37563900	-0.03408200
H	-2.59711700	1.84183100	-0.06851400

Zero-point correction = 0.222436
Thermal correction to Energy = 0.236779
Thermal correction to Enthalpy = 0.237723
Thermal correction to Gibbs Free Energy = 0.178970
Sum of electronic and zero-point Energies = -1050.799712
Sum of electronic and thermal Energies = -1050.785369
Sum of electronic and thermal Enthalpies = -1050.784425
Sum of electronic and thermal Free Energies = -1050.843178
E(RM06) = -1051.04535767

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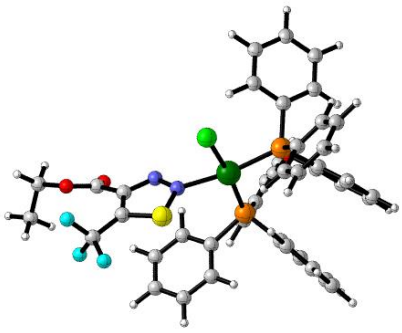

Cl	0.00902200	-3.19966700	-0.08583800
C	-4.11765000	-1.12645200	-0.71268100
C	-3.94482300	-0.88656000	0.62763700
S	-2.58857000	-1.17525200	-1.44705400
N	-1.83479100	-0.86819600	0.02102200
N	-2.64369800	-0.74519200	1.00080700
C	-4.99790400	-0.61644400	1.64971500
O	-4.86574500	0.19426500	2.53286400
O	-6.07857100	-1.35986600	1.42346500
C	-7.22960200	-1.09845300	2.24976100
C	-8.01527900	0.08599800	1.71817100
H	-6.89463600	-0.93257900	3.27599900
H	-7.80747800	-2.02221600	2.19960800
H	-8.92780400	0.21785300	2.30803200
H	-7.42466300	1.00328800	1.79115900
H	-8.29420300	-0.07581400	0.67360400
Rh	0.24938500	-0.81238500	0.04507000
P	2.50807300	-1.12499400	0.20436300
P	0.27608200	1.45625400	-0.16442000
C	3.06226800	-1.80149300	1.82360800
C	3.62197700	0.32425400	0.01549600
C	3.21449700	-2.27708500	-1.03943400
C	0.65636200	2.57861400	1.26297900
C	-1.38751100	2.07693600	-0.67993100
C	1.33568500	2.11605700	-1.51775200
C	4.34774200	-1.54677400	2.31564700
C	2.18822600	-2.58699000	2.58017400
C	4.55691500	0.47134300	-1.00991100
C	3.45799000	1.38348200	0.90980600
C	2.54467600	-2.45250800	-2.25282600
C	4.43198400	-2.93241900	-0.83465400
C	1.68956900	2.26627200	2.15800000
C	-0.09420600	3.72857800	1.53975500
C	-1.67117700	2.38930800	-2.01225000
C	-2.43671100	2.09372000	0.25012100
C	1.60207400	1.28130500	-2.60686200
C	1.81952400	3.42562400	-1.53271900
C	4.75559300	-2.07572300	3.53585400
H	5.03525500	-0.92371300	1.75040700
C	2.59967600	-3.11317400	3.80179900
H	1.19043300	-2.79334000	2.20772700
C	5.29943100	1.64185200	-1.13661500
H	4.69226400	-0.32990100	-1.72858700
O	2.52654100	1.20363500	1.91061200
C	4.20468600	2.55092300	0.81021700
C	3.09318500	-3.24824900	-3.25358400
H	1.57107400	-1.99302200	-2.39164900
C	4.97748600	-3.73354600	-1.83318300
H	4.95626400	-2.82430100	0.10985500
C	1.90591800	3.00067900	3.31794800
C	0.13154800	4.49111700	2.68180300
H	-0.88151000	4.02965300	0.85794800
C	-2.97329500	2.69143300	-2.40848100
H	-0.87826300	2.38958300	-2.75310600
C	-3.73465400	2.39625100	-0.14541900
H	-2.24686100	1.84686100	1.29062000
C	2.33358200	1.74621800	-3.69462300
H	1.23702400	0.25794300	-2.58567000
C	2.55909600	3.88898200	-2.61684400
H	1.62953600	4.08481600	-0.69076400
C	3.88094200	-2.86093200	4.28225600
H	5.75623700	-1.86911100	3.90460200
H	1.90996300	-3.72179900	4.37896600
C	5.12546900	2.67688300	-0.22408900
H	6.00880100	1.74409900	-1.95148600
H	4.05074200	3.35453500	1.52272900
C	4.31214100	-3.88774900	-3.04678000
H	2.55696600	-3.38391800	-4.18817800
H	5.92138800	-4.24193700	-1.65961900
C	1.11783400	4.11366400	3.58678700
H	2.70228000	2.68885800	3.98572400
H	-0.47464400	5.37228800	2.86664100
C	-4.00931200	2.68806300	-1.48039000
H	-3.17418200	2.92641000	-3.44960500
H	-4.52992100	2.38501400	0.59423600
C	2.81487600	3.05256400	-3.69999100
H	2.53639200	1.08323400	-4.53049200
H	2.93866100	4.90658000	-2.61281400
H	4.19720600	-3.27159000	5.23693900
H	5.70366900	3.59125300	-0.31711200
H	4.73726700	-4.51578500	-3.82442800
H	1.28587600	4.69022100	4.49117100
H	-5.02496400	2.91210500	-1.79261000
H	3.39334900	3.41693100	-4.54398900
C	-5.39065000	-1.24277700	-1.50279100
F	-6.03761300	-2.38041800	-1.25939700
F	-6.21600100	-0.22293700	-1.23199200
F	-5.11414700	-1.20364700	-2.81791200

Zero-point correction = 0.667906
Thermal correction to Energy = 0.717577
Thermal correction to Enthalpy = 0.718521
Thermal correction to Gibbs Free Energy = 0.579565
Sum of electronic and zero-point Energies = -3905.333273
Sum of electronic and thermal Energies = -3905.283601
Sum of electronic and thermal Enthalpies = -3905.282657
Sum of electronic and thermal Free Energies = -3905.421613
E(RM06) = -3906.19378845

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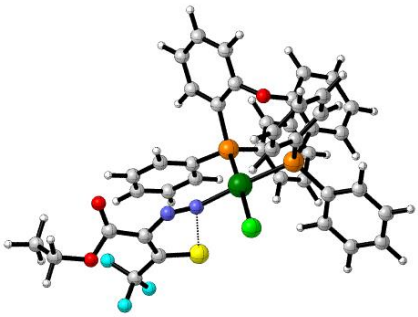

Cl	-0.19865200	-3.23614900	-0.30170400
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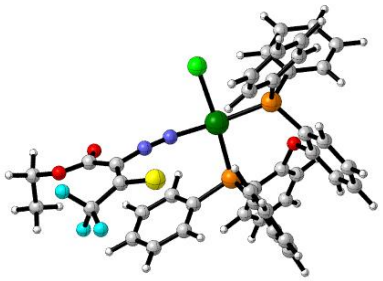
C	3.95142600	-1.08922800	-0.49390300
S	2.78243900	-1.04948600	1.92265200
N	1.63382800	-0.94086400	-0.38701100
N	2.66635800	-1.01531100	-0.91401400
C	4.94004700	-0.99238800	-1.59254300
O	4.70057200	-0.42824700	-2.63857700
O	6.08357200	-1.60847200	-1.30094000
C	7.16121700	-1.44652200	-2.23742300
C	7.87721000	-0.12580400	-2.01913000
H	6.76290000	-1.52404100	-3.25152300
H	7.81658600	-2.29570800	-2.03762400
H	8.74138300	-0.05835900	-2.68781200
H	7.20918200	0.71225500	-2.23629500
H	8.22483400	-0.04414400	-0.98606600
Rh	-0.27218800	-0.85331100	-0.19173500
P	-2.60608900	-1.10483000	-0.17912100
P	-0.20872900	1.44515500	0.07944400
C	-3.33579700	-1.66987700	-1.76556000
C	-3.63119400	0.36485800	0.20669100
C	-3.18057500	-2.29654100	1.08797100
C	-0.73215900	2.59877700	-1.27222200
C	1.50420900	2.03600600	0.40111300
C	-1.11222200	2.03071200	1.56390700
C	-4.66948100	-1.38127300	-2.07876700
C	-2.56015800	-2.39080100	-2.67686900
C	-4.45299100	0.48613700	1.32750200
C	-3.52551600	1.45644300	-0.65587100
C	-2.39308600	-2.51303600	2.22187700
C	-4.41669600	-2.93968700	0.98213800
C	-1.86909500	2.34233100	-2.05089100
C	0.01979600	3.73402600	-1.60299000
C	1.91410400	2.48143600	1.65827500
C	2.45226400	1.94059600	-0.62682000
C	-1.20212400	1.16093800	2.65529700
C	-1.64643500	3.31573400	1.66938100
C	-5.22196500	-1.81858500	-3.27777200
H	-5.28035200	-0.80333400	-1.39090600
C	-3.11710600	-2.82321300	-3.87734000
H	-1.52765400	-2.62356800	-2.44059700
C	-5.15034500	1.66608000	1.57115800
H	-4.53798000	-0.34265700	2.02224100
O	-2.69661400	1.28789800	-1.74375900
C	-4.23110300	2.63314400	-0.44000800
C	-2.84415800	-3.34139100	3.24402600
H	-1.40728300	-2.06310300	2.28538600
C	-4.86379300	-3.77348900	2.00262100
H	-5.03145600	-2.79949700	0.09849400
C	-2.19706400	3.12028600	-3.15456900
C	-0.31487900	4.53934200	-2.68721400
H	0.89266100	3.98734500	-1.01252100
C	3.25095400	2.80164400	1.88928300
H	1.20016800	2.56374900	2.47078100
C	3.78384800	2.25879100	-0.39464400
H	2.15417800	1.60258600	-1.61622400
C	-1.81875800	1.56782100	3.83318600
H	-0.78330900	0.16139500	2.57459400
C	-2.27042100	3.71978000	2.84597000
H	-1.58598400	4.00054600	0.82864000
C	-4.44548600	-2.54104800	-4.18012100
H	-6.25825200	-1.58922300	-3.50806700
H	-2.50432800	-3.38330100	-4.57711100
C	-5.04414400	2.73230000	0.68416500
H	-5.77402700	1.75004400	2.45509500
H	-4.12895200	3.46248800	-1.13196800
C	-4.08130500	-3.97077300	3.13728200
H	-2.21758500	-3.51068500	4.11438500
H	-5.82258500	-4.27415300	1.90655800
C	-1.41237500	4.22054600	-3.47964600
H	-3.07311600	2.85062400	-3.73515200
H	0.29406100	5.40775000	-2.91703900
C	4.18874300	2.68186500	0.87055600
H	3.55812800	3.13083500	2.87714200
H	4.50439100	2.14877500	-1.19918700
C	-2.35696700	2.84858800	3.92824900
H	-1.88318200	0.88184300	4.67230400
H	-2.69248800	4.71797100	2.91485600
H	-4.87520700	-2.87990500	-5.11835500
H	-5.59092600	3.65212200	0.86824700
H	-4.42965100	-4.62494200	3.93115200
H	-1.66674100	4.83132800	-4.34023000
H	5.23325700	2.90801000	1.05997900
H	-2.84528500	3.16702200	4.84452200
C	5.50018900	-0.94107600	1.50276700
F	6.17216800	-2.08892500	1.39242100
F	5.47580500	-0.61365200	2.79392400
F	6.19932800	0.02454100	0.87404400

Zero-point correction = 0.665600 (Hartree/Particle)
Thermal correction to Energy = 0.715447
Thermal correction to Enthalpy = 0.716391
Thermal correction to Gibbs Free Energy = 0.577038
Sum of electronic and zero-point Energies = -3905.300417
Sum of electronic and thermal Energies = -3905.250570
Sum of electronic and thermal Enthalpies = -3905.249626
Sum of electronic and thermal Free Energies = -3905.388979
E(RM06) = -3906.16542395

INT2l



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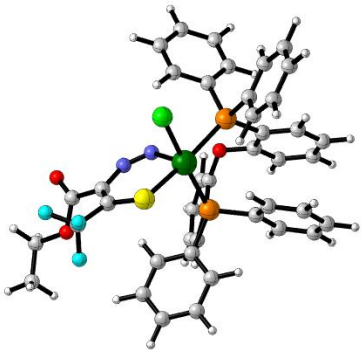
S	2.83865100	-1.66189000	1.93397700
N	1.44350700	-0.87846800	-1.03671100
N	2.55396500	-1.00397300	-0.89585900
C	4.73266200	-0.87131300	-1.68850500
O	4.31610200	-0.44957100	-2.74762600
O	5.99888800	-1.18862600	-1.44090500
C	6.96140400	-0.82630600	-2.44285600
C	7.33053700	0.64157800	-2.32267900
H	6.55487200	-1.05988300	-3.42922400
H	7.81534900	-1.47344700	-2.23721500
H	8.13158100	0.88520400	-3.02786000
H	6.46607200	1.27095400	-2.55265400
H	7.67461300	0.86446200	-1.30869200
Rh	-0.47022400	-0.66042800	-0.92662700
P	-2.69790100	-0.98850300	-0.32020000
P	-0.15396600	1.39435000	0.09195300
C	-3.95610600	-0.95809300	-1.65576600
C	-3.40700800	0.17560700	0.90172100
C	-2.90520300	-2.59632900	0.53206200
C	-0.96970700	2.91601600	-0.57801100
C	1.61945900	1.88150600	-0.00617500
C	-0.47778800	1.45876600	1.89388100
C	-5.29065700	-0.64716100	-1.36893100
C	-3.58688000	-1.23683600	-2.97401000
C	-3.79012300	-0.17102100	2.19695200
C	-3.48279100	1.51667800	0.52531100
C	-1.80996000	-3.15829000	1.19471800
C	-4.14569500	-3.23649300	0.59574300
C	-2.31930000	2.91664700	-0.95629600
C	-0.25689400	4.10780800	-0.76506200
C	2.43490200	1.97248200	1.12301000
C	2.18590400	2.07646000	-1.27347900
C	-0.36304400	0.27186900	2.62225800
C	-0.73631500	2.65463300	2.56799700
C	-6.24298000	-0.62938000	-2.38223400
H	-5.58959800	-0.40723000	-0.35232200
C	-4.54344800	-1.21394700	-3.98547000
H	-2.55665500	-1.48549000	-3.20480300
C	-4.22901600	0.80357500	3.08903600
H	-3.72583700	-1.20616400	2.51571100
O	-3.09604700	1.79880100	-0.76663200
C	-3.93566500	2.49909800	1.39504400
C	-1.95865400	-4.33153200	1.92673400
H	-0.83154000	-2.69482400	1.10683000
C	-4.29047500	-4.41391600	1.32336600
H	-5.00134100	-2.82427700	0.07004600
C	-2.91537900	4.01960500	-1.55544900
C	-0.84905500	5.22787000	-1.34047000
H	0.78409600	4.15999400	-0.46748600
C	3.79369000	2.25359900	0.98635500
H	2.02270500	1.80809300	2.11262200
C	3.53686800	2.37000900	-1.40614500
H	1.56935700	1.97978200	-2.16407200
C	-0.49828100	0.28041300	4.00672500
H	-0.16010800	-0.65770600	2.09826000
C	-0.87934900	2.66048200	3.95162500
H	-0.83137200	3.58313100	2.01227800
C	-5.87018500	-0.91294100	-3.69371400
H	-7.27538600	-0.38842600	-2.14645300
H	-4.24483300	-1.43359800	-5.00599800
C	-4.30328200	2.13286500	2.68594300
H	-4.50619200	0.52305500	4.09983700
H	-3.97862000	3.53397800	1.07184900
C	-3.19925500	-4.95981400	1.99411200
H	-1.09792600	-4.76325600	2.42818600
H	-5.25689800	-4.90778500	1.35998300
C	-2.17587500	5.17953900	-1.75441200
H	-3.95683200	3.94719900	-1.85083500
H	-0.26531600	6.13300000	-1.47384700
C	4.34550100	2.45482600	-0.27341100
H	4.42216600	2.29643300	1.87013300
H	3.96147700	2.49999300	-2.39599800
C	-0.75790500	1.47487700	4.67240300
H	-0.40150900	-0.64762000	4.56157500
H	-1.08563300	3.59360500	4.46746900
H	-6.61282800	-0.89592000	-4.48615100
H	-4.64390500	2.89488200	3.38020600
H	-3.31310400	-5.88077000	2.55837800
H	-2.63922100	6.04314200	-2.22112800
H	5.40688700	2.65913300	-0.37588200
H	-0.86638900	1.48287600	5.75298300
C	5.48876900	-1.20627200	1.40010000
F	6.05781300	-0.06326500	0.97266100
F	6.24749500	-2.23498600	1.00968100
F	5.52167100	-1.17148600	2.72959400

Zero-point correction = 0.665649
Thermal correction to Energy = 0.716438
Thermal correction to Enthalpy = 0.717382
Thermal correction to Gibbs Free Energy = 0.575504
Sum of electronic and zero-point Energies = -3905.306642
Sum of electronic and thermal Energies = -3905.255853
Sum of electronic and thermal Enthalpies = -3905.254908
Sum of electronic and thermal Free Energies = -3905.396787
E(RM06) = -3906.17159524

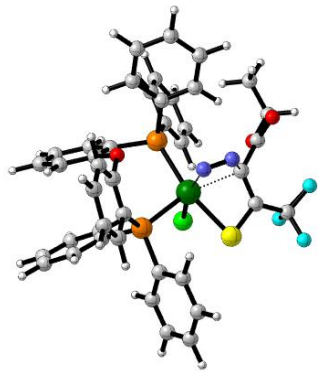
INT3l



Cl	0.51521900	-2.83109300	-1.80433200
C	-3.09377800	-1.25300100	-0.95793600
C	-3.00512200	-1.53132000	0.40494700
S	-1.86438100	-0.76839700	-1.98916100
N	-0.66555700	-1.41422700	0.94525200
N	-1.82196700	-1.63399000	1.09481600
C	-4.16876600	-1.77100900	1.30818000
O	-4.22053900	-2.60673800	2.17622600
O	-5.13795300	-0.87201600	1.07022900
C	-6.39033200	-1.10838200	1.72385900
C	-7.37396300	-0.09841600	1.17129000
H	-6.25418200	-1.00702600	2.80482100
H	-6.70354700	-2.13662200	1.51913400
H	-8.36059200	-0.25171600	1.61920000
H	-7.04870200	0.92269300	1.39449100
H	-7.45857700	-0.20727400	0.08662900
Rh	0.13554100	-0.70338600	-0.77959200
P	2.39718700	-0.94310900	-0.02043900
P	-0.18926900	1.52176800	-0.07615300
C	2.66948300	-2.21723600	1.27295200
C	3.22301500	0.51831500	0.71592500
C	3.56432500	-1.37213500	-1.36662800
C	-0.34879800	1.88078900	1.73201200
C	-1.70411600	2.32158300	-0.74092500
C	1.13597900	2.62447900	-0.69111900
C	3.70010800	-2.07905800	2.21077000
C	1.84877800	-3.34716900	1.32415900
C	4.37271800	1.13109700	0.21767100
C	2.62042300	1.06635600	1.84801400
C	3.26260500	-1.00832500	-2.68114800
C	4.78589100	-1.99591000	-1.09767400
C	0.44393200	1.22148700	2.68345700
C	-1.32083700	2.76435900	2.22198000
C	-1.64616300	3.30303800	-1.73144900
C	-2.95616700	1.89962400	-0.27654700
C	1.70984200	2.32240900	-1.92966100
C	1.54476000	3.77129500	-0.01010900
C	3.90802800	-3.05541800	3.17939200
H	4.34432300	-1.20490500	2.19312100
C	2.05936300	-4.31974500	2.29712500
H	1.05373200	-3.47291100	0.59881100
C	4.90594300	2.25307700	0.84653900
H	4.85009600	0.73416000	-0.67186600
O	1.48618000	0.42039500	2.28682000
C	3.14976800	2.17202800	2.50108000
C	4.17303600	-1.24183800	-3.70618100
H	2.29492100	-0.57544200	-2.91339800
C	5.69457600	-2.23517600	-2.12419700
H	5.02847600	-2.30262000	-0.08486800
C	0.21437500	1.34933400	4.04781500
C	-1.53548000	2.92899000	3.58639100
H	-1.93481500	3.32387600	1.52676400
C	-2.81984100	3.85170500	-2.24647300
H	-0.68951800	3.64912800	-2.10786500
C	-4.12299400	2.45348500	-0.78308800
H	-3.02906300	1.13322600	0.48936500
C	2.68519400	3.14779200	-2.47717700
H	1.38661300	1.43554200	-2.46870700
C	2.52582300	4.59422500	-0.55520600
H	1.10803800	4.01551900	0.95363800
C	3.08553100	-4.17772200	3.22567500
H	4.71157000	-2.93489800	3.90011400
H	1.41118000	-5.19009700	2.32705600
C	4.30039200	2.76396300	1.99007500
H	5.79476000	2.72558800	0.44125000
H	2.66016900	2.56905900	3.38408800
C	5.39238900	-1.85350300	-3.42858100
H	3.91937900	-0.96466700	-4.72484000
H	6.63750900	-2.72650200	-1.90370700
C	-0.78614300	2.19923800	4.50283700
H	0.83897500	0.78277800	4.73029800
H	-2.30141500	3.61781500	3.92770700
C	-4.05731500	3.43130000	-1.77381500
H	-2.75949500	4.61268500	-3.01863300
H	-5.08064100	2.10123300	-0.41558500
C	3.09685400	4.28468700	-1.78640200
H	3.12648500	2.89783500	-3.43706900
H	2.84832000	5.47719400	-0.01179800
H	3.24395300	-4.93810500	3.98492500
H	4.71954600	3.63335200	2.48761000
H	6.10044400	-2.04473200	-4.22951900
H	-0.96657300	2.30127400	5.56832200
H	-4.96970800	3.85937500	-2.17795100
H	3.86433800	4.92792100	-2.20639100
C	-4.45144300	-1.43626500	-1.65733300
F	-5.17156200	-2.42663700	-1.10519100
F	-4.29276100	-1.75339000	-2.94442600
F	-5.19043500	-0.31787100	-1.61972500

Zero-point correction = 0.666203
Thermal correction to Energy = 0.716172
Thermal correction to Enthalpy = 0.717116
Thermal correction to Gibbs Free Energy = 0.578725
Sum of electronic and zero-point Energies = -3905.324724
Sum of electronic and thermal Energies = -3905.274755
Sum of electronic and thermal Enthalpies = -3905.273811
Sum of electronic and thermal Free Energies = -3905.412201
E(RM06) = -3906.18561540

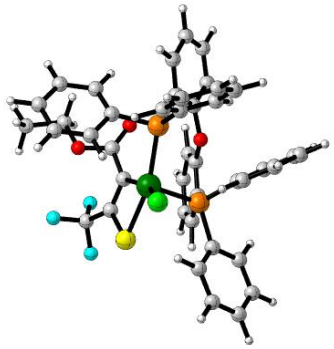
TS2l



Cl	-0.18288600	1.33850800	-2.29400400
C	-1.52472900	2.95748100	0.44194400
C	-1.96427300	1.73120400	0.94625000
S	0.14464900	3.17446500	0.37016400
N	-0.24823000	0.73145700	2.11501600
N	-1.28931500	1.27976400	2.33126200
C	-3.41934600	1.38046400	0.96529800
O	-4.06100700	1.23995200	1.98165900
O	-3.90582900	1.24008200	-0.26501300
C	-5.31688400	0.97460800	-0.37390200
C	-5.67078700	-0.45368500	0.00028100
H	-5.53393300	1.17489600	-1.42432800
H	-5.85082000	1.69567200	0.25112000
H	-6.73734300	-0.61885400	-0.18694700
H	-5.10199700	-1.16595000	-0.60165600
H	-5.47255700	-0.63942900	1.05780600
Rh	-0.13525600	0.81783600	0.14484200
P	-0.98771400	-1.42993300	-0.11230800
P	2.24957700	0.43574400	0.03968400
C	-1.62974900	-2.32765000	1.36810700
C	0.31258700	-2.56141800	-0.71296700
C	-2.35941800	-1.71594000	-1.30380000
C	2.97879500	-0.40320500	1.51271600
C	3.09178300	2.06335400	0.02977200
C	3.10353900	-0.44221100	-1.33426000
C	-1.28066000	-3.65772900	1.63101700
C	-2.55921600	-1.70638500	2.20281100
C	0.30538900	-3.20641600	-1.94802100
C	1.41566800	-2.73334900	0.12653600
C	-2.76470100	-0.73492900	-2.20956000
C	-2.99816100	-2.96528700	-1.31870900
C	2.41903300	-1.60279300	1.96494400
C	4.10784100	0.07001500	2.19188000
C	3.63028700	2.57093500	-1.15492300
C	3.10210600	2.86012300	1.18290600
C	2.46456600	-0.70152500	-2.54578000
C	4.44914100	-0.80363100	-1.17682800
C	-1.84149700	-4.33940400	2.70569000
H	-0.57301300	-4.17620500	0.99238000
C	-3.11959100	-2.38712700	3.27950900
H	-2.86691200	-0.68465200	2.03774300
C	1.38888000	-3.99026500	-2.33456700
H	-0.54166600	-3.08000000	-2.61445100
O	1.30612600	-2.11647600	1.34780800
C	2.50295900	-3.51305800	-0.24203900
C	-3.78312200	-1.00370900	-3.12323700
H	-2.28146400	0.23353100	-2.21258700
C	-4.01119100	-3.22929700	-2.23212500
H	-2.70771200	-3.73599700	-0.61150300
C	2.91630500	-2.28073400	3.07033600
C	4.62698000	-0.60598200	3.29171400
H	4.59010700	0.98224500	1.85937800
C	4.19048300	3.84513300	-1.17949200
H	3.60631500	1.97799400	-2.06301500
C	3.67596600	4.12629000	1.15682600
H	2.65488300	2.49363800	2.10286800
C	3.16265500	-1.31684900	-3.58401000
H	1.43141300	-0.40486100	-2.68474600
C	5.13776400	-1.42021200	-2.21229400
H	4.96377800	-0.60786700	-0.24139500
C	-2.76143000	-3.70552400	3.53661800
H	-1.55713500	-5.37110300	2.89144200
H	-3.83469500	-1.87333600	3.91425700
C	2.48396800	-4.13362200	-1.48735300
H	1.38412000	-4.47574900	-3.30492800
H	3.35327400	-3.61352300	0.42417100
C	-4.40563000	-2.24646400	-3.13965200
H	-4.08424100	-0.22950100	-3.82250500
H	-4.49639400	-4.20071100	-2.23127900
C	4.02428200	-1.77666600	3.74073900
H	2.41919700	-3.19123300	3.38757400
H	5.50084100	-0.21030100	3.79929100
C	4.22198800	4.62081600	-0.02519000
H	4.60098200	4.23035500	-2.10767500
H	3.68130100	4.73125000	2.05821700
C	4.49361400	-1.67932700	-3.42155400
H	2.65172600	-1.51315200	-4.52170000
H	6.17957800	-1.69544000	-2.07672200
H	-3.19650500	-4.23794300	4.37720000
H	3.33650000	-4.73004400	-1.79632700
H	-5.19924900	-2.45162900	-3.85238200
H	4.41725900	-2.30052500	4.60638300
H	4.66180200	5.61330500	-0.04743600
H	5.03268300	-2.15948800	-4.23323700
C	-2.45923100	3.98674000	-0.17735900
F	-1.92286500	5.20930200	-0.11440900
F	-3.62991100	4.02696200	0.48466900
F	-2.71946400	3.71430300	-1.45551500

Zero-point correction = 0.664683
Thermal correction to Energy = 0.714208
Thermal correction to Enthalpy = 0.715152
Thermal correction to Gibbs Free Energy = 0.580235
Sum of electronic and zero-point Energies = -3905.312021
Sum of electronic and thermal Energies = -3905.262496
Sum of electronic and thermal Enthalpies = -3905.261552
Sum of electronic and thermal Free Energies = -3905.396469
E(RM06) = -3906.16148400

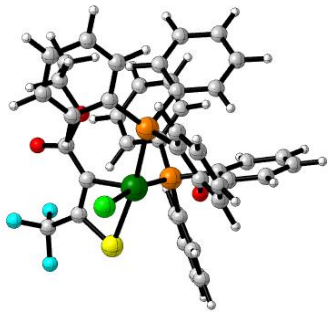
INT4l



C	-1.86598100	-2.14323200	0.73249100
C	-1.63518600	-0.97986900	0.10934800
S	-0.55690200	-2.51400400	1.85116900
C	-4.93946200	0.15556900	-0.94037200
H	-5.02599200	-0.44028100	-1.85540100
H	-4.73225800	1.18998000	-1.23027800
C	-2.63028200	-0.28537300	-0.72973400
O	-2.42662000	0.30428700	-1.77420700
O	-3.84759500	-0.34606700	-0.16873100
C	-6.17374300	0.04177100	-0.07143000
H	-7.05747300	0.37981800	-0.62200000
H	-6.32456600	-0.99617500	0.23799800
H	-6.06182100	0.65514800	0.82796500
Rh	0.01291700	-0.30658800	1.11207000
P	-0.08950100	1.90166300	0.25363000
P	1.54614500	-1.26469700	-0.19566200
C	-1.69779100	2.32829500	1.03756300
C	-0.26006000	2.37812500	-1.51142100
C	1.12257800	3.15624400	0.81495700
C	0.73136000	-1.93044300	-1.67763800
C	2.54325600	-2.62143300	0.52187800
C	2.91725800	-0.16729500	-0.72491100
C	-1.84730700	2.00128400	2.39627300
C	-2.80789300	2.79897700	0.33013400
C	-0.60890900	3.69194700	-1.84081500
C	-0.00848800	1.48260700	-2.55615700
C	2.19385600	3.47319100	-0.02633200
C	1.04398900	3.75669700	2.07374900
C	0.15818300	-0.97893600	-2.53354300
C	0.42388200	-3.27823700	-1.85281000
C	3.30472600	-3.40818400	-0.35054200
C	2.67954600	-2.79060100	1.90008000
C	3.59708600	0.56459400	0.25015400
C	3.38024100	-0.16102900	-2.04466400
C	-3.07331000	2.17039900	3.03261300
H	-1.00691900	1.60877200	2.96646300
C	-4.02870600	2.97157400	0.97497900
H	-2.73665600	2.99835000	-0.73273600
C	-0.75671900	4.08545500	-3.16562600
H	-0.76337300	4.41632000	-1.04594300
O	0.52278800	0.28627000	-2.19454300
C	-0.12140300	1.87127300	-3.88735700
C	3.16367700	4.38239600	0.38151600
H	2.28092400	3.00800600	-1.00387000
C	2.01372200	4.66853800	2.47695100
H	0.22781200	3.52098100	2.74644800
C	-0.68933600	-1.35184800	-3.56584300
C	-0.41872500	-3.66683100	-2.88942800
H	0.81340700	-4.01581800	-1.15889100
C	4.15821400	-4.38402900	0.15169600
H	3.23751400	-3.26044600	-1.42478000
C	3.54470800	-3.76083900	2.39654500
H	2.12763300	-2.15599800	2.58572800
C	4.72607400	1.30228900	-0.09648000
H	3.23662200	0.57465100	1.27527400
C	4.50222300	0.58509200	-2.38540100
H	2.86875700	-0.73808400	-2.80878400
C	-4.16584300	2.66039700	2.32473300
H	-3.17013400	1.90696200	4.08103000
H	-4.88203300	3.33918600	0.41216000
C	-0.51732100	3.16927700	-4.18641700
H	-1.03984300	5.10641400	-3.39947600
H	0.13217200	1.17148700	-4.67573000
C	3.07516800	4.98369000	1.63328200
H	3.99105900	4.61388000	-0.28254900
H	1.93919000	5.12941100	3.45703500
C	-0.96941900	-2.70542900	-3.73290400
H	-1.17411900	-0.60485700	-4.18110100
H	-0.66457800	-4.71495500	-3.02174800
C	4.27632200	-4.56423900	1.52731200
H	4.73501600	-4.99787600	-0.53344100
H	3.64157300	-3.88651900	3.47031000
C	5.17777900	1.31878600	-1.41129200
H	5.23778900	1.87796100	0.66822000
H	4.85210100	0.58939800	-3.41347600
H	-5.12391200	2.78878300	2.81945100
H	-0.60958900	3.47324200	-5.22458500
H	3.83153300	5.69492000	1.95188300
H	-1.64759500	-3.00742900	-4.52515300
H	4.94445600	-5.32482500	1.92030100
H	6.05601300	1.89866500	-1.68002400
Cl	1.40529900	0.34104900	2.99252200
C	-3.04165000	-3.07508700	0.58162500
F	-4.03365400	-2.79286600	1.44044900
F	-3.55814000	-3.03425600	-0.66164600
F	-2.67373200	-4.34620800	0.80950300

Zero-point correction = 0.656731
Thermal correction to Energy = 0.704966
Thermal correction to Enthalpy = 0.705911
Thermal correction to Gibbs Free Energy = 0.573255
Sum of electronic and zero-point Energies = -3795.891391
Sum of electronic and thermal Energies = -3795.843155
Sum of electronic and thermal Enthalpies = -3795.842211
Sum of electronic and thermal Free Energies = -3795.974866
E(RM06) = -3796.71125788

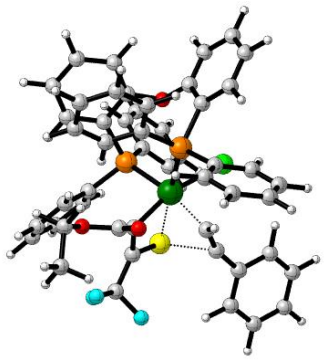
INT4l'



C	-2.20810600	-1.90469900	-1.41333200
C	-1.10726100	-1.85313400	-0.63963800
S	-2.25941000	-0.49456200	-2.43026100
C	-0.70753800	-2.85171800	0.35209800
O	-1.31182200	-3.88274400	0.57054600
O	0.42247100	-2.52707700	1.02088400
C	0.95992400	-3.54516300	1.87454500
C	0.32832000	-3.51428900	3.25432700
H	2.03243900	-3.33239700	1.91290000
H	0.81265700	-4.51786900	1.39970300
H	0.82833000	-4.23797800	3.90721000
H	0.41121500	-2.51954200	3.70482600
H	-0.73055800	-3.77413000	3.18852900
Cl	0.89125000	-0.99665800	-3.13536000
Rh	-0.23801700	-0.14257800	-1.21045100
C	2.78384900	1.05975400	-1.38026600
C	1.99661000	2.04678900	-1.97530300
C	2.46144500	2.84373100	-3.00727100
C	3.77987400	2.69182700	-3.42920500
C	4.60018100	1.74416100	-2.82614900
C	4.10042600	0.92423200	-1.81768900
O	0.66752100	2.16685200	-1.55501800
C	-4.49597300	2.90987800	-1.44920000
C	-5.55662000	2.76376800	-0.55501200
C	-5.36479200	2.07492000	0.63519000
C	-4.11789300	1.52728700	0.93840500
C	-3.05910000	1.65727100	0.04162900
P	-1.35313900	1.06038100	0.38203000
C	-0.51461900	2.68889200	0.46204500
P	1.94842900	-0.10125400	-0.22326400
C	3.02534300	-1.58309100	-0.19945500
C	2.28510000	0.63666200	1.42823500
C	-1.45275500	0.38181000	2.07239700
H	1.79098600	3.55358800	-3.48013600
H	4.15784500	3.30646700	-4.23987700
H	5.62448100	1.61883700	-3.16193400
H	4.72843700	0.14706100	-1.39447600
H	-3.98626100	1.00360500	1.87846300
H	-6.18378900	1.95888700	1.33853300
H	-6.52866700	3.18676800	-0.79006000
H	-4.63802300	3.44301300	-2.38401900
C	-0.85617300	3.63124000	1.43944800
C	-0.24042300	4.87293700	1.48935700
C	0.70618900	5.20494300	0.52303200
C	1.01826000	4.31151900	-0.49262400
H	-1.61846700	3.37939500	2.17069800
H	-0.50637500	5.58188300	2.26632200
H	1.19108100	6.17605600	0.54302400
H	1.73957900	4.58067500	-1.25475100
C	-0.78046000	0.91804300	3.16948600
C	-0.93698400	0.34980300	4.43230900
C	-1.76004700	-0.75614700	4.60844300
C	-2.41691200	-1.31113500	3.51121400
C	-2.26073400	-0.75239600	2.24990000
H	-0.11434100	1.76601200	3.05023900
H	-0.40253900	0.77625000	5.27591200
H	-1.88202700	-1.19448900	5.59446400
H	-3.04548600	-2.18773000	3.63110200
H	-2.77503400	-1.19999200	1.40477100
C	2.13691800	-0.15756900	2.56973100
C	2.39873800	0.35851200	3.83296800
C	2.77667900	1.69053300	3.98034100
C	2.91327000	2.49456600	2.85201800
C	2.68811400	1.96569900	1.58376500
H	1.81392600	-1.18480000	2.46777100
H	2.28520200	-0.27968400	4.70414900
H	2.97045500	2.09835700	4.96807800
H	3.21409000	3.53306400	2.95175700
H	2.84023600	2.59692100	0.71570400
C	4.20819100	-1.58445300	0.54979500
C	5.01838600	-2.71596800	0.58672600
C	4.65097000	-3.85758300	-0.11988400
C	3.47730100	-3.86011100	-0.86923600
C	2.66713300	-2.73040600	-0.91307500
H	4.49768300	-0.70578100	1.11846600
H	5.93251000	-2.70395400	1.17274900
H	5.27807900	-4.74368500	-0.08596200
H	3.18368000	-4.74633100	-1.42311500
H	1.75941400	-2.73661900	-1.50430200
C	-3.25850100	2.35861900	-1.15426700
H	-2.44232200	2.46493000	-1.86388800
C	0.40679100	3.05919500	-0.52134500
C	-3.31377100	-2.93308400	-1.44315600
F	-4.25633500	-2.58800600	-2.33390200
F	-3.92477400	-3.01766800	-0.24410400
F	-2.88102400	-4.15117200	-1.77620000

Zero-point correction = 0.658030
Thermal correction to Energy = 0.705537
Thermal correction to Enthalpy = 0.706481
Thermal correction to Gibbs Free Energy = 0.576910
Sum of electronic and zero-point Energies = -3795.903445
Sum of electronic and thermal Energies = -3795.855939
Sum of electronic and thermal Enthalpies = -3795.854994
Sum of electronic and thermal Free Energies = -3795.984565
E(RM06) = -3796.72814431

TS3l

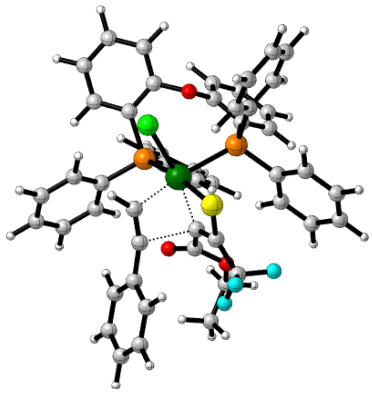


C	2.28466100	-0.89944000	1.18237000
C	1.15255700	-0.22937200	1.42273900
S	2.56022300	-0.96974400	-0.57172200
C	0.70182300	0.24040700	2.75347400
O	0.74702600	1.40252100	3.09533800
O	0.20305200	-0.73945300	3.52472200
C	-0.24896700	-0.35520500	4.83327400
C	0.90919600	-0.27665400	5.81089800
H	-0.95704200	-1.13827100	5.11353400
H	-0.78145400	0.59602300	4.75973300
H	0.53171300	-0.05204600	6.81401500
H	1.45014900	-1.22632700	5.84498100
H	1.60404500	0.51341400	5.51644800
Cl	0.16110500	1.01680400	-2.76338500
Rh	0.46912800	0.25889100	-0.42502400
C	-2.61100000	2.05695100	-1.20075500
C	-3.17672700	1.00438300	-1.92407600
C	-4.16049400	1.20894000	-2.88209600
C	-4.64067400	2.49310500	-3.10886000
C	-4.13049700	3.55538600	-2.37110800
C	-3.12663600	3.33681600	-1.43260700
O	-2.71801800	-0.27320700	-1.72100300
C	0.36361200	-2.74365800	-4.65605100
C	-0.65379100	-3.58911500	-5.08766800
C	-1.70496900	-3.90145900	-4.22938800
C	-1.73537700	-3.37151900	-2.94384400
C	-0.71918600	-2.51617700	-2.50671700
P	-0.69845400	-1.89674700	-0.78228400
C	-2.45116600	-2.05699400	-0.27206200
P	-1.29935200	1.73974000	0.06834800
C	-0.65857100	3.42659800	0.36692900
C	-2.37695800	1.39271000	1.51517900
C	0.12320500	-3.27174500	0.11656200
H	-4.53023300	0.35374700	-3.43808800
H	-5.40974900	2.65991500	-3.85651500
H	-4.50286100	4.56238700	-2.53048800
H	-2.73203800	4.18455100	-0.88463000
H	-2.55465700	-3.62811400	-2.27887800
H	-2.50268400	-4.56089300	-4.55869300
H	-0.62980000	-4.00230100	-6.09194200
H	1.18218800	-2.48750800	-5.32152800
C	-2.97452600	-2.98860900	0.62359100
C	-4.30146100	-2.89997800	1.03894500
C	-5.11281200	-1.87646900	0.55799100
C	-4.62427300	-0.95696200	-0.36543500
H	-2.33838900	-3.77661800	1.01268300
H	-4.69659600	-3.62605200	1.74233800
H	-6.14137900	-1.79314400	0.89556500
H	-5.25366100	-0.16221500	-0.75004600
C	0.12611500	-3.26810400	1.51689500
C	0.79865300	-4.25171200	2.23032300
C	1.49275000	-5.25174300	1.55359000
C	1.50388600	-5.26114400	0.16350600
C	0.82288800	-4.27899200	-0.55290300
H	-0.37874100	-2.48051800	2.06541000
H	0.79865300	-4.21904900	3.31550300
H	2.03132800	-6.01371500	2.10904600
H	2.04820100	-6.03247500	-0.37290900
H	0.84591300	-4.29932300	-1.63713600
C	-2.35620100	0.13895000	2.11818600
C	-3.24496800	-0.17438800	3.14315600
C	-4.15968900	0.77483400	3.58185700
C	-4.18766600	2.03654100	2.98744400
C	-3.30907700	2.34110700	1.95598300
H	-1.65054900	-0.60504700	1.77670300
H	-3.22116500	-1.16573100	3.58479600
H	-4.85484200	0.53551300	4.38128900
H	-4.90143300	2.78223000	3.32451800
H	-3.34869500	3.32182400	1.49103400
C	-0.47859100	3.92353900	1.65821900
C	0.11274100	5.17053900	1.85012800
C	0.53128400	5.92489700	0.75953100
C	0.37201000	5.42424600	-0.53195800
C	-0.21073500	4.17816600	-0.72962500
H	-0.77206200	3.33215200	2.51776800
H	0.25255500	5.54505700	2.85948600
H	0.99210600	6.89616900	0.91350000
H	0.71326700	5.99839200	-1.38798600
H	-0.29726300	3.76962500	-1.73356300
C	0.33137300	-2.20504600	-3.37312800
H	1.11409800	-1.52720500	-3.05625500
C	-3.30370900	-1.07177300	-0.78146600
C	4.41504400	2.29611900	-2.45214100
C	5.65306900	2.61872800	-2.99700600
C	6.82181900	2.19068900	-2.37208600
C	6.75566900	1.43903300	-1.19824400
C	5.52457000	1.12183800	-0.64182700
C	4.34552300	1.55703700	-1.26200000
H	3.49087200	2.59822900	-2.93530400
H	5.70490300	3.19439900	-3.91617900
H	7.78801100	2.43643000	-2.80324100
H	7.66832800	1.10176600	-0.71640400
H	5.45804800	0.53366000	0.26667100
C	3.04374500	1.28540200	-0.70592300
C	1.86444000	1.71900500	-0.38536200
H	1.67742800	2.77557900	-0.21441400
C	3.34109100	-1.38778400	2.11817000

F	2.91566200	-1.41476700	3.39111300
F	3.75696700	-2.62305700	1.80031100
F	4.43881000	-0.59658500	2.09517000

Zero-point correction = 0.769869
Thermal correction to Energy = 0.824712
Thermal correction to Enthalpy = 0.825656
Thermal correction to Gibbs Free Energy = 0.678664
Sum of electronic and zero-point Energies = -4104.081327
Sum of electronic and thermal Energies = -4104.026484
Sum of electronic and thermal Enthalpies = -4104.025540
Sum of electronic and thermal Free Energies = -4104.172532
E(RM06) = -4104.98990324

TS4l



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C	1.67146300	-0.71881400	-0.03957000
S	0.84002300	-2.07044700	-2.03678300
C	2.23473400	-0.30325600	1.25532100
O	2.50065600	0.84247800	1.56112700
O	2.37078300	-1.33163300	2.11517100
C	2.99439700	-1.02961300	3.37139500
C	4.50511900	-0.97559100	3.22655200
H	2.68508700	-1.84538900	4.02900500
H	2.59271300	-0.08574400	3.74943000
H	4.96882000	-0.81071500	4.20479400
H	4.88158200	-1.91469100	2.81227100
H	4.79496000	-0.15794400	2.56115000
C	4.85817400	-0.39594300	-1.85473300
C	6.23528400	-0.36114800	-1.68525200
C	6.81466800	0.63208800	-0.89673000
C	6.01672300	1.59580100	-0.28255400
C	4.63762800	1.56988300	-0.44957800
C	4.04947000	0.57099300	-1.23879200
H	4.39404700	-1.17148500	-2.45577600
H	6.85763800	-1.11039600	-2.16444800
H	7.89225100	0.65515500	-0.76196700
H	6.47119000	2.37069200	0.32745700
H	3.99962600	2.30530200	0.02515300
C	2.62455000	0.54471400	-1.43472000
C	1.52599900	0.85873000	-2.01932800
H	1.39473000	1.47002100	-2.90516800
Cl	-1.40456100	0.74589000	-2.97307100
Rh	-0.01404600	-0.01996100	-1.10751600
C	-2.07226800	2.90727400	-0.51088200
C	-3.27486600	2.19656500	-0.55179000
C	-4.47352800	2.79260200	-0.91634100
C	-4.49915600	4.14976500	-1.21722300
C	-3.32561800	4.89165100	-1.14644100
C	-2.12680800	4.27394500	-0.80054800
O	-3.26887800	0.85289300	-0.27033200
C	-3.68298700	-2.81871600	-3.47952000
C	-4.92847500	-3.20837100	-2.99868600
C	-5.23066700	-3.04556100	-1.64852600
C	-4.28803600	-2.49838300	-0.78561100
C	-3.03315500	-2.10330300	-1.26316100
P	-1.75811000	-1.48053200	-0.10048600
C	-2.78361000	-0.81140500	1.26941400
P	-0.51242600	2.03730500	-0.03514500
C	0.75100700	3.31591900	-0.38734600
C	-0.66286900	2.07871700	1.79525400
C	-1.12183400	-3.03478400	0.64635800
H	-5.36676500	2.17879800	-0.96443100
H	-5.43309200	4.62282000	-1.50417900
H	-3.33450200	5.95361500	-1.37070100
H	-1.22138600	4.86893500	-0.76645000
H	-4.53017400	-2.38246000	0.26661200
H	-6.20133800	-3.34603300	-1.26489100
H	-5.66504100	-3.63417500	-3.67402800
H	-3.44270700	-2.93000400	-4.53231200
C	-2.95148500	-1.38453700	2.53011800
C	-3.64504500	-0.70803800	3.52988800
C	-4.17609200	0.55258400	3.27522000
C	-4.06271100	1.12560500	2.01273200
H	-2.52045300	-2.35675500	2.74176100
H	-3.75712500	-1.16099100	4.50981400
H	-4.69438200	1.09499500	4.06006600
H	-4.48480300	2.10175100	1.80074700
C	-0.27721100	-2.96186000	1.75795100
C	0.20865100	-4.11503700	2.36274000
C	-0.12655200	-5.36382300	1.85025600
C	-0.94581000	-5.44828200	0.72848400
C	-1.44350400	-4.29395700	0.13100400
H	0.01319300	-2.00008300	2.16295400
H	0.86882100	-4.03206800	3.22065800
H	0.25866300	-6.26676300	2.31456400
H	-1.20418100	-6.41811200	0.31387200
H	-2.08437900	-4.37861200	-0.73992100
C	-0.41482400	0.93950400	2.55440900
C	-0.55331900	0.96001600	3.93814500
C	-0.93497200	2.13335900	4.57868600
C	-1.18322900	3.28248100	3.82985100
C	-1.05295800	3.25466300	2.44679000
H	-0.13311500	0.02429000	2.05155500
H	-0.37428600	0.05377200	4.50896400
H	-1.04618100	2.15370500	5.65885600
H	-1.48518900	4.20107600	4.32401800
H	-1.26063400	4.15193800	1.87102500
C	1.65388800	3.74907800	0.58309200

C	2.64195800	4.67574400	0.25355200
C	2.73874200	5.16887100	-1.04318500
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C	0.85614700	3.81063000	-1.69407200
H	1.60595700	3.35039300	1.58967000
H	3.34031200	5.00639400	1.01696000
H	3.51151900	5.88851800	-1.29683800
H	1.91207500	5.11185200	-3.03364300
H	0.15989800	3.46800800	-2.45678500
C	-2.73906700	-2.26555000	-2.61818800
H	-1.78722300	-1.93401600	-3.01277100
C	-3.38794100	0.42432700	1.02100500
C	2.92113300	-2.98157200	-0.40248600
F	4.00641500	-2.44962500	0.18188700
F	3.33480500	-3.57100900	-1.53690000
F	2.45397900	-3.94251600	0.39739500

Zero-point correction = 0.769602
Thermal correction to Energy =0.824143
Thermal correction to Enthalpy = 0.825087
Thermal correction to Gibbs Free Energy = 0.680191
Sum of electronic and zero-point Energies = -4104.078181
Sum of electronic and thermal Energies = -4104.023641
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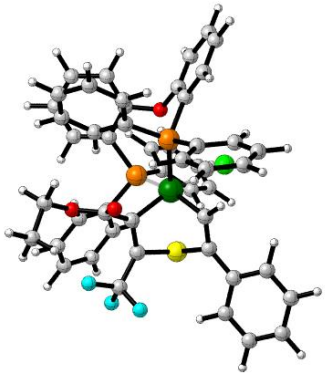
E(RM06) = -4104.98713292

INT5l



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S	2.49689400	-1.05273800	-0.76919200
C	0.82757200	0.16057800	2.66380200
O	1.05531200	1.29140300	3.03373100
O	0.23609400	-0.76766900	3.42810200
C	-0.08099100	-0.37783000	4.77584000
C	1.12650700	-0.52601300	5.68265500
H	-0.88822700	-1.05296900	5.06763900
H	-0.45853600	0.64698100	4.76781200
H	0.84412300	-0.29014900	6.71397900
H	1.51129000	-1.54911400	5.65041000
H	1.92143200	0.15760100	5.37529800
Cl	-0.05605800	0.88778600	-2.83078300
Rh	0.39271200	0.19585400	-0.51718800
C	-2.53768600	2.26792000	-1.02923300
C	-3.28405000	1.26045400	-1.64537400
C	-4.36385800	1.54435500	-2.47190600
C	-4.75828000	2.86317800	-2.65982900
C	-4.06779200	3.88390500	-2.01531200
C	-2.97079100	3.58594200	-1.21398700
O	-2.92022600	-0.05206500	-1.47213600
C	-0.30807800	-2.87441500	-4.64371100
C	-1.45880000	-3.56785500	-5.00703600
C	-2.48999100	-3.72945800	-4.08558400
C	-2.36875100	-3.20184800	-2.80402100
C	-1.21893700	-2.49799800	-2.43562600
P	-0.99352000	-1.87887700	-0.72731500
C	-2.69708800	-1.87061000	-0.05644200
P	-1.09605700	1.88012400	0.06464400
C	-0.19538700	3.46880500	0.11935900
C	-1.98667700	1.77020300	1.66746800
C	-0.20760100	-3.31332600	0.10861800
H	-4.87711700	0.72070000	-2.95718300
H	-5.60198100	3.08962900	-3.30411200
H	-4.37203100	4.91784300	-2.14319300
H	-2.43527000	4.39945700	-0.73797000
H	-3.17426300	-3.34232700	-2.08945600
H	-3.39050700	-4.27004900	-4.36198600
H	-1.55353800	-3.97948100	-6.00771400
H	0.49655200	-2.73539400	-5.35903500
C	-3.21613600	-2.74505200	0.89725800
C	-4.48047300	-2.52733500	1.44166700
C	-5.23339000	-1.43198200	1.02963100
C	-4.75030200	-0.56251200	0.05565100
H	-2.62317300	-3.59051100	1.23012000
H	-4.87245400	-3.21151000	2.18751800
H	-6.21194400	-1.25000300	1.46342500
H	-5.33530900	0.29063400	-0.26872800
C	-0.07026400	-3.29360000	1.50217800
C	0.58625900	-4.32100900	2.16722900
C	1.13062800	-5.38175200	1.44728300
C	1.00755300	-5.40787000	0.06271100
C	0.34042900	-4.38256800	-0.60514900
H	-0.45819100	-2.46106700	2.07899600
H	0.69234200	-4.27659500	3.24686200
H	1.65719400	-6.17875800	1.96367300
H	1.43232200	-6.22852400	-0.50756200
H	0.25205400	-4.42106400	-1.68564300
C	-2.23776800	0.52224000	2.23276200
C	-3.04247600	0.40198700	3.36271500
C	-3.58945600	1.53639000	3.94997800
C	-3.33665300	2.79179700	3.39756000
C	-2.55093400	2.90792100	2.25799200
H	-1.80885200	-0.36618400	1.78937600
H	-3.23820200	-0.58371200	3.77334200
H	-4.21428200	1.44749900	4.83387000
H	-3.76030200	3.68256200	3.85154400
H	-2.37417800	3.88923900	1.82829500
C	0.37610200	3.92105300	1.31090000
C	1.19495300	5.04772900	1.30754500

C	1.45637800	5.72293400	0.11961100
C	0.90864900	5.25981500	-1.07536300
C	0.09453000	4.13270500	-1.08030400
H	0.21745400	3.37722000	2.23550800
H	1.63821500	5.38741000	2.23849400
H	2.09787800	6.59920200	0.12086500
H	1.12635400	5.76679300	-2.01049900
H	-0.28763200	3.74468700	-2.02006700
C	-0.18900200	-2.33639900	-3.36613300
H	0.69972100	-1.77587500	-3.10130900
C	-3.49337700	-0.80154900	-0.48573000
C	4.65552900	2.22348100	-2.03867000
C	5.94591100	2.58102600	-2.40850000
C	7.01588500	1.73077800	-2.13596300
C	6.78285500	0.52120400	-1.48796800
C	5.49311800	0.16497900	-1.10750300
C	4.41470900	1.01439800	-1.37197900
H	3.81858600	2.87310200	-2.27779600
H	6.11521900	3.52136100	-2.92530000
H	8.02333200	2.00695900	-2.43296600
H	7.60948900	-0.14913600	-1.27116100
H	5.32806000	-0.77222700	-0.58581000
C	3.04009300	0.68219500	-0.96945000
C	1.97633500	1.43954700	-0.71493200
H	1.98313400	2.52462800	-0.72956800
C	3.30140900	-1.62325100	1.89466400
F	2.94580600	-1.58936000	3.18921100
F	4.47401100	-0.96613800	1.78799600
F	3.55270400	-2.90369800	1.57394000

Zero-point correction = 0.772459
Thermal correction to Energy = 0.827174
Thermal correction to Enthalpy = 0.828118
Thermal correction to Gibbs Free Energy = 0.680605
Sum of electronic and zero-point Energies = -4104.113654
Sum of electronic and thermal Energies = -4104.058938
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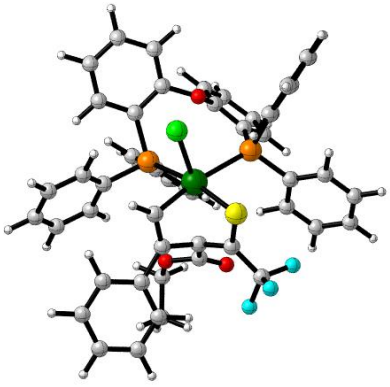
Sum of electronic and thermal Free Energies = -4104.205508
E(RM06) = -4105.01766431

INT6l

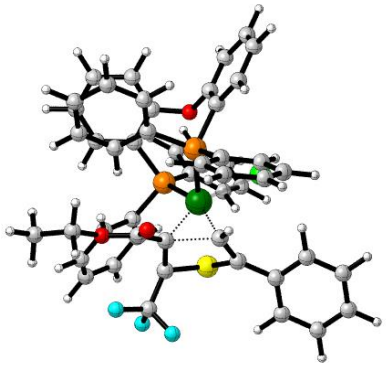


Rh	-0.00885200	-0.12331900	-1.11649900
Cl	-0.96415500	1.07742300	-2.95941300
C	1.04726300	-2.58540900	-0.81384800
C	1.63567600	-1.42797700	-0.18938300
S	0.10574600	-2.27392800	-2.15076100
C	1.95217000	-1.45210500	1.25674300
O	1.50193100	-2.23788600	2.06914700
O	2.76283400	-0.43465000	1.58643900
C	3.23415000	-0.38930400	2.93712300
C	4.45822700	-1.27302100	3.09651700
H	2.42862000	-0.68763300	3.61169900
H	3.47107800	0.66289300	3.11044700
H	4.87041000	-1.16573300	4.10539900
H	4.19008000	-2.32208300	2.94215200
H	5.22584800	-0.99773900	2.36724900
C	4.62802800	-1.95662500	-0.60382200
C	6.01458600	-2.07141600	-0.56754100
C	6.81843200	-1.02653300	-1.01494700
C	6.22206800	0.13543400	-1.50183800
C	4.83846100	0.25159000	-1.53409700
C	4.02181100	-0.79448800	-1.08923300
H	4.01744700	-2.78076700	-0.25120700
H	6.46651900	-2.98362200	-0.18833400
H	7.90042900	-1.11555200	-0.98275600
H	6.83774000	0.96139400	-1.84737700
H	4.37722000	1.16897500	-1.88507400
C	2.55524300	-0.62419000	-1.12206800
C	1.81086700	0.13825500	-1.90385800
H	2.08268800	0.75808200	-2.74943400
C	-0.83500800	3.36645800	-0.48472400
C	-2.21431000	3.14889700	-0.53608600
C	-3.10820700	4.14763400	-0.89570900
C	-2.63237100	5.42365800	-1.17413500
C	-1.26957200	5.68360500	-1.08257600
C	-0.38327900	4.66438600	-0.74581300
O	-2.70516100	1.89912000	-0.25611100
C	-4.50448200	-1.27515900	-3.47834600
C	-5.80641700	-1.10706600	-3.01890200
C	-6.03439300	-0.82616600	-1.67348800
C	-4.96364200	-0.71780500	-0.79346300
C	-3.65082400	-0.88265800	-1.24900200
P	-2.24042900	-0.83799900	-0.07580900
C	-2.91237100	0.18632900	1.29479000
P	0.29424600	1.97152500	-0.04038800
C	1.93511200	2.70733800	-0.40279600
C	0.20116100	2.01870200	1.79080700
C	-2.31271800	-2.51662600	0.66927200
H	-4.16412800	3.90512400	-0.95129800
H	-3.32520900	6.21032500	-1.45596500
H	-0.88691200	6.67902900	-1.28434700
H	0.67579000	4.88836100	-0.69736300
H	-5.15191100	-0.50814900	0.25530700
H	-7.04813400	-0.69348900	-1.30686900
H	-6.64261300	-1.19084500	-3.70705900
H	-4.31603100	-1.48331200	-4.52701200
C	-3.27928400	-0.26398500	2.56291700
C	-3.63234100	0.63838200	3.56275500

C	-3.62181400	2.00425300	3.30031900
C	-3.30601000	2.47695800	2.03044200
H	-3.26796500	-1.32571300	2.78165000
H	-3.90195900	0.27238300	4.54827400
H	-3.87177200	2.71308400	4.08386100
H	-3.30891400	3.53933800	1.81345900
C	-1.52820400	-2.78717700	1.79522700
C	-1.60465800	-4.01696500	2.43790800
C	-2.44694900	-5.00862800	1.94448300
C	-3.20424000	-4.76340200	0.80301500
C	-3.14476800	-3.52387700	0.17154500
H	-0.83899400	-2.04412800	2.17883400
H	-0.98062700	-4.20406500	3.30600800
H	-2.50188800	-5.97425700	2.43844300
H	-3.85322300	-5.53650900	0.40241900
H	-3.75563200	-3.34295600	-0.70649200
C	0.02434500	0.84070900	2.50988900
C	-0.07212300	0.86206400	3.89804800
C	0.01584500	2.07063700	4.57912900
C	0.19597800	3.25718000	3.86873500
C	0.28356000	3.23323800	2.48258700
H	-0.05221400	-0.09900700	1.97804100
H	-0.22365600	-0.06782000	4.43747800
H	-0.06130300	2.09258400	5.66218300
H	0.26182300	4.20389900	4.39654200
H	0.41187300	4.16302900	1.93581400
C	2.94888400	2.75947100	0.55269200
C	4.18601100	3.31744600	0.23577100
C	4.41791800	3.82948200	-1.03540500
C	3.41627100	3.75864800	-2.00390100
C	2.18643600	3.19054300	-1.69439200
H	2.77735900	2.36524800	1.54792000
H	4.96845200	3.34770600	0.98770400
H	5.38009200	4.27038800	-1.27859300
H	3.59443500	4.14076100	-3.00449900
H	1.41090600	3.12441400	-2.45418200
C	-3.43065500	-1.16005400	-2.59932300
H	-2.42094500	-1.26039500	-2.97775600
C	-2.97711100	1.55901600	1.04065500
C	1.26449600	-4.04665300	-0.40508800
F	2.34383200	-4.20140300	0.37244500
F	0.22017600	-4.58021000	0.21731100
F	1.48206900	-4.76515900	-1.51964300

Zero-point correction = 0.772031
Thermal correction to Energy = 0.826706
Thermal correction to Enthalpy = 0.827650
Thermal correction to Gibbs Free Energy = 0.681274
Sum of electronic and zero-point Energies = -4104.118469
Sum of electronic and thermal Energies = -4104.063793
Sum of electronic and thermal Enthalpies = -4104.062849
Sum of electronic and thermal Free Energies = -4104.209226
E(RM06) = -4105.02316537

TS5l



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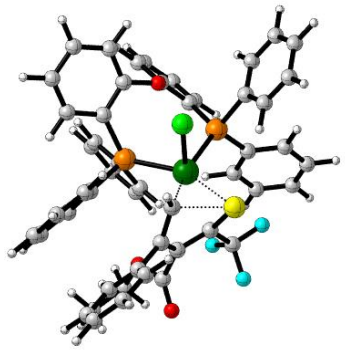
C	1.28193000	-0.44931400	1.46431100
S	2.66249400	-1.05437500	-0.51454600
C	0.76516900	-0.20693800	2.83771800
O	0.84117300	0.84425400	3.43380100
O	0.15768200	-1.29252200	3.33949500
C	-0.35783700	-1.17327000	4.67078100
C	-0.92002500	-2.52909000	5.04152700
H	-1.12353100	-0.39149700	4.68716400
H	0.45373200	-0.87064000	5.33855900
H	-1.34087400	-2.49894700	6.05122800
H	-1.71178900	-2.82460200	4.34512700
H	-0.13454300	-3.29007000	5.01317400
Rh	0.53181800	0.20890900	-0.29643400
C	4.09208100	2.66953800	-1.26372200
C	5.17398500	3.29474400	-1.87164200
C	6.37980000	2.61297400	-2.02222800
C	6.50414800	1.30201800	-1.56539900
C	5.42468500	0.67322000	-0.95723500
C	4.21348200	1.35636500	-0.79296600
H	3.13429700	3.17057900	-1.17026400
H	5.07280300	4.31052900	-2.24176500
H	7.22285200	3.10136300	-2.50238000
H	7.44406500	0.77102200	-1.68146200
H	5.52079900	-0.34286100	-0.58467200
C	3.08192400	0.72860100	-0.11616300
C	2.12357200	1.19499800	0.68408600
H	2.11147500	2.15596200	1.18080600
C	-2.15722700	2.51233900	-0.94016800
C	-2.81196500	1.71096900	-1.87868300
C	-3.65998900	2.24331700	-2.83955000
C	-3.90113900	3.61223800	-2.85933200
C	-3.28932200	4.43054300	-1.91683500
C	-2.42526800	3.88449100	-0.97212600
O	-2.56745900	0.36078100	-1.90196800
C	0.37536200	-1.85191600	-5.06243900
C	-0.68067400	-2.51926300	-5.67495600
C	-1.79458700	-2.89155600	-4.92540100
C	-1.84839300	-2.59918400	-3.56708400
C	-0.79080500	-1.92565000	-2.94748300
P	-0.79965800	-1.62380700	-1.14260000
C	-2.58296400	-1.63452300	-0.72604200

P	-1.05033500	1.76956800	0.33969600
C	-0.21243500	3.24940600	1.01371400
C	-2.29578600	1.31169900	1.60684600
C	-0.20706200	-3.22142400	-0.46854900
H	-4.10968800	1.57293200	-3.56438400
H	-4.56223500	4.03463000	-3.60955100
H	-3.47111600	5.50056900	-1.91937300
H	-1.94308500	4.54450500	-0.26018000
H	-2.71633100	-2.89882600	-2.98655000
H	-2.62254400	-3.41185300	-5.39810500
H	-0.63928100	-2.74612000	-6.73642900
H	1.24121700	-1.54798700	-5.64249500
C	-3.25790600	-2.61523100	-0.00049500
C	-4.58360800	-2.42174800	0.38115800
C	-5.24065000	-1.24282000	0.04024000
C	-4.59952600	-0.26602500	-0.71605200
H	-2.73952800	-3.52451500	0.28551200
H	-5.09787300	-3.18754700	0.95315100
H	-6.26667400	-1.08068800	0.35614500
H	-5.10694900	0.65092700	-0.99538700
C	-0.22656900	-3.41882000	0.91765300
C	0.26206300	-4.59288700	1.47651300
C	0.80348800	-5.58034400	0.65818400
C	0.84810000	-5.38641500	-0.71842300
C	0.34485700	-4.21556100	-1.28124000
H	-0.60427600	-2.64511500	1.57647300
H	0.24669900	-4.71771800	2.55481700
H	1.20189000	-6.49189000	1.09362600
H	1.27605700	-6.14826400	-1.36310800
H	0.38483700	-4.08151900	-2.35712100
C	-2.37232400	0.00430100	2.07736700
C	-3.36850000	-0.36870600	2.97599000
C	-4.29180800	0.57036200	3.41962500
C	-4.22162400	1.88403800	2.95680100
C	-3.23531300	2.25114300	2.05066500
H	-1.66020500	-0.73002900	1.72575900
H	-3.42534500	-1.39852400	3.31480100
H	-5.07031400	0.28178700	4.11972400
H	-4.94179400	2.62172000	3.29768700
H	-3.19834700	3.27276200	1.68373200
C	-0.21349500	3.54784100	2.37549500
C	0.52873100	4.62688900	2.85345400
C	1.27206300	5.40969700	1.97795300
C	1.28186100	5.10927800	0.61555800
C	0.55127100	4.03118900	0.13365700
H	-0.76435600	2.92838100	3.07359200
H	0.53021800	4.84412800	3.91703400
H	1.85135900	6.24755800	2.35457800
H	1.86960000	5.70959000	-0.07262100
H	0.58526900	3.76990100	-0.92165500
C	0.32171300	-1.55176300	-3.70393500
H	1.13271400	-1.00141300	-3.24141700
C	-3.28440800	-0.48601800	-1.10517600
Cl	0.62978000	1.52551600	-2.43237900
C	3.09790700	-2.24752200	1.94381700
F	2.62197900	-2.49932400	3.17409800
F	3.39507500	-3.42652600	1.36772000
F	4.28701500	-1.61117400	2.11592700

Zero-point correction = 0.770042
Thermal correction to Energy = 0.824582
Thermal correction to Enthalpy = 0.825526
Thermal correction to Gibbs Free Energy = 0.677900
Sum of electronic and zero-point Energies = -4104.083004
Sum of electronic and thermal Energies = -4104.028464
Sum of electronic and thermal Enthalpies = -4104.027520
Sum of electronic and thermal Free Energies = -4104.175146
E(RM06) = -4104.99298160

TS6l



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Cl	-0.76334300	1.14187700	-2.90036400
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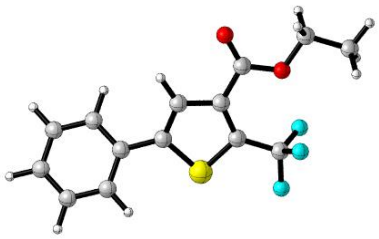
C	2.20139300	-1.76115100	-0.30633400
S	0.25515400	-2.26436300	-2.20070400
C	3.00787300	-2.15596400	0.90132600
O	3.76059200	-3.09424400	0.94519300
O	2.78492900	-1.29416000	1.89890800
C	3.42575700	-1.56970000	3.15612600
C	4.85827900	-1.06933500	3.17215300
H	3.37679400	-2.64507600	3.34557000
H	2.80602600	-1.04252800	3.88475900
H	5.28866100	-1.21388300	4.16850800
H	5.46564000	-1.61988600	2.44908100
H	4.89368700	-0.00275200	2.92938200
C	5.07081500	-0.41946900	-0.56701700
C	6.41292700	-0.21217700	-0.86240500
C	6.85892900	-0.26722300	-2.17969500
C	5.94825900	-0.53383300	-3.19958600
C	4.60747500	-0.75362900	-2.90317200
C	4.15177900	-0.70076800	-1.58102400
H	4.72540200	-0.30723000	0.45457300
H	7.10849700	0.01037400	-0.05799300
H	7.90712100	-0.10285800	-2.41122100
H	6.28424000	-0.58294500	-4.23130900
H	3.90701500	-0.98504400	-3.70096400
C	2.71521800	-0.90879000	-1.29365900
C	1.66725900	-0.37996600	-2.04722300
H	1.83211500	0.14136400	-2.98914100
C	-0.25592200	3.26411600	-0.16328300

C	-1.58520800	3.39277200	-0.58122400
C	-2.09008000	4.58798200	-1.07597500
C	-1.27720800	5.71464500	-1.11070800
C	0.02971200	5.63420700	-0.64195200
C	0.53320700	4.42086700	-0.18304900
O	-2.42465300	2.30818800	-0.51727000
C	-4.32557200	-0.95611900	-3.90644200
C	-5.61630200	-0.48403300	-3.68704200
C	-5.96897300	0.01078500	-2.43411800
C	-5.03495100	0.02985200	-1.40324500
C	-3.73494100	-0.43583800	-1.61917800
P	-2.50000400	-0.51543600	-0.26568600
C	-3.19038800	0.67422100	0.96415400
P	0.42823200	1.60813000	0.29308900
C	2.21630200	2.00550700	0.32230000
C	0.00843400	1.40834800	2.06432000
C	-2.91725800	-2.11757200	0.53378300
H	-3.11754300	4.61208800	-1.42331100
H	-1.66746200	6.65182400	-1.49528800
H	0.66901900	6.51127700	-0.64667700
H	1.56316800	4.37586000	0.15111400
H	-5.32308900	0.40794600	-0.42699400
H	-6.97453700	0.38066100	-2.25606000
H	-6.34600200	-0.49905100	-4.49151600
H	-4.04042500	-1.33670400	-4.88245600
C	-3.86241900	0.33555800	2.14119900
C	-4.29701500	1.31609100	3.02826100
C	-4.08078700	2.65901200	2.73941600
C	-3.44522900	3.02646100	1.55942900
H	-4.04500400	-0.70634900	2.37584000
H	-4.80650500	1.02640700	3.94165700
H	-4.41639100	3.42870100	3.42808700
H	-3.28016700	4.07050000	1.31678100
C	-2.39480300	-2.40121400	1.80073500
C	-2.67385500	-3.60620800	2.43275200
C	-3.46603900	-4.55886600	1.79756800
C	-3.97950700	-4.29250600	0.53286800
C	-3.71393600	-3.07741900	-0.09409700
H	-1.77128600	-1.66911900	2.30303600
H	-2.25975200	-3.80598500	3.41663300
H	-3.67777700	-5.50599100	2.28487400
H	-4.59525400	-5.03088400	0.02797500
H	-4.12977100	-2.88411000	-1.07706300
C	0.08575600	0.12487700	2.61148900
C	-0.18925500	-0.08414200	3.95937400
C	-0.56334900	0.98571500	4.76859700
C	-0.64794200	2.26577000	4.22787100
C	-0.35539900	2.47887400	2.88405800
H	0.36449000	-0.71418900	1.98328500
H	-0.12663100	-1.08847900	4.36952000
H	-0.79383700	0.82178800	5.81714500
H	-0.94643900	3.10263800	4.85200200
H	-0.42453900	3.48000900	2.46932200
C	2.97128500	2.05180100	1.49390000
C	4.30572900	2.45507400	1.45072300
C	4.89525200	2.79982700	0.23938900
C	4.15205500	2.73431500	-0.93767200
C	2.82221500	2.33802700	-0.89697700
H	2.51790900	1.79115800	2.44498700
H	4.88122300	2.50574500	2.37092800
H	5.93651300	3.10553800	0.20688700
H	4.61363200	2.97639800	-1.88956600
H	2.23596200	2.31182900	-1.81248000
C	-3.38639100	-0.92656400	-2.88012500
H	-2.37715000	-1.27803600	-3.06213400
C	-3.01331700	2.03221600	0.68785700
C	0.50196800	-3.50717500	0.28762400
F	1.36272600	-4.53194500	0.14620700
F	0.50784700	-3.18956200	1.60658300
F	-0.70254800	-3.97837600	-0.02111700

Zero-point correction = 0.771791
Thermal correction to Energy = 0.825752
Thermal correction to Enthalpy = 0.826697
Thermal correction to Gibbs Free Energy = 0.682640
Sum of electronic and zero-point Energies = -4104.103704
Sum of electronic and thermal Energies = -4104.049742
Sum of electronic and thermal Enthalpies = -4104.048798
Sum of electronic and thermal Free Energies = -4104.192855
E(RM06) = -4105.00827653

3l

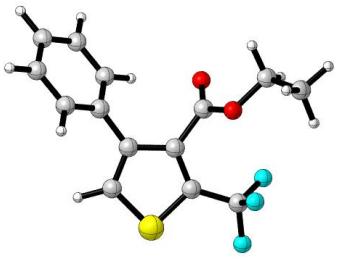


C	-0.67903000	-0.61719900	0.03181800
C	-0.75231800	0.75307500	-0.06399700
S	0.81806000	1.45944500	-0.11609400
C	-1.79626800	-1.59717500	0.10290300
O	-2.98933400	-1.00806500	0.10670800
O	-1.62346100	-2.79438300	0.15245900
C	-4.13867200	-1.86520100	0.16221600
H	-4.08559300	-2.46737200	1.07419600
H	-4.11135000	-2.54724200	-0.69286800
C	-5.35515600	-0.96475300	0.13897000
H	-6.26679400	-1.56849300	0.17701400
H	-5.34761000	-0.28640000	0.99651200
H	-5.37000200	-0.36357000	-0.77423500
C	0.66335600	-1.08521100	0.07112700
H	0.90299200	-2.13651800	0.17150700
C	1.59272700	-0.08494600	0.00665700
C	3.05935500	-0.20707200	0.01856800
C	3.66729000	-1.32335800	-0.56801800
C	3.86730100	0.76865700	0.61304900
C	5.04952500	-1.46392900	-0.54982200

H	3.05163800	-2.07343400	-1.05539700
C	5.25049800	0.63054300	0.62032200
H	3.41093400	1.63134000	1.09111900
C	5.84586000	-0.48682900	0.04208700
H	5.50647300	-2.33494300	-1.00949100
H	5.86359000	1.39488800	1.08787900
H	6.92604100	-0.59526400	0.05107400
C	-1.94523400	1.66800100	-0.13384500
F	-2.72383800	1.41357800	-1.19172500
F	-2.70639300	1.60300300	0.96452600
F	-1.53002700	2.94651400	-0.24895100

Zero-point correction = 0.227421
Thermal correction to Energy = 0.245523
Thermal correction to Enthalpy = 0.246467
Thermal correction to Gibbs Free Energy = 0.178167
Sum of electronic and zero-point Energies = -1387.746815
Sum of electronic and thermal Energies = -1387.728713
Sum of electronic and thermal Enthalpies = -1387.727769
Sum of electronic and thermal Free Energies = -1387.796069
E(RM06) = -1388.12498562

4l



C	-0.15984800	-0.27997000	0.17149900
C	-1.22717700	-1.13671700	0.09437000
S	-0.73242500	-2.76513200	-0.15653300
C	-0.32908800	1.18640800	0.40634200
O	-1.21361000	1.69982200	-0.44903000
O	0.23321200	1.81894100	1.26854800
C	-1.61965100	3.05726600	-0.20908200
H	-0.76570600	3.71737200	-0.38777400
H	-1.90775600	3.15368900	0.84165200
C	-2.77513800	3.34178900	-1.14399800
H	-3.14102700	4.36044300	-0.98386400
H	-2.46457300	3.24381300	-2.18798700
H	-3.59313300	2.64043100	-0.95894800
C	1.10077700	-0.95338900	0.01482300
C	0.91448100	-2.29522700	-0.18416900
H	1.68902900	-3.03801600	-0.32017600
C	2.45070600	-0.33786800	-0.01263100
C	2.91430600	0.47393400	1.02742100
C	3.30252100	-0.61726000	-1.08720700
C	4.20339600	0.99416200	0.98668700
H	2.25910800	0.70334800	1.85898100
C	4.59178800	-0.09754500	-1.12358000
H	2.94167500	-1.23392500	-1.90588100
C	5.04539200	0.71045500	-0.08505600
H	4.55136200	1.62301900	1.80061400
H	5.23903500	-0.31937700	-1.96685700
H	6.05082900	1.11997600	-0.11223700
C	-2.68899800	-0.80996300	0.18702500
F	-2.93278600	0.11238700	1.13119100
F	-3.18755700	-0.34573300	-0.96664400
F	-3.39495400	-1.91056600	0.50391900

Zero-point correction = 0.227673
Thermal correction to Energy = 0.245581
Thermal correction to Enthalpy = 0.246525
Thermal correction to Gibbs Free Energy = 0.179621
Sum of electronic and zero-point Energies = -1387.741795
Sum of electronic and thermal Energies = -1387.723886
Sum of electronic and thermal Enthalpies = -1387.722942
Sum of electronic and thermal Free Energies = -1387.789847
E(RM06) = -1388.11816620